Supporting Information

Ring-Strain Enabled Transannulation of *N*-Aryl Bicyclo[1.1.0]butane Carboxamides via Rhodium (II)Carbene Intermediate

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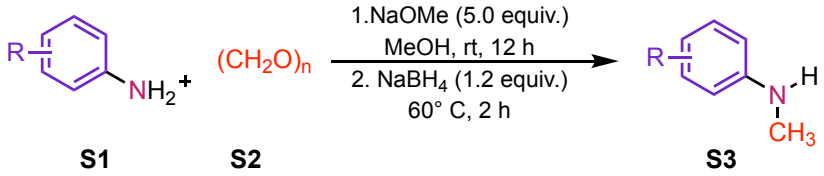
1.0 General Information.

All chemicals were purchased from Aldrich, TCI, GLR Innovations and Avra chemicals in analytical grade and were used as supplied. All reaction were carried out under nitrogen atmosphere using oven dried reaction vials. Dry solvents were prepared by distilling over sodium metal with benzophenone, Calcium hydride and stored over molecular sieves 4 Å under N_2 atmosphere. All compounds were purified by column chromatography using silica gel (60-120 mesh). Thin layer chromatography was performed on 0.25 mm thick aluminum-baked silica gel plates purchased from Merck and visualized with ultraviolet (λ = 254 nm). ^{1}H, $^{13}C\{^{1}H\}$ and ^{19}F NMR spectra were recorded on JEOL ECZ500R/S1 (500, 126, 471 MHz respectively) instrument. ^{1}H signals are referenced to residual $CHCl_3$ at 7.26 ppm. ^{13}C signals are referenced to $CDCl_3$ at 77.16 ppm. IR spectra were recorded on Bruker Alpha II compact FT-IR spectrophotometer. High resolution mass spectra quadrupole time-of-flight (HRMS-QTOF) was obtained in ESI mode. The single-crystal XRD data was collected and integrated using a Bruker SMART APEX CCD diffractometer with a Mo-Kα (λ = 0.71073 Å) sealed tube. All the heating reactions are conducted in an oil bath.

2.0 Synthesis of Starting Materials.

General procedure 2.1: *N*-Methyl amines were prepared according to the literature procedure.[1]

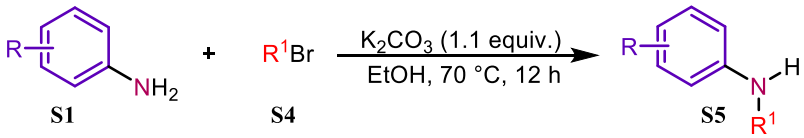


S1 **S2** **S3**

Step-1: Substituted aniline **S1** (10 mmol, 1.0 equiv.) and *p*-formaldehyde **S2** (13 mmol 1.3 equiv.) was dissolved in methanol (30 mL) in a 100 mL round-bottom (RB) flask equipped with a stirring bar. Then, sodium methoxide (5.0 equiv.) was added portion wise. The reaction mixture was stirred for 12 h at room temperature, and the reaction was monitored by TLC. After complete conversion of the starting material, the crude reaction mixture was used for the next step without further purification.

Step-2: In the crude reaction mixture of step-1, sodium borohydride (1.2 equiv.) was added at 0 °C slowly. After the addition of $NaBH_4$, warm the reaction mixture to rt, then reflux at 60 °C and stir it for 2-3 h, the reaction was monitored by TLC. The reaction mixture was quenched by saturated solution of NH_4Cl, then the solvent was evaporated under reduced pressure. The crude compound was dissolved in ethyl acetate and then extracted and then work up with H_2O, the procedure was repeated 2 times. The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude compound **S3** was used for the next step.

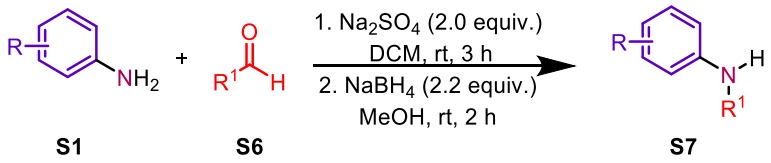
General procedure 2.2: *N*-Alkyl amines were prepared according to the literature procedure.[1]



S1 **S4** **S5**

To a solution of aniline **S1** (10 mmol, 1.0 equiv.) in ethanol (20 mL), add alkyl bromide **S4** (11 mmol, 1.1 equiv.) and potassium carbonate (11 mmol, 1.1 equiv.) at room temperature. Then reaction mixture was refluxed at 70 °C for 12 h. After complete conversion of aniline, the solvent was evaporated under reduced pressure. The crude compound was dissolved in ethyl acetate and then extracted and then work up with H_2O, the procedure was repeated 2 times. The organic layer was washed with brine and dried over Na_2SO_4. Filter the solution, concentrated using a rotatory evaporator under reduced pressure and purified by column chromatography.

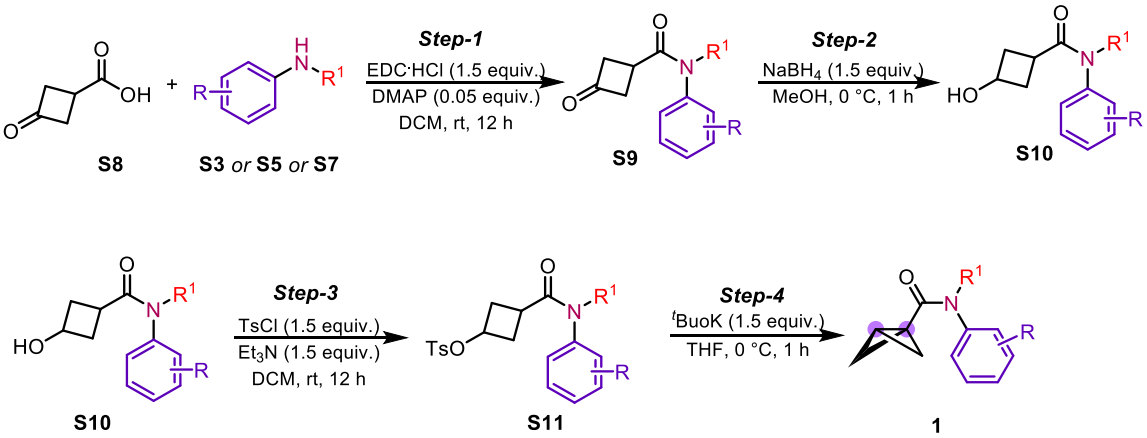
General procedure 2.3: *N*-Benzyl amines were prepared according to the literature procedure.[1]



Step-1: To a solution of aniline **S1** (10.1 mmol, 1.1 equiv.) in DCM (15 mL), sodium sulphate (2.0 equiv.) and aldehyde **S6** (9.42 mmol, 1.0 equiv.) were added with continuous stirring. Keep the reaction mixture stirring for 5-6 h at room temperature. The progress of the reaction was monitored by using TLC, after complete conversion of the starting material. The reaction mixture was filtered and concentrated under reduced pressure. The crude residue was used for the next step without further purification.

Step-2: The crude compound **S7** was dissolved in 15 mL methanol and stirred for a few minutes at 0 °C, then sodium borohydride (2.2 equiv.) was added portion wise with stirring, then the reaction mixture was stirred at room temperature for 2-3 h. The progress of the reaction was monitored by using TLC After complete conversion of the starting material, the reaction mixture was quenched with saturated solution of NH_4Cl, then the solvent was evaporated under reduced pressure. The crude compound was dissolved in ethyl acetate and then extracted and then work up with H_2O, the procedure was repeated 2 times. The organic layer was dried over Na_2SO_4, filtered, and organic residue was concentrated at reduced pressure. The crude reaction mixture was purified by column chromatography using ethyl acetate and hexanes to get the desired product **S7**.

General procedure 2.4: Bicyclobutanes **1** were prepared according to the literature procedure.[2]



Step-1: To an oven dried RB flask 3-oxocyclobutane-1-carboxylic acid **S8** (1.0 equiv.) was dissolved in dry DCM (0.3 M), *N*-alkyl aniline **S3** *or* **S5** *or* **S7** (1.0 equiv.), 4-dimethylaminopyridine (DMAP, 0.05 equiv.), and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC·HCl, 1.5 equiv.) were

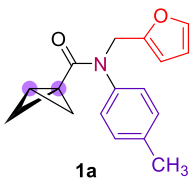
added sequentially. The reaction mixture was stirred for 12 h. After complete conversion of starting material monitored by TLC analysis and the reaction was quenched by water. The crude compound was diluted with DCM then extracted with DCM and H_2O the procedure was repeated 2 times. The organic layer was dried over Na_2SO_4, filtered, and organic residue was concentrated at reduced pressure and the crude compound **S9** was used for next step without further purification.

Step-2: The crude **S9** (1.0 equiv.) was dissolved in MeOH (0.3 M) and cooled to 0 °C. Then $NaBH_4$ (1.5 equiv.) was added portion wise. The reaction mixture was stirred for 1 h at 0 °C, the progress of the reaction was monitored by using TLC After complete conversion of the starting material, the reaction mixture was quenched with saturated solution of NH_4Cl, then the solvent was evaporated under reduced pressure. The crude compound was dissolved in ethyl acetate and then extracted and then work up with H_2O, the procedure was repeated 2 times. The organic layer was dried over Na_2SO_4, filtered, and organic residue was concentrated at reduced pressure and the crude compound **S10** was used for next step without further purification.

Step-3: The crude compound **S10** (1.0 equiv.) was dissolved in dry DCM (1.0 M), *p*-toluenesulfonyl chloride (TsCl) (1.5 equiv.) and Et_3N (1.5 equiv.) were added at 0 °C. The reaction mixture was stirred at room temperature for 12 hours. After complete conversion of starting material monitored by TLC analysis and the reaction was quenched by water. The crude compound was diluted with DCM then extracted with DCM and H_2O the procedure was repeated 2 times. The organic layer was dried over Na_2SO_4, filtered, and organic residue was concentrated at reduced pressure. The crude reaction mixture was purified by column chromatography column chromatography (Hexanes: ethyl acetate = 10:1 to 3:1) to afford **S11**.

Step-4: The solution of **S11** (1.0 equiv.) in dry THF (0.3 M) was cooled to 0 °C, and *t*BuOK (1.0 M in THF solution, 1.5 equiv.) was added dropwise under N_2 atmosphere. The reaction mixture was stirred for 1 h. The progress of the reaction was monitored by using TLC After complete conversion of the starting material, the reaction mixture was quenched with saturated solution of NH_4Cl, then organic residue was extracted with ethyl acetate and H_2O, the procedure was repeated 2 times. The organic layer was dried over Na_2SO_4, filtered, and organic residue was concentrated at reduced pressure. The residue was purified by column chromatography (Hexanes: ethyl acetate = 10:1 to 4:1) to afford **1**.

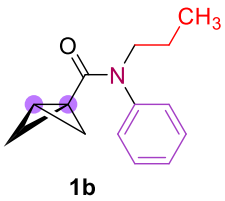
N-(Furan-2-ylmethyl)-*N*-(-tolyl)bicyclo[1.1.0]butane-1-carboxamide (**1a**)



1a

1a was prepared according to the general procedure **2.4** in 37% yield over 4 steps (436 mg) isolated yield. colorless oil. **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.30 (dd, *J* = 1.8, 2.7 Hz, 1H), 7.11-7.09 (m, 2H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.25-6.24 (m, 1H), 6.14-6.13 (m, 1H), 4.89 (s, 2H), 2.32 (s, 3H), 2.04-2.03 (m, 1H), 1.80 (s, 2H), 0.75 (s, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 171.7, 151.1, 142.0, 140.8, 136.8, 129.7, 127.6, 110.3, 108.7, 46.5, 37.1, 21.1, 17.0, 10.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{17}H_{18}NO_2$ 268.1332, Found 268.1340.

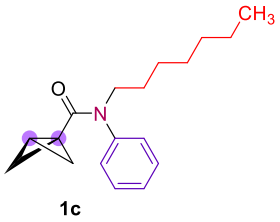
N-Phenyl-*N*-propylbicyclo[1.1.0]butane-1-carboxamide (**1b**)



1b

1b was prepared according to the general procedure **2.4** in 64% yield over 4 steps (601 mg) isolated yield. colorless oil. **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.39-7.36 (m, 2H), 7.29-7.24 (m, 3H), 3.75 (t, *J* = 7.6 Hz, 2H), 2.04-2.02 (m, 1H), 1.79 (d, *J* = 2.8 Hz, 2H), 1.59-1.54 (m, 2H), 0.89 (t, *J* = 7.4 Hz, 3H), 0.75 (d, *J* = 2.7 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 171.4, 143.7, 129.1, 127.9, 126.6, 51.5, 37.1, 20.9, 16.8, 11.3, 10.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{14}H_{18}NO$ 216.1383, Found 216.1383.

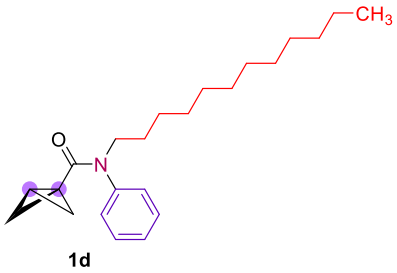
N-Heptyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide (**1c**)



1c

1c was prepared according to the general procedure **2.4** in 67% yield over 4 steps (800 mg) isolated yield. colorless oil. **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.40-7.37 (m, 2H), 7.27-7.24 (m, 3H), 3.77 (t, *J* = 7.5 Hz, 2H), 2.03-2.02 (m, 1H), 1.79 (d, *J* = 2.8 Hz, 2H), 1.57-1.52 (m, 2H), 1.27-1.24 (m, 8H), 0.86 (t, *J* = 7.3 Hz, 3H), 0.75 (s, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 171.3, 143.8, 129.1, 127.9, 126.6, 50.1, 37.1, 31.8, 29.1, 27.7, 26.9, 22.6, 16.8, 14.1, 10.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{26}NO$ 272.2009, Found 272.2011.

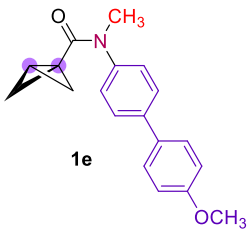
N-Dodecyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide (**1d**)



1d

1d was prepared according to the general procedure **2.4** in 50% yield over 4 steps (715 mg) isolated yield. colorless oil. **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.5; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.30-7.29 (m, 2H), 7.18-7.15 (m, 3H), 3.69 (t, *J* = 7.4 Hz, 2H), 1.94-1.93 (m, 1H), 1.71 (d, *J* = 2.9 Hz, 2H), 1.49-1.43 (m, 2H), 1.21-1.15 (m, 18H), 0.79 (t, *J* = 7.1 Hz, 3H), 0.66 (d, *J* = 1.7 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 171.1, 143.6, 128.9, 127.7, 126.4, 49.9, 36.9, 31.8, 29.5, 29.47, 29.42, 29.2, 27.6, 26.7, 16.5, 14.0, 10.0; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{23}H_{36}NO$ 342.2791, Found 342.2799.

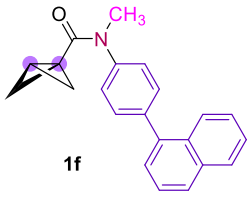
N-(4'-Methoxy-[1,1'-biphenyl]-4-yl)-*N*-methyl bicyclo[1.1.0]butane-1-carboxamide (**1e**)



1e

1e was prepared according to the general procedure **2.4** in 47% yield over 4 steps (654 mg) isolated yield. colorless oil. **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.25; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.55-7.52 (m, 4H), 7.30 (d, *J* = 7.9 Hz, 2H), 6.98 (d, *J* = 8.1 Hz, 2H), 3.85 (s, 3H), 3.37 (s, 3H), 2.05 (s, 1H), 1.82 (s, 2H), 0.84 (s, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 171.9, 159.4, 143.9, 138.9, 132.7, 128.1, 127.3, 127.2, 114.4, 55.5, 38.0, 37.4, 17.2, 10.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{20}NO_2$ 294.1489, Found 294.1485.

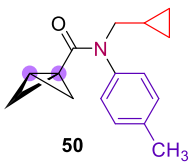
N-Methyl-*N*-(4-(naphthalen-1-yl)phenyl)bicyclo[1.1.0]butane-1-carboxamide (**1f**)



1f

1f was prepared according to the general procedure **2.4** in 18% yield over 4 steps (246 mg) isolated yield. colorless oil. **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.93-7.84 (m, 4H), 7.55-7.52 (m, 1H), 7.51 (d, *J* = 8.3 Hz, 2H), 7.47-7.42 (m, 2H), 7.39 (d, *J* = 8.3 Hz, 2H), 3.45 (s, 3H), 2.14-2.12 (m, 1H), 1.95 (d, *J* = 3.2 Hz, 2H), 0.91 (d, *J* = 3.2 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 172.0, 144.2, 139.3, 139.0, 133.9, 131.6, 130.8, 128.5, 128.0, 127.0, 126.7, 126.3, 126.0, 125.7, 125.4, 38.1, 37.4, 17.4, 10.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{22}H_{20}NO$ 314.1539, Found 314.1539.

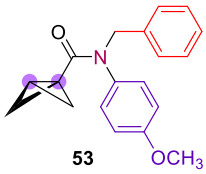
N-(Cyclopropylmethyl)-*N*-(p-tolyl)bicyclo[1.1.0]butane-1-carboxamide (**50**)



50

50 was prepared according to the general procedure **2.4** in 65% yield over 4 steps (686.1 mg) isolated yield. colorless oil. **TLC** (10% ethyl acetate in hexanes): R_f = 0.3; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.15-7.11 (m, 4H), 3.60 (d, *J* = 7.1 Hz, 2H), 2.34 (s, 3H), 2.04-1.98 (m, 1H), 1.77 (s, 2H), 1.0-0.95 (m, 1H), 0.72 (s, 2H), 0.39-0.37 (m, 2H), 0.12-0.09 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 171.5, 141.3, 136.5, 129.7, 128.1, 54.4, 37.0, 21.1, 16.4, 10.2, 9.9, 3.7; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{20}NO$ 242.1539, Found 242.1541.

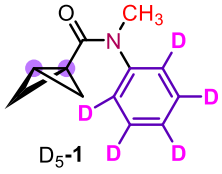
N-Benzyl-*N*-(4-methoxyphenyl)bicyclo[1.1.0]butane-1-carboxamide (**53**)



53

53 was prepared according to the general procedure **2.4** in 61% yield over 4 steps (782 mg) isolated yield. colorless oil. **TLC** (20% ethyl acetate in hexanes): R_f = 0.4; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.13-7.09 (m, 5H), 6.91 (d, *J* = 7.4 Hz, 2H), 6.69 (d, *J* = 7.8 Hz, 2H), 4.85 (s, 2H), 3.61 (s, 3H), 1.99 (s, 1H), 1.75 (s, 2H), 0.68 (s, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 171.2, 157.7, 137.3, 135.8, 128.6, 128.1, 127.9, 126.8, 113.8, 54.8, 53.2, 36.7, 16.2, 9.7; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{20}NO_2$ 294.1489, Found 294.1491.

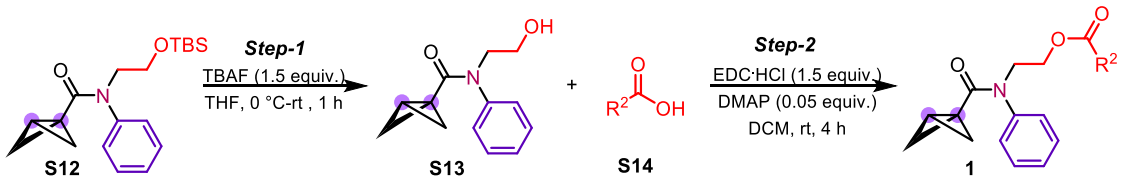
N-Methyl-*N*-(phenyl-D_5)bicyclo[1.1.0]butane-1-carboxamide (D_5-**1**)



D_5-**1**

D_5-**1** was prepared according to the general procedure **2.4** in 30% yield over 4 steps (230 mg) isolated yield. colorless oil. **TLC** (10% ethyl acetate in hexanes): R_f = 0.3; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 3.34 (s, 3H), 2.02-2.01 (m, 1H), 1.80 (d, *J* = 3.2 Hz, 2H), 0.77 (d, *J* = 3.2 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 171.8, 145.0, 129.1, 126.3, 115.1, 38.0, 37.1, 16.9, 10.0; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_9D_5NO$ 193.1384, Found 193.1392.

General procedure 2.5: Bicyclobutanes **1** were prepared according to the literature procedure.[2]

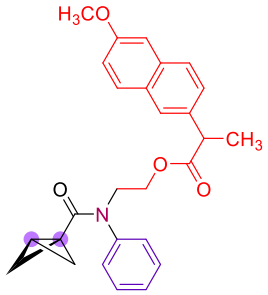


Step-1: *N*-(2-((Tert-butyldimethylsilyl)oxy)ethyl)-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **S12** (1.0 equiv.) in dry THF (0.3 M) was cooled to 0 °C, and TBAF (1.0 M in THF, 1.2 equiv.) was added dropwise. The reaction mixture was stirred at room temperature for 1 hour until TLC shows complete conversion of the **S12**. Then the reaction was quenched with saturated solution of NH_4Cl and extracted with ethyl acetate and water. The organic phase was dried over anhydrous Na_2SO_4, filtrated and concentrated under reduced

pressure. The crude reaction mixture was purified by column chromatography (Hexanes: ethyl acetate = 4:1 to 2:1) to afford **S13**.

Step-2: *N*-(2-Hydroxyethyl)-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **S13** (1.0 equiv.) was dissolved in DCM (0.3 M), carboxylic acid **S14** (1.2 equiv.), DMAP (0.05 equiv.) and EDC·HCl (1.5 equiv.) were added. The reaction mixture was stirred for 4 hours. After complete conversion of starting material monitored by TLC analysis and the reaction was quenched by water. The crude compound was diluted with DCM then extracted with DCM and H_2O the procedure was repeated 2 times. The organic layer was dried over Na_2SO_4, filtered, and organic residue was concentrated at reduced pressure and the residue was purified by column chromatography (Hexanes:ethyl acetate = 10:1 to 3:1) to afford **1**.

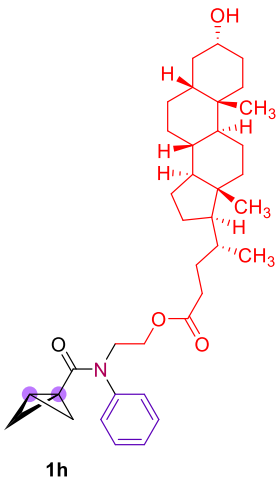
2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido) ethyl 2-(6-methoxynaphthalen-2-yl) propanoate (**1g**)



1g

1g was prepared according to the general procedure **2.5** in 63% yield (310 mg) isolated yield. colorless oil. **TLC** (20% ethyl acetate in hexanes): R_f = 0.45; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.67 (t, *J* = 8.5 Hz, 2H), 7.60 (s, 1H), 7.35-7.31 (m, 1H), 7.18-7.12 (m, 4H), 7.10 (d, *J* = 2.5 Hz, 1H), 7.06-7.02 (m, 2H), 4.30-4.21 (m, 2H), 4.06-3.92 (m, 2H), 3.89 (s, 3H), 3.73 (q, *J* = 7.2 Hz, 1H), 1.98-1.97 (m, 1H), 1.75-1.66 (m, 2H), 1.49 (d, *J* = 7.2 Hz, 3H), 0.71-0.68 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 174.4, 171.9, 157.7, 143.7, 135.6, 133.7, 129.3, 129.1, 128.9, 127.6, 127.2, 126.6, 126.3, 126.0, 119.0, 105.6, 62.2, 55.3, 48.8, 45.4, 37.1, 18.4, 17.4, 10.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{27}H_{28}NO_4$ 430.2013, Found 430.1219.

2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 3-hydroxy-10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)pentanoate (**1h**)

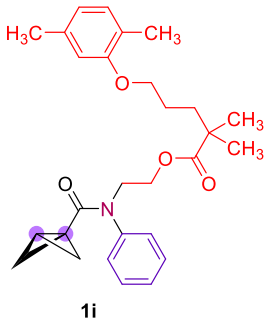


1h

1h was prepared according to the general procedure **2.5** in 35% yield (231 mg) isolated yield. colorless oil. **TLC** (30% ethyl acetate in hexanes): R_f = 0.2; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.37-7.35 (m, 2H), 7.26-7.23 (m, 3H), 4.26 (t, *J* = 5.9 Hz, 2H), 4.01 (t, *J* = 6.1 Hz, 2H), 3.63-3.59 (m, 1H), 2.18-2.14 (m, 1H), 2.07-2.02 (m, 2H), 1.95-1.91 (m, 1H), 1.83- 1.74 (m, 7H), 1.67-1.63 (m, 3H), 1.41-1.33 (m, 6H), 1.26-1.20 (m, 6H), 1.13-1.10 (m, 5H), 0.90 (s, 3H), 0.84 (d, *J* = 6.5 Hz, 3H), 0.76 (d, *J* = 2.0 Hz, 2H), 0.61 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 174.1, 172.0, 144.0, 129.9, 127.7, 126.8, 71.9, 61.9, 56.6, 56.0, 49.0, 42.8, 42.2, 40.5, 40.2, 37.2, 36.5, 35.9, 35.4, 35.3, 34.6, 31.1, 30.8, 30.6, 28.3, 27.3, 26.5, 24.3, 23.4, 20.9, 18.3, 17.6, 12.1, 10.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd

for $C_{37}H_{54}NO_4$ 576.4047, Found 576.4041.(Stereochemistry of **1h** same as the stereochemistry of commercial available lithocholic acid.)

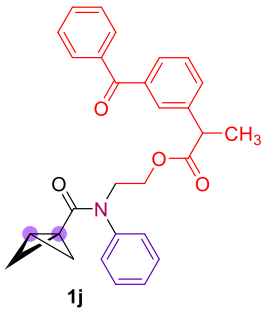
2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (**1i**)



1i

1i was prepared according to the general procedure **2.5** in 58% yield (299 mg) isolated yield. colorless oil. **TLC** (20% ethyl acetate in hexanes): R_f = 0.4; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.38-7.34 (m, 2H), 7.28-7.23 (m, 3H), 7.0 (d, *J* = 7.5 Hz, 1H), 6.65 (d, *J* = 7.5 Hz, 1H), 6.59 (s, 1H), 4.26 (t, *J* = 6.2 Hz, 2H), 4.05 (t, *J* = 6.0 Hz, 2H), 3.86 (t, *J* = 6.0 Hz, 2H), 2.30 (s, 3H), 2.16 (s, 3H), 2.08-2.05 (m, 1H), 1.79 (d, *J* = 1.9 Hz, 2H), 1.66-1.59 (m, 4H), 1.09 (s, 6H), 0.77 (d, *J* = 1.8 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.6, 172.0, 156.9, 143.7, 136.4, 130.3, 129.3, 127.7, 126.8, 123.5, 120.7, 111.9, 67.9, 62.2, 48.9, 42.0, 37.2, 36.9, 25.1, 25.0, 21.4, 17.5, 15.8, 10.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{36}NO_4$ 450.2639, Found 450.2641.

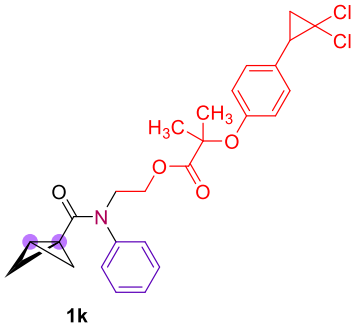
2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 2-(3-benzoylphenyl)propanoate (**1j**)



1j

1j was prepared according to the general procedure **2.5** in 53% yield (277 mg) isolated yield. colorless oil. **TLC** (20% ethyl acetate in hexanes): R_f = 0.6; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.78-7.76 (m, 2H), 7.67-7.66 (m, 2H), 7.60-7.56 (m, 1H), 7.48-7.45 (s, 3H), 7.42-7.39 (m, 1H), 7.31-7.27 (m, 2H), 7.22-7.18 (m, 1H), 7.13-7.11 (m, 2H), 4.32-4.19 (m, 2H), 4.08-3.94 (m, 2H), 3.64 (q, *J* = 7.2 Hz, 1H), 2.02-2.00 (m, 1H), 1.75-1.71 (m, 2H), 1.42 (d, *J* = 7.2 Hz, 3H), 0.72 (d, *J* = 5.1 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 196.5, 173.8, 172.0, 143.8, 140.8, 137.9, 137.5, 132.6, 131.7, 130.1, 129.3, 129.2, 129.1, 128.6, 128.4, 127.6, 126.8, 62.5, 48.8, 45.3, 37.2, 18.4, 17.7, 10.1 ; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{29}H_{28}NO_4$ 454.2013, Found 454.2010.

2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 2-(4-(2,2-dichlorocyclopropyl)phenoxy)-2-methylpropanoate (**1k**)

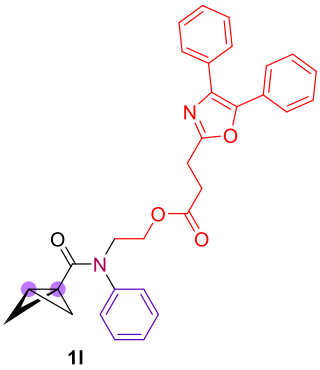


1k

1k was prepared according to the general procedure **2.5** in 47% yield (281 mg) isolated yield. colorless oil. **TLC** (20% ethyl acetate in hexanes): R_f = 0.5; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.32-7.29 (m, 2H), 7.22-7.20 (m, 3H), 7.06 (d, *J* = 8.1 Hz, 2H), 6.74 (d, *J* = 8.0 Hz, 2H), 4.33 (t, *J* = 5.5 Hz, 2H), 3.98 (t, *J* = 6.2 Hz, 2H), 2.81-2.77 (m, 1H), 2.02-1.96 (m, 1H), 1.92-1.89 (m, 1H), 1.76-1.71 (m, 3H), 1.46 (s, 6H), 0.72 (s, 2H); **^{13}C NMR** (126 MHz,

$CDCl_3$): δ 173.9, 172.0, 154.8, 143.7, 129.6, 129.2, 128.2, 127.7, 126.8, 118.8, 63.0, 60.9, 48.9, 37.1, 34.8, 25.8, 25.3, 25.2, 17.6, 10.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{26}H_{28}Cl_2NO_4$ 488.1390, Found 488.1386.

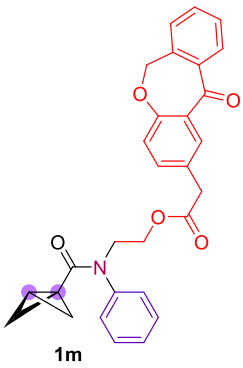
2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 3-(4,5-diphenyloxazol-2-yl)propanoate (**1l**)



1l

1l was prepared according to the general procedure **2.5** in 46% yield (315 mg) isolated yield. colorless oil. **TLC** (40% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.62-7.60 (m, 2H), 7.56-7.54 (m, 2H), 7.36-7.30 (m, 8H), 7.26-7.20 (m, 3H), 4.33 (t, *J* = 5.7 Hz, 2H), 4.04 (t, *J* = 5.7 Hz, 2H), 3.06 (t, *J* = 7.2 Hz, 2H), 2.76 (t, *J* = 7.1 Hz, 2H), 2.06-2.04 (m, 1H), 1.78 (d, *J* = 3.3 Hz, 2H), 0.75 (d, *J* = 2.1 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 172.0, 171.7, 161.7, 145.4, 143.8, 135.1, 132.4, 129.2, 128.9, 128.6, 128.59, 128.50, 128.1, 127.9, 127.7, 126.8, 126.4, 62.3, 48.8, 37.2, 30.9, 23.3, 17.6, 10.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{29}N_2O_4$ 493.2122, Found 493.2125.

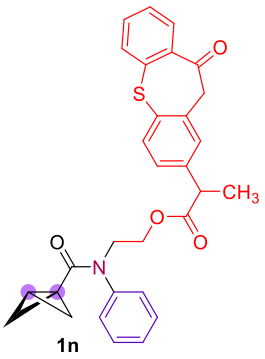
2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 2-(11-oxo-6,11-dihydrodibenzo[b,e]oxepin-2-yl)acetate (**1m**)



1m

1m was prepared according to the general procedure **2.5** in 38% yield (245 mg) isolated yield. colorless oil. **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.35; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.01 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.54-7.50 (m, 1H), 7.43 (t, *J* = 7.4 Hz, 1H), 7.35-7.29 (m, 4H), 7.23-7.18 (m, 3H), 6.97 (d, *J* = 7.3 Hz, 1H), 5.14 (s, 2H), 4.28 (t, *J* = 5.7 Hz, 2H), 4.01 (t, *J* = 5.9 Hz, 2H), 3.45 (s, 2H), 2.03-2.01 (m, 1H), 1.75 (d, *J* = 3.1 Hz, 2H), 0.73 (d, *J* = 1.9 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 190.8, 172.0, 171.1, 160.4, 143.8, 140.4, 136.4, 135.5, 132.8, 132.4, 129.4, 129.27, 129.25, 127.8, 127.63, 127.60, 126.7, 125.0, 121.0, 73.5, 62.5, 48.8, 39.9, 37.1, 17.7, 10.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{29}H_{26}NO_5$ 468.1805, Found 468.1803.

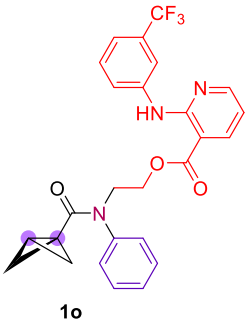
2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 2-(10-oxo-10,11-dihydrodibenzo[b,f]thiepin-2-yl)propanoate (**1n**)



1n

1n was prepared according to the general procedure **2.5** in 44% yield (304 mg) isolated yield. colorless oil. **TLC** (20% ethyl acetate in hexanes): R_f = 0.4; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.17 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.58-7.54 (m, 2H), 7.42-7.39 (m, 1H), 7.31-7.25 (m, 4H), 7.20-7.17 (m, 1H), 7.11-7.04 (m, 3H), 4.33 (s, 2H), 4.28-4.17 (m, 2H), 4.04-3.90 (m, 2H), 3.54 (q, *J* = 7.1 Hz, 1H), 2.01-1.99 (m, 1H), 1.75-1.67 (m, 2H), 1.37 (d, *J* = 7.15 Hz, 3H), 0.71 (d, *J* = 1.9 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 191.3, 173.7, 172.0, 143.7, 142.6, 140.2, 137.9, 136.2, 133.3, 132.6, 131.6, 131.5, 130.9, 129.2, 128.7, 127.6, 126.9, 126.8, 126.5, 62.5, 51.1, 48.7, 45.1, 37.2, 18.3, 17.6, 10.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{28}SNO_4$ 498.1734, Found 498.1743.

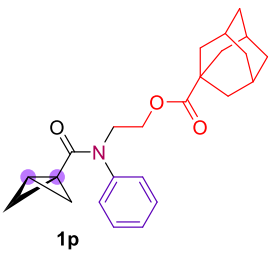
2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 2-((3-(trifluoromethyl)phenyl)amino)nicotinate (**1o**)



1o

1o was prepared according to the general procedure **2.5** in 55% yield (303 mg) isolated yield. colorless oil. **TLC** (30% ethyl acetate in hexanes): R_f = 0.3; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 10.2 (s, 1H), 8.33 (dd, J = 2.0, 4.7 Hz, 1H), 8.05 (s, 1H), 7.81-7.76 (m, 2H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.33-7.29 (m, 2H), 7.26-7.20 (m, 4H), 6.63 (dd, *J* = 4.7, 7.8 Hz, 1H), 4.51 (t, *J* = 5.3 Hz, 2H), 4.19 (t, *J* = 5.2 Hz, 2H), 2.07-2.04 (m, 1H), 1.77 (d, *J* = 3.2 Hz, 2H), 0.76 (d, *J* = 2.4 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 172.2, 167.2, 155.7, 153.1, 143.9, 140.4, 140.3, 131.2 (q, *J* = 32.3 Hz), 129.4, 129.2, 127.6, 126.8, 125.3 (q, *J* = 272.9 Hz), 123.5, 119.0 (q, *J* = 4.1 Hz), 117.1 (q, *J* = 4.6 Hz), 114.0, 107.2, 63.4, 48.7, 37.3, 17.9, 10.2; **^{19}F NMR** (471 MHz, $CDCl_3$): δ -62.49; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{26}H_{23}F_3N_3O_3$ 482.1686, Found 482.1694.

2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl (1*S*,3*S*)-adamantane-1-carboxylate (**1p**)

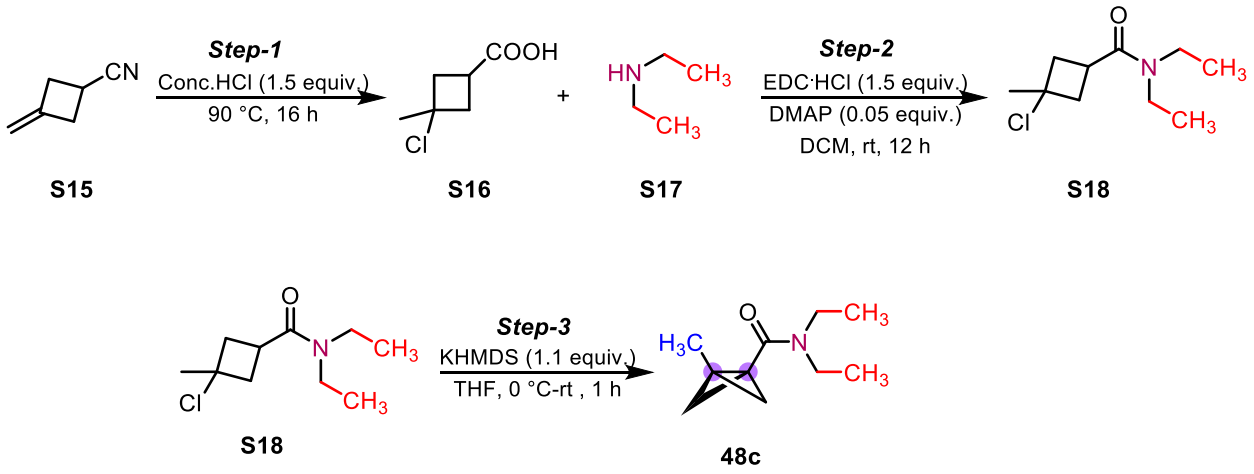


1p

1p was prepared according to the general procedure **2.5** in 67% yield (293 mg) isolated yield. colorless oil. **TLC** (20% ethyl acetate in hexanes): R_f = 0.4; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.37-7.34 (m, 2H), 7.27-7.22 (m, 3H), 4.23 (t, *J* = 6.2 Hz, 2H), 4.02 (t, *J* = 6.0 Hz, 2H), 2.04-2.02 (m, 1H), 1.94-1.89 (m, 3H), 1.78 (d, *J* = 2.1 Hz, 2H), 1.75-1.71 (m, 6H), 1.68-1.60 (m, 6H), 0.75 (d, *J* = 1.9 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.5, 171.9, 144.0, 129.9, 127.8, 126.7, 62.0,

49.0, 40.6, 38.6, 37.2, 36.5, 27.9, 17.3, 10.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{24}H_{30}NO_3$ 380.2220, Found 380.2218.

General procedure 2.6: 47c were prepared according to the literature procedure.[2]



Step-1: To a 100 mL RB flask equipped with a magnetic stir bar 3-methylenecyclobutanecarbonitrile **S15** (0.93 g, 10.0 mmol, 1.0 equiv.) and conc.HCl solution (10 mL) were added. The reaction mixture was heated to 90 °C (reflux) for 16 h, then cooled to room temperature, the solution was diluted with H_2O (25 mL). The organic residue was extracted with diethyl ether. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filter and concentrated using rotatory evaporator under reduced pressure to afford **S16** colorless oil, which was used directly used for next step without further purification.

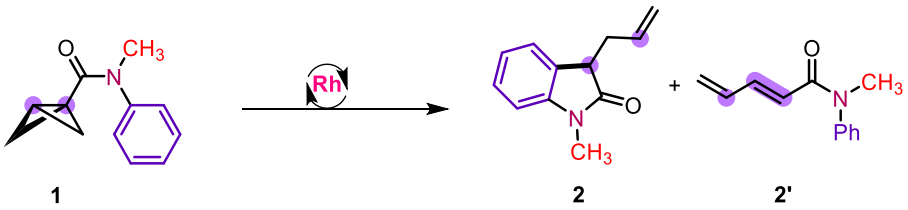
Step-2: To a 100 mL RB flask containing the above compound **S16** was added DCM (20 mL), and diethylamine **S17** (803 mg, 11 mmol, 1.1 equiv.), DMAP (61 mg, 0.5 mmol, 0.05 equiv.), EDC·HCl (2.9 g, 15 mmol, 1.5 equiv.) were added and the solution was stirred at room temperature for 12 h. The organic residue was extracted with DCM. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filter and concentrated using rotatory evaporator under reduced pressure to afford **S18** yellow oil, which was used directly in next step without purification.

Step-3: The above crude residue **S17** (10 mmol, 1.0 equiv.) was dissolved in THF (20 mL) then KHMDS (1.0 M in THF solution, 11 mL, 1.1 equiv.) was added dropwise to this solution at 0 °C. After stirring at room temperature for 1 hour, the reaction quenched with saturated solution of NH_4Cl (10 mL) and water (10 mL), and the organic residue was extracted with ethyl acetate. The combined organic layers were dried over anhydrous Na_2SO_4, filter and concentrated using rotatory evaporator under reduced pressure. The reaction mixture was purified by silica gel column chromatography (Hexanes: ethyl acetate = 90:10) to

afford *N*, *N*-diethyl-3-methylbicyclo[1.1.0]butane-1-carboxamide **47c** (568 mg, 34% yield over three steps) as a pale-yellow oil.

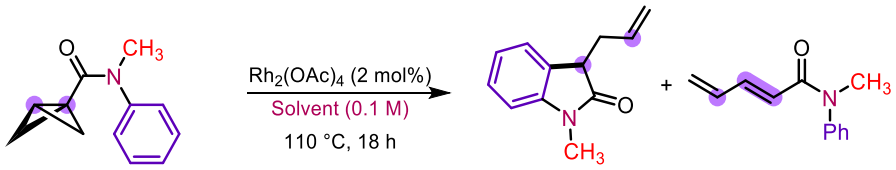
^{1}H NMR (500 MHz, $CDCl_3$): δ 3.61 (d, *J* = 6.5 Hz, 2H), 3.37 (t, *J* = 6.5 Hz, 2H), 1.99 (s, 2H), 1.52 (s, 3H), 1.16-1.10 (m, 8H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 170.3, 42.5, 39.7, 38.8, 22.6, 14.8, 13.2, 11.8, 10.9; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{10}H_{18}NO$ 168.1383, Found 168.1382.

3.0 Reaction Optimization.



1 **2** **2'**

3.1 Solvent optimization.



1 **2** **2'**

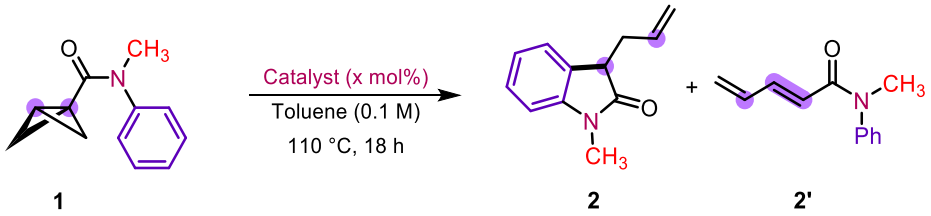
To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **1** (18.7 mg, 0.1 mmol, 1.0 equiv.) and $Rh_2(OAc)_4$ (0.88 mg, 0.002 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by solvent (0.1 M, 1 mL) was added under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 110 °C (using oil bath) for 18 h, the residue was diluted with ethyl acetate (5 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue was submitted for ^{1}H NMR analysis to determine the yield. The yield was determined by using CH_2Br_2 as internal standard.

Entry	Solvent	Yield of **2** (%) [a]	Yield of **3** (%) [a]
1	**Toluene**	**36%**	**12%**
2	ACN	17%	16%
3	1,4-Dioxane	28%	17%
4	Mesitylene	23%	10%

5	THF	ND	ND
6	DMF	ND	ND
7	DCM	16%	14%
8	DCE	32%	20%
9	Benzene	13%	9
10	CF_3-Benzene	28%	12%
11	HFIP	ND	ND
12	Chloro-Benzene	26%	18%
13	Xylene	30%	16%
14	HFIP:Toluene (1:1)	12%	14%

Reaction condition: **1** (0.1 mmol, 1.0 equiv.), $Rh_2(OAc)_4$ (2 mol%), Solvent (0.1 M, 1 mL), 110 °C for 18 h. [a]Yield determined by ^{1}H NMR using CH_2Br_2 as internal standard. ND = Not detected.

3.2 Catalyst optimization.



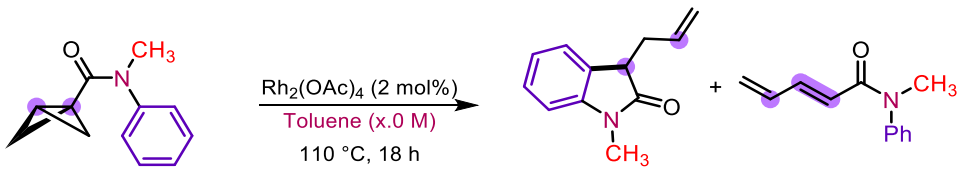
1 **2** **2'**

To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **1** (18.7 mg, 0.1 mmol, 1.0 equiv.) and Catalyst were added in glove box (argon atmosphere) followed by toluene (0.1 M, 1 mL) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 110 °C (using oil bath) for 18 h, the residue was diluted with ethyl acetate (5 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue was submitted for ^{1}H NMR analysis to determine the yield. The yield was determined by using CH_2Br_2 as internal standard.

Entry	Catalyst	Yield of **2** (%)[a]	Yield of **3** (%)[a]
1	$Cu(OTf)_2$ (10 mol%)	14%	12%
2	$Cu(CH_3CN)_4$ PF_6 (10 mol	ND	ND
3	CuI (10 mol%)	ND	ND
4	CuTC (10 mol%)	ND	ND
5	**$Rh_2(OAc)_4$ (2 mol%)**	**36%**	**12%**

Reaction condition: **1** (0.1 mmol, 1.0 equiv.), Catalyst (x mol%), Toluene (0.1 M, 1 mL), 110 °C for 18 h. [a]Yield determined by ^{1}H NMR using CH_2Br_2 as internal standard. ND = Not detected.

3.3 Concentration optimization.

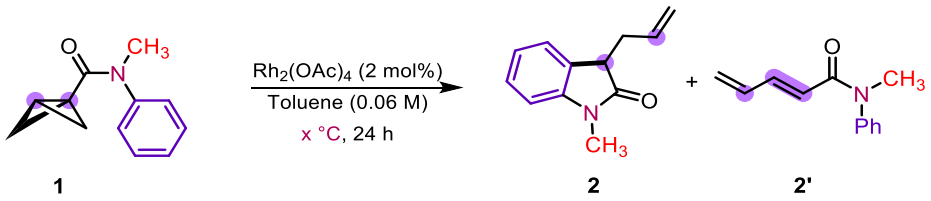


To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **1** (18.7 mg, 0.1 mmol, 1.0 equiv.) and $Rh_2(OAc)_4$ (0.88 mg, 0.002 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by toluene (x.0 M) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 110 °C (using oil bath) for 18 h, the residue was diluted with ethyl acetate (5 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue was submitted for ^{1}H NMR analysis to determine the yield. The yield was determined by using CH_2Br_2 as internal standard.

Entry	Concentration	Yield of **2** (%)[a]	Yield of **3** (%)[a]
1	0.1 M	36%	12%
2	0.05 M	40%	15%
3	0.06 M	50	22%
4 [b]	**0.06 M**	**60%**	**24%**

Reaction condition: **1** (0.1 mmol, 1.0 equiv.), $Rh_2(OAc)_4$ (2 mol%), Toluene, 110 °C for 18 h. [a]Yield determined by ^{1}H NMR using CH_2Br_2 as internal standard. ND = Not detected. [b]24 h.

3.4 Temperature optimization.



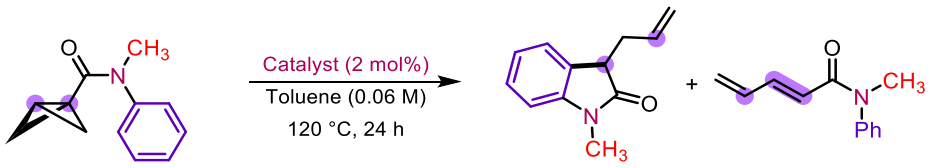
To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **1** (18.7 mg, 0.1 mmol, 1.0 equiv.) and $Rh_2(OAc)_4$ (0.88 mg, 0.002 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by toluene (1.5 mL, 0.06 M) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at x °C (using oil bath) for 24 h, the residue was diluted with ethyl acetate (5 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue

was submitted for ^{1}H NMR analysis to determine the yield. The yield was determined by using CH_2Br_2 as internal standard.

Entry	Temperature (x °C)	Yield of **2** (%)[a]	Yield of **3** (%)[a]
1	Room Temperature	NR	NR
2	40 °C	NR	NR
3	60 °C	NR	NR
4	80 °C	NR	NR
5	100 °C	39%	7%
5	110 °C	60%	24%
6	**120 °C**	**66%**	**24%**
7	130 °C	62%	30%
8	150 °C	54%	22%

Reaction condition: **1** (0.1 mmol, 1.0 equiv.), $Rh_2(OAc)_4$ (2 mol%), Toluene (0.06 M, 1.5 mL), x °C for 24 h. [a]Yield determined by ^{1}H NMR using CH_2Br_2 as internal standard. ND = Not detected. NR no reaction.

3.5 Catalyst optimization.



1 **2** **2'**

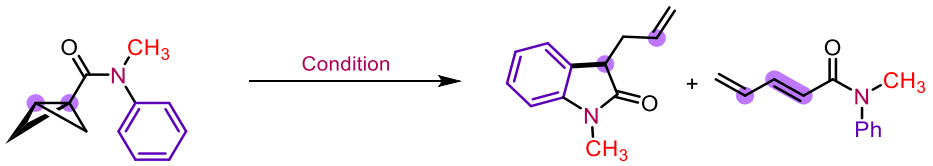
To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **1** (18.7 mg, 0.1 mmol, 1.0 equiv.) and Catalyst (2 mol%) were added in glove box (argon atmosphere) followed by toluene (0.06 M, 1.5 mL) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 110 °C (using oil bath) for 18 h, the residue was diluted with ethyl acetate (5 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue was submitted for ^{1}H NMR analysis to determine the yield. The yield was determined by using CH_2Br_2 as internal standard.

Entry	Catalyst	Yield of **2** (%)[a]	Yield of **3** (%)[a]
1	$Rh(PPh_3)_3Cl$	31%	16%
2	$Rh_2(esp)_2$	28%	24%
3	Rh_2 (Octonate)$_4$	38%	32%
4	$Rh_2(TFA)_4$	12%	8%
5	**$Rh_2(OAc)_4$**	**66%**	**24%**

6	$Rh(CO)_2Cl]_2$ (2 mol%), DPPE (4 mol %)	ND	ND
7	Without Catalyst	ND	ND

Reaction condition: **1** (0.1 mmol, 1.0 equiv.), Catalyst (2 mol%), Toluene (0.06 M, 1.5 mL), 120 °C for 24 h. [a]Yield determined by ^1H NMR using CH_2Br_2 as internal standard. ND = Not detected.

3.6 Nickel catalyst optimization.



1 **2** **2'**

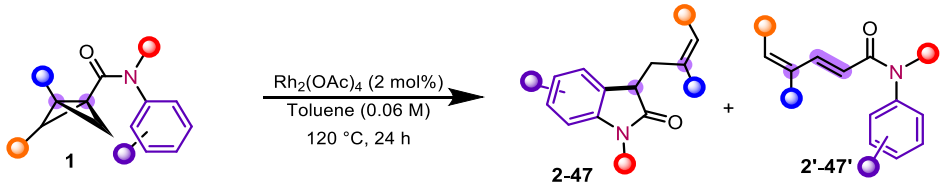
To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **1** (37.4 mg, 0.2 mmol, 1.0 equiv.) and Catalyst (2 mol%) were added in glove box (argon atmosphere) followed by toluene (0.06 M, 3 mL) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 24 h, the residue was diluted with ethyl acetate (5 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure to get the crude residue, purifications done by using column chromatography on silica gel.

Entry	**Condition**	Yield of **2**[a]	Yield of **2'**[a]
1	$Ni(COD)_2$ (10 mol%),	NR	NR
2	$Ni(COD)_2$ (10 mol%) *p*-tolyl phosphine (15 mol%) NaH (3.0 equiv.)	N.D	N.D
3	$Ni(COD)_2$ (10 mol%), p-tolyl phosphine (15 mol%) LiO^tBu (3.0 equiv.)	N.D	N.D
4	$Ni(COD)_2$ (10 mol%), Cs_2CO_3 (3.0 equiv.)	NR	NR
5	$Ni(COD)_2$ (10 mol%), *p*-tolyl phosphine (15 mol%), Cs_2CO_3 (3.0 equiv.)	NR	NR
6	$Ni(COD)_2$ (10 mol%), *p*-tolyl phosphine (15 mol%)	NR	NR
7	$Ni(COD)_2$ (10 mol%), PCy_3 (15 mol%, Cs_2CO_3 (3.0 equiv.)	NR	NR
8	$NiCl_2Dmg$ (10 mol%),	NR	NR

9	$NiCl_2$ glyme (10 mol%), *p*-tolyl phosphine (15 mol%), Cs_2CO_3 (3.0 equiv.)	NR	NR
10	$NiBr_2$ (10 mol%), Toluene (0.06 M)	Trace	Trace
11	$NiBr_2$ (10 mol%), *p*-tolyl phosphine (15 mol%, Cs_2CO_3 (3.0 equiv.)	27%	12%
12	$NiBr_2$ (10 mol%), Cs_2CO_3 (3.0 equiv.)	Trace	Trace
13	$NiBr_2$ (10 mol%), PCy_3(15 mol%, Cs_2CO_3 (3.0 equiv.)	20%	15%
14	**$NiBr_2$ (10 mol%), RuPhos (15 mol%, Cs_2CO_3 (3.0 equiv.)**	**29%**	**20%**
15	$NiBr_2$ (10 mol%), IPr NHC (15 mol%)	Trace	Trace
16	$NiBr_2$ (10 mol%), IPr-NHC (15 mol%, Cs_2CO_3 (3.0 equiv.)	15%	8%
17[b]	$Ni(COD)_2$ (10 mol%),	NR	NR
18[b]	$NiBr_2$ (10 mol%), PCy_3(15 mol%, Cs_2CO_3 (3.0 equiv.)	NR	NR
19[c]	$Ni(COD)_2$ (10 mol%)	NR	NR

Reaction condition: **1** (0.2 mmol, 1.0 equiv.), Catalyst (2 mol%), Toluene (0.06 M, 3.0 mL), 120 °C for 24 h. [a]Isolated Yield . ND = Not detected. NR = No reaction. [b]30 °C, [c]80 °C.

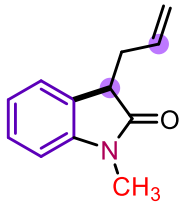
4.0 General procedure for Ring-Strain Enabled Transannulation of *N*-Aryl Bicyclo[1.1.0]butane Carboxamides via Rhodium (II)Carbene Intermediate



To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, bicyclobutane-1-carboxamide **1** (0.2 mmol, 1.0 equiv.) and $Rh_2(OAc)_4$ (1.8 mg, 0.004 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by addition of toluene (0.06 M, 3 mL) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 24 h, the residue was diluted with ethyl acetate (10 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue was purified by column chromatography on silica gel using ethyl acetate and hexanes as eluent to give the product **2-47** and **2'-47'**.

Spectral data of isolated compounds.

3-Allyl-1-methylindolin-2-one (**2**)



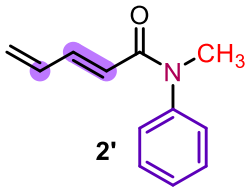
2

2 was prepared according to the general procedure **4** in 63% (23.5 mg) isolated yield. Yellow liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 93:7) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3

IR (neat); 3061, 2923, 1712, 1614, 1470, 1365, 1260 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.27-7.25 (m, 2H), 7.03-7.00 (m, 1H), 6.81 (d, *J* = 7.5 Hz, 1H), 5.75-5.69 (m, 1H), 5.10-5.01 (m, 2H), 3.47 (dd, *J* = 2.7, 6.9 Hz, 1H), 3.18 (s, 3H), 2.84-2.78 (m, 1H), 2.56-2.51 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.2, 144.3, 134.1, 128.7, 128.0, 124.2, 122.3, 118.0, 108.0, 45.2, 34.9, 26.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{14}NO$ 188.1070, Found 188.1079.

The Spectral data matched with the reported literature.[3]

(*E*)-*N*-Methyl-*N*-phenylpenta-2,4-dienamide (**2'**)

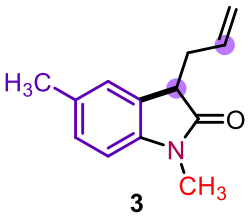


2'

2' was prepared according to the general procedure **4** in 18% (6.7 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 92:8) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.25

IR (neat); 3061, 2923, 1707, 1614, 1470, 1365, 1260 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.43-7.39 (m, 2H), 7.35-7.32 (m, 1H), 7.29-7.26 (m, 1H), 7.18-7.17 (m, 2H), 6.28-6.21 (m, 1H), 5.84 (d, *J* = 14.9 Hz, 1H), 5.54-5.50 (m, 1H), 5.36-5.32 (m, 1H), 3.35 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 166.2, 143.7, 142.1, 135.2, 129.7, 127.6, 127.4, 124.1, 122.7, 37.6; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{14}NO$ 188.1070, Found 188.1073.

3-Allyl-1,5-dimethylindolin-2-one (**3**)

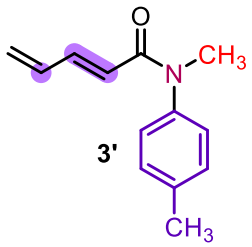


3

3 was prepared according to the general procedure **4** in 74% (29.7 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.35

IR (neat); 3079, 2915, 1708, 1622, 1497, 1355, 1259 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.10-7.06 (m, 2H), 6.71 (d, *J* = 7.5 Hz, 1H), 5.79-5.70 (m, 1H), 5.13-5.02 (m, 2H), 3.45 (dd, *J* = 2.7, 7.6 Hz, 1H), 3.17 (s, 3H), 2.83-2.78 (m, 1H), 2.56-2.50 (m, 1H), 2.33 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.2, 142.0, 134.3, 131.8, 128.8, 128.2, 125.1, 117.9, 107.7, 45.3, 35.0, 26.2, 21.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{16}NO$ 202.1226, Found 202.1232.

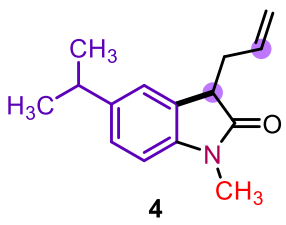
(*E*)-*N*-Methyl-*N*-(p-tolyl)penta-2,4-dienamide (**3'**)



3' was prepared according to the general procedure **4** in 14% (5.6 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 91:9) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3

IR (neat); 2922, 1724, 1651, 1592, 1425, 1373, 1270cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.23 (d, *J* = 3.9 Hz, 1H), 7.19 (d, *J* = 7.9 Hz, 2H), 7.04 (d, *J* = 8.3 Hz, 2H), 6.27-6.19 (m, 1H), 5.83 (d, *J* = 14.9 Hz, 1H), 5.49 (dd, *J* = 16.9, 0.7 Hz, 1H), 5.31 (d, *J* = 11.2 Hz, 1H), 3.31 (s, 3H), 2.37 (s, 3H).; **^{13}C NMR** (126 MHz, $CDCl_3$): 166.2, 141.8, 141.0, 137.5, 135.2, 130.2, 127.1, 123.9, 122.8, 37.5, 21.1.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{16}NO$ 202.1226, Found 202.1228.

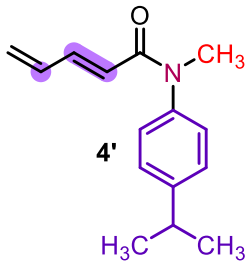
3-Allyl-5-isopropyl-1-methylindolin-2-one (**4**)



4 was prepared according to the general procedure **4** in 68% (31.1 mg) isolated yield. colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 95:5) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3079, 2935, 1734, 1624, 1495, 1352, 1284 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.16-7.11 (m, 2H), 6.74 (d, *J* = 7.5 Hz, 1H), 5.82-5.73 (m, 1H), 5.12-5.08 (m, 1H), 5.06-50.4 (m, 1H), 3.46 (dd, *J* = 2.7, 7.6 Hz, 1H), 3.18 (s, 3H), 2.91-2.80 (m, 2H), 2.55-2.49 (m, 1H), 1.24 (d, *J* = 2.2 Hz, 3H), 1.23 (d, *J* = 2.2 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.4, 143.2, 142.3, 134.5, 128.8, 125.7, 122.6, 117.9, 107.7, 45.4, 35.1, 34.0, 26.3, 24.4(3), 24.4(1); **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{20}NO$ 230.1539, Found 230.1542.

(*E*)-*N*-(4-isopropylphenyl)-*N*-methylpenta-2,4-dienamide (**4'**)

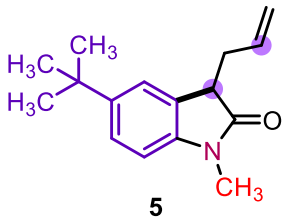


4' was prepared according to the general procedure **4** in 20% (9.1 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.35

IR (neat); 2960, 1657, 1623, 1599, 1510, 1382, 1278 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.25 (d, *J* = 7.6 Hz, 3H), 7.09 (d, *J* = 7.9 Hz, 2H), 6.27 (dd, *J* = 17.6, 9.4 Hz, 1H), 5.87 (d, *J* = 14.8 Hz, 1H), 5.52 (d, *J* = 16.9 Hz, 1H), 5.33 (d, *J* = 9.9 Hz, 1H), 3.34 (s, 3H), 2.95 (dt, *J* = 13.4, 6.6 Hz, 1H), 1.28 (d, *J* = 6.9 Hz, 6H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 166.3, 148.4,

141.9, 141.2, 136.3, 127.6, 127.2, 123.9, 122.8, 37.6, 33.8, 24.0. ; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{20}NO$ 230.1539, Found 230.1550.

3-Allyl-5-(tert-butyl)-1-methylindolin-2-one (**5**)

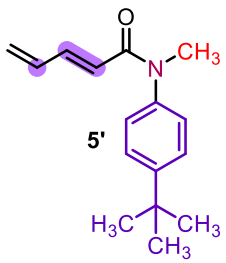


5

5 was prepared according to the general procedure **4** in 70% (34.0 mg) isolated yield. colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 95:5) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3076, 2958, 1709, 1621, 1498, 1368, 1267 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.34-7.33 (m, 1H), 7.31-7.28 (m, 1H), 6.74 (d, *J* = 7.4 Hz, 1H), 5.83-5.75 (m, 1H), 5.12-5.06 (m, 2H), 3.46 (dd, *J* = 2.7, 7.6 Hz, 1H), 3.18 (s, 3H), 2.87-2.81 (m, 1H), 2.54-2.48 (m, 1H), 1.31 (s, 9H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.4, 145.5, 142.0, 134.6, 128.5, 124.4, 121.7, 117.9, 107.3, 45.5, 35.2, 34.6, 31.7, 26.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{22}NO$ 244.1696, Found 244.1698.

(*E*)-*N*-(4-(tert-butyl)phenyl)-*N*-methylpenta-2,4-dienamide (**5'**)

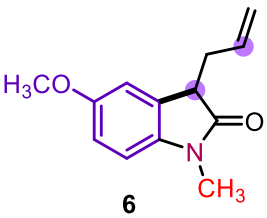


5'

5' was prepared according to the general procedure **4** in 17% (8.2 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.35

IR (neat); 2962, 1650, 1617, 1592, 1510, 1365, 1273 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.40 (d, *J* = 8.7 Hz, 2H), 7.31-7.21 (m, 1H), 7.08 (d, *J* = 8.1 Hz, 2H), 6.27 (dt, *J* = 16.9, 10.5 Hz, 1H), 5.87 (d, *J* = 15.0 Hz, 1H), 5.55-5.47 (m, 1H), 5.36 - 5.27 (m, 1H), 3.33 (s, 3H), 1.34 (s, 9H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 166.3, 150.7, 141.9, 140.9, 136.3, 126.8, 126.5, 123.9, 122.9, 37.5, 34.7, 31.4 ; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{22}NO$ 244.1696, Found 244.1696.

3-Allyl-5-methoxy-1-methylindolin-2-one (**6**)



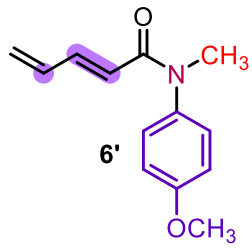
6

6 was prepared according to the general procedure **4** in 58% (25.1 mg) isolated yield. yellow liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 92:8) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.2

IR (neat); 3062, 2918, 1712, 1618, 1472, 1365, 1262 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 6.91 (dd, *J* = 2.7, 8.1 Hz, 1H), 6.80-6.78 (m, 1H), 6.71 (d, *J* = 7.3 Hz, 1H), 5.79-5.70 (m, 1H), 5.12-5.03 (m, 2H), 3.78 (s, 3H), 3.45 (dd, *J* = 2.7, 7.6 Hz, 1H), 3.17 (s, 3H), 2.84-2.79 (m, 1H), 2.55-2.50 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 176.9, 155.8, 138.0, 134.2, 130.1, 118.1, 112.07, 112.06, 108.1,

55.9, 45.6, 35.0, 26.3, ; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{16}NO_2$ 218.1176, Found 218.1178.

(*E*)-*N*-(4-Methoxyphenyl)-*N*-methylpenta-2,4-dienamide (**6'**)

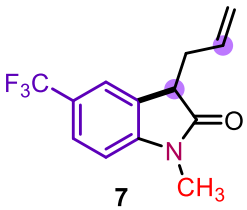


6'

6' was prepared according to the general procedure **4** in 16% (6.9 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 91:9) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.40

IR (neat); 2975, 1637, 1563, 1469, 1433, 1368, 1253 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.27 (dd, *J* = 12.2, 9.2 Hz, 1H), 7.11 (d, *J* = 8.2 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 6.33-6.20 (m, 1H), 5.85 (d, *J* = 14.9 Hz, 1H), 5.53 (d, *J* = 16.9 Hz, 1H), 5.35 (d, *J* = 9.9 Hz, 1H), 3.85 (s, 3H), 3.33 (s, 3H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 166.4, 158.9, 141.9, 136.4, 136.3, 128.5, 123.9, 122.7, 114.8, 55.6, 37.7.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{16}NO_2$ 218.1176, Found 218.1178.

3-Allyl-1-methyl-5-(trifluoromethyl)indolin-2-one (**7**)

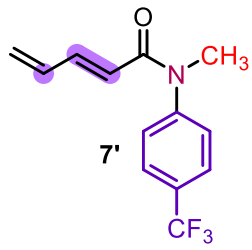


7

7 was prepared according to the general procedure **4** in 65% (33.1 mg) isolated yield. colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.35

IR (neat); 3076, 2919, 1722, 1624, 1504, 1375, 1287 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.57-7.55 (m, 1H), 7.51 (s, 1H), 6.89 (d, *J* = 8.7 Hz, 1H), 5.77-5.68 (m, 1H), 5.13-5.06 (m, 2H), 3.53 (dd, *J* = 2.7, 7.5 Hz, 1H), 3.23 (s, 3H), 2.87-2.82 (m, 1H), 2.59-2.50 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.1, 147.3, 133.5, 129.2, 125.9 (q, J_{CF} = 4.5 Hz), 124.7 (q, J_{CF} = 32.4 Hz), 123.4 (q, J_{CF} = 277.9 Hz), 121.2 (q, J_{CF} = 3.8 Hz), 118.7, 107.7, 45.0, 34.8, 26.5; **^{19}F NMR** (471 MHz, $CDCl_3$): δ -61.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{13}F_3NO$ 256.0944, Found 256.0945.

(*E*)-*N*-Methyl-*N*-(4-(trifluoromethyl)phenyl)penta-2,4-dienamide (**7'**)



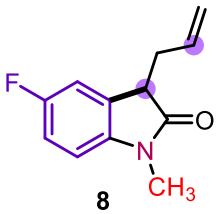
7'

7' was prepared according to the general procedure **4** in 16% (8.1 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 93:7) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.40

IR (neat); 2931, 1724, 1655, 1609, 1416, 1333, 1242 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.63 (d, *J* = 7.7 Hz, 2H), 7.27-7.21 (m, 3H), 6.34-6.15 (m, 1H), 5.78 (d,

J = 14.8 Hz, 1H), 5.51 (d, J = 16.9 Hz, 1H), 5.34 (d, J = 9.9 Hz, 1H), 3.33 (s, 3H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 166.0, 146.9, 143.1, 135.0, 129.6 (q, J = 10.0 Hz), 127.6, 126.8 (q, J = 3.6 Hz), 124.9, 122.1, 37.4.; **^{19}F NMR** (471 MHz, $CDCl_3$): δ -62.4; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{13}F_3NO$ 256.0944, Found 256.0942.

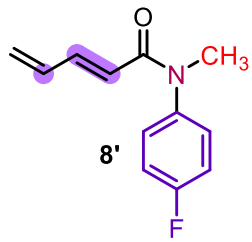
3-Allyl-5-fluoro-1-methylindolin-2-one (**8**)



8

8 was prepared according to the general procedure **4** in 61% (25.0 mg) isolated yield. colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.35 **IR** (neat); 3082, 2922, 1708, 1624, 1492, 1370, 1251 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.05-7.02 (m, 1H), 6.99-6.95 (m, 1H), 6.72 (dd, J = 5.5, 8.4 Hz, 1H), 5.77-5.69 (m, 1H), 5.13-5.06 (m, 2H), 3.47 (dd, J = 2.7, 7.5 Hz, 1H), 3.19 (s, 3H), 2.85-2.79 (m, 1H), 2.55-2.49 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 176.9, 160.1 (d, J_{CF} = 240.5 Hz), 140.3, 133.8, 130.3 (d, J_{CF} = 8.5 Hz), 118.5, 114.3 (d, J_{CF} = 23.5 Hz), 112.6 (d, J_{CF} = 24.8 Hz), 108.3, 45.5, 34.9, 26.4; **^{19}F NMR** (471 MHz, $CDCl_3$): δ -120.9; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{13}FNO$ 206.0976, Found 206.0980.

(*E*)-*N*-(4-fluorophenyl)-*N*-methylpenta-2,4-dienamide (**8'**)

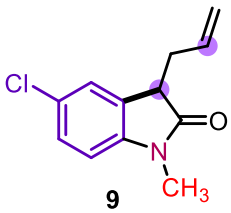


8'

8' was prepared according to the general procedure **4** in 28% (11.4 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 93:7) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.40

IR (neat); 2917, 1704, 1637, 1604, 1417, 1343, 1262 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.28-7.21 (m, 1H), 7.17-7.12 (m, 2H), 7.11-7.06 (m, 2H), 6.24 (dt, J = 16.9, 10.5 Hz, 1H), 5.77 (d, J = 14.8 Hz, 1H), 5.54-5.48 (m, 1H), 5.34 (dd, J = 10.0, 0.5 Hz, 1H), 3.31 (s, 3H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 166.1, 162.4 (d, J = 246.2 Hz), 142.5, 139.7 (d, J = 3.0 Hz), 135.1, 129.1 (d, J = 8.4 Hz), 124.4, 122.2, 116.6 (d, J = 35.1 Hz), 37.6.; **^{19}F NMR** (471 MHz, $CDCl_3$): δ -113.5; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{13}FNO$ 206.0976, Found 206.0976.

3-Allyl-5-chloro-1-methylindolin-2-one (**9**)

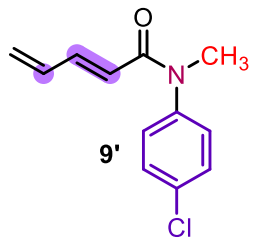


9

9 was prepared according to the general procedure **4** in 73% (32.2 mg) isolated yield. colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 95:5) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3073, 2927, 1713, 1610, 1488, 1366, 1265 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.26-7.24 (m, 2H), 6.74 (d, *J* = 7.4 Hz, 1H), 5.76-5.68 (m, 1H), 5.14-5.05 (m, 2H), 3.47 (dd, *J* = 2.6, 7.6 Hz, 1H), 3.18 (s, 3H), 2.84-2.78 (m, 1H), 2.56-2.50 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 176.7, 143.0, 133.7, 130.4, 128.0, 127.7, 124.7, 118.6, 108.9, 45.3, 34.8, 26.4; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{13}ClNO$ 222.0680, Found 222.0684.

(*E*)-*N*-(4-chlorophenyl)-*N*-methylpenta-2,4-dienamide (**9'**)

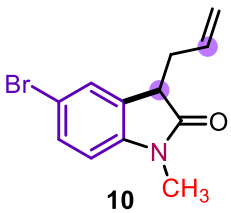


9'

9' was prepared according to the general procedure **4** in 17% (7.5 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): R_f = 0.40

IR (neat); 2912, 1701, 1627, 1468, 1346, 1245 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.38 (d, *J* = 7.9 Hz, 2H), 7.25 (t, *J* = 12.9 Hz, 1H), 7.12 (d, *J* = 7.8 Hz, 2H), 6.34-6.21 (m, 1H), 5.81 (d, *J* = 14.3 Hz, 1H), 5.53 (d, *J* = 16.9 Hz, 1H), 5.36 (d, *J* = 9.9 Hz, 1H), 3.32 (s, 3H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 166.1, 142.6, 142.2, 135.1, 133.4, 129.9, 128.7, 124.6, 122.2, 37.5.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{13}ClNO$ 222.0680, Found 222.0688.

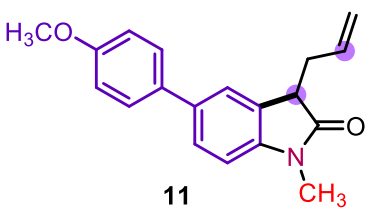
3-Allyl-5-bromo-1-methylindolin-2-one (**10**)



10

10 was prepared according to the general procedure **4** in 71% (37.6 mg) isolated yield. White solid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 95:5) as the eluent, **TLC** (10% ethyl acetate in hexanes): R_f = 0.4 **M.P.** 97-98 °C; **IR** (neat); 3082, 2922, 1713, 1689, 1487, 1364, 1265 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.41-7.38 (m, 2H), 6.68 (d, *J* = 7.5 Hz, 1H), 5.75-5.67 (m, 1H), 5.13-5.06 (m, 2H), 3.48 (dd, *J* = 2.8, 7.5 Hz, 1H), 3.17 (s, 3H), 2.83-2.77 (m, 1H), 2.56-2.49 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 176.6, 143.4, 133.6, 130.9, 130.7, 127.4, 118.6, 115.0, 109.4, 45.2, 34.8, 26.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{13}BrNO$ 266.0175, Found 266.0178.

3-Allyl-5-(4-methoxyphenyl)-1-methylindolin-2-one (**11**)



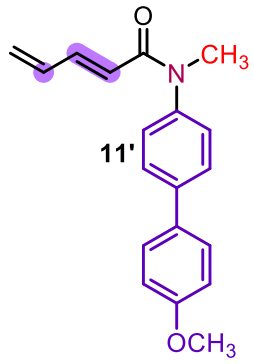
11

11 was prepared according to the general procedure **4** in 46% (8.9 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 92:8) as the eluent, **TLC** (20% ethyl acetate in hexanes): R_f = 0.5

IR (neat); 3067, 2928, 1712, 1622, 1475, 1341, 1257 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.48-7.44 (m, 4H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 7.9 Hz, 1H), 5.83-5.75 (m, 1H),

5.15-5.11 (m, 1H), 5.08-5.06 (m, 1H), 3.85 (s, 3H), 3.54 (dd, *J* = 3.8, 6.9 Hz, 1H), 3.23 (s, 3H), 2.90-2.84 (m, 1H), 2.61-2.54 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.3, 159.0, 143.3, 135.5, 134.3, 133.7, 129.3, 127.9, 126.4, 122.9, 118.2, 114.4, 108.2, 55.5, 45.4, 35.1, 26.4; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{20}NO_2$ 294.1489, Found 294.1490.

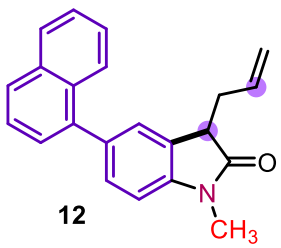
(*E*)-*N*-(4'-methoxy-[1,1'-biphenyl]-4-yl)-*N*-methylpenta-2,4-dienamide (**11'**)



11' was prepared according to the general procedure **4** in 19% (11.1 mg) isolated yield. White solid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 90:10) as the eluent, **TLC** (20% ethyl acetate in hexanes): R_f = 0.55

M.P. 122-124 °C; **IR** (neat); 2951, 1647, 1612, 1586, 1496, 1354, 1245 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.55 (d, *J* = 7.9 Hz, 2H), 7.51 (d, *J* = 7.9 Hz, 2H), 7.25 (dd, *J* = 10.9, 7.8 Hz, 1H), 7.18 (d, *J* = 7.8 Hz, 2H), 6.97 (d, *J* = 7.9 Hz, 2H), 6.31-6.22 (m, 1H), 5.91 (d, *J* = 14.8 Hz, 1H), 5.50 (d, *J* = 16.9 Hz, 1H), 5.32 (d, *J* = 9.9 Hz, 1H), 3.83 (s, 3H), 3.35 (s, 3H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 166.2, 159.5, 142.2, 142.1, 140.1, 135.2, 132.5, 128.1, 127.7, 127.6, 124.1, 122.8, 114.4, 55.4, 37.5.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{14}NO$ 294.1489, Found 294.1493.

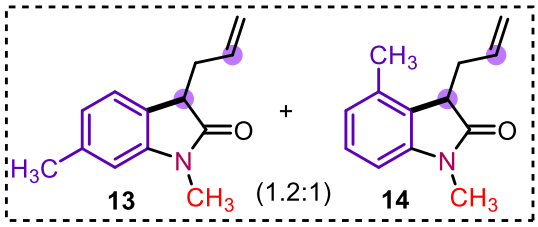
3-Allyl-1-methyl-5-(naphthalen-1-yl)indolin-2-one (**12**)



12 was prepared according to the general procedure **4** in 37% (23.17 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 90:10) as the eluent, **TLC** (20% ethyl acetate in hexanes): R_f = 0.4

IR (neat); 3024, 2961, 1708, 1614, 1484, 1353, 1278 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.92-7.85 (m, 3H), 7.53-7.49 (m, 2H), 7.42-7.40 (m, 4H), 6.95 (d, *J* = 7.9 Hz, 1H), 5.86-5.75 (m, 1H), 5.16-5.12 (m, 1H), 5.06-5.04 (m, 1H), 3.59 (dd, *J* = 4.2, 6.9 Hz, 1H), 3.28 (s, 3H), 2.90-2.85 (m, 1H), 2.65-2.59 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.4, 143.7, 140.0, 135.0, 134.2, 134.0, 131.8, 129.7, 128.7, 128.5, 127.7, 127.0, 126.2, 126.1, 126.0, 125.9, 125.5, 118.2, 107.8, 45.4, 35.2, 26.4; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{22}H_{20}NO$ 314.1539, Found 314.1539.

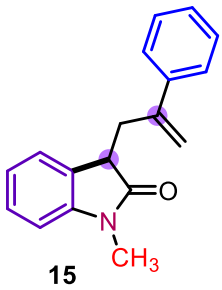
3-Allyl-1,6-dimethylindolin-2-one (**13**) and 3-Allyl-1,4-dimethylindolin-2-one (**14**)



13&14 (1.2:1) was prepared according to the general procedure **4** in 74% (29.7 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 96:4) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.5

IR (neat); 3074, 2956, 1714, 1620, 1496, 1358, 1251 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.19-7.14 (m, 1H), 6.83 (d, *J* = 7.5 Hz, 1H), 6.64 (t, *J* = 7.1 Hz, 1H), 5.79-5.70 (m, 0.4H), 5.45-5.36 (m, 0.52H), 5.11-5.00 (m, 1.48H), 4.88-4.85 (m, .53H), 3.54 (dd, *J* = 2.7, 7.4 Hz, 0.54H), 3.47 (dd, *J* = 2.7, 7.4 Hz, 0.43H), 3.18 (s, 3H), 2.91-2.78 (m, 1.5H), 2.53-2.44 (m, 0.5H), 2.38 (s, 1.3H), 2.34 (s, 1.7H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.6, 177.4, 144.6, 144.5, 138.1, 134.4, 134.3, 132.8, 128.0, 126.1, 125.7, 124.3, 124.0, 122.8, 117.9, 109.0, 105.6; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{16}NO$ 202.1226, Found 202.1226.

1-Methyl-3-(2-phenylallyl)indolin-2-oneone (**15**)

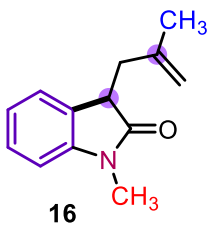


15

15 was prepared according to the general procedure **4** in 63% (33.15 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 84:16) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3014, 2928, 1716, 1622, 1470 1357, 1242 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.49-7.47 (m, 2H), 7.37-7.33 (m, 2H), 7.30-7.28 (m, 1H), 7.24-7.22 (m, 1H), 7.17 (d, *J* = 7.2 Hz, 1H), 6.98-6.96 (m, 1H), 6.78 (d, *J* = 7.1 Hz, 1H), 5.39 (s, 1H), 5.11 (s, 1H), 3.52-3.45 (m, 2H), 3.14 (s, 3H), 2.66-2.60 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.5, 145.5, 144.2, 139.8, 128.9, 128.6, 127.9, 126.7, 124.8, 122.1, 115.7, 107.9, 43.6, 37.2, 26.2 (2 aromatic carbons overlapped); **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{18}NO$ 264.1383, Found 264.1389.

1-Methyl-3-(2-phenylallyl)indolin-2-oneone (**16**)

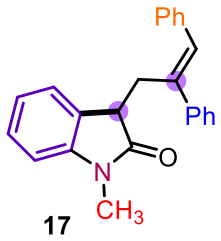


16

16 was prepared according to the general procedure **4** in 53% (22.4 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 92:8) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3029, 2978, 1709, 1614, 1457 1331, 1290 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.31-7.25 (m, 2H), 7.03 (t, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 7.7 Hz, 1H), 4.95 (s, 1H), 4.77 (s, 1H), 3.56 (dd, *J* = 4.4, 7.8 Hz, 1H), 3.23 (s, 3H), 2.86-2.83 (m, 1H), 2.37-2.32 (m, 1H), 1.83 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.6, 144.1, 142.0, 129.0, 127.9, 124.5, 122.2, 113.5, 107.9, 43.5, 39.1, 26.3, 22.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{16}NO$ 202.1226, Found 202.1226.

1-Methyl-3-(2-phenylallyl)indolin-2-oneone (**17**)

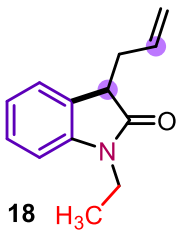


17

17 was prepared according to the general procedure **4** in 46% (31.2 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 93:7) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3017, 2932, 1718, 1634, 1468, 1361, 1268 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.33 (d, *J* = 7.4 Hz, 1H), 7.28 (dd, *J* = 6.9, 1.4 Hz, 3H), 7.26 -7.23 (m, 1H), 7.20-7.17 (m, 2H), 7.10 (d, *J* = 7.3 Hz, 3H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.95-6.91 (m, 2H), 6.78 (d, *J* = 7.7 Hz, 1H), 6.47 (s, 1H), 3.44-3.36 (m, 2), 3.10 (s, 3H), 2.79 (dd, *J* = 15.5, 10.8 Hz, 1H).; **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.4, 144.4, 139.2, 137.0, 129.6, 129.26, 129.23, 129.1, 128.8, 128.7, 128.0, 127.9, 127.5, 126.7, 124.8, 122.1, 108.0, 43.5, 41.7, 26.2 ; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{24}H_{22}NO$ 340.1696, Found 340.1698.

3-Allyl-1-ethylindolin-2-one (**18**)

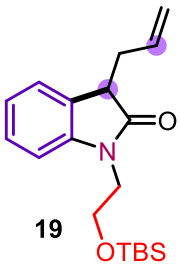


18

18 was prepared according to the general procedure **4** in 78% (31.3 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

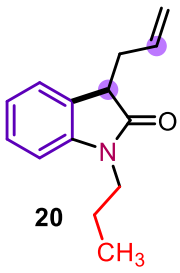
IR (neat); 3058, 2914, 1707, 1625, 1478, 1352, 1266 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.29-7.24 (m, 2H), 7.03-7.00 (m, 1H), 6.83 (d, *J* = 7.5 Hz, 1H), 5.75-5.67 (m, 1H), 5.11-5.01 (m, 2H), 3.79-3.71 (m, 2H), 3.48-3.45 (m, 1H), 2.84-2.79 (m, 1H), 2.59-2.52 (m, 1H), 1.24 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 176.9, 143.5, 134.0, 128.9, 127.9, 124.4, 122.1, 118.0, 108.1, 45.2, 35.0, 34.7, 12.8; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{16}NO$ 202.1226, Found 202.1228.

3-Allyl-1-(2-((tert-butyldimethylsilyl)oxy)ethyl)indolin-2-one (**19**)



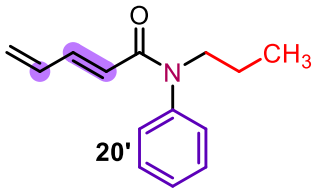
19 was prepared according to the general procedure **4** in 57% (37.5 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4 **IR** (neat); 3054, 2930, 1713, 1613, 1489, 1383, 1254 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.24-7.21 (m, 2H), 7.01-6.95 (m, 2H), 5.78-5.70 (m, 1H), 5.12-5.07 (m, 1H), 5.04-5.01 (m, 1H), 3.83-3.82 (m, 4H), 3.46 (dd, *J* = 2.9, 7.5 Hz, 1H), 2.85-2.79 (m, 1H), 2.58-2.51 (m, 1H), 0.81 (s, 9H), -0.04 (s, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.4, 144.4, 134.2, 128.5, 127.8, 124.1, 122.1, 118.0, 109.3, 61.1, 45.2, 42.7, 35.1, 25.9, 18.3, -5.3, -5.4; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{30}SiNO_2$ 332.2040, Found 332.2045.

3-Allyl-1-propylindolin-2-one (**20**)



20 was prepared according to the general procedure **4** in 57% (24.5 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4 **IR** (neat); 3057, 2958, 1708, 1612, 1487, 1375, 1235 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.28-7.23 (m, 2H), 7.02-6.99 (m, 1H), 6.82 (d, *J* = 8.3 Hz, 1H), 5.75-5.67 (m, 1H), 5.11-5.07 (m, 1H), 5.03-5.00 (m, 1H), 3.73-3.60 (m, 2H), 3.47 (dd, *J* = 3.0, 7.5 Hz 1H), 2.85-2.79 (m, 1H), 2.59-2.53 (m, 1H), 1.73-1.66 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.2, 143.8, 134.0, 128.8, 127.9, 124.3, 122.0, 118.0, 108.3, 45.2, 41.5, 35.0, 20.8, 11.4; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{14}H_{18}NO$ 216.1383, Found 216.1384.

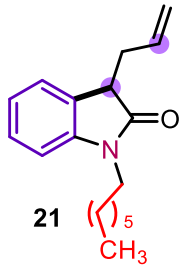
(*E*)-N-phenyl-*N*-propylpenta-2,4-dienamide (**20'**)



20' was prepared according to the general procedure **4** in 23% (9.8 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 93:7) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.30.

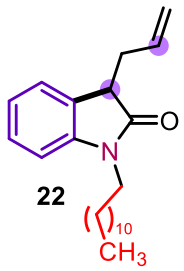
IR (neat); 2994, 1624, 1615, 1568, 1498, 1398, 1267 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.41 (t, *J* = 7.3 Hz, 2H), 7.34 (t, *J* = 7.1 Hz, 1H), 7.27-7.22 (m, 1H), 7.15 (d, *J* = 7.3 Hz, 2H), 6.26-6.18 (m, 1H), 5.74 (d, *J* = 14.7 Hz, 1H), 5.50 (d, *J* = 16.9 Hz, 1H), 5.31 (d, *J* = 9.9 Hz, 1H), 3.74 (t, *J* = 7.4 Hz, 2H), 1.55 (dd, *J* = 14.6, 7.3 Hz, 2H), 0.89 (t, *J* = 7.3 Hz, 2H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 165.8, 142.3, 142.1, 136.2, 129.6, 128.4, 127.7, 123.9, 123.1, 51.1, 21.1, 11.4.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{14}H_{18}NO$ 216.1383, Found 216.1389.

3-Allyl-1-heptylindolin-2-one (**21**)



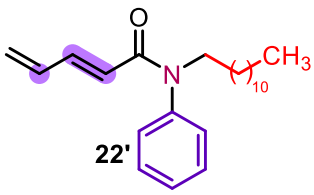
21 was prepared according to the general procedure **4** in 66% (35.7 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4 **IR** (neat); 3076, 2940, 1707, 1614, 1461, 1370, 1242 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.28-7.24 (m, 2H), 7.03-7.00 (m, 1H), 6.82 (d, *J* = 7.8 Hz, 1H), 5.74-5.67 (m, 1H), 5.11-5.07 (m, 1H), 5.03-5.01 (m, 1H), 3.75-3.61 (m, 2H), 3.47 (dd, *J* = 3.0, 7.7 Hz 1H), 2.85-2.79 (m, 1H), 2.59-2.53 (m, 1H), 1.66-1.63 (m, 2H), 1.34-1.25 (m, 8H), 0.86 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.2, 143.9, 134.1, 128.9, 127.9, 124.3, 122.0, 118.1, 108.3, 45.2, 40.0, 35.0, 31.8, 29.1, 27.5, 27.0, 22.7, 14.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{26}NO$ 272.2009, Found 272.2012.

3-Allyl-1-dodecylindolin-2-one (**22**)



22 was prepared according to the general procedure **4** in 77% (52.5 mg) isolated yield. White solid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 93:7) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.35 **M.P.** 112-114 °C; **IR** (neat); 3070, 2952, 1714, 1618, 1454, 1375, 1265 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.28-7.23 (m, 2H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.81 (d, *J* = 7.5 Hz, 1H), 5.78-5.67 (m, 1H), 5.11-5.07 (m, 1H), 5.03-5.01 (m, 1H), 3.75-3.60 (m, 2H), 3.47 (dd, *J* = 2.9, 7.5 Hz, 1H), 2.85-2.79 (m, 1H), 2.59-2.53 (m, 1H), 1.68-1.62 (m, 2H), 1.33-1.24 (m, 18H), 0.87 (t, *J* = 6.8 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.1, 143.9, 134.1, 128.9, 127.9, 124.3, 122.0, 118.1, 108.3, 45.2, 40.0, 35.0, 32.0, 29.7(7), 29.7(5), 29.7(0), 29.6, 29.4(7), 29.4(3), 27.5, 27.0, 22.8, 14.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{23}H_{36}NO$ 342.2791, Found 342.2793.

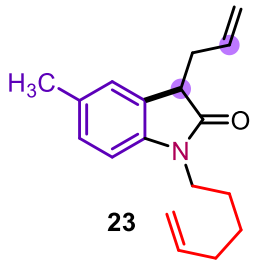
(*E*)-*N*-Phenyl-*N*-propylpenta-2,4-dienamide (**22'**)



22' was prepared according to the general procedure **4** in 8% (5.4 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 92:8) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.35 **IR** (neat); 2907, 1623, 1617, 1545, 1437, 1414, 1376, 1261 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.41 (t, *J* = 7.1 Hz, 2H), 7.34 (t, *J* = 6.9 Hz, 1H), 7.27-7.22 (m, 1H), 7.15 (d, *J* = 7.3 Hz, 2H), 6.29-6.17 (m, 1H), 5.74 (d, *J* = 14.7 Hz, 1H), 5.50 (d, *J* = 16.9 Hz, 1H), 5.32 (d, *J* = 9.9 Hz, 1H), 3.76 (t, *J* = 7.1 Hz, 2H), 1.52 (s, 2H) 1.22 (s, 18H), 0.87 (t, *J* = 6.6 Hz, 3H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 165.7, 142.4, 142.0, 135.3,

129.6, 128.4, 127.7, 123.9, 123.2, 49.7, 32.0, 29.75, 29.70, 29.6, 29.4, 27.9, 27.0, 22.8, 14.2.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{23}H_{36}NO$ 342.2791, Found 342.2791.

3-Allyl-1-(hex-5-en-1-yl)-5-methylindolin-2-one (**23**)

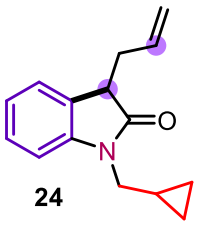


23

23 was prepared according to the general procedure **4** in 64% (34.4 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 93:7) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3041, 2915, 1712, 1624, 1454, 1362, 1262 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.10 (s, 1H), 7.08-7.04 (m, 1H), 6.71 (d, *J* = 7.9 Hz, 1H), 5.75-5.65 (m, 2H), 5.10 (d, *J* = 17.0 Hz, 1H), 5.04-4.91 (m, 3H), 3.72 (dt, *J* = 14.7, 7.5 Hz, 1H), 3.63 (dt, *J* = 13.9, 7.0 Hz, 1H), 3.47-3.42 (m, 1H), 2.86-2.75 (m, 1H), 2.56 (dt, *J* = 14.2, 7.7 Hz, 1H), 2.33 (s, 3H), 2.08 (dt, *J* = 7.5, 3.9 Hz, 2H), 1.71-1.61 (m, 2H), 1.49-1.41 (m, 2H).; **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.1, 141.4, 138.4, 134.2, 131.6, 128.1, 125.2, 118.0, 114.9, 108.0, 45.3, 39.8, 35.0, 33.4, 26.9, 26.2, 21.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{24}NO$ 270.1852, Found 270.1858**.**

3-Allyl-1-(cyclopropylmethyl)indolin-2-one (**24**)

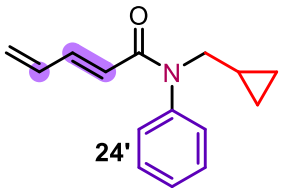


24

24 was prepared according to the general procedure **4** in 62% (28.16 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3057, 2923, 1709, 1612, 1487, 1380, 1266 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.29-7.24 (m, 2H), 7.04-7.00 (m, 1H), 6.91 (d, *J* = 8.0 Hz, 1H), 5.76-5.68 (m, 1H), 5.11-5.07 (m, 1H), 5.04-5.01 (m, 1H), 3.63-3.54 (m, 2H), 3.49 (dd, *J* = 2.7, 7.5 Hz, 1H), 2.85-2.79 (m, 1H), 2.61-2.54 (m, 1H), 1.18-1.11 (m, 1H), 0.51-0.48 (m, 2H), 0.39-0.34 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.2, 144.0, 134.0, 128.8, 127.9, 124.3, 122.0, 118.0, 108.4, 45.3, 44.2, 36.0, 9.7, 4.0, 3.8; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{18}NO$ 228.1383, Found 228.1385.

(*E*)-*N*-(cyclopropylmethyl)-*N*-phenylpenta-2,4-dienamide (**24'**)

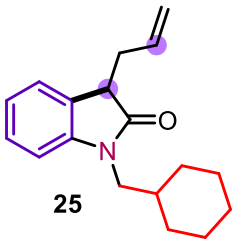


24'

24' was prepared according to the general procedure **4** in 19% (8.6 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 95:5) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.35

IR (neat); 2927, 1617, 1605, 1534, 1446, 1402, 1383, 1264 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.47-7.43 (m, 2H), 7.42-7.37 (m, 1H), 7.31 (dd, *J* = 8.8, 6.2 Hz, 1H), 7.28-7.23 (m, 2H), 6.27 (dt, *J* = 16.9, 10.5 Hz, 1H), 5.79 (d, *J* = 14.9 Hz, 1H), 5.60-5.50 (m, 1H), 5.40-5.32 (m, 1H), 3.70 (d, *J* = 7.1 Hz, 2H), 1.10-0.99 (m, 1H), 0.50-0.41 (m, 2H), 0.23-0.16 (m, 2H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 165.8, 142.4, 142.1, 136.3, 129.5, 128.7, 127.8, 123.9, 123.0, 53.8, 10.0, 3.8.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{14}NO$ 228.1383, Found 228.1389.

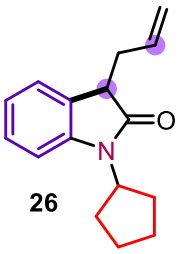
3-Allyl-1-(cyclohexylmethyl)indolin-2-one (**25**)



25

25 was prepared according to the general procedure **4** in 65% (34.9 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 93:8) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.2 **IR** (neat); 3065, 2923, 1709, 1612, 1487, 1381, 1266 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.89-7.26 (m, 1H), 7.25-7.23 (m, 1H), 7.01 (t, *J* = 7.1 Hz, 1H), 6.83 (d, *J* = 7.9 Hz, 1H), 5.76-5.69 (m, 1H), 5.12-5.08 (m, 1H), 5.04-5.01 (m, 1H), 3.59-3.54 (m, 1H), 3.50-3.44 (m, 2H), 2.85-2.80 (m, 1H), 2.59-2.53 (m, 1H), 1.82-1.75 (m, 1H), 1.72-1.67 (m, 5H), 1.20-1.10 (m, 3H), 1.07-1.10 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.5, 144.4, 134.2, 128.8, 127.9, 124.3, 122.0, 118.1, 108.6, 46.4, 45.2, 36.3, 35.1, 31.1, 31.0, 26.3, 25.87, 25.84; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{24}NO$ 270.1852, Found 270.1854.

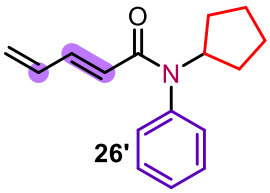
3-Allyl-1-cyclopentylindolin-2-one (**26**)



26

26 was prepared according to the general procedure **4** in 70% (33.7 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4 **IR** (neat); 3069, 2955, 1706, 1609, 1485, 1361, 1232 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.29-7.27 (m, 1H), 7.24-7.21 (m, 1H), 7.02-6.99 (m, 1H), 6.91 (d, *J* = 7.8 Hz, 1H), 5.75-5.67 (m, 1H), 5.10-5.00 (m, 2H), 4.81-4.76 (m, 1H), 3.44 (dd, *J* = 2.9, 7.1 Hz, 1H), 2.83-2.78 (m, 1H), 2.58-2.52 (m, 1H), 2.09-2.02 (m, 2H), 1.92-1.84 (m, 4H), 1.73-1.69 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.2, 142.8, 134.1, 129.2, 127.6, 124.4, 121.7, 117.9, 109.7, 52.1, 45.2, 36.1, 27.6, 27.5, 25.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{20}NO$ 242.1539, Found 242.1539.

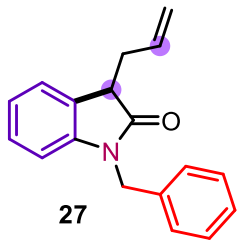
(*E*)-*N*-Cyclopentyl-*N*-phenylpenta-2,4-dienamide (**26'**)



26' was prepared according to the general procedure **4** in 12% (5.8 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 93:7) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.30

IR (neat); 2978, 1639, 1609, 1517, 1445, 1407, 1314, 1260 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.43-7.39 (m, 3H), 7.25-7.19 (m, 1H), 7.14-7.06 (m, 2H), 6.19 (dt, *J* = 17.0, 10.5 Hz, 1H), 5.60-5.44 (m, 1H), 5.30 (d, *J* = 10.1 Hz, 1H), 5.02 – 4.89 (m, 1H), 4.91-4.93 (m, 1H), 1.97-1.85 (m, 2H), 1.58-1.48 (m, 4H), 1.40 -1.23 (m, 2H).; **^{13}C NMR** (126 MHz, $CDCl_3$): δ 166.2, 141.8, 139.1, 135.3, 130.6, 129.3, 128.3, 123.9, 123.7, 57.2, 29.7, 22.9.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{20}NO$ 242.1539, Found 242.1547.

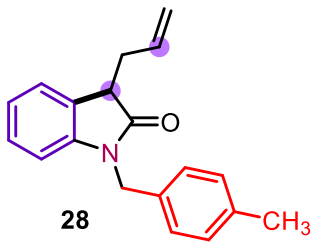
3-Allyl-1-benzylindolin-2-one (**27**)



27 was prepared according to the general procedure **4** in 81% (42.6 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 90:10) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.6

IR (neat); 3033, 2924, 1712, 1618, 1472, 1363, 1265 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.31-7.28 (m, 5H), 7.26-7.23 (m, 1H), 7.17-6.13 (m, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 6.71 (d, *J* = 8.1 Hz, 1H), 5.81-5.71 (m, 1H), 5.16-5.11 (m, 1H), 5.07-5.05 (m, 1H), 4.98 (d, *J* = 15.7 Hz, 1H), 4.83 (d, *J* = 15.6 Hz, 1H), 3.60 (dd, *J* = 2.7, 7.7 Hz, 1H), 2.91-2.85 (m, 1H), 2.68-2.64 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.3, 143.5, 136.0, 134.0, 128.8, 128.6, 128.0, 127.6, 127.4, 124.3, 122.3, 118.3, 109.1, 45.3, 43.8, 35.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{18}NO$ 264.1383, Found 264.1385.

3-Allyl-1-(4-methylbenzyl)indolin-2-one (**28**)

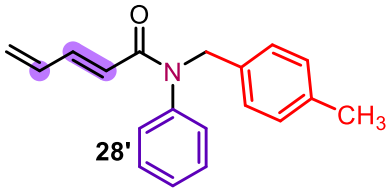


28 was prepared according to the general procedure **4** in 75% (55.4 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 90:10) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.5

IR (neat); 3026, 2978, 1712, 1620, 1458, 1351, 1260 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.28-7.26 (m, 1H), 7.19-7.14 (m, 3H), 7.15-7.09 (m, 2H), 7.00-6.97 (m, 1H), 6.71 (d, *J* = 7.9 Hz, 1H), 5.79-5.70 (m, 1H), 5.15-5.11 (m, 1H), 5.07-5.04 (m, 1H), 4.95 (d, *J* = 15.5 Hz, 1H), 4.79 (d, *J* = 15.6 Hz, 1H), 3.58 (dd, *J* = 3.1, 7.9 Hz, 1H), 2.89-2.86 (m, 1H), 2.66-2.63

(m, 1H), 2.30 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.3, 143.6, 137.3, 134.1, 133.0, 129.5, 128.7, 127.9, 127.4, 124.2, 122.3, 118.2, 109.1, 45.3, 43.5, 35.1, 21.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{20}NO$ 278.1539, Found 278.1543.

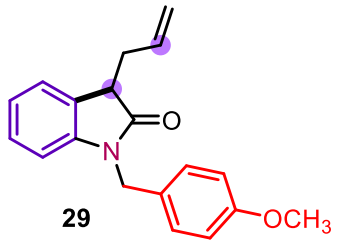
(*E*)-*N*-Cyclopentyl-*N*-phenylpenta-2,4-dienamide (**28'**)



28' was prepared according to the general procedure **4** in 11% (6.1 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 89:11) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.45

IR (neat); 2912, 1651, 1602, 1515, 1488, 1417, 1375, 1232 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.28 (dd, *J* = 13.6, 8.5 Hz, 4H), 7.09-6.98 (m, 4H), 6.96 (d, J = 7.4 Hz, 2H), 6.26-6.15 (m, 1H), 5.75 (d, *J* = 14.7 Hz, 1H), 5.48 (d, *J* = 16.9 Hz, 1H), 5.29 (d, *J* = 9.9 Hz, 1H), 4.89 (s, 2H), 2.25 (s, 3H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ165.9, 142.6, 142.1, 137.0, 135.2, 134.5, 129.5, 129.1, 128.7, 128.5, 127.8, 124.2, 122.8, 53.0, 21.2.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{20}NO$ 278.1539, Found 278.1539.

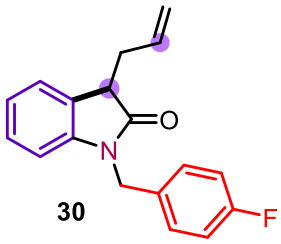
3-Allyl-1-(4-methoxybenzyl)indolin-2-one (**29**)



29 was prepared according to the general procedure **4** in 87% (51.0 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 90:10) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3079, 2957, 1709, 1621, 1496, 1377, 1231 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.28-7.27 (m, 1H), 7.22 (d, *J* = 8.8 Hz, 2H), 7.17-7.14 (m, 1H), 7.01-6.97 (m, 1H), 6.82 (d, *J* = 8.7 Hz, 2H), 6.73 (d, *J* = 7.9 Hz, 1H), 5.77-5.69 (m, 1H), 5.14-5.11 (m, 1H), 5.06-5.03 (m, 1H), 4.91 (d, *J* = 15.9 Hz, 1H), 4.76 (d, *J* = 15.6 Hz, 1H), 3.76 (s, 3H), 3.57 (dd, *J* = 2.7, 7.1 Hz, 1H), 2.90-2.84 (m, 1H), 2.67-2.60 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.3, 159.1, 143.5, 134.0, 128.8, 128.7, 128.1, 127.9, 124.2, 122.3, 118.2, 114.2, 109.1, 55.3, 45.3, 43.2, 35.0; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{20}NO_2$ 294.1489, Found 294.1491.

3-Allyl-1-(4-fluorobenzyl)indolin-2-one (**30**)

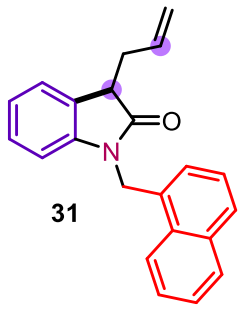


30

30 was prepared according to the general procedure **4** in 73% (41.0 mg) isolated yield. yellow solid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 92:8) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.6

M.P. 66-68 °C; **IR** (neat); 3065, 2924, 1707, 1609, 1510, 1335, 1222 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.29-7.27 (m, 2H), 7.19-7.15 (m, 1H) 7.03-6.96 (m, 4H), 6.69 (d, *J* = 7.5 Hz, 1H), 5.75-5.67 (m, 1H), 5.14-5.10 (m, 1H), 5.05-5.02 (m, 1H), 4.95 (d, *J* = 15.5 Hz, 1H), 4.78 (d, *J* = 15.5 Hz, 1H), 3.59 (dd, *J* = 2.6, 7.8 Hz, 1H), 2.90-2.84 (m, 1H), 2.67-2.63 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.3, 163.2 (d, J_{CF} = 246.5 Hz), 143.2, 133.8, 131.7 (d, J_{CF} = 3.4 Hz), 129.1 (d, J_{CF} = 8.3 Hz), 128.6, 127.9, 124.3, 122.4, 118.3, 115.8 (d, J_{CF} = 21.7 Hz), 108.8, 45.2, 43.0, 35.0; **^{19}F NMR** (471 MHz, $CDCl_3$): δ -114.7; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{17}FNO$ 282.1289, Found 282.1292.

3-Allyl-1-(naphthalen-1-ylmethyl)indolin-2-one (**31**)

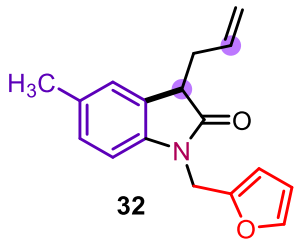


31

31 was prepared according to the general procedure **4** in 42% (26.3 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 90:10) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.5

IR (neat); 3060, 2954, 1709, 1622, 1490, 1345, 1242 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.80-7.73 (m, 4H), 7.46-7.44 (m, 2H), 7.41 (dd, *J* = 1.8, 7.9 Hz, 1H), 7.30-7.28 (m, 1H), 7.13-7.10 (m, 1H), 7.01-6.97 (m, 1H), 6.74 (d, *J* = 8.3 Hz, 1H), 5.80-5.72 (m, 1H), 5.18-5.14 (m, 2H), 5.09 (d, *J* = 15.5 Hz, 1H), 4.98 (d, *J* = 16.0 Hz, 1H), 3.64 (dd, *J* = 2.6, 7.9 Hz, 1H), 2.94-2.88 (m, 1H), 2.73-2.67 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.4, 143.5, 134.0, 133.5, 133.4, 132.9, 128.8, 128.6, 128.0, 127.8, 126.4, 126.2, 126.1, 125.4, 124.3, 122.4, 118.4, 109.2, 45.4, 44.0, 35.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{22}H_{20}NO$ 314.1539, Found 314.1541.

3-Allyl-1-(furan-2-ylmethyl)-5-methylindolin-2-one (**32**)



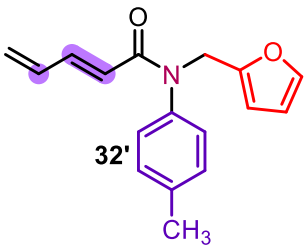
32

32 was prepared according to the general procedure **4** in 57% (30.4 mg) isolated yield. White solid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 90:10) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.5

M.P. 85-87 °C; **IR** (neat); 3017, 2923, 1697, 1617, 1494, 1355, 1242 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.31 (dd, *J* = 0.85, 1.8 Hz, 1H), 7.09 (d, *J* =

7.9 Hz, 1H) 7.04-7.01 (m, 1H), 6.81 (d, J = 8.0 Hz, 1H), 6.28-6.24 (m, 2H), 5.77-5.68 (m, 1H), 5.12-5.07 (m, 1H), 5.03-5.01 (m, 1H), 4.90 (d, J = 16.0 Hz, 1H), 4.84 (d, J = 16.0 Hz, 1H), 3.50 (dd, J = 3.1, 7.5 Hz, 1H), 2.84-2.78 (m, 1H), 2.62-2.56 (m, 1H), 2.31 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 176.9, 149.6, 142.3, 140.9, 134.0, 131.9, 128.6, 128.2, 125.1, 118.0, 110.5, 108.6, 108.3, 45.2, 36.8, 35.0, 21.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{17}H_{18}NO_2$ 268.1332, Found 268.1335.

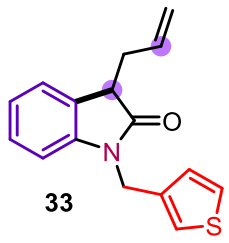
(*E*)-*N*-(furan-2-ylmethyl)-*N*-(p-tolyl)penta-2,4-dienamide (**32'**)



32' was prepared according to the general procedure **4** in 10% (5.4 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 88:12) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.40

IR (neat); 2932, 1647, 1657, 1542, 1490, 1442, 1381, 1278 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.23 (dd, J = 14.8, 2.1 Hz, 2H), 7.10 (d, J = 7.2 Hz, 2H), 6.88 (d, J = 7.1 Hz, 2H), 6.26-6.04 (m, 3H), 5.72 (d, J = 14.8 Hz, 1H), 5.46 (d, J = 16.9 Hz, 1H), 5.27 (d, J = 9.8 Hz, 1H), 4.86 (s, 2H), 2.31 (s, 3H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 166.0, 151.0, 142.6, 142.2, 139.2, 137.9, 135.2, 130.1, 128.1, 124.2, 122.7, 110.4, 108.9, 45.8, 21.2.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{17}H_{18}NO_2$ 268.1332, Found 268.1330.

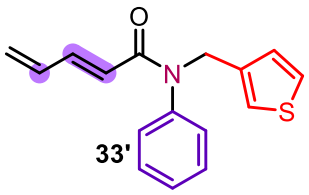
3-Allyl-1-(furan-2-ylmethyl)-5-methylindolin-2-one (**33**)



33 was prepared according to the general procedure **4** in 68% (36.5 mg) isolated yield. White solid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 90:10) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.5

M.P. 78-80 °C; **IR** (neat); 3026, 2944, 1705, 1621, 1498, 1364, 1244 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.29-7.26 (m, 2H), 7.19 (t, J = 7.6 Hz, 1H) 7.14 (s, 1H), 7.03-6.99 (m, 2H), 6.78 (d, J = 7.9 Hz, 1H), 5.75-5.67 (m, 1H), 5.13-5.09 (m, 1H), 5.04 (d, J = 10.1 Hz, 1H), 4.97 (dd, J = 6.8, 10.6 Hz, 1H), 4.82 (d, J = 15.6 Hz, 1H), 3.56 (dd, J = 3.2, 6.9 Hz, 1H), 2.88-2.83 (m, 1H), 2.66-2.60 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 171.1, 143.4, 136.7, 133.9, 128.6, 128.0, 127.1, 126.5, 124.3, 122.5, 122.4, 118.4, 108.8, 45.3, 39.2, 35.0; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{16}SNO$ 270.0947, Found 270.0948.

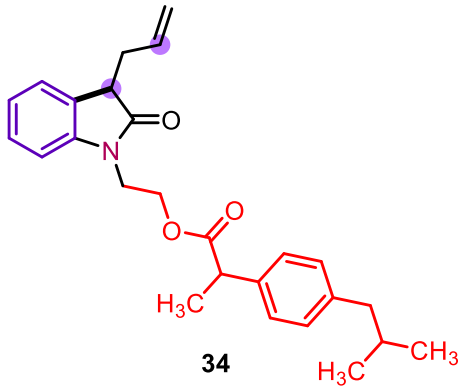
(*E*)-*N*-Phenyl-*N*-(thiophen-3-ylmethyl)penta-2,4-dienamide (**33'**)



33' was prepared according to the general procedure **4** in 12% (6.7 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 88:12) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.40

IR (neat); 2929, 1652, 1621, 1591, 1493, 1432, 1378, 1267 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.37-7.30 (m, 4H), 7.27-7.20 (m, 1H), 7.05-6.97 (m, 4H), 6.34-6.11 (m, 1H), 5.79 (t, *J* = 33.4 Hz, 1H), 5.53 (d, *J* = 16.9 Hz, 1H), 5.34 (d, *J* = 9.9 Hz, 1H), 4.95 (s, 2H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 166.8, 142.6, 142.0, 138.1, 135.2, 129.5, 128.5, 128.4, 127.9, 125.8, 124.3, 123.6, 122.8, 48.2.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{16}NOS$ 270.0947, Found 270.0952.

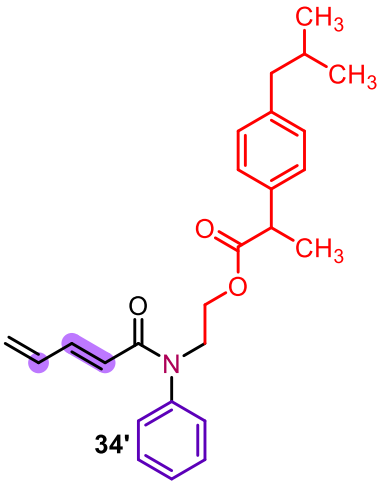
2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(4-isobutylphenylpropanoate (**34**)



34 was prepared according to the general procedure **4** in 66% (dr = 1:1, 53.4 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 90:10) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.25

IR (neat); 3065, 2980, 1734, 1707, 1608, 1486, 1394, 1265 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 7.27-7.21 (m, 2H), 7.09 (dd, *J* = 1.6, 6.8 Hz, 2H), 7.02 (d, *J* = 8.1 Hz, 3H), 6.81(dd, *J* = 1.8, 7.1 Hz, 1H), 5.74-5.61 (m, 1H), 5.11-5.06 (m, 1H), 5.03-4.97 (m, 1H), 4.35-4.29 (m, 1H), 4.27-4.19 (m, 1H), 4.02-3.93 (m, 1H), 3.90-3.82 (m, 1H), 3.62-3.57 (m, 1H), 3.44 (dd, *J* = 2.8, 6.9 Hz, 1H), 2.82-2.76 (m, 1H), 2.56-2.51 (m, 1H), 2.43 (d, *J* = 7.1 Hz, 2H), 1.83 (Sept, *J* = 6.8 Hz, 1H), 1.41 (d, J = 7.1 Hz, 3H), 0.89 (d, *J* = 4.9 Hz, 3H), 0.87 (d, *J* = 4.8 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): (Inseparable mixture of diastereomers) δ 177.3, 174.67, 174.66, 143.6, 140.69, 140.68, 137.4, 133.97, 133.90, 129.4, 128.6(1), 128.6, 128.0, 127.2, 124.38, 124.34, 122.3, 118.5, 108.4(5), 108.4(4), 61.86, 61.8, 45.1, 45.0, 38.8, 35.0, 34.9, 30.2, 22.5, 18.4(4), 18.4(5) (some of the ^{13}C peaks are overlapped) ; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{26}H_{32}NO_3$ 406.2377, Found 406.2384.

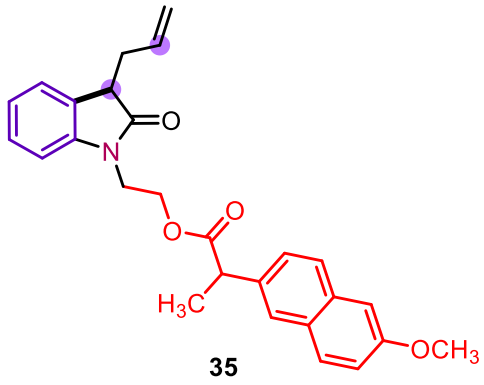
(*E*)-2-(*N*-phenylpenta-2,4-dienamido)ethyl 2-(4-isobutylphenyl)propanoate (**34'**)



34' was prepared according to the general procedure **4** in 14% (11.3 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 88:12) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 2975, 1697, 1635, 1612, 1507, 1412, 1365, 1232 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.36-7.30 (m, 3H), 7.28-7.23 (m, 1H), 7.13 (d, *J* = 7.4 Hz, 2H), 7.05 (d, *J* = 7.5 Hz, 2H), 6.97 (d, *J* = 5.6 Hz, 2H), 6.28-6.17 (m, 1H), 5.69 (d, *J* = 14.8 Hz, 1H), 5.54 (d, *J* = 16.9 Hz, 1H), 5.36 (d, *J* = 9.9 Hz, 1H), 4.27-4.21 (m, 1H), 4.15 (dd, *J* = 11.1, 3.6 Hz, 1H), 4.11-4.05 (m, 1H), 3.99-3.92 (m, 1H), 3.58 (q, *J* = 6.5 Hz, 1H), 2.42 (d, *J* = 7.0 Hz, 2H), 1.82 (dt, *J* = 12.9, 6.4 Hz, 1H), 1.40 (d, *J* = 6.9 Hz, 3H), 0.87 (d, *J* = 6.5 Hz, 6H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 174.6, 166.2, 142.5, 141.9, 140.6, 137.7, 135.2, 129.6, 129.4, 128.3, 127.9, 127.3, 124.4, 122.7, 62.1, 48.0, 45.16, 45.13, 30.2, 22.5, 18.3.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{26}H_{32}NO_3$ 406.2377, Found 406.2381.

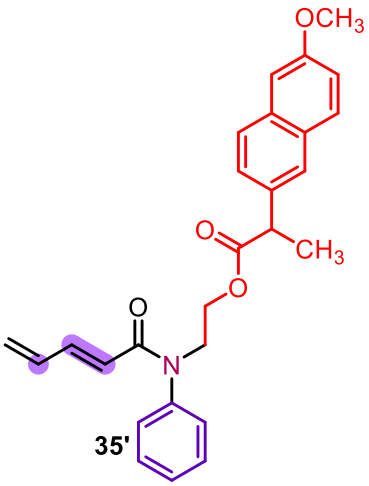
2-(3-allyl-2-oxoindolin-1-yl) ethyl 2-(6-methoxynaphthalen-2-yl) propanoate (**35**)



35 was prepared according to the general procedure **4** in 54% (dr = 1:1, 46.3 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 88:12) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3050, 2954, 1728, 1712, 1610, 1472, 1380, 1243 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 7.65-7.62 (m, 2H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.30-7.27 (m, 1H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.14-7.08 (m, 3H), 6.98 (t, *J* = 7.2 Hz, 1H), 6.75 (t, *J* = 7.5 Hz, 1H), 5.72-5.56 (m, 1H), 5.07-4.93 (m, 2H), 4.36-4.24 (m, 2H), 4.00-3.94 (m, 1H), 3.91 (s, 3H), 3.87-3.74 (m, 2H), 3.38 (dd, *J* = 3.1, 6.9 Hz, 1H), 2.79-2.70 (m, 1H), 2.52-2.42 (m, 1H), 1.50 (d, *J* = 7.0 Hz, 1.5H), 1.48 (d, *J* = 7.1 Hz, 1.5H); **^{13}C NMR** (126 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 177.3(9), 177.3(7), 174.6, 157.8, 143.5(9), 143.5(8), 135.4, 135.3, 134.0, 133.9, 133.8, 129.4, 129.0, 128.6, 127.9(5), 127.9(4) 127.2, 126.2(5), 126.2(1), 126.1(4), 126.1(2), 124.3, 122.3(8), 122.3(4), 119.1, 118.1, 118.0, 108.3(8), 108.3(7), 105.7, 62.0, 61.9, 55.4, 45.4(8), 45.4(5), 45.0(8), 45.0(4), 38.9, 35.0, 34.9, 18.4(7), 18.4(6) (some of the ^{13}C peaks are overlapped); **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{27}H_{28}NO_4$ 430.2013, Found 430.2017.

(*E*)-2-(N-phenylpenta-2,4-dienamido)ethyl 2-(6-methoxynaphthalen-2-yl)propanoate (**35'**)

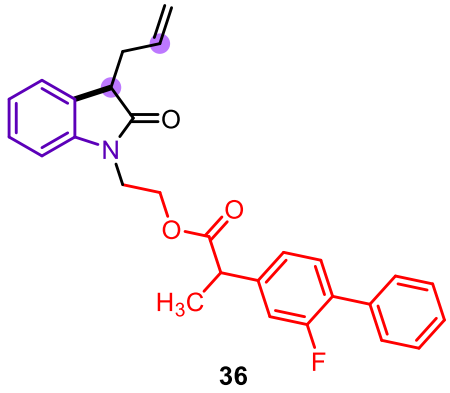


35'

35' was prepared according to the general procedure **4** in 12% (10.3 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 86:14) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3

IR (neat); 2934, 1730, 1657, 1593, 1490, 1392, 1264 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.72-7.63 (m, 2H), 7.59 (s, 1H), 7.32 (d, *J* = 7.9 Hz, 1H), 7.25-7.08 (m, 8H), 6.92 (d, *J* = 6.6 Hz, 2H), 6.24-6.16 (m, 1H), 5.63 (d, *J* = 14.7 Hz, 1H), 5.53 (d, *J* = 16.9 Hz, 1H), 5.35 (d, *J* = 9.9 Hz, 1H), 4.26 (s, 1H), 4.18 (s, 1H), 4.09 (d, *J* = 13.7 Hz, 1H), 3.94 (d, *J* = 7.0 Hz, 1H), 3.91 (s, 3H), 3.74 (d, *J* = 6.8 Hz, 1H), 1.50 (d, *J* = 7.1 Hz, 3H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 174.4, 166.1, 157.6, 142.3, 141.8, 135.5, 135.1, 133.6, 129.4, 129.3, 128.9, 128.1, 127.7, 127.1, 126.2, 125.9, 124.2, 122.5, 118.9, 105.5, 62.2, 55.3, 48.0, 45.3, 18.2.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{27}H_{28}NO_4$ 430.2013, Found 430.2021.

2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl) propanoate (**36**)

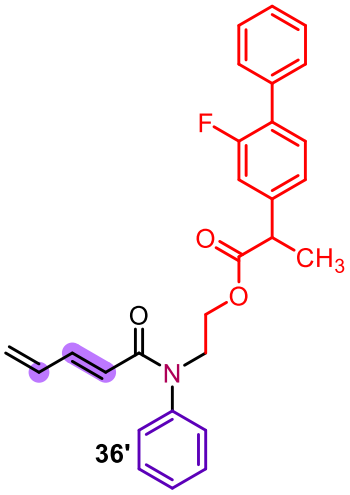


36

36 was prepared according to the general procedure **4** in 59% (dr = 1:1 52.2 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 88:12) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3062, 2980, 1738, 1708, 1611, 1486, 1381, 1268 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 7.51 (d, *J* = 7.8 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.38-7.34 (m, 2H), 7.27-7.21 (m, 2H), 7.05-6.95 (m, 3H), 6.82 (d, *J* = 7.1 Hz, 1H), 5.74-5.62 (m, 1H), 5.10-4.97 (m, 2H), 4.41-4.26 (m, 2H), 4.01-3.87 (m, 2H), 3.66 (q, *J* = 5.1 Hz, 1H), 3.46 (dd, *J* = 2.8, 7.5 Hz, 1H), 2.83-2.76 (m, 1H), 2.58-2.50 (m, 1H), 1.47 (d, *J* = 7.2 Hz, 1.5H), 1.45 (d, *J* = 7.2 Hz, 1.5H); **^{13}C NMR** (126 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 177.4, 177.3, 173.8, 160.7 (d, J_{CF} = 248.4 Hz), 143.5, 141.5 (d, J_{CF} = 7.9 Hz), 135.5, 133.9, 133.8, 130.9 (d, J_{CF} = 8.9 Hz), 129.06, 129.03, 128.5, 127.9, 127.7, 124.4 (d, J_{CF} = 4.9 Hz), 123.6 (d, J_{CF} = 6.8 Hz), 122.4, 118.1, 115.4 (d, J_{CF} = 23.8 Hz), 108.3, 108.2, 62.1(9), 62.1 45.1, 45.0(6), 45.0(1), 38.9, 35.0, 34.9, 18.3 (some of the ^{13}C peaks are overlapped); **^{19}F NMR** (471 MHz, $CDCl_3$): δ -117.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{27}FNO_3$ 444.1969, Found 444.1969.

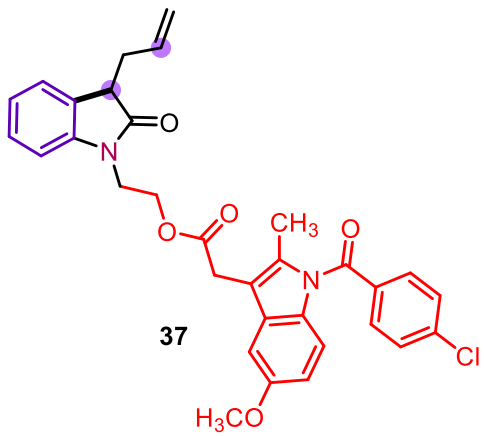
(*E*)-2-(*N*-phenylpenta-2,4-dienamido)ethyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (**36'**)



36' was prepared according to the general procedure **4** in 15% (13.2 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 86:14) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.35

IR (neat); 2924, 1737, 1662, 1571, 1454, 1374, 1251 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.51 (d, *J* = 7.4 Hz, 2H), 7.43 (t, *J* = 7.2 Hz, 2H), 7.34 (dt, *J* = 9.2, 7.0 Hz, 5H), 7.29-7.23 (m, 1H), 7.10-7.00 (m, 4H), 6.25-6.12 (m, 1H), 5.71 (d, *J* = 14.9 Hz, 1H), 5.52 (d, *J* = 16.9 Hz, 1H), 5.34 (d, *J* = 10.0 Hz, 1H), 4.30 (d, *J* = 11.2 Hz, 1H), 4.23 (dd, *J* = 11.2, 3.5 Hz, 1H), 4.16-4.09 (m, 1H), 4.04-3.96 (m, 1H), 3.64 (q, *J* = 6.6 Hz, 1H), 1.45 (d, *J* = 7.1 Hz, 3H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 173.7, 166.1, 160.3 (d, *J* = 247.1 Hz), 142.5, 141.9, 141.6 (d, *J* = 36.2 Hz), 135.4, 135.0, 130.8 (d, *J* = 36.4 Hz), 129.6, 128.9 (d, *J* = 7.1 Hz), 128.4, 128.1, 127.8, 127.6, 124.3, 123.6, 122.4, 115.3 (d, *J* = 24.5 Hz), 62.4, 48.0, 44.9, 18.1.; **^{19}F NMR** (471 MHz, $CDCl_3$): δ -117.4;**HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{27}FNO_3$ 444.1969, Found 444.1973.

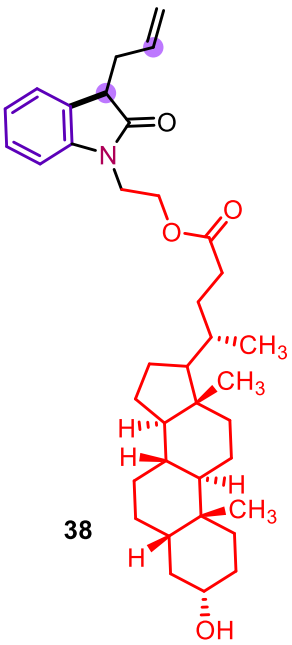
2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl) propanoate (**37**)



37 was prepared according to the general procedure **4** in 39% (43.3 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 80:20) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.2

IR (neat); 3054, 2949, 1740, 1711, 1613, 1483, 1398, 1259 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.65 (d, *J* = 8.6 Hz, 2H), 7.46 (d, *J* = 8.7 Hz, 2H), 7.21-7.17 (m, 1H), 7.02-6.99 (m, 1H), 6.89 (d, *J* = 2.5 Hz, 1H), 6.86 (d, *J* = 9.0 Hz, 1H), 6.79 (d, *J* = 7.8 Hz, 1H), 5.74-5.65 (m, 1H), 5.09-5.00 (m, 2H), 4.37-4.33 (m, 2H), 3.97 (q, *J* = 5.0 Hz, 2H), 3.80 (s, 3H), 3.60 (d, *J* = 2.0 Hz, 2H), 3.39 (dd, *J* = 3.1, 7.5 Hz, 1H), 2.81-2.75 (m, 1H), 2.55-2.49 (m, 1H), 2.28 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.5, 170.8, 168.4, 156.2, 143.4, 139.3, 136.1, 134.0, 133.9, 131.3, 130.9, 130.7, 129.2, 128.6, 128.0, 124.5, 122.4, 118.2, 115.1, 112.2, 111.7, 108.0, 101.4, 61.8, 55.8, 45.0, 38.9, 35.0, 30.2, 13.4; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{32}H_{30}ClNO_5$ 557.1838, Found 557.1842.

2-(3-Allyl-2-oxoindolin-1-yl) ethyl 3-hydroxy-10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)pentanoate (**38**)

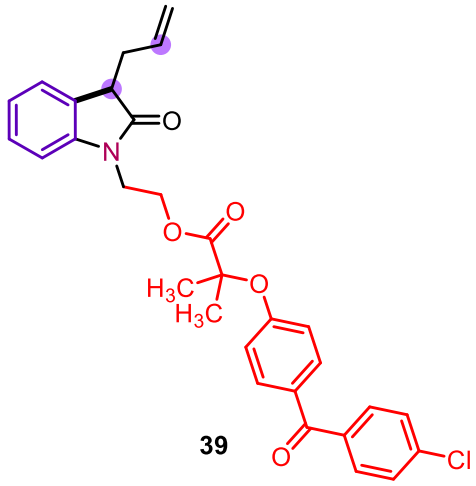


38

38 was prepared according to the general procedure **4** in 46% (dr = 1:1 52.9 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 70:30) as the eluent, **TLC** (40% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3

IR (neat); 3079, 2928, 1740, 1714, 1613, 1491, 1357, 1245 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 7.30-7.26 (m, 2H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 7.8 Hz, 1H), 5.74-5.67 (m, 1H), 5.11-5.01 (m, 2H), 4.30-4.25 (m, 3H), 3.99-3.92 (m, 2H), 3.64-3.59 (m, 1H), 3.49 (dd, *J* = 3.1, 7.5 Hz, 1H), 2.84-2.79 (m, 1H), 2.59-2.54 (m, 1H), 2.29-2.23 (m, 1H), 2.15-2.11 (m, 1H), 1.94-1.91 (m, 1H), 1.81-1.74 (m,5H), 1.69-1.64 (m, 3H), 1.39-1.33 (m, 6H), 1.26-1.20 (m, 5H), 1.05-1.01 (m, 4H), 0.90 (s, 6H), 0.85 (d, *J* = 6.4 Hz, 4H), 0.61 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ (inseparable mixture of diastereomers)177.4, 174.2, 143.6, 133.9, 128.6, 128.0, 124.4, 122.4, 118.2, 108.3, 72.0, 61.02, 56.9, 55.9, 45.1, 42.8, 40.5, 40.2, 38.9, 36.7, 36.5, 35.9, 35.4, 35.0, 34.6, 31.1, 30.8, 30.6, 28.2, 27.3, 26.5, 24.8, 24.3, 23.5, 20.9, 18.3, 12.1 (most of the ^{13}C peaks are overlapped); **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{37}H_{54}NO_4$ 576.4047, Found 576.4051**.** (The absolute configuration draw same as the stereo of commercially available lithocholic acid)

2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl) propanoate (**39**)



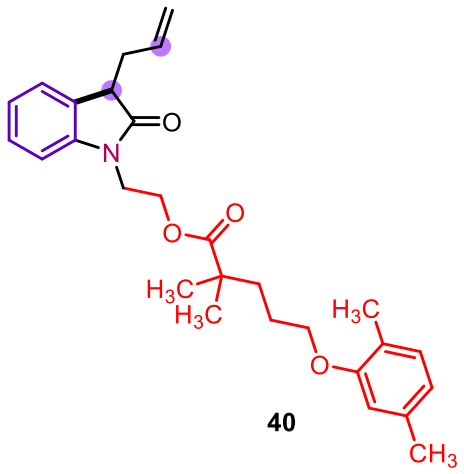
39

39 was prepared according to the general procedure **4** in 52% (53.8 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 86:14) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3

IR (neat); 3052, 2932, 1745, 1732, 1712, 1622, 1474, 1384, 1263 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.68 (d, *J* = 8.7 Hz, 2H), 7.65 (d, *J* = 8.9 Hz, 2H), 7.45 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 7.2 Hz, 2H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.67 (d, *J* = 8.9 Hz, 2H), 5.72-5.63 (m, 1H), 5.08-5.04 (m, 1H), 5.01-4.99 (m, 1H), 4.41-4.34 (m, 2H), 3.94 (t, *J* = 7.1 Hz, 2H), 3.40 (dd, *J* = 2.8, 7.5 Hz, 1H), 2.80-2.74 (m, 1H), 2.54-2.48 (m, 1H), 1.58 (s, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 194.2, 177.3, 173.6, 159.5, 143.2, 138.5, 136.4, 133.8, 132.1, 131.2, 130.5, 128.6, 128.5, 128.0, 124.5, 122.5, 118.2, 117.3, 108.3, 79.3,

62.7, 45.0, 38.7, 34.9, 25.5, 25.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{29}ClNO_5$ 518.1729, Found 518.1729.

2-(3-Allyl-2-oxoindolin-1-yl)ethyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (**40**)

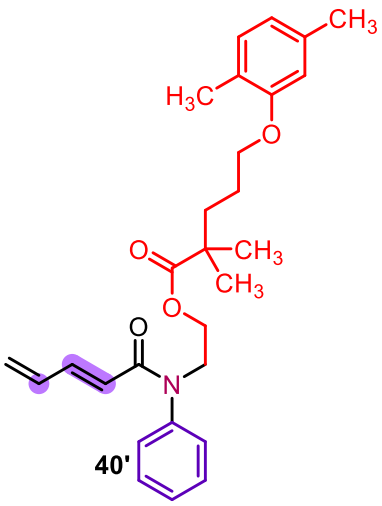


40

40 was prepared according to the general procedure **4** in 74% (66.5 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 82:18) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3

IR (neat); 3022, 2972, 1738, 1732, 1709, 1612, 1453, 1368, 1250 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.27-7.24 (m, 2H), 7.03-6.98 (m, 2H), 6.91 (d, *J* = 8.2 Hz, 1H), 6.66 (d, *J* = 8.1 Hz, 1H), 6.57 (s, 1H), 5.72-5.65 (m, 1H), 5.10-5.0 (m, 2H), 4.33-4.26 (m, 2H), 3.97 (m, 2H), 3.82-3.79 (m, 2H), 3.48 (dd, *J* = 2.8, 7.0 Hz, 1H), 2.83-2.77 (m, 1H), 2.58-2.52 (m, 1H), 2.30 (s, 3H), 2.15 (s, 3H), 1.64-1.63 (m, 4H), 1.14 (s, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.7, 177.3, 157.0, 143.6, 136.5, 133.9, 130.4, 128.0, 124.4, 123.6, 122.4, 120.8, 118.1, 112.1, 108.4, 67.9, 61.4, 45.1, 42.1, 38.8, 37.0, 35.0, 25.17, 25.15, 25.12, 21.5, 15.8; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{36}NO_4$ 450.2639, Found 450.2647.

(*E*)-2-(*N*-phenylpenta-2,4-dienamido)ethyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (**40'**)

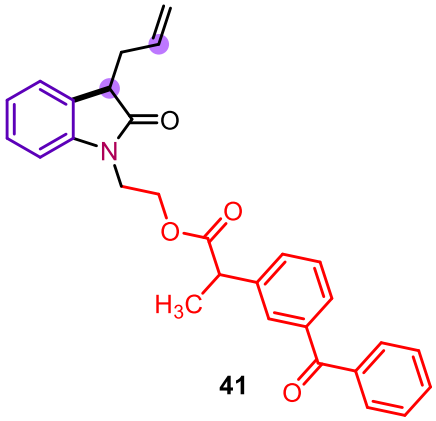


40'

40' was prepared according to the general procedure **4** in 12% (10.8 mg) isolated yield. Colorless oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 80:20) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.25

IR (neat); 2994, 1702, 1641, 1534, 1447, 1348, 1259 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.40 (t, *J* = 6.8 Hz, 2H), 7.34 (d, *J* = 6.8 Hz, 1H), 7.24 (s, 1H), 7.19 (d, *J* = 7.3 Hz, 2H), 6.99 (d, *J* = 6.3 Hz, 1H), 6.65 (d, *J* = 6.3 Hz, 1H), 6.58 (s, 1H), 6.26-6.18 (m, 1H), 5.76 (d, *J* = 15.2 Hz, 1H), 5.52 (d, *J* = 17.0 Hz, 1H), 5.34 (d, *J* = 9.9 Hz, 1H), 4.25 (s, 2H), 4.06 (s, 2H), 3.85 (s, 2H), 2.30 (s, 3H), 2.15 (s, 3H), 1.65 (s, 2H), 1.26 (s, 2H), 1.11 (s, 6H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ 177.5, 166.1, 156.9, 142.5, 142.0, 136.4, 135.0, 130.2, 129.6, 128.2, 127.8, 124.3, 123.5, 122.4, 120.6, 111.9, 67.8, 62.0, 48.2, 41.9, 36.9, 25.08, 25.04, 21.4, 15.7.; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{36}NO_4$ 450.2639, Found 450.2641.

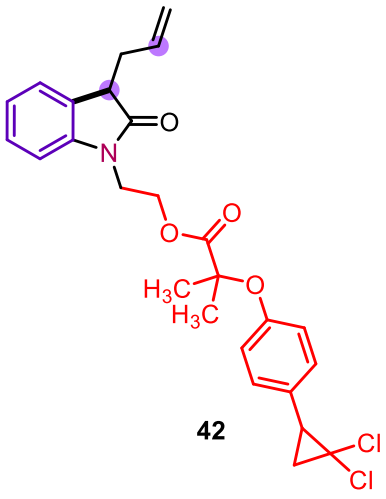
2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(3-benzoylphenyl) propanoate (**41**)



41

41 was prepared according to the general procedure **4** in 44% (dr = 1:1, 39.8 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 88:12) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4 **IR** (neat); 3028, 2926, 1724, 1709, 1608, 1447, 1371, 1265 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 7.78 (d, *J* = 7.1 Hz, 2H), 7.66-7.63 (m, 2H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.44-7.42 (m, 1H), 7.39-7.36 (m, 1H), 7.25 (d, *J* = 6.1 Hz, 1H), 7.20 (t, *J* = 7.1 Hz, 1H), 7.01-6.98 (m,1H), 6.80 (dd, *J* = 3.8, 7.8 Hz, 1H), 5.71-5.61 (m, 1H), 5.09-4.97 (m, 2H), 4.39-4.23 (m, 2H), 4.01-3.85 (m, 2H), 3.72-3.67 (m, 1H), 3.45 (dd, *J* = 2.8, 7.2 Hz, 1H), 2.81-2.74 (m, 1H), 2.56-2.48 (m, 1H), 1.45 (d, *J* = 6.3 Hz, 1.5H), 1.44 (d, *J* = 6.3 Hz, 1.5H); **^{13}C NMR** (126 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 196.5, 177.4, 177.3, 174.0, 143.5, 140.5, 138.0, 137.5, 133.9, 133.8, 132.6, 131.6, 130.2, 129.3, 129.2, 128.6, 128.4, 128.0, 124.4(8), 124.4(5), 122.4, 118.2, 108.2, 62.0(9), 62.0(4), 45.3, 45.1, 45.0, 38.8, 35.0(3), 35.0 18.4 (some of the ^{13}C peaks are overlapped); **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{29}H_{28}NO_4$ 454.2013, Found 454.2017.

2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(4-(2,2-dichlorocyclopropyl) phenoxy)-2-methylpropanoate (**42**)



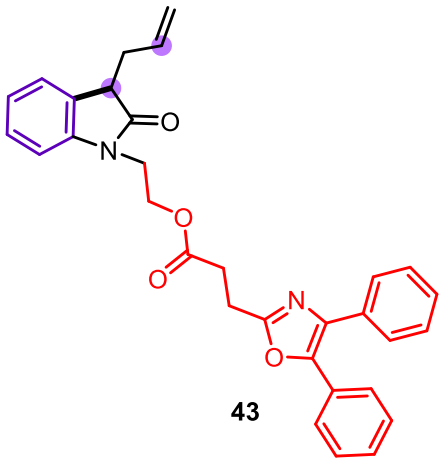
42

42 was prepared according to the general procedure **4** in 35% (dr = 1:1, 34.0 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 88:12) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 2991, 2924, 1740, 1709, 1612, 1464, 1380, 1243 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 7.23 (t, *J* = 7.5 Hz, 2H), 7.06-7.00 (m, 3H), 6.84 (d, *J* = 8.1 Hz, 1H), 6.73 (dd, *J* = 1.8, 8.6 Hz, 2H), 5.72-5.64 (m, 1H), 5.09-5.05 (m, 1H), 5.02-4.99 (m, 1H), 4.40-4.32 (m, 2H), 3.93 (t, *J* = 5.7 Hz, 2H), 3.43 (dd, *J* = 2.9, 7.4 Hz, 1H), 2.82-2.75 (m, 2H), 2.56-2.50 (m, 1H), 1.93 (dd, J = 3.3, 7.4 Hz, 1H), 1.77-1.74 (m, 1H), 1.50 (s, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 177.3, 174.1, 174.0, 154.8, 143.3, 133.8, 129.7, 128.5, 128.3, 128.0, 126.6, 124.4(4), 124.4(2), 122.5, 121.7, 118.8, 118.2, 108.5, 62.4(3), 62.4(0), 60.9, 45.0,

38.7, 35.0, 34.9, 29.8, 27.8, 25.9, 25.5, 25.4, 25.3(6), 25.3(3) (some of the ^{13}C peaks are overlapped); **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{26}H_{28}Cl_2NO_4$ 488.1390, Found 488.1390.

2-(3-Allyl-2-oxoindolin-1-yl) ethyl 3-(4,5-diphenyloxazol-2-yl) propanoate (**43**)

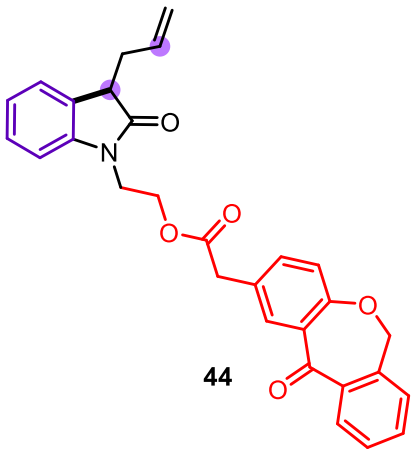


43

43 was prepared according to the general procedure **4** in 44% (43.3 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 75:25) as the eluent, **TLC** (40% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3068, 2924, 1740, 1709, 1611, 1486, 1352, 1282 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.61 (d, *J* = 6.7 Hz, 2H), 7.56 (d, *J* = 7.0 Hz, 2H), 7.35-7.31 (m, 6H), 7.24 (t, *J* = 7.4 Hz, 2H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 7.8 Hz, 1H), 5.74-5.66 (m, 1H), 5.10-5.07 (m, 1H), 5.03-5.01 (m, 1H), 4.36 (t, *J* = 5.8 Hz, 2H), 4.01-3.94 (m, 2H), 3.48 (dd, *J* = 2.4, 4.9 Hz, 1H), 3.11 (t, *J* = 7.1 Hz, 2H), 2.84 (t, *J* = 7.5 Hz, 2H), 2.81-2.78 (m, 1H), 2.59-2.53 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.4, 171.9, 161.6, 145.5, 143.5, 135.2, 133.9, 132.5, 129.0, 128.7, 128.68, 128.65, 128.5, 128.1, 128.08, 128.02, 126.5, 124.5, 122.4, 118.2, 108.2, 61.7, 45.1, 38.9, 35.0, 31.0, 23.4; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{29}N_2O_4$ 493.2122, Found 493.2124.

2-(3-Allyl-2-oxoindolin-1-yl)ethyl 2-(11-oxo-6,11-dihydrodibenzo[b,e]oxepin-2-yl)acetate (**44**)



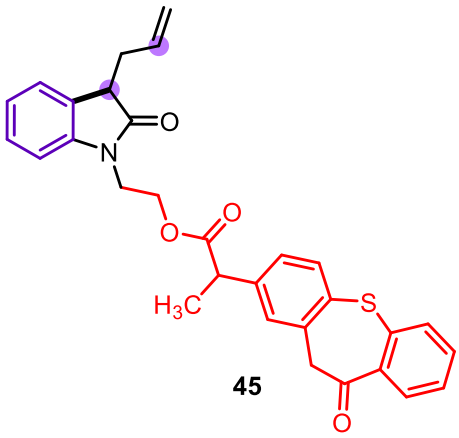
44

44 was prepared according to the general procedure **4** in 51% (47.6 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 80:20) as the eluent, **TLC** (30% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.5

IR (neat); 3052, 2974, 1734, 1712, 1608, 1472, 1378, 1265 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.03 (d, *J* = 2.3 Hz, 1H), 7.89 (d, *J* = 7.7 Hz, 1H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 8.1 Hz, 1H), 7.29 (dd, *J* = 2.4, 8.4 Hz, 1H), 7.27-7.24 (m, 2H), 7.01 (t, *J* = 7.5 Hz, 1H), 6.97 (d, *J* = 8.4 Hz, 1H), 6.85 (d, *J* = 8.2 Hz, 1H), 5.72-5.65 (m, 1H), 5.17 (s, 2H), 5.10-5.06 (m, 1H), 5.03-5.02 (m, 1H), 4.36 (t, *J* = 5.8 Hz, 2H), 4.01-3.92 (m, 2H), 3.55 (s, 2H), 3.48 (dd, *J* = 2.8, 7.6 Hz, 1H), 2.82-2.77 (m, 1H), 2.57-2.51 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 190.9, 177.4, 171.3, 160.6, 143.5, 140.5, 136.4, 135.6, 133.9, 132.9, 132.6, 129.6, 129.3, 128.6, 128.0, 127.9, 127.4, 125.2, 124.4, 122.4, 121.1, 118.2, 73.7,

61.9, 45.1, 40.0, 38.9, 35.0; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{29}H_{26}NO_5$ 468.1805, Found 468.1806.

2-(3-Allyl-2-oxoindolin-1-yl)ethyl 2-(10-oxo-10,11-dihydrodibenzo[b,f]thiepin-2-yl)propanoate (**45**)

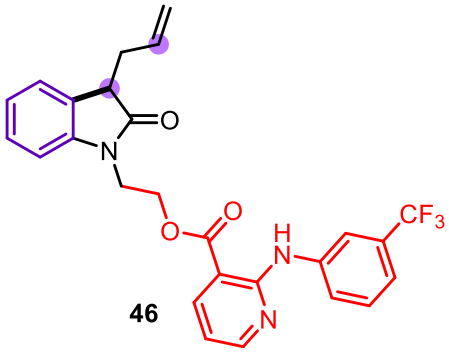


45

45 was prepared according to the general procedure **4** in 28% (dr = 1:1, 27.8 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 80:20) as the eluent, **TLC** (30% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.5

IR (neat); 3058, 2980, 1737, 1708, 1612, 1486, 1382, 1283 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 8.20 (d, *J* = 7.9 Hz, 1H), 7.60 (d, *J* = 7.5 Hz, 1H), 7.51 (dd, *J* = 2.5, 8.0 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.31 (t, *J* = 7.2 Hz, 2H), 7.24 (d, *J* = 7.3 Hz, 1H), 7.19-7.16 (m, 1H), 7.03-6.97 (m, 2H), 6.76 (dd, *J* = 2.2, 7.6 Hz, 1H), 5.71-5.59 (m, 1H), 5.09-4.96 (m, 2H), 4.30 (s, 2H), 4.27-4.20 (m, 2H), 3.99-3.83 (m, 2H), 3.63-3.58 (m, 1H), 3.43 (dd, *J* = 2.8, 7.6 Hz, 1H), 2.80-2.72 (m, 1H), 2.54-2.47 (m, 1H), 1.39 (d, J = 7.1 Hz, 1.5H), 1.38 (d, J = 7.1 Hz, 1.5H); **^{13}C NMR** (126 MHz, $CDCl_3$): (inseparable mixture of diastereomers) δ 191.4, 177.4, 177.3, 173.8, 143.5, 142.3, 140.2, 138.0, 136.2, 133.9, 133.8, 133.4, 132.6, 131.6, 131.5, 130.9, 128.7(3), 128.7(1), 128.5, 127.9, 127.0, 126.4, 124.4(5), 124.4(2), 122.4, 118.2, 108.2(7), 108.2(6), 62.1, 62.0, 51.1, 45.1, 45.0, 38.8, 35.0, 34.9, 18.4 (some of the ^{13}C peaks are overlapped); **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{28}SNO_4$ 498.1734, Found 498.1733.

2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-((3-(trifluoromethyl) phenyl) amino) nicotinate (**46**)



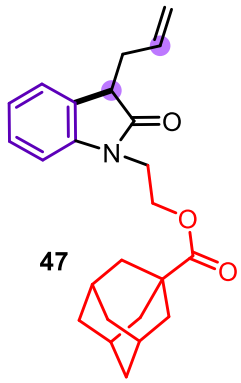
46

46 was prepared according to the general procedure **4** in 57% (54.9 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 80:20) as the eluent, **TLC** (30% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

IR (neat); 3027, 2921, 1732, 1714, 1624, 1457, 1397, 1252 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 10.2 (s, 1H), 8.38 (dd, *J* = 2.0, 4.7 Hz, 1H), 8.10 (dd, *J* = 1.9, 7.8 Hz, 1H), 8.04 (s, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.43-7.40 (m, 1H), 7.30 (d, *J* = 7.7 Hz, 3H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 7.8 Hz, 1H), 6.70 (dd, *J* = 2.1, 7.8 Hz, 1H) 5.71-5.63 (m, 1H), 5.08-5.03 (m, 1H), 4.97-4.95 (m, 1H), 4.56 (t, *J* = 5.5 Hz, 2H), 4.24-4.07 (m, 2H), 3.53 (dd, *J* = 2.8, 6.9 Hz, 1H), 2.86-

2.77 (m, 1H), 2.61-2.56 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.5, 167.4, 155.8, 153.4, 143.3, 140.6, 140.3, 133.7, 131.3, 131.1, 129.3, 128.6 (q, J_{CF} = 31.2 Hz), 128.0, 124.6, 123.7, 122.6, 119.3 (q, J_{CF} = 4.1 Hz), 118.3, 117.4 (q, J_{CF} = 4.1 Hz), 114.2, 108.1, 107.0, 62.2, 45.2, 38.8, 35.0; **^{19}F NMR** (471 MHz, $CDCl_3$): δ -62.5; **HRMS** (ESI/Q-TOF) *m/z*: $[M+Na]^+$ Calcd for $C_{26}H_{23}N_3F_3O_3$ 482.1686, Found 482.1686.

2-(3-Allyl-2-oxoindolin-1-yl) ethyl (1s,3s)-adamantane-1-carboxylate (**47**)

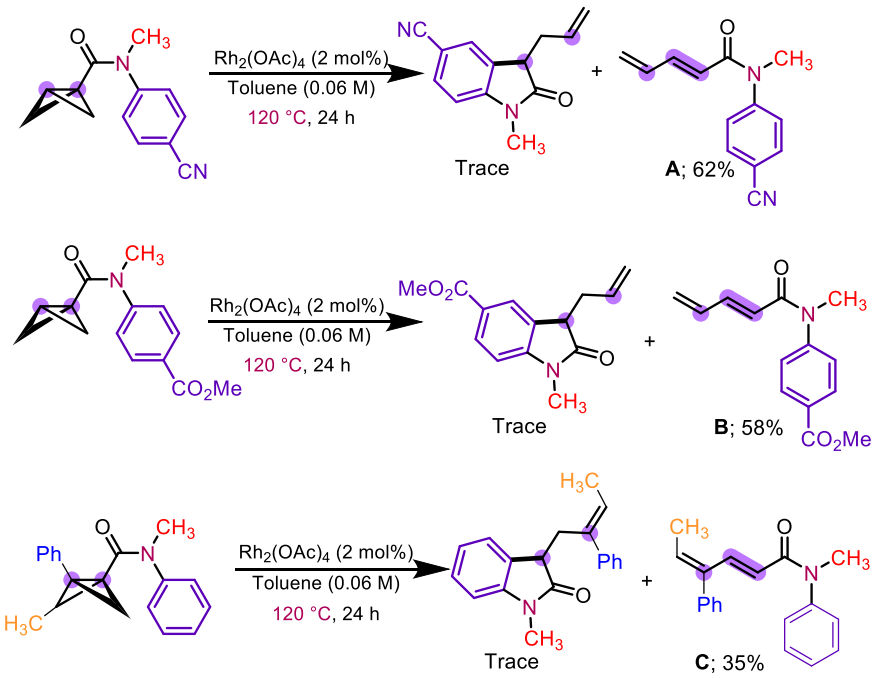


47

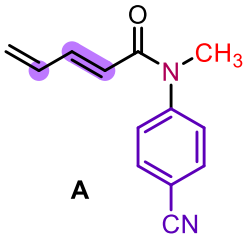
47 was prepared according to the general procedure **4** in 76% (57.6 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 88:12) as the eluent, **TLC** (20% ethyl acetate in hexanes): R_f = 0.4

IR (neat); 3062, 2935, 1729, 1709, 1613, 1489, 1382, 1271 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.26 (t, *J* = 7.5 Hz, 2H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 7.7 Hz, 1H), 5.73-5.66 (m, 1H), 5.10-5.06 (m, 1H), 5.03-5.00 (m, 1H), 4.29-4.22 (m, 2H), 4.01-3.91 (m, 2H), 3.49 (dd, *J* = 4.9, 7.4 Hz, 1H), 2.83-2.78 (m, 1H), 2.59-2.53 (m, 1H), 2.01 (s, 1H), 1.98-1.94 (m, 3H), 1.91 (d, J = 2.7 Hz, 1H), 1.78-1.74 (m, 6H), 1.72-1.69 (m, 2H), 1.63-1.60 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.6, 177.3, 143.6, 133.9, 128.6, 127.9, 124.4, 122.4, 118.2, 108.6, 61.2, 45.1,40.7, 38.9, 38.7, 36.56, 36.53, 35.0, 27.9; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{24}H_{30}NO_3$ 380.2220, Found 380.2221.

4.1 Unsuccessful Substrate



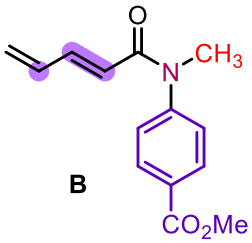
(*E*)-*N*-(4-cyanophenyl)-*N*-methylpenta-2,4-dienamide (**A**)



A was prepared according to the general procedure **4** in 62% (26.3 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 86:14) as the eluent, **TLC** (20% ethyl acetate in hexanes): R_f = 0.4

IR (neat); 2927, 1658, 1636, 1471, 1432, 1260 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.76-7.67 (m, 2H), 7.31-7.27 (m, 3H), 6.29-6.27 (m, 1H), 5.83 (d, *J* = 14.9 Hz, 1H), 5.58 (dd, *J* = 16.9, 0.7 Hz, 1H), 5.46-5.38 (m, 1H), 3.39 (s, 3H).; **^{13}C NMR** (126 MHz, $CDCl_3$): δ 165.9, 147.8, 143.5, 134.9, 133.6, 127.7, 125.3, 121.8, 118.2, 111.0, 37.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{13}N_2O$ 213.1022, Found 213.1028.

Methyl (*E*)-4-(*N*-methylpenta-2,4-dienamido)benzoate (**B**)

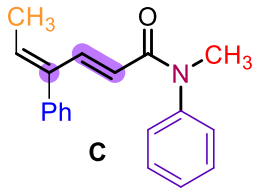


B was prepared according to the general procedure **4** in 58% (28.4 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 85:15) as the eluent, **TLC** (20% ethyl acetate in hexanes): R_f = 0.3

IR (neat); 2945, 1734, 1645, 1608, 1456, 1414, 1244 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.19-7.91 (m, 2H), 7.29 (dd, *J* = 13.6, 9.9 Hz, 2H), 7.24 (d, *J* = 0.7 Hz,

1H), 6.26 (m,1H), 5.84 (d, J = 14.9 Hz, 1H), 5.55 (d, J = 16.9 Hz, 1H), 5.38 (d, J = 10.0 Hz, 1H), 3.94 (s, 3H), 3.38 (s, 3H).; **^{13}C NMR** (126 MHz, $CDCl_3$): δ 166.3, 166.0, 147.8, 142.8, 135.0, 131.0, 129.1, 127.0, 124.8, 122.3, 52.4, 37.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{14}H_{16}NO_3$ 246.1125, Found 246.1129.

(2*E*,4*E*)-*N*-Methyl-*N*,4-diphenylhexa-2,4-dienamide (**C**)

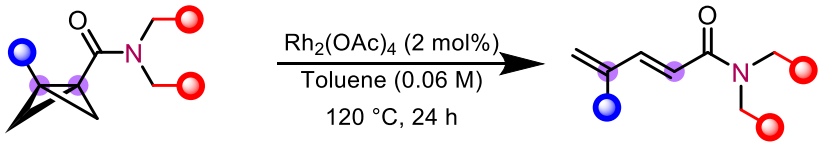


C

C was prepared according to the general procedure **4** in 35% (19.4 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 90:10) as the eluent, **TLC** (20% ethyl acetate in hexanes): R_f = 0.45

IR (neat); 2932, 1654, 1618, 1598, 1435, 1397, 1260 cm^{-1}; **^{1}H NMR** (700 MHz, $CDCl_3$): δ 7.34 (t, J = 7.8 Hz, 2H), 7.27 (d, J = 10.7 Hz, 2H), 7.18-7.07 (m, 4H), 6.92 (s, 2H), 5.56 (s, 1H), 5.28 (s, 1H), 5.14 (s, 1H), 3.32 (s, 3H), 2.21 (s, 3H).; **^{13}C NMR** (126 MHz, $CDCl_3$): δ 167.8, 151.9, 147.1, 143.9, 140.2, 129.5, 128.4, 128.0, 127.3, 127.1, 123.5, 115.7, 36.8, 16.7 (2 aromatic carbons overlapped) ; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{20}NO$ 278.1539, Found 278.1545.

5.0 Synthesis of *α, β, γ, δ*-unsaturated amides *via* [1,2]–*H* migration

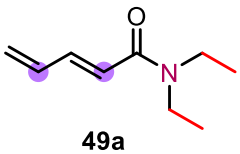


48 **49**

5.1 General Procedure for Synthesis of α, β, γ, *δ*-unsaturated amides *via* [1,2]–*H* migration.

To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, bicyclobutane-1-carboxamide **47** (0.2 mmol, 1.0 equiv.) and $Rh_2(OAc)_4$ (1.8 mg, 0.004 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by addition of toluene (0.06 M, 3 mL) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 24 h, the residue was diluted with ethyl acetate (10 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue was purified by column chromatography on silica gel using ethyl acetate and hexanes as eluent.

(*E*)-*N*,*N*-Diethylpenta-2,4-dienamide (**49a**)

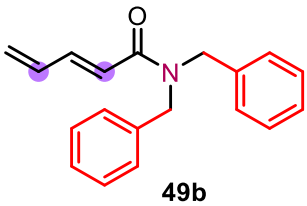


49a

49a was prepared according to the general procedure **5.1** in 54% (16.5 mg) isolated yield. Yellow oil. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 70:30) as the eluent, **TLC** (30% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3

IR (neat); 2970, 2924, 1660, 1508, 1487, 1463, 1275 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.30-7.25 (m, 1H), 6.51-6.43 (m, 1H), 6.29 (dd, *J* = 1.5, 14.1 Hz, 1H), 5.56-5.52 (m, 1H), 5.41-5.38 (m, 1H), 3.44 (q, *J* = 7.2 Hz, 2H), 3.38 (q, *J* = 7.2 Hz, 2H), 1.21 (t, *J* = 6.2 Hz, 3H), 1.14 (t, *J* = 6.2 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 166.7, 142.6, 135.4, 123.9, 121.8, 42.3, 41.0, 15.0, 13.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_9H_{16}NO$ 154.1226, Found 154.1228.

(*E*)-*N*,*N*-Dibenzylpenta-2,4-dienamide (**49b**)

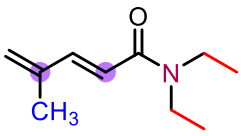


49b

49b was prepared according to the general procedure **5.1** in 58% (32.1 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 88:12) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.3

IR (neat); 2972, 2936, 1661, 1614, 1485, 1463, 1288 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.46-7.41 (m, 1H), 7.38-7.28 (m, 8H), 7.18 (d, *J* = 7.8 Hz, 2H), 6.44-6.36 (m, 2H), 5.61-5.57 (m, 1H), 5.43-5.41 (m, 1H), 4.66 (s, 2H), 4.52 (s, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 167.3, 144.1, 137.4, 136.7, 135.2, 129.0, 128.7, 128.4, 127.8, 127.5, 126.6, 124.7, 121.3, 50.0, 48.7; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{20}NO$ 278.1539, Found 278.1541.

(*E*)-*N*,*N*-Diethyl-4-methylpenta-2,4-dienamide (**49c**)



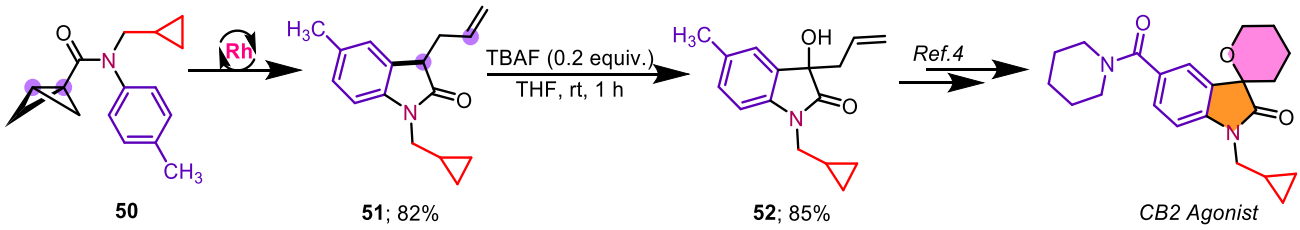
49c

49c was prepared according to the general procedure **5.1** in 62% (20.7 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 90:10) as the eluent, **TLC** (10% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.4

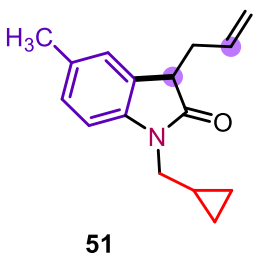
IR (neat); 3029, 2922, 1600, 1603, 1495, 1453, 1261 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.36 (d, *J* = 15.2 Hz, 1H), 6.23 (d, *J* = 15.2 Hz, 1H), 5.30-5.24 (m, 2H), 3.42-3.34 (m, 4H), 1.88 (s, 3H), 1.19-1.11 (m, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 166.1, 144.7, 140.7, 122.9, 118.0, 42.3, 41.0, 18.4, 15.0, 13.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{10}H_{18}NO$ 168.1383, Found 168.1383.

6.0 Synthesis of bioactive molecule percussors

6.1 Synthesis of *CB2 Agonist*



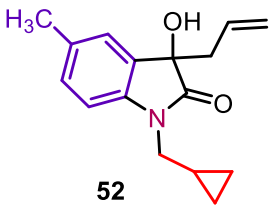
3-Allyl-1-(cyclopropylmethyl)-5-methylindolin-2-one (**51**)


51

51 was prepared according to the general procedure **4** in 82% (39.5 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 94:6) as the eluent, **TLC** (10% ethyl acetate in hexanes): $R_f = 0.4$

IR (neat); 3051, 2928, 1708, 1614, 1487, 1378, 1254 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.10 (s, 1H), 7.07 (d, J = 7.9 Hz, 1H), 6.79 (d, J = 8.1 Hz, 1H), 5.76-5.65 (m, 1H), 5.12-5.07 (m, 1H), 5.03-5.01 (m, 1H), 3.61-3.52 (m, 2H), 3.46 (dd, J = 2.9, 7.5 Hz, 1H), 2.82-2.77 (m, 1H), 2.60-2.54 (m, 1H), 2.33 (s, 3H), 1.17-1.05 (m, 1H), 0.52-0.45 (m, 2H), 0.40-0.32 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.2, 141.7, 134.1, 131.5, 128.9, 128.1, 125.2, 117.9, 108.1, 45.4, 44.2, 35.0, 21.2, 9.7, 4.0, 3.8; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{20}NO$ 242.1539, Found 242.1539.

3-Allyl-1-(cyclopropylmethyl)-3-hydroxy-5-methylindolin-2-one (**52**)

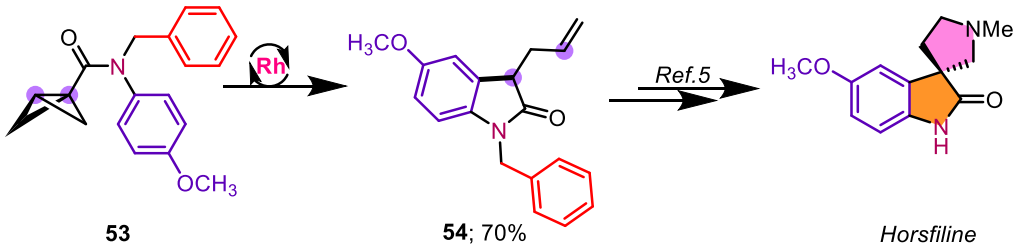

52

To a solution of 3-allyl-1-(cyclopropyl methyl)-5-methylindolin-2-one **50** (48.2 mg, 0.2 mmol, 1.0 equiv.) in THF (2 mL) tetrabutylammonium fluoride (0.04 mmol, 20 mol%) was added, the mixture was kept stirring for 1 hour at room temperature. The mixture was quenched with saturated Solution of NH_4Cl, extracted with diethyl ether, the combined organic layers were dried over Na_2SO_4. The reaction mixture was concentrated under reduce pressure and the residue was purified by column chromatography (hexanes: ethyl acetate 80:20) to give the pure product **52** in 85% yield (43.7 mg) as a white solid. Spectral data matched with the reported literature.[4]

IR (neat); 3050, 2920, 1709, 1608, 1486, 1368, 1252 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.21 (s, 1H), 7.10 (d, J = 8.0 Hz, 1H), 6.79 (d, J = 8.1 Hz, 1H), 5.60-5.52 (m, 1H), 5.10 (d, J = 17.1 Hz, 1H), 5.03 (d, J

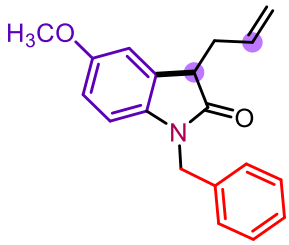
= 10.1 Hz, 1H), 3.64 (s, 1H), 3.58 (dd, *J* = 2.9, 7.1 Hz, 1H), 3.45 (dd, *J* = 2.9, 7.1 Hz, 1H), 2.78 (dd, *J* = 2.8, 6.4 Hz, 1H), 2.64 (dd, *J* = 2.8, 6.4 Hz, 1H), 2.33 (s, 3H), 1.13-1.10 (m, 1H), 0.52-0.43 (m, 2H), 0.38-0.30 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.9, 140.6, 132.5, 130.7, 129.9, 129.8, 125.0, 120.1, 108.6, 76.2, 44.3, 43.1, 21.1, 9.6, 4.0, 3.8; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{20}NO_2$ 258.1489, Found 258.1488.

6.2 Synthesis of *Horsfiline*



53 **54**; 70% *Horsfiline*

3-Allyl-1-benzyl-5-methoxyindolin-2-one (**54**)



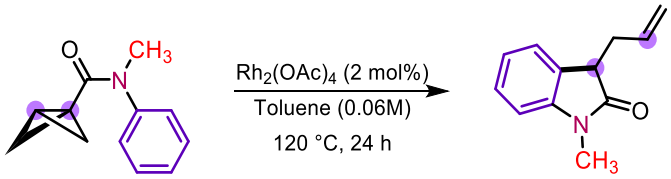
54

54 was prepared according to the general procedure **4** in 70% (41.0 mg) isolated yield. Colorless liquid. Purification done by column chromatography on silica gel using (hexanes: EtOAc = 92:8) as the eluent, **TLC** (20% ethyl acetate in hexanes): $\boldsymbol{R_f}$ = 0.5

IR (neat); 3057, 2935, 1706, 1600, 1490, 1392, 1248 cm^{-1}; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.31-7.27 (m, 4H), 6.91-6.82 (m, 2H), 6.70-6.65 (m, 1H), 6.58 (d, *J* = 8.0 Hz, 1H), 5.79-5.70 (m, 1H), 5.16-5.05 (m, 2H), 4.98 (d, *J* = 15.6 Hz, 1H), 4.81 (d, *J* = 16.0 Hz, 1H), 3.74 (s, 3H), 3.58 (dd, *J* = 4.1, 6.8 Hz, 1H), 2.90-2.84 (m, 1H), 2.67-2.62 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 176.9, 155.8, 136.9, 136.0, 133.9, 130.0, 128.7, 127.6, 127.3, 118.3, 112.0, 111.9, 109.2, 55.8, 45.6, 43.8, 35.0; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{20}NO_2$ 294.1489, Found 294.1491. Spectral data matched with the reported literature.[5]

7.0 Synthetic utility of 3-allyl oxindole

7.1 Scale-up reaction.

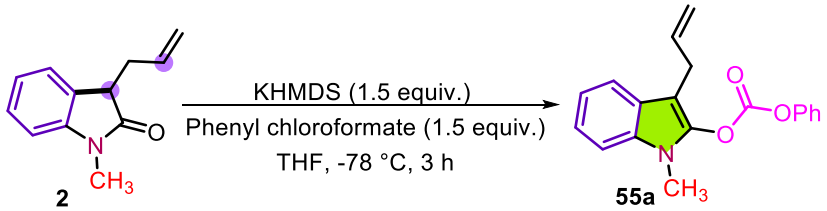


1 (2 mmol) **2**; 60%

Procedure for Scale-up reaction

To an oven dried round bottom flask (50 mL) equipped with magnetic stir bar, *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **1** (374.1 mg, 2.0 mmol, 1.0 equiv.) and $Rh_2(OAc)_4$ (17.6 mg, 0.04 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by toluene (30 mL, 0.06 M) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 24 h, the residue was diluted with ethyl acetate (10 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue was purified by column chromatography (hexanes:ethyl acetate 93:7) to give the pure product **2** in 60% yield (224.5 mg) as a yellow liquid.

7.2 Synthesis of 3-allyl-1-methyl-1H-indol-2-yl phenyl carbonate (**55a**).

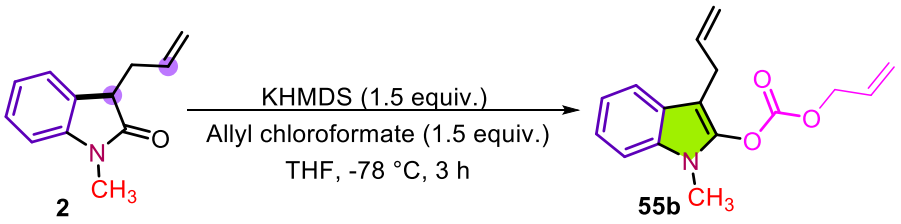


Compound **55a** was synthesized by using reported literature procedure.[5]

3-Allyl-1-methylindolin-2-one **2** (37.4 mg, 0.2 mmol, 1.0 equiv.) was dissolved in THF (0.1 M, 2 mL) and add the solution of KHMDS (0.3 mL, 1.0 M in THF, 0.3 mmol, 1.5 equiv.) at -78 °C and stirred for 30 minutes. Then the solution of phenyl chloroformate (46.9 mg, 0.3 mmol, 1.5 equiv.) in 2 mL THF was added dropwise at -78 °C and the resulting solution allowed to warm slowly to rt and continued stirring for further 3 h. Upon complete conversion of **2**. Then the reaction mixture was poured into 0.1 N aqueous HCl (5 mL) and extracted with diethyl ether. The combined organic layers were dried over Na_2SO_4. The reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography (hexanes:ethyl acetate 92:8) to give the pure product **55a** in 88% yield (54.0 mg) as a white solid. Spectral data matched with the reported literature.[5]

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.62 (d, J = 8.2 Hz, 1H), 7.46-7.44 (m, 2H), 7.34-7.29 (m, 5H), 7.19-7.16 (m, 1H), 6.10-6.02 (m, 1H), 5.25-5.21 (m, 1H), 5.13-5.10 (m, 1H), 3.68 (s, 3H), 3.54 (d, J = 6.3 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 151.0, 139.2, 136.3, 132.7, 129.8, 126.7, 125.8, 121.9, 121.0, 120.7, 119.8, 119.3, 115.4, 109.1, 98.6, 28.4, 27.7; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{18}NO_3$ 308.1281, Found 308.1279.

7.3 Synthesis of allyl (3-allyl-1-methyl-1H-indol-2-yl) carbonate (**55b**).

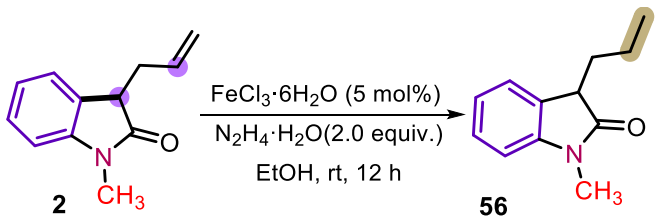


Compound **55b** was synthesized by using reported literature procedure.[5]

3-Allyl-1-methylindolin-2-one **2** (37.4 mg, 0.2 mmol, 1.0 equiv.) was dissolved in THF (0.1 M, 2 mL) and add the solution of KHMDS (0.3 mL, 1.0 M in THF, 0.3 mmol, 1.5 equiv.) at -78 °C and stirred for 30 minutes. Then the solution of Allyl chloroformate (36.15 mg, 0.3 mmol, 1.5 equiv.) in 2 mL THF was added dropwise at -78 °C and the resulting solution allowed to warm slowly to rt and continued stirring for further 3 h. Upon complete conversion of **2**. Then the reaction mixture was poured into 0.1 N aqueous HCl (5 mL) and extracted with diethyl ether. The combined organic layers were dried over Na_2SO_4. The reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography (hexanes:ethyl acetate 93:7) to give the pure product **55b** in 84% yield (45.5 mg) as a colorless liquid.

^{1}H NMR (500 MHz, $CDCl_3$): δ NMR (500 MHz,) δ 7.58-7.55 (m, 1H), 7.29-7.20 (m, 2H), 7.13 (dd, J = 8.0, 1.3 Hz, 1H), 6.08-5.91 (m, 2H), 5.46-4.45 (m, 1H), 5.42-5.36 (m, 1H), 5.14 (dq, J = 17.0, 1.7 Hz, 1H), 5.04 (dq, J = 10.0, 1.5 Hz, 1H), 4.83-4.77 (m, 2H), 3.59 (s, 3H), 3.43 (dt, J = 6.3, 1.5 Hz, 2H).; **^{13}C NMR** (126 MHz, $CDCl_3$): δ 152.5, 139.4, 136.3, 132.7, 130.7, 125.8, 121.7, 120.1, 119.7, 119.3, 115.2, 109.1, 98.7, 70.0, 28.3, 27.6; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{18}NO_3$ 272.1281, Found 272.1287.

7.4 Synthesis of 1-methyl-3-propylindolin-2-one (**56**).



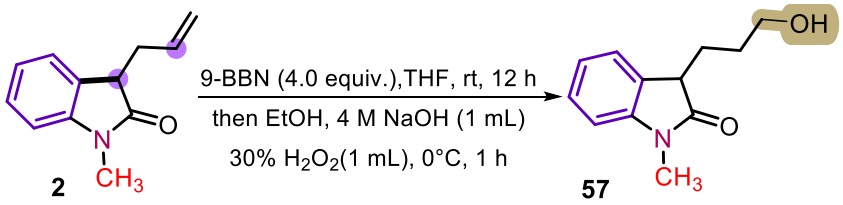
Compound **56** was synthesized by using reported literature procedure.[6]

A mixture of **2** (37.4 mg, 0.2 mmol, 1.0 equiv.) $FeCl_3$.$6H_2O$ (2.7 mg, 5 mol %) were dissolved in ethanol (1 mL), immediately followed by addition of 80 % hydrazine hydrate (20.4 mg, 0.4 mmol). The reaction mixture was then stirred at room temperature in air for 12 h. The reaction mixture was extracted with DCM (5 mL ×3) and dried over sodium sulfate, and concentrated under reduced pressure. The resulting residue

was purified by column chromatography (hexanes:ethyl acetate 94:6) to give the product **56** in 78% (29.5 mg) as colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.27-7.24 (m 2H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.80 (d, *J* = 7.8 Hz, 1H), 3.41 (t, *J* = 6.1 Hz, 1H), 3.19 (s, 3H), 1.96-1.86 (m, 2H), 1.44-1.33 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (126 MHz $CDCl_3$): δ 178.1, 144.4, 129.4, 127.8, 123.9, 122.2, 107.9, 45.5, 32.9, 26.1, 19.3, 14.0; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{16}NO$ 190.1226, Found 190.1232.

7.5 Synthesis of 3-(3-hydroxypropyl)-1-methylindolin-2-one (**57**).

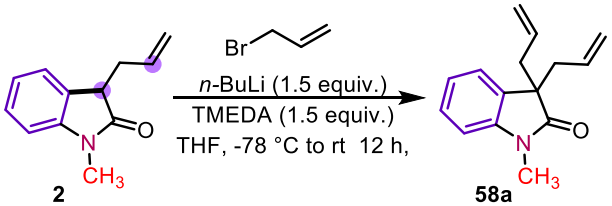


Compound **57** was synthesized by using reported literature procedure.[7]

To a solution of 3-Allyl-1-methylindolin-2-one **2** (37.4 mg, 0.2 mmol, 1.0 equiv.) in THF (1 mL), 9-BBN (0.5 M in THF, 4.0 equiv.) was added under nitrogen atmosphere. Then the resulting solution was stirred for 12 h at room temperature. The reaction was diluted with EtOH (3 mL) and treated with 4 M NaOH (1 mL). Then 30% H_2O_2 (1 mL) was added dropwise at 0 °C. Then it was stirred at 0 °C for 1 h, and was quenched by addition of saturated aq. NH_4Cl. The mixture was extracted with Et_2O (3×10 mL). The combined organic phase was washed with brine, dried over Na_2SO_4, and concentrated in vacuum. The resulting residue was purified by column chromatography (hexanes:ethyl acetate 50:50)to give the product **57** in 72% (29.5 mg) as colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.31-7.27 (m, 1H), 7.25-7.24 (m, 1H), 7.10-7.03 (m, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 3.69-3.59 (m, 2H), 3.50 (t, *J* = 6.0 Hz, 1H), 3.21 (s, 3H), 2.12-2.00 (m, 2H), 1.67-1.59 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 178.2, 144.4, 129.1, 128.1, 123.9, 122.6, 108.1, 62.5, 45.2, 29.0, 26.8, 26.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{16}NO_2$ 206.1176, Found 206.1172.

7.6 Synthesis of 3,3-diallyl-1-methylindolin-2-one (**58a**).

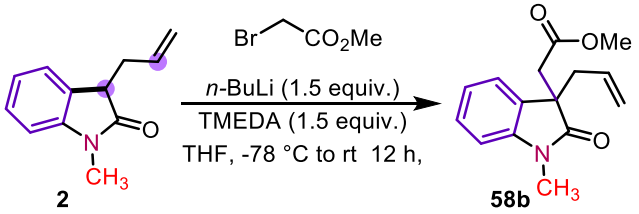


Compound **58a** was synthesized by using reported literature procedure.[8]

3-Allyl-1-methylindolin-2-one **2** (37.4 mg, 0.2 mmol, 1.0 equiv.) and tetramethylethylenediamine (TMEDA) (34.8 mg, 0.3 mmol, 1.5 equiv.) was dissolved in THF (0.1 M, 3 mL) then *n*BuLi (1.6 M in Hexane, 0.3 mmol, 1.5 equiv.) was added at -78 °C The mixture was kept stirring for 30 minutes before the addition of allyl bromide (24.1 mg, 0.2 mmol, 1.0 equiv.). The reaction mixture was stirred overnight and warmed to room temperature slowly. The reaction mixture was quenched with saturated NH_4Cl, extracted with DCM, the combined organic layers were dried over Na_2SO_4. The organic residue was concentrated under reduce pressure and the residue was purified by column chromatography (hexanes:ethyl acetate 95:5) to give the pure product **58a** in 85% yield (38.61 mg) as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.27-7.24 (m, 1H), 7.19 (d, J = 6.6 Hz, 1H), 7.07-7.04 (m, 1H), 6.80 (d, J = 7.7 Hz, 1H), 5.42-5.35 (m, 2H), 5.0-4.95 (m, 2H), 4.93-4.87 (m, 2H), 3.17 (s, 3H), 2.56-2.54 (m, 4H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 179.0, 143.8, 132.4, 131.4, 127.9, 123.4, 122.3, 118.8, 107.9, 52.7, 41.3, 26.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{18}NO$ 228.1383, Found 228.1383.

7.7 Synthesis of methyl 2-(3-allyl-1-methyl-2-oxoindolin-3-yl)acetate (**58b**).



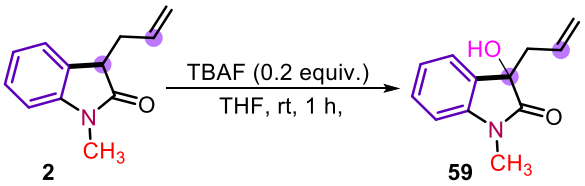
Compound **58b** was synthesized by using reported literature procedure.[8]

3-Allyl-1-methylindolin-2-one **2** (37.4 mg, 0.2 mmol, 1.0 equiv.) and tetramethylethylenediamine (TMEDA) (34.8 mg, 0.3 mmol, 1.5 equiv.) was dissolved in THF (0.1 M, 3 mL) then ^{n}BuLi (1.6 M in Hexane, 0.3 mmol, 1.5 equiv.) was added at -78 °C The reaction mixture was kept stirring for 30 minutes before the methyl bromoacetate (30.6 mg, 0.2 mmol, 1.0 equiv.) was added. The reaction mixture was stirred overnight and warmed to room temperature slowly. The reaction mixture was quenched with saturated solution of NH_4Cl, the organic residue was extracted with DCM, the combined organic layers were dried over Na_2SO_4. The organic residue was concentrated under reduced pressure and the residue was purified by column chromatography (hexanes:ethyl acetate 92:8) to give the pure product **58b** in 73% yield (37.8 mg) as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.30-7.27 (m, 1H), 7.17 (d, J = 6.8 Hz, 1H), 7.03 (t, J = 7.8 Hz, 1H), 6.84 (d, J = 7.8 Hz, 1H), 5.48-5.40 (m, 1H), 5.03-4.96 (m, 2H), 3.43 (s, 3H), 3.23 (s, 3H), 3.03 (d, J = 16.4 Hz, 1H), 2.90 (d, J = 16.2 Hz, 1H), 2.51-2.46 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 178.9, 170.4, 144.2,

131.5, 130.8, 128.4, 122.9, 122.3, 119.6, 108.1, 51.7, 49.5, 42.1, 40.2, 26.4; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{18}NO_3$ 260.1281, Found 260.1287.

7.8 Synthesis of 3-allyl-3-hydroxy-1-methylindolin-2-one (**59**).

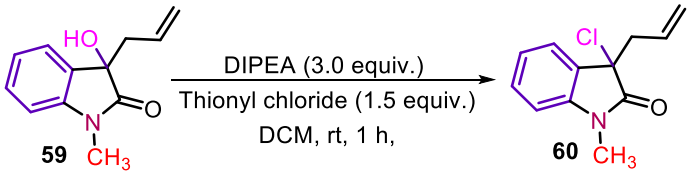


Compound **59** was synthesized by using reported literature procedure.[9]

To a solution of 3-Allyl-1-methylindolin-2-one **2** (37.4 mg, 0.2 mmol, 1.0 equiv.) in THF (2 mL) tetrabutylammonium fluoride (0.04 mmol, 20 mol%) was added and the reaction mixture was kept stirring for 1 hour at room temperature. The reaction mixture was quenched with saturated NH_4Cl, extracted with diethyl ether, the combined organic layers were dried over Na_2SO_4. The organic residue was concentrated under reduced pressure and the residue was purified by column chromatography (hexanes:ethyl acetate 80:20) to give the pure product **59** in 81% yield (32.9 mg) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.37 (d, J = 7.5 Hz, 1H), 7.32 (t, J = 7.87 Hz, 1H), 7.09 (t, J = 7.5 Hz, 1H), 6.83 (d, J = 7.8 Hz, 1H), 5.66-5.60 (m, 1H), 5.12-5.06 (m, 2H), 3.29 (s, 1H), 3.17 (s, 3H), 2.76-2.71 (m, 1H), 2.62-2.58 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.9, 143.3, 130.6, 129.8, 129.6, 124.2, 123.1, 120.5, 108.5, 75.9, 43.0, 26.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{14}NO_2$ 204.1019, Found 204.1019

7.9 Synthesis of 3-allyl-3-chloro-1-methylindolin-2-one (**60**).



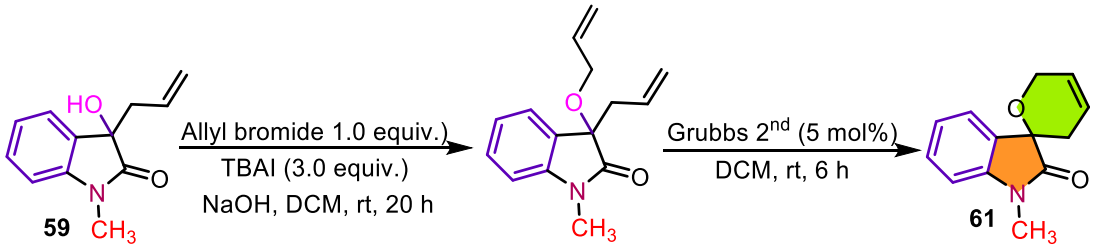
Compound **60** was synthesized by using reported literature procedure.[5]

To a solution of 3-allyl-3-hydroxy-1-methylindolin-2-one **59** (40.6 mg, 0.2 mmol, 1.0 equiv.) in DCM (2 mL) was added *N, N*-Diisopropylethylamine (77.5 mg, 0.6 mmol, 3.0 equiv.) and thionyl chloride (35.6 mg, 0.3 mmol, 1.5 equiv.) the mixture was kept stirring for 1 hour at room temperature. The reaction mixture was quenched with saturated $NaHCO_3$, extracted with diethyl ether, the combined organic layers were dried over Na_2SO_4. The organic residue was concentrated under reduced pressure and the residue was purified

by column chromatography (hexanes:ethyl acetate 95:5) to give the pure product **60** in 69% yield (30.5 mg) as a yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.40 (d, *J* = 7.5 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.11 (t, *J* = 7.7 Hz, 1H), 6.84 (d, *J* = 7.9 Hz, 1H), 5.75-5.50 (m, 1H), 5.11-5.05 (m, 2H), 3.21 (s, 3H), 3.03-2.99 (m, 1H), 2.93-2.89 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 173.6, 142.7, 130.29, 130.26, 129.1, 124.6, 123.3, 121.0, 108.7, 64.0, 43.3, 26.7; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{13}ClNO$ 222.0680, Found 222.0679.

7.10 Synthesis of 1-methyl-3',4'-dihydrospiro[indoline-3,2'-pyran]-2-one (**61**).



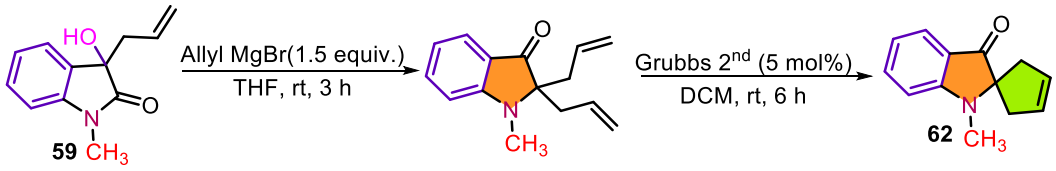
Compound **61** was synthesized by using reported literature procedure.[10]

3-allyl-3-hydroxy-1-methylindolin-2-one **59** (40.7 mg, 0.2 mmol, 1.0 equiv.) and tetrabutylammonium iodide (3.7 mg, 0.01 mmol, 5 mol%) was dissolved in DCM (0.1 M, 2 mL), NaOH (aq. 50%), 2 mL and allyl bromide (24.1 mg, 0.2 mmol, 1.0 equiv.) was added at room temperature and the reaction mixture was stirred for 16 h and then concentrated. The reaction mixture was quenched with water, extracted with DCM, the combined organic layers were dried over Na_2SO_4. The crude residue was used in the next step without purification.

Grubbs 2nd generation catalyst (8.4 mg, 0.01 mmol, 5 mol%), was added to crude residue of 3-allyl-3-(allyloxy)-1-methylindolin-2-one (48.6 mg, 0.2 mmol, 1.0 equiv.) in anhydrous DCM (0.02 M, 10 mL), the reaction mixture was stirred at room temperature for 6 h and then concentrated. Purification of the crude reaction mixture was done by column chromatography (hexanes:ethyl acetate 95:5) to give the pure product **61** in 66% yield (28.4 mg) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.43 (d, *J* = 8.0 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.04 (t, *J* = 7.5 Hz, 1H), 6.85 (d, *J* = 8.0 Hz, 1H), 6.03-5.94 (m, 2H), 4.59-4.53 (m, 1H), 4.42-4.37 (m, 1H), 3.19 (s, 3H), 2.73-2.68 (m, 1H), 2.19-2.14 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 175.1, 143.6, 129.8, 129.6, 125.9, 124.4, 122.8, 121.6, 108.5, 74.1, 62.6, 30.0, 26.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{14}NO_2$ 216.1019, Found 216.1019. Spectral data matched with the reported literature.[5]

7.11 Synthesis of 1'-methylspiro[cyclopentane-1,2'-indolin]-3-en-3'-one (**62**).



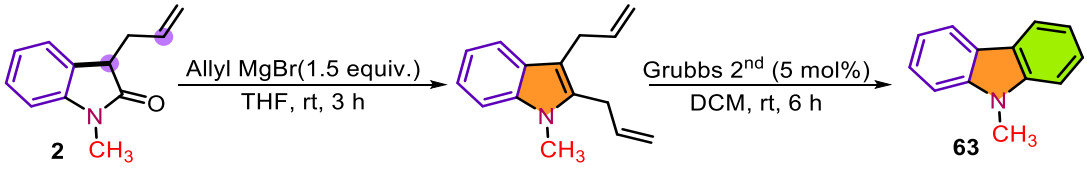
Compound **62** was synthesized by using reported literature procedure.[11]

To a solution of 3-allyl-3-hydroxy-1-methylindolin-2-one **59** (40.6 mg, 0.2 mmol, 1.0 equiv.) in THF (2 mL), allyl magnesium bromide (0.3 mmol, 1.0 M in THF, 1.5 equiv.) was added dropwise at room temperature. The resulting reaction mixture was then stirred at room temperature for 3 h. The reaction mixture was quenched with aqueous NH_4CI solution, extracted with EtOAc, the combined organic layers were dried over Na_2SO_4. Purification of the crude mixture was done by column chromatography (hexanes: ethyl acetate 99:1) to give the pure product 2,2-diallyl-1-methylindolin-3-one in 86% yield (39.0 mg) as a yellow oil.

Grubbs 2nd generation catalyst (7.1 mg, 0.008 mmol, 5 mol%), was added to a solution of 2,2-diallyl-1-methylindolin-3-one (39.0 mg, 0.17 mmol, 1.0 equiv.) in anhydrous DCM (0.02 M, 8.5 mL), the reaction mixture was stirred at room temperature for 6 h and then concentrated. Purification of the crude mixture was done by column chromatography (hexanes:ethyl acetate 98:2) to give the pure product **64** in 68% yield (23.01 mg) as a yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.60-7.57 (m, 1H), 7.45 (dd, J = 7.1, 1.2 Hz, 1H), 6.69 (dd, J = 7.5, 2.1 Hz, 2H), 5.80 (s, 2H), 2.92 (s 3H), 2.83 (d, J = 16.4 Hz, 2H), 2.51-2.41 (m, 2H).; **^{13}C NMR** (126 MHz, $CDCl_3$): δ 204.8, 159.8, 137.6, 128.8, 124.9, 119.2, 116.8, 107.9, 75.0, 42.0, 27.6; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for$C_{13}H_{14}NO$ $[M+H]^+$: 200.1070; Found: 200.1074 Spectral data matched with the reported literature.[11]

7.12 Synthesis of 9-methyl-9H-carbazole (**63**).



Compound **63** was synthesized by using reported literature procedure.[12]

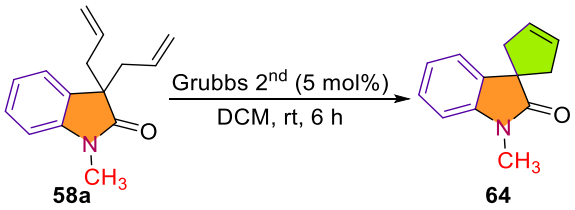
To a solution of 3-Allyl-1-methylindolin-2-one **2** (74.8 mg, 0.4 mmol, 1.0 equiv.) in THF (4 mL), allyl magnesium bromide (0.6 mmol, 1 M in THF, 1.5 equiv.) was added dropwise at room temperature. The resulting reaction mixture was then stirred at room temperature for 3 h. The reaction mixture was quenched

with aqueous NH_4CI solution, extracted with EtOAc, the combined organic layers were dried over Na_2SO_4. Purification of the crude mixture was done by column chromatography (hexanes:ethyl acetate 99:1) to give the pure product 2,3-diallyl-1-methyl-1H-indole in 79% yield (0.31 mmol, 66.7 mg) as a colorless liquid.

Grubbs 2nd generation catalyst (13.0 mg, 0.015 mmol, 5 mol%), was added to a solution of 2,3-diallyl-1-methyl-1H-indole (66.7 mg, 0.31 mmol, 1.0 equiv.) in anhydrous DCM (0.02 M, 15 mL), the reaction mixture was stirred at room temperature for 6 h and then concentrated. Purification of the crude mixture was done by column chromatography (hexanes:ethyl acetate 99:1) to give the pure product **63** in 87% yield (48.8 mg) as a white solid.

^{1}H NMR (700 MHz, $CDCl_3$): δ ^{1}H NMR (700 MHz, $CDCl_3$) δ 8.07 (s, 2H), 7.44 (d, *J* = 7.4 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 2H), 7.20 (d, *J* = 7.8 Hz, 2H), 3.75 (s, 3H).; **^{13}C NMR** (176 MHz, $CDCl_3$): δ141.0, 122.8, 120.4, 118.9, 108.5, 29.0; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for$C_{13}H_{12}N$ $[M+H]^+$: 182.0970; Found: 182.0968. Spectral data matched with the reported literature.[12]

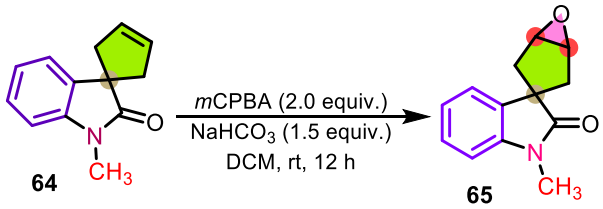
7.13 Synthesis of 1'-methylspiro[cyclopentane-1,3'-indolin]-3-en-2'-one (**64**).



Compound **64** was synthesized by using reported literature procedure.[10]
Grubbs 2nd generation catalyst (8.4 mg, 0.01 mmol, 5 mol%), was added to a solution of 3,3-diallyl-1-methylindolin-2-one **58a** (45.4 mg, 0.2 mmol, 1.0 equiv.) in anhydrous DCM (0.02 M, 10 mL), the reaction mixture was stirred at room temperature for 6 h and then concentrated. Purification of the crude mixture was done by column chromatography (hexanes:ethyl acetate 95:5) to give the pure product **64** in 77% yield (30.6 mg) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.25-7.2 (m, 2H), 7.01 (d, *J* = 7.7 Hz, 1H), 6.82 (d, *J* = 7.9 Hz, 1H), 5.83 (s, 2H), 3.22 (s, 3H), 3.01 (d, *J* = 14.6 Hz, 2H), 2.60 (d, *J* = 14.8 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 181.5, 142.6, 137.5, 129.0, 127.7, 122.9, 121.7, 107.9, 52.1, 45.0, 26.4; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{14}NO$ 200.1070, Found 200.1070. Spectral data matched with the reported literature.[5]

7.14 Synthesis of 1'-methyl-6-oxaspiro[bicyclo[3.1.0]hexane-3,3'-indolin]-2'-one (**65**).

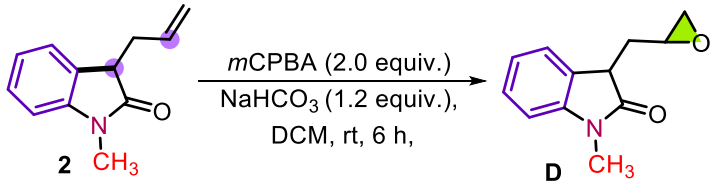


Compound **65** was synthesized by using reported literature procedure.[13]

1'-methylspiro[cyclopentane-1,3'-indolin]-3-en-2'-one **64** (39.8 mg, 0.2 mmol, 1.0 equiv.) was dissolved in DCM (0.05 M, 4 mL) then *m*CPBA (68.9 mg, 0.4 mmol, 2.0 equiv.) and $NaHCO_3$ (25.2 mg, 0.3 mmol, 1.5 equiv.) were added then the reaction mixture was continued stirred for 12 h at room temperature. The reaction progress was monitored by TLC. The reaction mixture extracted by DCM and water twice. The combined organic layers were dried over Na_2SO_4. The reaction mixture was concentrated under reduced. pressure and the residue was purified by column chromatography (hexanes:ethyl acetate 60:40) to give the compound **65** in 64% yield (27.5 mg) as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$):δ 7.63 (d, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 7.7 Hz, 1H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.80 (d, *J* = 7.7 Hz, 1H), 3.71 (s, 2H), 3.21 (s, 3H), 2.41 (d, *J* = 14.4 Hz, 2H), 2.14 (d, *J* = 14.4 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 180.5, 143.3, 136.6, 127.6, 126.5, 123.5, 107.7, 57.7, 50.5, 39.8, 26.6; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{14}NO_2$ 216.1019, Found 216.1025.

7.15 Synthesis of 1-methyl-3-(oxiran-2-ylmethyl)indolin-2-one (**D**).

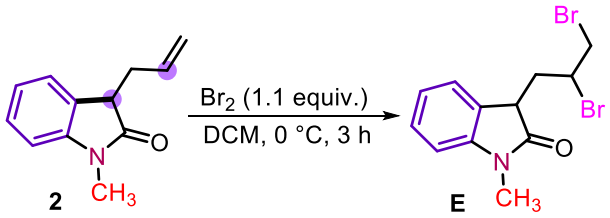


Compound **D** was synthesized by using reported literature procedure.[13]

3-Allyl-1-methylindolin-2-one **2** (37.4 mg, 0.2 mmol, 1.0 equiv.) was dissolved in DCM (0.05 M, 4 mL) then *m*CPBA (68.9 mg, 0.4 mmol, 2.0 equiv.) and $NaHCO_3$ (20.16 mg, 0.24 mmol, 1.2 equiv.) were added then the reaction mixture was continued stirred for 6 h at room temperature. The reaction progress was monitored by TLC. The reaction mixture extracted by DCM and water twice. The combined organic layers were dried over Na_2SO_4. The reaction mixture was concentrated under reduced. pressure and the residue was purified by column chromatography (hexanes:ethyl acetate 80:20) to give the compound **D** in 65% yield (26.5 mg) dr; 1:1 as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35-7.27 (m, 2H), 7.09-7.05 (m, 1H), 6.84 (t, *J* = 7.7 Hz, 1H), 3.63-3.57 (m, 1H), 3.22 (s, 1H), 3.20-3.17 (m, 0.5H), 3.06-3.03 (m, 0.5H), 2.79-2.76 (m, 1H), 2.59 (dd, *J* = 2.6, 5.0 Hz, 0.5H), 2.50 (dd, *J* = 2.6, 5.0 Hz, 0.5H), 2.36-2.31 (m, 0.5H), 2.29-2.24 (m, 0.5H), 1.98-1.90 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.3, 177.2, 144.3, 144.2, 130.2, 129.8, 128.36, 128.33, 124.4, 124.3, 122.6, 108.3, 108.2, 50.3, 49.6, 47.69, 47.61, 43.8, 43.1, 34.1, 33.5, 26.3; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{12}NO_2$ 204.1019, Found 204.1017

7.16 Synthesis of 3-(2,3-dibromopropyl)-1-methylindolin-2-one (**E**).



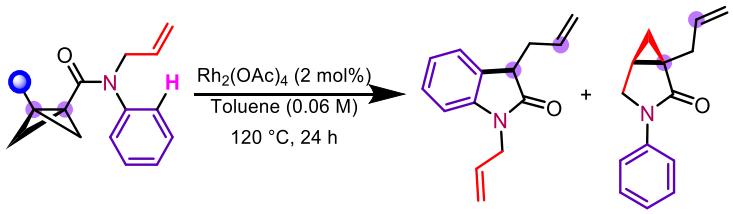
Compound **E** was synthesized by using reported literature procedure.[14]

A solution of Br_2 (21 µL, 0.41 mmol, 1.1 equiv.) in dry DCM (2 mL) was added to a solution of 3-Allyl-1-methylindolin-2-one **2** (37.4 mg, 0.2 mmol, 1.0 equiv.) compound in dry DCM (0.1 M, 2 mL) under N_2 atmosphere in an ice-bath. The resulting mixture was stirred at 0 °C for 3 h. The reaction mixture was washed with water and brine. The organic layer was dried over $MgSO_4$, filtered and the reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography (hexanes:ethyl acetate 90:10) to give the mixture of diastereomers 3:1 **57** in 61% (42.0 mg) yield as a yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.58 (d, *J* = 8.1 Hz, 0.32H), 7.52-7.46 (m, 2.36H), 6.78 (d, *J* = 8.2 Hz, 1H), 6.74 (d, *J* = 8.2 Hz, 0.4H), 4.02-3.99 (m, 0.26H), 3.79-3.75 (m, 0.75H), 3.73-3.69 (m, 1H), 3.56-3.52 (m, 1H), 3.49 (dd, *J* = 4.0, 8.9 Hz, 0.76H), 3.43 (dd, *J* = 4.0, 8.9 Hz, .25H), 3.24 (s, 0.75H), 3.22 (m, 2.25H), 3.03 (dd, *J* = 4.3, 10.8 Hz, .0.75H), 2.95 (dd, *J* = 4.3, 10.8 Hz, 0.25H); **^{13}C NMR** (126 MHz $CDCl_3$): δ 173.3, 172.6, 142.1, 141.3, 133.7, 133.4, 131.3, 129.3, 128.6, 127.9, 116.0, 115.9, 110.8, 110.5, 53.0, 52.7, 45.8, 45.5, 45.3, 44.5, 37.0, 36.6, 27.2, 27.1; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{14}Br_2NO$ 345.9437, Found 345.9439.

8.0 Control experiments.

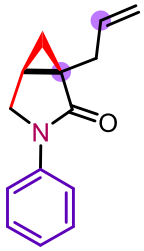
8.1 Intramolecular Rh(II)-carbene trapping.



66 **67**; 28% **68**; 25%

To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-allyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **66** (42.6 mg, 0.2 mmol, 1.0 equiv.) and $Rh_2(OAc)_4$ (1.8 mg, 0.004 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by toluene (0.06 M, 3 mL) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 24 h, the residue was diluted with ethyl acetate (10 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue purified by column chromatography on silica gel using (hexanes:ethyl acetate 93:7) we get the mixture of compounds **67 & 68** and some amount of pure compound **68**. Then we repeat the same reaction and the crude residue was submitted for ^{1}H NMR analysis to determine the yield, and we get the transannulation product **67** and cyclopropanation **68** in 28% and 25% yield respectively. Yield was determined by using CH_2Br_2 as internal standard.

1-Allyl-3-phenyl-3-azabicyclo[3.1.0]hexan-2-one (**68**)

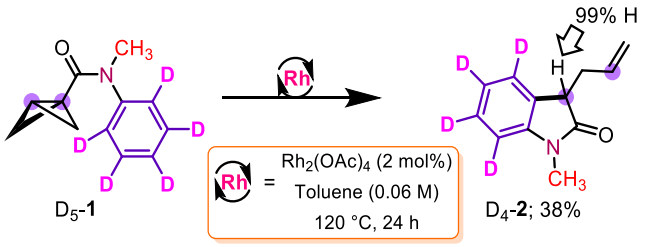


68

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.57-7.56 (m, 2H), 7.32 (t, *J* = 7.8 Hz, 2H), 7.11-7.07 (m, 1H), 5.86-5.77 (m, 1H), 5.11-5.04 (m, 1H), 3.99 (dd, J = 5.7, 6.8 Hz, 1H), 3.67 (d, *J* = 9.9 Hz, 1H), 2.83 (dd, *J* = 6.7, 7.1 Hz, 1H), 2.31 (dd, *J* = 6.7, 7.1 Hz, 1H), 1.88-1.84 (m, 1H), 1.08 (dd, *J* = 4.7, 7.5 Hz, 1H), 0.81 (t, *J* = 4.4 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ175.1, 139.7, 134.6, 128.9, 124.1, 119.5, 117.2, 49.4, 32.8, 31.1, 17.4, 15.8; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{14}H_{16}NO$ 214.1226, Found 214.1232.

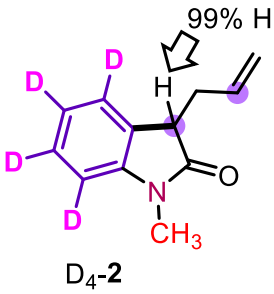
8.2 Deuterium trapping experiments.

Procedure for *N*-methyl-*N*-(phenyl-D_5)bicyclo[1.1.0]butane-1-carboxamide D_5-1



To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-methyl-*N*-(phenyl-D_5)bicyclo[1.1.0]butane-1-carboxamide D_5-**1** (38.4 mg, 0.2 mmol, 1.0 equiv.) and $Rh_2(OAc)_4$ (1.8 mg, 0.004 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by toluene (0.06 M, 3 mL) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 24 h, the residue was diluted with ethyl acetate (10 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue purified by column chromatography on silica gel using (hexanes:ethyl acetate 93:7) to give the pure product D_4-**2** in 38% yield (14.5 mg) as a yellow oil.

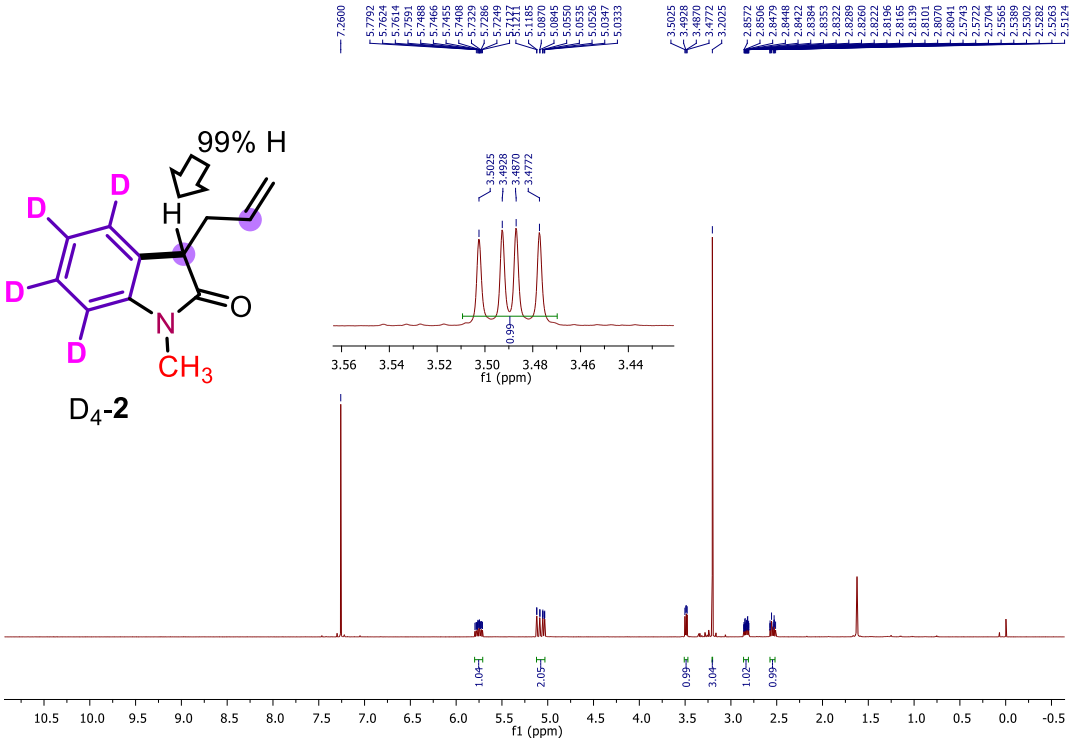
3-Allyl-1-methylindolin-2-one-4,5,6,7-D_4 (D_4-**2**)



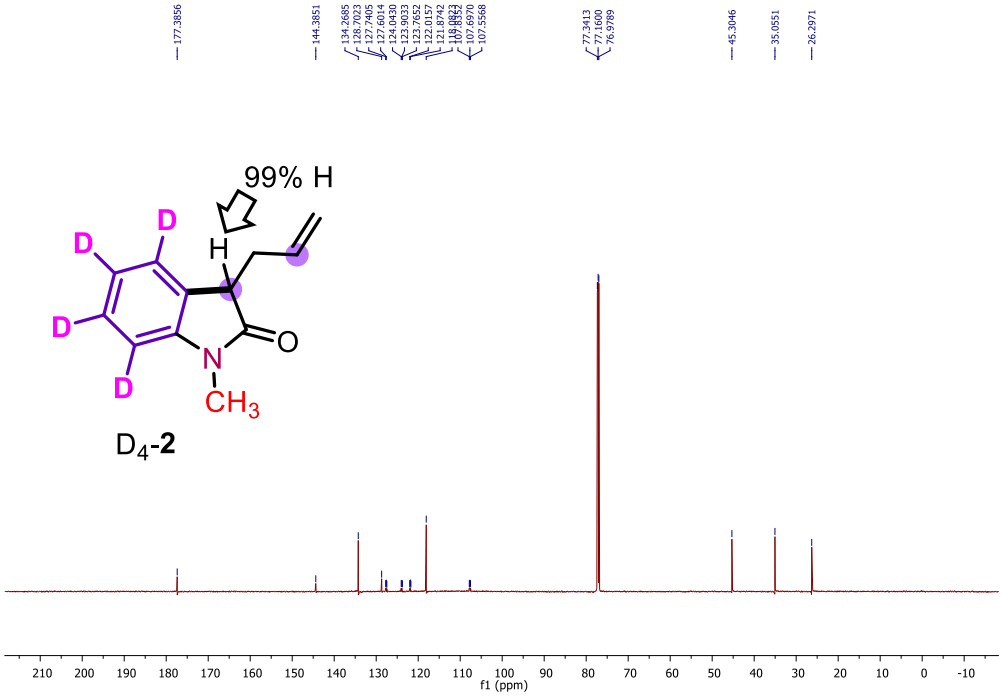
^{1}H NMR (500 MHz, $CDCl_3$): δ 5.79-5.71 (m, 1H), 5.12-5.03 (m, 2H), 3.48 (dd, J = 4.2, 7.1 Hz, 1H), 3.20 (s, 3H), 2.86-2.80 (m, 1H), 2.57-2.51 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.3, 144.3, 134.2, 128.7, 127.6 (t, $J_{C\text{-}D}$ = 17.5 Hz), 123.9 (t, $J_{C\text{-}D}$ = 17.7 Hz), 121.8 (t, $J_{C\text{-}D}$ = 17.5 Hz), 118.0, 107.6 (t, $J_{C\text{-}D}$ = 17.5Hz), 45.3, 35.0, 26.2; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{10}D_4NO$ 192.1321, Found 192.1320.

3-Allyl-1-methylindolin-2-one-4,5,6,7-D_4 (D_4-**2**)

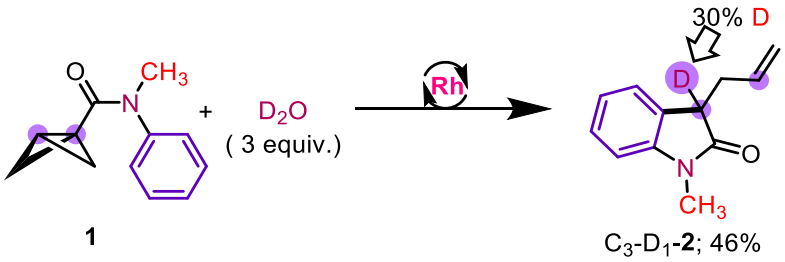
^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)



^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

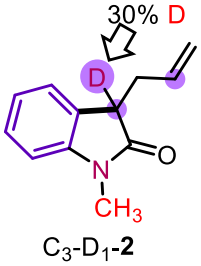


Procedure for *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide 1 with D_2O



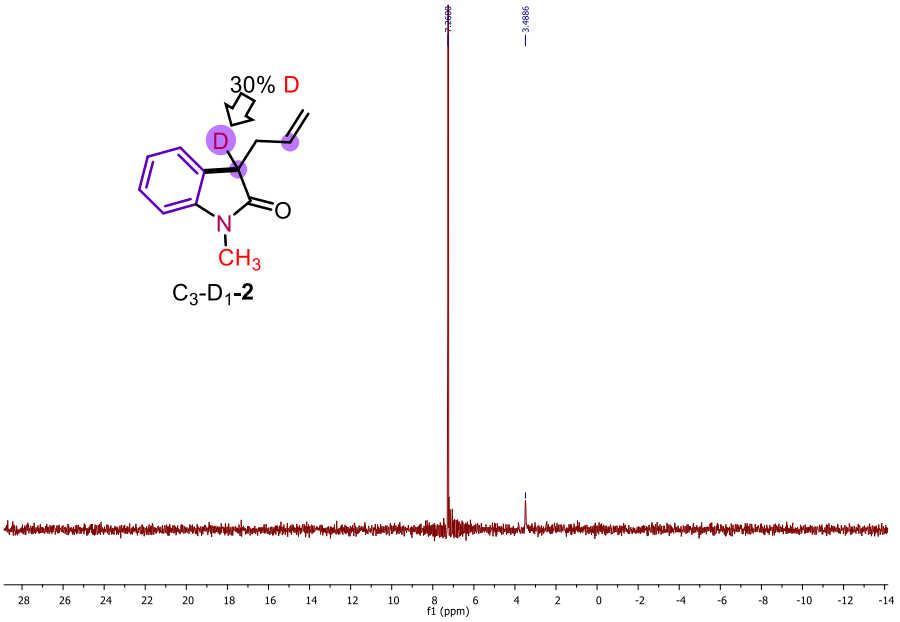
To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **1** (37.4 mg, 0.2 mmol, 1.0 equiv.), and $Rh_2(OAc)_4$ (1.8 mg, 0.004 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by toluene (0.06 M, 3 mL) and D_2O (12.0 mg, 0.6 mmol, 3.0 equiv.) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 24 h, the residue was diluted with ethyl acetate (10 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue purified by column chromatography on silica gel using (hexanes:ethyl acetate 93:7) to give the pure product C_3-D_1-**2** in 46% yield (17.3 mg) as a yellow oil.

3-Allyl-1-methylindolin-2-one-3-D (C_3-D_1-**2**)



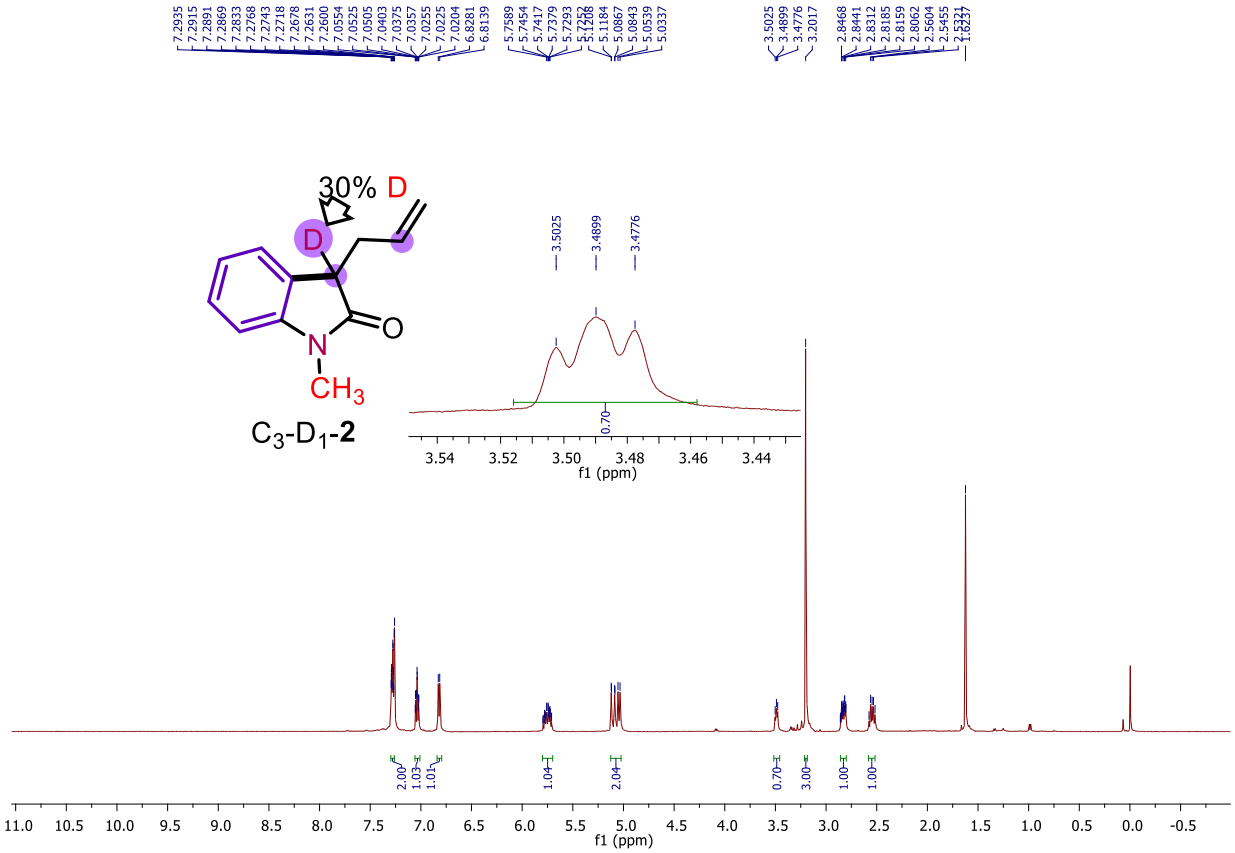
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.29-7.26 (m, 2H), 7.05-7.02(m, 1H), 6.81 (d, *J* = 7.1 Hz, 1H), 5.79-5.70 (m, 1H), 5.12-5.03 (m, 2H),3.48 (t, *J* = 6.3 Hz, **0.7H**), 3.20 (s, 3H), 2.85-2.80 (m, 1H), 2.57-2.51 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 177.3, 144.4, 134.2, 128.8, 128.0, 124.2, 122.3, 118.0, 108.0, 45.4 (C-D), 45.3, 35.0, 26.0; **HRMS** (ESI/Q-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{14}NO$ 188.1070, Found 188.1076 and $[M+H]^+$ Calcd for $C_{12}H_{13}DNO$ 189.1133, Found 188.1123.

^{2}H-NMR (76.7 MHz, $CDCl_3$, 24 °C)

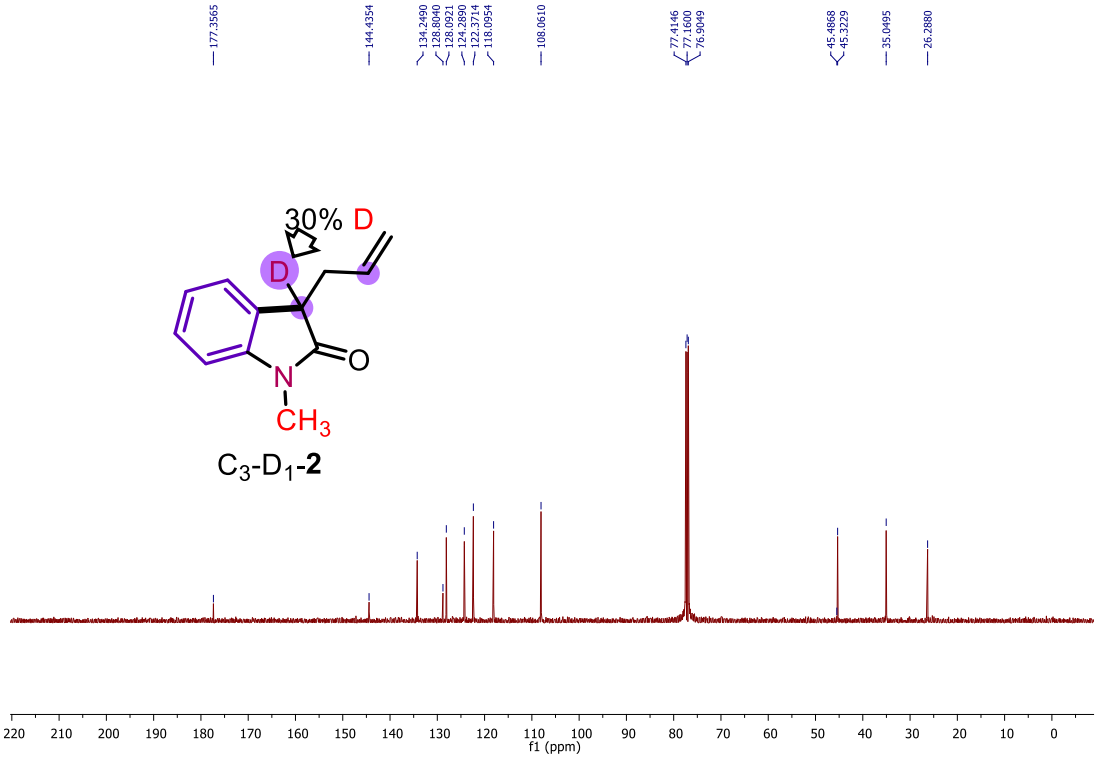


3-Allyl-1-methylindolin-2-one-3-D (C_3-D_1-**2**)

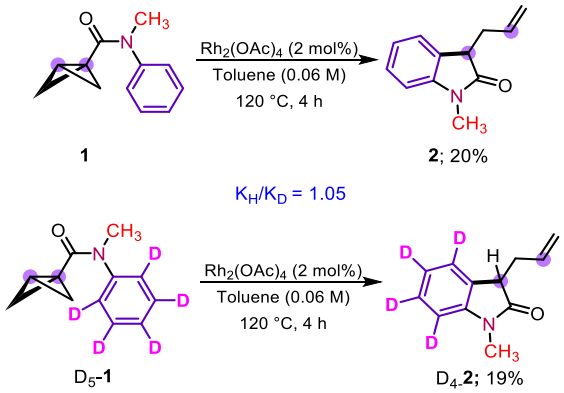
^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)



$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)



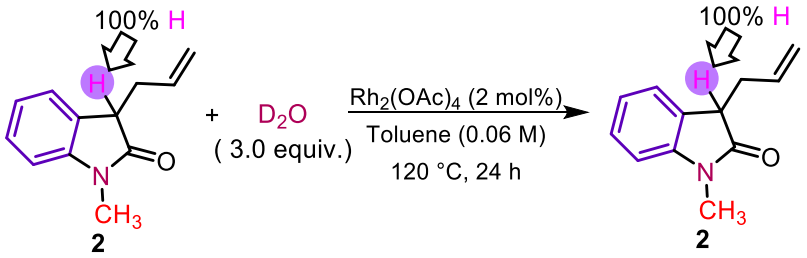
Procedure for kinetic isotopic effect (KIE) D_5-1 and H_5-1



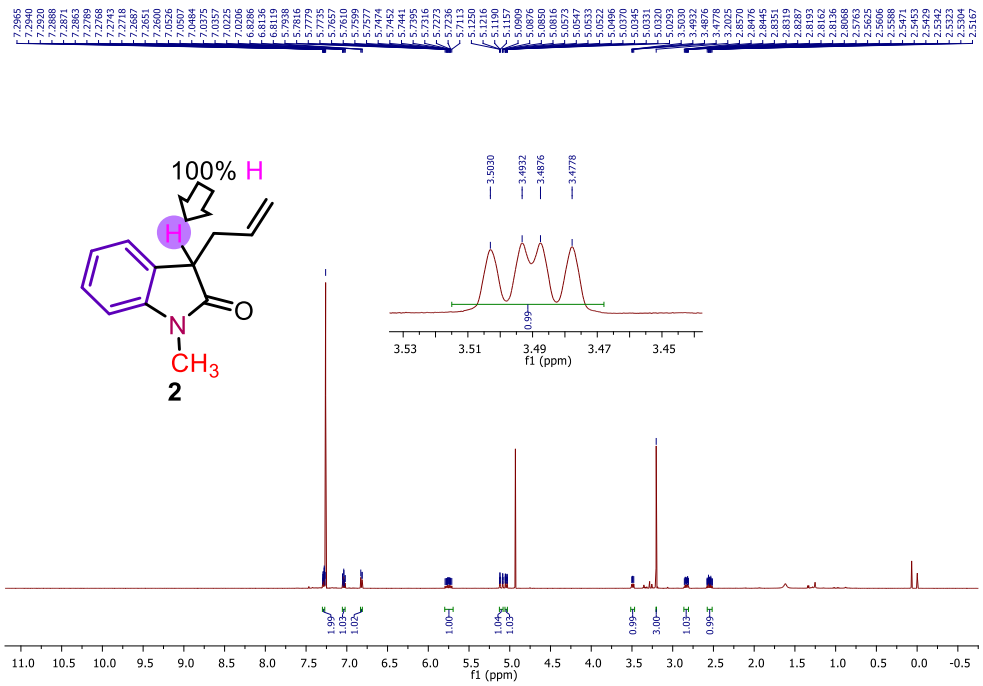
To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **1** (18.7 mg, 0.1 mmol, 1.0 equiv.), and $Rh_2(OAc)_4$ (0.9 mg, 0.002 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by toluene (0.06 M, 1.5 mL) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 4 h, the residue was diluted with ethyl acetate (5 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue submitted for ^{1}H NMR analysis to determine the yield, we get the product **2** in 20% yield.

To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-methyl-*N*-(phenyl-D_5) bicyclo[1.1.0]butane-1-carboxamide D_5-**1** (19.2 mg, 0.1 mmol, 1.0 equiv.), and $Rh_2(OAc)_4$ (0.9 mg, 0.002 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by toluene (0.06 M, 1.5 mL) under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 4 h, the residue was diluted with ethyl acetate (5 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue submitted for ^{1}H NMR analysis to determine the yield, we get the product D_4-**2** in 19% yield. For the competition of **1** and D_5-**1**, K_H/K_D = 1.05. Yield was determined by using CH_2Br_2 as internal standard.

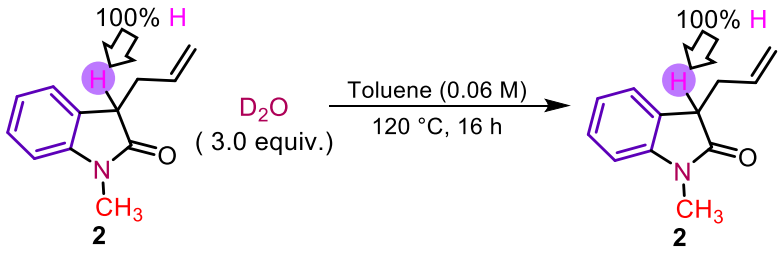
Procedure for deuterium trapping of 2 reaction of D_2O with $Rh_2(OAc)_4$ catalyst



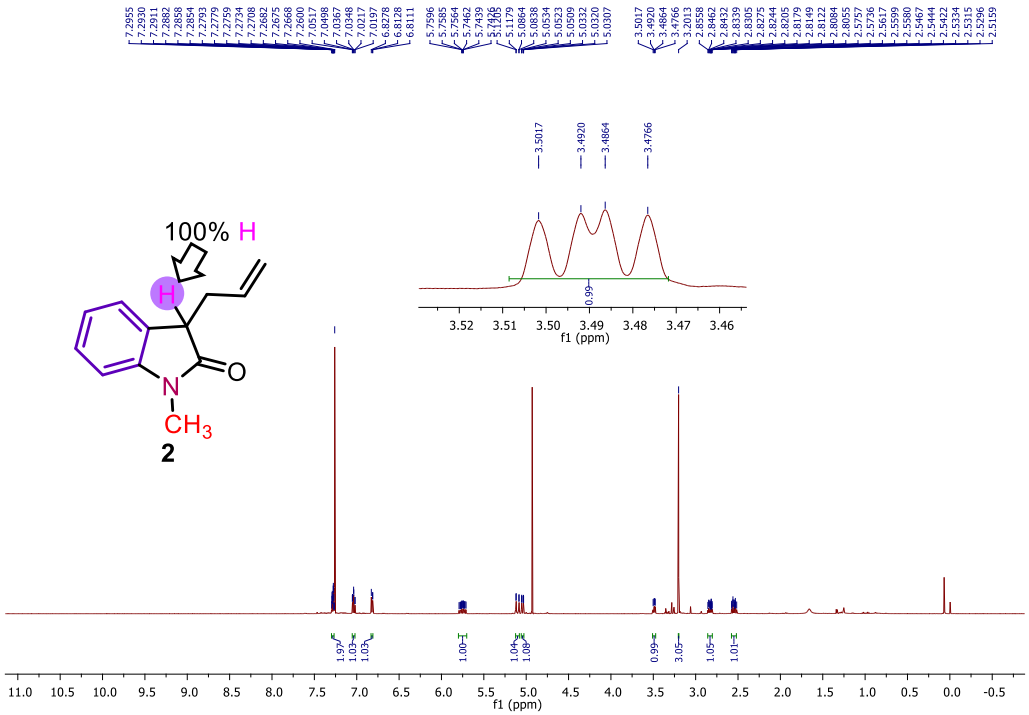
To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, 3-allyl-1-methylindolin-2-one **2** (18.7 mg, 0.1 mmol, 1.0 equiv.) and $Rh_2(OAc)_4$ (0.88 mg, 0.002 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by toluene (0.06 M, 1.5 mL) and D_2O (6.0 mg, 0.3 mmol, 3.0 equiv.) were added under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 24 h, the residue was diluted with ethyl acetate (10 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue submitted for ^{1}H and ^{2}H NMR analysis to check the hydrogen to deuterium exchange take place or not, here we observe that there is no H to D exchange take place and 100 % H was intact.



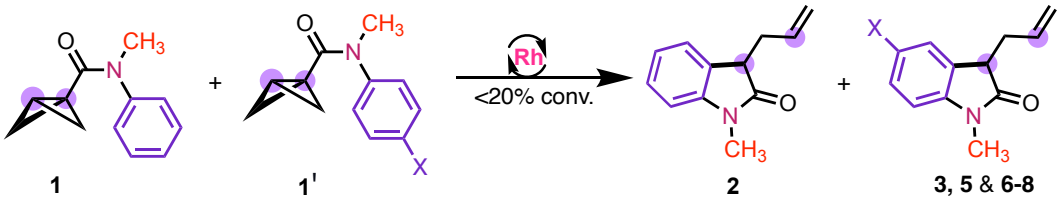
Procedure for deuterium trapping of 2 reaction of D_2O without $Rh_2(OAc)_4$ catalyst



To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, 3-allyl-1-methylindolin-2-one **2** (18.7 mg, 0.1 mmol, 1.0 equiv.), toluene (0.06 M, 1.5 mL) and D_2O (12.0 mg, 0.6 mmol, 3.0 equiv.) were added under nitrogen atmosphere and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 16 h, the residue was diluted with ethyl acetate (10 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue submitted for ^1H and ^2H NMR analysis to check the hydrogen to deuterium exchange take place or not, here we observe that there is no H to D exchange take place and 100 % hydrogen was intact.



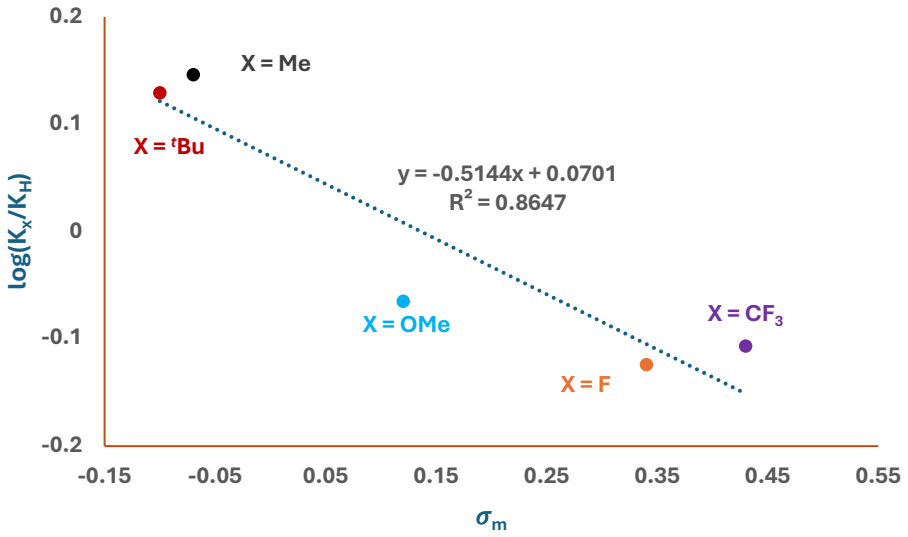
8.3 Hammett Study.[15]



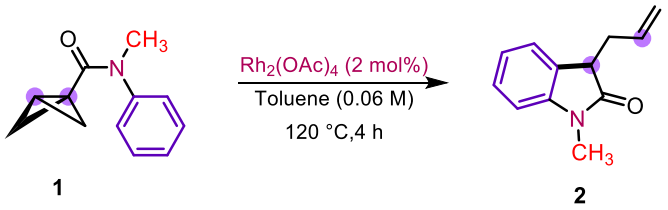
X	σ_m	Ratio	log (K_X/K_H)
OMe	0.12	0.86:1	-0.065
Me	-0.07	1.40:1	0.146
^{t}Bu	-0.01	1.35:1	0.130
F	0.34	0.75:1	-0.124
CF_3	0.43	0.78:1	-0.107

To an oven dried reaction tube (10 mL) equipped with magnetic stir bar, *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **1** (18.7 mg, 0.1 mmol, 1.0 equiv.), **1'** (0.1 mmol, 1.0 equiv.)

and $Rh_2(OAc)_4$ (1.76 mg, 0.004 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by solvent (0.06 M, 3 mL) was added under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 4 h, the residue was diluted with ethyl acetate (5 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure and residue was submitted for ^{1}H NMR analysis to determine the yield. The yield was determined by using CH_2Br_2 as internal standard.



8.4 $^{12}C/^{13}C$ KIE Experiment.



1 2

To an oven dried round bottom flask (100 mL) equipped with magnetic stir bar, *N*-methyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide **1a** (374.1 mg, 2.0 mmol, 1.0 equiv.) and $Rh_2(OAc)_4$ (17.7 mg, 0.04 mmol, 0.02 equiv.) were added in glove box (argon atmosphere) followed by solvent (0.06 M, 30 mL) was added under nitrogen atmosphere outside the glove box and closed the reaction tube with stopper. The reaction mixture was stirred at 120 °C (using oil bath) for 4 h, the residue was diluted with ethyl acetate (20 mL) and filtered using celite, solvent was removed using rotatory evaporator under reduced pressure to get the crude product. The conversion of the reaction was determined by ^{1}H NMR analysis by using CH_2Br_2 as

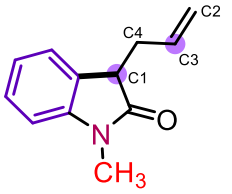
internal standard. Further purification done by column chromatography on silica gel Purification done by column chromatography on silica gel using (hexanes: EtOAc = 93:7) as the eluent give the product **2**.

Conversion = 13%

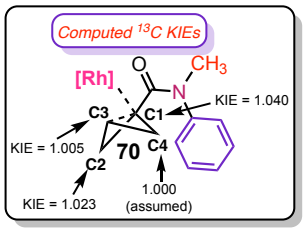
The sample was analyzed by quantitative ^{13}C NMR spectroscopy on JEOL 500 MHz spectrometer and proceeds with Mest Renova software. The KIE values were derived using the following equation.[16]

$$KIE = \frac{\ln (1-F)}{\ln [1-F(R/R_0)]}$$

Where F denotes the conversion of starting material, R denotes the peak area of site where reaction occurred while R_0 represent the peak area of the site that remains intact without C-C bond cleavage or formation.



2



δ (ppm)	**R_1**	**R_1/R_0**	**KIE**
45.3 (C1)	927.8	0.928	1.042
34.9 (C4)	1000	1.000	1.000
117.9 (C2)	958.7	0.959	1.018
134.1 (C3)	988.8	0.989	1.006

9.0 Computational Methods:

All calculations were conducted using a DFT method as implemented in the Gaussian 16 suite of programs.[17] For geometry optimization and frequency analysis, the B3LYP functional[18] in addition to including the Grimme dispersion corrections including Becke-Johnson damping (D3BJ)[19] was employed. Geometry optimizations utilized the def2-SVP[20] split-valence plus single polarization basis set for non-metals and the Stuttgart/Dresden small-core relativistic effective core potential

(RECP) with a valence double-ζ basis set (SDD)[21] for rhodium. No symmetry constraints were imposed during geometry optimizations. Single-point energy refinements were performed using the hybrid-meta-GGA M06 functional[22] with the def2-TZVP[20] basis set for non-metals and SDD for rhodium. Solvation energies were calculated implicitly for all intermediates and transition states using a self-consistent reaction field (SCRF) approach in dichloromethane solvent (ε = 8.93) and the SMD continuum solvation model.[23] Free energies (ΔG) reported throughout the article, unless stated otherwise, were determined at the M06(SMD, Toluene)/SDD(Rh)/def2-TZVP//B3LYP-D3(BJ)/SDD/def2-SVP level. The ΔG values were obtained by adding the in-solvent electronic energy (ΔE) at M06(SMD, toluene)/SDD(Rh)/def2-TZVP to the free energy corrections computed at B3LYP-D3(BJ)/SDD(Rh)/def2-SVP in the gas phase.

Influence of *para*-substituents on the phenyl ring.

A comparative DFT investigation was carried out to examine the influence of para-substituents on the phenyl ring of NAr-BCB carboxamides. Three representative substituents, namely –CF_3, –CN, –CO_2Me, were selected to evaluate the key transition states governing the formation of either the oxindole or the [1,2]–H migration product. To understand the origin of product selectivity, the free energy profiles of the para-substituted BCB carboxamides were computed and are presented in the figure below. The calculations reveal that the initial step proceeds via a common Rh-catalyzed C–C bond cleavage, involving the concerted transition state **TS1_R**, with activation barriers of 26–27 kcal/mol for all substrates. Subsequent product distribution is determined by the competition between intramolecular cyclization and the 1,2-hydride shift pathway.

Experimentally, substrates bearing p–CF_3 substituent predominantly afforded the cyclized products. Consistent with these observations, the calculated activation barriers for cyclization via **TS2_R** (**R**= CF_3) were lower, at 24.5 kcal/mol for the –CF_3 substrate. In contrast, the competing 1,2-hydride shift transition states, **TS3_R,** showed relatively higher barriers of 28.3 kcal/mol in the corresponding system.

On the other hand, para-substituted –CN and –CO_2Me substrates experimentally favored the formation of the 1,2-hydride shift products over the cyclized analogs. Under the experimental reaction conditions (120 °C), the computed free energy differences between **TS2_R** and **TS3_R** for these substrates were very small, indicating that both pathways are energetically accessible. These results suggest that the observed product distribution arises from a delicate balance between the cyclization and hydride-shift pathways, influenced by the electronic nature of the para substituent, e.g., whereas a strong electron-withdrawing effect dominated by the mesomeric (-M) effect is observed with the cyano (CN) and methoxycarbonyl (CO_2Me) groups, which is more significant than that of the trifluoromethyl group.

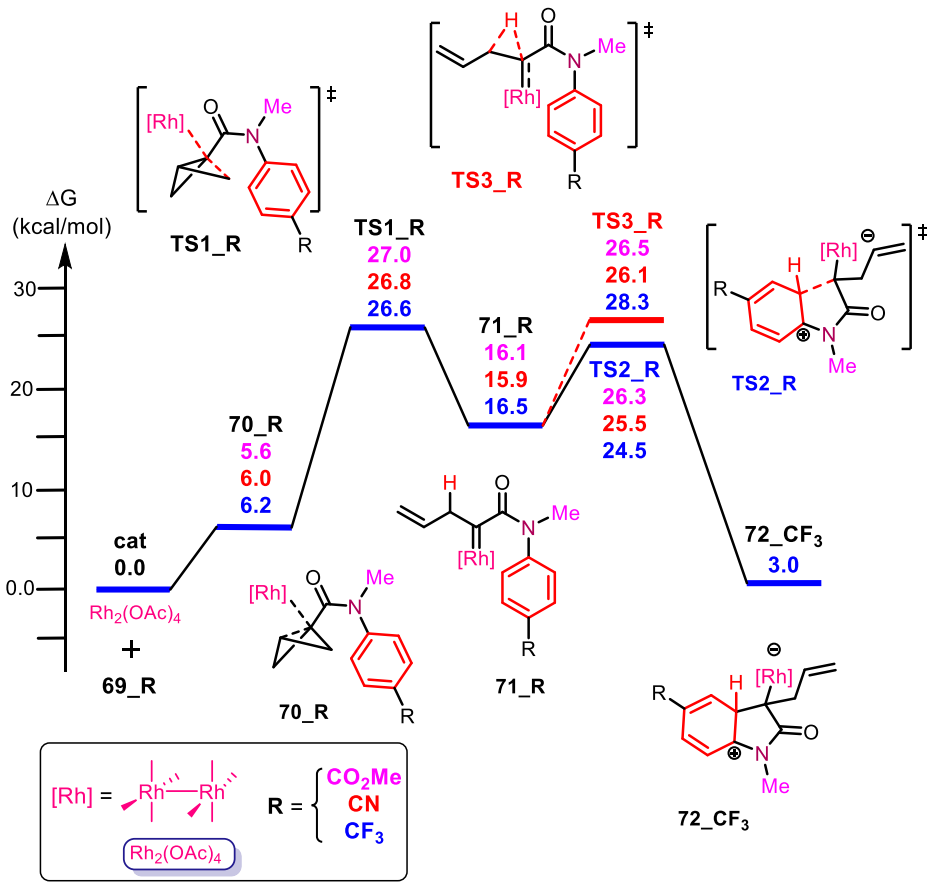
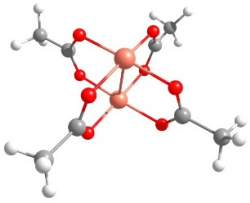


Figure-3: Free energy profiles for the [$Rh_2(OAc)_4$] with para-substituents on the phenyl ring of NAr-BCB carboxamides, **69_R** (**R**= –CF_3, –CN, –CO_2Me). (Method: M06/SDD/def2TZVP//B3LYP-D3(BJ)/ SDD/def2SVP).

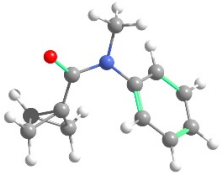
Table X. Cartesian coordinates (Å) of the optimized structures of all intermediate and transition states at B3LYP-D3(BJ)/SDD(Rh)/def2-SVP level of theory. E_e^S represents the absolute electronic energy in Hartree at the M06(SMD)/SDD(Rh)/def2-TZVP level of theory in toluene solvent.



Cat. $Rh_2(OAc)_4$

E_e^S = -1135.0589013

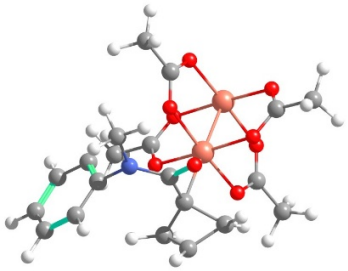
O	-1.458967000	1.441293000	-1.126672000
O	-1.453181000	-1.458449000	1.126748000
O	1.448040000	-1.452843000	1.126693000
C	1.865628000	-1.860773000	0.000131000
C	-1.871336000	-1.865878000	0.000178000
O	1.447829000	-1.453155000	-1.126469000
O	-1.453395000	-1.458456000	-1.126458000
C	-2.975984000	-2.890183000	0.000513000
H	-2.918966000	-3.513060000	0.902321000
H	-3.941845000	-2.359351000	0.008334000
H	-2.927978000	-3.504532000	-0.907570000
C	2.969949000	-2.885596000	0.000165000
H	3.936269000	-2.355539000	0.000085000
H	2.917138000	-3.504145000	0.905164000
H	2.917062000	-3.504287000	-0.904731000
C	-1.866430000	1.859361000	-0.000117000
C	-2.891134000	2.963731000	0.000045000
O	1.442333000	1.447059000	-1.126731000
C	1.860038000	1.854933000	-0.000219000
C	2.964012000	2.880199000	-0.000053000
O	1.442237000	1.447392000	1.126398000
O	-1.459064000	1.441313000	1.126496000
H	2.905854000	3.503993000	0.901071000
H	3.930434000	2.350412000	0.009308000
H	2.916495000	3.493543000	-0.908851000
H	-2.360598000	3.929756000	0.007531000
H	-3.505547000	2.915455000	-0.907996000
H	-3.513872000	2.906932000	0.901975000
Rh	-0.005818000	-0.006187000	-1.194972000
Rh	-0.005752000	-0.006010000	1.195027000



69

E_e^S = -594.8192756

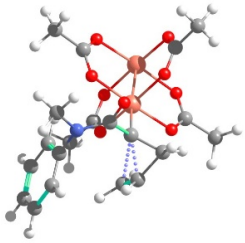
C	2.491462000	-1.403330000	0.990062000
C	2.898537000	-1.475043000	-0.438099000
C	1.036598000	-1.724949000	0.851523000
C	1.661971000	-0.706830000	-0.053751000
H	2.769271000	-2.418240000	-0.988979000
H	3.757387000	-0.867227000	-0.737589000
H	0.364847000	-1.348315000	1.629075000
H	0.731913000	-2.692652000	0.425666000
H	3.012049000	-0.926333000	1.819326000
C	1.515252000	0.764592000	-0.173139000
O	2.494133000	1.477154000	-0.340648000
N	0.237757000	1.289435000	-0.042652000
C	0.102902000	2.738541000	0.064324000
H	1.065215000	3.185314000	-0.211295000
H	-0.150330000	3.051187000	1.091594000
H	-0.684641000	3.096064000	-0.615654000
C	-0.951622000	0.514334000	-0.098511000
C	-1.156123000	-0.414112000	-1.130968000
C	-2.330314000	-1.165475000	-1.178197000
C	-3.328407000	-0.981985000	-0.216229000
C	-3.140133000	-0.038135000	0.796534000
C	-1.959168000	0.704474000	0.858837000
H	-0.386342000	-0.543350000	-1.892825000
H	-2.472510000	-1.890138000	-1.983517000
H	-4.250256000	-1.566028000	-0.260618000
H	-1.810379000	1.427833000	1.662339000
H	-3.914521000	0.117843000	1.551470000



70

E_e^S = **-1729.8928935**

O	-1.457647000	1.499643000	-1.234023000
O	-1.619274000	-1.490954000	0.975833000
O	1.257960000	-1.498233000	1.165190000
C	1.741702000	-1.884263000	0.053919000
C	-1.966421000	-1.864522000	-0.185804000
O	1.401358000	-1.450198000	-1.082791000
O	-1.498639000	-1.419078000	-1.273820000
C	-3.051949000	-2.909172000	-0.279968000
H	-3.197583000	-3.406605000	0.686364000
H	-3.990754000	-2.414473000	-0.576751000
H	-2.802740000	-3.638863000	-1.062541000
C	2.833824000	-2.922670000	0.111024000
H	3.785089000	-2.416427000	0.341953000
H	2.632176000	-3.642992000	0.915237000
H	2.931928000	-3.431962000	-0.855510000
C	-1.933781000	1.897210000	-0.132668000
C	-2.977729000	2.985617000	-0.160296000
O	1.425209000	1.458563000	-1.039697000
C	1.776262000	1.834602000	0.119175000
C	2.880858000	2.856396000	0.216207000
O	1.296178000	1.404102000	1.210128000
O	-1.618282000	1.447613000	1.012512000
H	2.741320000	3.479340000	1.109212000
H	3.841392000	2.324866000	0.314145000
H	2.915972000	3.470063000	-0.692831000
H	-2.668998000	3.802272000	0.508539000
H	-3.124008000	3.360470000	-1.180100000
H	-3.927057000	2.584342000	0.227668000
Rh	-0.028689000	0.022002000	-1.228295000
Rh	-0.180547000	-0.021927000	1.183622000
C	0.259824000	-0.760360000	4.856877000
C	1.212049000	-0.107578000	3.956512000
C	-0.649937000	-1.452708000	3.937273000
C	-0.289603000	0.017365000	3.605909000
H	1.798048000	-0.720636000	3.266904000
H	1.682204000	0.817359000	4.295264000
H	-1.657420000	-1.679982000	4.281385000
H	-0.234607000	-2.179040000	3.231628000
H	-0.013993000	-0.403543000	5.850132000
C	-0.960899000	1.335033000	3.892482000
O	-0.258595000	2.330017000	4.002062000
N	-2.329813000	1.400835000	4.006850000

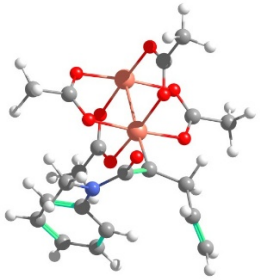


TS1

E_e^S = **-1729.859978**

O	-1.355335000	1.483343000	-1.297554000
O	-1.611531000	-1.455385000	0.970428000
O	1.252689000	-1.465240000	1.293991000
C	1.782899000	-1.878265000	0.209214000
C	-1.905850000	-1.862413000	-0.198579000
O	1.496113000	-1.478808000	-0.949682000
O	-1.399280000	-1.448577000	-1.275728000
C	-2.984405000	-2.916406000	-0.301778000
H	-3.111478000	-3.441145000	0.653125000
H	-3.933718000	-2.422352000	-0.565182000
H	-2.743863000	-3.622591000	-1.107698000
C	2.871166000	-2.915539000	0.348771000
H	3.807479000	-2.404667000	0.625944000
H	2.624749000	-3.623303000	1.152033000
H	3.024775000	-3.441596000	-0.601392000
C	-1.863720000	1.915567000	-0.228585000
C	-2.859646000	3.046426000	-0.322476000
O	1.525961000	1.438873000	-1.010076000
C	1.825657000	1.848111000	0.147267000
C	2.856055000	2.944819000	0.261046000
O	1.317062000	1.438318000	1.236543000
O	-1.603413000	1.495303000	0.945345000
H	3.470355000	2.796855000	1.159205000
H	3.478733000	2.983931000	-0.641354000
H	2.328724000	3.905892000	0.372223000
H	-3.710708000	2.857191000	0.347178000
H	-2.370600000	3.972673000	0.018647000
H	-3.201223000	3.177646000	-1.356283000
Rh	0.074939000	-0.003901000	-1.226029000
Rh	-0.177376000	0.025334000	1.214500000
C	-0.137442000	-1.000678000	4.681260000
C	0.978944000	-0.207683000	4.087271000
C	-0.817522000	-1.854010000	3.852884000
C	-0.229072000	0.218565000	3.328463000
H	1.718077000	-0.756893000	3.495786000
H	1.404227000	0.544124000	4.759033000
H	-1.810057000	-2.223938000	4.118735000
H	-0.365567000	-2.232321000	2.936240000
H	-0.586581000	-0.669913000	5.620256000
C	-0.945628000	1.439851000	3.838372000
O	-0.251881000	2.445527000	3.915854000
N	-2.286009000	1.441049000	4.118047000
C	-2.936643000	2.714035000	4.406610000

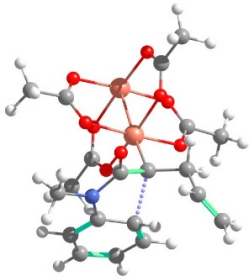
C	-2.962254000	2.710923000	4.074707000
H	-3.578253000	2.801675000	4.984282000
H	-3.611843000	2.864570000	3.196852000
H	-2.174110000	3.471983000	4.087375000
C	-3.214421000	0.280309000	4.015405000
C	-3.723337000	-0.237017000	2.820850000
C	-4.594638000	-1.327719000	2.852850000
C	-4.970652000	-1.895990000	4.072943000
C	-4.479696000	-1.364026000	5.270374000
C	-3.608378000	-0.273577000	5.241522000
H	-3.395957000	0.204622000	1.882530000
H	-4.974549000	-1.742230000	1.916733000
H	-5.649382000	-2.751911000	4.093034000
H	-3.210645000	0.151121000	6.166134000
H	-4.775033000	-1.800924000	6.227208000
H	-3.519617000	2.646160000	5.338271000
H	-3.619661000	2.989141000	3.585488000
H	-2.162848000	3.483581000	4.507037000
C	-3.132382000	0.291749000	4.061500000
C	-3.604034000	-0.185718000	2.836756000
C	-4.435103000	-1.308188000	2.806070000
C	-4.808483000	-1.944630000	3.992140000
C	-4.355949000	-1.449814000	5.221463000
C	-3.523158000	-0.330527000	5.256015000
H	-3.282483000	0.312177000	1.924604000
H	-4.784696000	-1.691660000	1.845914000
H	-5.456798000	-2.823525000	3.962611000
H	-3.158747000	0.065106000	6.207048000
H	-4.651370000	-1.938640000	6.152807000



71

E_e^S **= -1729.873467**

O	-1.556143000	1.466317000	-1.141616000
O	-1.694934000	-1.355597000	1.147849000
O	1.190954000	-1.506483000	1.258993000
C	1.640247000	-1.926955000	0.140578000
C	-2.068938000	-1.798896000	0.014571000
O	1.296612000	-1.513140000	-0.997268000
O	-1.609131000	-1.445004000	-1.104352000
C	-3.179328000	-2.820142000	0.026148000
H	-3.048487000	-3.513186000	0.867170000
H	-4.135526000	-2.296273000	0.176995000
H	-3.209580000	-3.357708000	-0.929440000
C	2.699922000	-2.999779000	0.214352000
H	3.655624000	-2.531285000	0.499357000
H	2.443113000	-3.733524000	0.990817000
H	2.818680000	-3.489337000	-0.759806000
C	-1.955488000	1.926063000	-0.040270000
C	-3.020874000	2.996453000	-0.060002000
O	1.359238000	1.402405000	-1.111849000
C	1.789600000	1.783028000	0.008543000
C	2.883717000	2.820811000	0.043841000
O	1.375716000	1.374447000	1.142686000
O	-1.559803000	1.559521000	1.114427000
H	2.492057000	3.736216000	0.513343000
H	3.712652000	2.461806000	0.671139000
H	3.238132000	3.041804000	-0.969895000



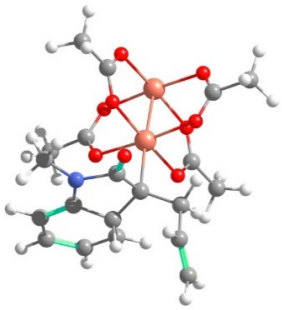
TS2

E_e^S **= -1729.865741**

O	-1.494663000	1.617822000	-1.049644000
O	-1.595465000	-1.443304000	0.981331000
O	1.311565000	-1.522001000	1.068480000
C	1.734384000	-1.855275000	-0.086901000
C	-1.992934000	-1.755614000	-0.186716000
O	1.369497000	-1.352348000	-1.183135000
O	-1.547753000	-1.286381000	-1.268060000
C	-3.101199000	-2.778222000	-0.263673000
H	-2.796651000	-3.690292000	0.269460000
H	-3.992622000	-2.385294000	0.247755000
H	-3.339320000	-3.008505000	-1.308763000
C	2.742734000	-2.979159000	-0.129852000
H	3.274892000	-2.980477000	-1.088974000
H	3.448096000	-2.890314000	0.707693000
H	2.207681000	-3.936255000	-0.019734000
C	-1.941151000	1.924384000	0.088404000
C	-3.029956000	2.968984000	0.162697000
O	1.415196000	1.562874000	-1.015896000
C	1.812231000	1.870389000	0.139883000
C	2.910180000	2.898255000	0.266739000
O	1.377973000	1.379390000	1.231582000
O	-1.579130000	1.415104000	1.197444000
H	3.823413000	2.402946000	0.632343000
H	3.112149000	3.368814000	-0.702833000
H	2.623784000	3.654036000	1.012125000

H	-2.756837000	3.800265000	0.641828000
H	-3.148864000	3.395939000	-1.073095000
H	-3.972047000	2.554603000	0.277409000
Rh	-0.124679000	-0.024301000	-1.182300000
Rh	-0.180709000	0.033326000	1.283125000
C	0.900539000	-0.384890000	5.521184000
C	0.973704000	-0.460271000	4.022313000
C	0.872365000	-1.455234000	6.319739000
C	-0.104559000	0.201236000	3.246634000
H	1.105278000	-1.487512000	3.647685000
H	1.879300000	0.072255000	3.653268000
H	0.816774000	-1.356605000	7.407136000
H	0.910398000	-2.471737000	5.913247000
H	0.862383000	0.623027000	5.947414000
C	-0.791538000	1.373607000	3.847557000
O	-0.061775000	2.334990000	4.073827000
N	-2.145881000	1.375585000	3.999966000
C	-2.806377000	2.649591000	4.236070000
H	-3.692077000	2.497802000	4.867614000
H	-3.106915000	3.121389000	3.285983000
H	-2.095028000	3.316734000	4.738717000
C	-2.900007000	0.208650000	3.741548000
C	-4.086129000	0.272707000	2.996041000
C	-4.817518000	-0.888732000	2.756032000
C	-4.367806000	-2.124575000	3.234218000
C	-3.184217000	-2.188399000	3.968622000
C	-2.462382000	-1.025280000	4.245358000
H	-4.424733000	1.228211000	2.595862000
H	-5.743903000	-0.830444000	2.179220000
H	-4.943783000	-3.031277000	3.037493000
H	-1.592285000	-1.066261000	4.901886000
H	-2.829286000	-3.144585000	4.359620000

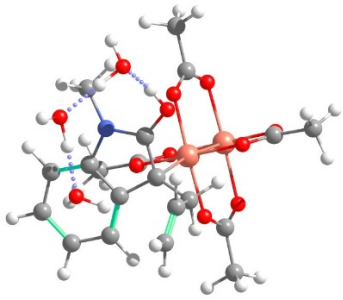
H	-2.884398000	3.602748000	1.048040000
H	-3.045473000	3.573621000	-0.752397000
H	-4.001809000	2.459079000	0.264447000
Rh	-0.059774000	0.140795000	-1.227406000
Rh	-0.117842000	-0.043741000	1.227115000
C	1.467730000	-0.112345000	5.346507000
C	1.359333000	-0.144249000	3.849932000
C	1.952229000	-1.114636000	6.087872000
C	-0.023216000	-0.033020000	3.280459000
H	1.860829000	-1.020615000	3.412835000
H	1.867109000	0.738131000	3.410157000
H	1.996777000	-1.053137000	7.178640000
H	2.333424000	-2.031684000	5.625144000
H	1.096313000	0.796669000	5.832815000
C	-0.944080000	0.969420000	3.891726000
O	-0.612503000	2.116626000	4.125087000
N	-2.249468000	0.491356000	4.066455000
C	-3.350699000	1.422184000	4.201667000
H	-4.062580000	1.071800000	4.962892000
H	-3.870227000	1.552657000	3.238561000
H	-2.926415000	2.387552000	4.504782000
C	-2.401278000	-0.862459000	3.889731000
C	-3.597019000	-1.491231000	3.506084000
C	-3.573997000	-2.848370000	3.204425000
C	-2.374340000	-3.588731000	3.221778000
C	-1.197762000	-2.980416000	3.624585000
C	-1.202578000	-1.623555000	4.029863000
H	-4.520477000	-0.918551000	3.419751000
H	-4.503306000	-3.342457000	2.910500000
H	-2.384043000	-4.645946000	2.949734000
H	-0.506254000	-1.356020000	4.832990000
H	-0.272688000	-3.554436000	3.709855000



72

E_e^S **= -1729.900318**

O	-1.421914000	1.769712000	-1.091504000
O	-1.739939000	-1.231134000	0.983070000
O	1.172611000	-1.587071000	0.951495000
C	1.557385000	-1.934854000	-0.211312000
C	-2.171509000	-1.550051000	-0.172548000
O	1.197490000	-1.409122000	-1.298738000
O	-1.714746000	-1.135165000	-1.269270000

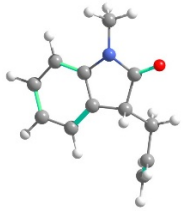
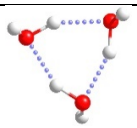
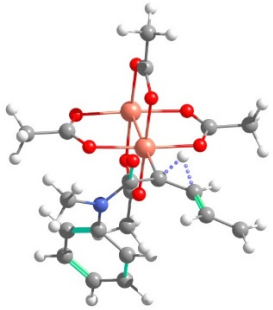
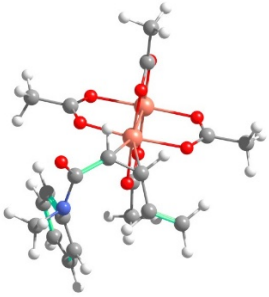


72_1

E_e^S **= -1959.262422**

O	-1.337932000	2.408329000	-0.617579000
O	-1.677534000	-0.774825000	1.134474000
O	1.210412000	-1.223300000	0.932733000
C	1.489743000	-1.490654000	-0.277107000
C	-2.185947000	-0.943311000	-0.014397000
O	1.110211000	-0.831757000	-1.286243000
O	-1.758375000	-0.438298000	-1.092954000
C	-3.427601000	-1.798969000	-0.083409000

C	-3.317594000	-2.533599000	-0.205710000
H	-2.937680000	-3.527096000	0.081046000
H	-4.079977000	-2.247897000	0.532587000
H	-3.752703000	-2.588236000	-1.210729000
C	2.559737000	-3.063851000	-0.276467000
H	3.553013000	-2.667654000	-0.010864000
H	2.305718000	-3.843368000	0.455478000
H	2.603780000	-3.483153000	-1.289028000
C	-1.800162000	2.128096000	0.058442000
C	-2.798231000	3.259029000	0.147057000
O	1.469553000	1.487244000	-1.106177000
C	1.921845000	1.764872000	0.040992000
C	3.101823000	2.703867000	0.122052000
O	1.488381000	1.309417000	1.144910000
O	-1.440883000	1.606516000	1.159853000
H	2.941374000	3.434512000	0.927186000
H	4.001758000	2.121545000	0.376411000
H	3.259400000	3.210896000	-0.837533000
H	-2.612653000	3.857238000	1.049097000
H	-2.751234000	3.883261000	-0.754001000
H	-3.811355000	2.830865000	0.221226000
Rh	-0.115459000	0.186539000	-1.290677000
Rh	-0.117330000	0.020776000	1.156769000
C	1.595630000	-0.379354000	5.296652000
C	1.455442000	-0.203532000	3.809821000
C	2.095832000	-1.463861000	5.899942000
C	0.002299000	-0.271636000	3.371207000
H	2.033841000	-0.967176000	3.268489000
H	1.847262000	0.776357000	3.499627000
H	2.142329000	-1.549255000	6.989353000
H	2.498579000	-2.301111000	5.318641000
H	1.204426000	0.443387000	5.908498000
C	-0.884301000	0.799692000	3.800005000
O	-0.715120000	1.961127000	4.087729000
N	-2.246579000	0.206891000	3.837424000
C	-3.422650000	1.041210000	3.937536000
H	-4.079431000	0.705029000	4.753667000
H	-3.973716000	1.030500000	2.985055000
H	-3.068658000	2.060743000	4.138835000
C	-2.199931000	-1.106476000	3.722772000
C	-3.263290000	-2.038330000	3.637119000
C	-2.948438000	-3.333750000	3.294910000
C	-1.611332000	-3.755797000	2.983357000
C	-0.567072000	-2.889710000	3.090114000
C	-0.781538000	-1.546043000	3.673223000
H	-4.297509000	-1.722337000	3.776976000
H	-3.755799000	-4.066121000	3.209792000
H	-1.448224000	-4.781975000	2.648579000
H	-0.528716000	-1.758073000	4.749542000
H	0.457003000	-3.184676000	2.859932000
H	-3.467382000	-2.336361000	-1.040041000
H	-3.454968000	-2.495160000	0.764833000
H	-4.310091000	-1.141135000	-0.026156000
C	2.323780000	-2.725233000	-0.521390000
H	2.780279000	-2.691043000	-1.518241000
H	3.092547000	-2.824675000	0.256985000
H	1.667010000	-3.608144000	-0.462147000
C	-1.629123000	2.675586000	0.581895000
C	-2.489043000	3.890939000	0.837813000
O	1.536228000	2.016341000	-0.815289000
C	2.067764000	2.153500000	0.323766000
C	3.311792000	3.003485000	0.416978000
O	1.663369000	1.615822000	1.400523000
O	-1.242933000	2.029086000	1.604056000
H	3.329942000	3.545479000	1.371969000
H	4.191684000	2.340557000	0.386389000
H	3.367310000	3.698419000	-0.430154000
H	-1.834343000	4.726846000	1.132499000
H	-3.038001000	4.174315000	-0.068639000
H	-3.182436000	3.697324000	1.667861000
Rh	-0.114412000	0.802937000	-1.030432000
Rh	0.003752000	0.393716000	1.364213000
C	2.191460000	-0.368140000	5.316992000
C	1.839517000	-0.305591000	3.854854000
C	2.626409000	-1.455024000	5.968048000
C	0.341271000	-0.205060000	3.667417000
H	2.206730000	-1.193850000	3.322350000
H	2.320961000	0.568457000	3.393194000
H	2.858517000	-1.432753000	7.036972000
H	2.784993000	-2.403848000	5.444576000
H	2.040962000	0.565888000	5.873691000
C	-0.412131000	0.910069000	4.109543000
O	0.058233000	2.108093000	4.347195000
N	-1.725681000	0.555737000	4.300267000
C	-2.848403000	1.458143000	4.437045000
H	-3.266155000	1.406719000	5.453903000
H	-3.619823000	1.192556000	3.699076000
H	-2.510540000	2.477685000	4.221991000
C	-1.851509000	-0.822984000	4.102012000
C	-2.981134000	-1.630687000	4.199572000
C	-2.818541000	-3.000305000	3.953500000
C	-1.561464000	-3.528894000	3.615826000
C	-0.436057000	-2.705019000	3.507217000
C	-0.576916000	-1.335334000	3.746224000
H	-3.955743000	-1.218318000	4.466154000
H	-3.681532000	-3.665319000	4.032011000
H	-1.463228000	-4.601712000	3.434407000
H	-1.001928000	-1.756614000	6.169167000
H	0.533102000	-3.115035000	3.219039000
O	-0.524926000	-1.312334000	6.888475000
H	-1.356246000	0.095835000	7.261204000
H	0.386397000	-1.246419000	6.546081000
H	-1.999979000	0.800716000	8.484639000
H	-1.330556000	2.324468000	6.934618000

	O -1.885975000 0.895169000 7.529966000 H -1.823562000 3.690187000 6.363104000 H -0.430923000 2.587520000 5.093121000 O -1.036804000 3.133693000 6.428126000
 **73** E_e^S **= -594.8790666** C 2.764372000 -1.456667000 5.012384000 C 1.945707000 -0.270110000 4.600077000 C 3.288306000 -2.361268000 4.181217000 C 0.523598000 -0.273471000 5.197540000 H 1.878873000 -0.212746000 3.501616000 H 2.429258000 0.659498000 4.947973000 H 3.884847000 -3.200273000 4.549547000 H 3.140926000 -2.292514000 3.098489000 H 2.928034000 -1.567283000 6.092786000 C -0.168539000 1.079186000 4.953833000 O 0.262608000 2.178970000 5.225108000 N -1.382490000 0.820117000 4.335380000 C -2.306902000 1.852602000 3.937165000 H -3.281149000 1.728006000 4.438507000 H -2.470019000 1.839310000 2.846451000 H -1.870018000 2.817333000 4.226576000 C -1.563638000 -0.551857000 4.121301000 C -2.642808000 -1.193840000 3.520045000 C -2.592884000 -2.592715000 3.415465000 C -1.499446000 -3.313905000 3.899729000 C -0.419504000 -2.648847000 4.506446000 C -0.452881000 -1.265156000 4.615869000 H -3.498834000 -0.633177000 3.141251000 H -3.426191000 -3.121941000 2.946960000 H -1.482392000 -4.401950000 3.807468000 H 0.606102000 -0.395328000 6.293085000 H 0.437049000 -3.210802000 4.881639000	 **3 H_2O** E_e^S **= -229.3005959** H -0.532811000 -0.414371000 5.271138000 O -0.232436000 -0.125478000 6.143460000 H -1.577804000 0.181595000 7.290925000 H -0.156895000 0.855365000 6.064389000 H -1.837588000 0.612363000 8.744854000 H -1.315724000 2.135877000 7.065665000 O -2.160382000 0.754681000 7.844320000 H -1.272674000 2.931709000 5.749720000 O -0.691837000 2.543706000 6.418278000
	

TS3 E_e^S = -1729.853973				74 E_e^S = -1729.909528			
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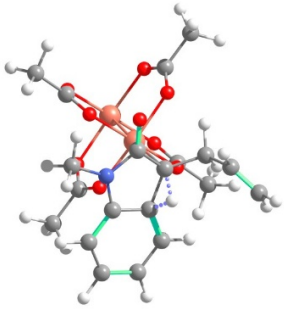
O	-1.622871000	-1.503372000	1.310506000	O	-1.102492000	-1.517989000	1.479783000
O	1.275898000	-1.491094000	1.291884000	O	1.759814000	-1.544514000	1.408932000
C	1.686717000	-1.947574000	0.172967000	C	2.169743000	-2.140743000	0.366078000
C	-2.033539000	-1.991460000	0.211919000	C	-1.478761000	-2.176418000	0.465166000
O	1.261078000	-1.608543000	-0.961558000	O	1.752842000	-1.928769000	-0.808631000
O	-1.652903000	-1.646787000	-0.942239000	O	-1.122149000	-1.953610000	-0.732071000
C	-3.095384000	-3.061532000	0.296362000	C	-2.421716000	-3.331525000	0.685458000
H	-3.019967000	-3.604979000	1.245931000	H	-2.594506000	-3.492510000	1.754420000
H	-4.082263000	-2.574592000	0.262047000	H	-3.377090000	-3.118614000	0.183711000
H	-3.013869000	-3.742473000	-0.560682000	H	-1.997601000	-4.232802000	0.218688000
C	2.803163000	-2.962637000	0.235007000	C	3.254828000	-3.170777000	0.554696000
H	3.749916000	-2.433547000	0.430004000	H	4.191481000	-2.655717000	0.820153000
H	2.634064000	-3.664245000	1.063653000	H	2.993843000	-3.835625000	1.390406000
H	2.886431000	-3.500486000	-0.717145000	H	3.405104000	-3.748608000	-0.364968000
C	-2.067120000	1.756573000	-0.010455000	C	-1.501527000	1.587540000	-0.312754000
C	-3.174536000	2.783828000	-0.047705000	C	-2.551274000	2.653142000	-0.505740000
O	1.212536000	1.304804000	-1.158004000	O	1.738338000	0.931706000	-1.324873000
C	1.653214000	1.767774000	-0.070408000	C	2.181529000	1.533671000	-0.303860000
C	2.675254000	2.876515000	-0.136310000	C	3.211574000	2.613104000	-0.518457000
O	1.294609000	1.400679000	1.094418000	O	1.810317000	1.322847000	0.893194000
O	-1.613928000	1.451939000	1.137964000	O	-1.053987000	1.429662000	0.863590000
H	3.137140000	2.916358000	-1.130382000	H	2.697593000	3.587864000	-0.529370000
H	2.165959000	3.833221000	0.061957000	H	3.930953000	2.622108000	0.311207000
H	3.435341000	2.738296000	0.644721000	H	3.721412000	2.473115000	-1.479585000
H	-4.141153000	2.256335000	0.000090000	H	-2.348377000	3.509024000	0.151720000
H	-3.103617000	3.461599000	0.812884000	H	-2.592632000	2.967215000	-1.555937000
H	-3.141255000	3.346247000	-0.989615000	H	-3.532318000	2.236265000	-0.226328000
Rh	-0.223256000	-0.178650000	-1.140610000	Rh	0.294622000	-0.519695000	-1.106386000
Rh	-0.180836000	-0.024608000	1.303758000	Rh	0.324152000	-0.055391000	1.261525000
C	0.731852000	-0.857553000	5.624793000	C	0.488349000	-1.201792000	4.617209000
C	0.643223000	-0.817909000	4.165096000	C	0.939766000	-0.074373000	3.814552000
C	1.366439000	-1.850856000	6.266183000	C	1.136531000	-2.377718000	4.632255000
C	-0.098917000	0.088776000	3.395786000	C	0.335100000	1.142867000	3.678370000
H	1.173015000	-1.597056000	3.601539000	H	1.916505000	-0.198970000	3.341074000
H	1.162434000	0.260343000	3.497118000	H	0.868712000	1.924037000	3.134629000
H	1.402659000	-1.894825000	7.357306000	H	0.787551000	-3.212130000	5.245402000
H	1.862078000	-2.656499000	5.715517000	H	2.021128000	-2.538848000	4.010252000
H	0.248765000	-0.048831000	6.180680000	H	-0.407213000	-1.060923000	5.222868000
C	-0.706102000	1.290162000	4.055528000	C	-0.714856000	1.727705000	4.577040000
O	0.033500000	2.202471000	4.409664000	O	-0.458352000	2.821823000	5.059191000
N	-2.071272000	1.353335000	4.140779000	N	-1.828987000	1.013857000	4.984135000
C	-2.668885000	2.653107000	4.420657000	C	-2.577747000	1.609780000	6.093815000
H	-3.602913000	2.515565000	4.981905000	H	-3.239670000	0.847740000	6.524435000
H	-2.880914000	3.202110000	3.487932000	H	-3.190679000	2.463095000	5.754849000
H	-1.957799000	3.242949000	5.010907000	H	-1.878194000	1.974441000	6.855528000
C	-2.918221000	0.263862000	3.802348000	C	-2.605620000	0.189704000	4.109443000
C	-3.986326000	0.449959000	2.913065000	C	-3.056375000	0.696435000	2.887329000
C	-4.838613000	-0.610445000	2.611982000	C	-3.924406000	-0.056259000	2.094536000
C	-4.632868000	-1.869709000	3.184027000	C	-4.371043000	-1.304084000	2.529540000

C	-3.571353000	-2.056319000	4.069878000
C	-2.728010000	-0.992150000	4.391894000
H	-4.134304000	1.423335000	2.448515000
H	-5.667129000	-0.453912000	1.916727000
H	-5.300744000	-2.699294000	2.942300000
H	-1.932558000	-1.130768000	5.124105000
H	-3.406299000	-3.031980000	4.532896000
C	-3.920076000	-1.814202000	3.751178000
C	-3.036680000	-1.074295000	4.535748000
H	-2.722889000	1.680620000	2.563223000
H	-4.266491000	0.343480000	1.137137000
H	-5.067489000	-1.882076000	1.918321000
H	-2.691886000	-1.464707000	5.495439000
H	-4.259651000	-2.793913000	4.095746000



TS4

E_e^S **= -1729.87164**

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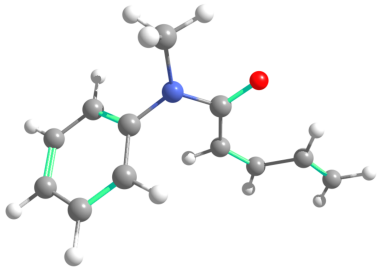
O	-1.832285000	-1.434171000	0.738945000
O	1.043499000	-1.638550000	0.354201000
C	1.268293000	-1.871934000	-0.874904000
C	-2.411938000	-1.624807000	-0.373799000
O	0.772110000	-1.234733000	-1.846984000
O	-2.102026000	-1.068020000	-1.466514000
C	-3.584613000	-2.572408000	-0.372780000
H	-4.497572000	-1.997112000	-0.148608000
H	-3.703895000	-3.036106000	-1.360295000
H	-3.455901000	-3.330082000	0.410987000
C	2.179968000	-3.031597000	-1.192215000
H	1.587815000	-3.960525000	-1.158644000
H	2.603552000	-2.923624000	-2.198369000
H	2.975649000	-3.108915000	-0.439177000
C	-2.103538000	2.026636000	0.234852000
C	-3.019355000	3.178667000	0.564624000
O	0.994868000	1.635932000	-1.376563000
C	1.578022000	1.816383000	-0.267527000
C	2.738035000	2.779548000	-0.233858000
O	1.286267000	1.234569000	0.822064000
O	-1.611256000	1.388793000	1.214184000
H	3.675287000	2.201979000	-0.282918000
H	2.698174000	3.461307000	-1.092246000
H	2.735347000	3.337646000	0.712092000
H	-2.400845000	4.077036000	0.721743000
H	-3.711089000	3.371616000	-0.265046000
H	-3.564813000	2.978679000	1.496105000
Rh	-0.559199000	0.296205000	-1.491897000
Rh	-0.259186000	-0.124167000	0.871289000
C	2.309543000	-0.855915000	4.614018000
C	1.739343000	-0.610651000	3.241421000



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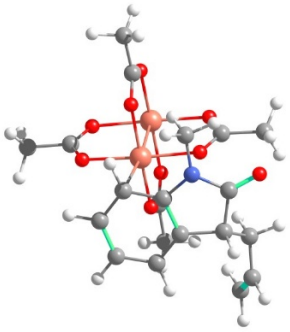
E_e^S **= -594.8409032**

C	1.732403000	-0.931765000	5.651244000
C	0.844303000	-1.375308000	4.588063000
C	2.791722000	-1.660083000	6.045952000
C	-0.256974000	-0.753156000	4.107169000
H	1.104116000	-2.338021000	4.130514000
H	-0.811323000	-1.245469000	3.307612000
H	3.454105000	-1.318646000	6.845284000
H	3.030935000	-2.621457000	5.578470000
H	1.505428000	0.031136000	6.111656000
C	-0.763349000	0.566502000	4.571550000
O	-0.111393000	1.330414000	5.273516000
N	-2.026630000	0.920420000	4.112897000
C	-2.539885000	2.245993000	4.433318000
H	-3.352722000	2.185758000	5.177303000
H	-2.934319000	2.737901000	3.530599000
H	-1.716942000	2.837365000	4.850558000
C	-2.937226000	0.000226000	3.518268000
C	-3.405744000	0.217271000	2.214975000
C	-4.317649000	-0.669594000	1.640010000
C	-4.763195000	-1.784258000	2.357256000
C	-4.298213000	-2.003068000	3.657072000
C	-3.398061000	-1.109556000	4.240950000
H	-3.038615000	1.078307000	1.652634000
H	-4.674077000	-0.494999000	0.622075000
H	-5.472360000	-2.480409000	1.903751000
H	-3.038356000	-1.265739000	5.259773000
H	-4.645242000	-2.869568000	4.224931000

C	3.007815000	-1.941024000	4.963337000
C	0.224596000	-0.665120000	3.241204000
H	2.134446000	-1.332660000	2.513084000
H	2.012892000	0.392198000	2.883462000
H	3.371341000	-2.087571000	5.984061000
H	3.251143000	-2.719642000	4.232041000
H	2.079626000	-0.088516000	5.363478000
C	-0.623547000	0.421169000	3.771985000
O	-0.323632000	1.564772000	4.058005000
N	-1.927847000	-0.124234000	3.902723000
C	-3.059546000	0.690239000	4.275148000
H	-3.531735000	0.321943000	5.200136000
H	-3.805508000	0.700701000	3.465002000
H	-2.683848000	1.708941000	4.434842000
C	-1.966982000	-1.465765000	3.638221000
C	-3.049035000	-2.347463000	3.633693000
C	-2.816193000	-3.675037000	3.270690000
C	-1.533848000	-4.126217000	2.896896000
C	-0.446034000	-3.264088000	2.890108000
C	-0.653607000	-1.924155000	3.287754000
H	-4.049959000	-2.002409000	3.895763000
H	-3.650275000	-4.380493000	3.272189000
H	-1.395055000	-5.170146000	2.608426000
H	0.060061000	-1.564127000	4.235017000
H	0.550146000	-3.594229000	2.595507000

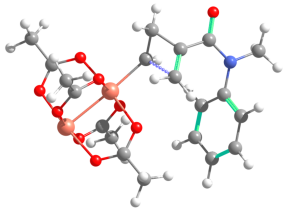


76

E_e^S **= -1729.948744**

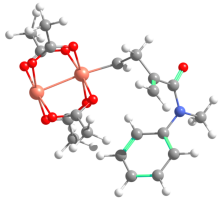
O	-1.878772000	1.197808000	-1.180434000
O	-2.556162000	-2.093570000	0.286006000
O	0.142122000	-2.151773000	1.399928000
C	0.969618000	-2.330147000	0.455976000
C	-2.466829000	-2.262583000	-0.968761000
O	1.000235000	-1.676465000	-0.629061000
O	-1.675056000	-1.643911000	-1.739247000
C	-3.385685000	-3.289344000	-1.582286000
H	-3.202709000	-4.266776000	-1.111120000
H	-4.429962000	-3.013908000	-1.371217000
H	-3.225940000	-3.356880000	-2.664766000
C	2.007083000	-3.410295000	0.633200000
H	3.010161000	-2.959581000	0.593086000
H	1.866933000	-3.931553000	1.587008000

H	1.935421000	-4.120984000	-0.203519000
C	-2.712497000	1.378603000	-0.247729000
C	-3.794069000	2.407229000	-0.461256000
O	0.805084000	1.175870000	-0.076446000
C	0.751596000	1.329237000	1.178529000
C	1.688690000	2.323942000	1.812222000
O	-0.018496000	0.684759000	1.958202000
O	-2.729947000	0.747856000	0.856325000
H	1.318995000	2.633329000	2.798342000
H	2.670042000	1.839563000	1.943358000
H	1.827836000	3.186768000	1.147412000
H	-3.943024000	2.993722000	0.456078000
H	-3.543504000	3.062243000	-1.304263000
H	-4.738954000	1.884463000	-0.679513000
Rh	-0.410337000	-0.224040000	-0.964714000
Rh	-1.322274000	-0.723066000	1.210274000
C	2.764884000	-1.451257000	5.008690000
C	1.931055000	-0.285019000	4.573014000
C	3.262783000	-2.384144000	4.192719000
C	0.526657000	-0.263637000	5.209891000
H	1.819268000	-0.276500000	3.479693000
H	2.422956000	0.658514000	4.867515000
H	3.876165000	-3.208338000	4.566881000
H	3.069918000	-2.352284000	3.116824000
H	2.966883000	-1.520611000	6.086033000
C	-0.167403000	1.083330000	4.950412000
O	0.289191000	2.189564000	5.149055000
N	-1.421115000	0.815738000	4.421009000
C	-2.324945000	1.853061000	3.979268000
H	-3.309450000	1.741517000	4.461721000
H	-2.453452000	1.812982000	2.887913000
H	-1.884453000	2.815356000	4.268979000
C	-1.571002000	-0.540692000	4.156530000
C	-2.609643000	-1.180985000	3.465524000
C	-2.552307000	-2.592933000	3.369580000
C	-1.488440000	-3.308213000	3.903725000
C	-0.425691000	-2.637081000	4.543118000
C	-0.460603000	-1.258853000	4.656604000
H	-3.481413000	-0.631353000	3.109817000
H	-3.351161000	-3.112265000	2.838734000
H	-1.458144000	-4.394351000	3.800417000
H	0.632270000	-0.363194000	6.305842000
H	0.429179000	-3.197181000	4.924400000



TS1'

E_e^S **= -1729.851406**



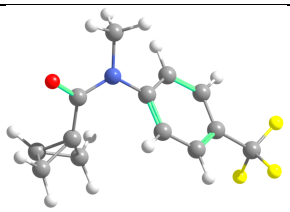
71'

E_e^S **= -1729.865163**

O	-1.905776000	0.855238000	-0.118230000

O	-1.819320000	1.230174000	-0.490902000	O	-1.827471000	0.242327000	3.418855000
O	-1.710368000	-1.112629000	2.328754000	O	1.010698000	-0.633812000	3.234140000
O	1.183068000	-1.347188000	2.044826000	C	1.046615000	-1.772198000	2.654750000
C	1.418282000	-2.034797000	0.998930000	C	-2.574776000	-0.663151000	2.920900000
C	-2.277243000	-1.722667000	1.365632000	O	0.414748000	-2.091063000	1.615579000
O	0.915628000	-1.847353000	-0.141919000	O	-2.381019000	-1.259624000	1.830470000
O	-1.972851000	-1.622837000	0.147036000	C	-3.803124000	-1.010673000	3.724760000
C	-3.440881000	-2.614752000	1.728358000	H	-4.251596000	-1.941040000	3.355775000
H	-3.561009000	-3.409025000	0.980522000	H	-3.541102000	-1.098342000	4.787740000
H	-3.301258000	-3.035070000	2.732388000	H	-4.534309000	-0.193059000	3.621155000
H	-4.359403000	-2.005406000	1.733775000	C	1.952017000	-2.802229000	3.285754000
C	2.359127000	-3.206711000	1.157756000	H	1.730825000	-3.800943000	2.890396000
H	2.944245000	-3.348570000	0.239580000	H	2.996607000	-2.544102000	3.049454000
H	3.018858000	-3.064260000	2.023000000	H	1.845236000	-2.783177000	4.379312000
H	1.759326000	-4.117984000	1.316661000	C	-1.926655000	1.982151000	0.441982000
C	-2.066412000	1.905098000	0.543168000	C	-2.727996000	3.082676000	-0.209609000
C	-3.022836000	3.066661000	0.413740000	O	0.866857000	-0.027850000	-0.388711000
O	1.063545000	0.987903000	-0.835476000	C	1.623378000	0.844116000	0.113386000
C	1.616673000	1.612294000	0.111076000	C	2.833366000	1.282418000	-0.674519000
C	2.695825000	2.608469000	-0.240624000	O	1.467331000	1.404237000	1.249178000
O	1.331494000	1.502209000	1.346453000	O	-1.305080000	2.300904000	1.511620000
O	-1.559214000	1.716303000	1.699169000	H	2.814984000	2.375390000	-0.797502000
H	2.257836000	3.619590000	-0.228808000	H	3.743446000	1.031738000	-0.108437000
H	3.496936000	2.581654000	0.510422000	H	2.853729000	0.789029000	-1.653381000
H	3.092466000	2.406622000	-1.243226000	H	-3.196941000	3.718507000	0.553300000
H	-3.635141000	3.162421000	1.320740000	H	-2.041399000	3.713039000	-0.797456000
H	-2.435591000	3.992866000	0.305116000	H	-3.481528000	2.657934000	-0.884164000
H	-3.655838000	2.945555000	-0.473917000	Rh	-0.777878000	-0.695330000	0.659676000
Rh	-0.464318000	-0.335062000	-0.434655000	Rh	-0.131354000	0.893681000	2.441119000
Rh	-0.167449000	0.212195000	1.939247000	C	0.320086000	1.996797000	3.941952000
C	0.258350000	0.697135000	3.904429000	C	-0.573507000	2.941116000	4.635481000
C	0.079673000	1.968398000	4.647627000	C	-2.341759000	1.914669000	6.080318000
C	-1.719891000	0.379866000	4.731012000	C	-1.057922000	2.244879000	5.904518000
C	-0.681169000	0.940169000	5.434838000	H	-1.423053000	3.239511000	4.007765000
H	-0.519997000	2.726227000	4.130967000	H	0.010822000	3.824995000	4.954173000
H	0.939492000	2.366675000	5.193845000	H	-2.689901000	1.447435000	7.002695000
H	-2.199277000	-0.554224000	5.017199000	H	-3.080024000	2.105730000	5.299226000
H	-2.155157000	0.921366000	3.889968000	H	1.265578000	1.784152000	4.474511000
H	1.013867000	0.018647000	4.319623000	C	0.003953000	2.070779000	6.958978000
C	-0.054694000	0.452709000	6.723989000	O	0.850345000	2.942620000	7.106503000
O	0.609669000	1.244424000	7.375221000	N	-0.037649000	0.947821000	7.757790000
N	-0.288054000	-0.830727000	7.166935000	C	0.919531000	0.868006000	8.858651000
C	0.244172000	-1.181415000	8.483885000	H	1.213155000	1.883380000	9.147517000
H	0.247716000	-0.290929000	9.122891000	H	1.824977000	0.313301000	8.556882000
H	1.279131000	-1.557440000	8.407765000	H	0.462398000	0.349617000	9.712861000
H	-0.381690000	-1.966458000	8.928765000	C	-0.678713000	-0.271904000	7.375079000
C	-0.724886000	-1.920595000	6.347439000	C	-1.601475000	-0.875952000	8.239764000
C	-1.933121000	-2.567840000	6.644364000	C	-2.218083000	-2.075403000	7.879559000
C	-2.369777000	-3.630080000	5.851431000	C	-1.922674000	-2.676247000	6.651160000
C	-1.610464000	-4.044482000	4.751194000	C	-0.998392000	-2.075542000	5.792662000
C	-0.405407000	-3.403453000	4.458437000	C	-0.367485000	-0.884705000	6.155978000
C	0.048579000	-2.361673000	5.268298000	H	-1.844553000	-0.391394000	9.188045000
H	-2.532220000	-2.218738000	7.488264000	H	-2.939915000	-2.537685000	8.556929000
H	-3.313167000	-4.128621000	6.085791000	H	-2.412179000	-3.609819000	6.364896000

H	-1.960399000	-4.866916000	4.123499000
H	0.999147000	-1.879184000	5.044130000
H	0.190097000	-3.702250000	3.594688000

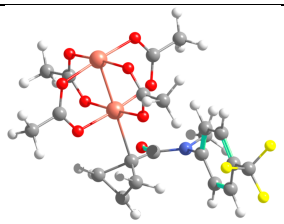


69_CF$_3$

E_e^S = -931.8994165

C	0.807799000	-0.441233000	4.539808000
C	1.014426000	-0.034175000	3.125452000
C	-0.450116000	-1.236943000	4.391976000
C	-0.347440000	0.115412000	3.751560000
H	1.143236000	-0.808184000	2.355007000
H	1.562002000	0.897371000	2.954868000
H	-1.094117000	-1.319804000	5.273216000
H	-0.458287000	-2.126783000	3.745153000
H	1.239891000	-0.005102000	5.439419000
C	-1.008322000	1.410966000	4.032943000
O	-0.375343000	2.454498000	4.019885000
N	-2.360487000	1.381154000	4.367495000
C	-2.940310000	2.597465000	4.931602000
H	-3.034469000	2.535711000	6.029152000
H	-3.935583000	2.774289000	4.499773000
H	-2.272670000	3.431303000	4.686243000
C	-3.213181000	0.276863000	4.141422000
C	-3.167043000	-0.440527000	2.932759000
C	-4.018436000	-1.519329000	2.719882000
C	-4.951616000	-1.887642000	3.696793000
C	-5.028095000	-1.157515000	4.885754000
C	-4.166665000	-0.084306000	5.106987000
H	-2.462279000	-0.141199000	2.157244000
H	-3.976165000	-2.066295000	1.776515000
H	-4.227418000	0.470256000	6.043944000
H	-5.763291000	-1.430477000	5.644207000
C	-5.833774000	-3.086583000	3.479538000
F	-6.168379000	-3.232684000	2.184658000
F	-5.221108000	-4.228358000	3.852959000
F	-6.974346000	-3.006673000	4.187391000

H	0.355810000	-0.433462000	5.477520000
H	-0.767422000	-2.532872000	4.828494000

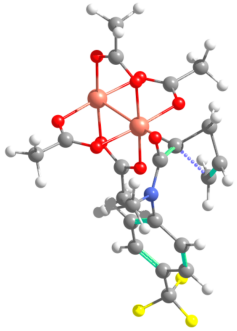


70_CF$_3$

E_e^S = -2066.972486

O	-1.547089000	1.459969000	-1.188633000
O	-1.665791000	-1.466487000	1.139621000
O	1.203180000	-1.495285000	1.219352000
C	1.636887000	-1.934106000	0.106480000
C	-2.048260000	-1.893472000	0.007161000
O	1.257985000	-1.539212000	-1.031937000
O	-1.638589000	-1.469567000	-1.113131000
C	-3.069032000	-3.005069000	-0.011273000
H	-3.412346000	-3.252383000	0.999652000
H	-3.920424000	-2.709675000	-0.642357000
H	-2.616191000	-3.893959000	-0.476741000
C	2.712216000	-2.989396000	0.163950000
H	3.676149000	-2.495699000	0.367616000
H	2.513424000	-3.689258000	0.986906000
H	2.782319000	-3.520729000	-0.792980000
C	-1.970601000	1.913924000	-0.088491000
C	-2.994629000	3.020878000	-0.124215000
O	1.334958000	1.368085000	-1.092939000
C	1.728786000	1.787174000	0.036657000
C	2.849960000	2.795110000	0.054643000
O	1.278441000	1.409661000	1.160249000
O	-1.624461000	1.500223000	1.062433000
H	2.744167000	3.462728000	0.919609000
H	3.804981000	2.253906000	0.153455000
H	2.869295000	3.363668000	-0.883645000
H	-2.709973000	3.810298000	0.585785000
H	-3.091598000	3.428129000	-1.137577000
H	-3.968206000	2.618479000	0.199059000
Rh	-0.150078000	-0.047192000	-1.177911000
Rh	-0.214352000	0.000944000	1.236603000
C	0.381522000	-0.659672000	4.893133000
C	1.275534000	0.010100000	3.948171000
C	-0.545881000	-1.388133000	4.020165000
C	-0.244561000	0.087886000	3.658753000
H	1.848591000	-0.593286000	3.239912000
H	1.732405000	0.951070000	4.259382000
H	-1.530896000	-1.640890000	4.407767000
H	-0.140707000	-2.110297000	3.304949000
H	0.141680000	-0.298920000	5.893807000
C	-0.939901000	1.384036000	3.978129000

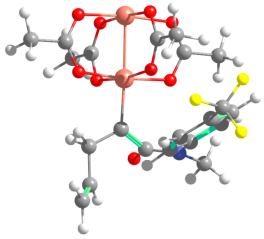
O	-0.260595000	2.392946000	4.094600000
N	-2.310071000	1.420341000	4.130939000
C	-2.958770000	2.720827000	4.252510000
H	-3.654884000	2.723573000	5.105827000
H	-3.525357000	2.956998000	3.335569000
H	-2.181497000	3.478228000	4.402616000
C	-3.190280000	0.302775000	4.029082000
C	-3.744289000	-0.048782000	2.794358000
C	-4.613239000	-1.131468000	2.703896000
C	-4.930831000	-1.873392000	3.846240000
C	-4.410124000	-1.504403000	5.090882000
C	-3.552062000	-0.407885000	5.180929000
H	-3.449458000	0.516561000	1.914164000
H	-5.032757000	-1.414567000	1.737396000
H	-3.134833000	-0.105865000	6.143783000
H	-4.674706000	-2.074735000	5.981899000
C	-5.799122000	-3.093918000	3.697724000
F	-6.904544000	-2.834587000	2.977100000
F	-5.140234000	-4.081122000	3.049714000
F	-6.191721000	-3.591943000	4.880208000



TS1_CF$_3$

E_e^S **= -2066.939352**

O	-1.437318000	1.440154000	-1.294347000
O	-1.665022000	-1.436826000	1.062113000
O	1.198464000	-1.446252000	1.332115000
C	1.709770000	-1.892632000	0.250900000
C	-1.968674000	-1.891020000	-0.087712000
O	1.407359000	-1.521307000	-0.912976000
O	-1.487527000	-1.499056000	-1.184905000
C	-3.009076000	-2.986273000	-0.141687000
H	-3.251715000	-3.361312000	0.859590000
H	-3.920616000	-2.588789000	-0.615573000
H	-2.645547000	-3.804467000	-0.779673000
C	2.790696000	-2.935279000	0.403104000
H	3.724839000	-2.431537000	0.699564000
H	2.526603000	-3.644428000	1.199793000
H	2.955679000	-3.459915000	-0.545752000
C	-1.919107000	1.914659000	-0.231842000
C	-2.903621000	3.053465000	-0.344256000
O	1.445044000	1.391419000	-1.047845000
C	1.775563000	1.822093000	0.093182000
C	2.887466000	2.839881000	0.166681000

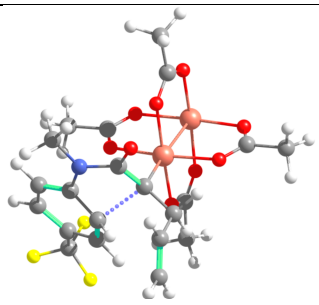


71_CF$_3$

E_e^S **= -2066.954123**

O	-1.620060000	1.438903000	-1.112650000
O	-1.688123000	-1.388281000	1.155848000
O	1.201366000	-1.498732000	1.235469000
C	1.652778000	-1.899373000	0.110141000
C	-2.050806000	-1.846318000	0.022490000
O	1.297538000	-1.476496000	-1.020598000
O	-1.602368000	-1.475931000	-1.095501000
C	-3.123947000	-2.904381000	0.033945000
H	-2.974350000	-3.595880000	0.872215000
H	-4.102574000	-2.422403000	0.176288000
H	-3.131260000	-3.443117000	-0.921360000
C	2.726050000	-2.958988000	0.167655000
H	3.667758000	-2.490546000	0.495580000
H	2.459881000	-3.725504000	0.908784000
H	2.873533000	-3.410025000	-0.820917000
C	-2.011763000	1.891244000	-0.006052000
C	-3.099132000	2.939283000	-0.012301000
O	1.294490000	1.439676000	-1.117433000
C	1.734175000	1.816374000	0.000498000
C	2.809486000	2.873278000	0.032352000
O	1.343789000	1.387256000	1.135730000
O	-1.592135000	1.531537000	1.143133000
H	2.409679000	3.774878000	0.521233000

O	1.272208000	1.456575000	1.200970000
O	-1.641749000	1.528168000	0.950917000
H	3.826817000	2.316725000	0.408379000
H	3.006583000	3.348073000	-0.798267000
H	2.686173000	3.560475000	0.970531000
H	-3.762374000	2.878515000	0.319875000
H	-2.409988000	3.978689000	-0.007414000
H	-3.237196000	3.176250000	-1.381576000
Rh	-0.014448000	-0.050892000	-1.201888000
Rh	-0.226638000	0.048982000	1.238936000
C	-0.105948000	-0.929507000	4.709421000
C	0.989531000	-0.126272000	4.091496000
C	-0.782624000	-1.798901000	3.893651000
C	-0.241980000	0.277921000	3.355794000
H	1.723552000	-0.669770000	3.488835000
H	1.417453000	0.635401000	4.750128000
H	-1.765247000	-2.186342000	4.169781000
H	-0.331255000	-2.177985000	2.977263000
H	-0.543301000	-0.600915000	5.654809000
C	-0.955094000	1.492702000	3.888489000
O	-0.272630000	2.504790000	3.959593000
N	-2.286564000	1.476745000	4.222023000
C	-2.930130000	2.735034000	4.585486000
H	-3.532073000	2.605341000	5.497807000
H	-3.592403000	3.079916000	3.773465000
H	-2.150174000	3.486042000	4.755188000
C	-3.136230000	0.339365000	4.091015000
C	-3.606805000	-0.044616000	2.833133000
C	-4.415179000	-1.171267000	2.711006000
C	-4.760215000	-1.913903000	3.843860000
C	-4.331658000	-1.504269000	5.112319000
C	-3.527058000	-0.371981000	5.233863000
H	-3.291687000	0.526134000	1.962424000
H	-4.763258000	-1.486435000	1.727127000
H	-3.175670000	-0.045040000	6.214801000
H	-4.620055000	-2.076116000	5.995035000
C	-5.539128000	-3.189410000	3.664994000
F	-6.575254000	-3.030232000	2.824600000
F	-4.757668000	-4.159230000	3.136300000
F	-6.022061000	-3.662258000	4.824314000
H	3.655119000	2.520570000	0.640653000
H	3.142871000	3.114223000	-0.983937000
H	-2.865673000	3.729319000	0.715217000
H	-3.220240000	3.363166000	-1.016324000
H	-4.046300000	2.466553000	0.293447000
Rh	-0.157230000	-0.019173000	-1.177871000
Rh	-0.190072000	0.021527000	1.285914000
C	0.916356000	-0.467722000	5.510235000
C	0.991609000	-0.512942000	4.010000000
C	0.868679000	-1.554708000	6.285170000
C	-0.081901000	0.173023000	3.249339000
H	1.119419000	-1.532429000	3.614364000
H	1.899328000	0.024854000	3.653359000
H	0.811191000	-1.478838000	7.374253000
H	0.893404000	-2.562612000	5.856854000
H	0.892991000	0.530997000	5.958816000
C	-0.738495000	1.354263000	3.867867000
O	0.004210000	2.303527000	4.093295000
N	-2.096231000	1.382046000	4.031723000
C	-2.728864000	2.672556000	4.259278000
H	-3.619156000	2.544644000	4.889439000
H	-3.014070000	3.145965000	3.305590000
H	-2.003649000	3.324428000	4.761547000
C	-2.871518000	0.237780000	3.763471000
C	-4.071244000	0.335182000	3.042631000
C	-4.817055000	-0.807643000	2.775704000
C	-4.368948000	-2.061563000	3.208527000
C	-3.175373000	-2.161716000	3.925350000
C	-2.441178000	-1.016311000	4.224079000
H	-4.407360000	1.303127000	2.673243000
H	-5.746181000	-0.730607000	2.208732000
H	-1.561131000	-1.090376000	4.863551000
H	-2.825949000	-3.135134000	4.272272000
C	-5.201307000	-3.288426000	2.958642000
F	-5.948741000	-3.169950000	1.843349000
F	-4.438452000	-4.390620000	2.815578000
F	-6.052359000	-3.535452000	3.972046000



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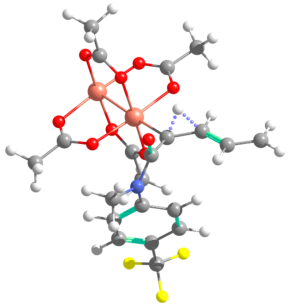

TS3_CF$_3$

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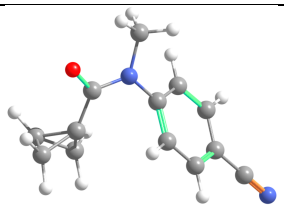
O	-1.932379000	-0.865748000	0.999565000	O	-1.776305000	1.280656000	-1.076562000
O	0.904032000	-1.482811000	1.303924000	O	-1.636064000	-1.504733000	1.303520000
C	1.275904000	-2.049719000	0.222264000	O	1.265323000	-1.454161000	1.255069000
C	-2.313015000	-1.236831000	-0.159145000	C	1.665011000	-1.897623000	0.126454000
O	1.074321000	-1.614240000	-0.941962000	C	-2.037662000	-1.995354000	0.200550000
O	-1.734900000	-0.966596000	-1.244104000	O	1.237798000	-1.533325000	-0.999377000
C	-3.544335000	-2.106748000	-0.224316000	O	-1.665762000	-1.629526000	-0.949851000
H	-3.240962000	-3.143823000	-0.013992000	C	-3.069637000	-3.093019000	0.273134000
H	-4.274194000	-1.802226000	0.536522000	H	-2.995249000	-3.640668000	1.219549000
H	-3.984321000	-2.064927000	-1.228222000	H	-4.072243000	-2.642599000	0.220354000
C	1.982922000	-3.374379000	0.370582000	H	-2.955922000	-3.770380000	-0.583112000
H	1.222813000	-4.157966000	0.515231000	C	2.724138000	-2.972906000	0.168459000
H	2.559471000	-3.604154000	-0.533779000	H	3.482689000	-2.729880000	0.925623000
H	2.632832000	-3.365702000	1.256124000	H	2.250119000	-3.923846000	0.460374000
C	-1.535872000	2.384901000	-0.257747000	H	3.187203000	-3.094238000	-0.818203000
C	-2.399703000	3.617598000	-0.374013000	C	-2.137900000	1.760589000	0.031369000
O	1.732888000	1.238905000	-1.064437000	C	-3.260652000	2.771530000	0.015977000
C	2.103491000	1.627540000	0.074977000	O	1.133553000	1.381724000	-1.154944000
C	3.335085000	2.495685000	0.163138000	C	1.592713000	1.822954000	-0.066301000
O	1.518370000	1.369593000	1.176720000	C	2.670917000	2.877239000	-0.127938000
O	-1.347376000	1.940596000	0.919686000	O	1.243770000	1.440883000	1.097126000
H	3.023638000	3.527752000	0.389723000	O	-1.667189000	1.450659000	1.172171000
H	3.977888000	2.155019000	0.987078000	H	3.645138000	2.395505000	0.053989000
H	3.883538000	2.483446000	-0.786363000	H	2.688573000	3.350601000	-1.117234000
H	-3.456747000	3.305492000	-0.373812000	H	2.514174000	3.623906000	0.662416000
H	-2.239806000	4.276410000	0.489678000	H	-4.218808000	2.230119000	0.077222000
H	-2.192055000	4.142239000	-1.314980000	H	-3.185657000	3.448554000	0.876877000
Rh	0.007357000	0.131575000	-1.236398000	H	-3.250824000	3.337330000	-0.924331000
Rh	-0.216040000	0.245752000	1.210653000	Rh	-0.273335000	-0.128697000	-1.141363000
C	1.052928000	0.676819000	5.419193000	Rh	-0.209340000	-0.006979000	1.302547000
C	1.053755000	0.615629000	3.919527000	C	0.808278000	-0.872824000	5.597056000
C	1.690858000	-0.195206000	6.207572000	C	0.685483000	-0.821298000	4.140322000
C	-0.279939000	0.428303000	3.257108000	C	1.458372000	-1.871608000	6.214206000
H	1.753778000	-0.142128000	3.535729000	C	-0.082859000	0.084677000	3.395910000
H	1.408667000	1.574498000	3.493654000	H	1.205478000	-1.592747000	3.557308000
H	1.649356000	-0.120943000	7.297580000	H	1.180510000	0.264224000	3.470152000
H	2.289251000	-1.010882000	5.786932000	H	1.518797000	-1.926411000	7.303755000
H	0.465845000	1.487803000	5.864688000	H	1.942836000	-2.670894000	5.644670000
C	-1.431986000	1.184837000	3.823656000	H	0.336604000	-0.070453000	6.171756000
O	-1.392396000	2.383263000	4.024818000	C	-0.680898000	1.279209000	4.074536000
N	-2.589550000	0.410781000	4.021294000	O	0.057429000	2.190013000	4.429555000
C	-3.874316000	1.060305000	4.195382000	N	-2.050493000	1.350079000	4.163013000
H	-4.451984000	0.565358000	4.989221000	C	-2.637204000	2.661629000	4.413589000
H	-4.451989000	1.045979000	3.256689000	H	-3.581969000	2.544375000	4.960884000
H	-3.677768000	2.103445000	4.472969000	H	-2.822947000	3.199073000	3.469042000
C	-2.431357000	-0.938844000	3.839493000	H	-1.928817000	3.249083000	5.008969000
C	-3.454792000	-1.823028000	3.455194000	C	-2.896664000	0.267948000	3.826648000
C	-3.108992000	-3.092816000	3.020552000	C	-3.999745000	0.466521000	2.982222000
C	-1.757450000	-3.496949000	2.943595000	C	-4.844243000	-0.592881000	2.670255000
C	-0.757927000	-2.679080000	3.444215000	C	-4.597583000	-1.868090000	3.191261000
C	-1.089575000	-1.407419000	3.957202000	C	-3.505302000	-2.070131000	4.037164000
H	-4.494020000	-1.496061000	3.431995000	C	-2.670654000	-1.005808000	4.365787000
H	-3.888835000	-3.778276000	2.684448000	H	-4.178807000	1.449673000	2.551784000
H	-0.471356000	-1.017724000	4.772871000	H	-5.692904000	-0.434436000	2.002846000

H	0.274936000	-3.020987000	3.480820000
C	-1.410241000	-4.792858000	2.271497000
F	-1.367544000	-4.640269000	0.922353000
F	-0.204400000	-5.256188000	2.639714000
F	-2.314164000	-5.755478000	2.517171000



69_CN

E_e^S **= -687.042143**

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C	-0.343581000	0.098508000	3.781364000
H	1.179060000	-0.857748000	2.443079000
H	1.583950000	0.862488000	3.009073000
H	-1.121497000	-1.298748000	5.323610000
H	-0.451970000	-2.143276000	3.830429000
H	1.205752000	0.022872000	5.507409000
C	-1.011437000	1.398380000	4.017670000
O	-0.382525000	2.443206000	3.992383000
N	-2.371695000	1.373547000	4.331361000
C	-2.953866000	2.596421000	4.880318000
H	-3.056394000	2.544231000	5.977489000
H	-3.944692000	2.772195000	4.438379000
H	-2.282156000	3.426136000	4.632515000
C	-3.222178000	0.272556000	4.101233000
C	-3.133096000	-0.482227000	2.916380000
C	-3.983711000	-1.557676000	2.696727000
C	-4.967922000	-1.893979000	3.645813000
C	-5.081537000	-1.122087000	4.815137000
C	-4.219629000	-0.052959000	5.037447000
H	-2.393177000	-0.213986000	2.162847000
H	-3.904737000	-2.136683000	1.775175000
H	-4.311103000	0.526639000	5.956345000
H	-5.845316000	-1.371426000	5.553543000
C	-5.849460000	-3.000703000	3.417177000
N	-6.562097000	-3.898964000	3.232927000

H	-1.851263000	-1.161710000	5.066199000
H	-3.312733000	-3.060340000	4.452486000
C	-5.543029000	-2.999365000	2.898530000
F	-6.133855000	-2.862670000	1.694399000
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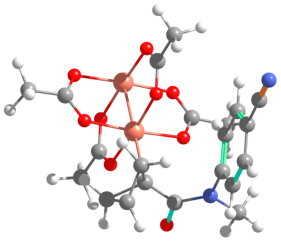

70_CN

E_e^S **= -1822.114736**

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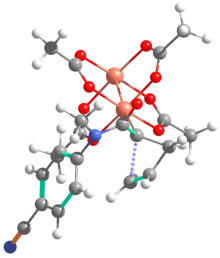
O	1.249127000	-1.503024000	1.163151000
C	1.729340000	-1.893625000	0.051341000
C	-1.969003000	-1.896139000	-0.167707000
O	1.383274000	-1.463600000	-1.085089000
O	-1.511269000	-1.448374000	-1.258494000
C	-3.032826000	-2.963117000	-0.254473000
H	-3.182477000	-3.447779000	0.717712000
H	-3.977094000	-2.496440000	-0.578062000
H	-2.756825000	-3.703162000	-1.018194000
C	2.821483000	-2.931264000	0.108162000
H	3.771420000	-2.425877000	0.346239000
H	2.616421000	-3.655438000	0.908091000
H	2.923741000	-3.436164000	-0.860146000
C	-1.951810000	1.884545000	-0.132782000
C	-2.982408000	2.985107000	-0.160320000
O	1.398014000	1.444409000	-1.056134000
C	1.754362000	1.828079000	0.098358000
C	2.856123000	2.853340000	0.184378000
O	1.280359000	1.401547000	1.194164000
O	-1.632610000	1.438340000	1.014374000
H	2.717622000	3.483025000	1.072815000
H	3.818263000	2.325042000	0.283959000
H	2.887185000	3.459826000	-0.729554000
H	-2.613115000	3.838189000	0.428404000
H	-3.191532000	3.298474000	-1.189780000
H	-3.907500000	2.631198000	0.320122000
Rh	-0.051260000	0.002070000	-1.228631000
Rh	-0.190913000	-0.029566000	1.182692000
C	0.301437000	-0.730935000	4.860698000
C	1.227253000	-0.089333000	3.926942000
C	-0.633105000	-1.437149000	3.976220000
C	-0.285426000	0.026659000	3.613826000
H	1.796735000	-0.710041000	3.230822000
H	1.703106000	0.841505000	4.240601000
H	-1.628199000	-1.662334000	4.356771000

H	-0.240402000	-2.174962000	3.269424000
H	0.055893000	-0.362417000	5.857103000
C	-0.955462000	1.340038000	3.910670000
O	-0.261135000	2.339990000	4.008016000
N	-2.324862000	1.398638000	4.069507000
C	-2.956650000	2.707457000	4.188381000
H	-3.598977000	2.749709000	5.082420000
H	-3.577041000	2.914973000	3.300230000
H	-2.165334000	3.461340000	4.265478000
C	-3.213505000	0.286000000	4.032578000
C	-3.675287000	-0.219353000	2.813519000
C	-4.548706000	-1.302932000	2.793764000
C	-4.982973000	-1.882548000	3.998603000
C	-4.541427000	-1.354875000	5.227300000
C	-3.665872000	-0.273385000	5.237492000
H	-3.310139000	0.229818000	1.893629000
H	-4.892502000	-1.714207000	1.844320000
H	-3.306972000	0.140342000	6.182068000
H	-4.884216000	-1.801748000	6.161816000
C	-5.872317000	-3.008758000	3.975109000
N	-6.588453000	-3.922169000	3.952062000



TS1_CN

E_e^S **= -1822.081185**

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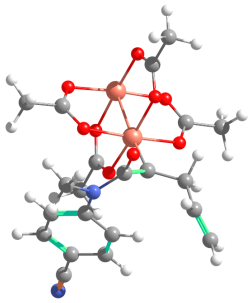
O	1.237406000	-1.443564000	1.308424000
C	1.772163000	-1.866634000	0.229071000
C	-1.908674000	-1.891956000	-0.178534000
O	1.485829000	-1.479062000	-0.933750000
O	-1.404516000	-1.482939000	-1.258222000
C	-2.964802000	-2.968712000	-0.272544000
H	-3.101639000	-3.473851000	0.691512000
H	-3.918222000	-2.503494000	-0.571414000
H	-2.693958000	-3.691106000	-1.054162000
C	2.861371000	-2.900225000	0.382604000
H	3.784953000	-2.391761000	0.703123000
H	2.591474000	-3.625262000	1.162855000
H	3.047920000	-3.407236000	-0.571803000
C	-1.900305000	1.898706000	-0.254430000
C	-2.897739000	3.026054000	-0.365028000
O	1.490597000	1.435343000	-1.026729000
C	1.797571000	1.850258000	0.126489000
C	2.896603000	2.878377000	0.236195000
O	1.279513000	1.460234000	1.219138000

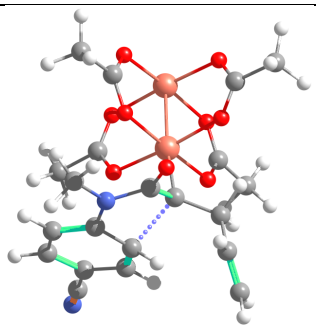


71_CN

E_e^S **= -1822.096323**

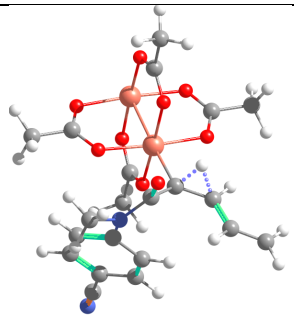
O	-1.570024000	1.476677000	-1.124334000
O	-1.733847000	-1.353299000	1.147461000
O	1.152433000	-1.522498000	1.264813000
C	1.604513000	-1.939366000	0.145342000
C	-2.098137000	-1.798055000	0.008903000
O	1.269749000	-1.512703000	-0.990229000
O	-1.628314000	-1.436935000	-1.103058000
C	-3.200631000	-2.826216000	0.005427000
H	-3.057440000	-3.549386000	0.818263000
H	-4.161861000	-2.320073000	0.181729000
H	-3.240130000	-3.335063000	-0.965043000
C	2.651111000	-3.024150000	0.217024000
H	3.602681000	-2.575611000	0.544405000
H	2.363504000	-3.777414000	0.963630000
H	2.791731000	-3.487118000	-0.767015000
C	-1.970810000	1.934433000	-0.023448000
C	-3.022122000	3.018422000	-0.042170000
O	1.342538000	1.401948000	-1.093282000
C	1.775480000	1.772296000	0.029089000

O	-1.639851000	1.493104000	0.926130000
H	3.838239000	2.360710000	0.480827000
H	3.023775000	3.406673000	-0.716856000
H	2.675808000	3.580652000	1.051024000
H	-3.745164000	2.851408000	0.313067000
H	-2.406539000	3.959429000	-0.047067000
H	-3.245065000	3.135684000	-1.399394000
Rh	0.052057000	-0.021205000	-1.225267000
Rh	-0.202957000	0.035387000	1.212098000
C	-0.116138000	-0.949341000	4.693241000
C	0.980535000	-0.149359000	4.074087000
C	-0.796428000	-1.817844000	3.879931000
C	-0.245857000	0.251627000	3.328345000
H	1.717604000	-0.695698000	3.477672000
H	1.405639000	0.616076000	4.730273000
H	-1.777789000	-2.203439000	4.164018000
H	-0.351411000	-2.200197000	2.961458000
H	-0.553570000	-0.617595000	5.637700000
C	-0.965869000	1.466758000	3.847207000
O	-0.288200000	2.481740000	3.916535000
N	-2.301447000	1.450111000	4.168027000
C	-2.948907000	2.709920000	4.521861000
H	-3.526723000	2.597513000	5.452049000
H	-3.633837000	3.029547000	3.718820000
H	-2.171252000	3.470345000	4.655895000
C	-3.145052000	0.306821000	4.071881000
C	-3.576314000	-0.154615000	2.825688000
C	-4.397068000	-1.276541000	2.746178000
C	-4.807277000	-1.937267000	3.916531000
C	-4.398819000	-1.450879000	5.174512000
C	-3.575288000	-0.332209000	5.245473000
H	-3.230799000	0.358712000	1.931096000
H	-4.715371000	-1.653936000	1.774672000
H	-3.243619000	0.048052000	6.213889000
H	-4.724836000	-1.959954000	6.082844000
C	-5.636129000	-3.105779000	3.830656000
N	-6.299821000	-4.055434000	3.758018000
C	2.876428000	2.801748000	0.073049000
O	1.357557000	1.357340000	1.160215000
O	-1.582666000	1.557972000	1.131806000
H	2.493787000	3.713708000	0.556396000
H	3.705769000	2.428379000	0.691418000
H	3.227882000	3.032941000	-0.939383000
H	-2.715154000	3.845391000	0.614384000
H	-3.185082000	3.381374000	-1.063779000
H	-3.964700000	2.608397000	0.353672000
Rh	-0.144961000	-0.019259000	-1.168686000
Rh	-0.207488000	0.025353000	1.293793000
C	0.913414000	-0.388756000	5.519549000
C	0.988681000	-0.444019000	4.019609000
C	0.896485000	-1.470860000	6.302638000
C	-0.108095000	0.198853000	3.255829000
H	1.153073000	-1.461197000	3.631618000
H	1.874391000	0.126174000	3.656539000
H	0.837113000	-1.388456000	7.391130000
H	0.950452000	-2.480812000	5.881927000
H	0.861862000	0.612226000	5.960696000
C	-0.788502000	1.377035000	3.856536000
O	-0.071023000	2.346342000	4.072431000
N	-2.150797000	1.379659000	4.008134000
C	-2.812188000	2.663032000	4.192628000
H	-3.705724000	2.535391000	4.818145000
H	-3.095740000	3.102648000	3.222603000
H	-2.104911000	3.342672000	4.683300000
C	-2.894794000	0.214561000	3.758615000
C	-4.102996000	0.269785000	3.044882000
C	-4.814142000	-0.894555000	2.788021000
C	-4.324770000	-2.139813000	3.226565000
C	-3.120405000	-2.192735000	3.945559000
C	-2.425539000	-1.022599000	4.231409000
H	-4.472798000	1.224381000	2.672932000
H	-5.750699000	-0.851905000	2.229378000
H	-1.546103000	-1.062741000	4.874822000
H	-2.745438000	-3.152069000	4.304834000
C	-5.044672000	-3.342461000	2.930641000
N	-5.618387000	-4.318672000	2.672701000



TS2_CN

E_e^S **= -1822.082492**



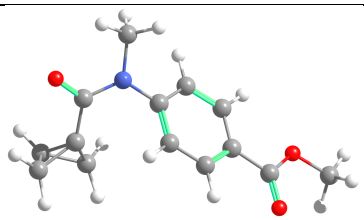
TS3_CN

E_e^S **= -1822.078411**

O	-1.710591000	1.270818000	-1.079736000

O	-1.516113000	1.585218000	-1.043003000	O	-1.652341000	-1.511985000	1.304759000
O	-1.596368000	-1.470652000	0.995449000	O	1.251538000	-1.500355000	1.309206000
O	1.299878000	-1.534419000	1.084966000	C	1.677668000	-1.938669000	0.187976000
C	1.727647000	-1.869650000	-0.069128000	C	-2.036685000	-2.001737000	0.194836000
C	-1.977966000	-1.803385000	-0.175175000	O	1.265511000	-1.580230000	-0.945264000
O	1.370034000	-1.360996000	-1.165135000	O	-1.639840000	-1.640727000	-0.948402000
O	-1.537139000	-1.323188000	-1.252695000	C	-3.078706000	-3.091613000	0.249077000
C	-3.040115000	-2.871478000	-0.260581000	H	-3.018528000	-3.645650000	1.193186000
H	-2.634423000	-3.824387000	0.112022000	H	-4.077845000	-2.633618000	0.187324000
H	-3.890505000	-2.601462000	0.381687000	H	-2.961967000	-3.765985000	-0.608861000
H	-3.372825000	-2.995785000	-1.297685000	C	2.792079000	-2.955277000	0.247973000
C	2.725645000	-3.001241000	-0.110798000	H	2.901525000	-3.462355000	-0.718184000
H	3.290913000	-2.978367000	-1.050591000	H	3.732910000	-2.434318000	0.487971000
H	3.401171000	-2.948913000	0.753632000	H	2.598735000	-3.683592000	1.047904000
H	2.175655000	-3.954684000	-0.054376000	C	-2.087206000	1.756522000	0.020356000
C	-1.965162000	1.895412000	0.092633000	C	-3.198168000	2.779833000	-0.017513000
C	-3.060888000	2.932696000	0.160369000	O	1.200747000	1.334099000	-1.105548000
O	1.392467000	1.555574000	-1.009863000	C	1.636509000	1.780441000	-0.009573000
C	1.789676000	1.866576000	0.144908000	C	2.656898000	2.891270000	-0.052255000
C	2.882302000	2.899558000	0.269608000	O	1.272697000	1.393023000	1.147855000
O	1.358917000	1.372696000	1.237152000	O	-1.640410000	1.443246000	1.170159000
O	-1.598898000	1.394025000	1.204814000	H	3.120777000	2.950186000	-1.044388000
H	3.803268000	2.404800000	0.616258000	H	2.146173000	3.843528000	0.162982000
H	3.069062000	3.381692000	-0.697300000	H	3.415656000	2.739193000	0.727499000
H	2.602082000	3.644962000	1.027513000	H	-4.163449000	2.249449000	0.025813000
H	-2.921102000	3.572529000	1.042280000	H	-3.132327000	3.457760000	0.843448000
H	-3.078970000	3.532543000	-0.757767000	H	-3.164250000	3.343895000	-0.958299000
H	-4.029552000	2.416764000	0.262307000	Rh	-0.225244000	-0.158512000	-1.115581000
Rh	-0.068607000	0.120357000	-1.214058000	Rh	-0.203889000	-0.034285000	1.328410000
Rh	-0.129173000	-0.057329000	1.235882000	C	0.746693000	-0.894611000	5.640998000
C	1.480113000	-0.135578000	5.350023000	C	0.644587000	-0.846831000	4.182592000
C	1.368154000	-0.156090000	3.853310000	C	1.380310000	-1.896741000	6.269860000
C	1.945513000	-1.153055000	6.083339000	C	-0.107367000	0.061610000	3.424360000
C	-0.019231000	-0.036966000	3.295121000	H	1.166464000	-1.624097000	3.609037000
H	1.863700000	-1.031976000	3.408936000	H	1.156641000	0.232210000	3.516948000
H	1.875832000	0.727649000	3.416846000	H	1.424928000	-1.948979000	7.360294000
H	1.990927000	-1.101251000	7.174507000	H	1.866743000	-2.701225000	5.709409000
H	2.311614000	-2.072535000	5.613341000	H	0.273410000	-0.087001000	6.207004000
H	1.126274000	0.776247000	5.844407000	C	-0.705951000	1.263314000	4.089380000
C	-0.917535000	0.988372000	3.899270000	O	0.031830000	2.168356000	4.457660000
O	-0.581357000	2.134750000	4.116634000	N	-2.078545000	1.350411000	4.145911000
N	-2.236533000	0.525210000	4.085459000	C	-2.654258000	2.672574000	4.366315000
C	-3.326366000	1.473400000	4.205532000	H	-3.614590000	2.574331000	4.889598000
H	-4.041852000	1.145448000	4.972899000	H	-2.806279000	3.201670000	3.411262000
H	-3.841246000	1.593746000	3.239160000	H	-1.953844000	3.256260000	4.974555000
H	-2.888132000	2.437181000	4.492917000	C	-2.925186000	0.277008000	3.794505000
C	-2.399459000	-0.819094000	3.916036000	C	-4.015910000	0.485177000	2.934435000
C	-3.607606000	-1.447842000	3.563322000	C	-4.857152000	-0.566703000	2.598881000
C	-3.593187000	-2.790898000	3.226762000	C	-4.624738000	-1.854669000	3.116026000
C	-2.380512000	-3.528828000	3.185375000	C	-3.542293000	-2.061217000	3.985963000
C	-1.190681000	-2.924721000	3.584219000	C	-2.713747000	-1.000945000	4.332882000
C	-1.192979000	-1.581706000	4.020472000	H	-4.186646000	1.472265000	2.509818000
H	-4.536713000	-0.879973000	3.521477000	H	-5.697247000	-0.402254000	1.921966000
H	-4.522262000	-3.289450000	2.945051000	H	-1.910009000	-1.161385000	5.050012000

H	-0.498263000	-1.344954000	4.837045000
H	-0.266522000	-3.502835000	3.625286000
C	-2.389954000	-4.887554000	2.732812000
N	-2.400552000	-5.980386000	2.339908000

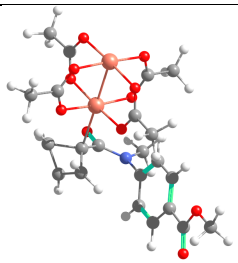


69_CO₂Me

E_e^S **= -822.673946**

C	0.969260000	-0.163947000	4.339959000
C	1.057069000	0.384499000	2.961131000
C	-0.196913000	-1.085536000	4.170029000
C	-0.279443000	0.319086000	3.652046000
H	1.234000000	-0.300034000	2.118867000
H	1.485966000	1.385185000	2.854309000
H	-0.783778000	-1.317920000	5.064325000
H	-0.137498000	-1.911112000	3.445420000
H	1.393924000	0.241091000	5.257483000
C	-1.068464000	1.499013000	4.075654000
O	-0.559238000	2.607263000	4.130552000
N	-2.388690000	1.281744000	4.463556000
C	-3.068532000	2.367966000	5.164692000
H	-3.087588000	2.202974000	6.255459000
H	-4.102091000	2.459368000	4.802137000
H	-2.517515000	3.293581000	4.962516000
C	-3.123042000	0.109209000	4.175093000
C	-3.054884000	-0.497347000	2.907062000
C	-3.790836000	-1.644109000	2.637676000
C	-4.632404000	-2.200942000	3.613419000
C	-4.726825000	-1.580423000	4.867009000
C	-3.980971000	-0.437664000	5.144953000
H	-2.423725000	-0.057316000	2.135030000
H	-3.742379000	-2.122794000	1.658214000
H	-4.051182000	0.026892000	6.129214000
H	-5.383067000	-2.005654000	5.626577000
C	-5.399317000	-3.426688000	3.265009000
O	-5.341267000	-3.993434000	2.197406000
O	-6.180373000	-3.851996000	4.278596000
C	-6.948175000	-5.025260000	4.024743000
H	-7.633291000	-4.868815000	3.177730000
H	-6.293699000	-5.877193000	3.785559000
H	-7.515150000	-5.225396000	4.942108000

H	-3.365863000	-3.053455000	4.403689000
C	-5.480441000	-2.944995000	2.753642000
N	-6.164133000	-3.832063000	2.446386000

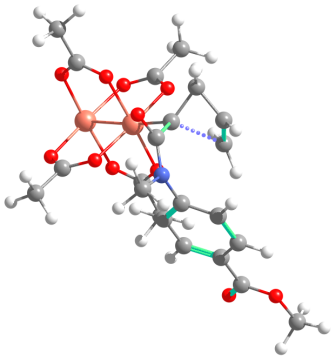


70_CO₂Me

E_e^S **= -1957.74673**

O	-1.584822000	1.225474000	-1.217092000
O	-1.566458000	-1.589312000	1.236862000
O	1.303302000	-1.482672000	1.319222000
C	1.761627000	-1.946023000	0.226657000
C	-1.921356000	-2.087403000	0.124950000
O	1.367035000	-1.620207000	-0.928388000
O	-1.530833000	-1.695643000	-1.013702000
C	-2.863856000	-3.266060000	0.160126000
H	-3.364988000	-3.348473000	1.131861000
H	-3.599152000	-3.181814000	-0.651874000
H	-2.277919000	-4.182144000	-0.018004000
C	2.889457000	-2.941655000	0.329558000
H	3.829232000	-2.389217000	0.491154000
H	2.735613000	-3.602634000	1.193173000
H	2.976866000	-3.521936000	-0.597130000
C	-2.028664000	1.708271000	-0.137129000
C	-3.103858000	2.762920000	-0.218087000
O	1.300320000	1.281535000	-1.122136000
C	1.675433000	1.766245000	-0.012436000
C	2.746593000	2.827027000	-0.040727000
O	1.245980000	1.415244000	1.127496000
O	-1.658937000	1.367541000	1.029961000
H	2.607750000	3.526066000	0.794238000
H	3.726689000	2.337740000	0.080627000
H	2.738838000	3.353975000	-1.003169000
H	-2.821115000	3.622673000	0.406350000
H	-3.264060000	3.077137000	-1.256159000
H	-4.041102000	2.352439000	0.190132000
Rh	-0.113164000	-0.207051000	-1.141089000
Rh	-0.182003000	-0.053543000	1.269710000
C	0.420489000	-0.496315000	4.958991000
C	1.299728000	0.139846000	3.977351000
C	-0.488593000	-1.295101000	4.129966000
C	-0.220933000	0.164376000	3.682816000
H	1.889612000	-0.488794000	3.305722000
H	1.732826000	1.108206000	4.234037000
H	-1.467550000	-1.548024000	4.533171000
H	-0.066017000	-2.047450000	3.457028000

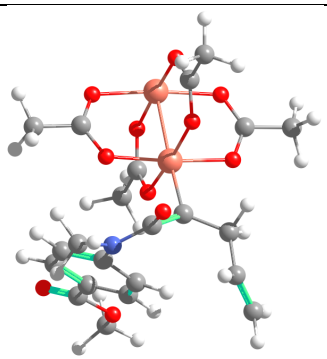
H	0.168886000	-0.084242000	5.936666000
C	-0.948574000	1.459452000	3.929904000
O	-0.296897000	2.492629000	3.966725000
N	-2.314422000	1.463846000	4.112570000
C	-3.002275000	2.747263000	4.182422000
H	-3.664000000	2.781544000	5.062214000
H	-3.613451000	2.906220000	3.277552000
H	-2.246487000	3.537359000	4.253786000
C	-3.155825000	0.311793000	4.112205000
C	-3.666026000	-0.190208000	2.912373000
C	-4.481017000	-1.319224000	2.920822000
C	-4.798108000	-1.952503000	4.129724000
C	-4.322773000	-1.420469000	5.339203000
C	-3.511898000	-0.289184000	5.329840000
H	-3.377896000	0.294357000	1.983172000
H	-4.866310000	-1.725426000	1.986556000
H	-3.122986000	0.128729000	6.260937000
H	-4.593461000	-1.918288000	6.271708000
C	-5.623262000	-3.192406000	4.182420000
O	-5.983763000	-3.736545000	5.200111000
O	-5.917067000	-3.663970000	2.953531000
C	-6.703971000	-4.852483000	2.911086000
H	-6.190515000	-5.678611000	3.425582000
H	-7.677602000	-4.693307000	3.398510000
H	-6.842462000	-5.090154000	1.849482000



TS1_CO_2Me

E_e^S = -1957.712445

O	-1.425684000	1.560230000	-1.283101000
O	-1.579044000	-1.439456000	0.924726000
O	1.285682000	-1.400487000	1.182789000
C	1.797341000	-1.781940000	0.077383000
C	-1.891664000	-1.830041000	-0.246090000
O	1.478297000	-1.361074000	-1.065066000
O	-1.420911000	-1.373772000	-1.323393000
C	-2.929635000	-2.922490000	-0.356851000
H	-3.844705000	-2.499228000	-0.800140000
H	-2.568811000	-3.701283000	-1.043839000
H	-3.173248000	-3.354738000	0.620607000
C	2.902131000	-2.806710000	0.170030000
H	3.832359000	-2.293505000	0.462726000
H	2.670563000	-3.548636000	0.946603000

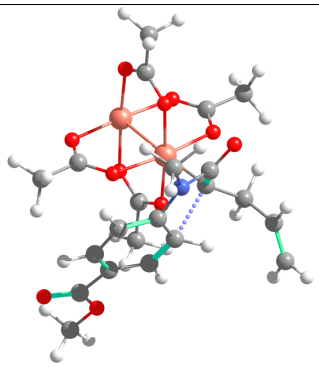


71_CO_2Me

E_e^S = -1957.729191

O	-1.653394000	1.259197000	-1.111773000
O	-1.620192000	-1.495358000	1.242944000
O	1.271147000	-1.503557000	1.318549000
C	1.731685000	-1.925775000	0.205284000
C	-1.977015000	-1.995453000	0.126675000
O	1.357159000	-1.555489000	-0.937654000
O	-1.545653000	-1.647197000	-1.005063000
C	-3.024714000	-3.080072000	0.172191000
H	-2.917946000	-3.682187000	1.082880000
H	-4.021925000	-2.613829000	0.189808000
H	-2.951568000	-3.707041000	-0.725222000
C	2.844729000	-2.941842000	0.292525000
H	3.775524000	-2.421580000	0.569878000
H	2.625968000	-3.676369000	1.079915000

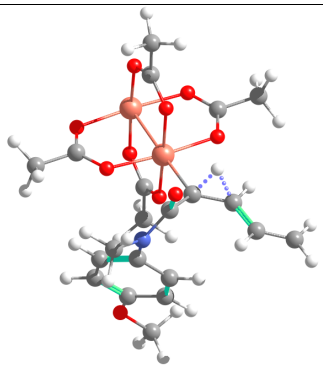
H	3.056966000	-3.293890000	-0.800352000	H	2.987049000	-3.439121000	-0.674492000
C	-1.917329000	1.962181000	-0.195260000	C	-2.055689000	1.735942000	-0.018902000
C	-2.939871000	3.071789000	-0.242994000	C	-3.191682000	2.729864000	-0.059522000
O	1.459956000	1.557675000	-1.056479000	O	1.261546000	1.354300000	-1.124536000
C	1.776071000	1.948575000	0.102701000	C	1.686601000	1.785749000	-0.020481000
C	2.789085000	3.061227000	0.218199000	C	2.722885000	2.881606000	-0.027447000
O	1.297217000	1.507282000	1.193442000	O	1.311260000	1.384320000	1.129398000
O	-1.622837000	1.522476000	0.964215000	O	-1.613869000	1.436299000	1.138807000
H	3.423030000	2.907601000	1.101637000	H	2.284347000	3.789632000	0.414208000
H	3.393643000	3.128282000	-0.694816000	H	3.573312000	2.589564000	0.605628000
H	2.247284000	4.010596000	0.357047000	H	3.058577000	3.087861000	-1.050620000
H	-3.809518000	2.807385000	0.376231000	H	-3.071600000	3.482836000	0.730983000
H	-2.493955000	3.981849000	0.187978000	H	-3.248289000	3.207468000	-1.045377000
H	-3.250153000	3.269098000	-1.275965000	H	-4.134116000	2.188055000	0.121778000
Rh	0.027575000	0.095066000	-1.273748000	Rh	-0.143604000	-0.150145000	-1.135642000
Rh	-0.171325000	0.066243000	1.169808000	Rh	-0.171632000	-0.029545000	1.326751000
C	-0.001984000	-1.054185000	4.599279000	C	0.880468000	-0.459342000	5.577025000
C	1.069208000	-0.205486000	3.999955000	C	0.959984000	-0.549811000	4.079203000
C	-0.677903000	-1.900257000	3.759138000	C	0.786133000	-1.520656000	6.382571000
C	-0.177984000	0.203700000	3.293649000	C	-0.076667000	0.163363000	3.290829000
H	1.806436000	-0.709701000	3.367701000	H	1.038456000	-1.585547000	3.714147000
H	1.490644000	0.537777000	4.683433000	H	1.896503000	-0.072093000	3.713593000
H	-1.649433000	-2.313211000	4.038060000	H	0.728062000	-1.411208000	7.468774000
H	-0.238672000	-2.233963000	2.819370000	H	0.770007000	-2.540632000	5.983380000
H	-0.432804000	-0.771328000	5.562372000	H	0.896489000	0.551942000	5.996780000
C	-0.911123000	1.379529000	3.883450000	C	-0.701323000	1.373939000	3.885073000
O	-0.251535000	2.404899000	3.980794000	O	0.069263000	2.303240000	4.100979000
N	-2.234112000	1.316868000	4.243143000	N	-2.058248000	1.443172000	4.043590000
C	-2.895832000	2.541266000	4.681488000	C	-2.655200000	2.753439000	4.251820000
H	-3.464704000	2.357947000	5.605799000	H	-3.557602000	2.656628000	4.870027000
H	-3.592502000	2.902645000	3.906389000	H	-2.913838000	3.227636000	3.290927000
H	-2.129252000	3.304152000	4.859073000	H	-1.918261000	3.388166000	4.759141000
C	-3.058726000	0.163740000	4.090202000	C	-2.858781000	0.317688000	3.771632000
C	-3.510583000	-0.215674000	2.824387000	C	-4.040806000	0.437406000	3.022979000
C	-4.286644000	-1.362786000	2.685044000	C	-4.781129000	-0.696398000	2.718166000
C	-4.631090000	-2.129161000	3.805297000	C	-4.356977000	-1.965598000	3.144294000
C	-4.219879000	-1.716631000	5.084649000	C	-3.192473000	-2.079040000	3.911499000
C	-3.438741000	-0.572298000	5.223800000	C	-2.459592000	-0.942684000	4.244831000
H	-3.206935000	0.375067000	1.963155000	H	-4.355694000	1.413134000	2.655470000
H	-4.623733000	-1.692863000	1.703000000	H	-5.693118000	-0.627088000	2.122789000
H	-3.095328000	-0.250807000	6.209623000	H	-1.605078000	-1.024902000	4.917025000
H	-4.502569000	-2.307553000	5.955966000	H	-2.871167000	-3.059657000	4.261622000
C	-5.411843000	-3.378890000	3.580225000	C	-5.160308000	-3.144509000	2.731170000
O	-5.689306000	-3.822603000	2.488989000	O	-6.165034000	-3.089839000	2.057728000
O	-5.770665000	-3.978652000	4.730107000	O	-4.629705000	-4.308169000	3.158676000
C	-6.508972000	-5.192309000	4.599944000	C	-5.327099000	-5.491308000	2.774336000
H	-7.452333000	-5.018288000	4.060999000	H	-6.358413000	-5.478606000	3.157245000
H	-5.927863000	-5.944880000	4.045924000	H	-5.365472000	-5.580714000	1.678148000
H	-6.710233000	-5.539209000	5.620594000	H	-4.768303000	-6.329972000	3.206821000



TS2_CO_2Me

E_e^S = -1957.717405

O	-1.313943000	1.648551000	-1.190366000
O	-1.980596000	-1.107502000	1.149744000
O	0.880548000	-1.675088000	1.307981000
C	1.203156000	-2.234766000	0.208164000
C	-2.416853000	-1.485770000	0.013613000
O	0.930617000	-1.807627000	-0.944422000
O	-1.896981000	-1.210091000	-1.100212000
C	-3.646961000	-2.360483000	0.014163000
H	-3.367817000	-3.379512000	0.324919000
H	-4.380165000	-1.983542000	0.739350000
H	-4.081868000	-2.400455000	-0.991756000
C	1.970053000	-3.529178000	0.332140000
H	2.172017000	-3.957236000	-0.656809000
H	2.917163000	-3.343975000	0.861414000
H	1.380809000	-4.229044000	0.942966000
C	-1.697551000	2.156725000	-0.100862000
C	-2.496491000	3.436153000	-0.163481000
O	1.531718000	1.064928000	-1.092557000
C	1.956097000	1.457441000	0.026496000
C	3.177632000	2.344023000	0.052634000
O	1.435008000	1.187633000	1.157043000
O	-1.451104000	1.706162000	1.063551000
H	3.881950000	1.990036000	0.818926000
H	3.658451000	2.367123000	-0.932595000
H	2.868942000	3.363505000	0.332934000
H	-3.263348000	3.444776000	0.622678000
H	-1.815368000	4.281222000	0.026323000
H	-2.948033000	3.560015000	-1.155507000
Rh	-0.180927000	-0.075930000	-1.177219000
Rh	-0.274319000	0.030941000	1.279686000
C	1.278758000	0.311376000	5.397219000
C	1.176078000	0.275502000	3.900350000
C	1.916360000	-0.608686000	6.129128000
C	-0.206285000	0.176723000	3.325523000
H	1.801702000	-0.516162000	3.460355000
H	1.557298000	1.219406000	3.463138000
H	1.952366000	-0.550711000	7.220339000
H	2.435905000	-1.450411000	5.658046000
H	0.770791000	1.146768000	5.892087000

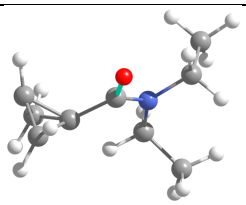


TS3_CO_2Me

E_e^S = -1957.710992

O	-1.748059000	1.167947000	-1.152425000
O	-1.577193000	-1.545800000	1.325030000
O	1.313726000	-1.462700000	1.278069000
C	1.728841000	-1.927876000	0.164438000
C	-1.973798000	-2.077702000	0.241008000
O	1.286178000	-1.621137000	-0.972654000
O	-1.621345000	-1.739232000	-0.923606000
C	-2.967196000	-3.207989000	0.365822000
H	-2.986713000	-3.800351000	-0.557180000
H	-2.707586000	-3.837117000	1.227984000
H	-3.969869000	-2.795531000	0.551128000
C	2.873940000	-2.910097000	0.235293000
H	2.742710000	-3.588554000	1.089570000
H	2.952670000	-3.475914000	-0.700983000
H	3.809382000	-2.348871000	0.391397000
C	-2.108324000	1.686434000	-0.060710000
C	-3.232401000	2.695012000	-0.110312000
O	1.158747000	1.285687000	-1.228578000
C	1.599573000	1.780336000	-0.154846000
C	2.590986000	2.914248000	-0.254078000
O	1.264670000	1.426343000	1.020782000
O	-1.634707000	1.419466000	1.088658000
H	3.047579000	2.940785000	-1.251081000
H	2.056280000	3.861605000	-0.079055000
H	3.357425000	2.817417000	0.526897000
H	-3.208134000	3.245293000	-1.059740000
H	-4.190502000	2.152767000	-0.056827000
H	-3.171919000	3.385324000	0.740989000
Rh	-0.237263000	-0.234212000	-1.166345000
Rh	-0.175174000	-0.027360000	1.274488000
C	0.745865000	-0.819956000	5.596610000
C	0.653727000	-0.788139000	4.136727000
C	1.375462000	-1.813476000	6.242533000
C	-0.083503000	0.120467000	3.363995000
H	1.176954000	-1.574479000	3.577260000
H	1.179747000	0.281257000	3.460057000
H	1.414981000	-1.850679000	7.333814000
H	1.864330000	-2.625751000	5.695510000
H	0.270440000	-0.004261000	6.148868000

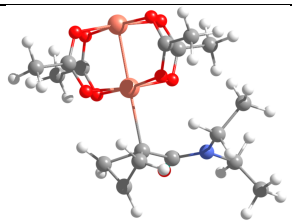
C	-1.276637000	0.978196000	3.979878000
O	-1.158082000	2.169423000	4.195846000
N	-2.457445000	0.263683000	4.242108000
C	-3.689487000	0.979070000	4.513955000
H	-4.240573000	0.498410000	5.334900000
H	-4.327599000	1.017525000	3.616065000
H	-3.416587000	2.003269000	4.797248000
C	-2.389208000	-1.089767000	4.030164000
C	-3.489274000	-1.903878000	3.706085000
C	-3.250058000	-3.182526000	3.233021000
C	-1.934495000	-3.674109000	3.055075000
C	-0.854702000	-2.921000000	3.502329000
C	-1.072996000	-1.640250000	4.049236000
H	-4.505158000	-1.512268000	3.754782000
H	-4.078050000	-3.823388000	2.926179000
H	-0.374233000	-1.294755000	4.818051000
H	0.154203000	-3.327826000	3.463513000
C	-1.773108000	-4.987038000	2.381715000
O	-2.686776000	-5.623939000	1.904517000
O	-0.489305000	-5.392834000	2.320675000
C	-0.258655000	-6.637091000	1.658741000
H	-0.797376000	-7.451709000	2.164867000
H	-0.598820000	-6.590120000	0.613625000
H	0.823443000	-6.809245000	1.701462000
C	-0.678758000	1.324233000	4.032019000
O	0.067602000	2.234969000	4.377831000
N	-2.038843000	1.370763000	4.157550000
C	-2.650703000	2.643156000	4.516516000
H	-3.520045000	2.466097000	5.165195000
H	-2.976154000	3.196958000	3.619624000
H	-1.904466000	3.250300000	5.042667000
C	-2.880315000	0.277456000	3.805088000
C	-3.915190000	0.450074000	2.871612000
C	-4.743338000	-0.609002000	2.534457000
C	-4.551464000	-1.874568000	3.114216000
C	-3.533907000	-2.052302000	4.057239000
C	-2.719143000	-0.971470000	4.406529000
H	-4.052873000	1.419950000	2.397512000
H	-5.547148000	-0.488766000	1.805797000
H	-1.951213000	-1.108337000	5.168542000
H	-3.366843000	-3.017595000	4.533373000
O	-5.391456000	-2.855845000	2.692338000
C	-5.265313000	-4.144459000	3.247490000
H	-4.271655000	-4.582209000	3.044333000
H	-5.432451000	-4.136349000	4.339470000
H	-6.033612000	-4.768306000	2.772278000



48a

E_e^S **= -481.7534713**

C	0.943424000	-0.262581000	4.807901000
C	1.179934000	0.223257000	3.424782000
C	-0.200791000	-1.193335000	4.560526000
C	-0.221573000	0.192806000	3.979710000
H	1.440880000	-0.494179000	2.632983000
H	1.623906000	1.218347000	3.325888000
H	-0.873214000	-1.381652000	5.405161000
H	-0.065050000	-2.057173000	3.891172000
H	1.267339000	0.186230000	5.745665000
C	-1.030052000	1.408745000	4.286217000
O	-0.461819000	2.463005000	4.544192000
N	-2.401021000	1.285825000	4.283955000
C	-3.188387000	2.435735000	4.724433000
H	-3.747302000	2.856970000	3.870392000
H	-2.463026000	3.197863000	5.033317000
C	-3.116434000	0.139433000	3.733181000
H	-2.376525000	-0.607695000	3.430549000
H	-3.734246000	-0.329355000	4.520189000
C	-3.993680000	0.486847000	2.529875000
H	-3.397894000	0.972154000	1.740822000



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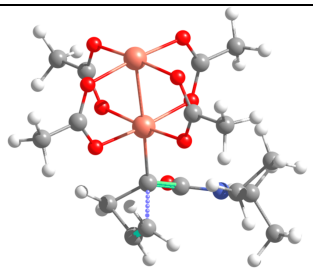
E_e^S **= -1616.830805**

O	-1.549276000	1.528607000	-1.113179000
O	-1.704089000	-1.318564000	1.282438000
O	1.183953000	-1.476948000	1.255954000
C	1.539439000	-1.969541000	0.137889000
C	-2.187592000	-1.717009000	0.176806000
O	1.122216000	-1.593811000	-0.993761000
O	-1.782910000	-1.368929000	-0.968313000
C	-3.367464000	-2.654888000	0.242147000
H	-3.357237000	-3.225435000	1.179585000
H	-4.290057000	-2.052844000	0.211083000
H	-3.370095000	-3.326293000	-0.626139000
C	2.567435000	-3.072502000	0.177339000
H	3.559177000	-2.621338000	0.342095000
H	2.364456000	-3.749850000	1.018080000
H	2.580662000	-3.621582000	-0.771970000
C	-1.914316000	2.014497000	-0.002960000
C	-2.919353000	3.138639000	-0.030710000
O	1.331849000	1.303727000	-1.150058000
C	1.783744000	1.747645000	-0.053414000

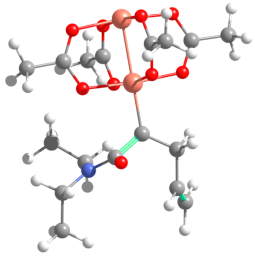
H	-4.822730000	1.160340000	2.794859000
H	-4.435583000	-0.431497000	2.112593000
C	-4.145935000	2.105410000	5.866468000
H	-4.926587000	1.387211000	5.568751000
H	-3.600225000	1.679488000	6.723299000
H	-4.655032000	3.020722000	6.206443000
C	2.941687000	2.711770000	-0.113206000
O	1.362832000	1.428442000	1.099933000
O	-1.532430000	1.614144000	1.138800000
H	2.864119000	3.445207000	0.700261000
H	3.876745000	2.145523000	0.026895000
H	2.977118000	3.209649000	-1.090156000
H	-2.855105000	3.731735000	0.890183000
H	-2.761892000	3.767500000	-0.916701000
H	-3.929470000	2.702921000	-0.099503000
Rh	-0.220104000	-0.038340000	-1.128210000
Rh	-0.175308000	0.075082000	1.286714000
C	0.677274000	-0.340384000	4.926387000
C	1.395716000	0.322309000	3.847842000
C	-0.250087000	-1.242746000	4.231543000
C	-0.152979000	0.200711000	3.696594000
H	1.969552000	-0.277246000	3.137691000
H	1.757627000	1.334980000	4.031694000
H	-1.155789000	-1.530089000	4.770265000
H	0.145934000	-2.009976000	3.557234000
H	0.484336000	0.105946000	5.902123000
C	-0.991779000	1.403535000	4.061482000
O	-0.409491000	2.451986000	4.317200000
N	-2.354694000	1.282404000	4.125799000
C	-3.109258000	2.448665000	4.579113000
H	-3.765676000	2.798829000	3.764683000
H	-2.373306000	3.239861000	4.760671000
C	-3.114258000	0.106264000	3.709556000
H	-2.438442000	-0.588431000	3.210953000
H	-3.524512000	-0.409522000	4.598713000
C	-4.248004000	0.412574000	2.733270000
H	-3.856454000	0.948190000	1.858469000
H	-5.055202000	1.010349000	3.182407000
H	-4.690766000	-0.535188000	2.390313000
C	-3.927021000	2.178628000	5.839765000
H	-4.701651000	1.411190000	5.682479000
H	-3.276480000	1.840646000	6.662070000
H	-4.436211000	3.099435000	6.165006000



TS5

E_e^S **= -1616.798762**

O	-1.463563000	1.514592000	-1.161358000
O	-1.713445000	-1.301863000	1.261436000
O	1.181424000	-1.458426000	1.363565000
C	1.594384000	-1.954862000	0.261958000

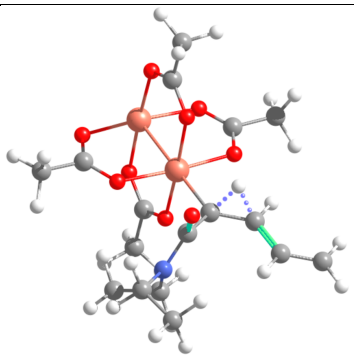


78

E_e^S **= -1616.811085**

O	-1.531186000	1.383781000	-1.273004000
O	-1.618390000	-1.289272000	1.255965000
O	1.286193000	-1.359763000	1.312626000
C	1.690526000	-1.895820000	0.226731000

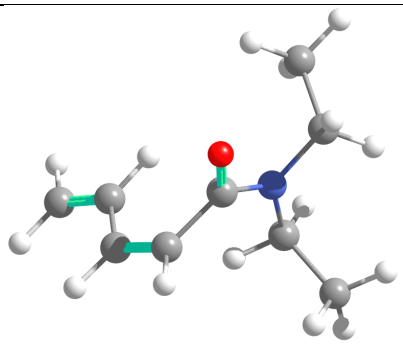
C	-2.142606000	-1.716446000	0.135210000	C	-2.049359000	-1.792535000	0.165438000
O	1.231963000	-1.595087000	-0.888037000	O	1.293030000	-1.608854000	-0.932385000
O	-1.687310000	-1.389428000	-0.992124000	O	-1.628136000	-1.519609000	-0.987151000
C	-3.326594000	-2.653514000	0.169200000	C	-3.190122000	-2.773006000	0.291519000
H	-3.309385000	-3.266680000	1.079864000	H	-3.079634000	-3.375915000	1.202728000
H	-4.247615000	-2.048137000	0.180947000	H	-4.130696000	-2.204399000	0.371962000
H	-3.341260000	-3.285120000	-0.727937000	H	-3.243177000	-3.413251000	-0.597639000
C	2.629494000	-3.048824000	0.367889000	C	2.762181000	-2.949727000	0.368239000
H	3.601317000	-2.590575000	0.612114000	H	3.720646000	-2.450359000	0.582363000
H	2.372400000	-3.739008000	1.183494000	H	2.534242000	-3.610475000	1.216152000
H	2.718456000	-3.587751000	-0.583083000	H	2.858077000	-3.526632000	-0.559458000
C	-1.878058000	2.006991000	-0.076396000	C	-1.932387000	1.914271000	-0.204276000
C	-2.896798000	3.118665000	-0.155565000	C	-2.984462000	2.993340000	-0.292928000
O	1.427810000	1.308127000	-1.074004000	O	1.376099000	1.280679000	-1.294324000
C	1.827068000	1.759664000	0.035534000	C	1.796858000	1.790120000	-0.221580000
C	2.921129000	2.799094000	0.021235000	C	2.881192000	2.835724000	-0.301342000
O	1.373954000	1.434843000	1.178510000	O	1.381429000	1.510124000	0.949872000
O	-1.542246000	1.629589000	1.091139000	O	-1.548377000	1.610511000	0.973685000
H	3.625546000	2.618820000	0.844760000	H	2.477832000	3.795667000	0.055926000
H	3.439857000	2.799885000	-0.945188000	H	3.709280000	2.560372000	0.367859000
H	2.464525000	3.788218000	0.185570000	H	3.239289000	2.941299000	-1.332236000
H	-3.902803000	2.669318000	-0.191312000	H	-2.704812000	3.840041000	0.349722000
H	-2.834862000	3.760239000	0.732764000	H	-3.114527000	3.320411000	-1.331397000
H	-2.752511000	3.702409000	-1.073782000	H	-3.938744000	2.591761000	0.083951000
Rh	-0.119311000	-0.048641000	-1.124030000	Rh	-0.120712000	-0.128475000	-1.218322000
Rh	-0.183723000	0.097034000	1.323060000	Rh	-0.125298000	0.143465000	1.234813000
C	0.324718000	-0.675305000	4.827606000	C	0.462341000	-0.356737000	5.533011000
C	1.230507000	0.215680000	4.055186000	C	0.832986000	-0.323446000	4.074604000
C	-0.313652000	-1.670297000	4.130148000	C	0.138766000	-1.470756000	6.193658000
C	-0.109234000	0.390495000	3.418024000	C	-0.113834000	0.395129000	3.183122000
H	1.975405000	-0.263126000	3.412730000	H	1.026120000	-1.323706000	3.655893000
H	1.594194000	1.082739000	4.612739000	H	1.788906000	0.223277000	3.919801000
H	-1.209606000	-2.146663000	4.536207000	H	-0.137638000	-1.448968000	7.251264000
H	0.100583000	-2.066309000	3.201614000	H	0.146142000	-2.448676000	5.700477000
H	-0.064329000	-0.334400000	5.790398000	H	0.445093000	0.611452000	6.045532000
C	-0.973094000	1.483601000	4.014823000	C	-0.894192000	1.500180000	3.787331000
O	-0.383277000	2.515883000	4.321986000	O	-0.215126000	2.515789000	3.943742000
N	-2.320824000	1.325849000	4.138723000	N	-2.196059000	1.345958000	4.099669000
C	-3.083352000	2.436597000	4.705827000	C	-2.928579000	2.475477000	4.659964000
H	-3.781284000	2.823168000	3.944200000	H	-3.773728000	2.722090000	3.995477000
H	-2.361296000	3.234697000	4.912929000	H	-2.237759000	3.328870000	4.636422000
C	-3.056130000	0.145469000	3.697251000	C	-3.420797000	2.225365000	6.083095000
H	-2.368737000	-0.509317000	3.161580000	H	-4.152531000	1.403651000	6.131624000
H	-3.427699000	-0.410565000	4.578930000	H	-2.579573000	1.973150000	6.747314000
C	-4.216654000	0.458030000	2.756489000	H	-3.911406000	3.128691000	6.477307000
H	-3.851551000	1.034091000	1.895816000	C	-2.869499000	0.071802000	3.874405000
H	-5.027272000	1.020095000	3.244522000	H	-2.125417000	-0.635018000	3.477156000
H	-4.643584000	-0.486474000	2.386064000	H	-3.207097000	-0.338416000	4.841615000
C	-3.840931000	2.057109000	5.975550000	C	-4.028996000	0.161823000	2.888447000
H	-4.607880000	1.287738000	5.793636000	H	-3.674690000	0.577149000	1.935407000
H	-3.150387000	1.674748000	6.744166000	H	-4.849407000	0.789571000	3.269485000
H	-4.351977000	2.941163000	6.387555000	H	-4.436010000	-0.843595000	2.704083000



TS6

E_e^S = **-1616.794029**

O	-1.604841000	1.109814000	-1.377388000
O	-1.711589000	-1.415272000	1.341422000
O	1.199726000	-1.428419000	1.433033000
C	1.619517000	-2.035196000	0.391857000
C	-2.123260000	-1.980750000	0.277366000
O	1.229449000	-1.831499000	-0.787179000
O	-1.692506000	-1.767365000	-0.887327000
C	-3.257143000	-2.965767000	0.435871000
H	-3.253286000	-3.690028000	-0.388359000
H	-3.192412000	-3.475280000	1.406322000
H	-4.207624000	-2.408686000	0.404380000
C	2.697826000	-3.069585000	0.611881000
H	3.644259000	-2.552544000	0.837210000
H	2.447009000	-3.698298000	1.477974000
H	2.829689000	-3.685017000	-0.286071000
C	-2.020937000	1.714549000	-0.352186000
C	-3.025970000	2.825216000	-0.540803000
O	1.300451000	1.039280000	-1.298979000
C	1.699618000	1.617904000	-0.251353000
C	2.824269000	2.616462000	-0.379888000
O	1.253697000	1.420736000	0.924512000
O	-1.666431000	1.481359000	0.848476000
H	3.760859000	2.136691000	-0.052959000
H	2.934755000	2.938240000	-1.422624000
H	2.641464000	3.476266000	0.279023000
H	-3.870131000	2.683910000	0.149774000
H	-2.548996000	3.783620000	-0.283004000
H	-3.378966000	2.856613000	-1.578422000
Rh	-0.190926000	-0.381584000	-1.186770000
Rh	-0.243858000	0.040588000	1.227977000
C	0.441685000	-0.348663000	5.636609000
C	0.481807000	-0.405826000	4.173806000
C	1.142590000	-1.205539000	6.394111000
C	-0.280552000	0.372133000	3.286411000
H	1.119523000	-1.171441000	3.712159000
H	0.958449000	0.662403000	3.493686000
H	1.083896000	-1.183828000	7.484937000
H	1.792009000	-1.962189000	5.942725000
H	-0.200236000	0.408858000	6.094957000

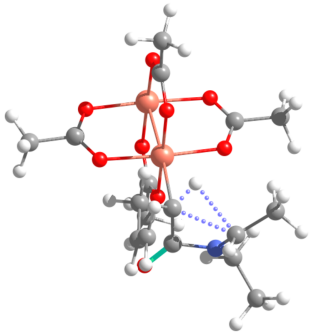


49a

E_e^S = **-481.7754692**

C	0.186486000	-0.421800000	4.806720000
C	0.413385000	0.348870000	3.590915000
C	0.829763000	-1.564608000	5.097648000
C	-0.241459000	1.474083000	3.242680000
H	1.195735000	-0.024912000	2.920534000
H	0.057078000	2.013274000	2.338847000
H	0.635222000	-2.110807000	6.023616000
H	1.576041000	-1.986573000	4.416871000
H	-0.550126000	-0.026155000	5.514106000
C	-1.221098000	2.221192000	4.102003000
O	-0.911707000	3.331224000	4.515377000
N	-2.425519000	1.637766000	4.403333000
C	-3.328638000	2.383802000	5.280043000
H	-4.363775000	2.149637000	4.986051000
H	-3.162861000	3.455845000	5.105087000
C	-2.946910000	0.433801000	3.762954000
H	-2.118057000	-0.241975000	3.525307000
H	-3.572982000	-0.093331000	4.501621000
C	-3.750846000	0.728187000	2.497063000
H	-3.109899000	1.199736000	1.735641000
H	-4.592267000	1.409202000	2.700626000
H	-4.161803000	-0.201625000	2.072400000
C	-3.099704000	2.059190000	6.754309000
H	-3.238992000	0.984225000	6.954673000
H	-2.076091000	2.338180000	7.045704000
H	-3.802855000	2.618515000	7.391955000

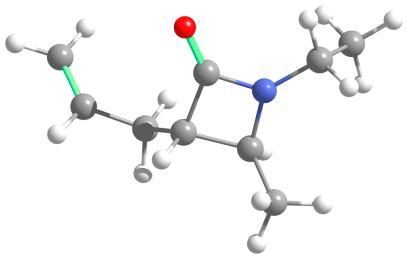
C	-1.047143000	1.523645000	3.868971000
O	-0.437161000	2.560477000	4.121095000
N	-2.375392000	1.355947000	4.088630000
C	-3.106912000	2.473784000	4.679164000
H	-4.157497000	2.397324000	4.363575000
H	-2.697480000	3.402050000	4.257024000
C	-3.077072000	0.098767000	3.845471000
H	-2.339011000	-0.662653000	3.561597000
H	-3.540433000	-0.235910000	4.791752000
C	-4.127335000	0.180647000	2.740930000
H	-3.652825000	0.489546000	1.801416000
H	-4.932310000	0.890928000	2.985814000
H	-4.588029000	-0.808434000	2.595907000
C	-3.000361000	2.504394000	6.203081000
H	-3.371300000	1.568441000	6.651695000
H	-1.952085000	2.648766000	6.504566000
H	-3.592032000	3.335603000	6.618225000



TS6'

E_e^S **= -1616.780868**

O	-2.022263000	1.548716000	-0.691367000
O	-2.089921000	-0.959453000	2.044710000
O	0.675689000	-1.692723000	1.407124000
C	0.689372000	-2.326940000	0.305705000
C	-2.851696000	-1.388267000	1.119208000
O	0.086963000	-1.979014000	-0.750154000
O	-2.661934000	-1.234558000	-0.118478000
C	-4.074693000	-2.157954000	1.555778000
H	-3.756032000	-3.117269000	1.993018000
H	-4.608015000	-1.598209000	2.337937000
H	-4.737898000	-2.348466000	0.703785000
C	1.524479000	-3.581798000	0.250655000
H	1.152346000	-4.256052000	-0.530896000
H	2.560288000	-3.298865000	0.002178000
H	1.533438000	-4.080032000	1.228960000
C	-2.055964000	2.174611000	0.408594000
C	-2.857584000	3.450681000	0.470285000
O	0.703184000	0.808069000	-1.307153000
C	1.459838000	1.249268000	-0.392906000
C	2.664432000	2.056667000	-0.804476000
O	1.280664000	1.088245000	0.853571000
O	-1.487722000	1.809899000	1.482286000
H	3.535165000	1.765647000	-0.200738000



79

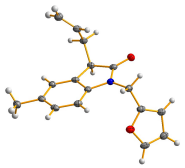
E_e^S **= -481.7756039**

C	-2.543211000	1.379401000	0.424334000
C	-3.411706000	0.753574000	-0.691228000
O	-3.816530000	1.085556000	-1.777653000
N	-3.598032000	-0.387657000	0.049472000
C	-4.392395000	-1.565991000	-0.194562000
H	-3.764264000	-2.467926000	-0.076592000
H	-4.690003000	-1.516944000	-1.253803000
C	-2.831945000	0.066986000	1.219093000
H	-3.479486000	0.249748000	2.096822000
C	-1.651413000	-0.806622000	1.605528000
H	-0.994463000	-0.978510000	0.738112000
H	-1.985366000	-1.787484000	1.981397000
H	-1.060667000	-0.328623000	2.403167000
C	-5.624106000	-1.659304000	0.705913000
H	-5.340441000	-1.701490000	1.770089000
H	-6.278604000	-0.785688000	0.561961000
H	-6.204000000	-2.567557000	0.478322000
C	-3.044111000	2.692643000	1.025495000
H	-4.113937000	2.597240000	1.277507000
H	-2.505782000	2.862429000	1.977040000
C	-2.834824000	3.869748000	0.115715000
H	-1.791541000	4.089035000	-0.146553000
C	-3.805797000	4.630685000	-0.391934000
H	-4.859747000	4.432849000	-0.171477000

H	2.870106000	1.928156000	-1.873967000
H	2.459049000	3.119304000	-0.599152000
H	-3.812740000	3.243135000	0.979275000
H	-2.316561000	4.199857000	1.064445000
H	-3.066945000	3.825977000	-0.538772000
Rh	-0.991952000	-0.225083000	-0.789462000
Rh	-0.373717000	0.079614000	1.528299000
C	2.619814000	0.730333000	5.161767000
C	2.034212000	0.288748000	3.845637000
C	3.360835000	-0.035664000	5.966673000
C	0.534550000	0.320512000	3.863246000
H	2.383155000	-0.717362000	3.570835000
H	2.369433000	0.972325000	3.043457000
H	3.753923000	0.341179000	6.915185000
H	3.612062000	-1.068235000	5.700043000
H	2.383468000	1.760447000	5.454831000
C	-0.221143000	1.541343000	4.127657000
O	0.078260000	2.708159000	3.968346000
N	-1.417605000	1.048968000	4.723294000
C	-2.759365000	1.538192000	4.449300000
H	-3.347914000	0.717276000	4.005806000
H	-2.640134000	2.298165000	3.666031000
C	-3.448820000	2.114976000	5.681703000
H	-3.562552000	1.357820000	6.474402000
H	-2.866995000	2.953985000	6.091891000
H	-4.453654000	2.483834000	5.421894000
C	-1.055895000	-0.104159000	5.359943000
H	-0.021587000	-0.586603000	3.589114000
H	-0.283022000	-0.030384000	6.129056000
C	-1.950222000	-1.297930000	5.383002000
H	-2.380263000	-1.486588000	4.389186000
H	-2.777696000	-1.141862000	6.100189000
H	-1.393872000	-2.184626000	5.718461000
H	-3.586870000	5.469756000	-1.057490000
H	-1.485873000	1.462515000	0.122304000

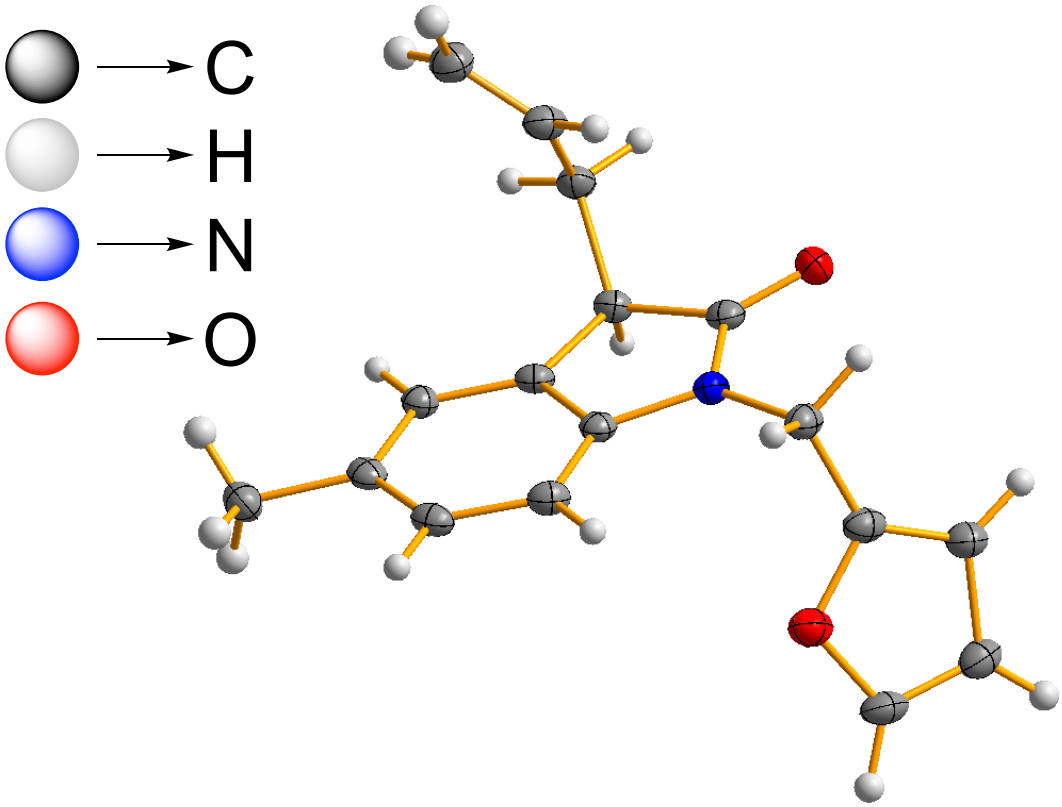
10.0 Single crystal XRD data.

Compound **31** was crystalized from 1: 4 mixtures of DCM: Hexane.

Data	**32**
Molecular Structure	
Formula	$C_{17}H_{17}NO_2$
Formula weight	267.32
Crystal system	Monoclinic
Space group	P 21/n
a (Å)	8.2701(19)
b (Å)	12.237(3)
c (Å)	13.439(3)
α (°)	90.000
β (°)	97.872(8)
γ (°)	90.000
Volume (Å^3)	1347.2(5)
Z	1
Crystal size, mm^3	0.145× 0.076 × 0.021
Density (g/cm^3)	1.318
λ (Å)	0.71073
Temp. (K)	100.00
Total reflns.	42122
Indepnt. reflns.	3459

Final R indices [I > 2σ(I)]	R_1 = 0.0481, wR_2 = 0.1176
R indices (all data)	R_1 = 0.0612, wR_2 = 0.1290
GOOF	1.051
CCDC	2487184

Crystal Structure of compound 32 (Thermal Ellipsoid Contour Probability 50%)



11.0 References.

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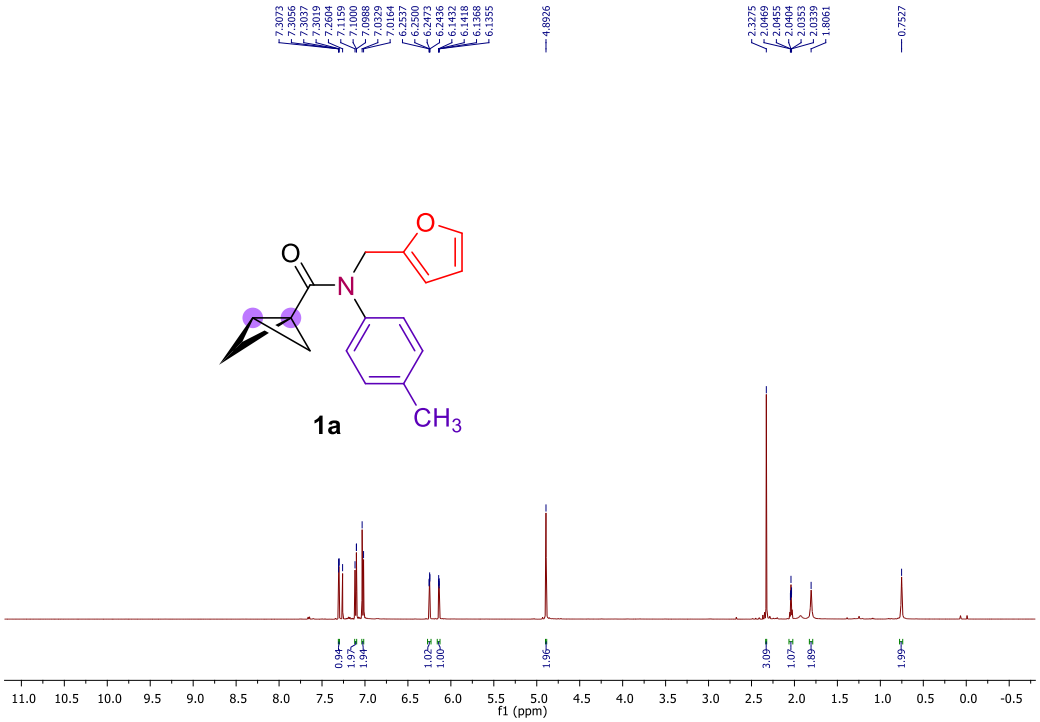
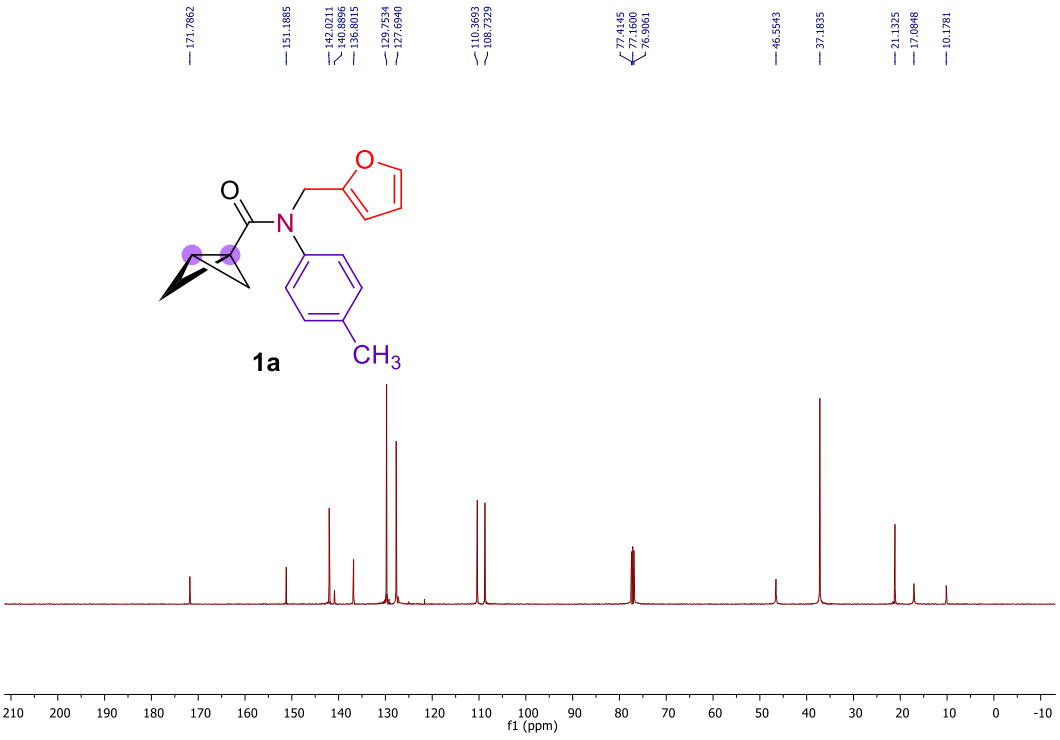
12.0 Spectral data.

N-(Furan-2-ylmethyl)-*N*-(-tolyl)bicyclo[1.1.0]butane-1-carboxamide (**1a**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

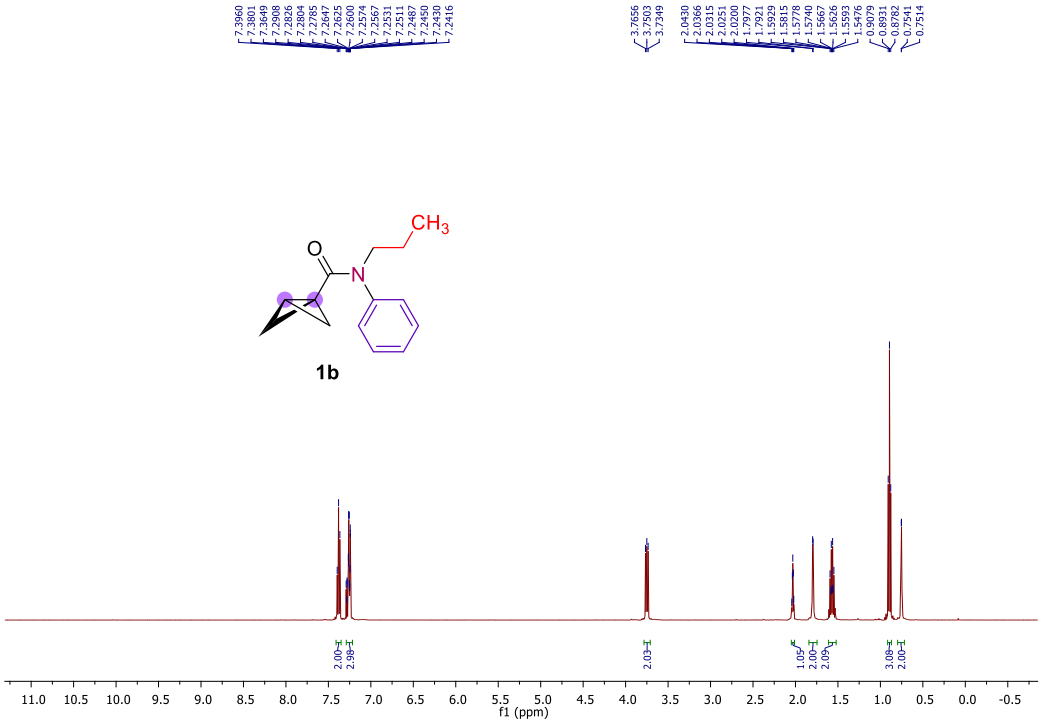


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

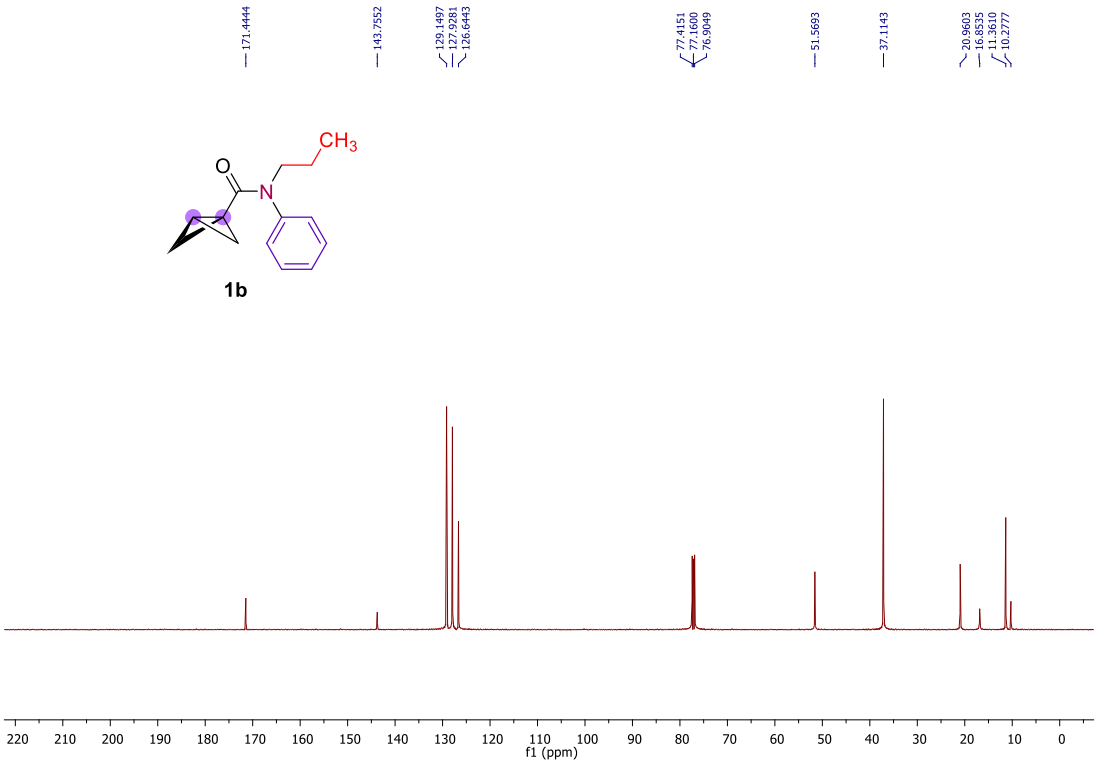


N-Phenyl-*N*-propylbicyclo[1.1.0]butane-1-carboxamide (**1b**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

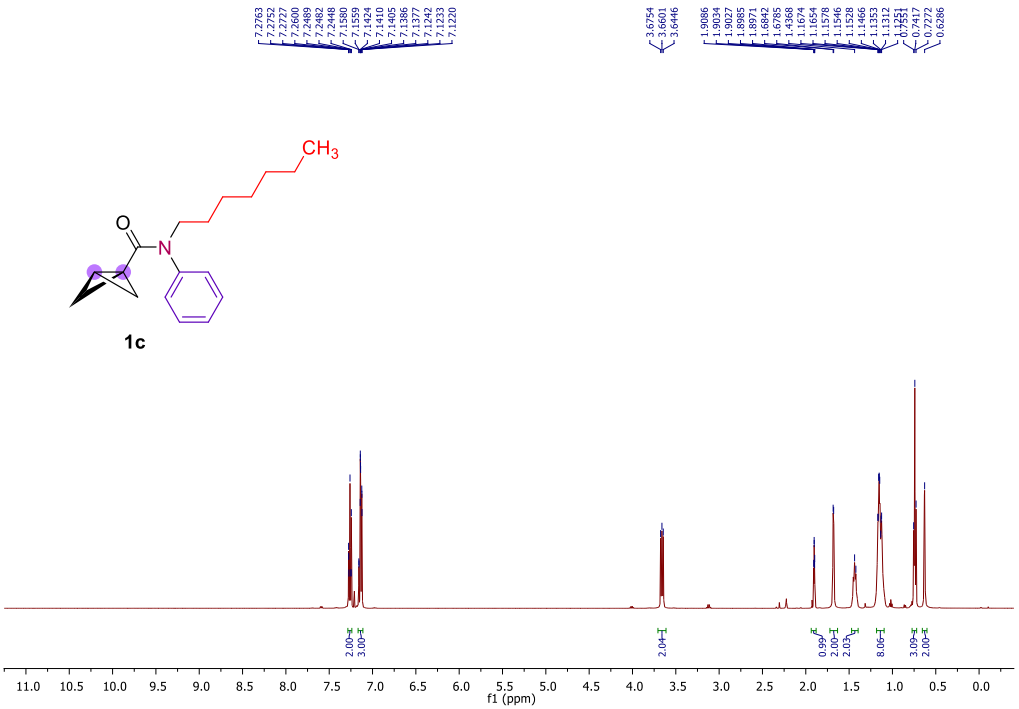


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

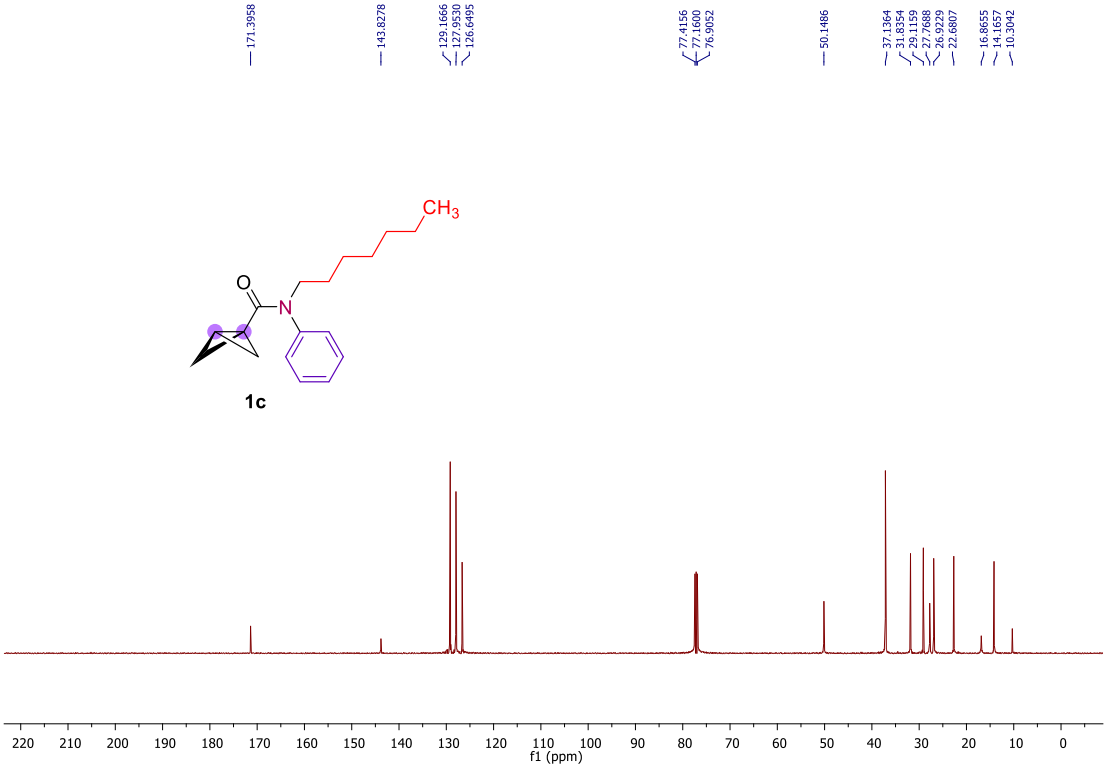


N-Heptyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide (**1c**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

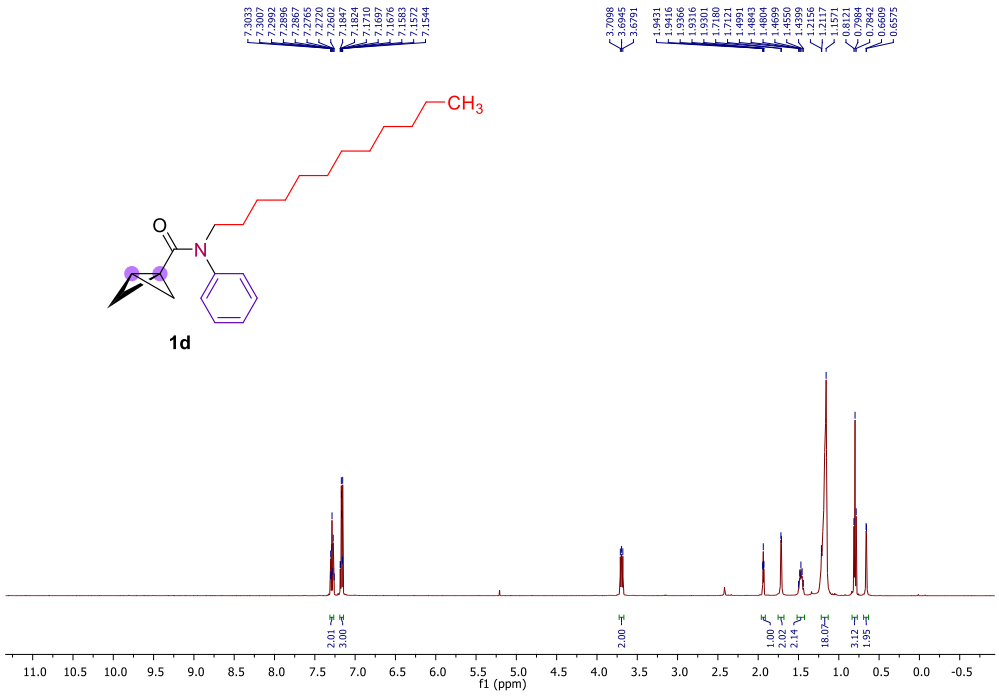


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

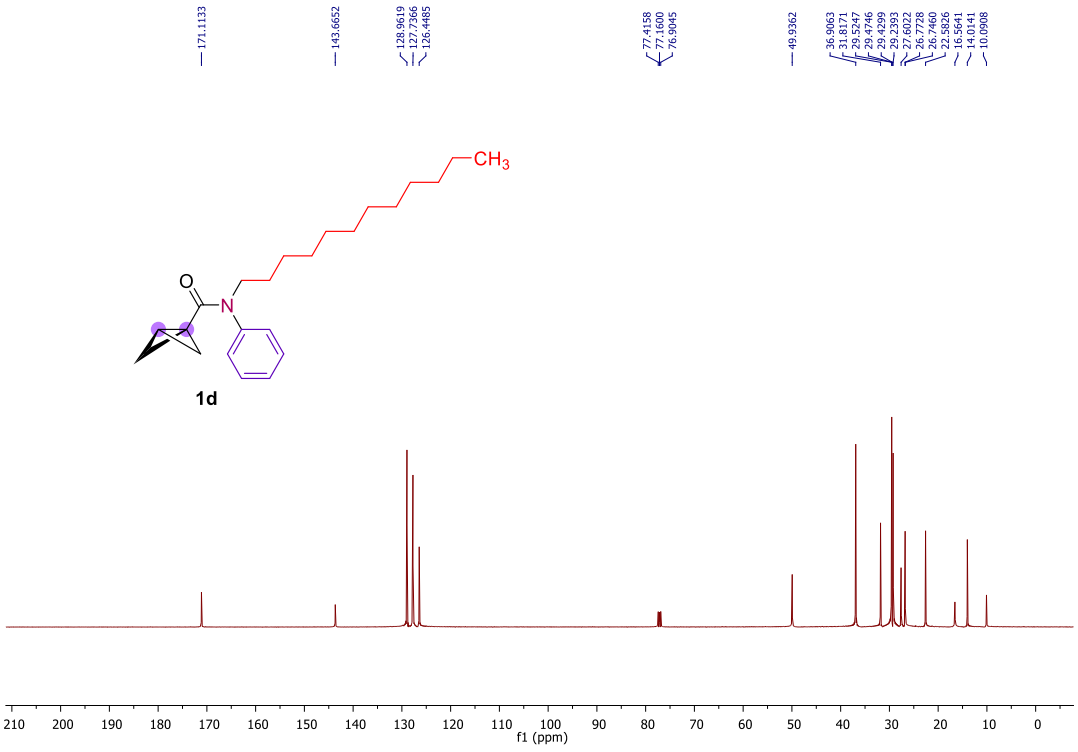


N-Dodecyl-*N*-phenylbicyclo[1.1.0]butane-1-carboxamide (**1d**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

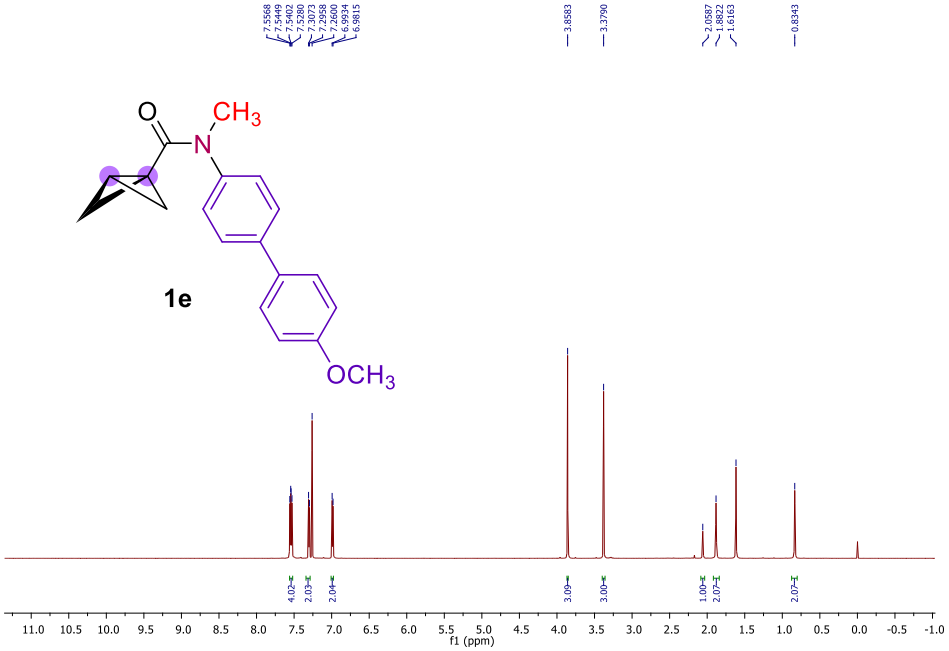


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

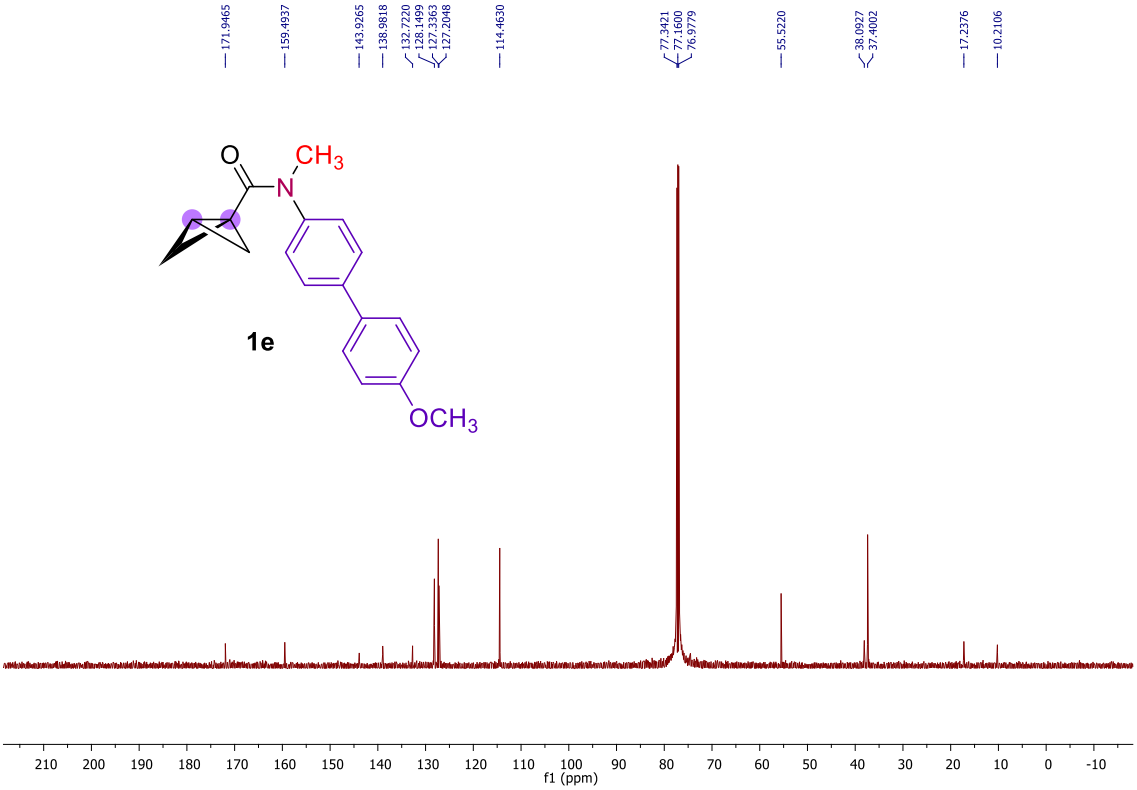


N-(4'-Methoxy-[1,1'-biphenyl]-4-yl)-*N*-methyl bicyclo[1.1.0]butane-1-carboxamide (**1e**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

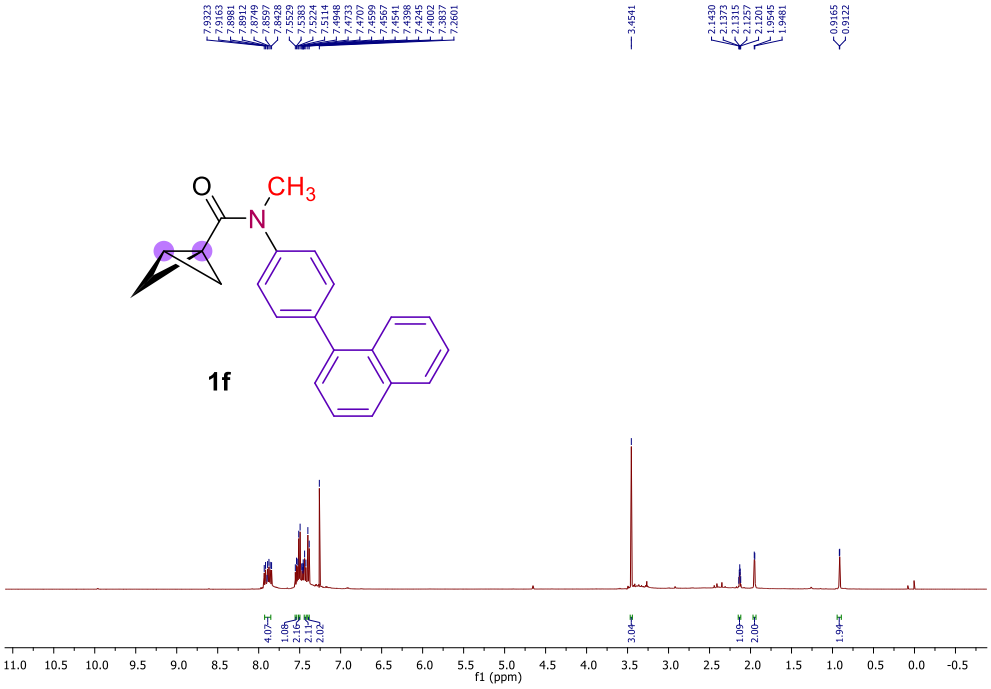


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

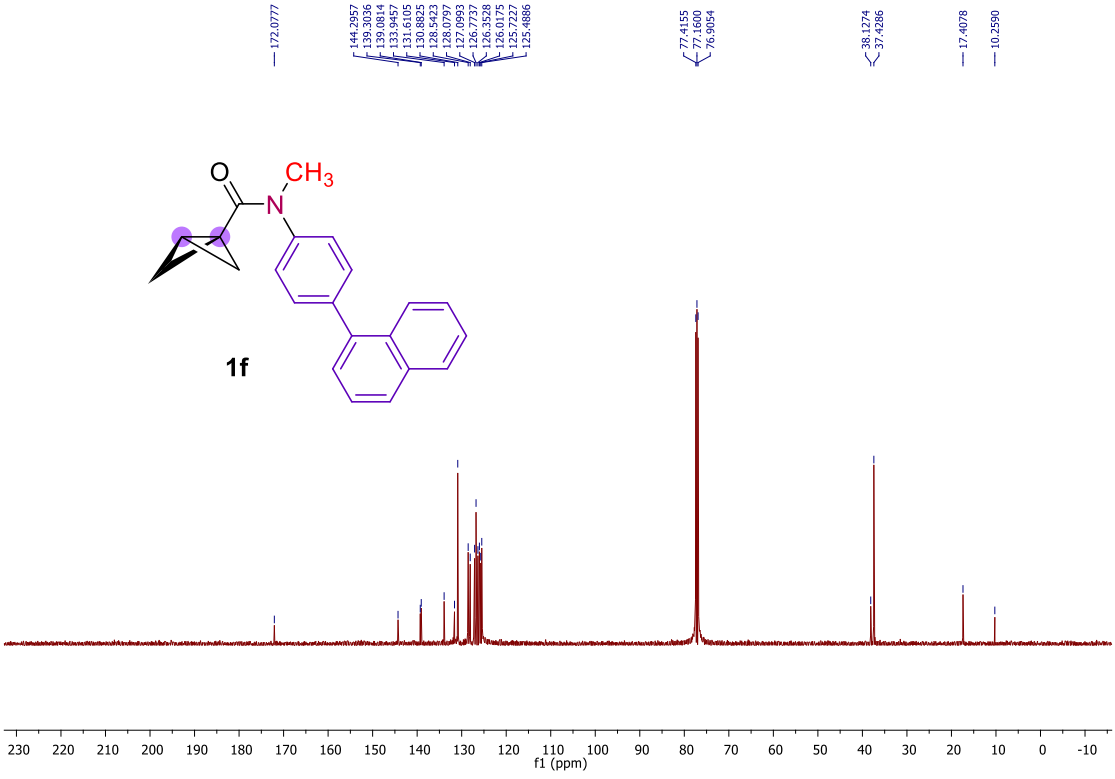


N-Methyl-*N*-(4-(naphthalen-1-yl)phenyl)bicyclo[1.1.0]butane-1-carboxamide (**1f**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

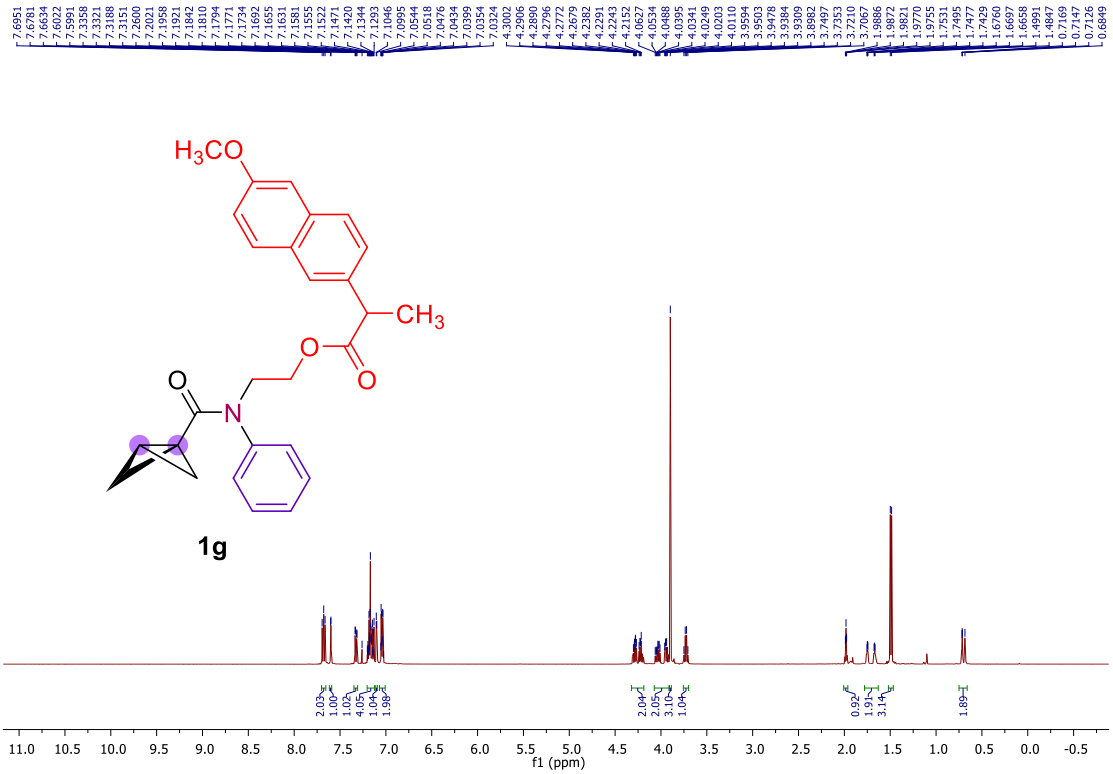


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

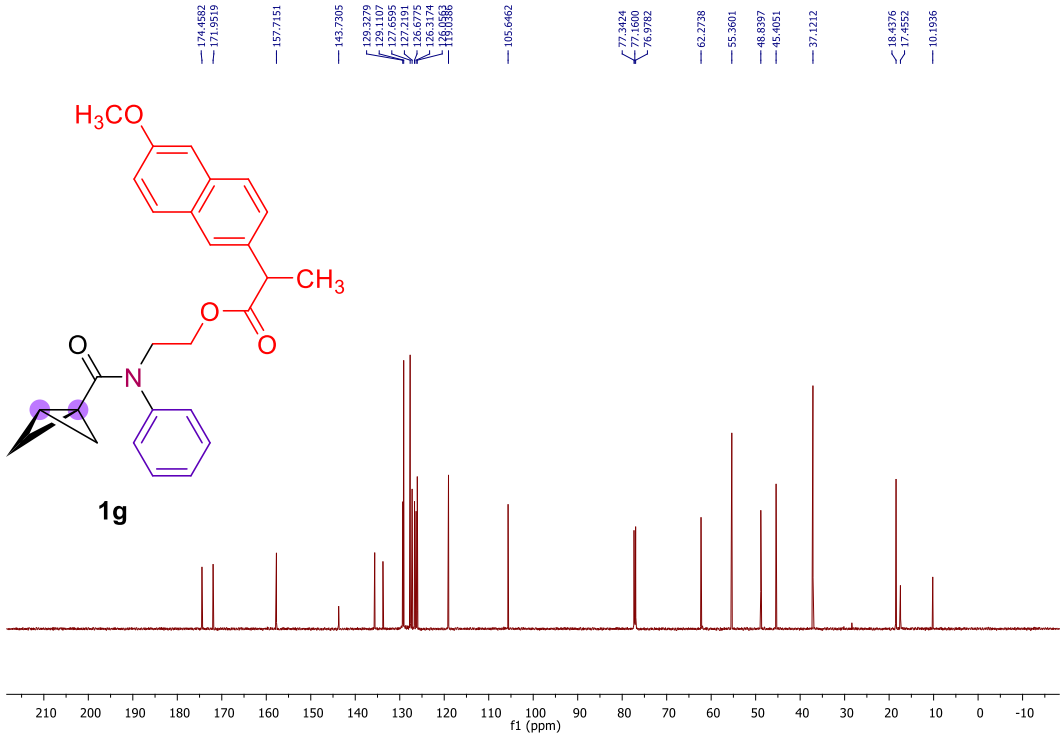


2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido) ethyl 2-(6-methoxynaphthalen-2-yl) propanoate (**1g**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

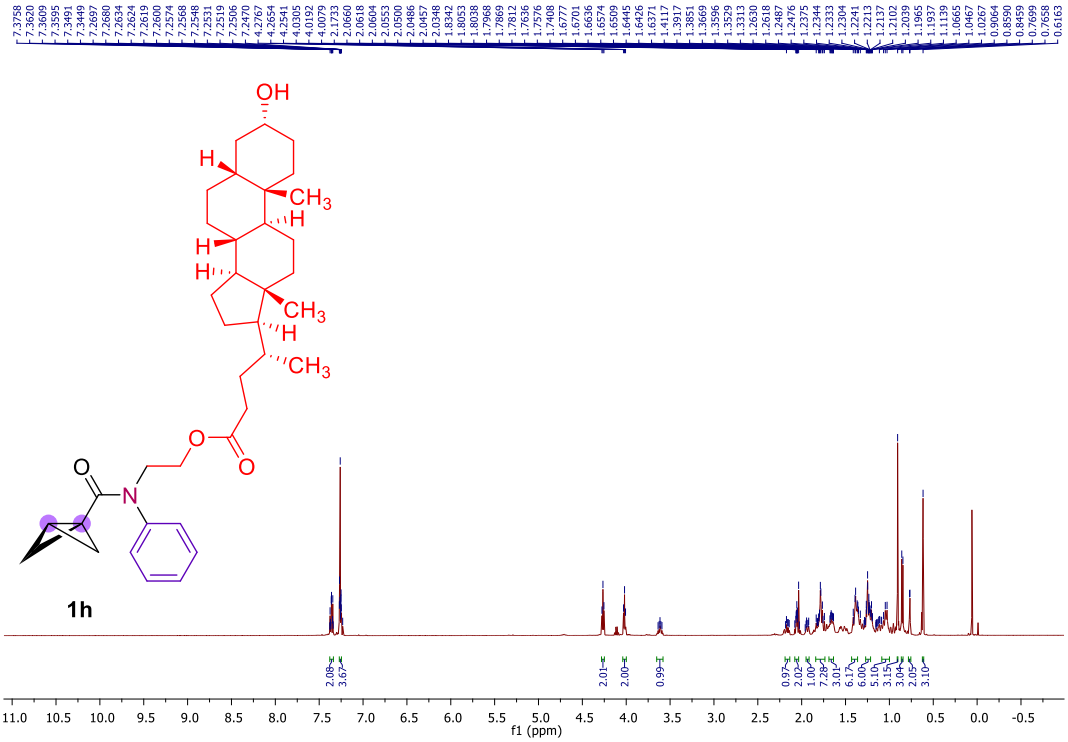


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

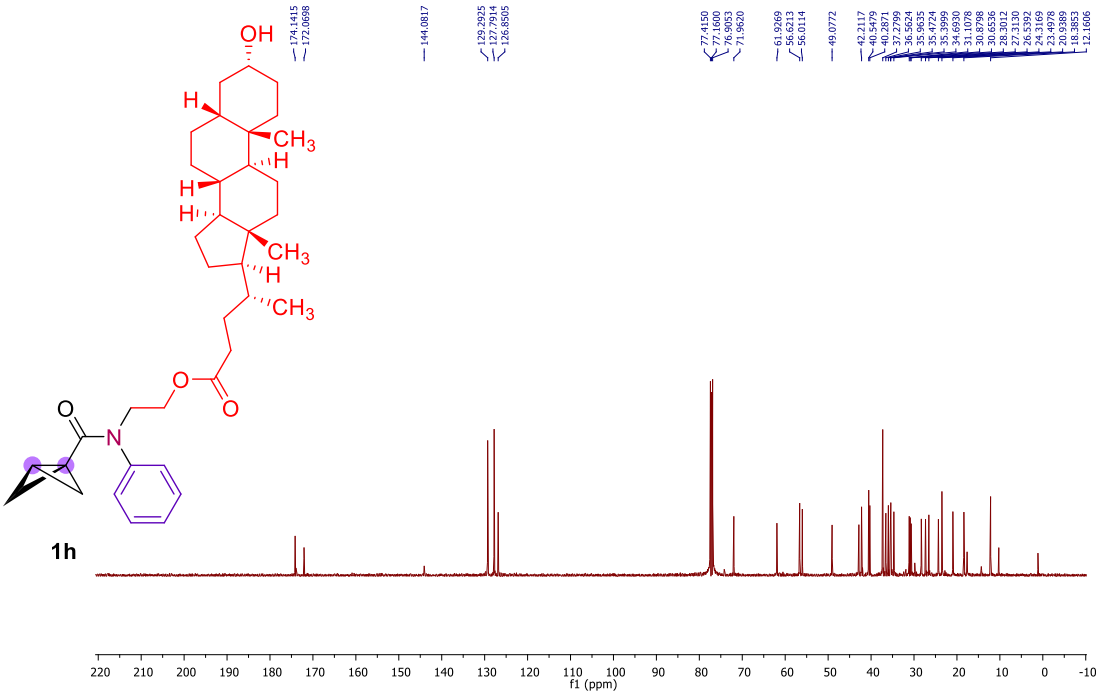


2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 3-hydroxy-10,13-dimethylhexadecahydro-1*H*-cyclopenta[a]phenanthren-17-yl)pentanoate (**1h**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

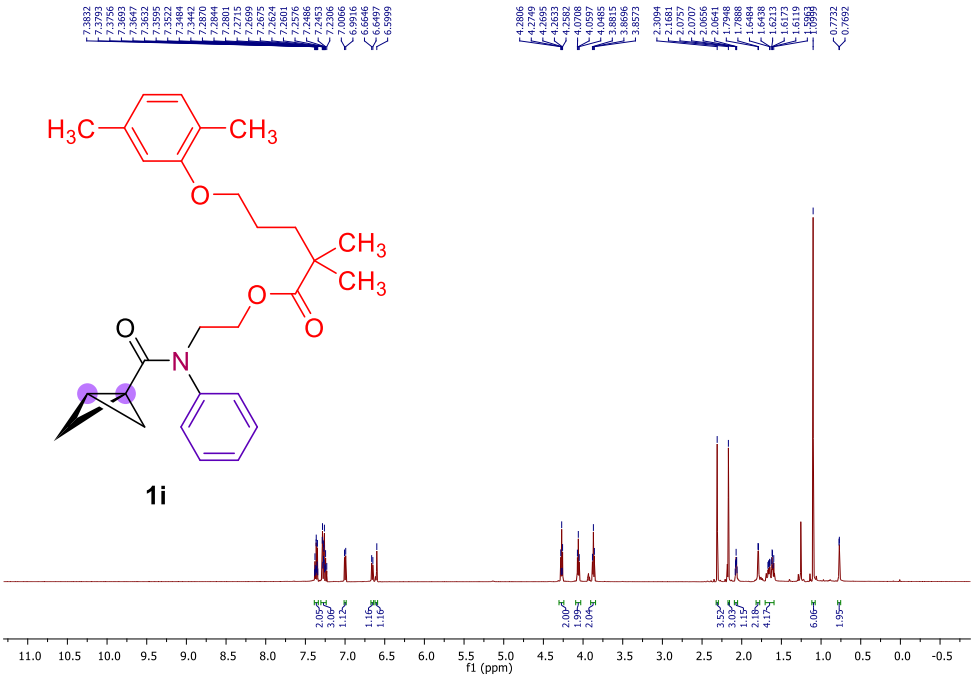


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

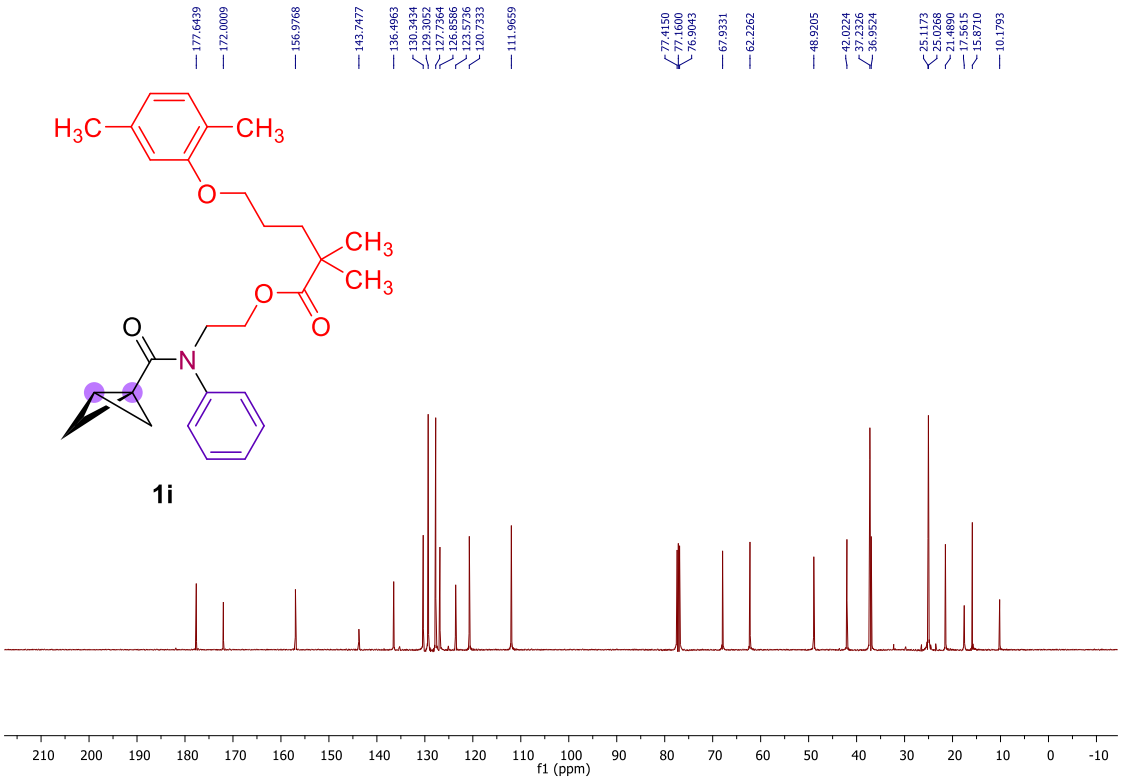


2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (**1i**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

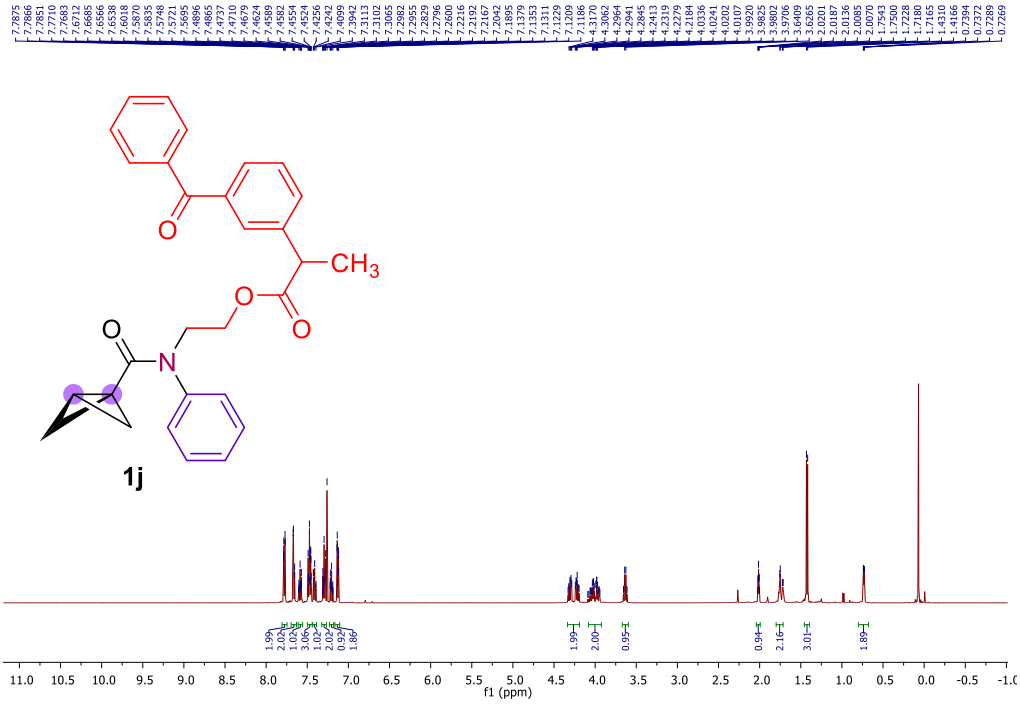


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

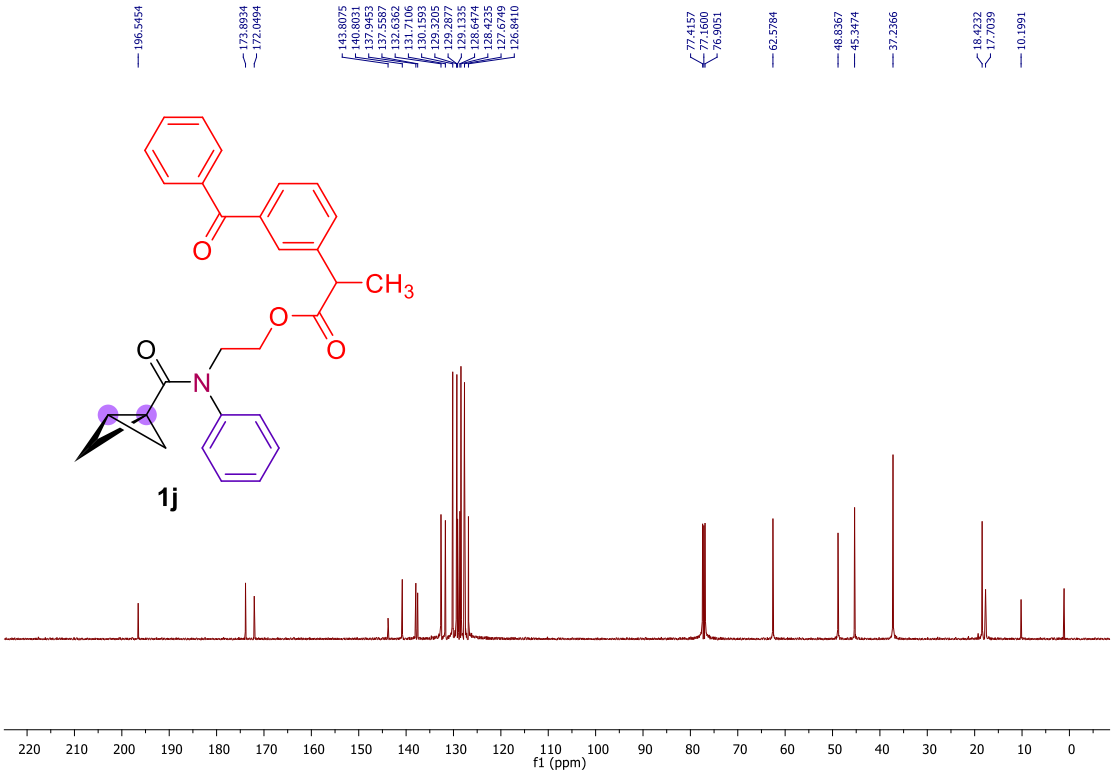


2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 2-(3-benzoylphenyl)propanoate (**1j**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

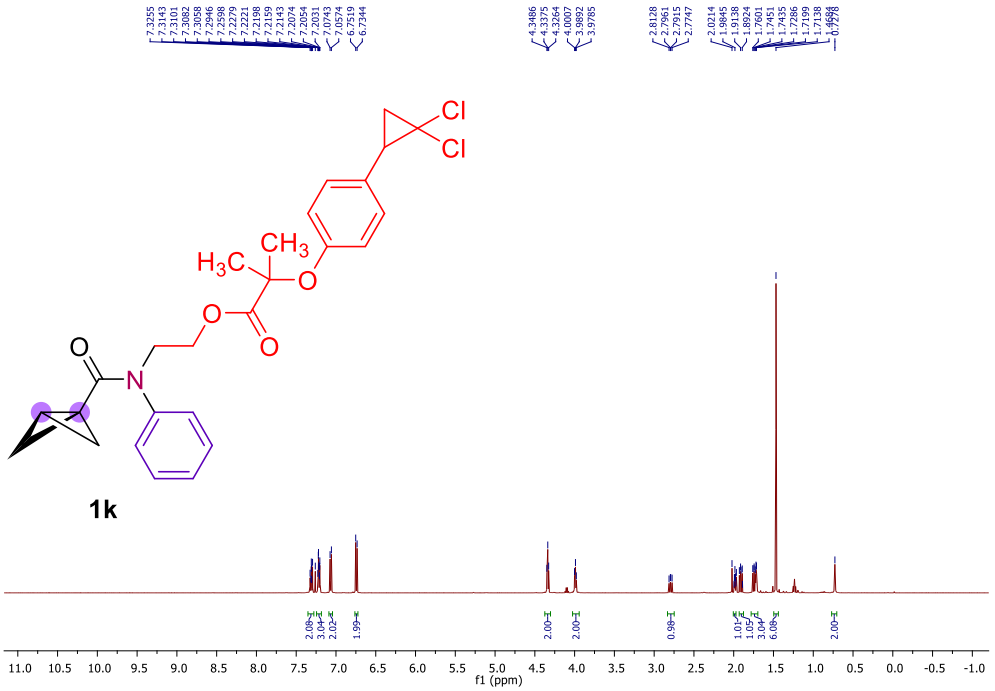


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

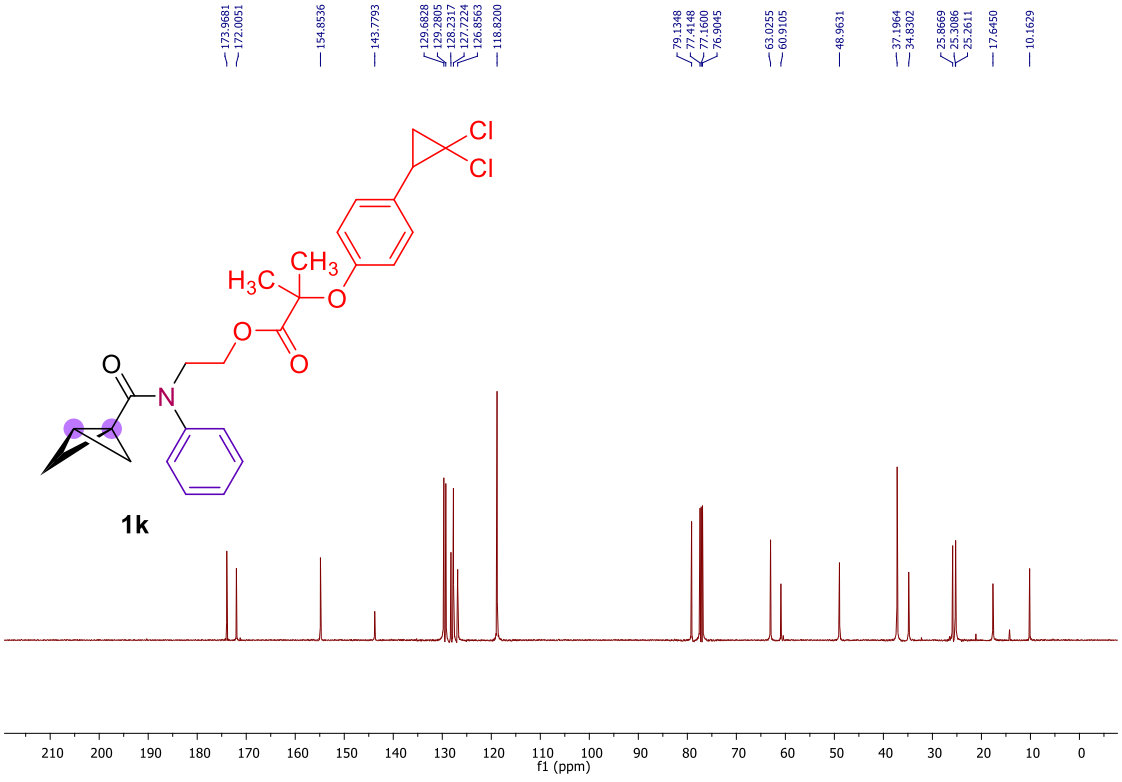


2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 2-(4-(2,2-dichlorocyclopropyl)phenoxy)-2-methylpropanoate (**1k**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

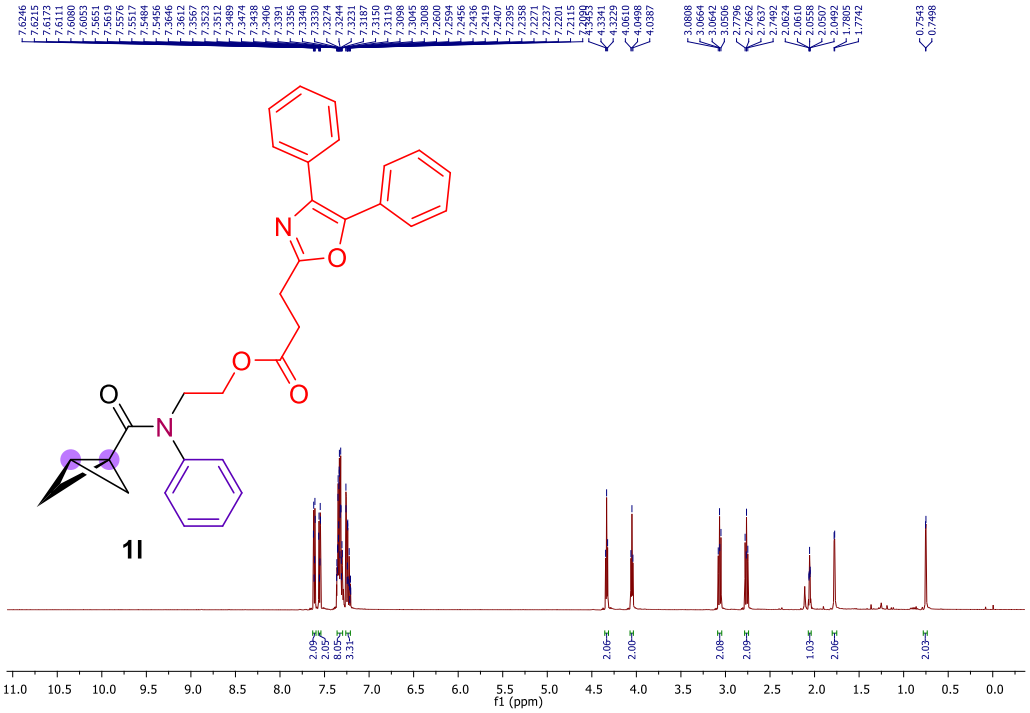


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

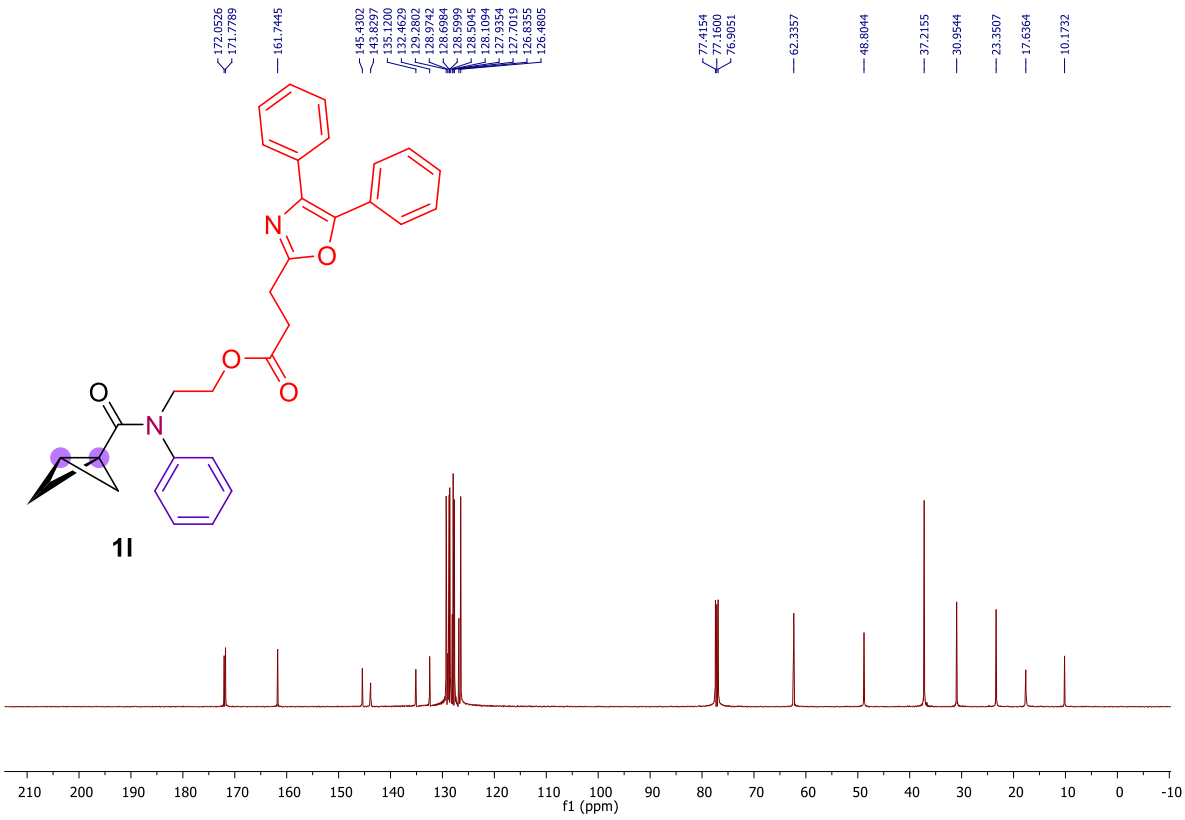


2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 3-(4,5-diphenyloxazol-2-yl)propanoate (**1l**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

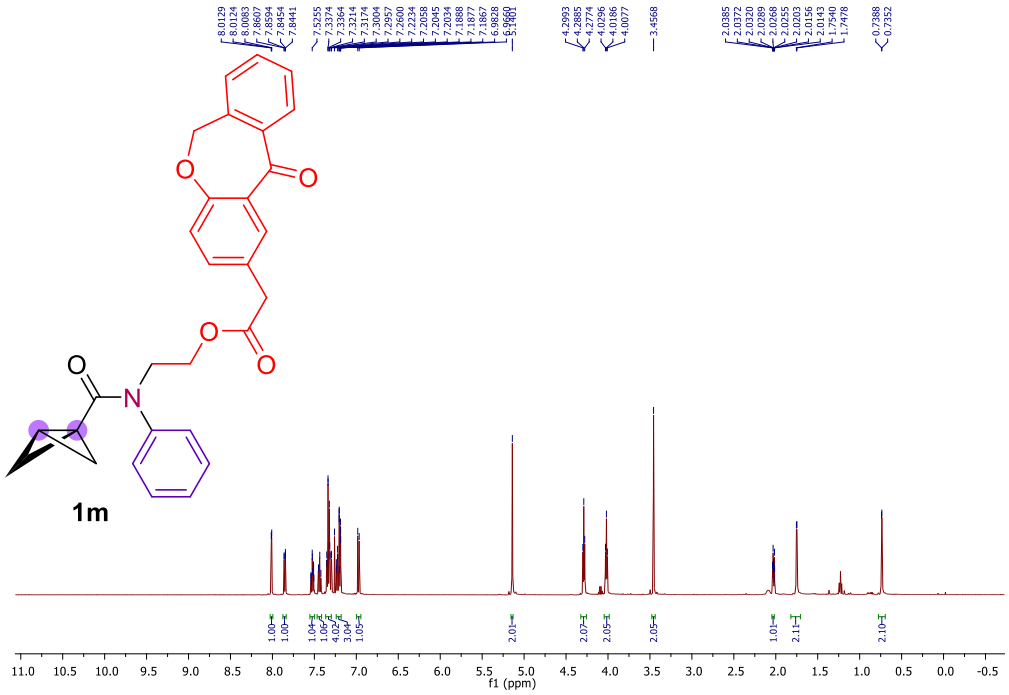


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

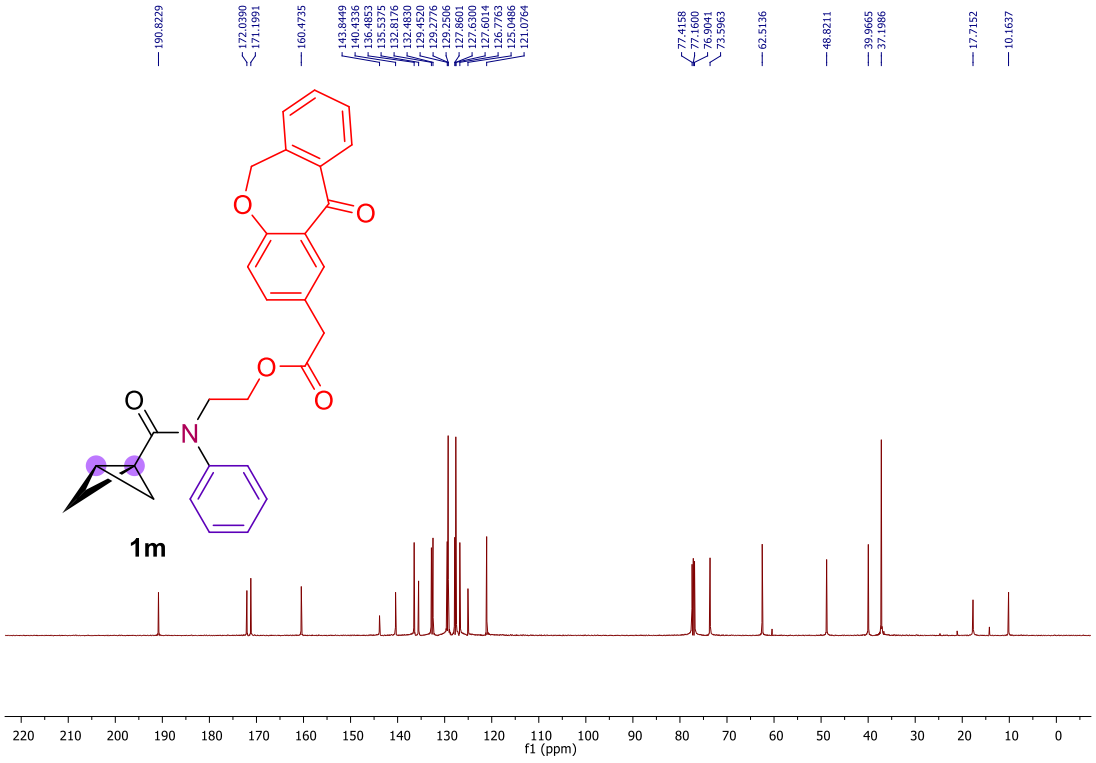


2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 2-(11-oxo-6,11-dihydrodibenzo[b,e]oxepin-2-yl)acetate (**1m**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

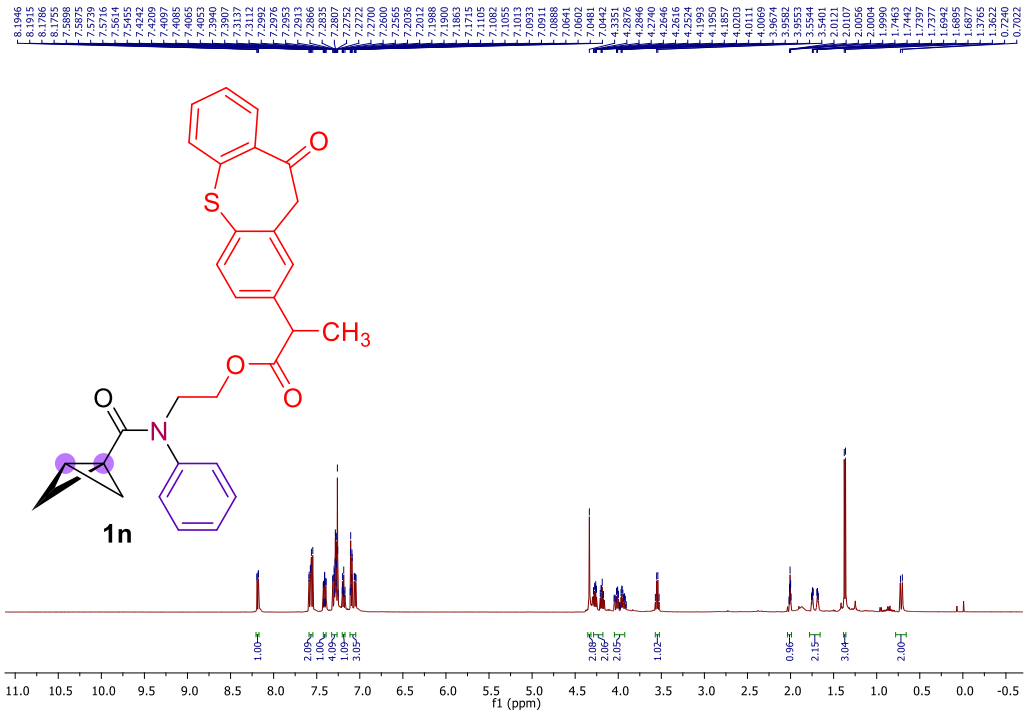


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

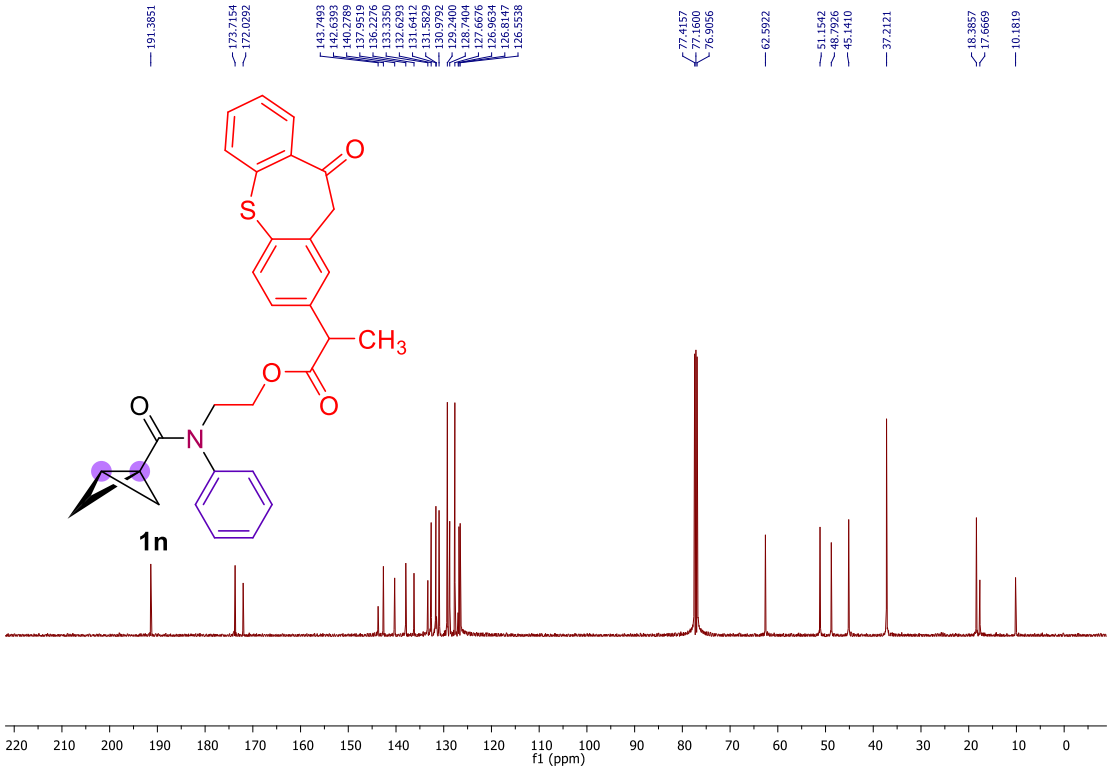


2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 2-(10-oxo-10,11-dihydrodibenzo[b,f]thiepin-2-yl)propanoate (**1n**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

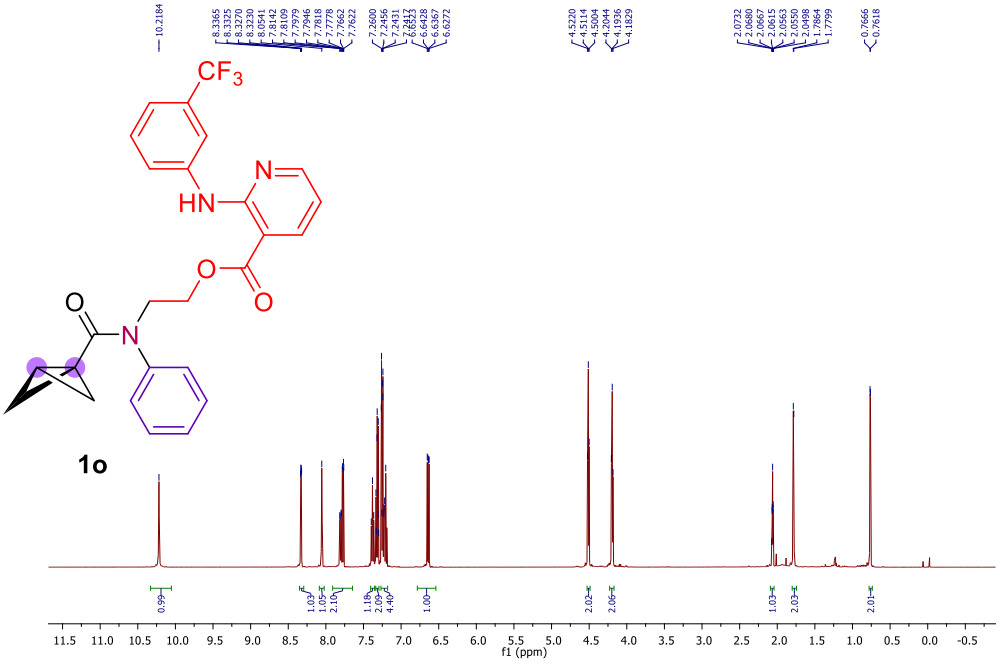


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

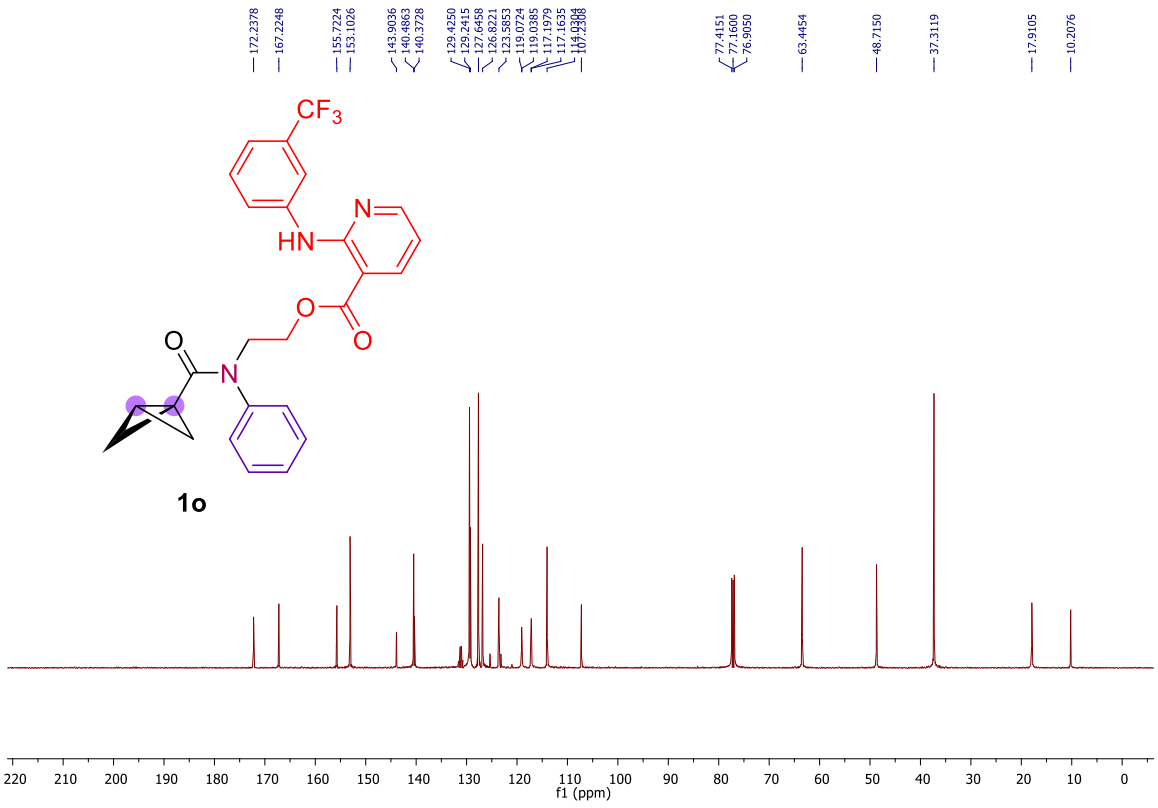


2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl 2-((3-(trifluoromethyl)phenyl)amino)nicotinate (**1o**)

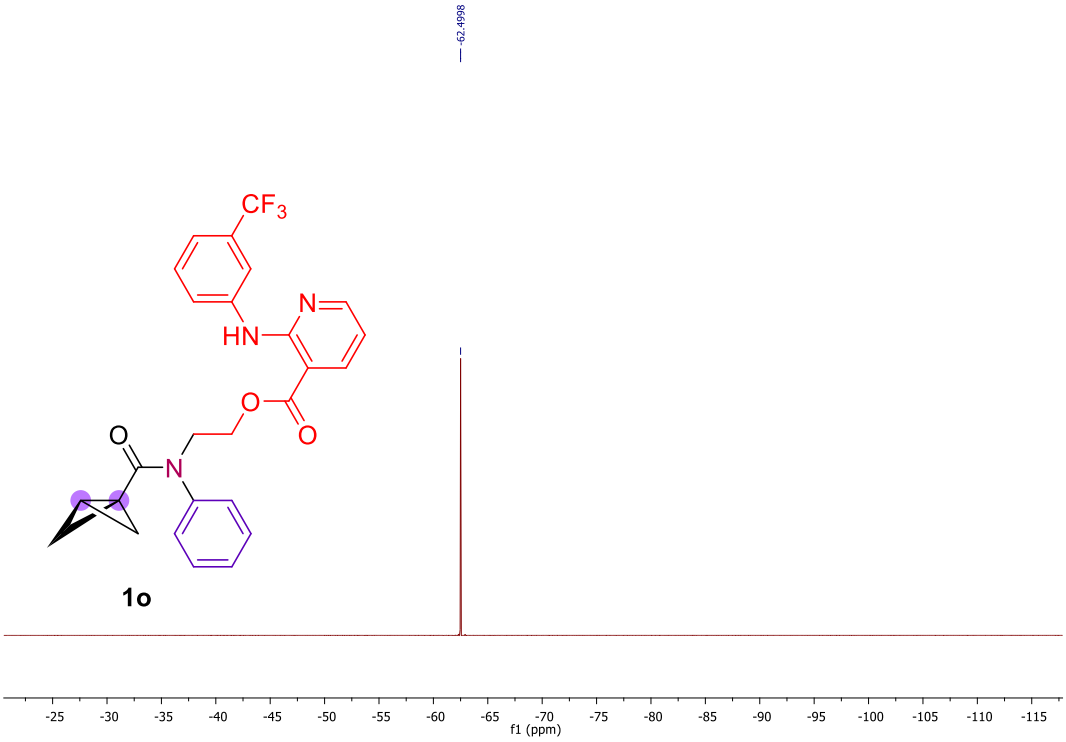
^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)



^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

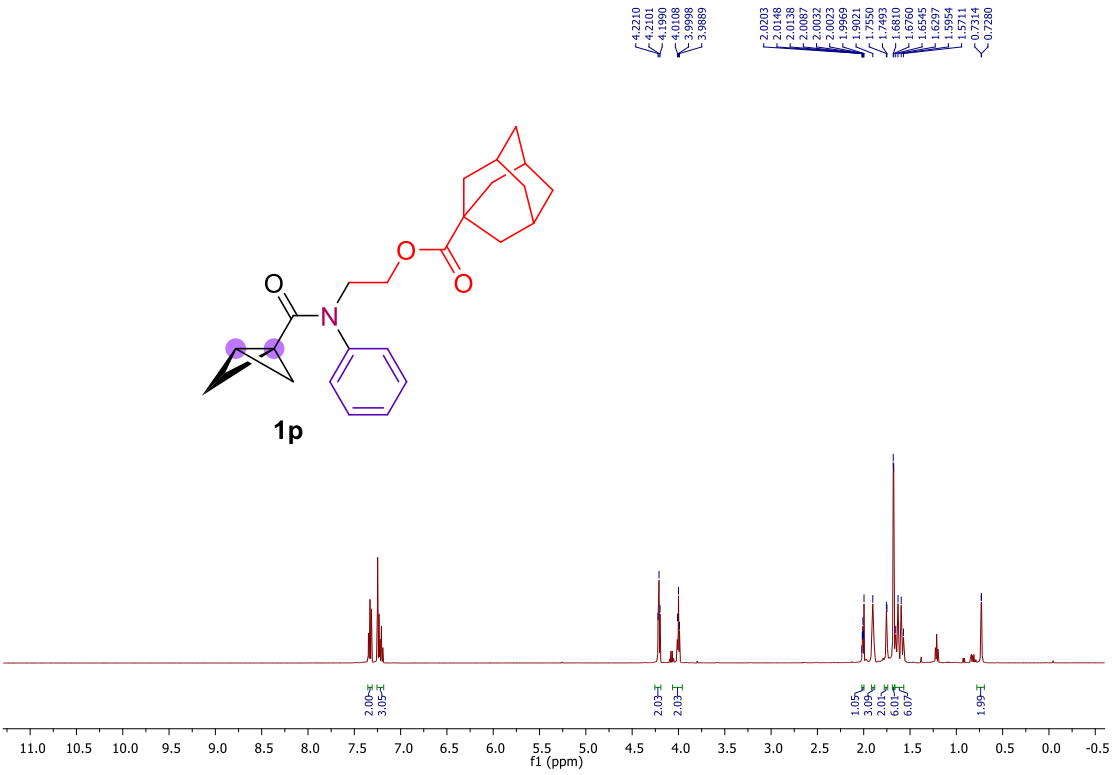


^{19}F NMR (471 MHz, $CDCl_3$, 24 °C)

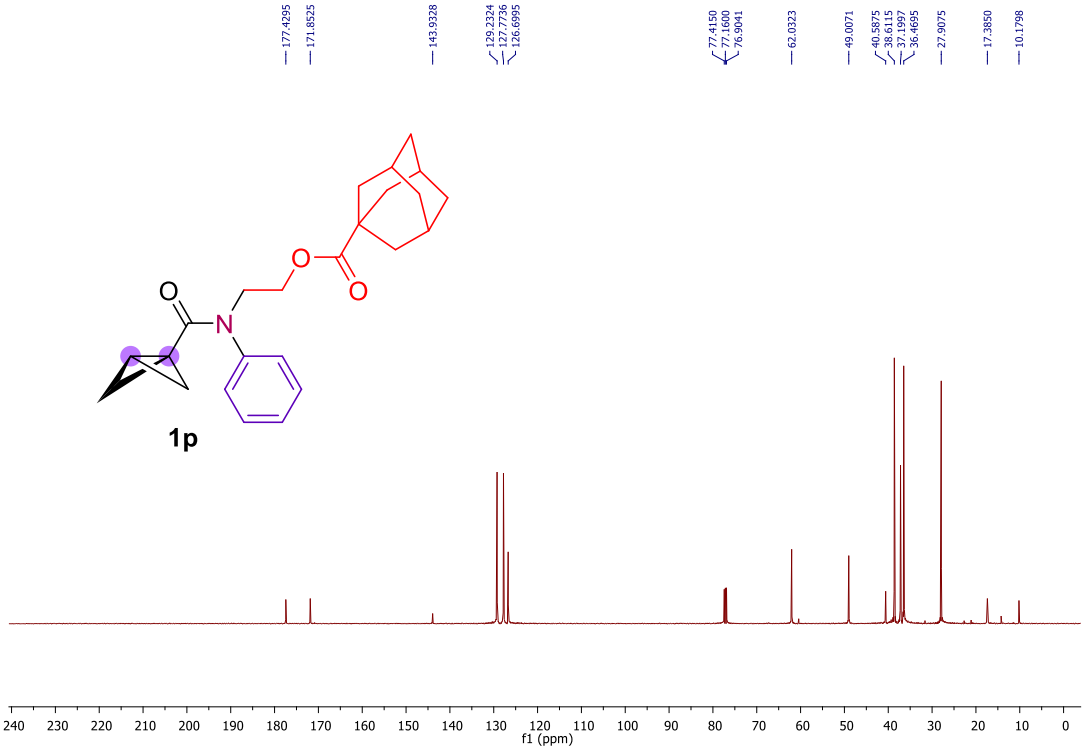


2-(*N*-Phenylbicyclo[1.1.0]butane-1-carboxamido)ethyl (1*S*,3*S*)-adamantane-1-carboxylate (**1p**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

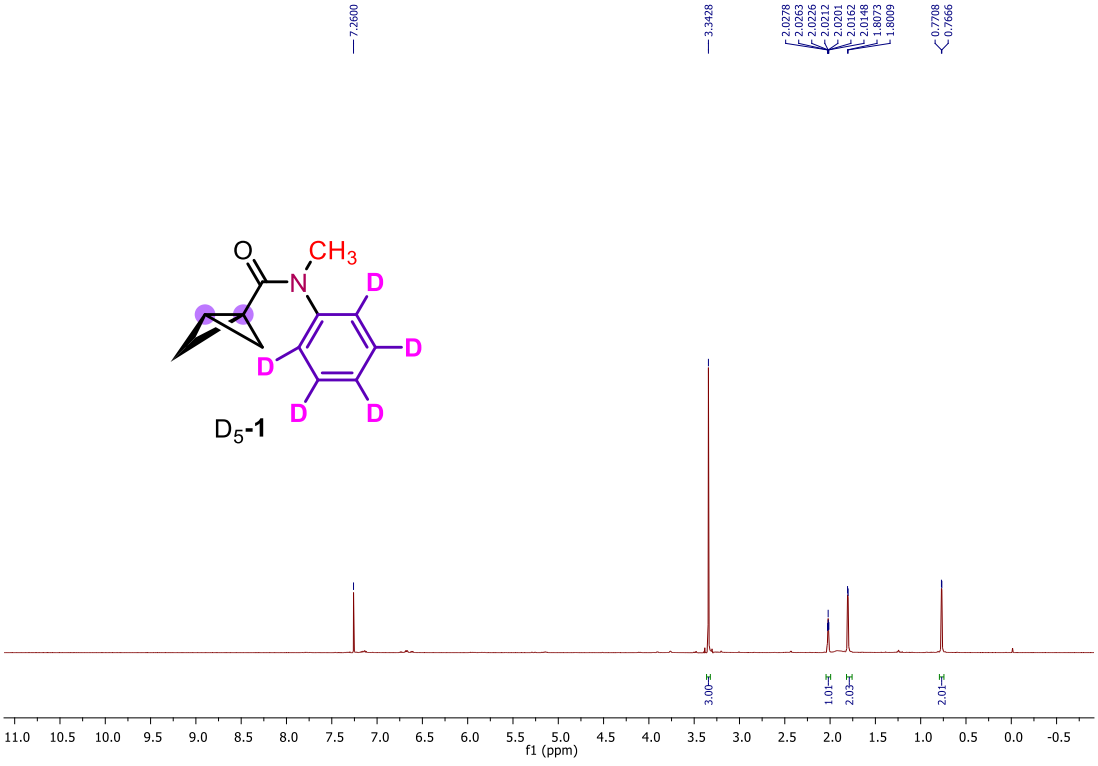


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

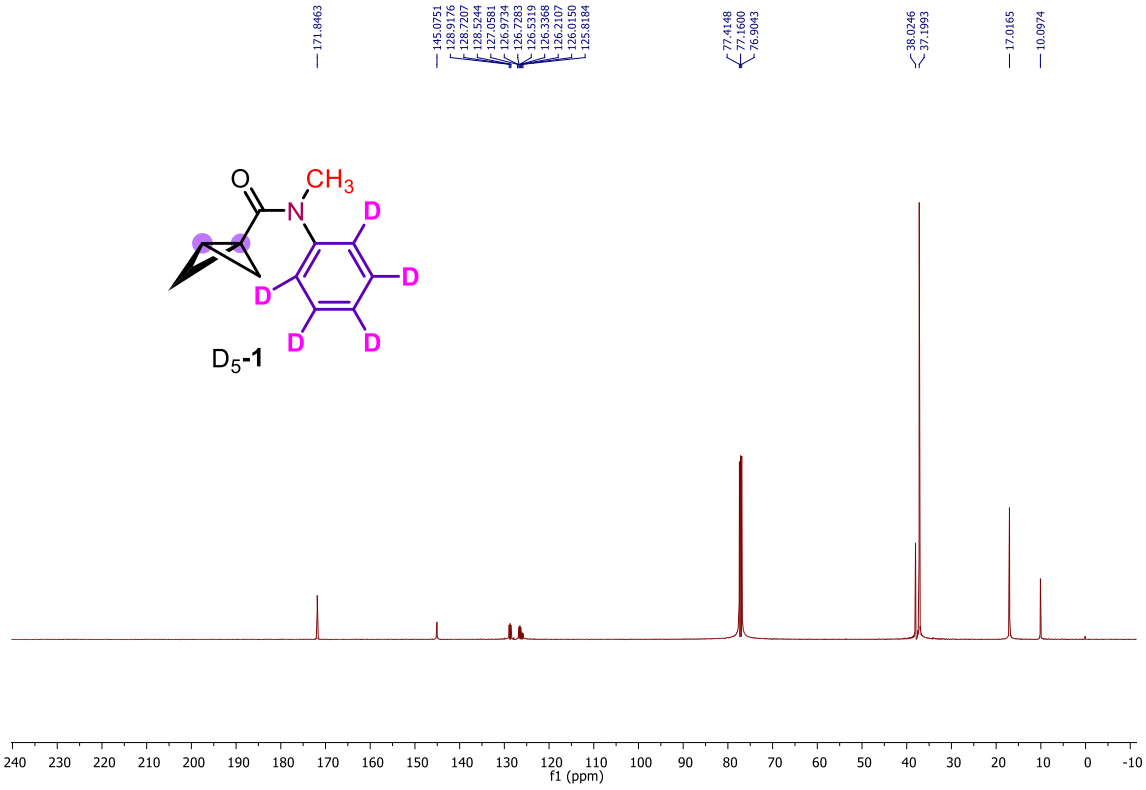


N-methyl-*N*-(phenyl-D_5)bicyclo[1.1.0]butane-1-carboxamide (D_5-**1**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

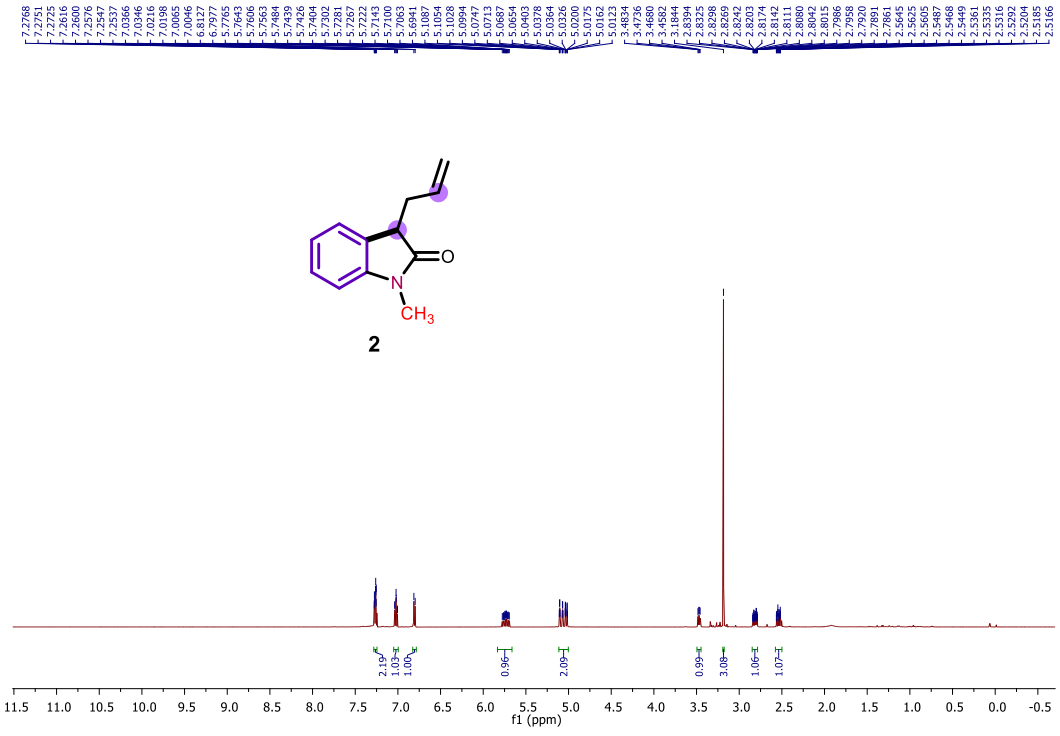


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

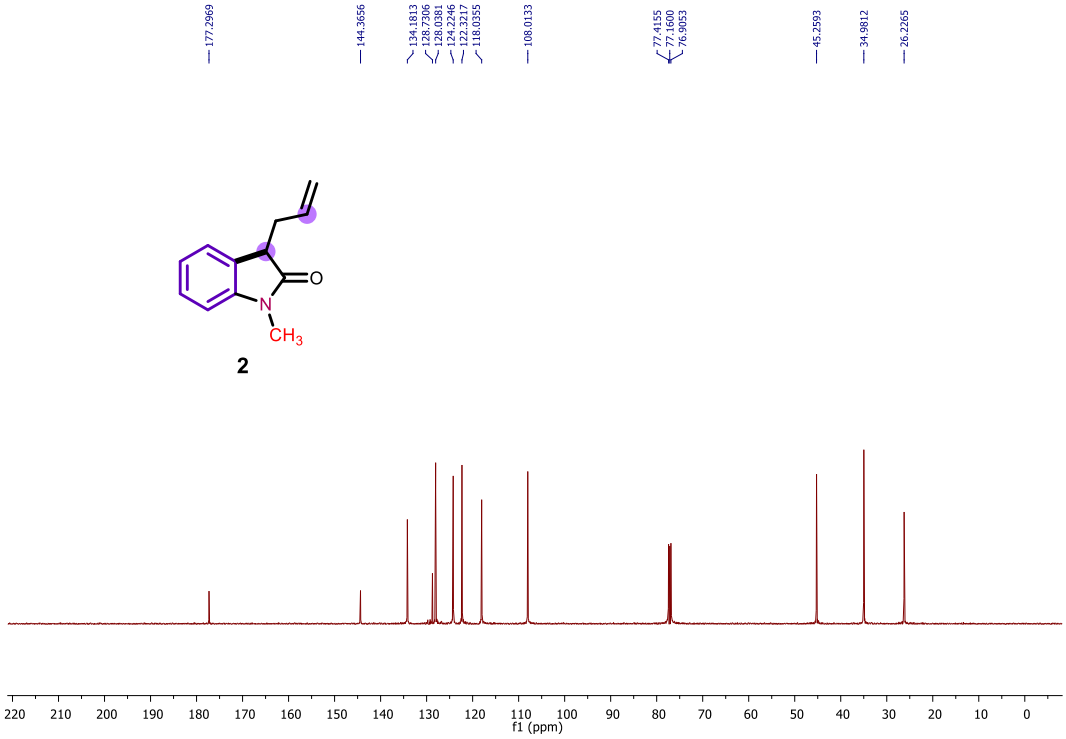


3-Allyl-1-methylindolin-2-one (**2**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

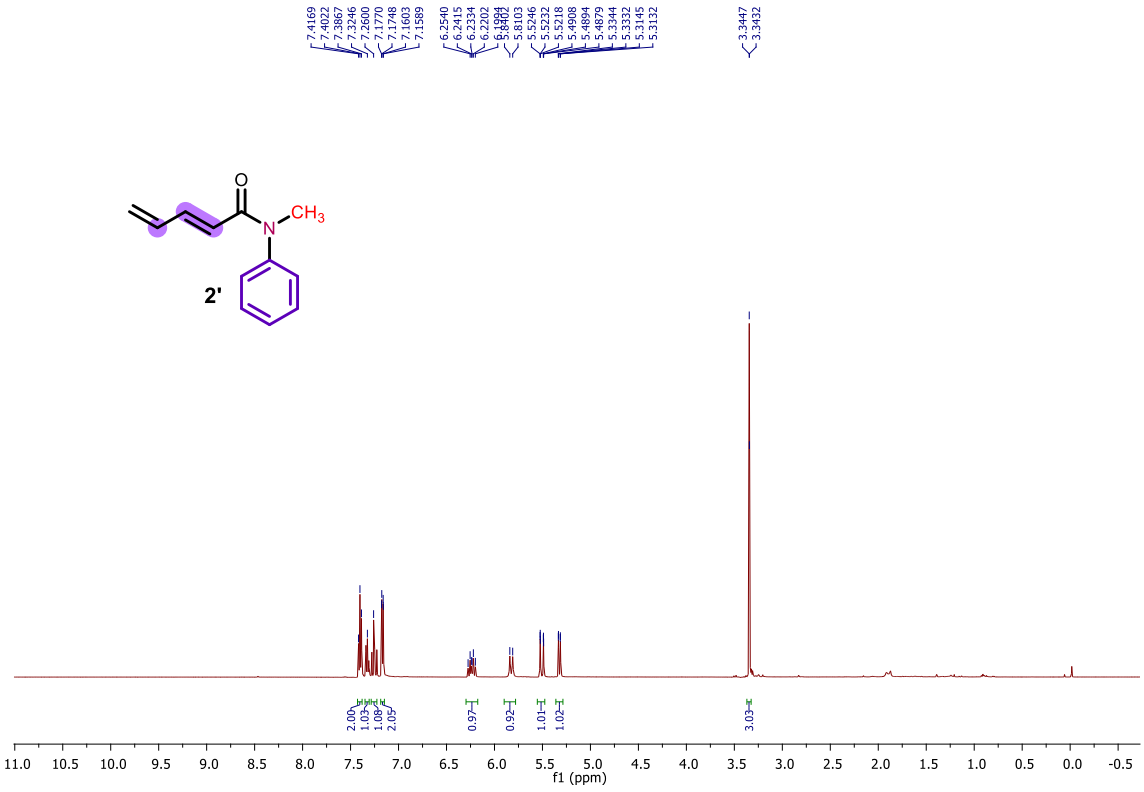


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

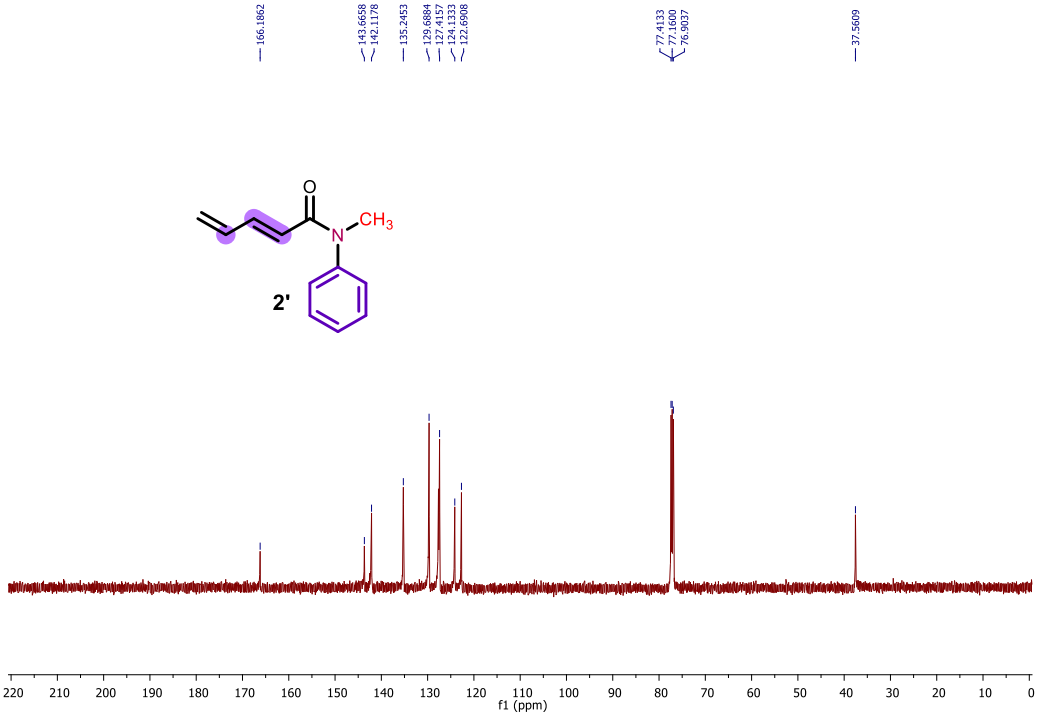


(*E*)-*N*-Methyl-*N*-phenylpenta-2,4-dienamide (**2'**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

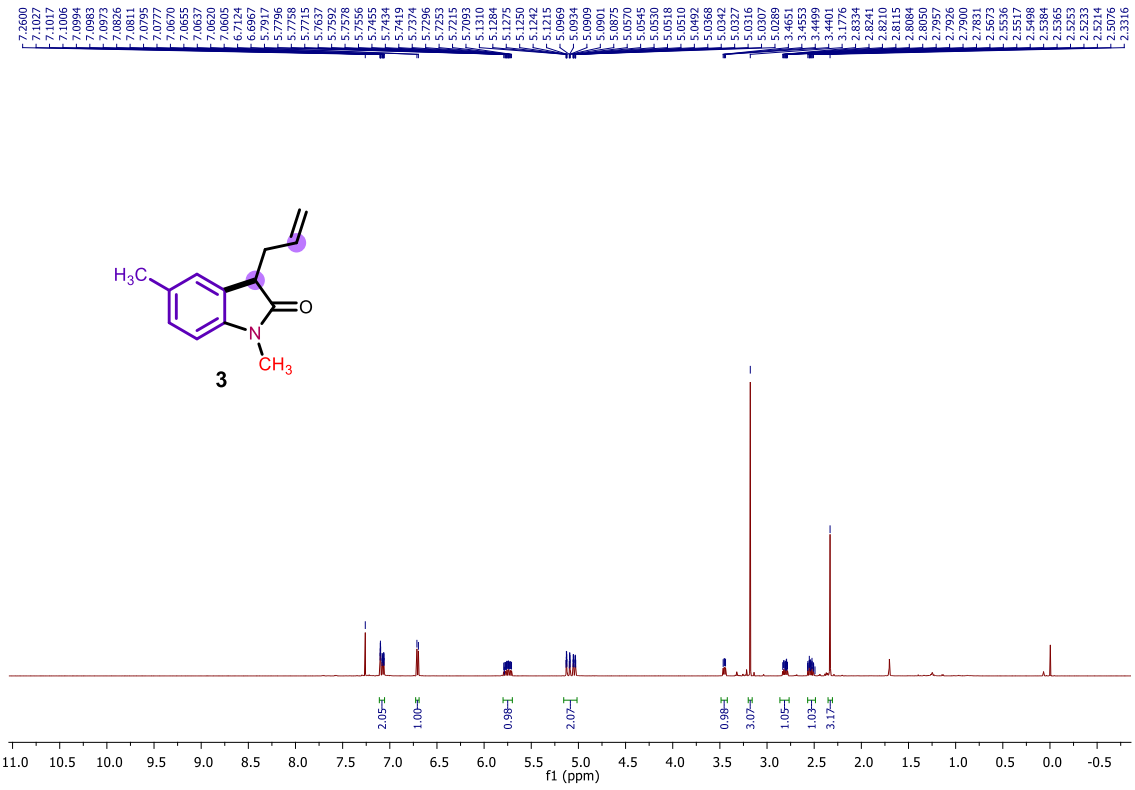


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

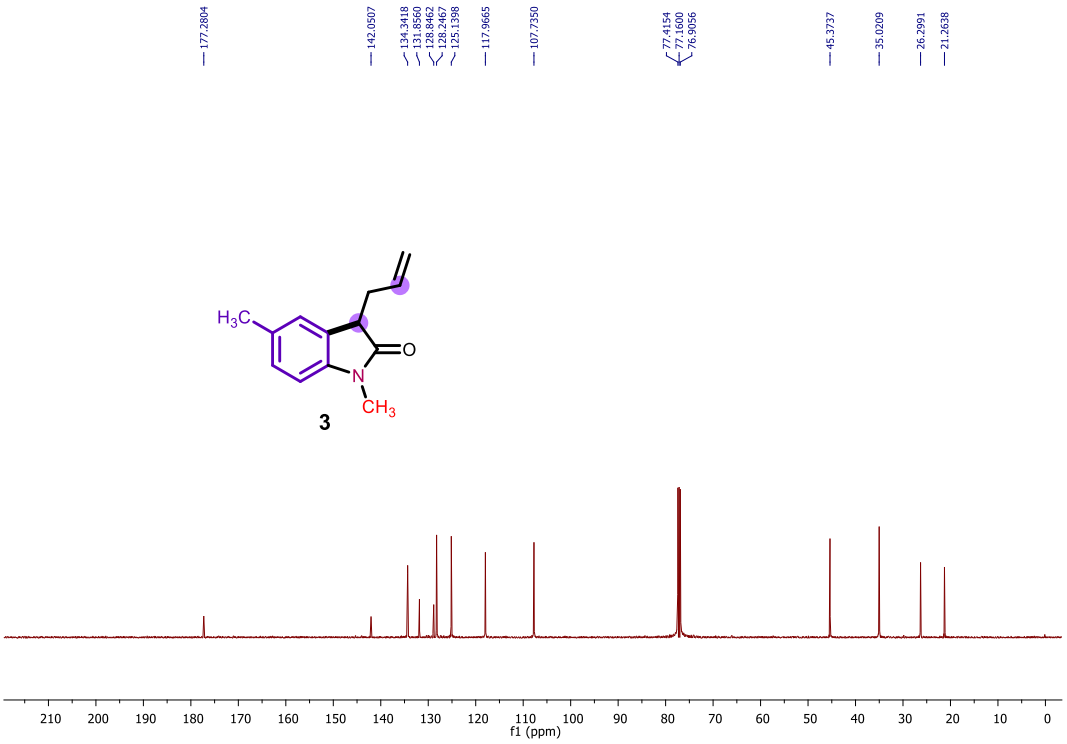


3-Allyl-1,5-dimethylindolin-2-one (**3**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

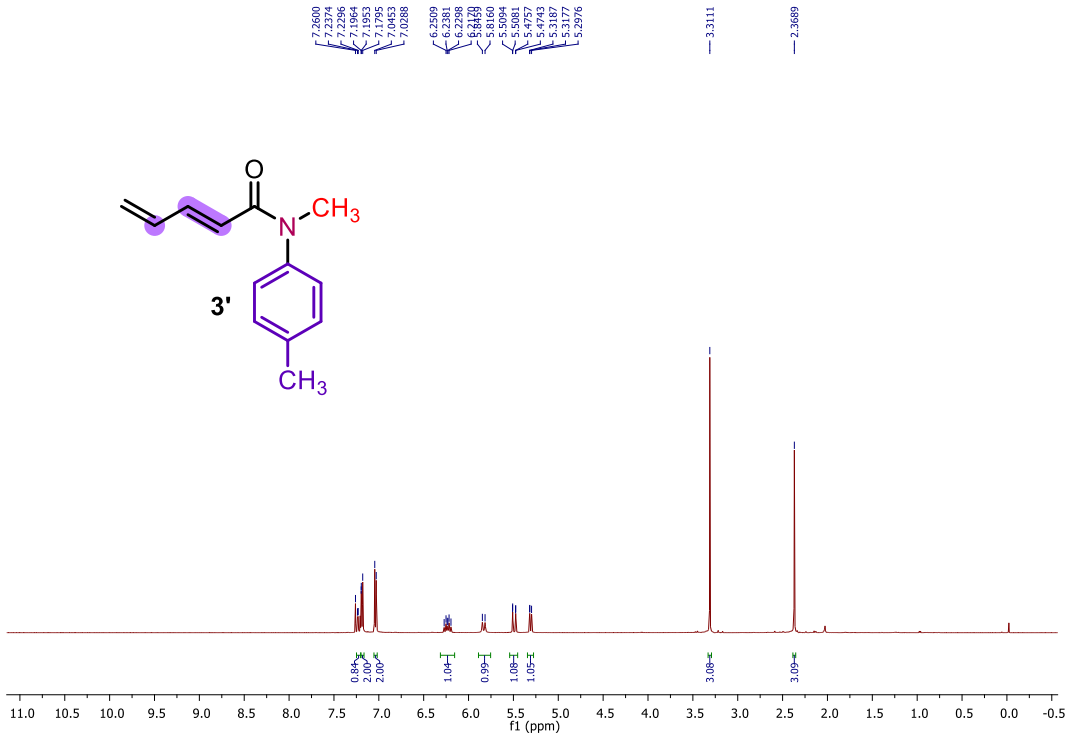


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

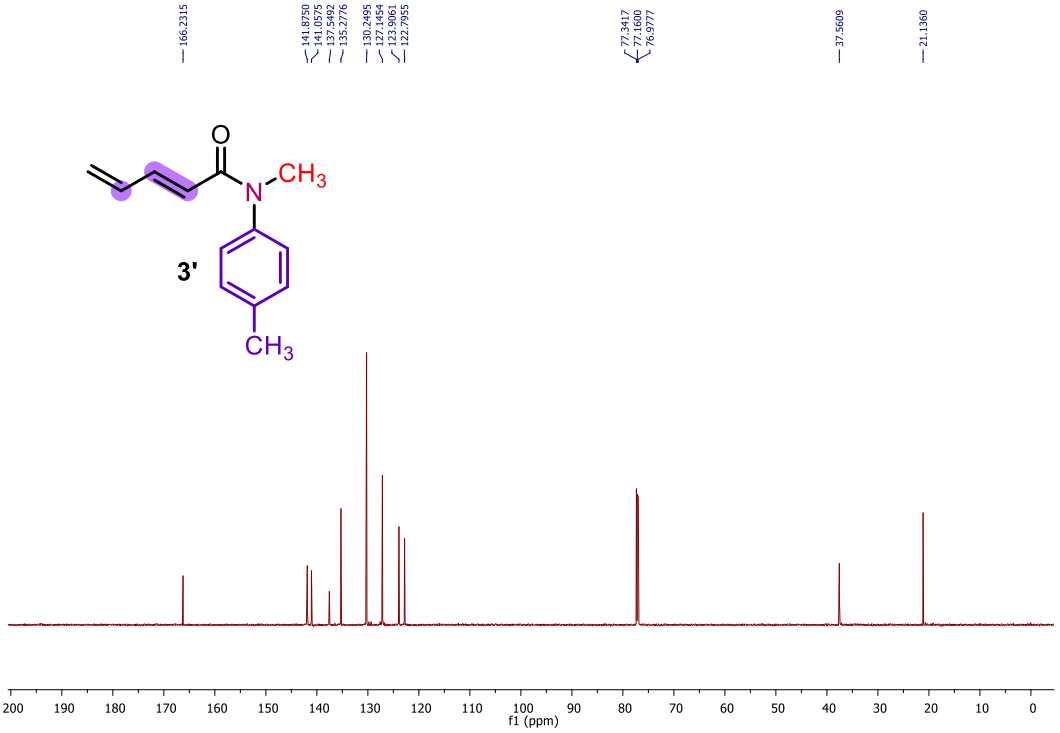


(*E*)-*N*-Methyl-*N*-(p-tolyl)penta-2,4-dienamide (**3'**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

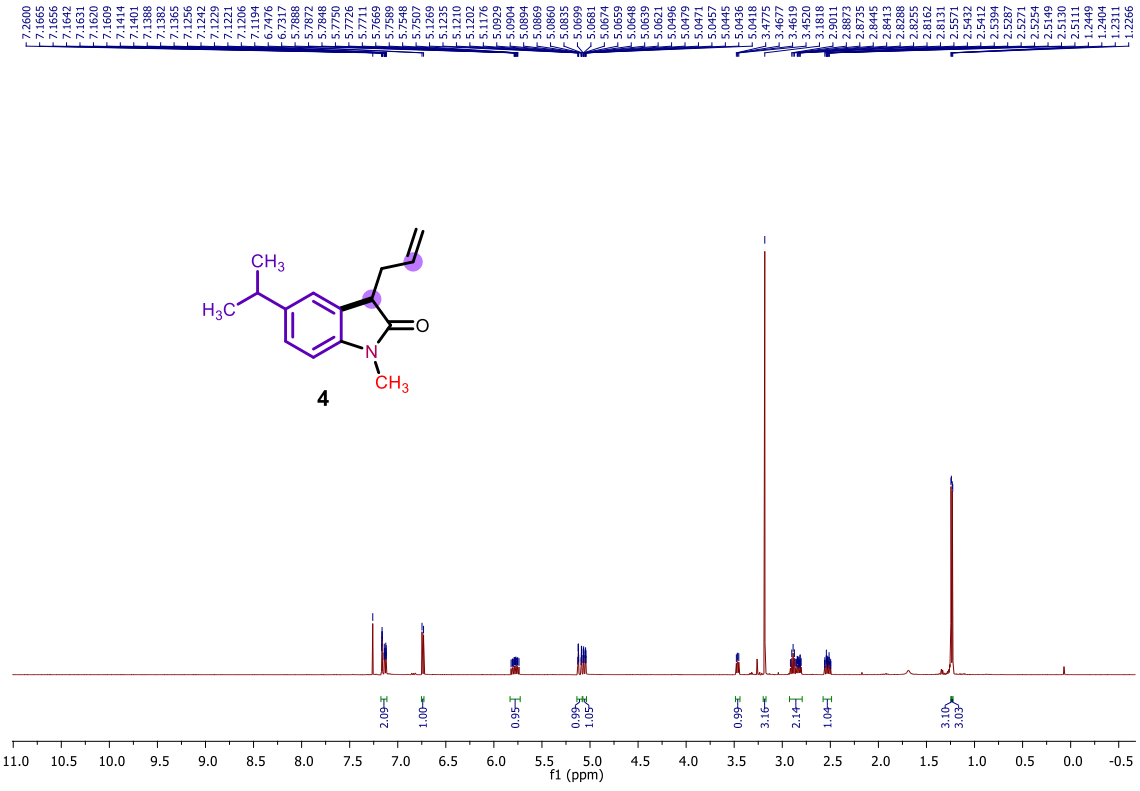


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

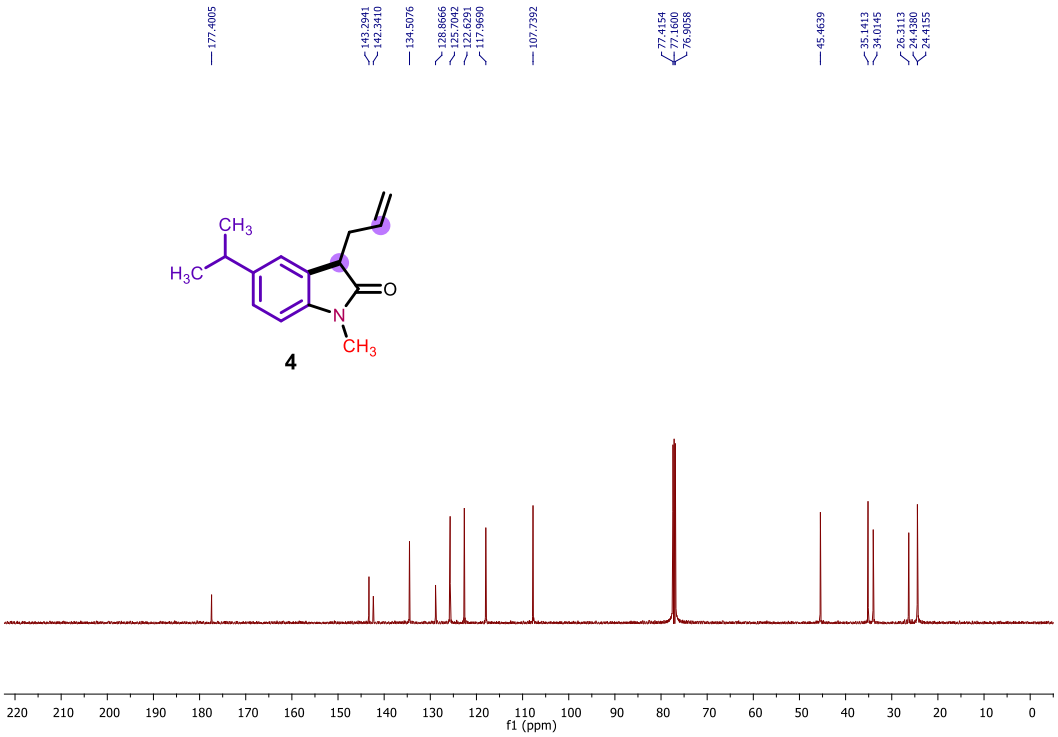


3-Allyl-5-isopropyl-1-methylindolin-2-one (**4**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

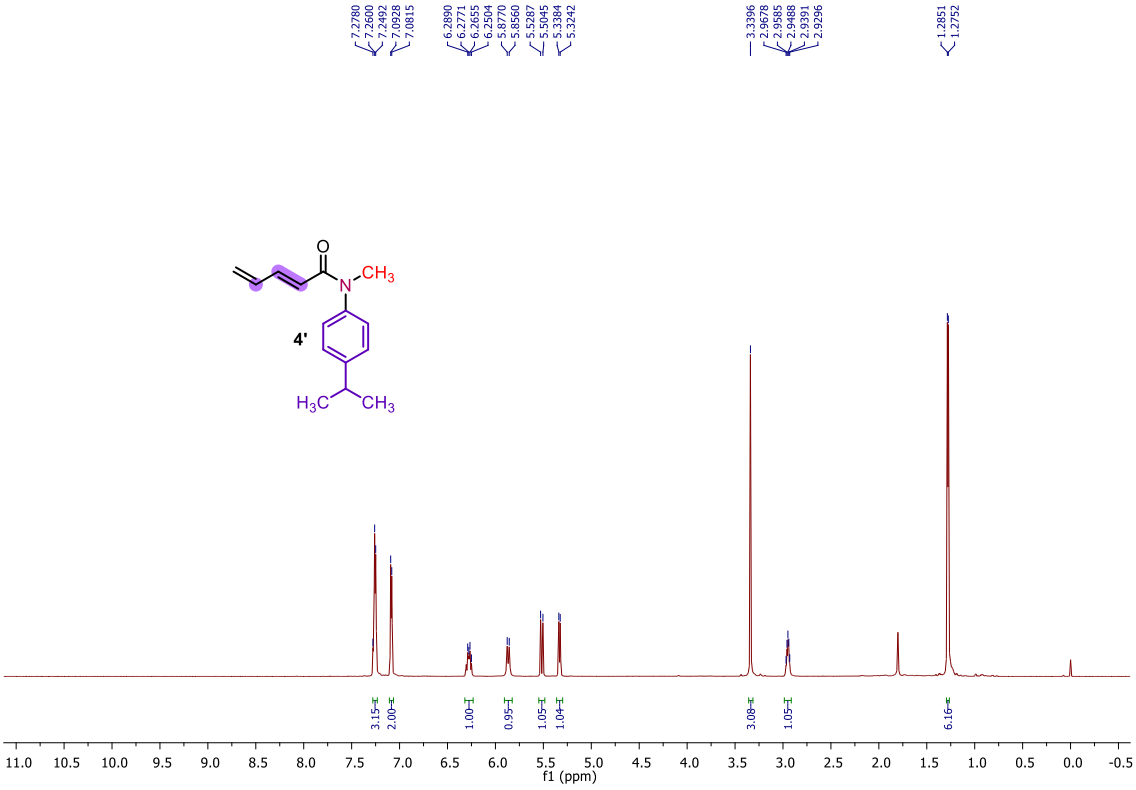


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

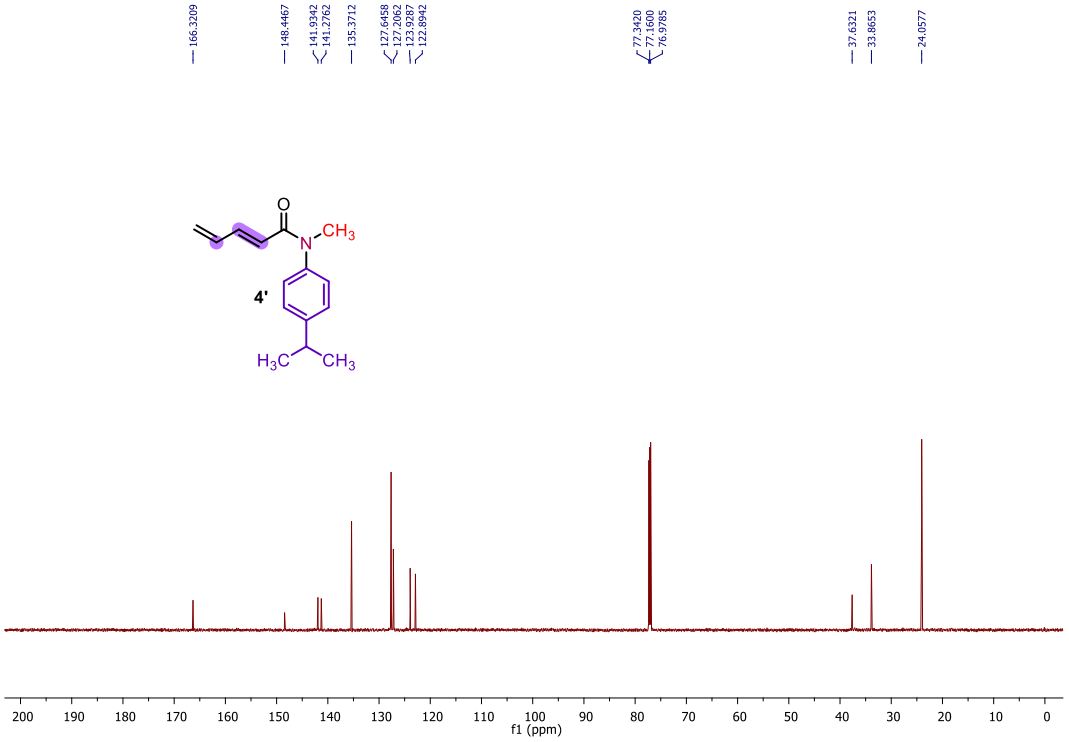


(*E*)-*N*-(4-isopropylphenyl)-*N*-methylpenta-2,4-dienamide (**4'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

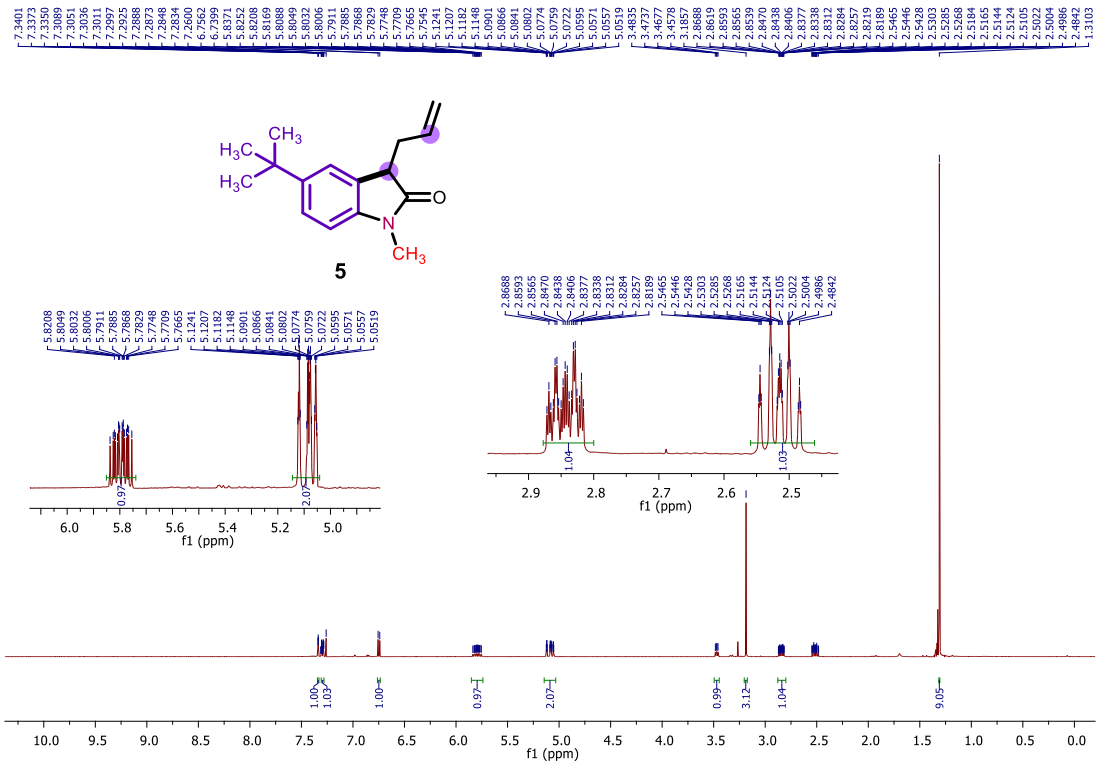


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

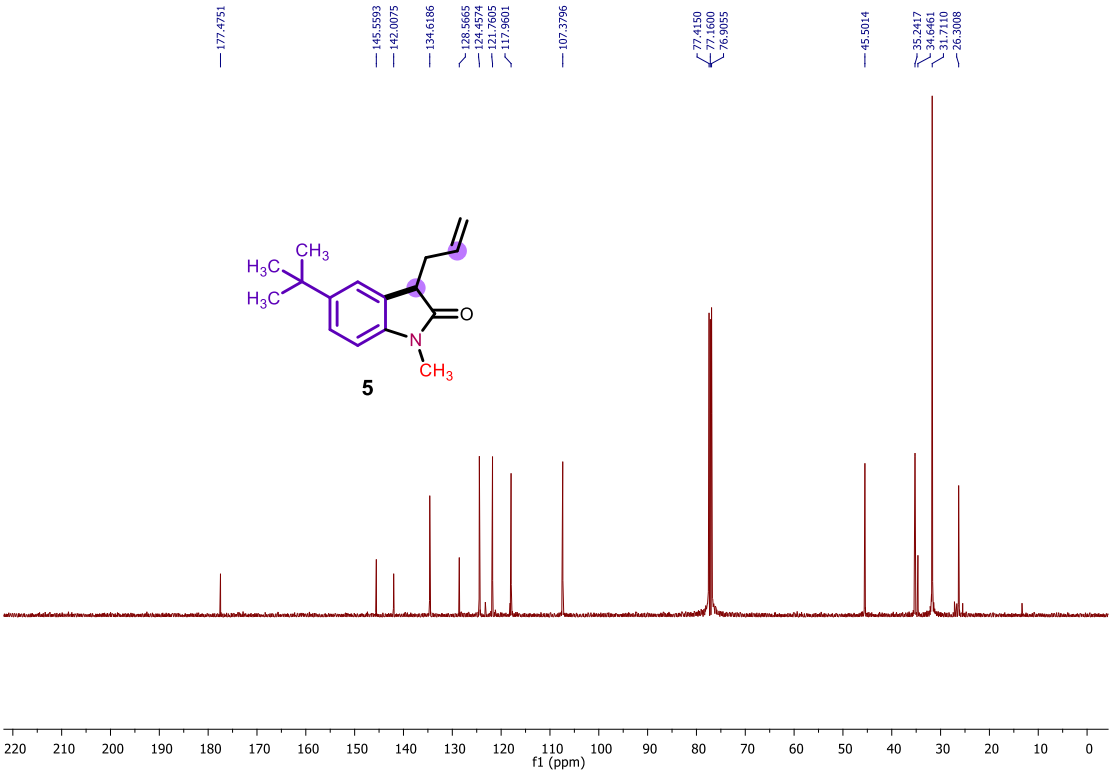


3-Allyl-5-(tert-butyl)-1-methylindolin-2-one (**5**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

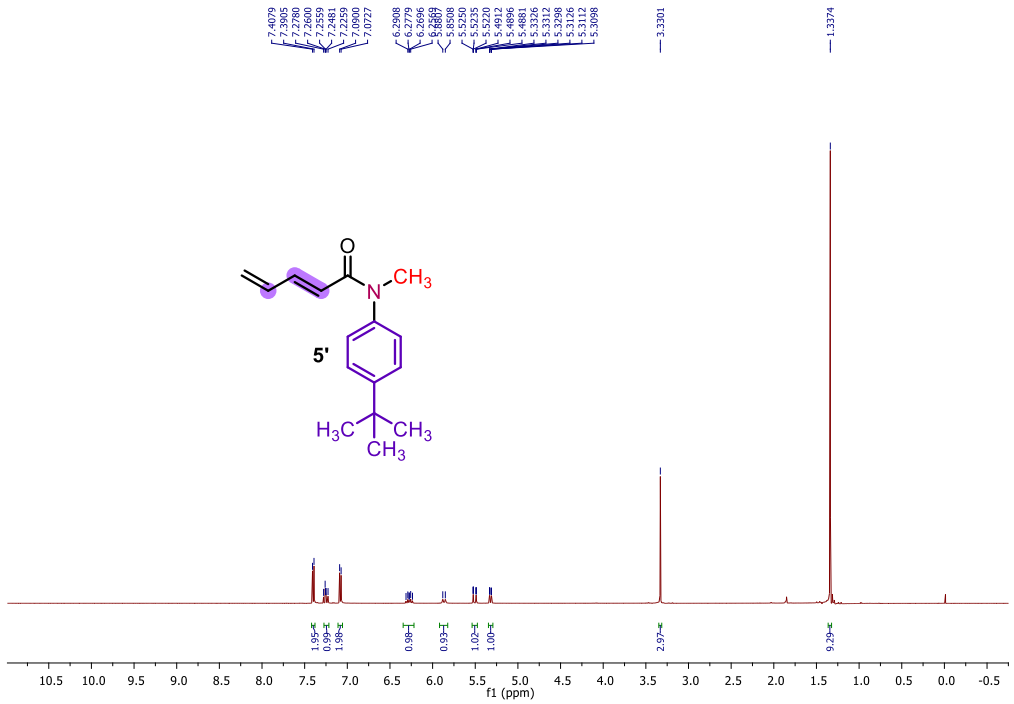


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

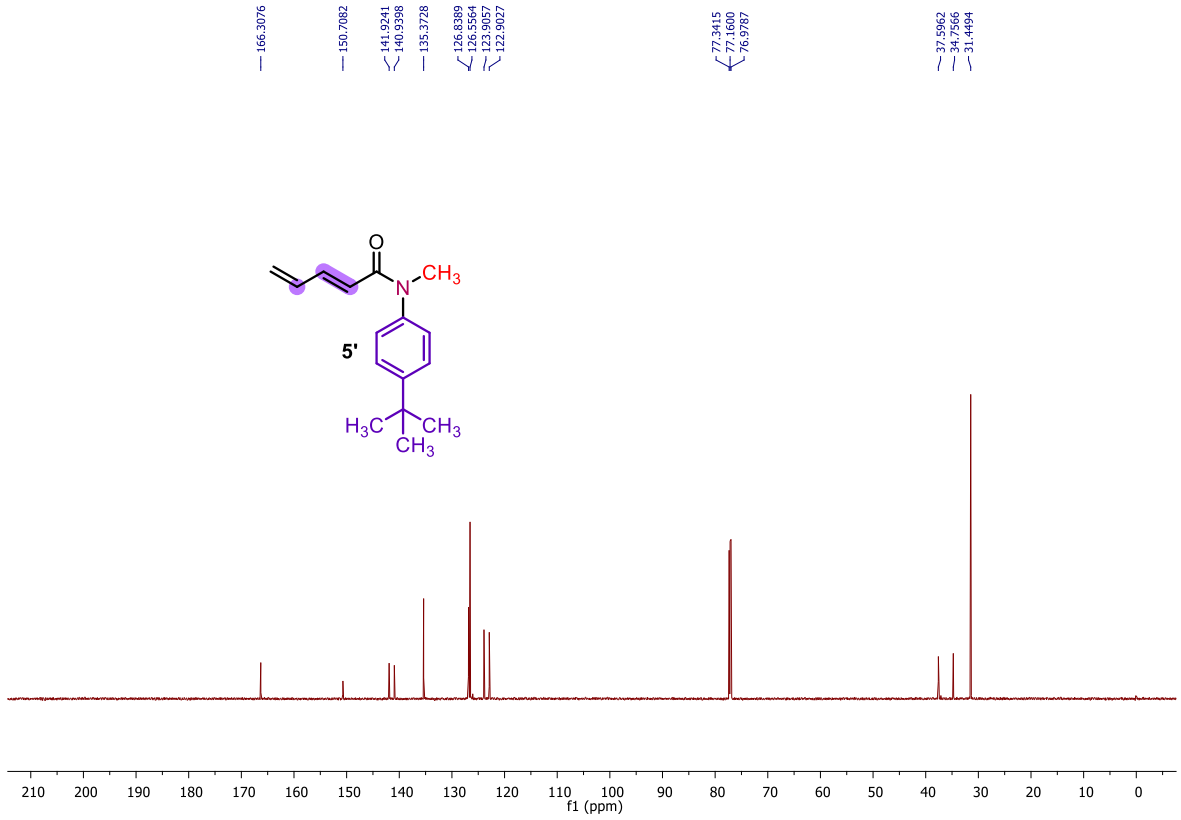


(*E*)-*N*-(4-(tert-butyl)phenyl)-*N*-methylpenta-2,4-dienamide (**5'**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

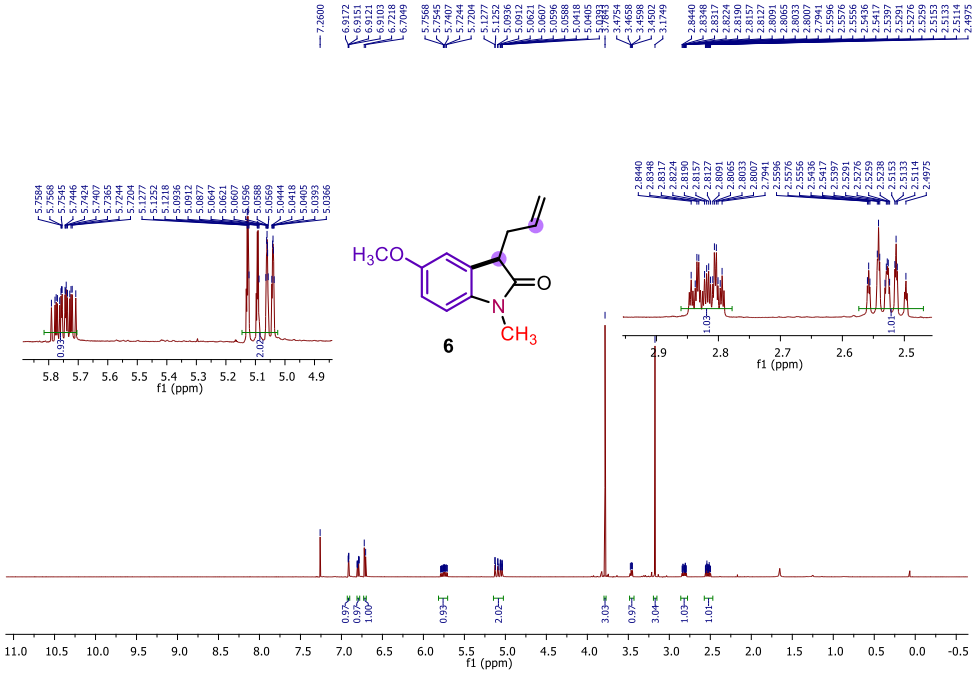


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

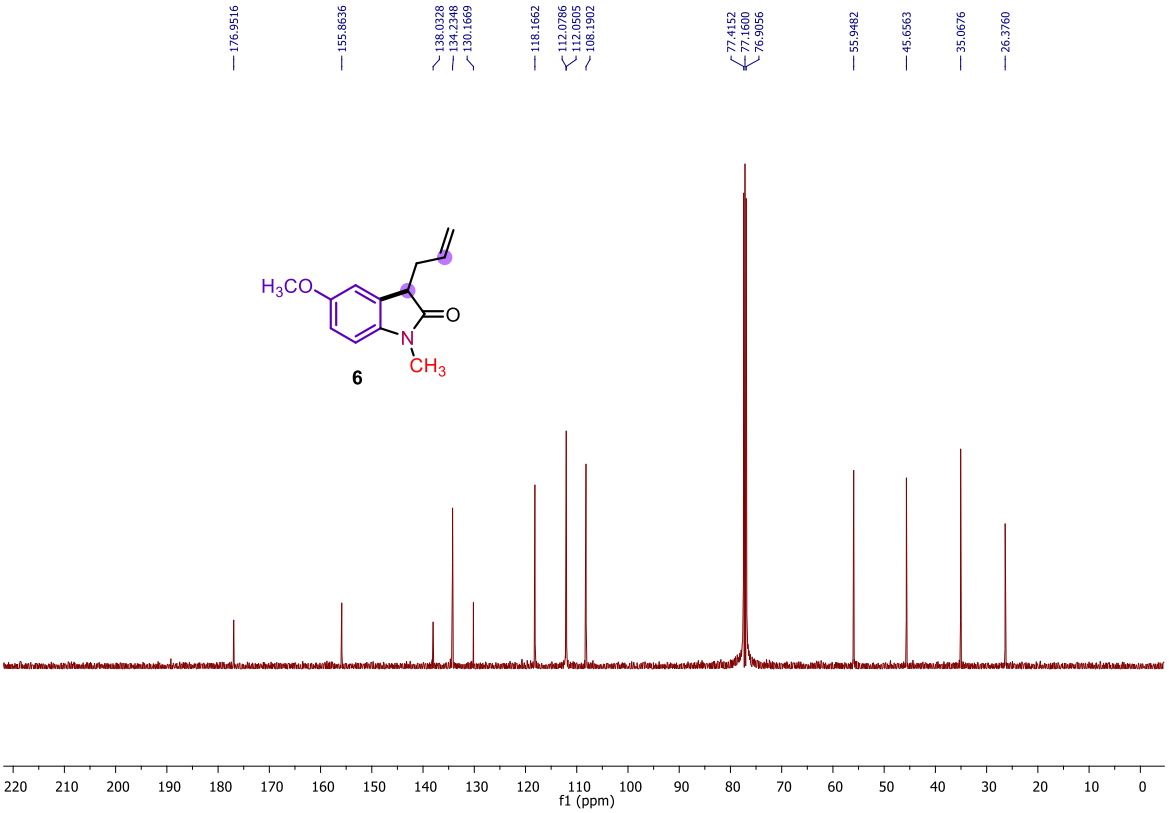


3-Allyl-5-methoxy-1-methylindolin-2-one (**6**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

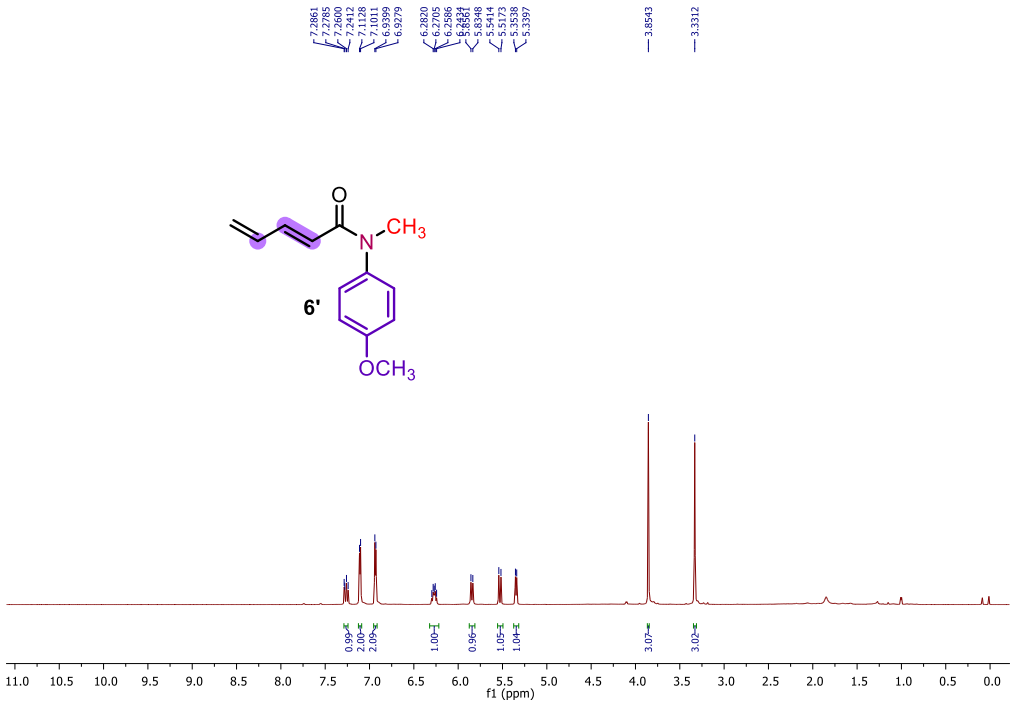


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

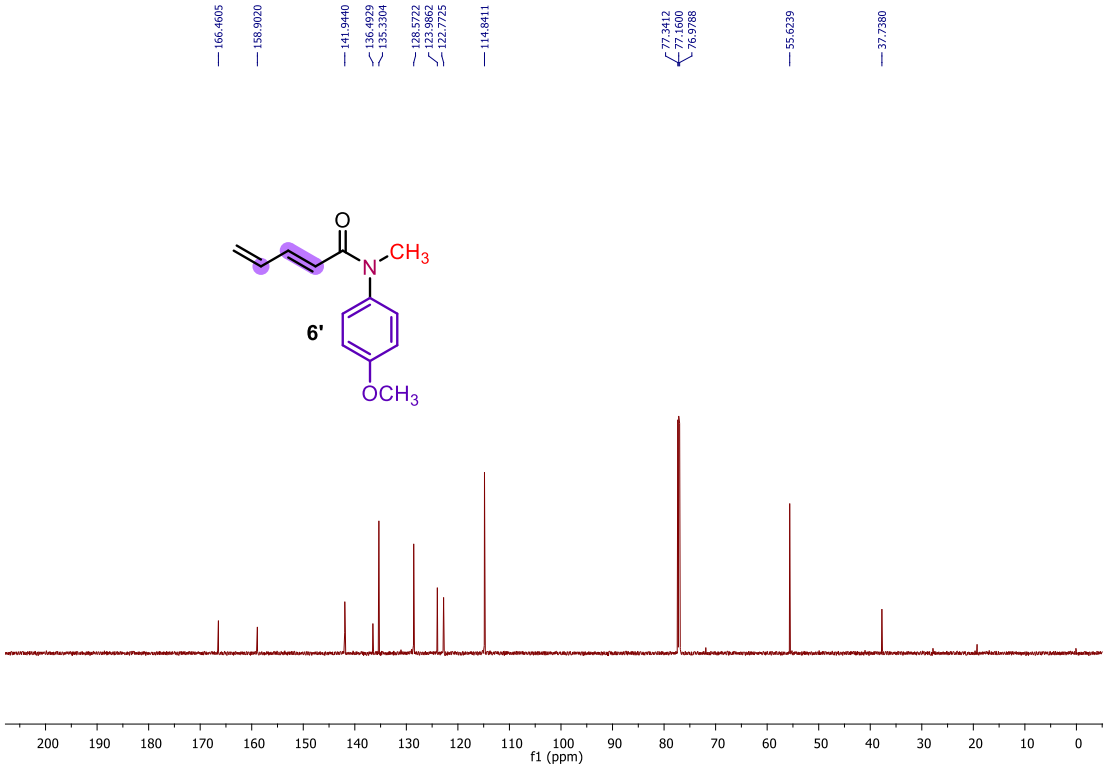


(*E*)-*N*-(4-Methoxyphenyl)-*N*-methylpenta-2,4-dienamide (**6'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

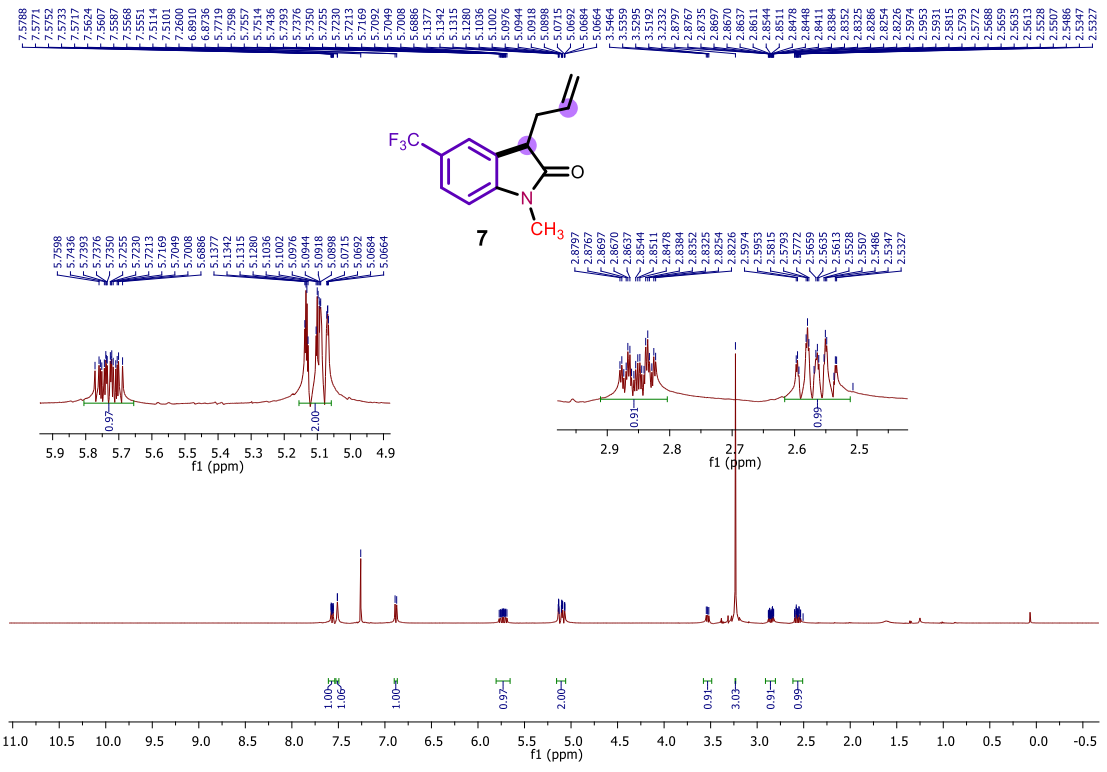


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

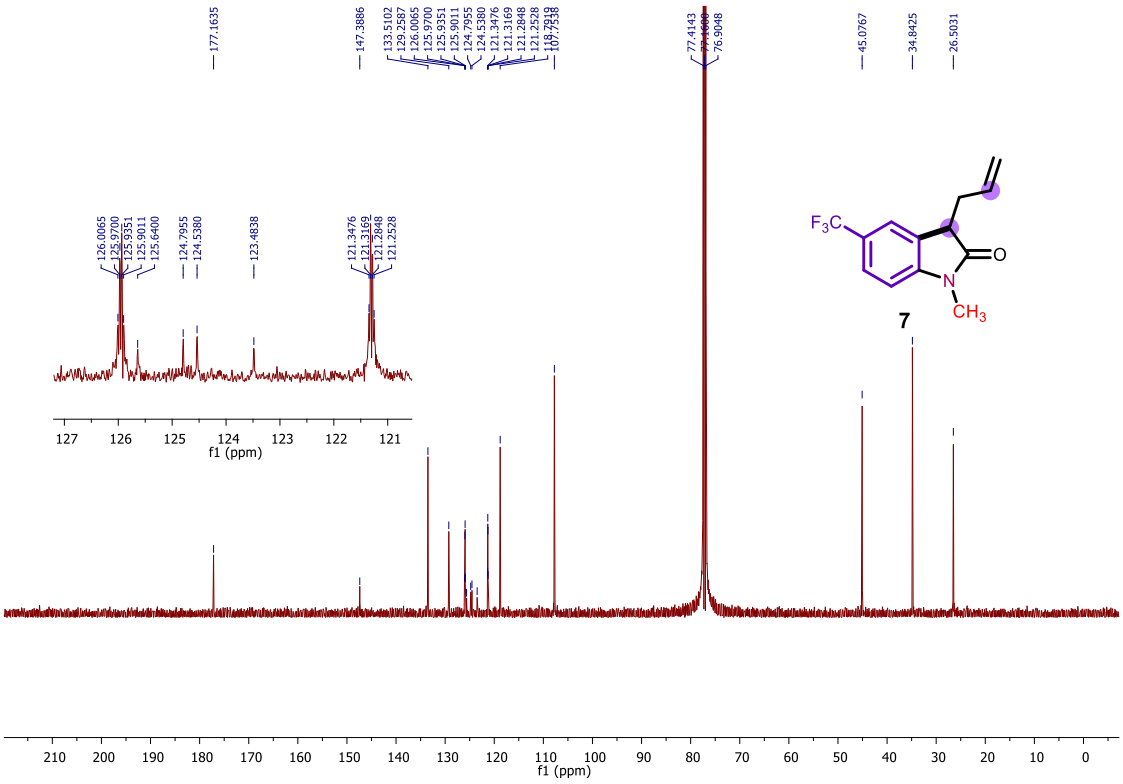


3-Allyl-1-methyl-5-(trifluoromethyl)indolin-2-one (**7**)

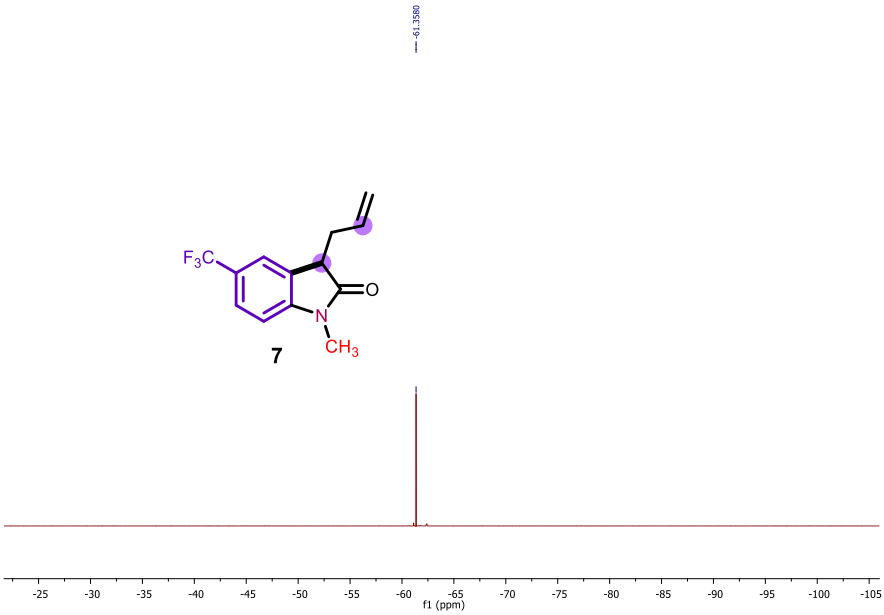
^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)



$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

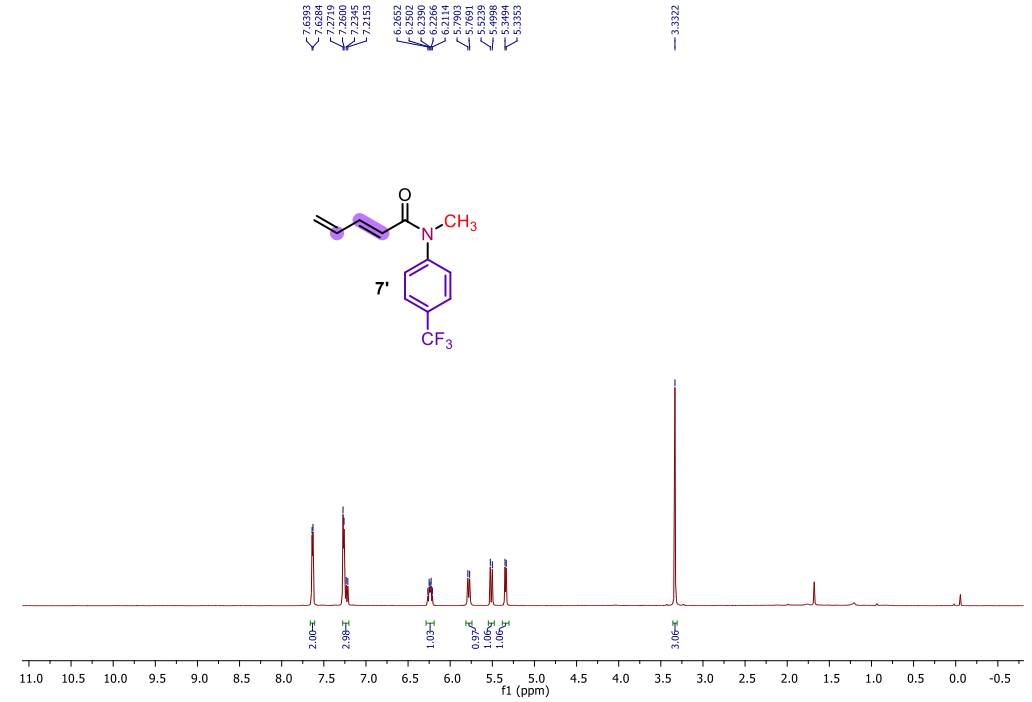


^{19}F NMR (471 MHz, $CDCl_3$, 24 °C)

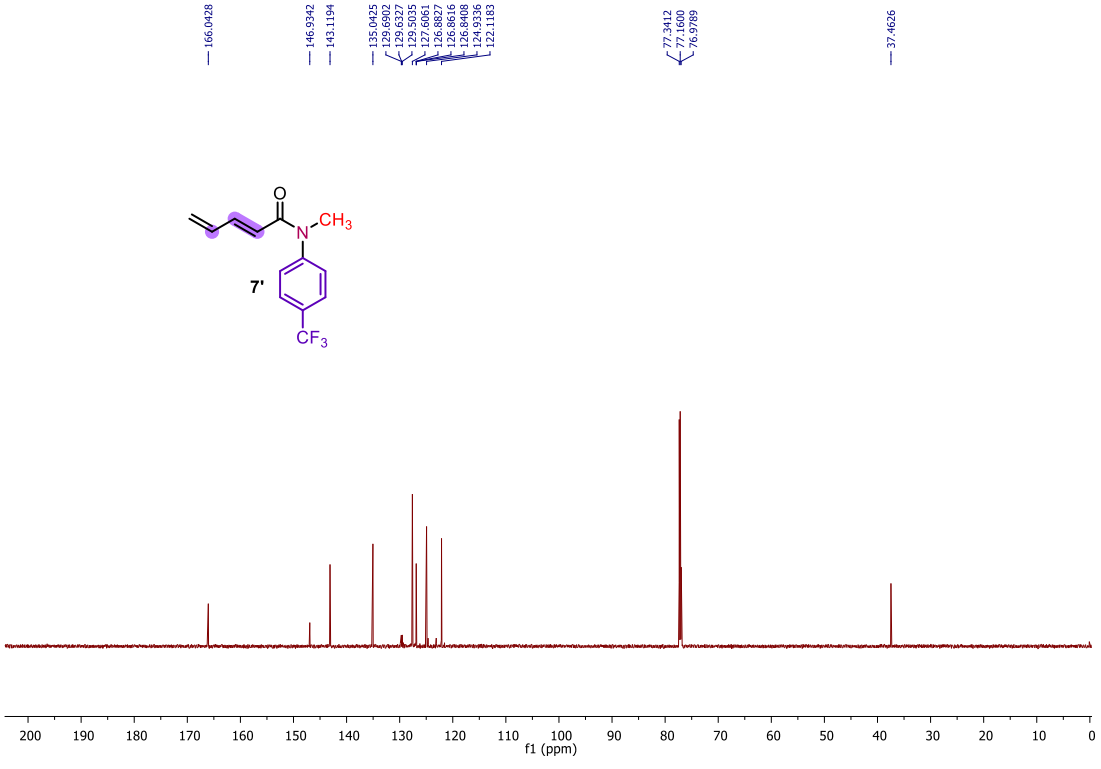


(*E*)-*N*-Methyl-*N*-(4-(trifluoromethyl)phenyl)penta-2,4-dienamide (**7'**)

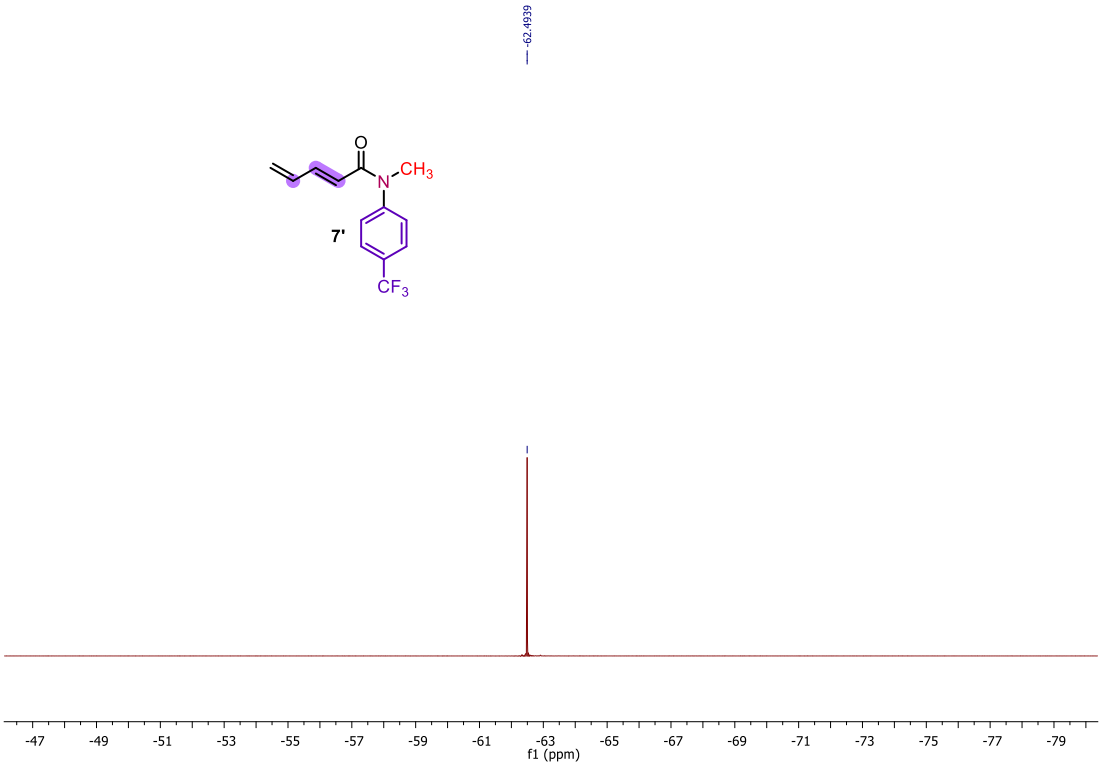
^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)



^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$, 24 °C)

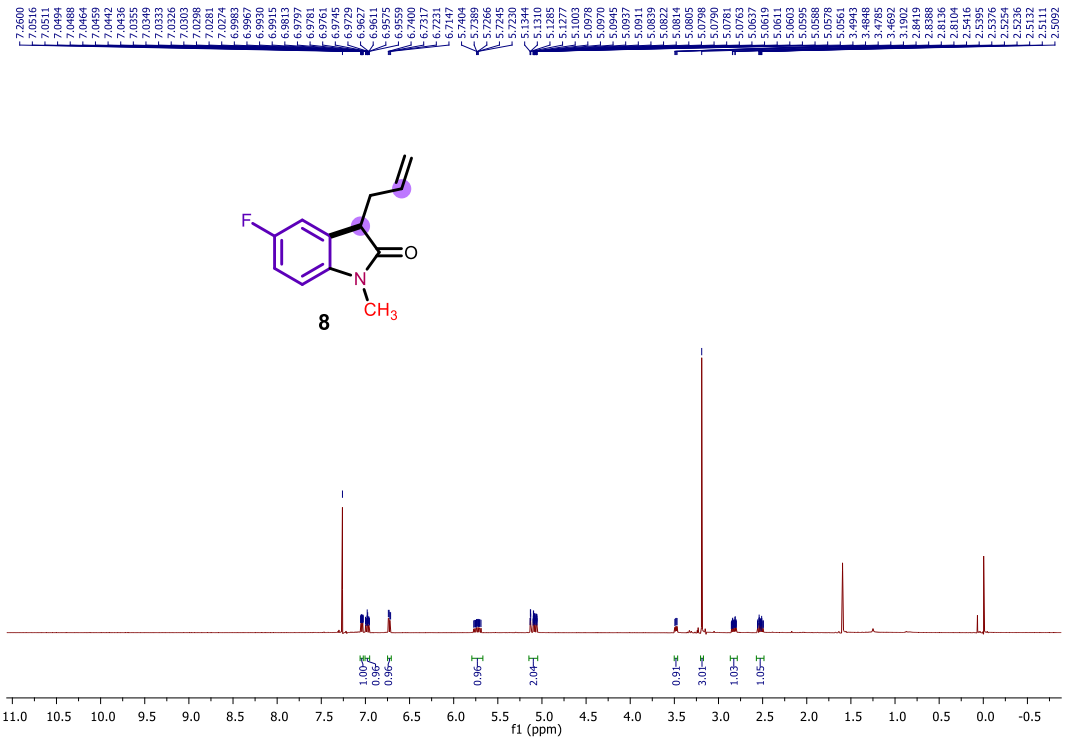


^{19}F NMR (471 MHz, $CDCl_3$, 24 °C)

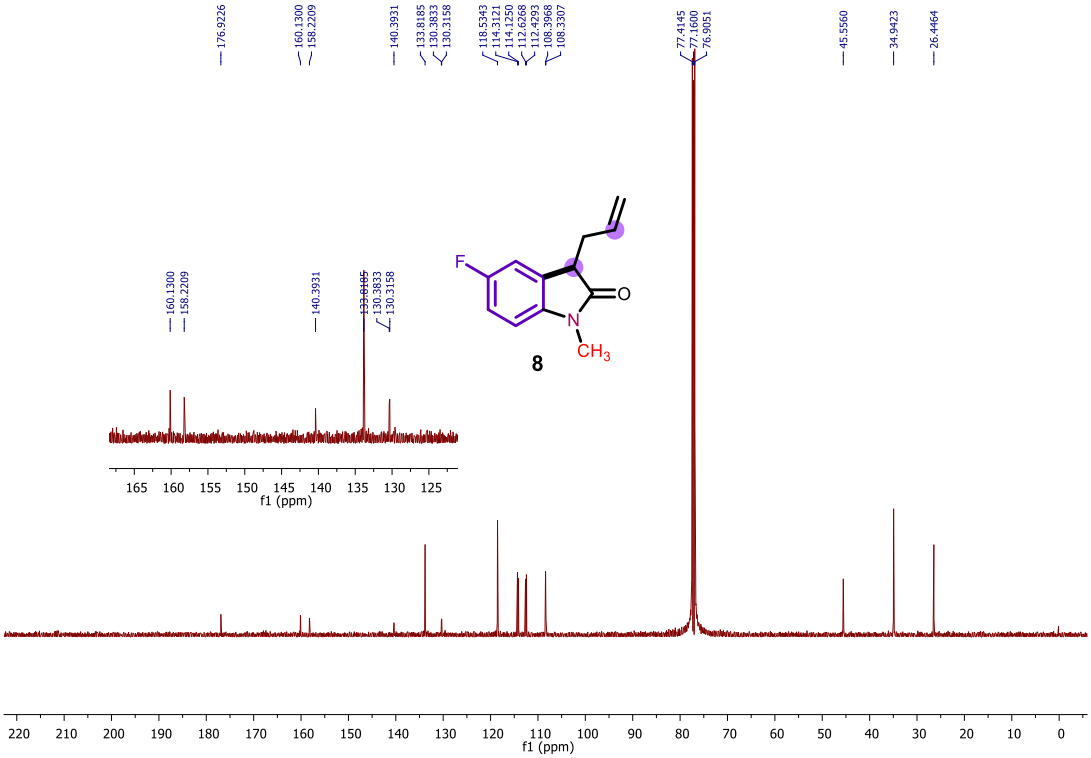


3-Allyl-5-fluoro-1-methylindolin-2-one (**8**)

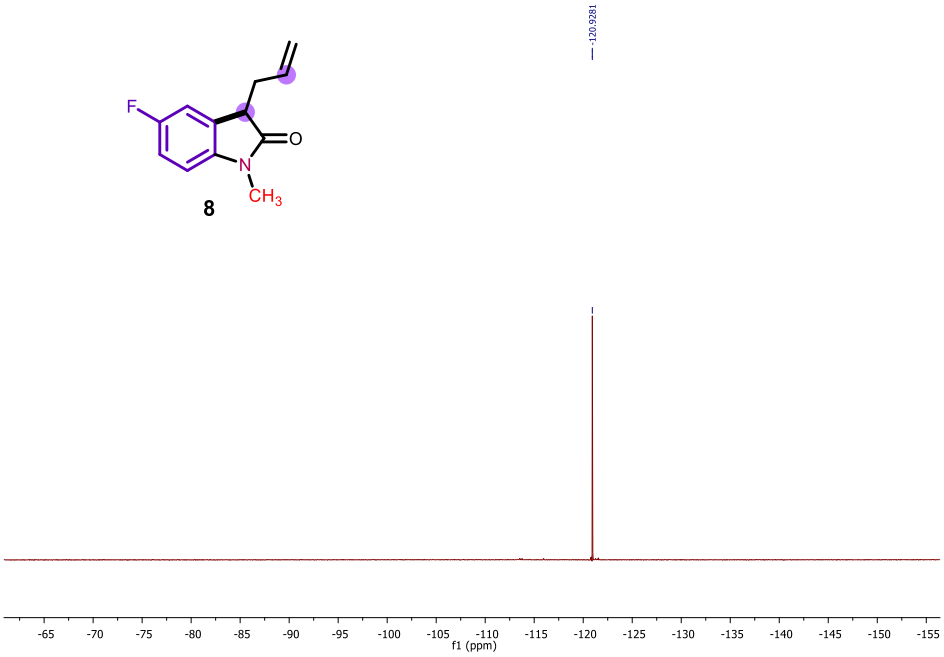
^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)



$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

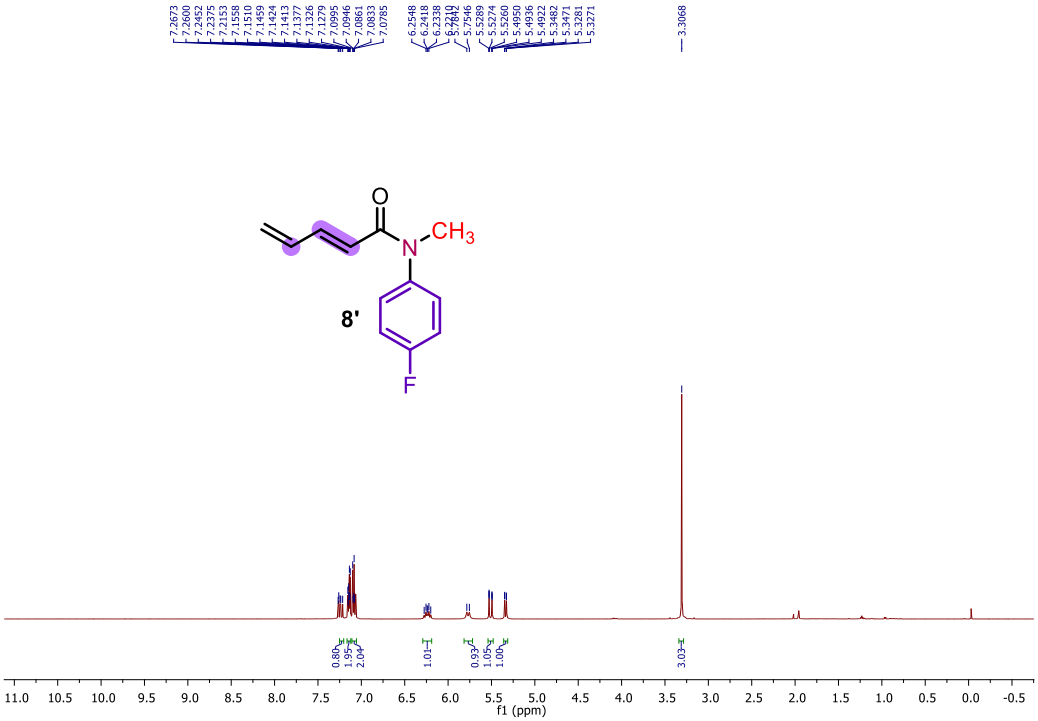


^{19}F NMR (471 MHz, $CDCl_3$, 24 °C)

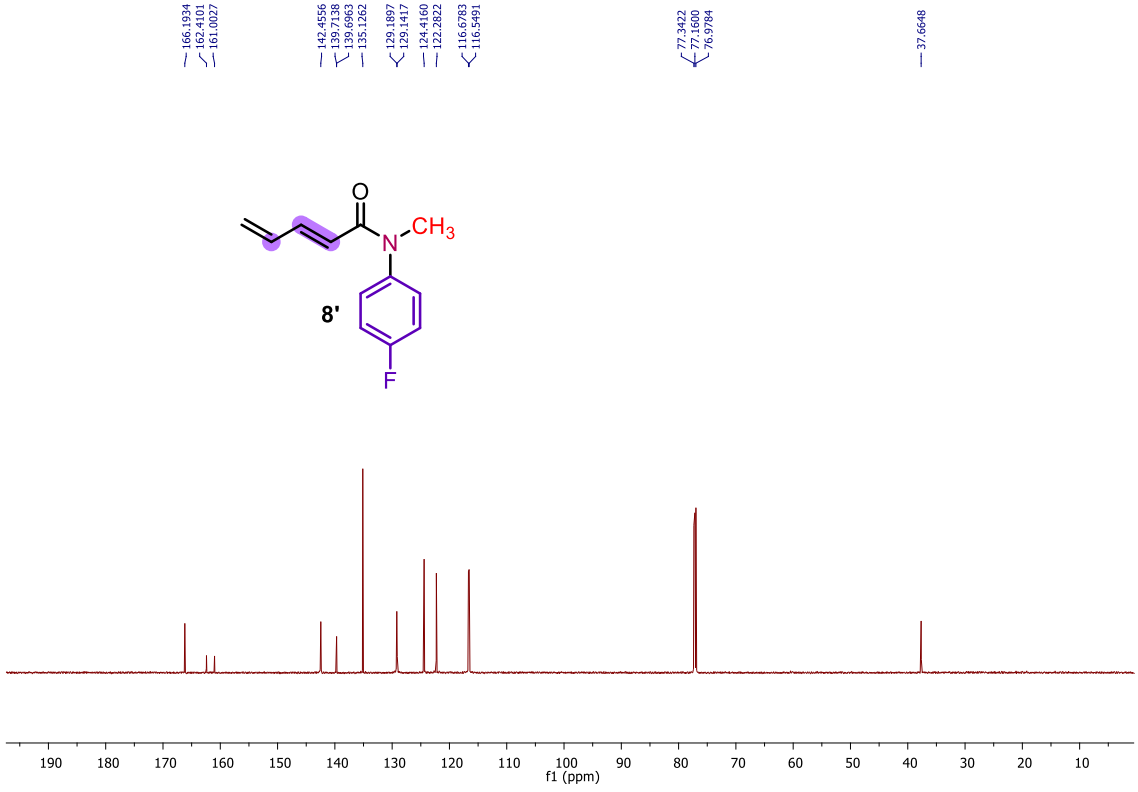


(*E*)-*N*-(4-fluorophenyl)-*N*-methylpenta-2,4-dienamide (**8'**)

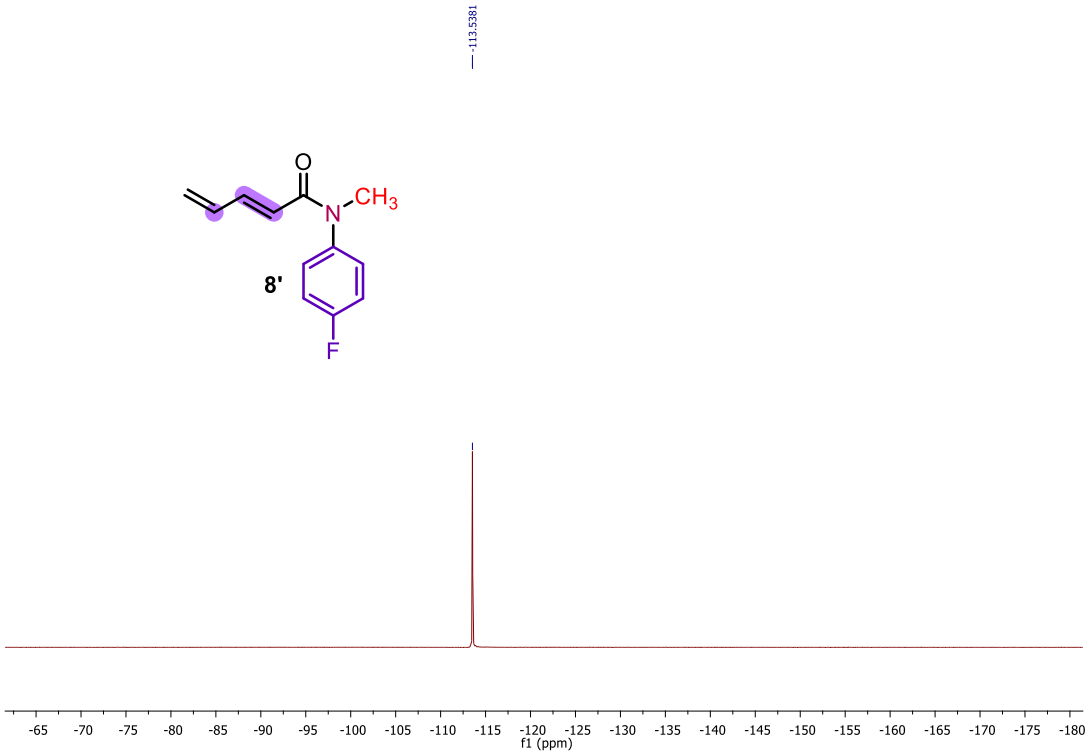
^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)



^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$, 24 °C)

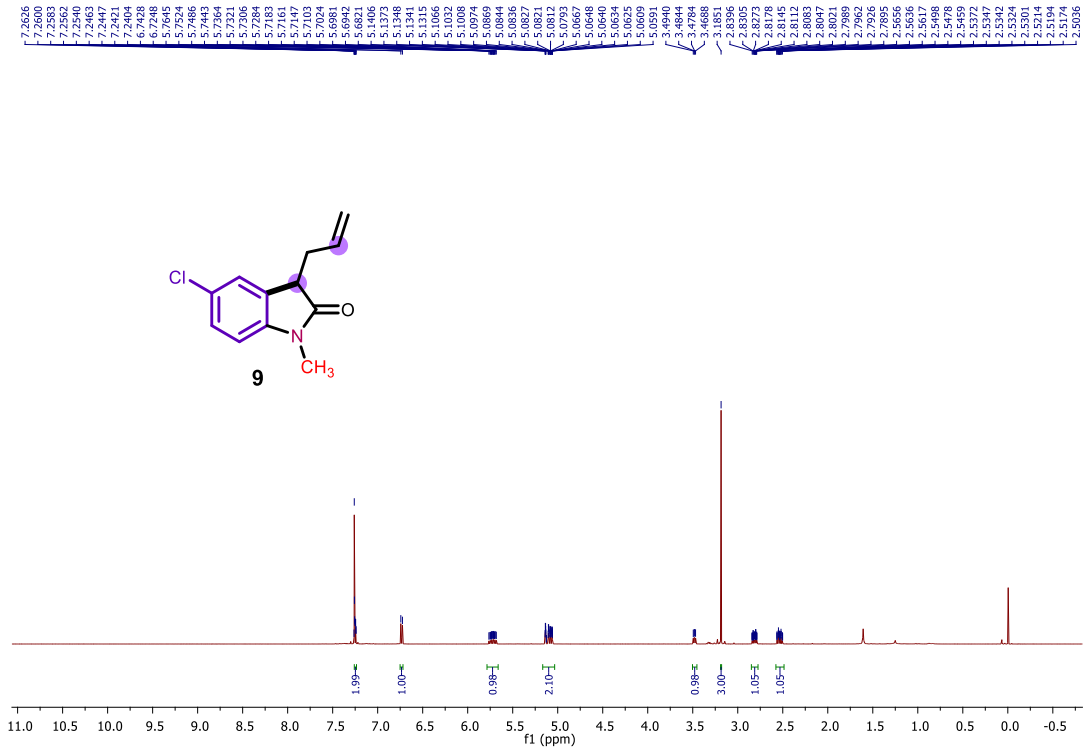


^{19}F NMR (471 MHz, $CDCl_3$, 24 °C)

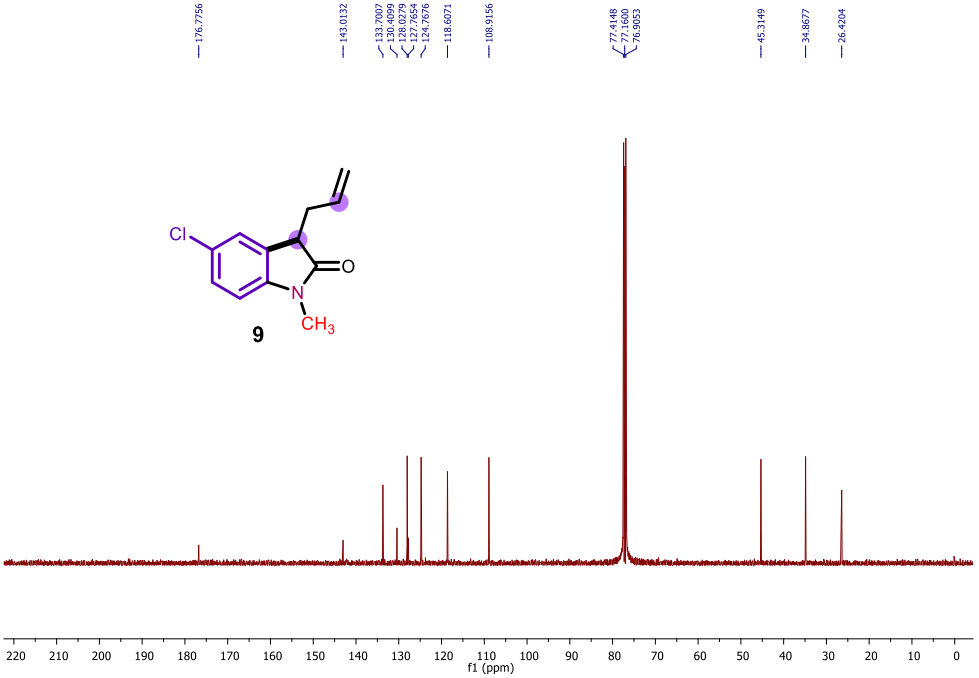


3-Allyl-5-chloro-1-methylindolin-2-one (**9**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

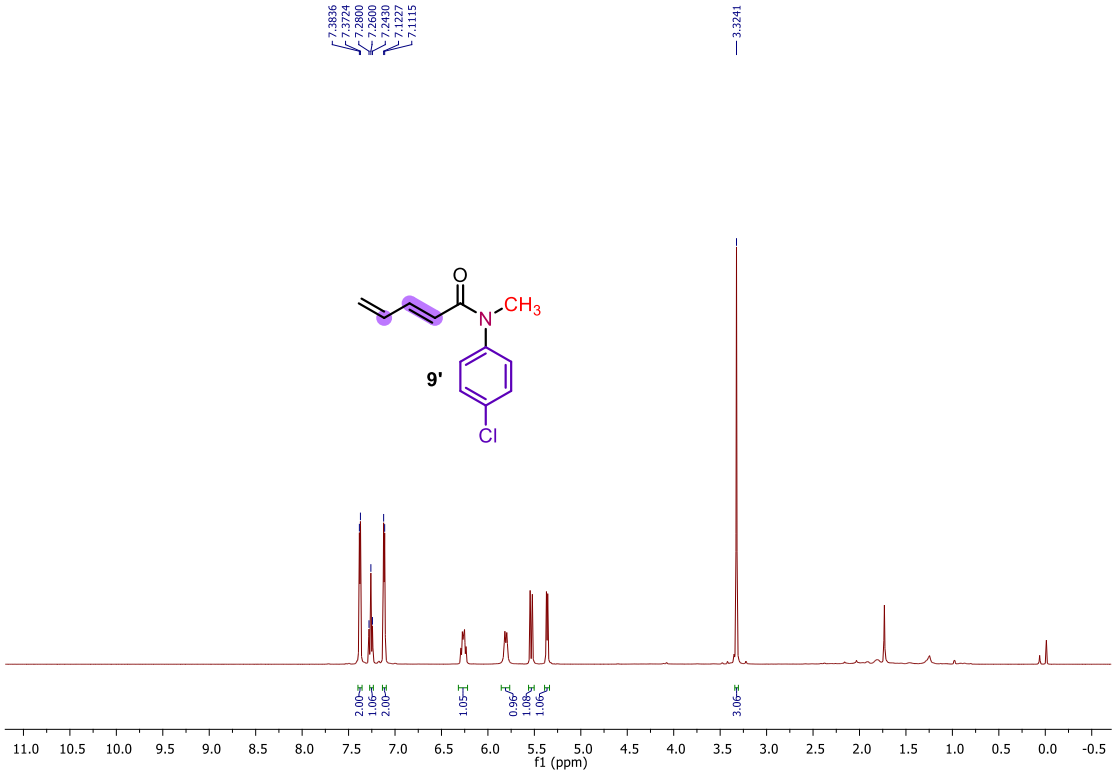


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

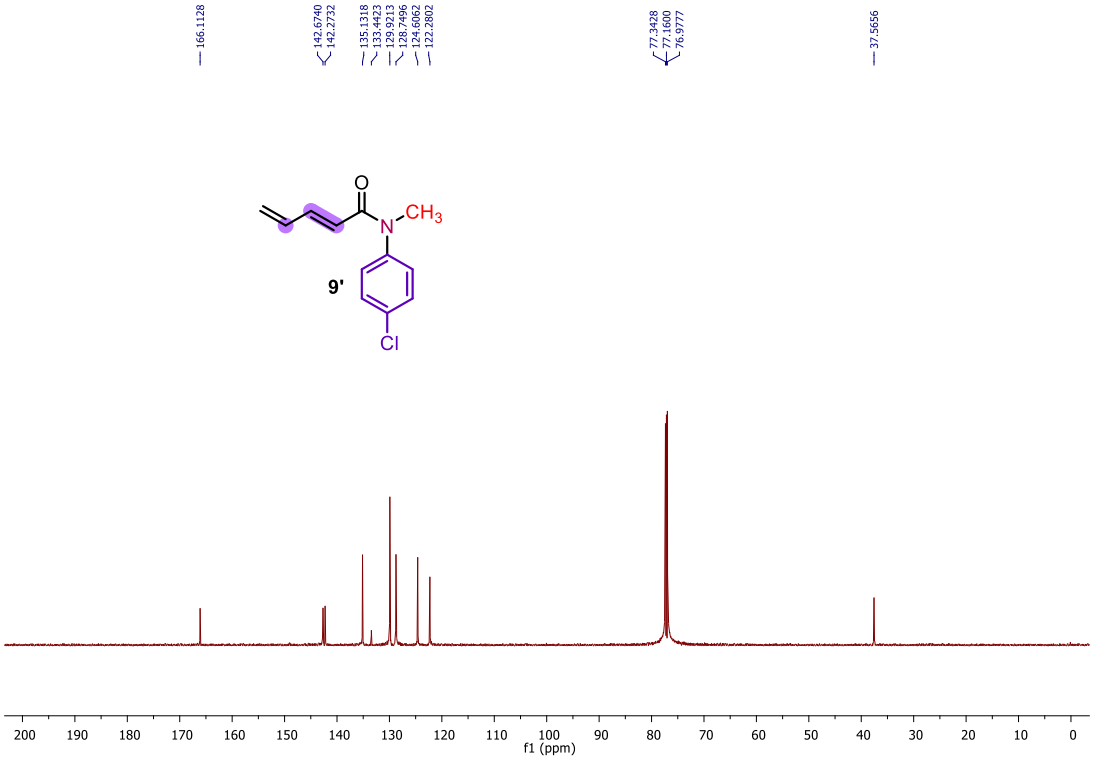


(*E*)-*N*-(4-chlorophenyl)-*N*-methylpenta-2,4-dienamide (**9'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

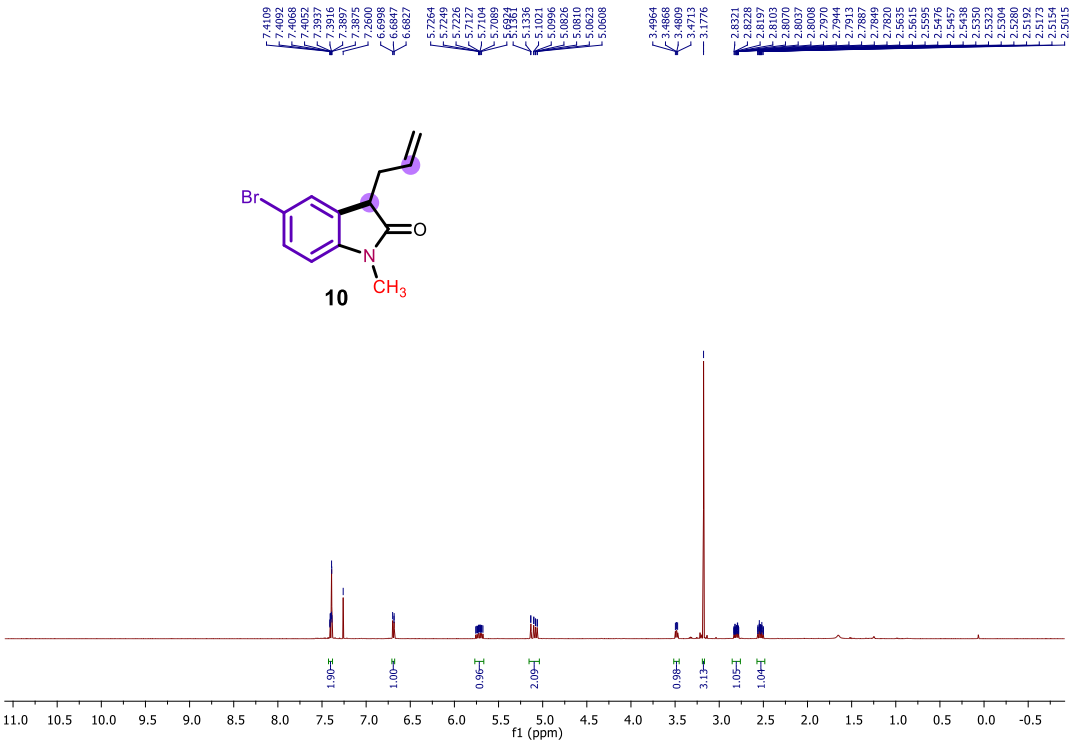


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

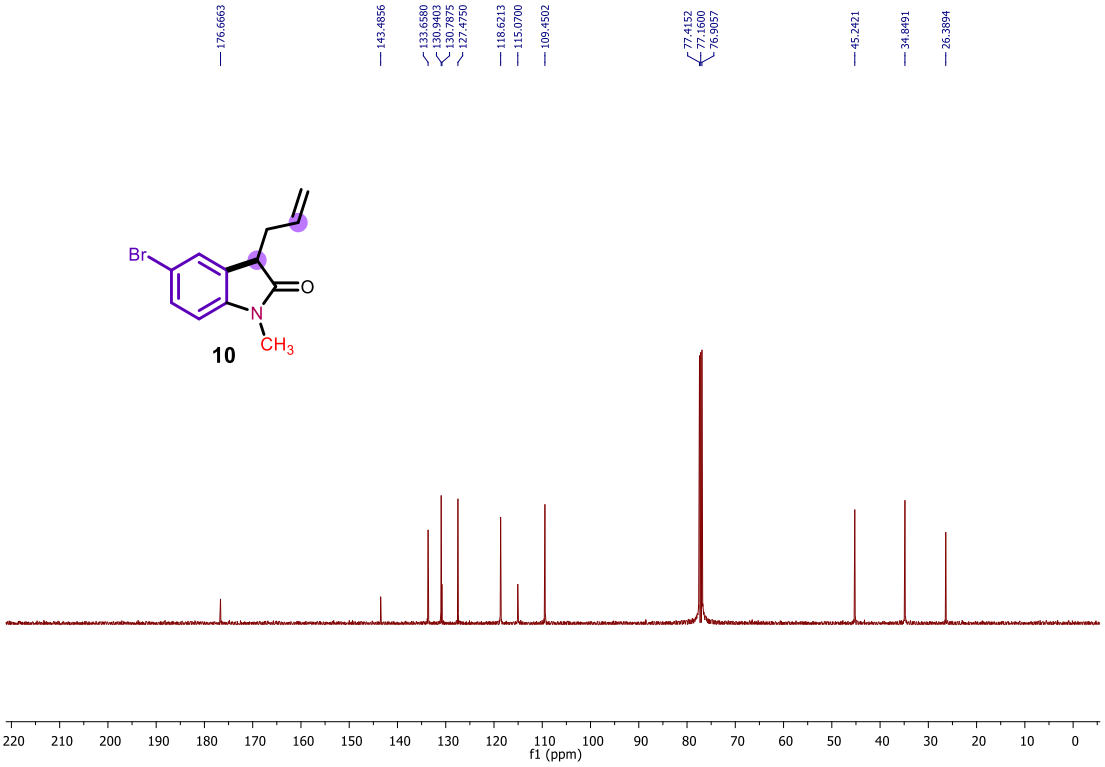


3-Allyl-5-bromo-1-methylindolin-2-one (**10**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

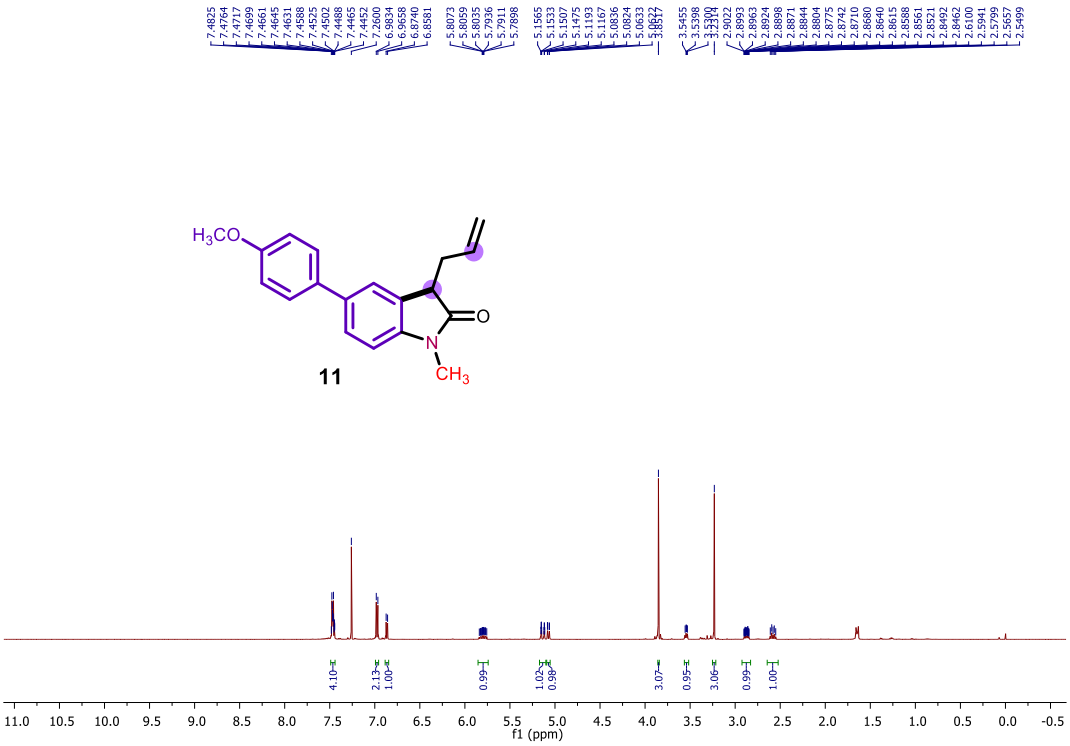


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

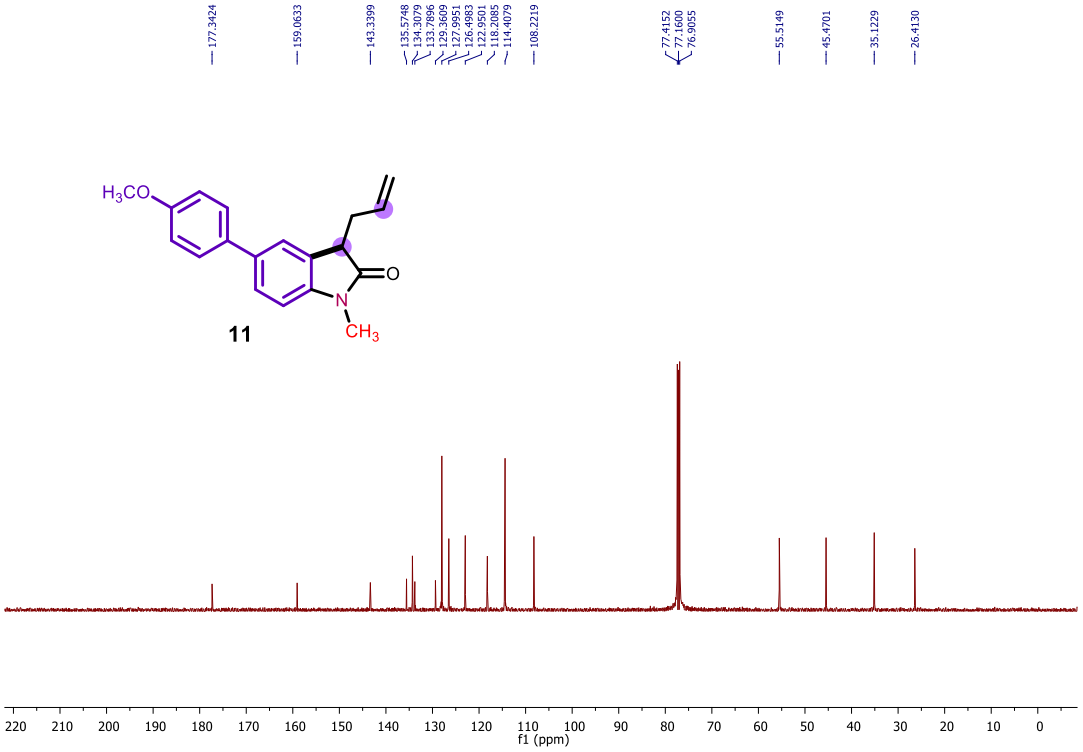


3-Allyl-5-(4-methoxyphenyl)-1-methylindolin-2-one (**11**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

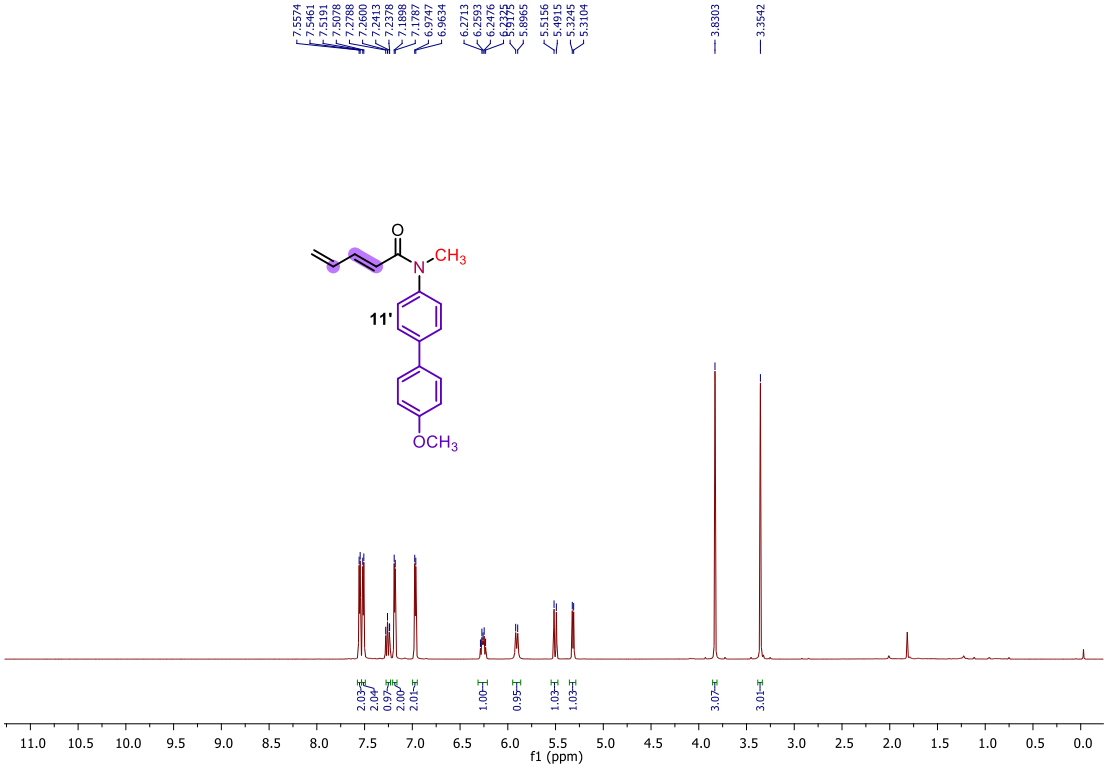


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

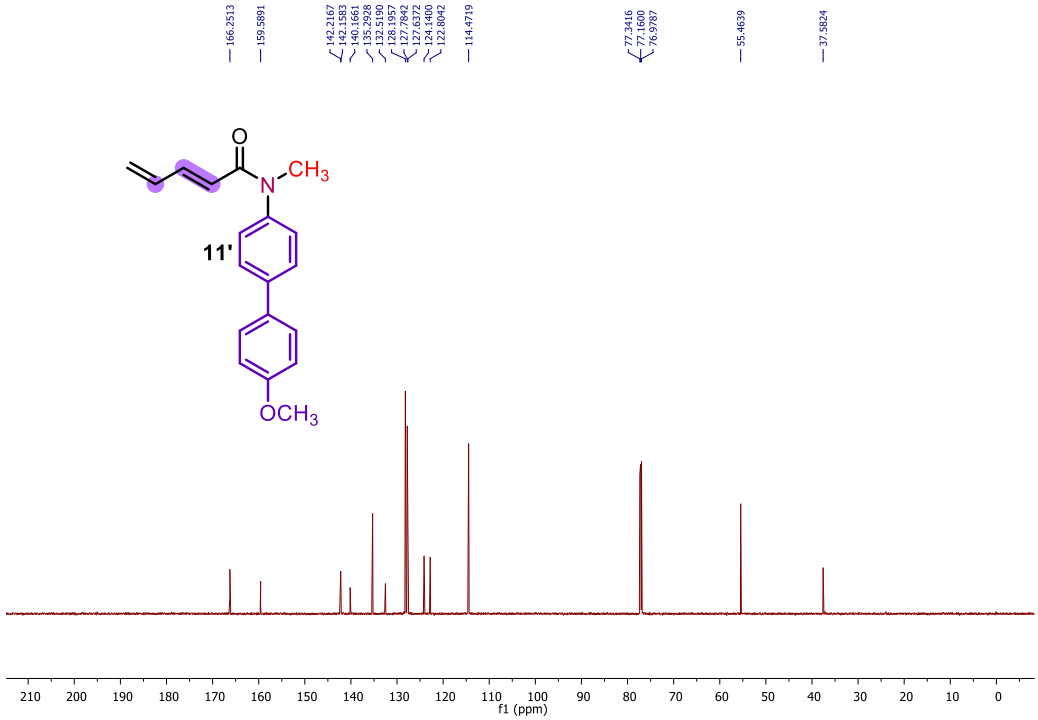


(*E*)-*N*-(4'-methoxy-[1,1'-biphenyl]-4-yl)-*N*-methylpenta-2,4-dienamide (**11'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

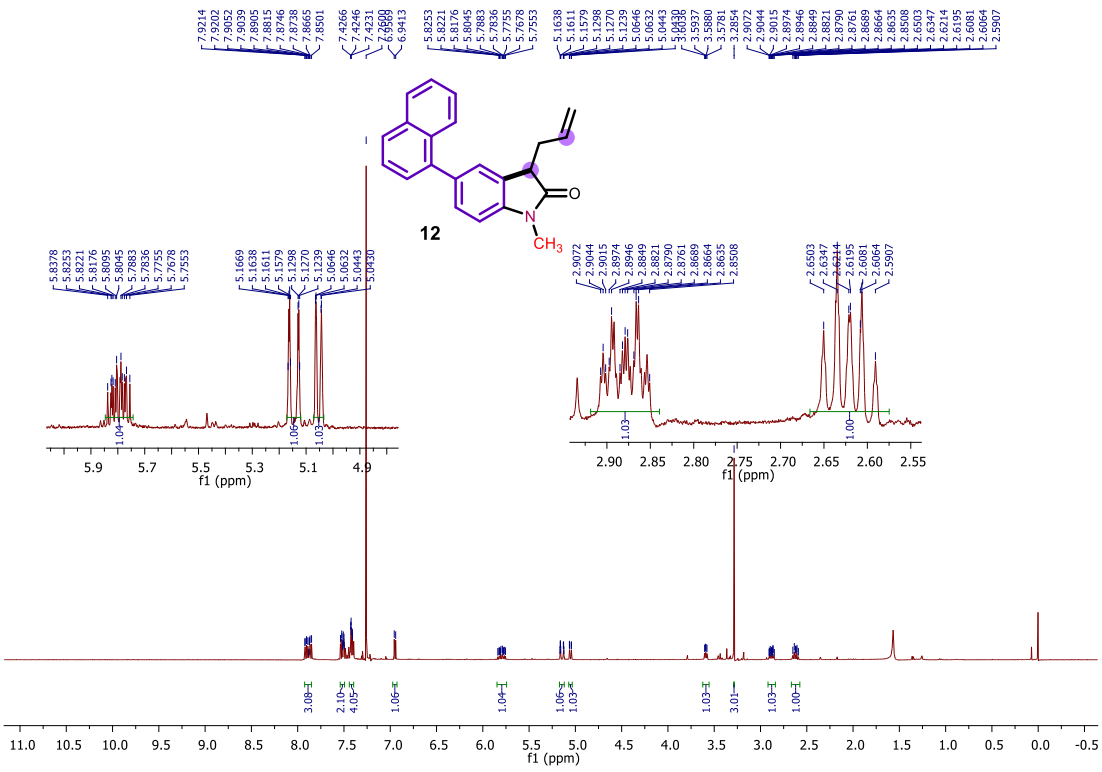


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

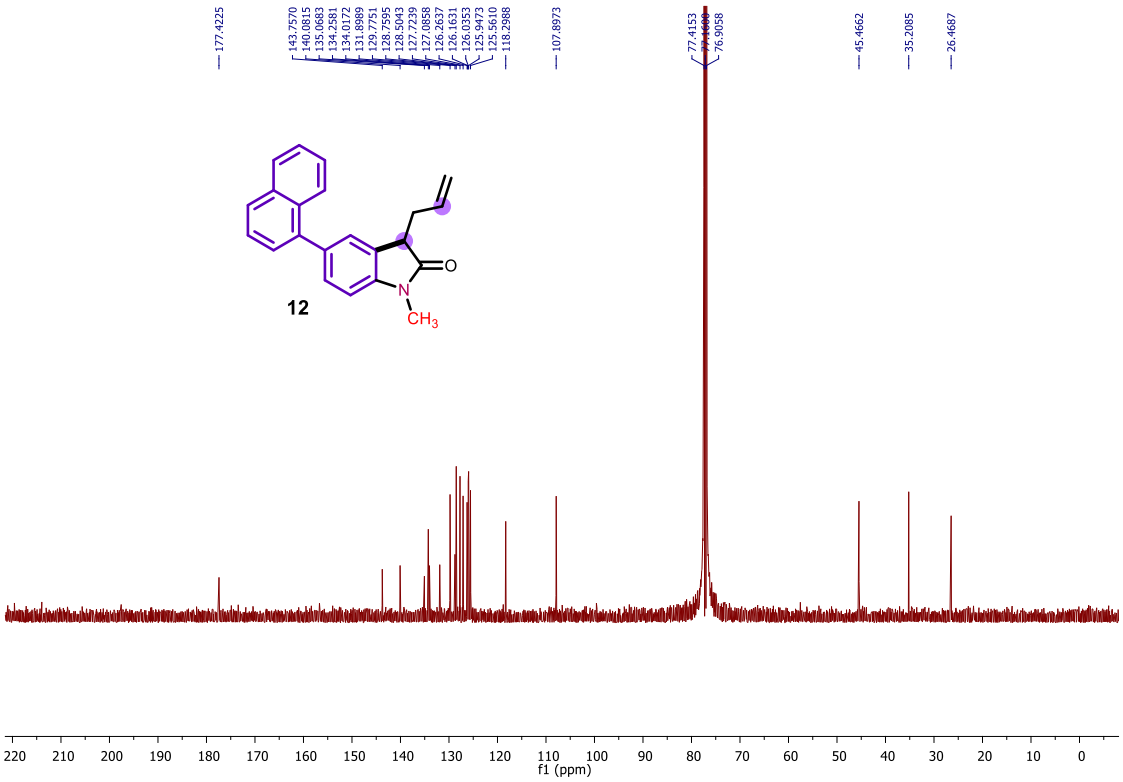


3-Allyl-1-methyl-5-(naphthalen-1-yl)indolin-2-one (**12**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

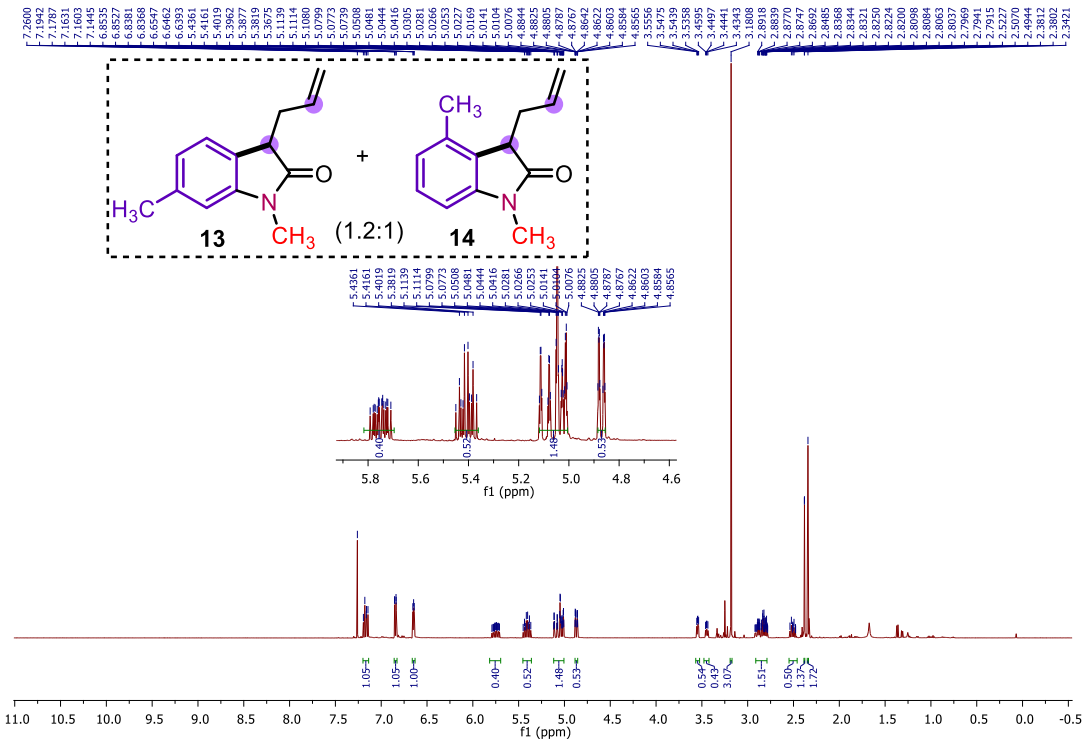


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

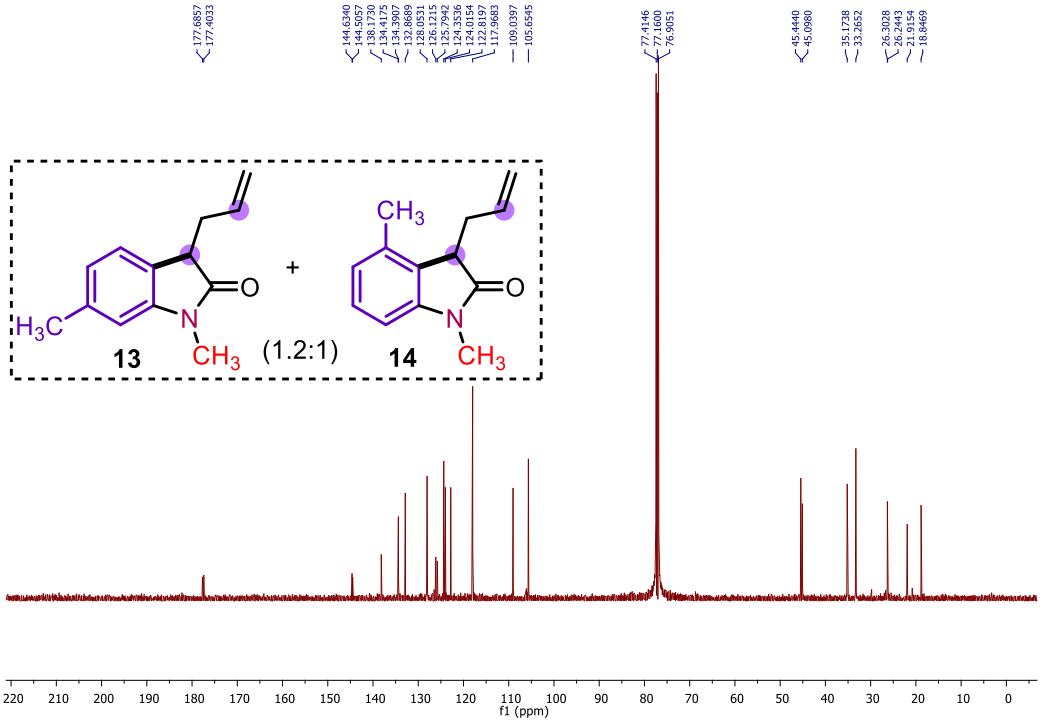


3-Allyl-1,6-dimethylindolin-2-one (**13**) and 3-Allyl-1,4-dimethylindolin-2-one (**14**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

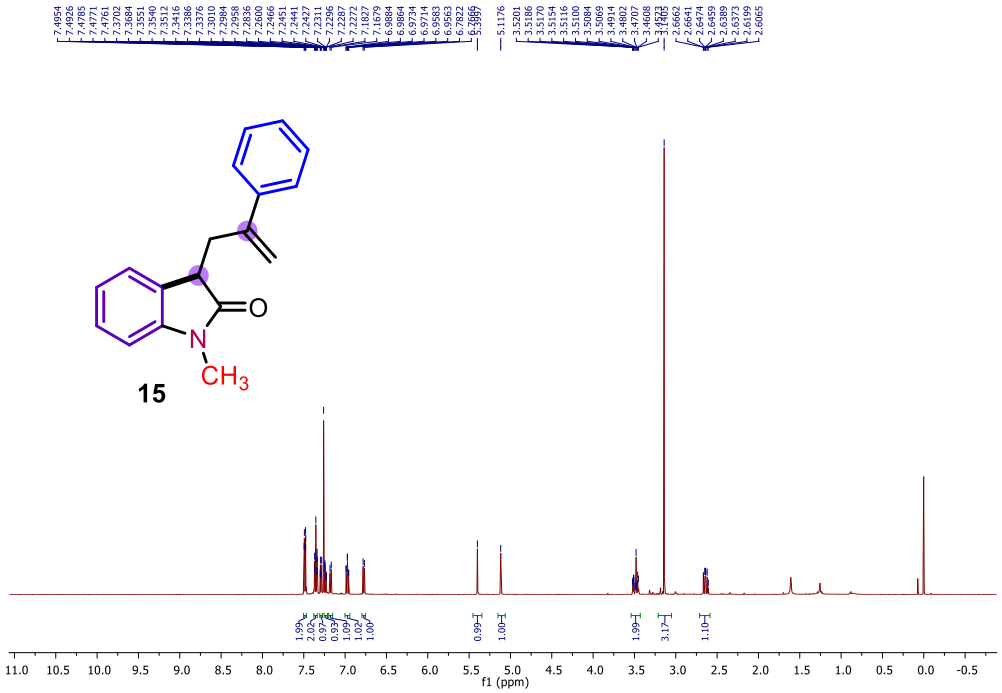


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

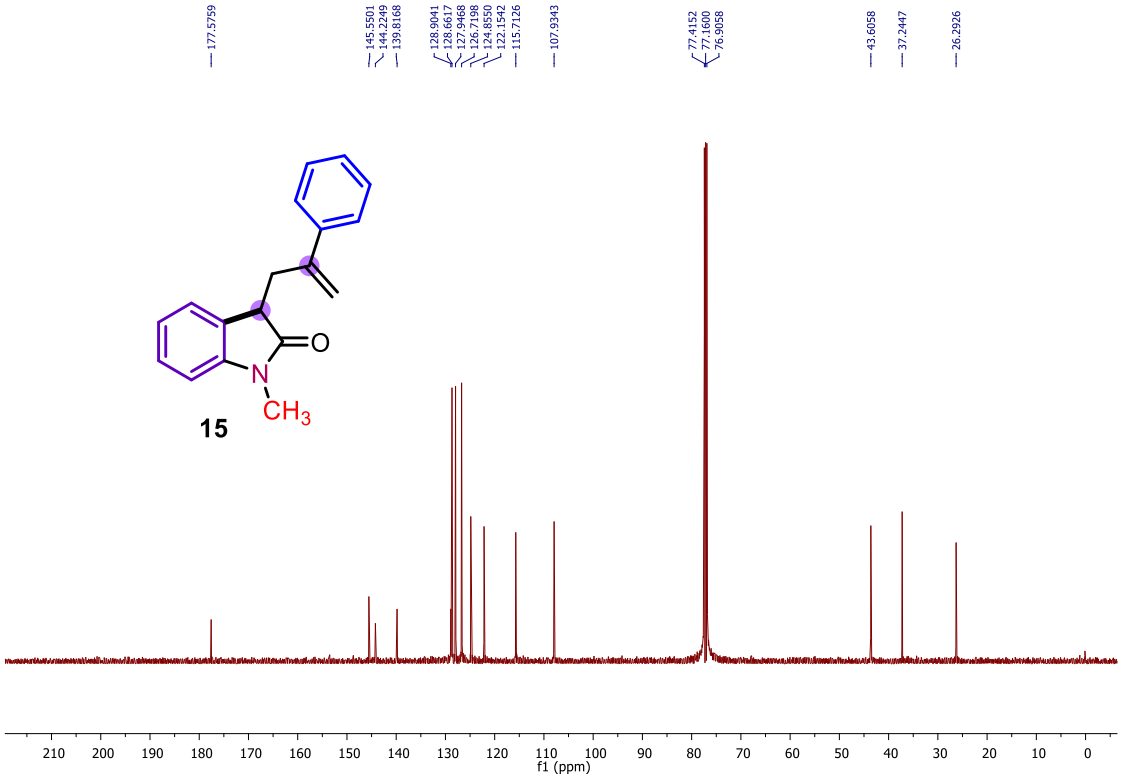


1-Methyl-3-(2-phenylallyl)indolin-2-oneone (**15**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

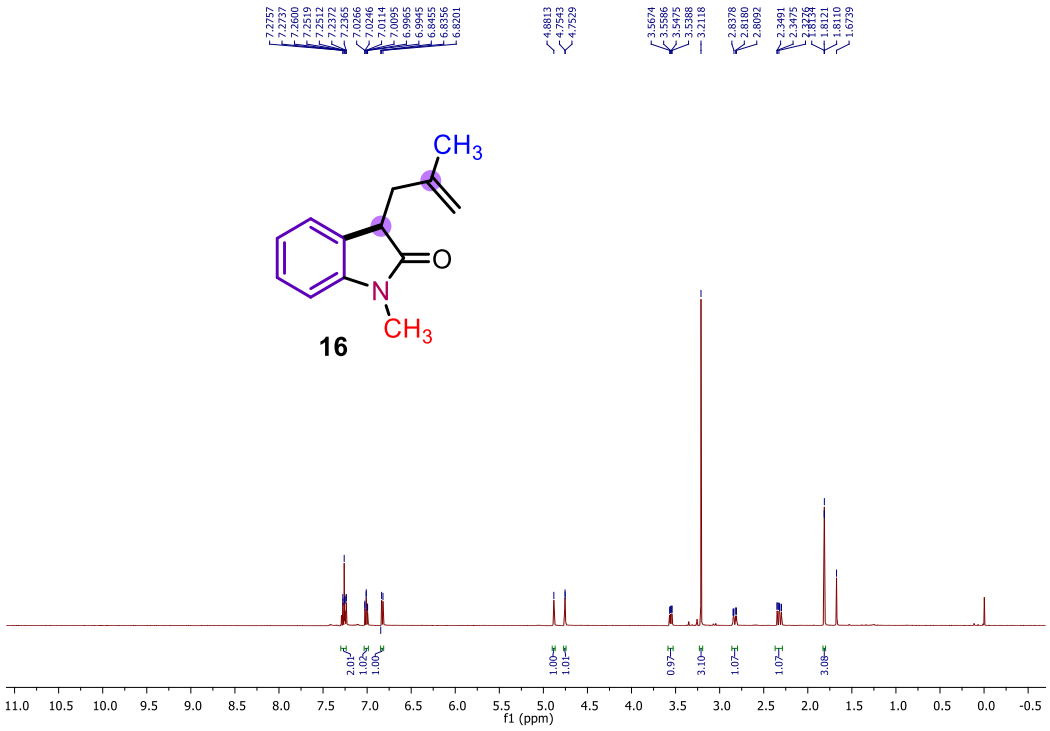


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

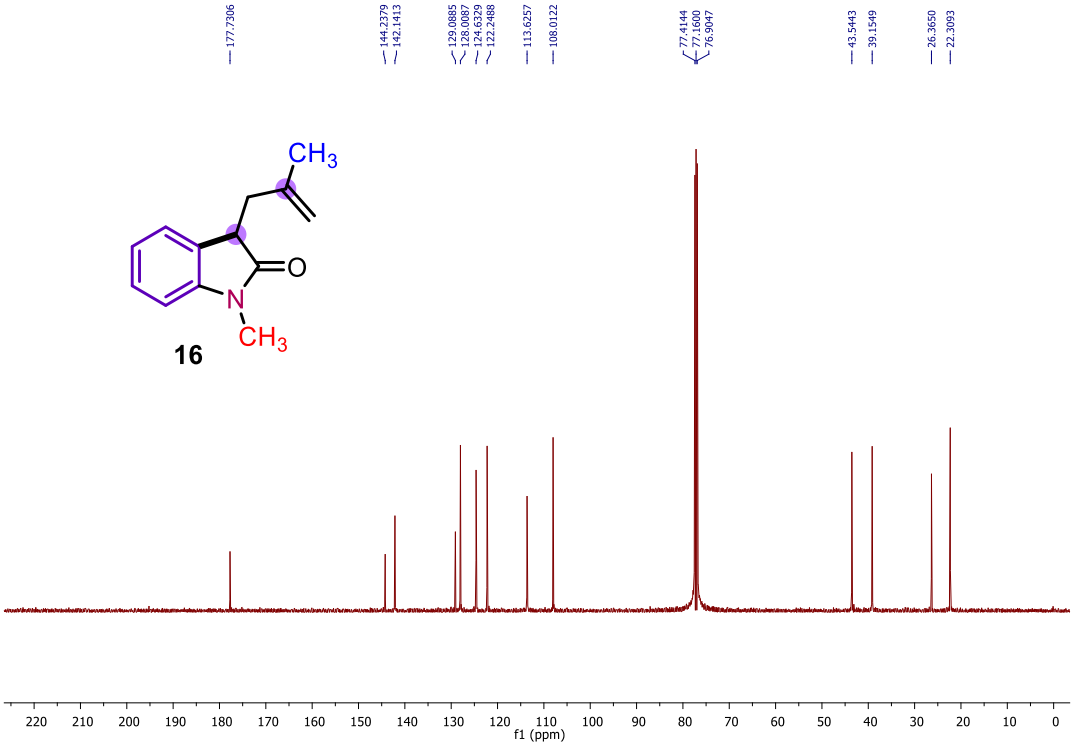


1-Methyl-3-(2-phenylallyl)indolin-2-oneone (**16**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

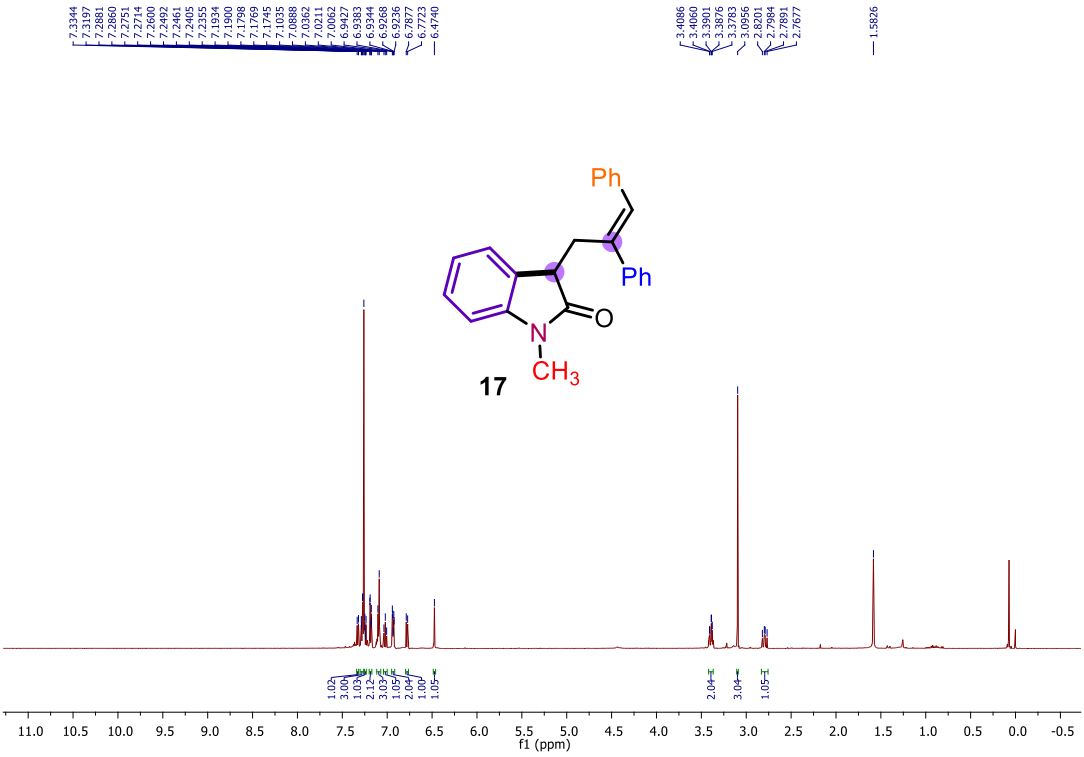


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

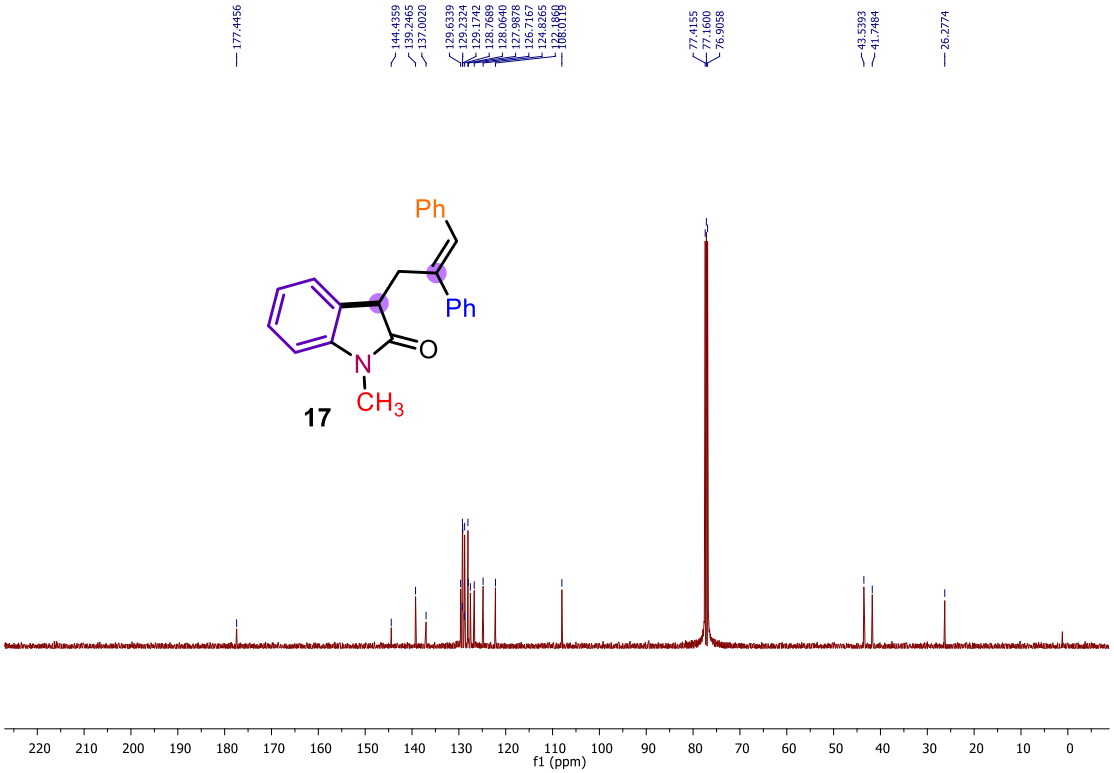


1-Methyl-3-(2-phenylallyl)indolin-2-oneone (**17**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

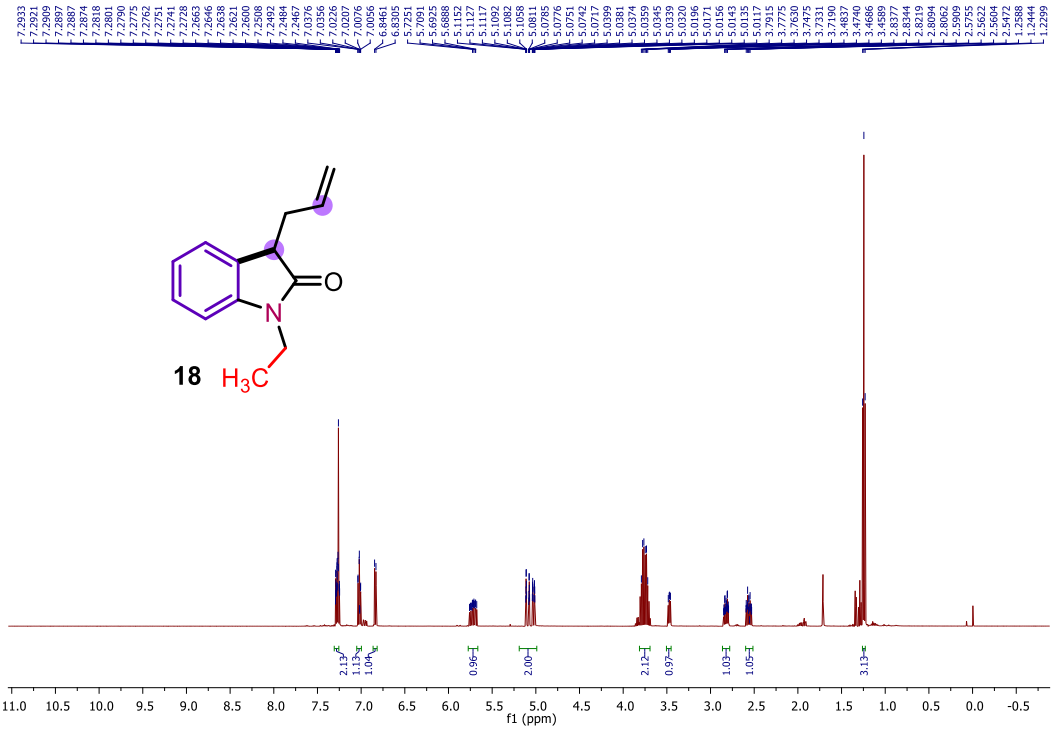


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

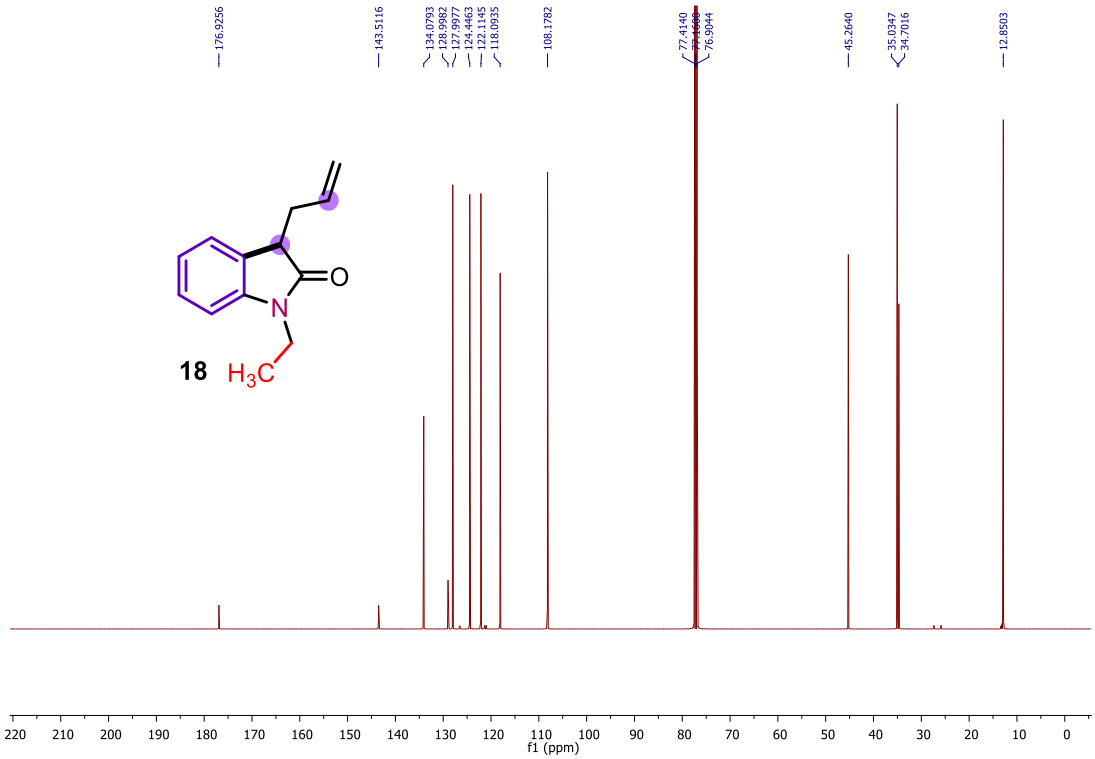


3-Allyl-1-ethylindolin-2-one (**18**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

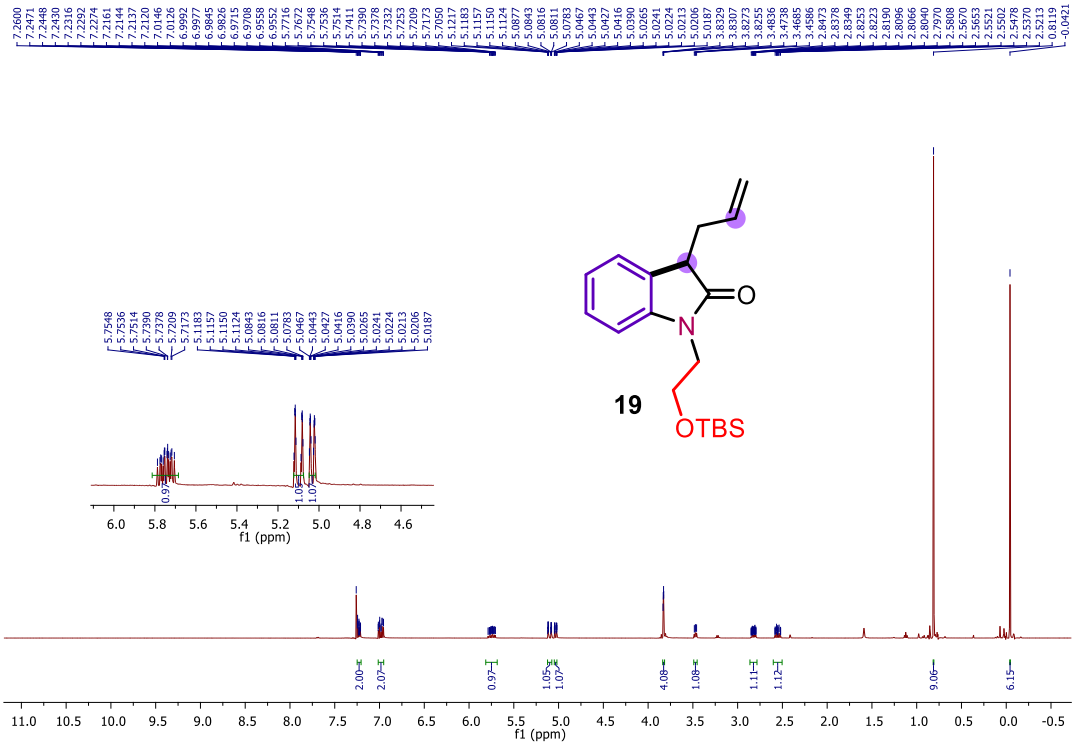


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

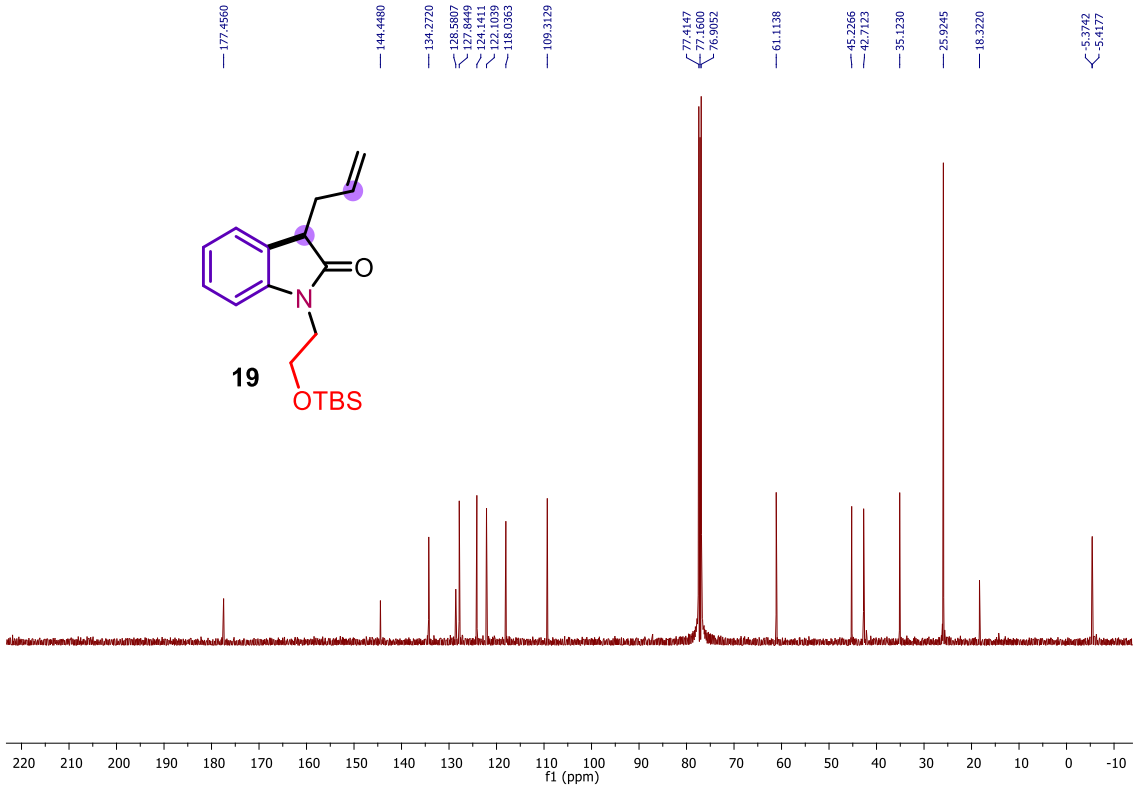


3-Allyl-1-(2-((tert-butyldimethylsilyl)oxy)ethyl)indolin-2-one (**19**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

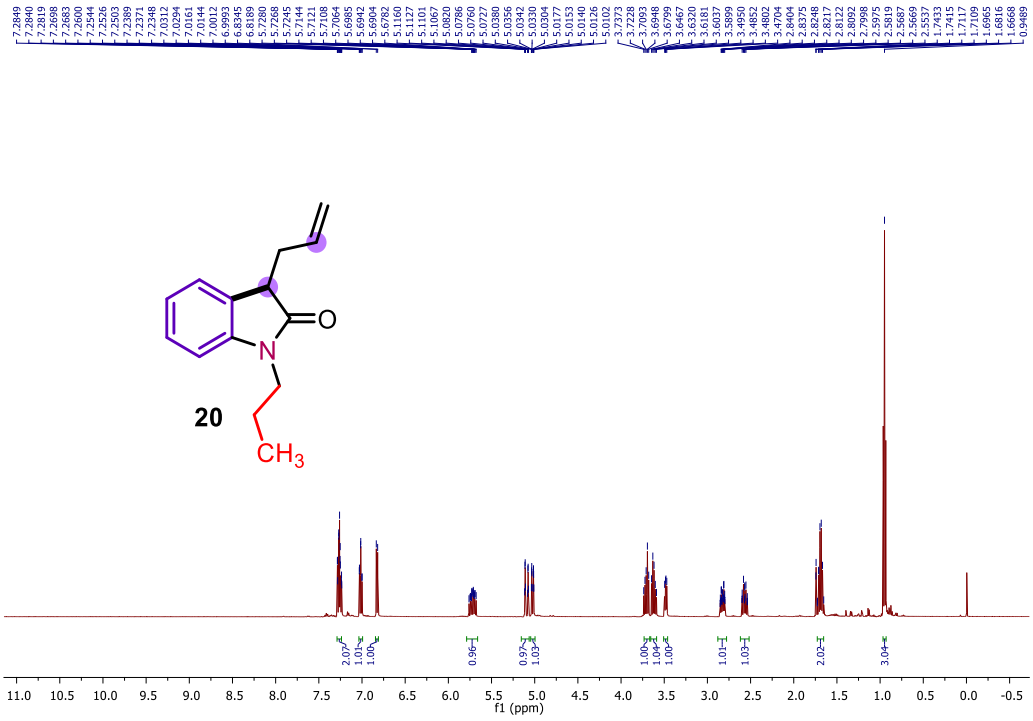


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

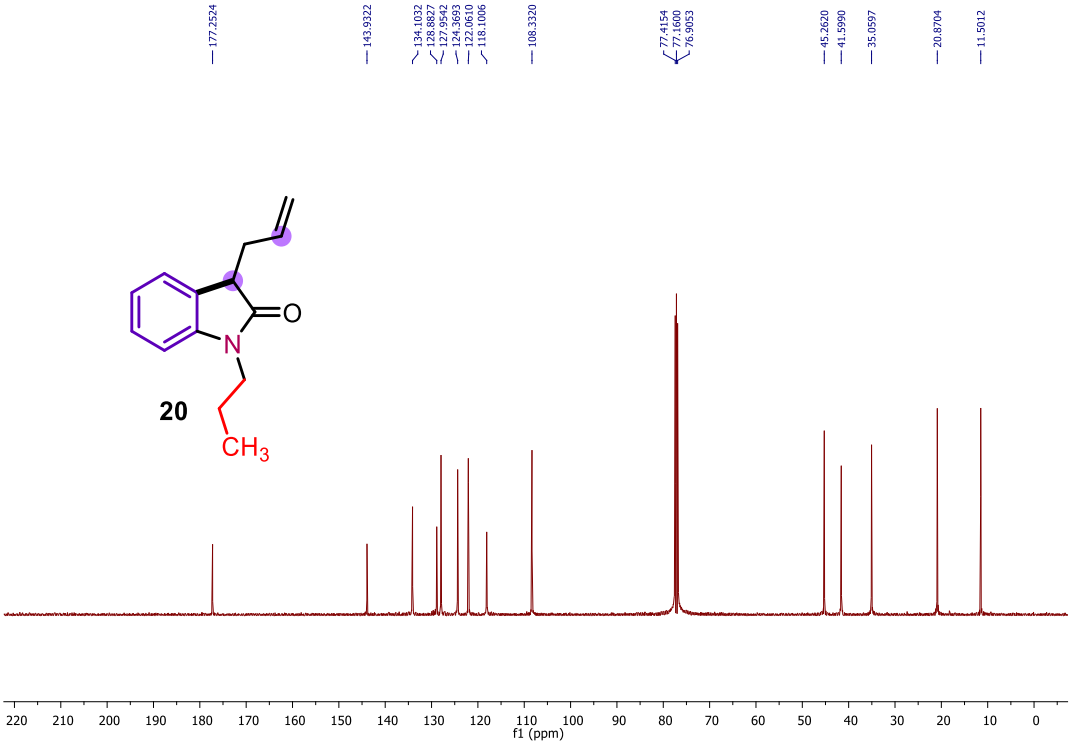


3-Allyl-1-propylindolin-2-one (**20**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

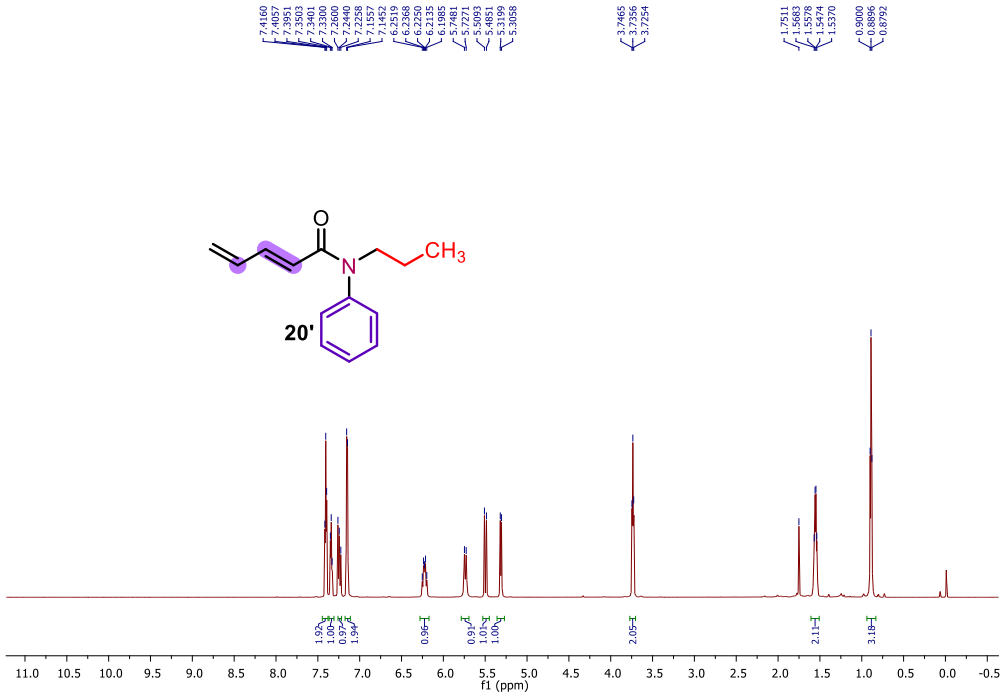


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

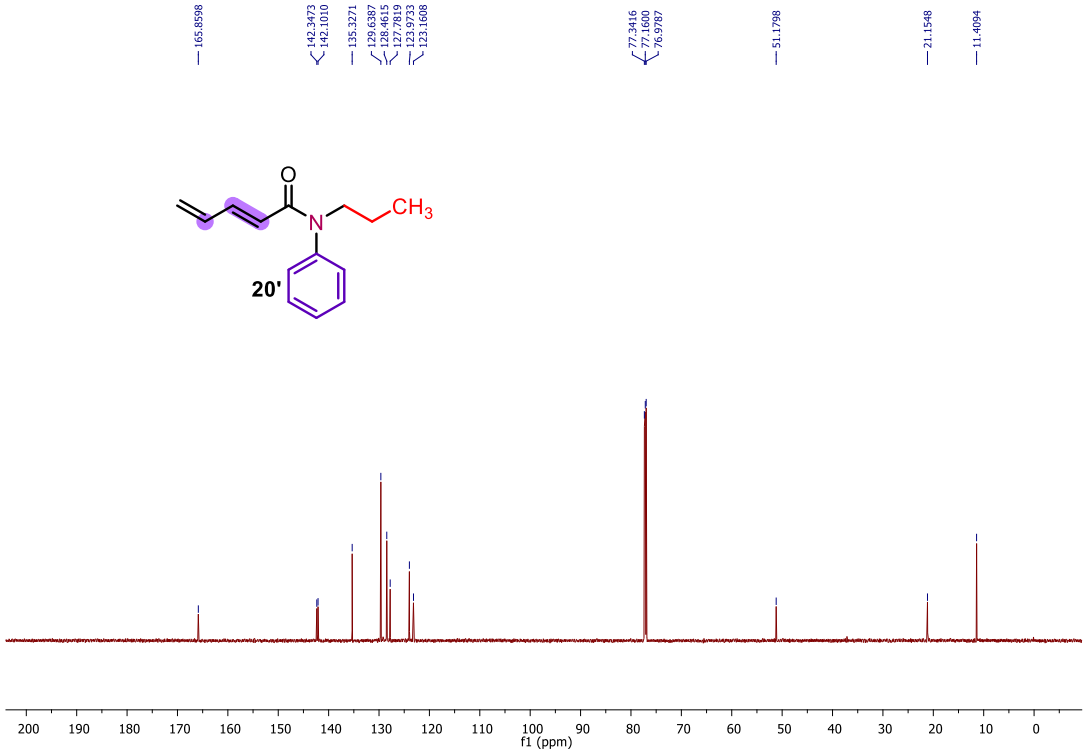


(*E*)-*N*-phenyl-*N*-propylpenta-2,4-dienamide (**20'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

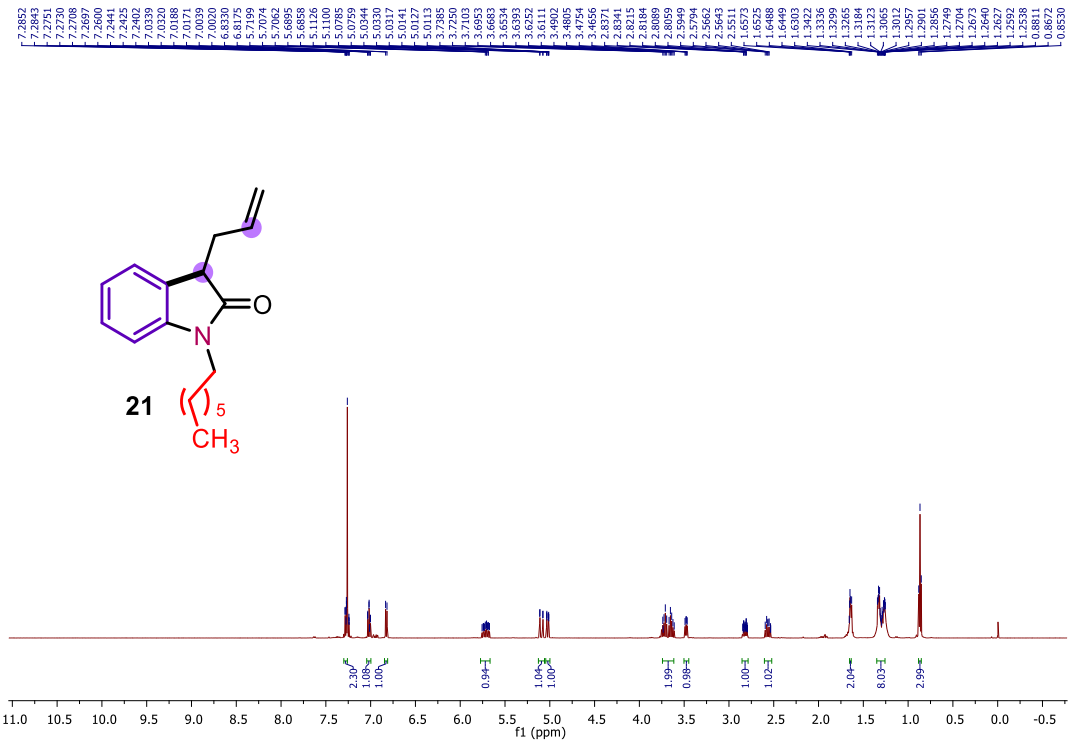


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

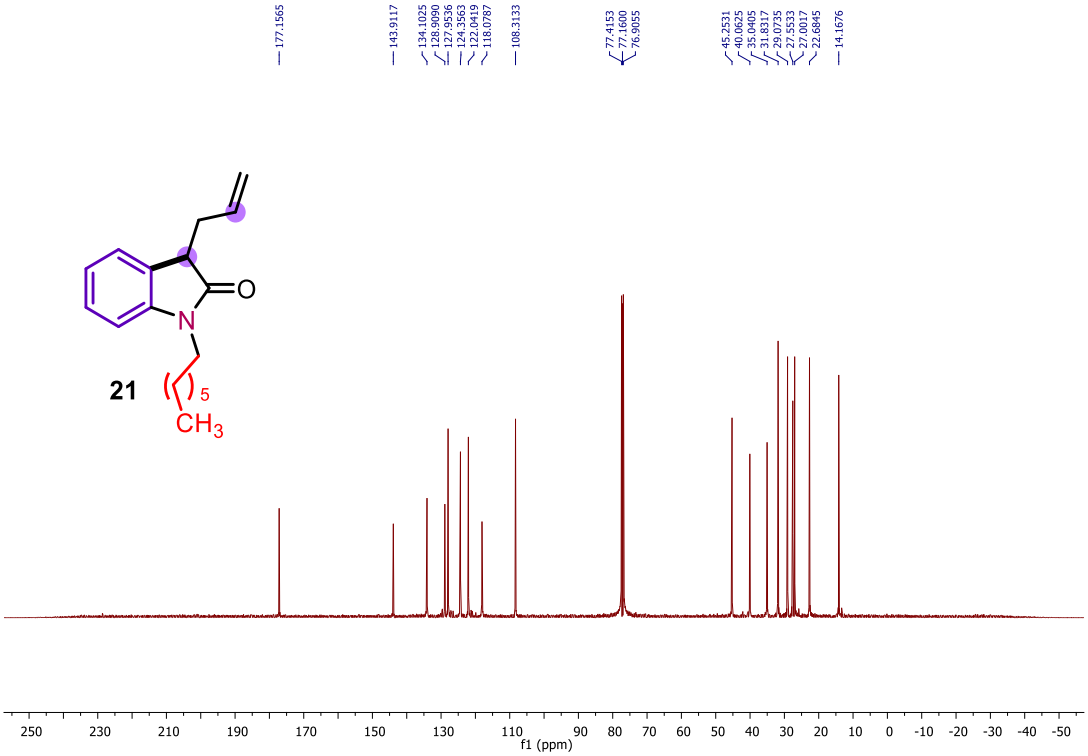


3-Allyl-1-heptylindolin-2-one (**21**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

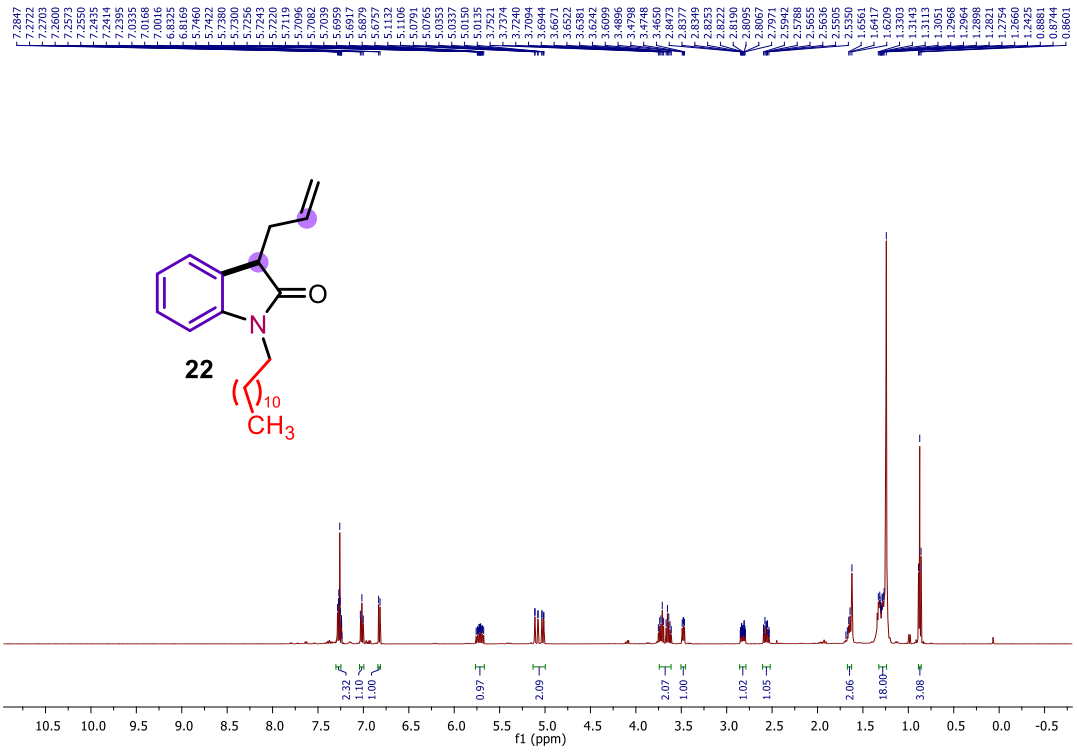


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

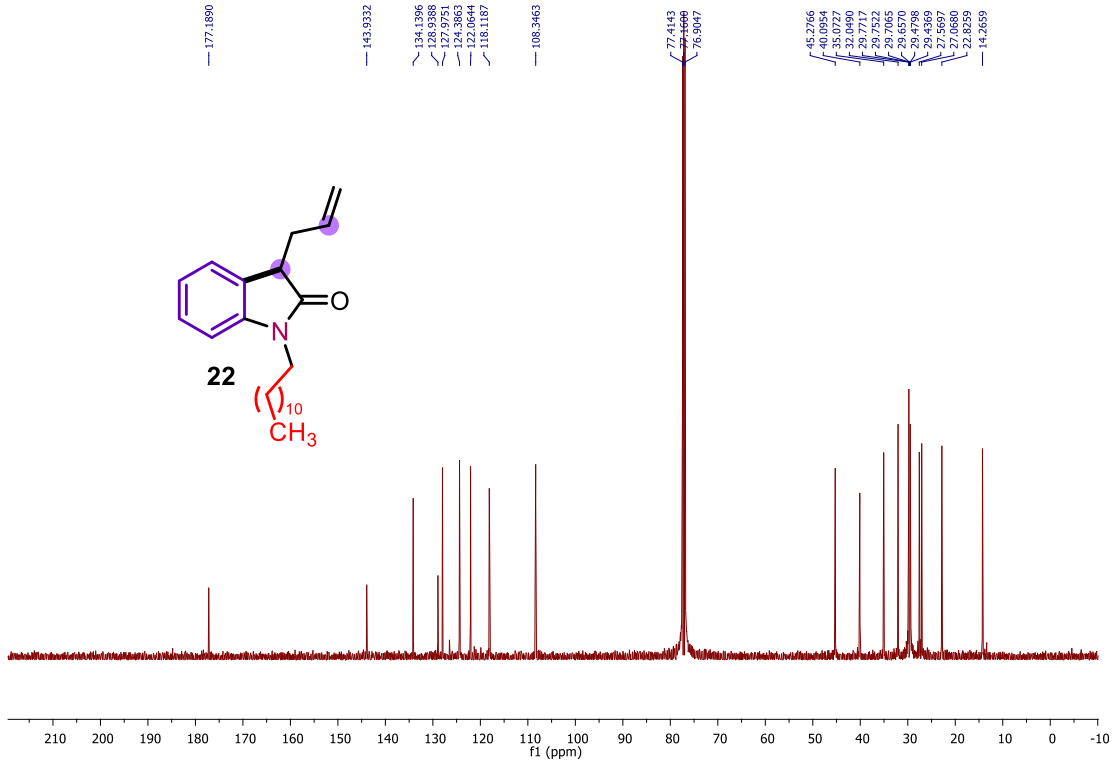


3-Allyl-1-dodecylindolin-2-one (**22**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

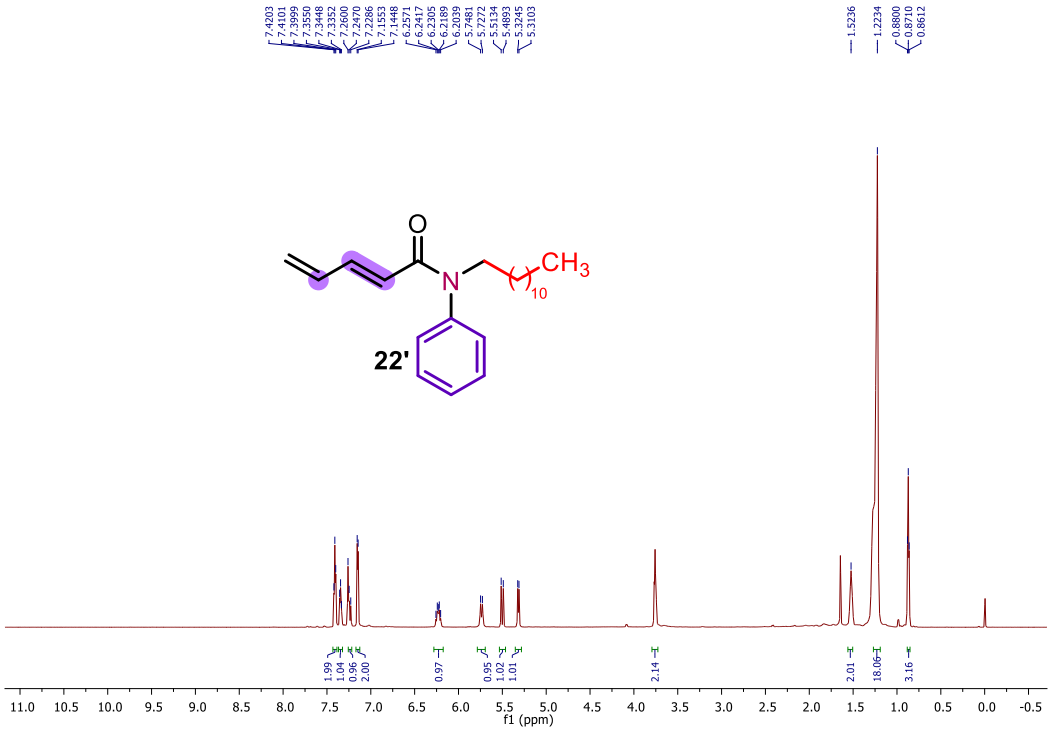


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

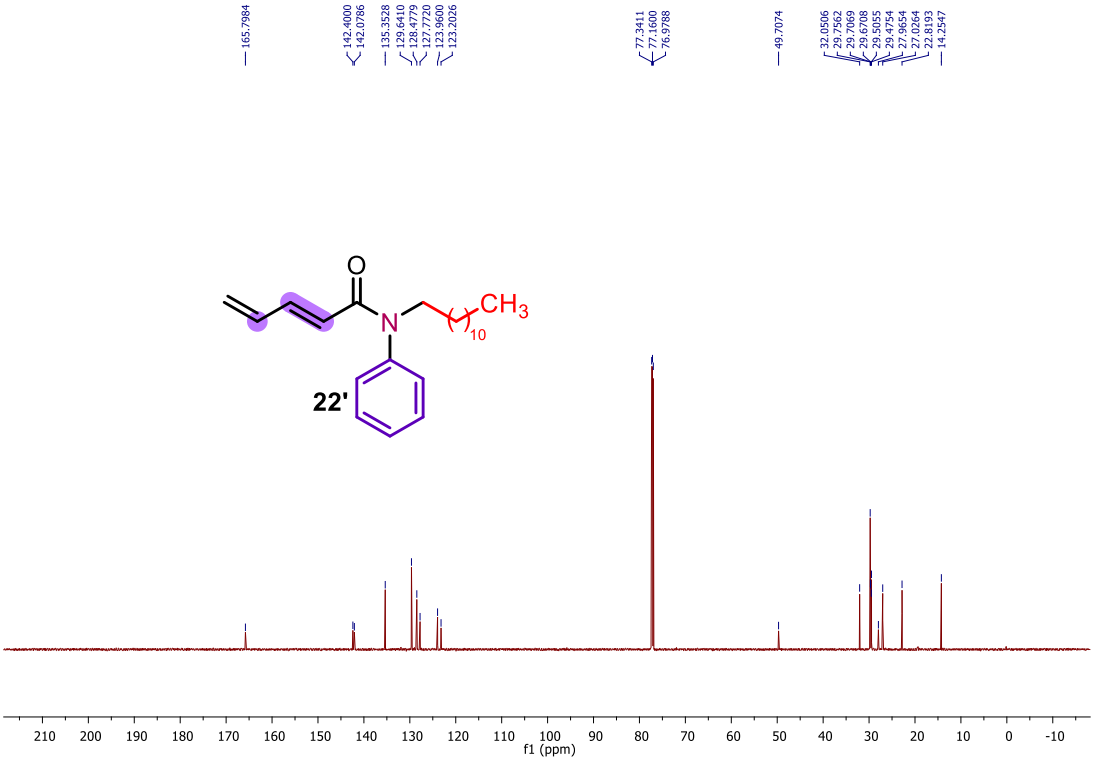


(*E*)-*N*-Phenyl-*N*-propylpenta-2,4-dienamide (**22'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

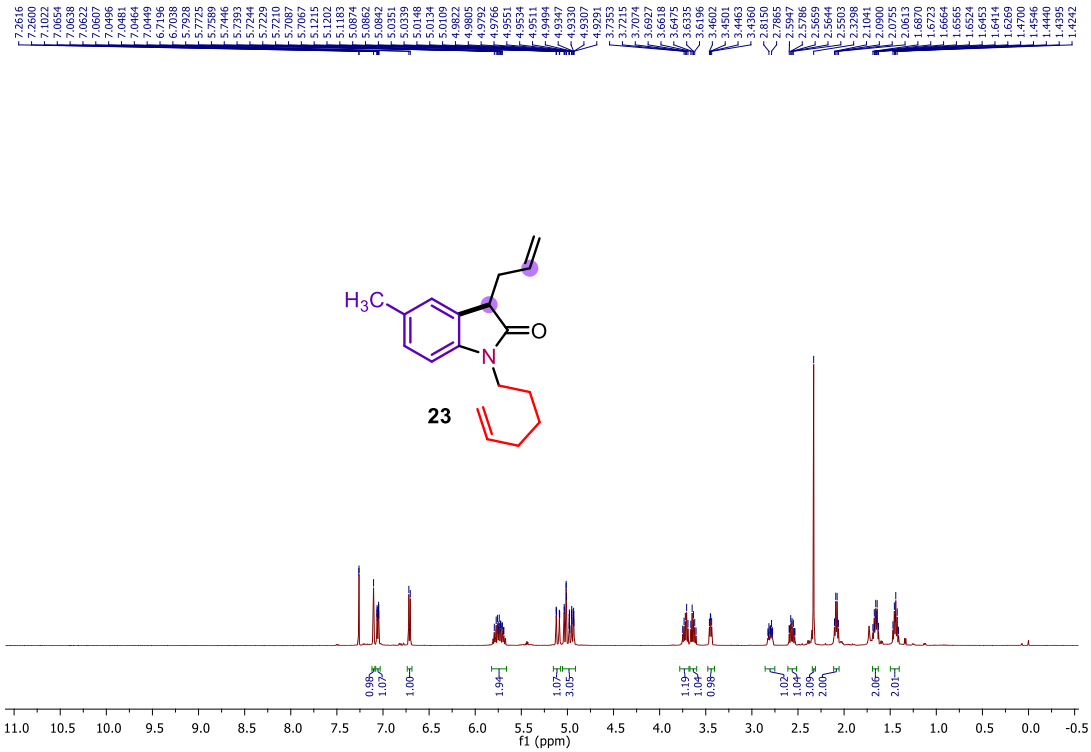


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

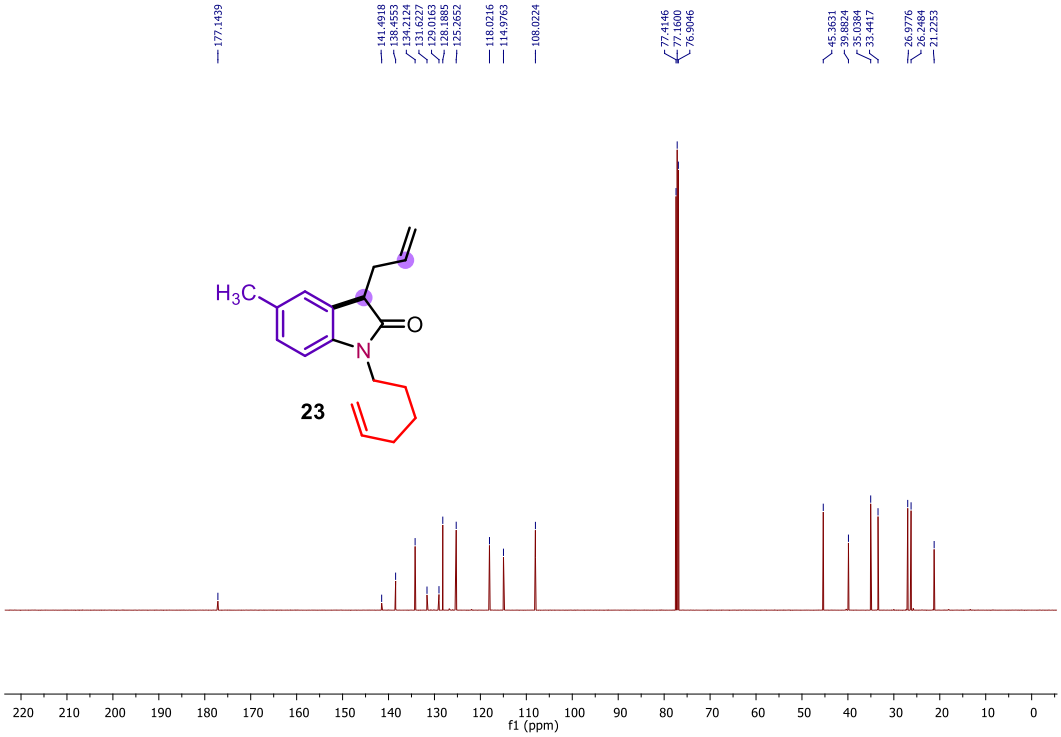


3-Allyl-1-(hex-5-en-1-yl)-5-methylindolin-2-one (**23**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

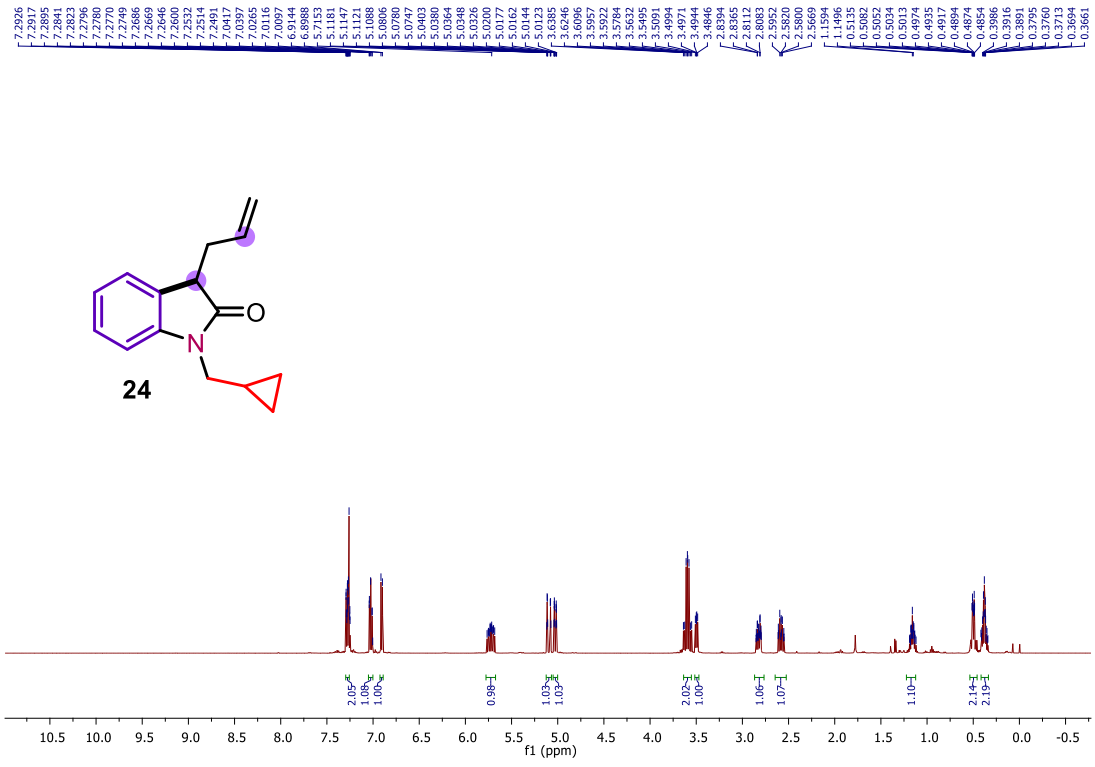


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

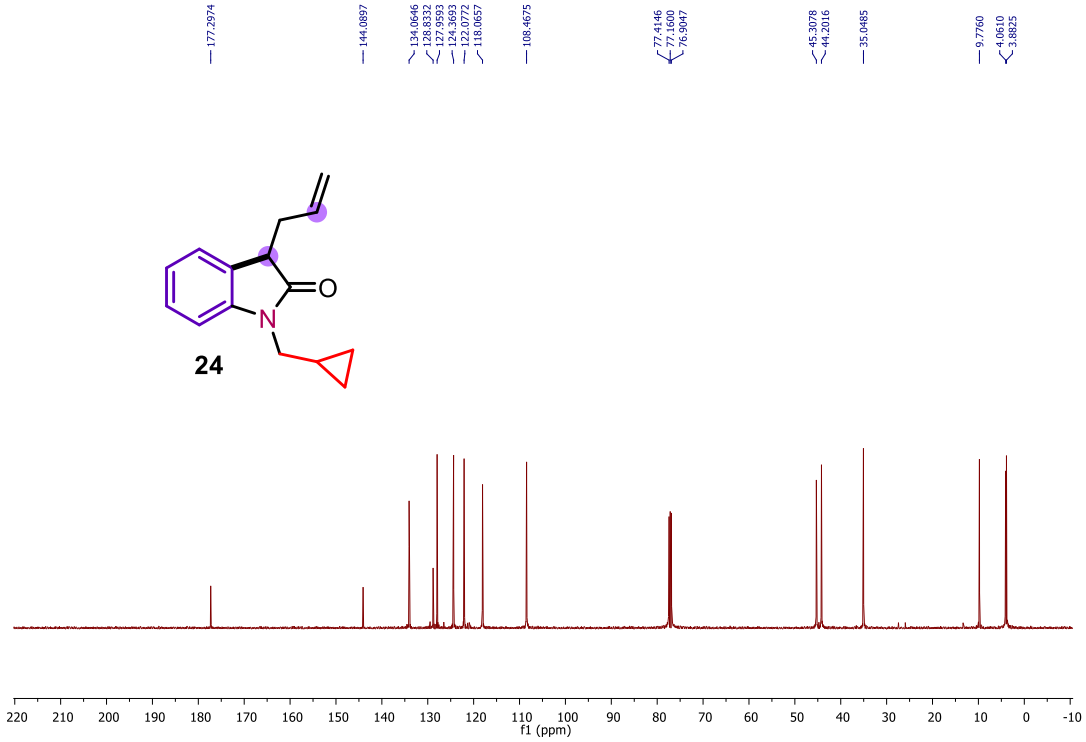


3-Allyl-1-(cyclopropylmethyl)indolin-2-one (**24**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

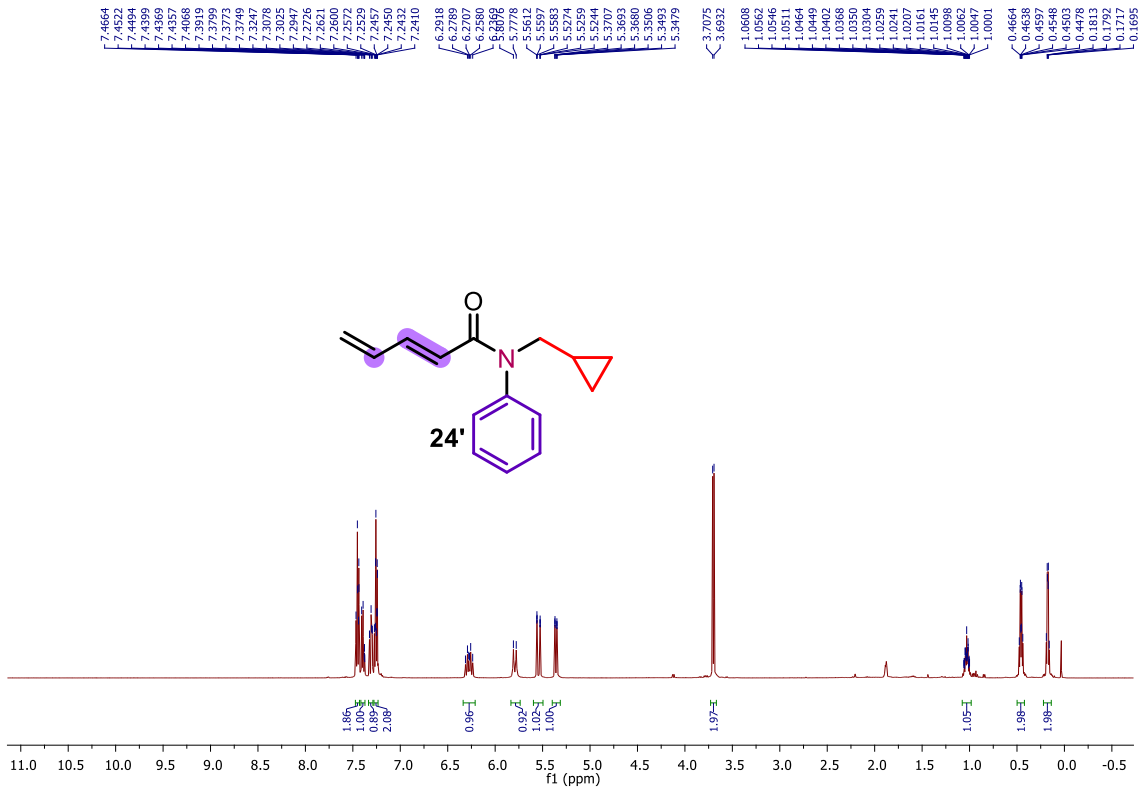


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

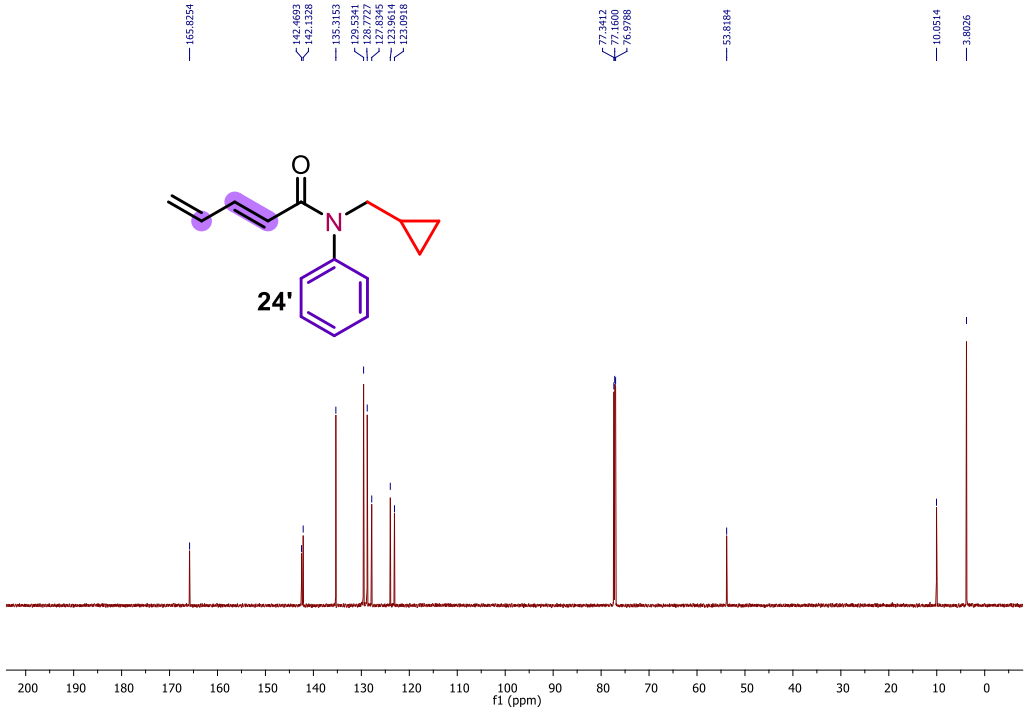


(*E*)-*N*-(cyclopropylmethyl)-*N*-phenylpenta-2,4-dienamide (**24'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

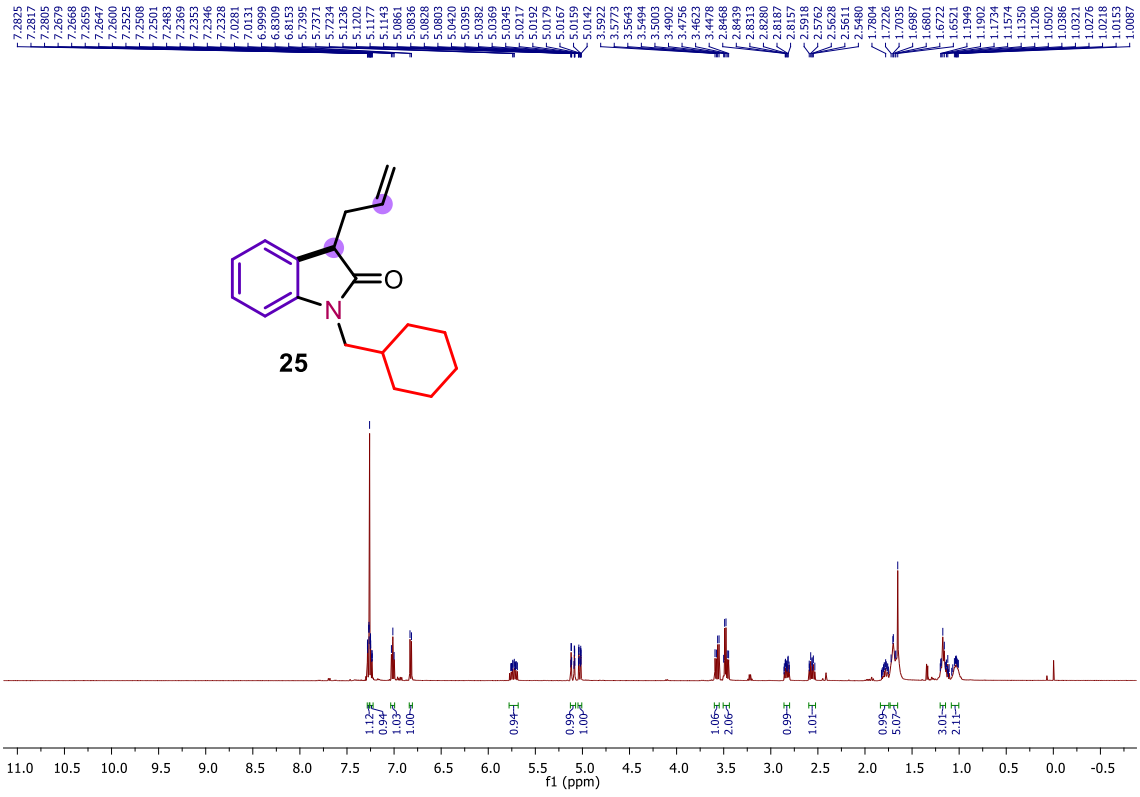


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

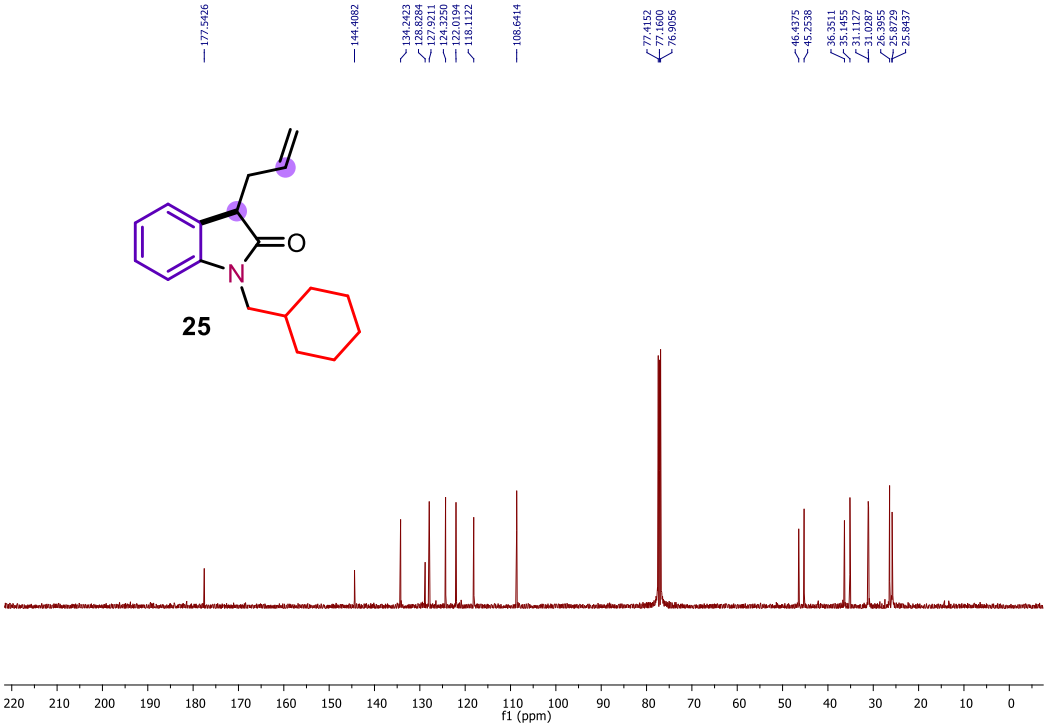


3-Allyl-1-(cyclohexylmethyl)indolin-2-one (**25**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

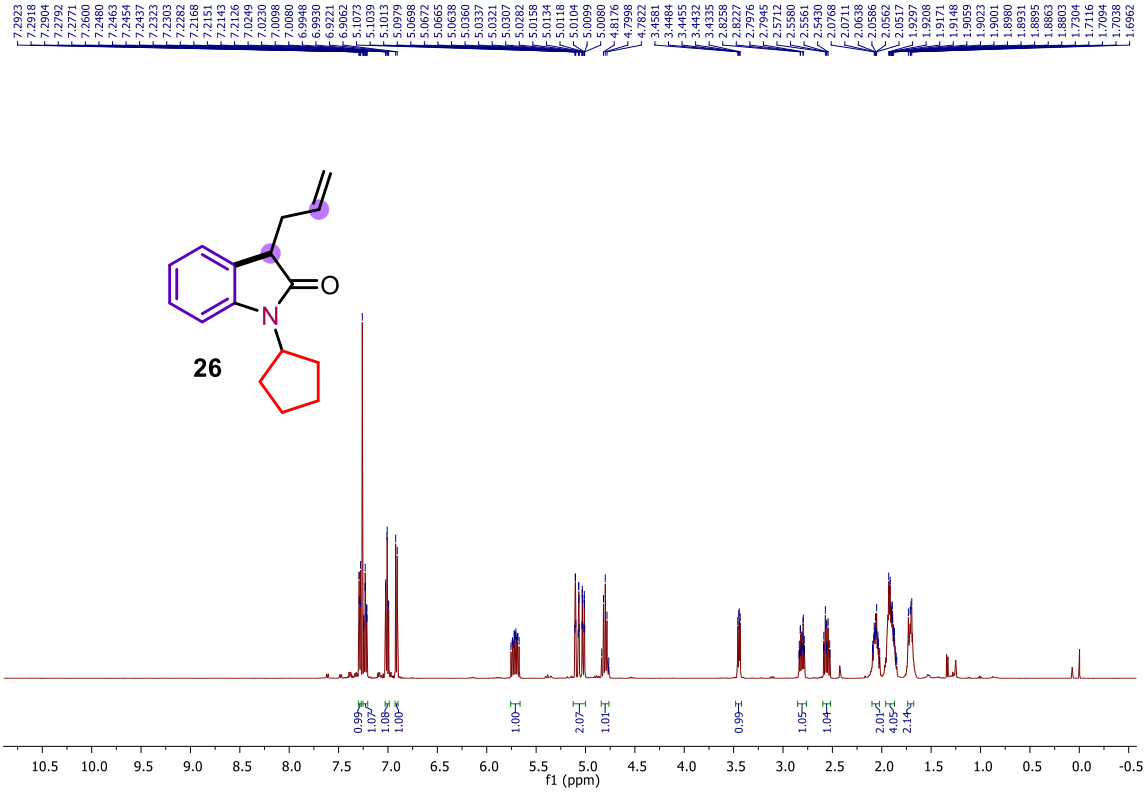


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

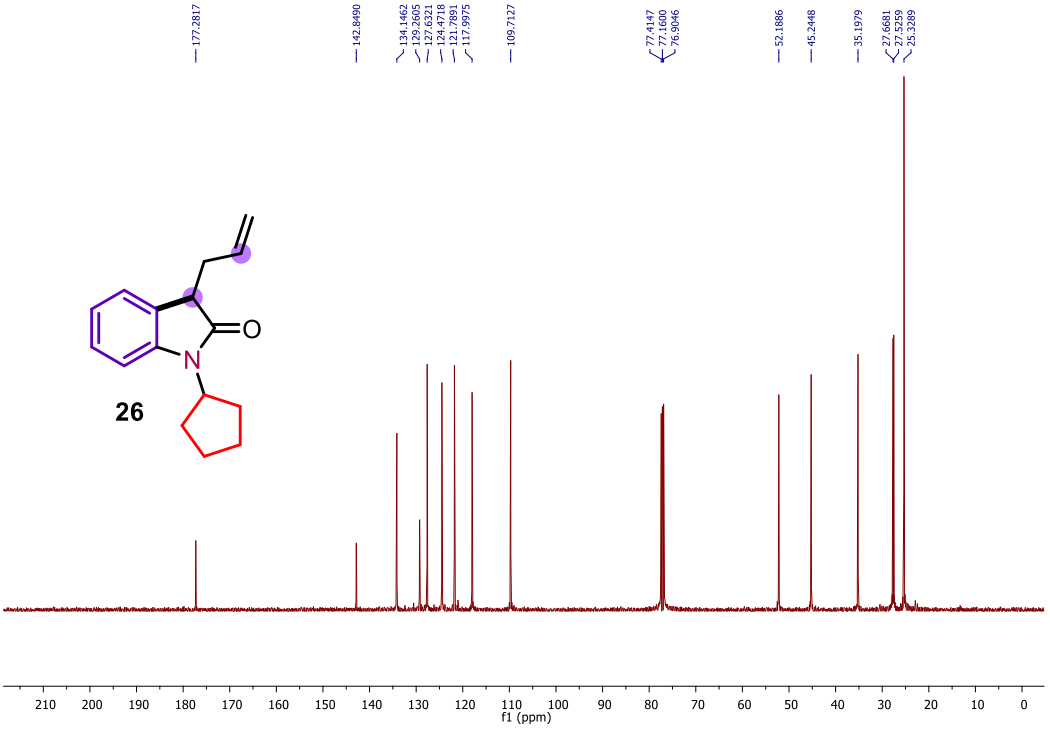


3-Allyl-1-cyclopentylindolin-2-one (**26**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

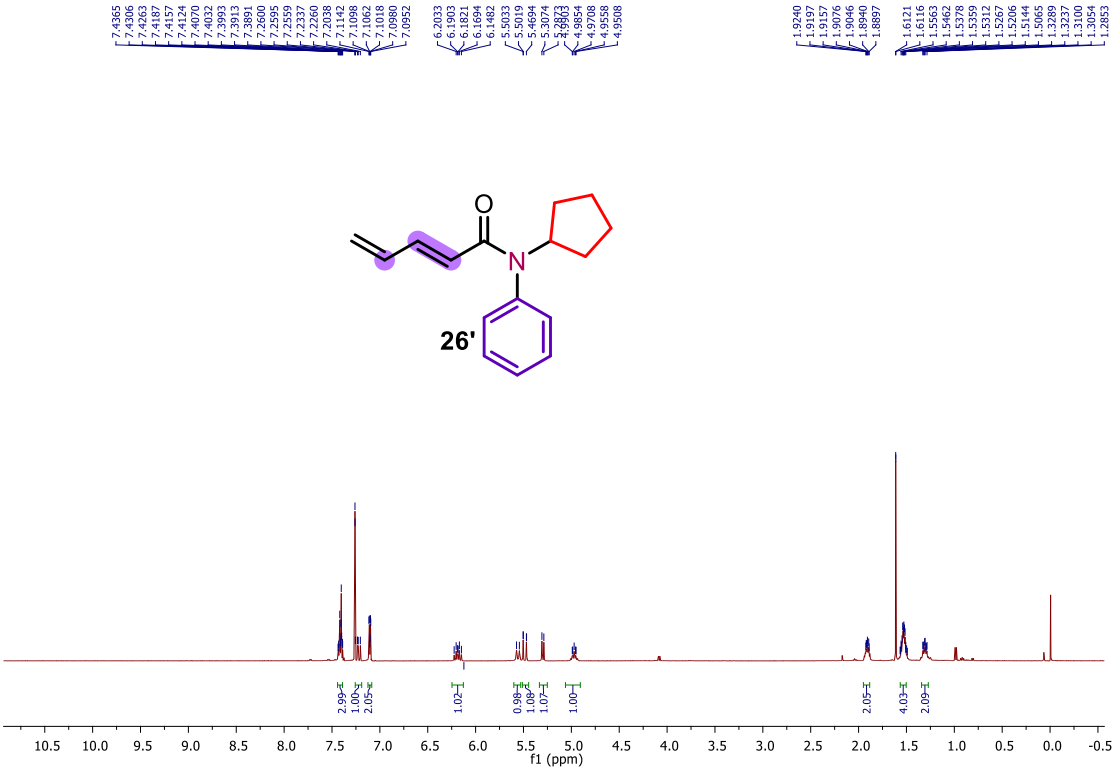


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

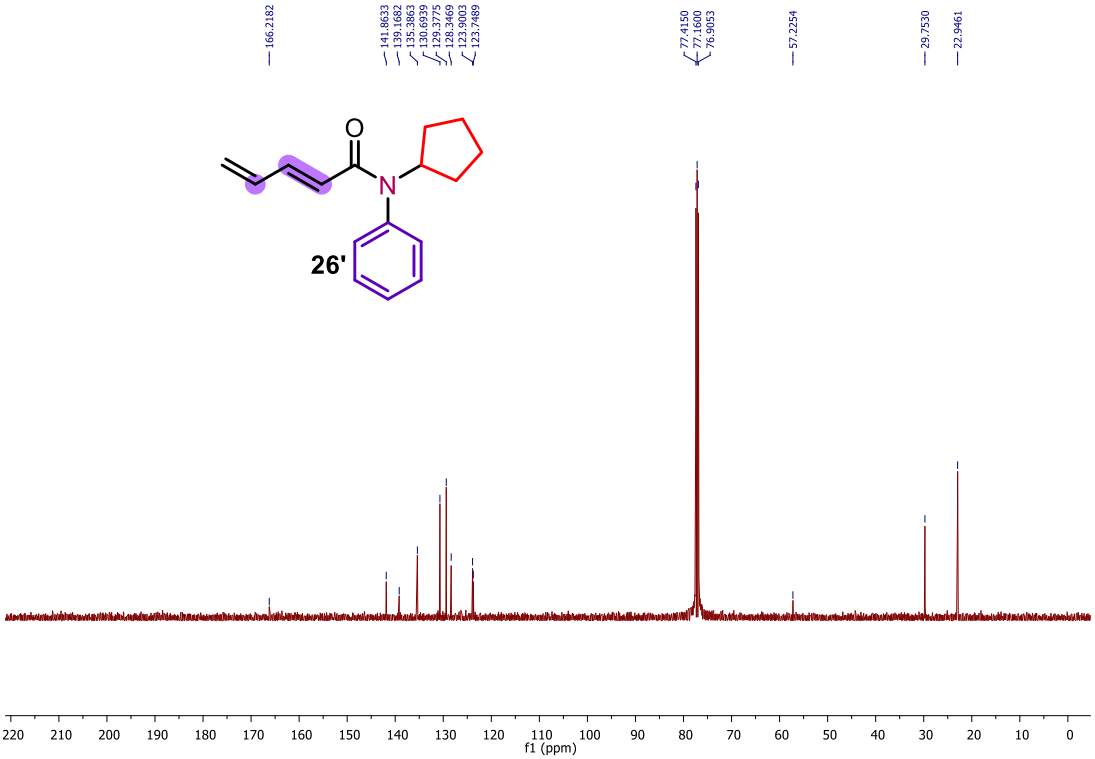


(*E*)-*N*-Cyclopentyl-*N*-phenylpenta-2,4-dienamide (**26'**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

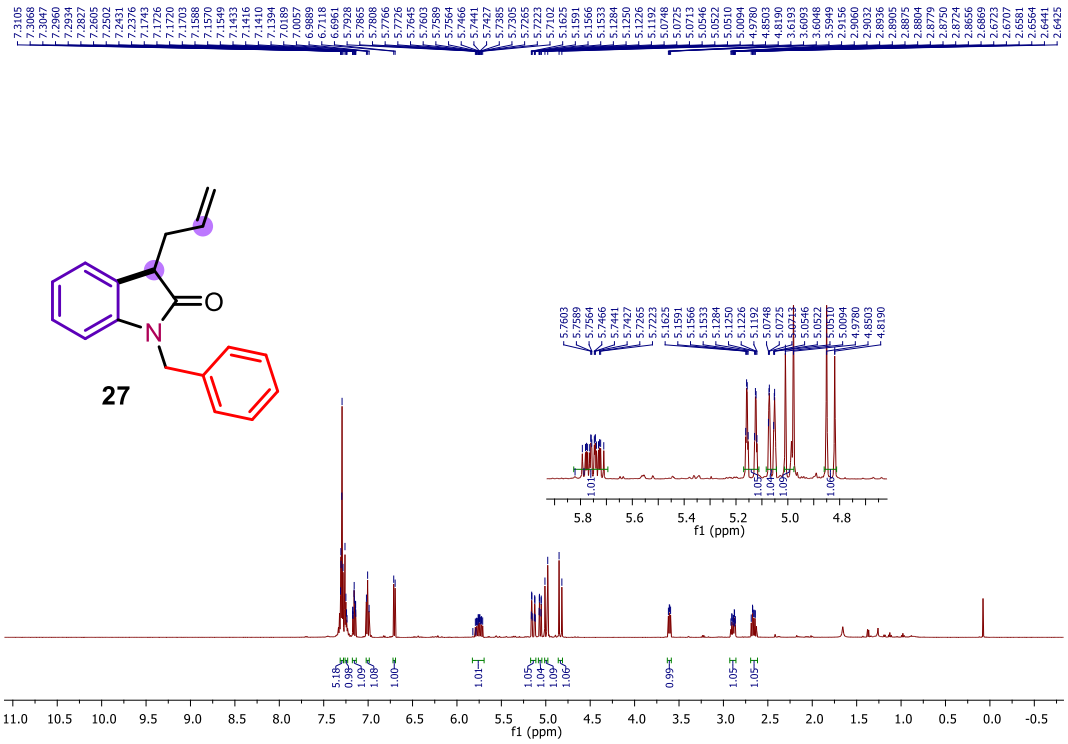


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

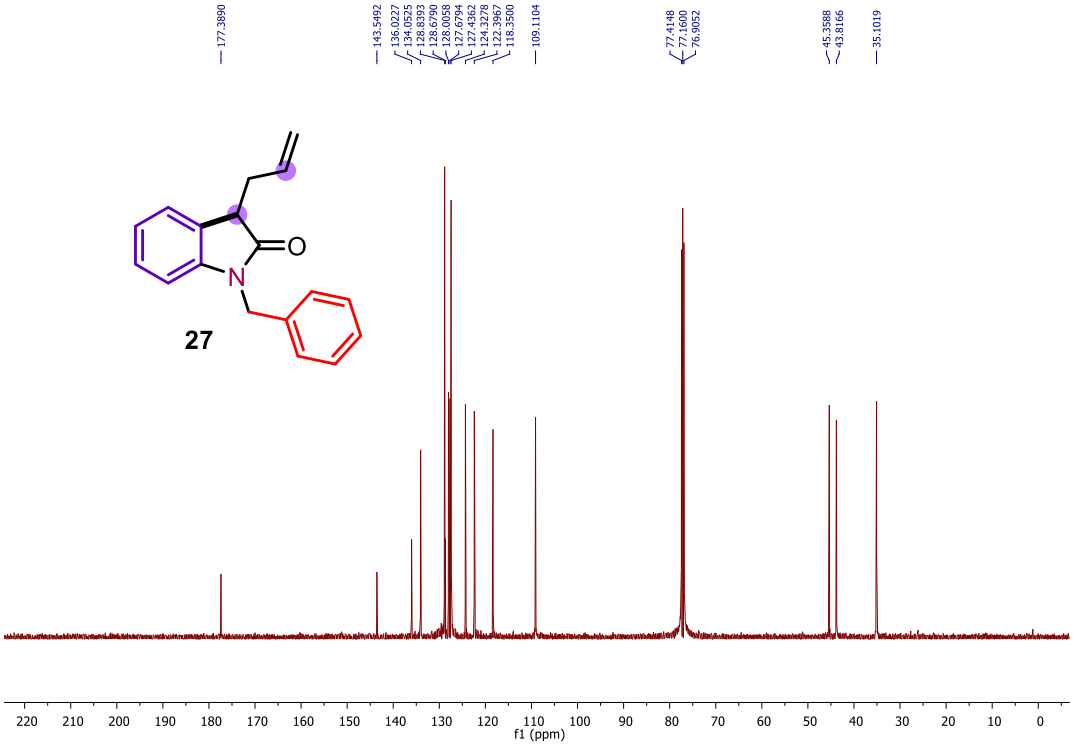


3-Allyl-1-benzylindolin-2-one (**27**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

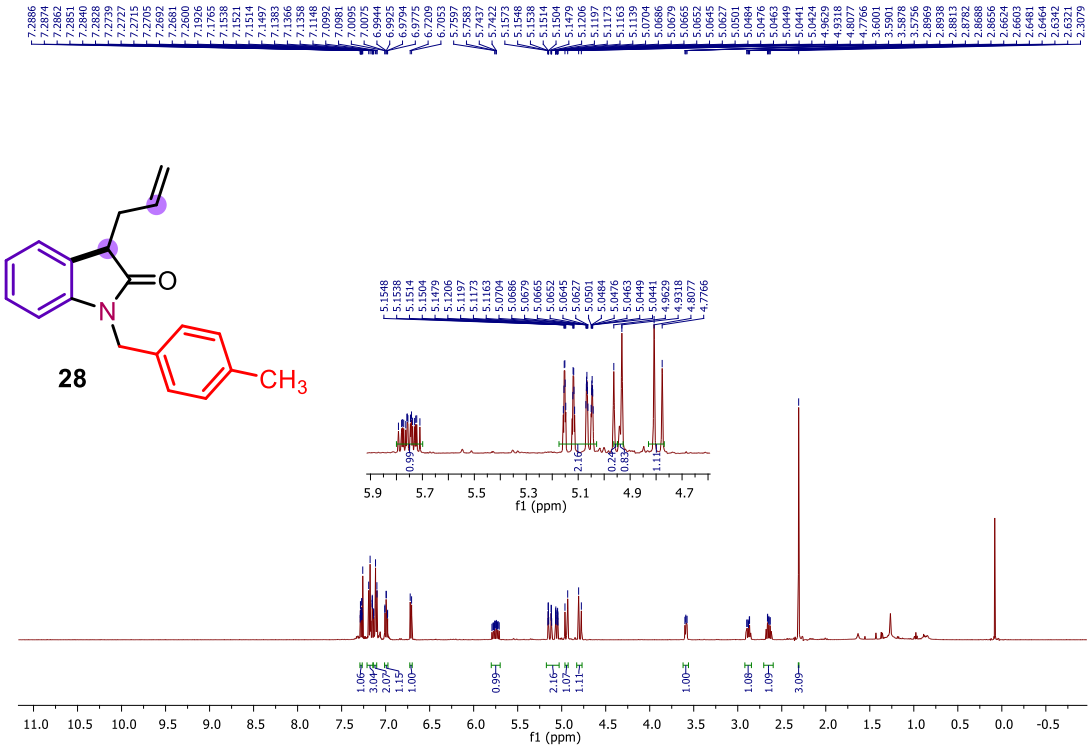


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

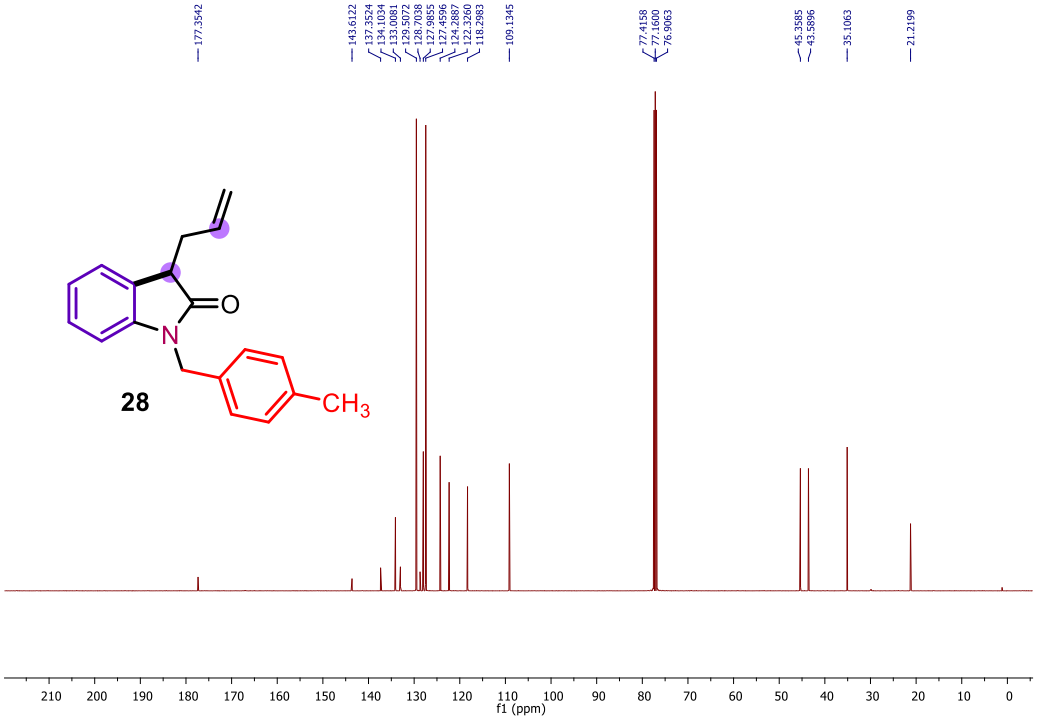


3-Allyl-1-(4-methylbenzyl)indolin-2-one (**28**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

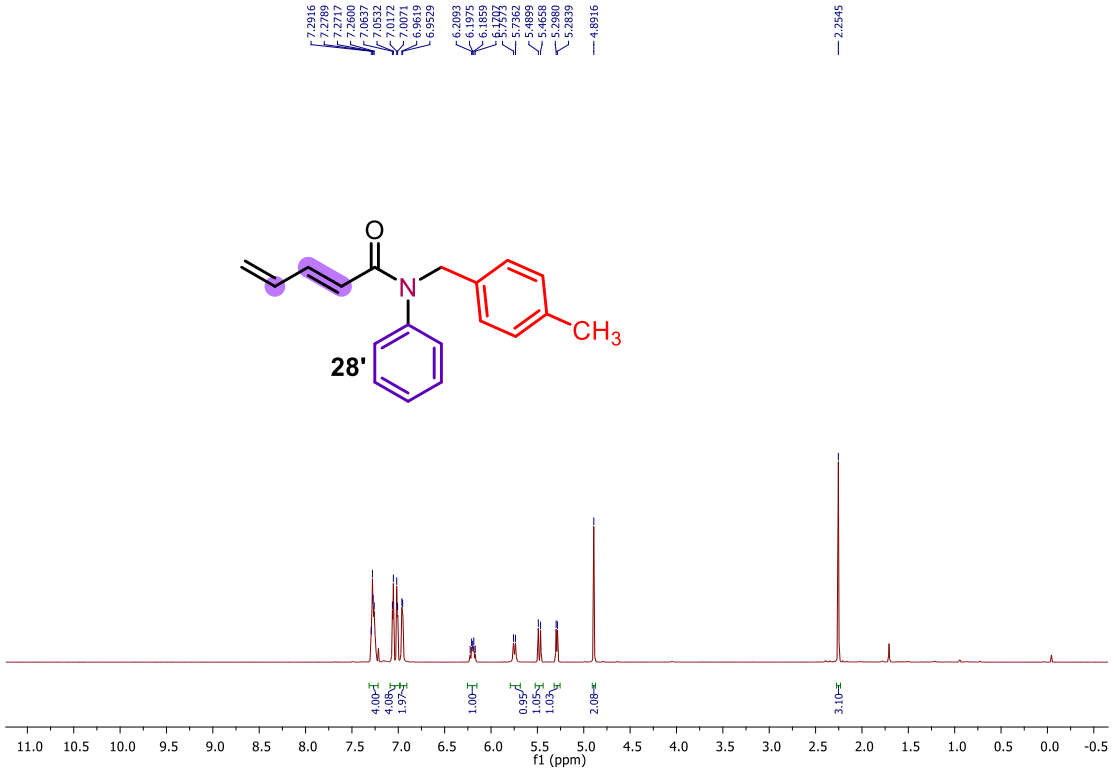


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

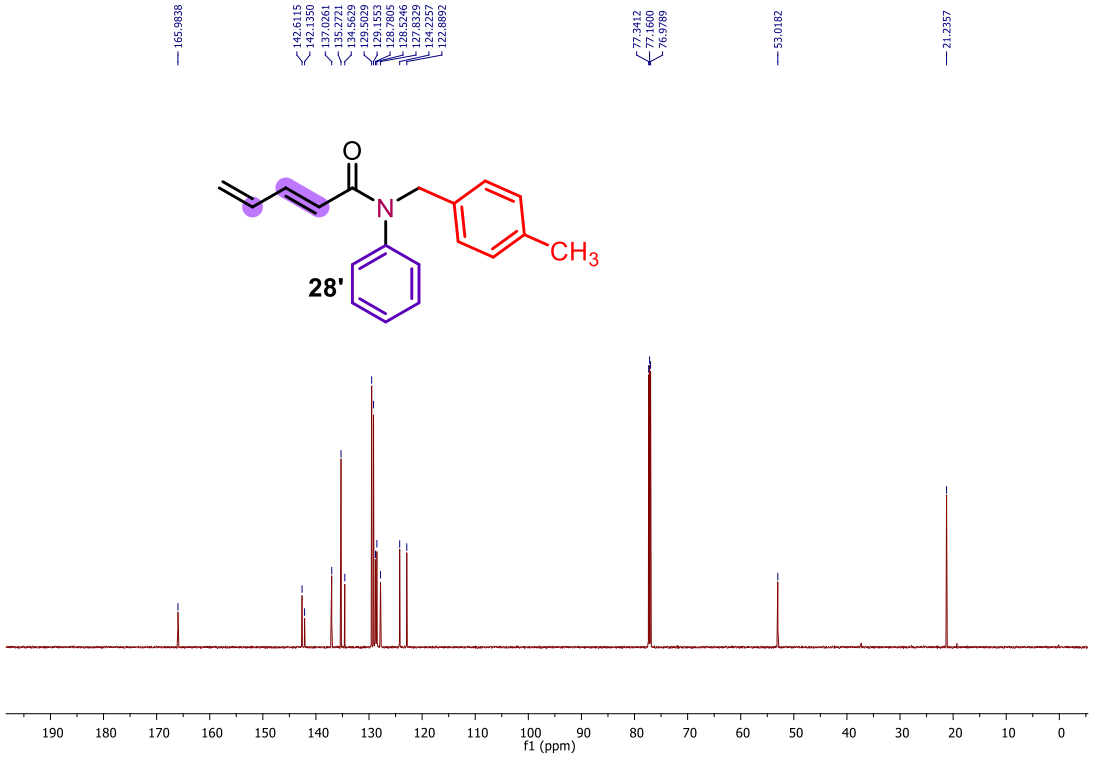


(*E*)-*N*-Cyclopentyl-*N*-phenylpenta-2,4-dienamide (**28'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

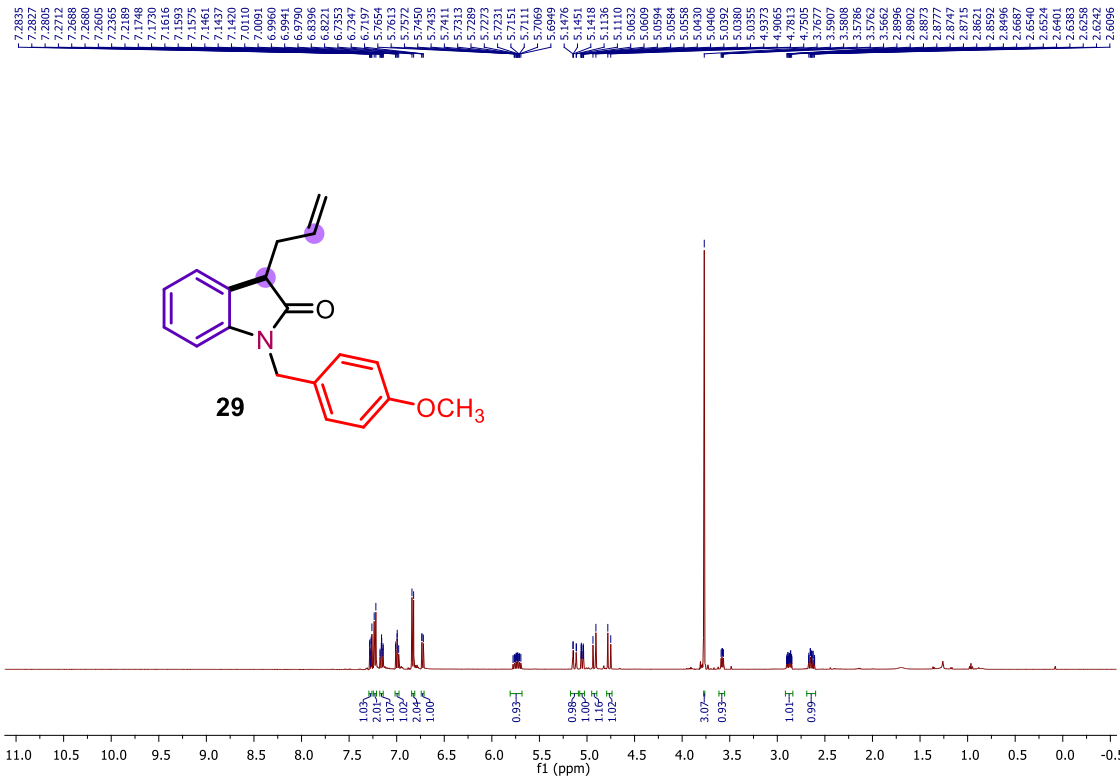


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

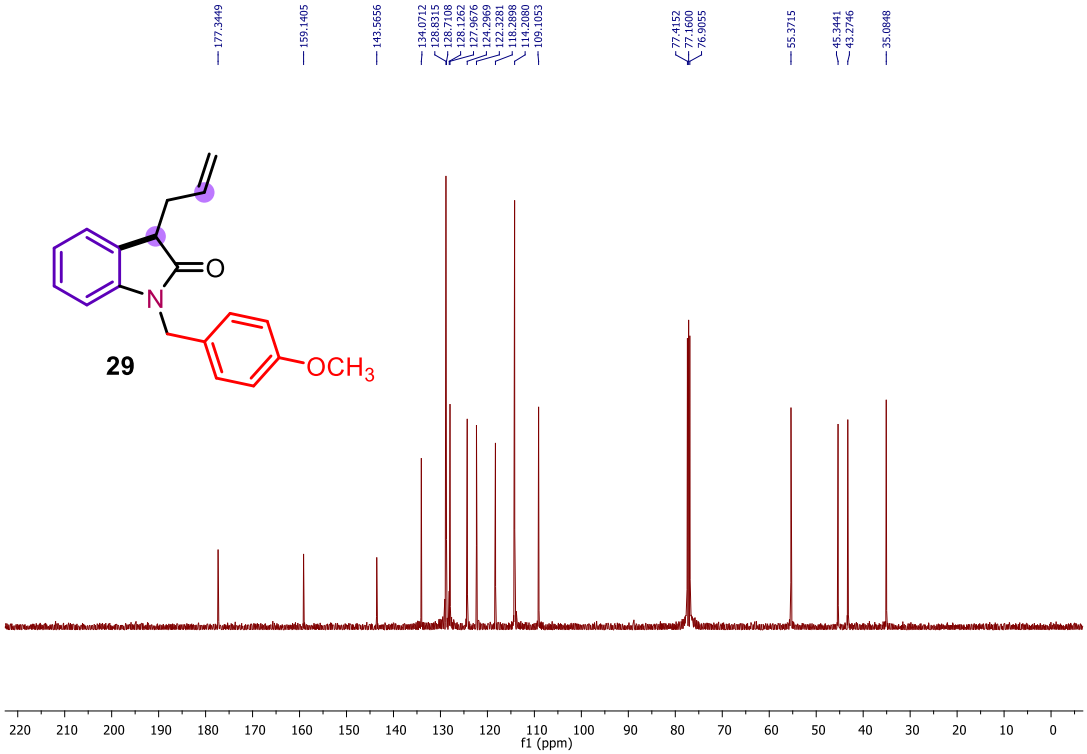


3-Allyl-1-(4-methoxybenzyl)indolin-2-one (**29**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

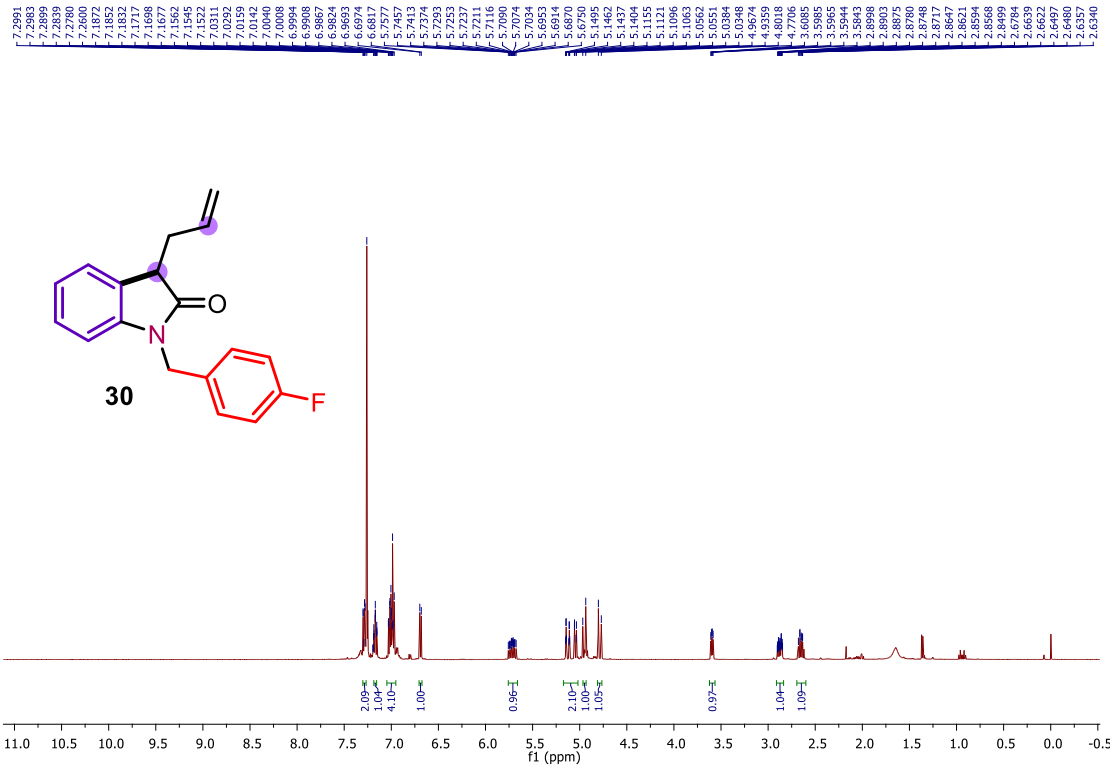


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

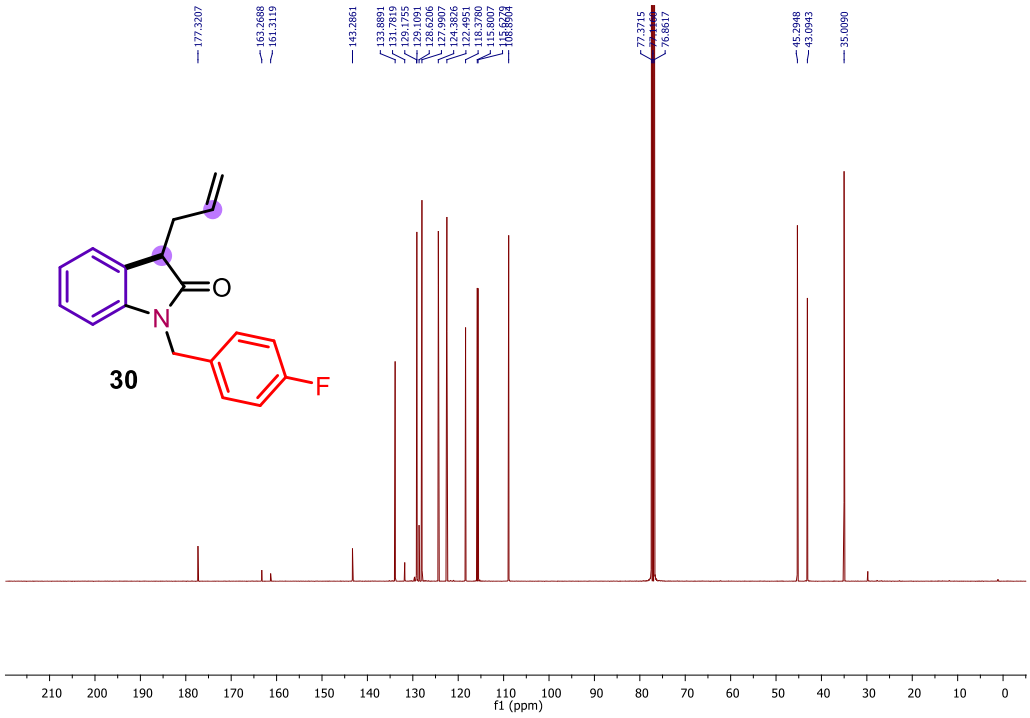


3-Allyl-1-(4-fluorobenzyl)indolin-2-one (**30**)

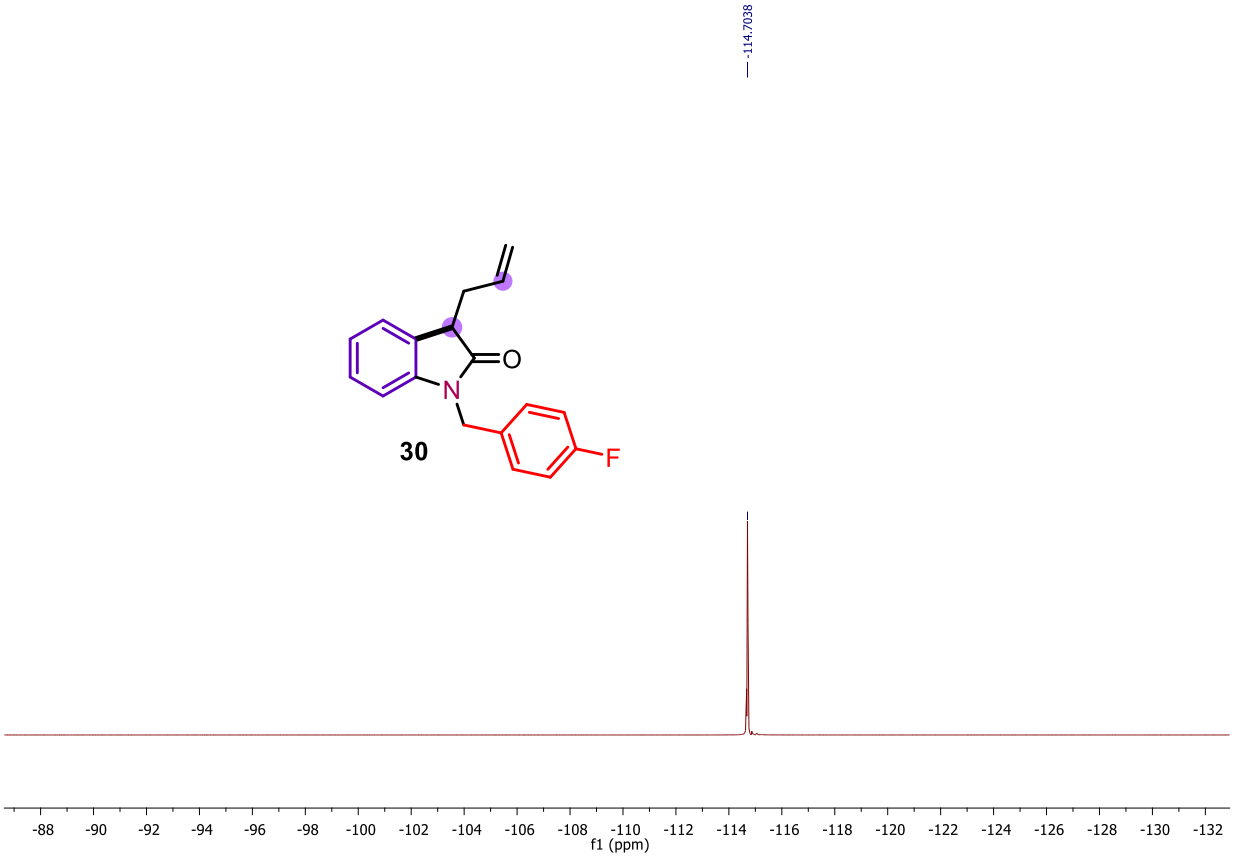
^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)



$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

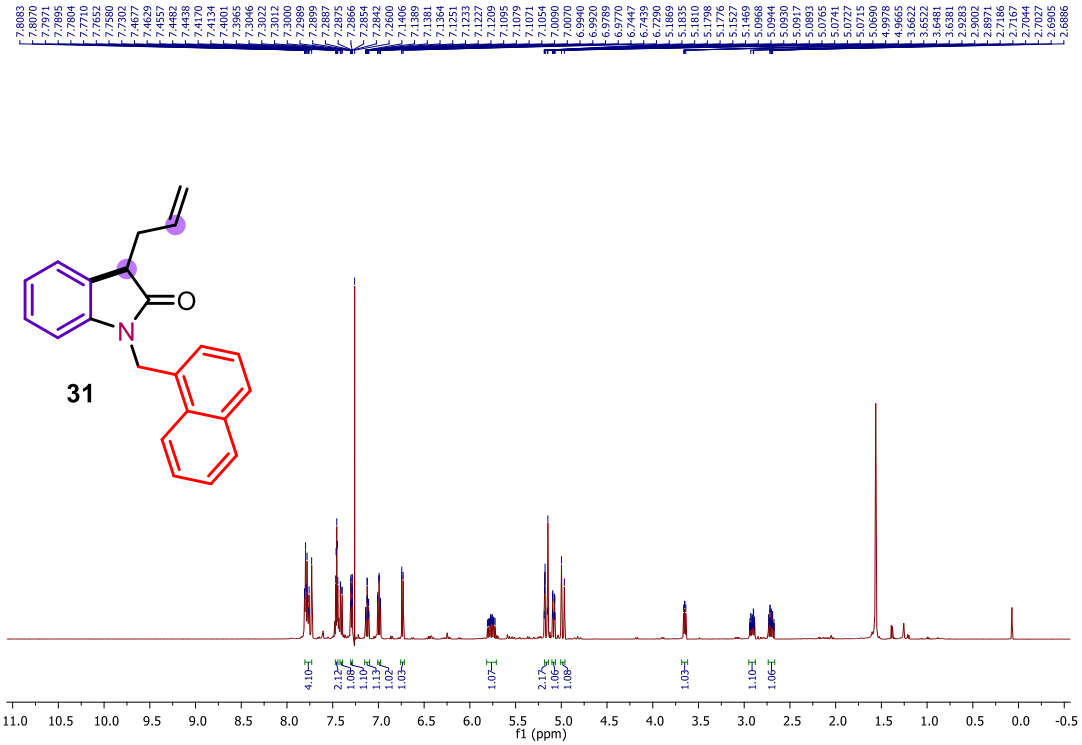


^{19}F NMR (471 MHz, $CDCl_3$, 24 °C)

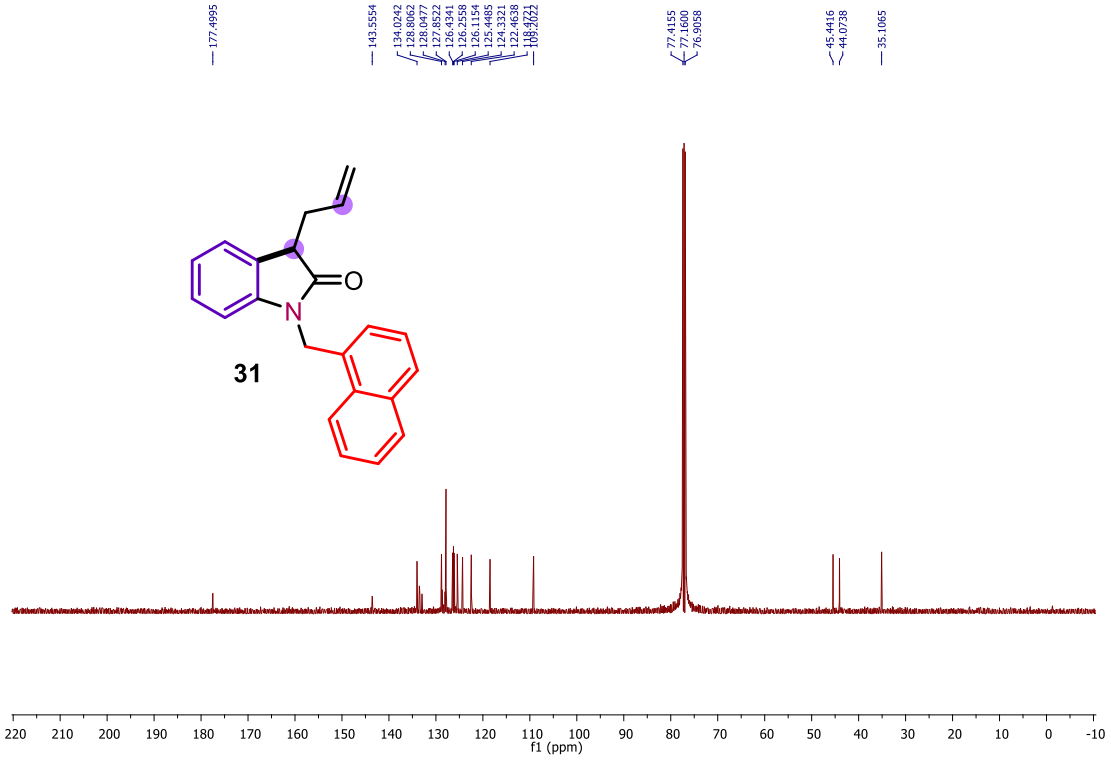


3-Allyl-1-(naphthalen-1-ylmethyl)indolin-2-one (**31**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

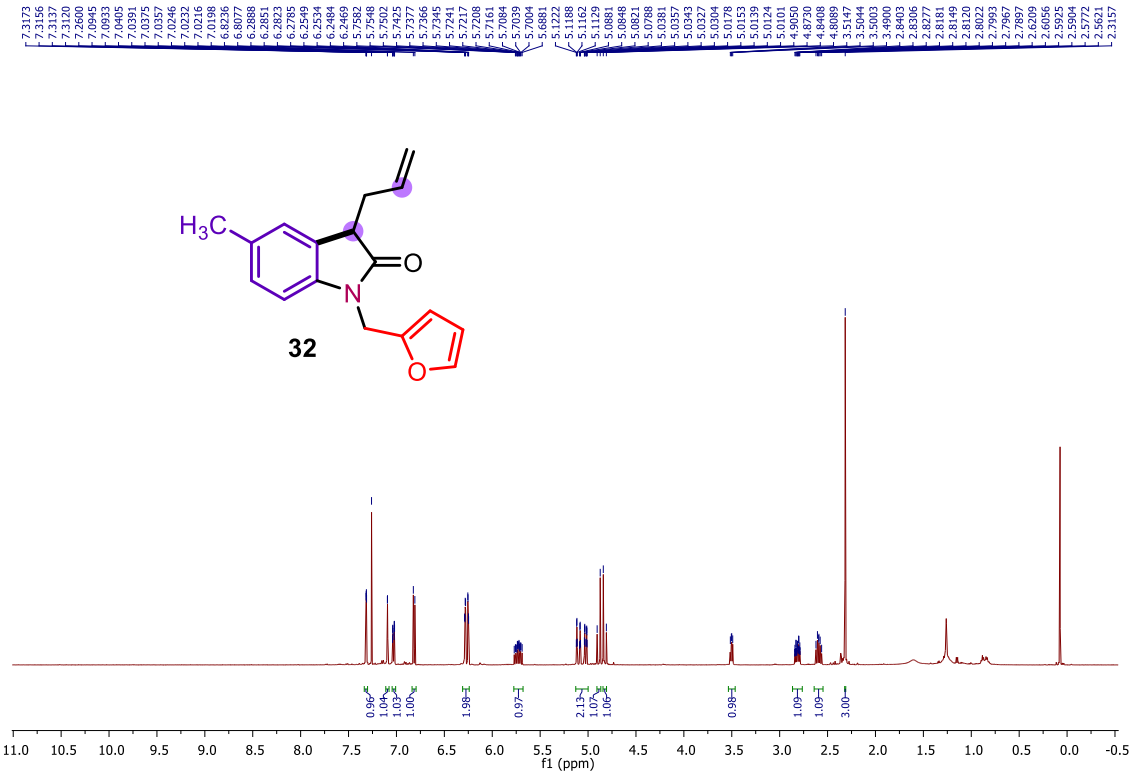


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

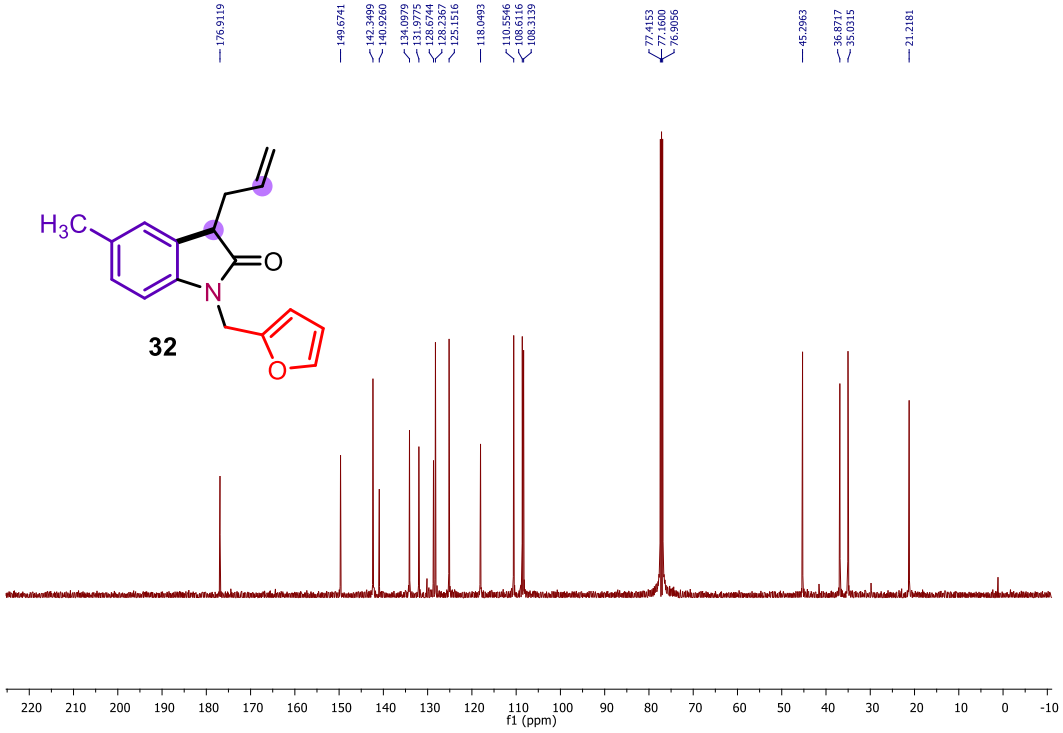


3-Allyl-1-(furan-2-ylmethyl)-5-methylindolin-2-one (**32**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

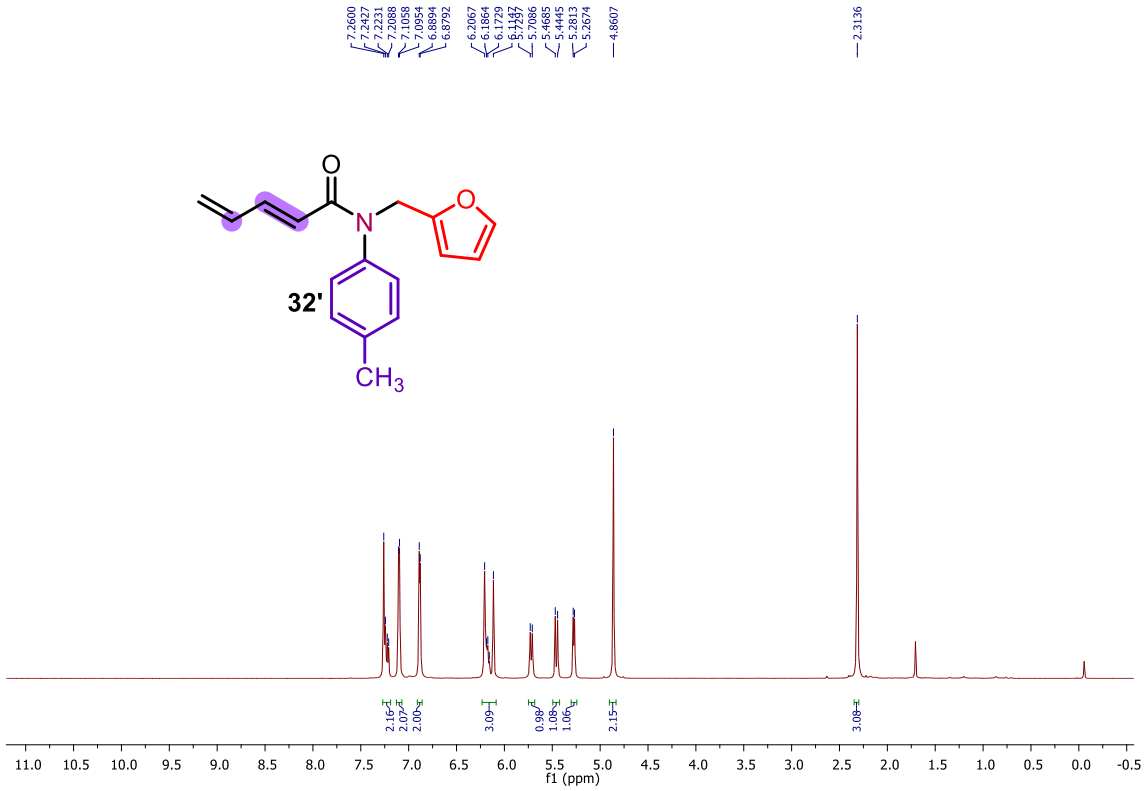


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

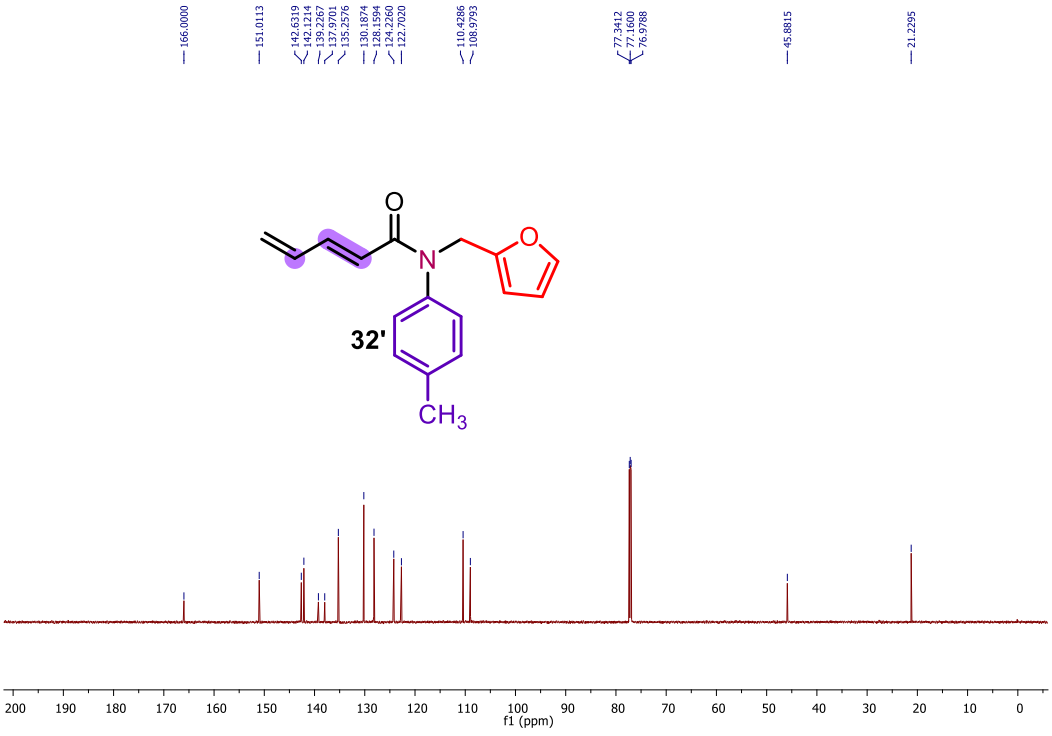


(*E*)-*N*-(furan-2-ylmethyl)-*N*-(p-tolyl)penta-2,4-dienamide (**32'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

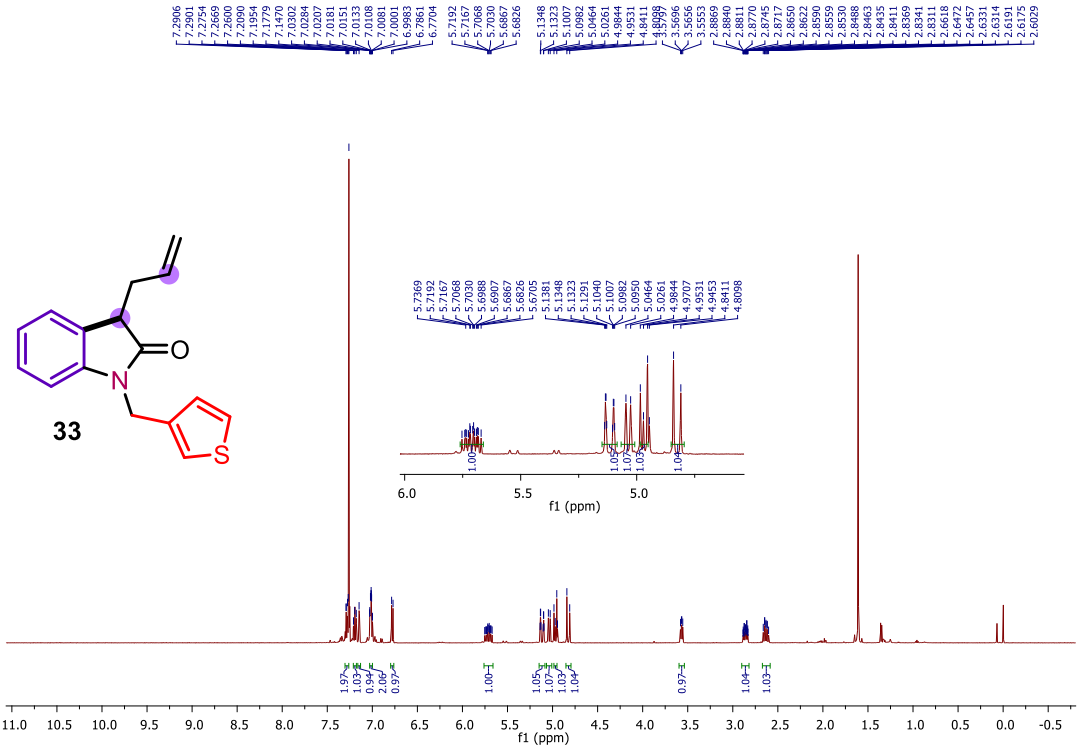


^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$, 24 °C)

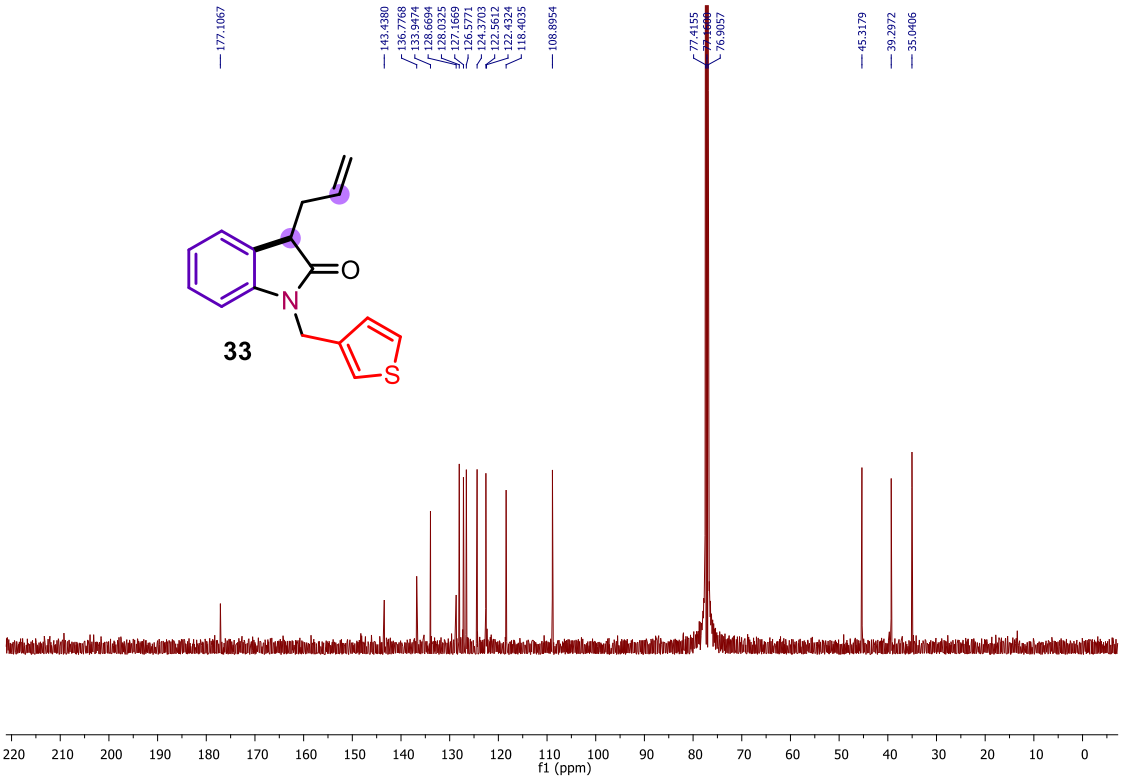


3-Allyl-1-(furan-2-ylmethyl)-5-methylindolin-2-one (**33**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

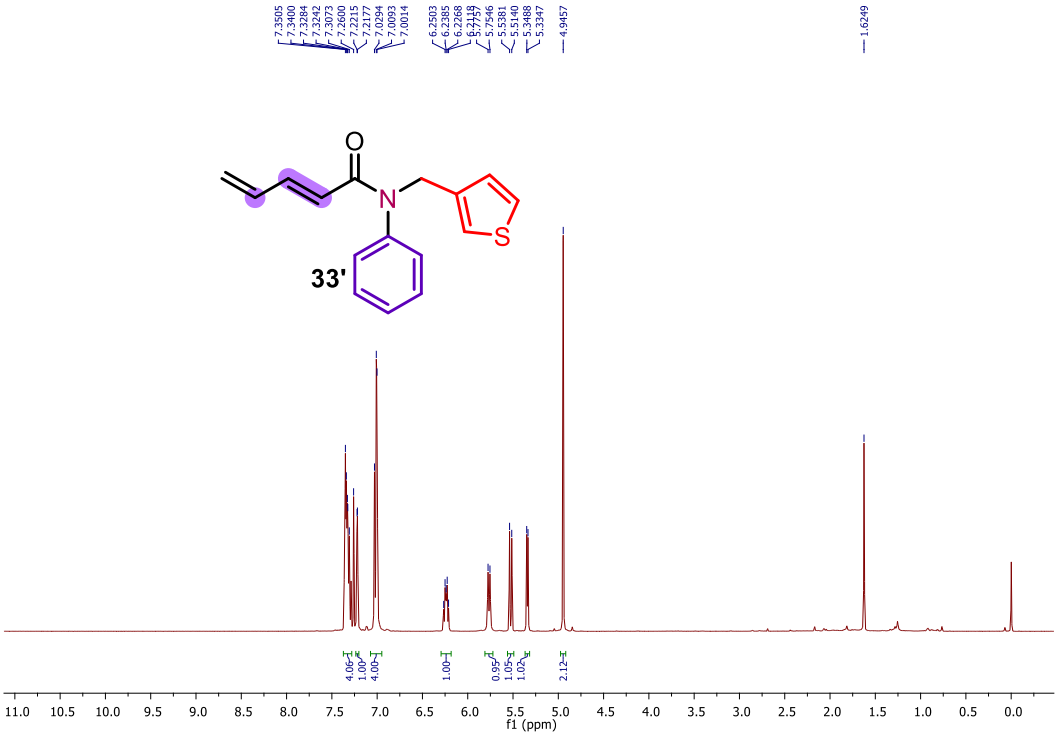


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

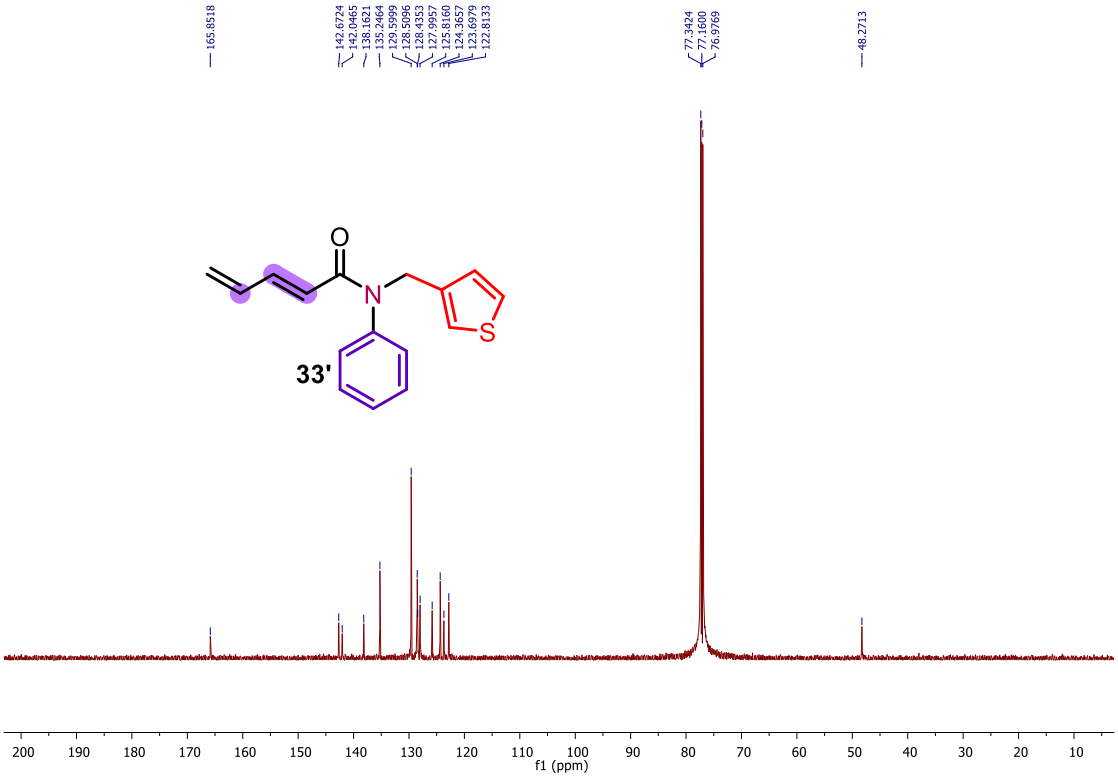


(*E*)-*N*-Phenyl-*N*-(thiophen-3-ylmethyl)penta-2,4-dienamide (**33'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

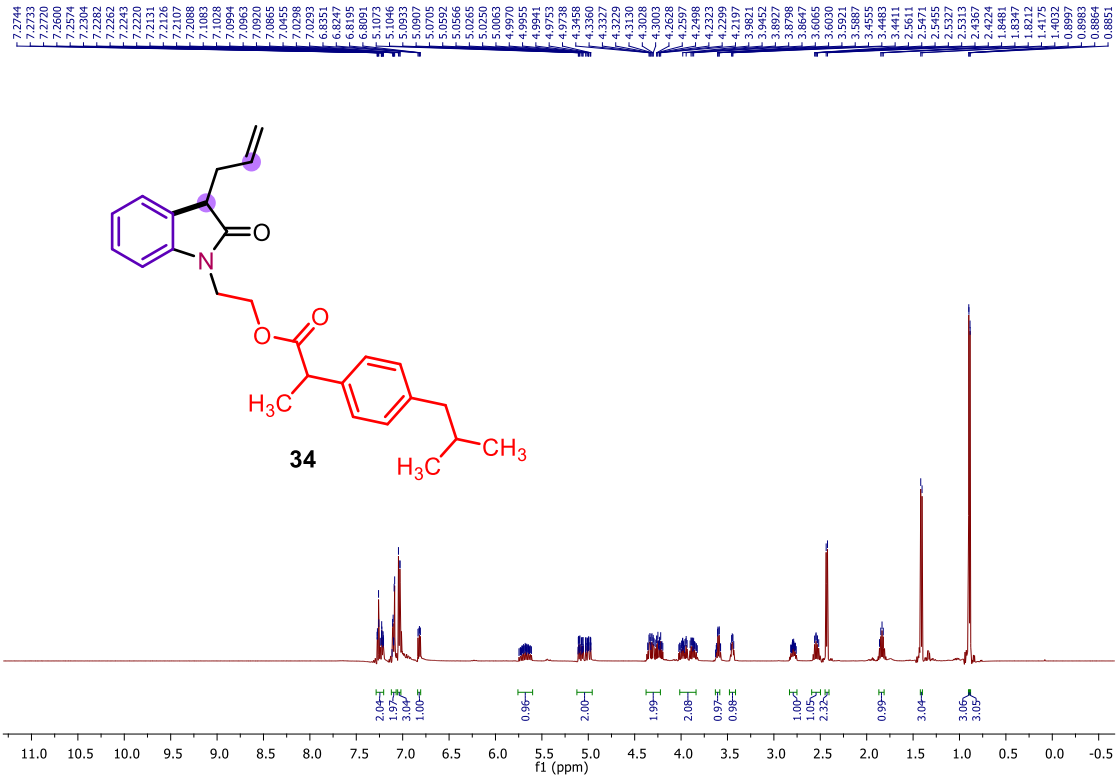


^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$, 24 °C)

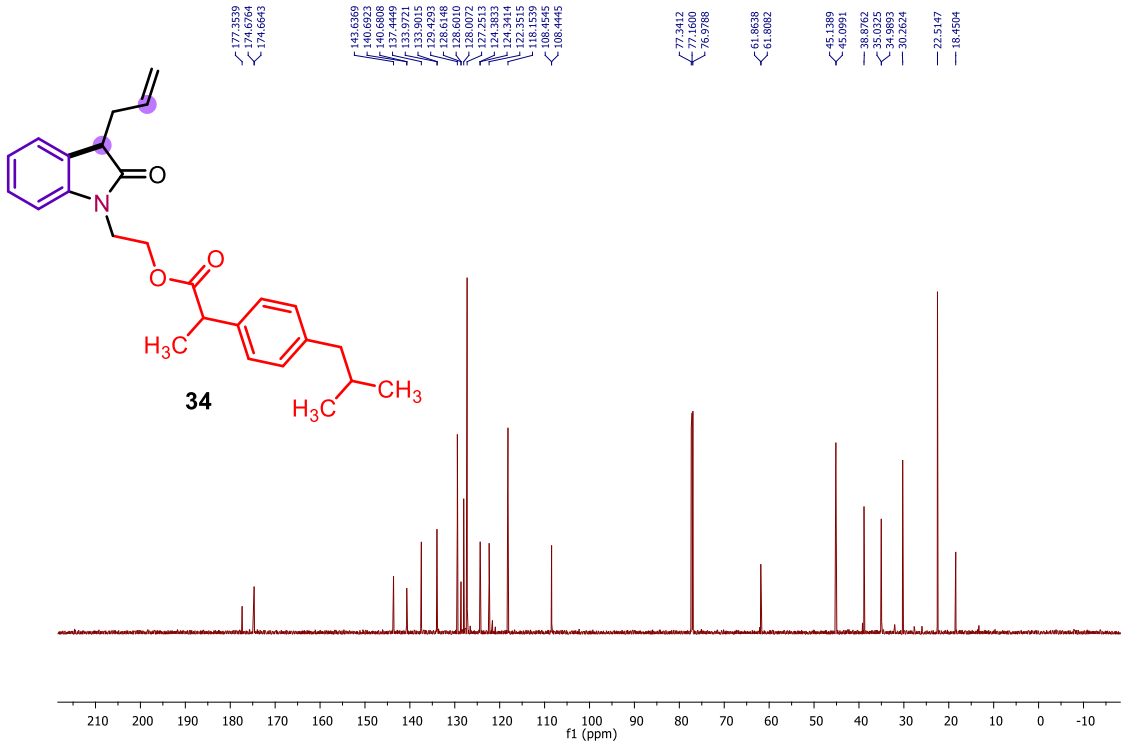


2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(4-isobutylphenylpropanoate (**34**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

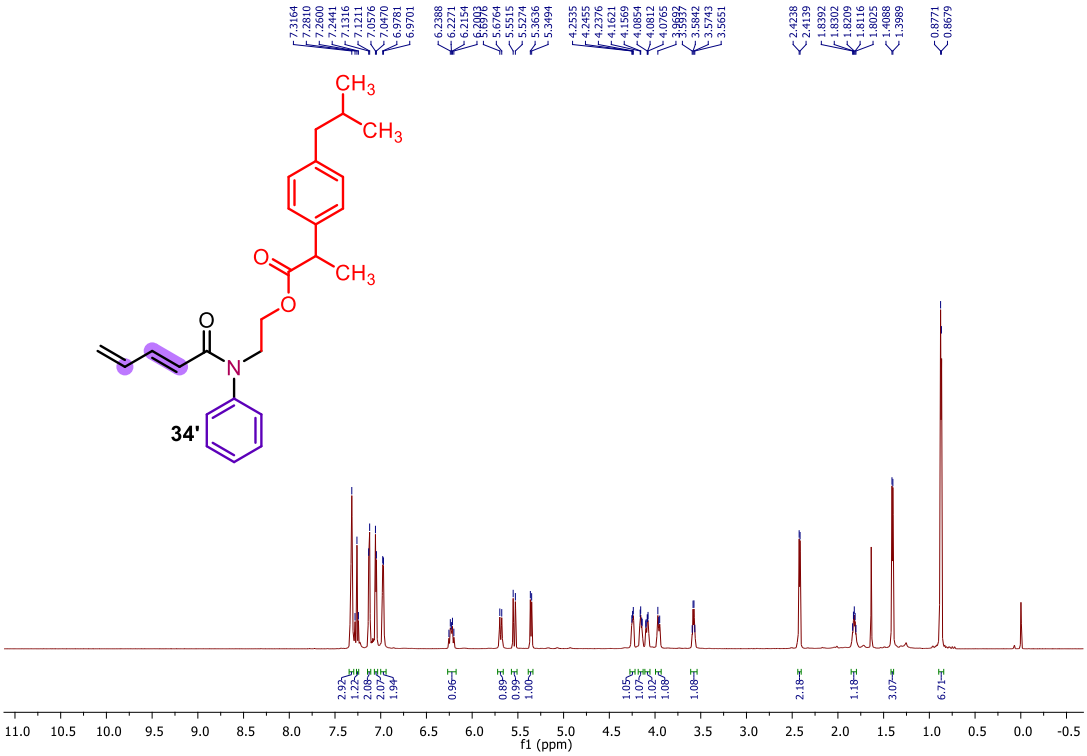


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

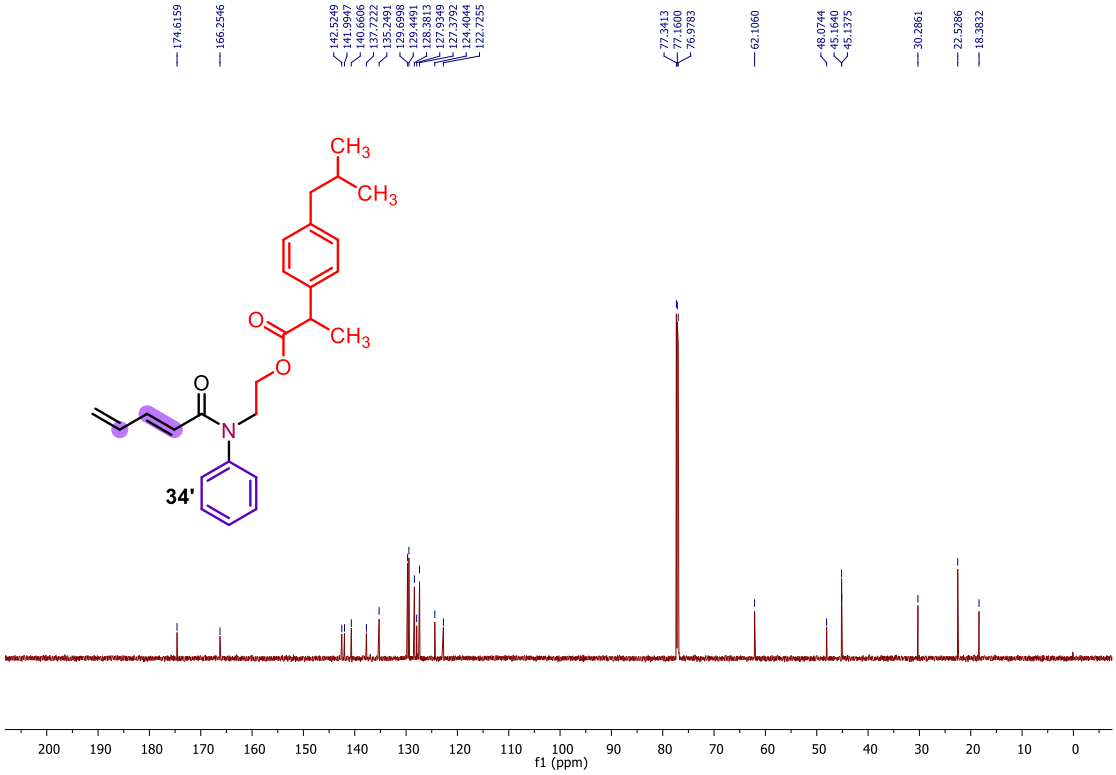


(*E*)-2-(*N*-phenylpenta-2,4-dienamido)ethyl 2-(4-isobutylphenyl)propanoate (**34'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

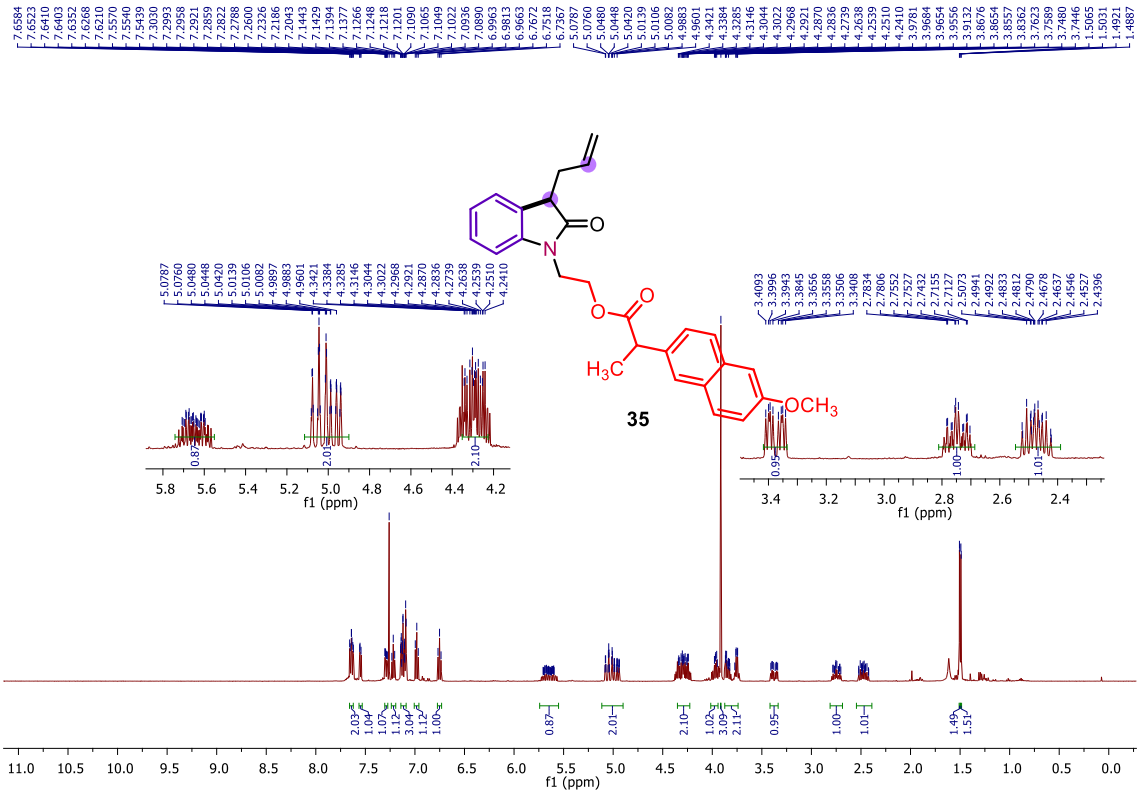


^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$, 24 °C)

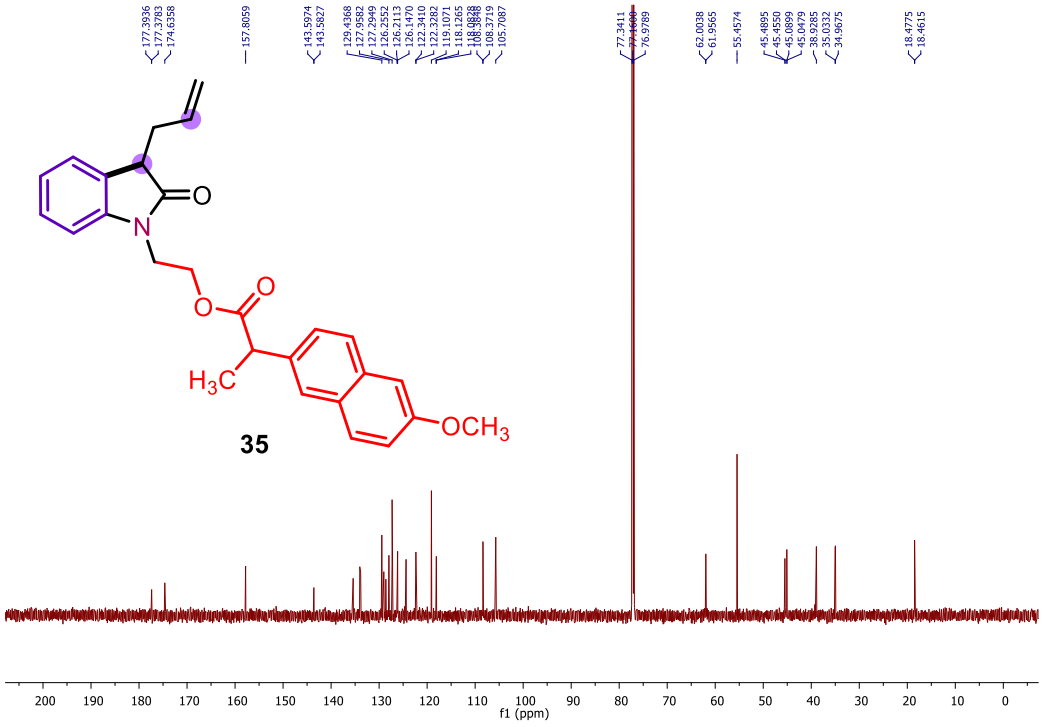


2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(6-methoxynaphthalen-2-yl) propanoate (**35**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

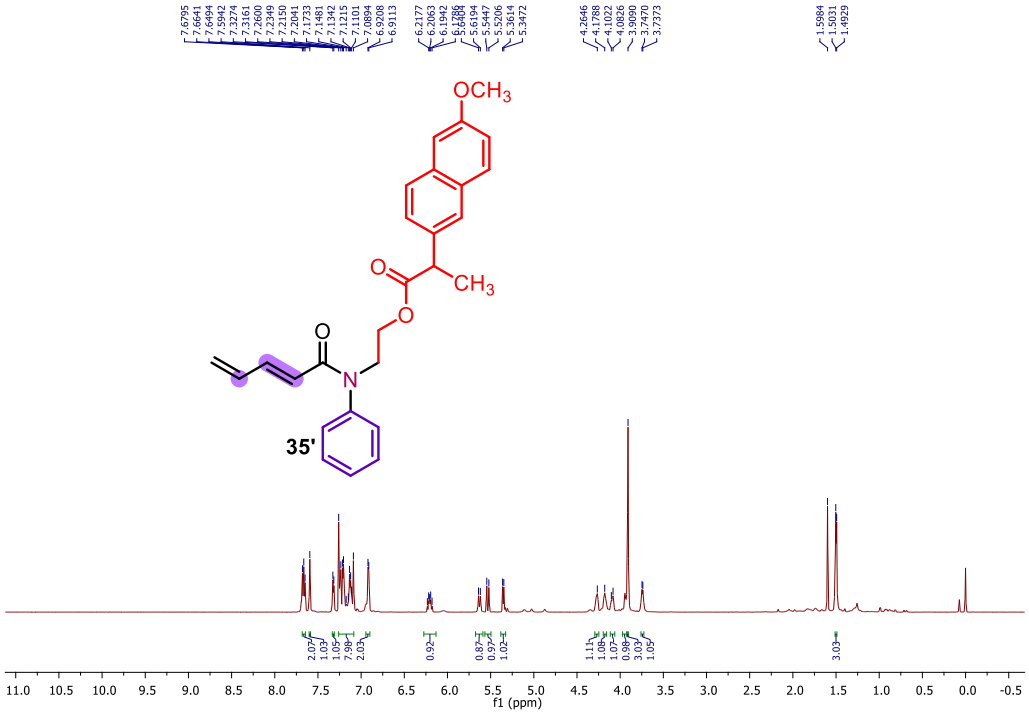


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

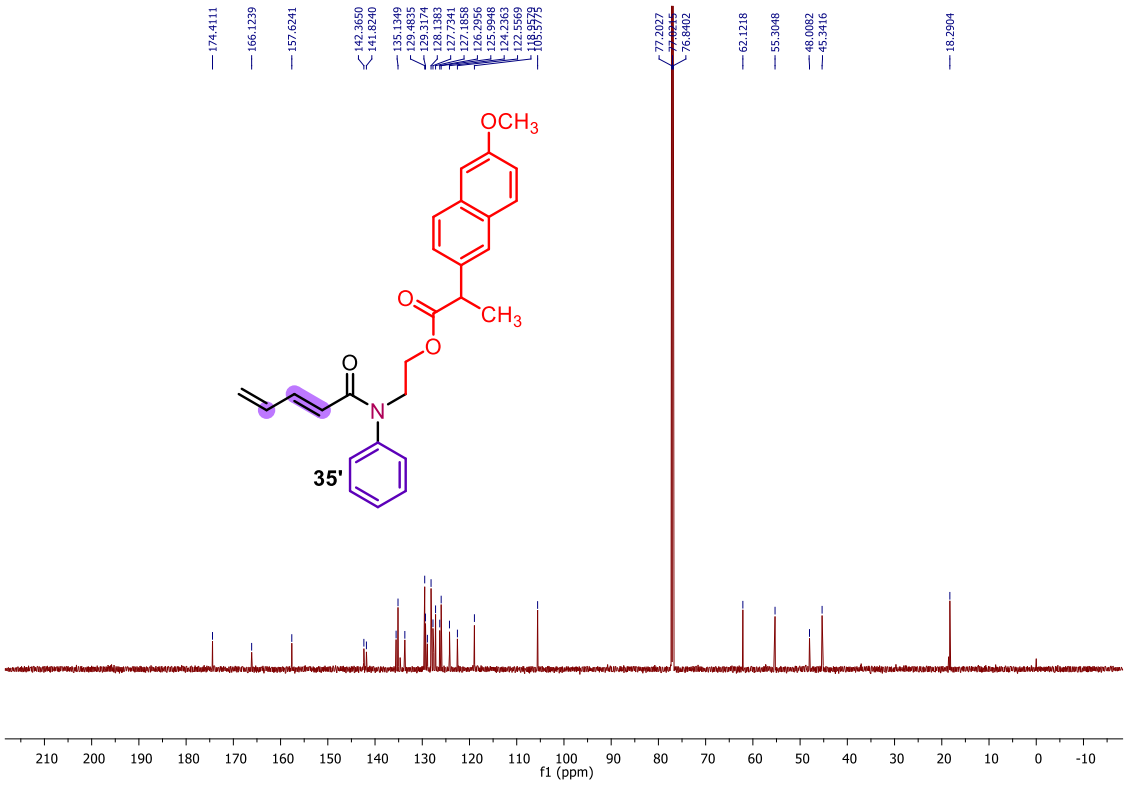


(*E*)-2-(N-phenylpenta-2,4-dienamido)ethyl 2-(6-methoxynaphthalen-2-yl)propanoate (**35'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

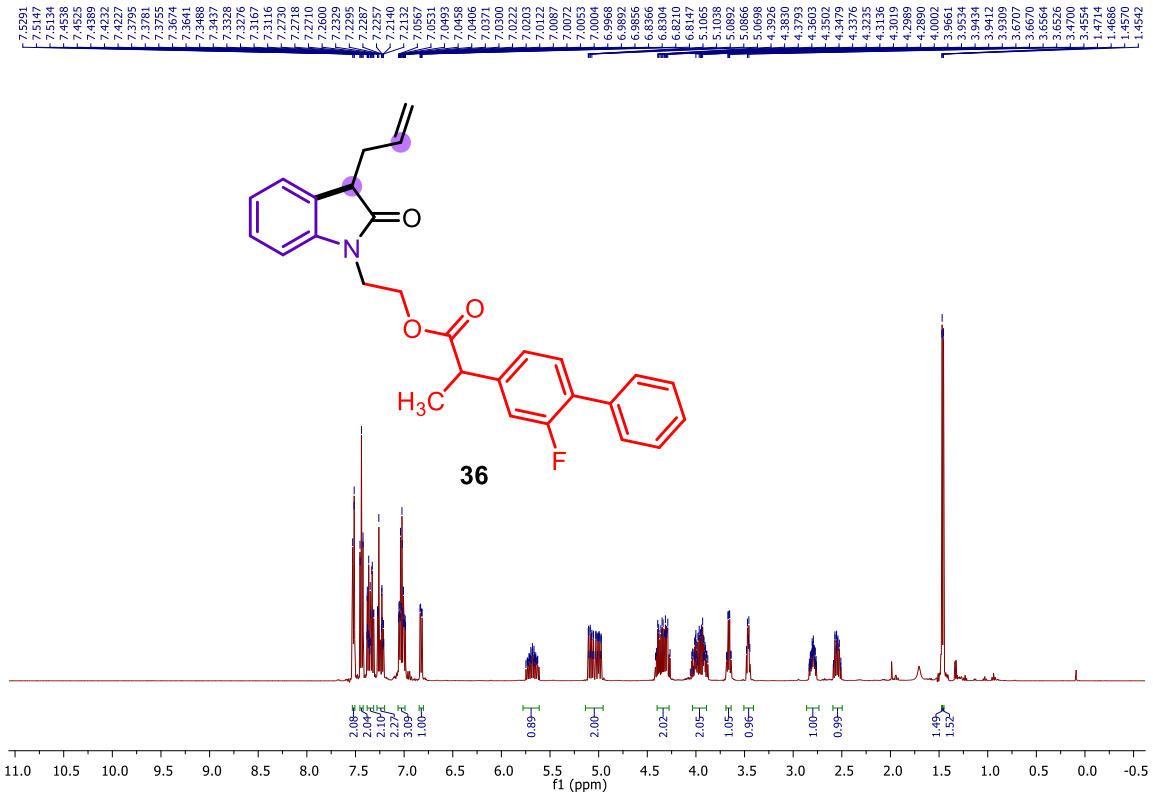


^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$, 24 °C)

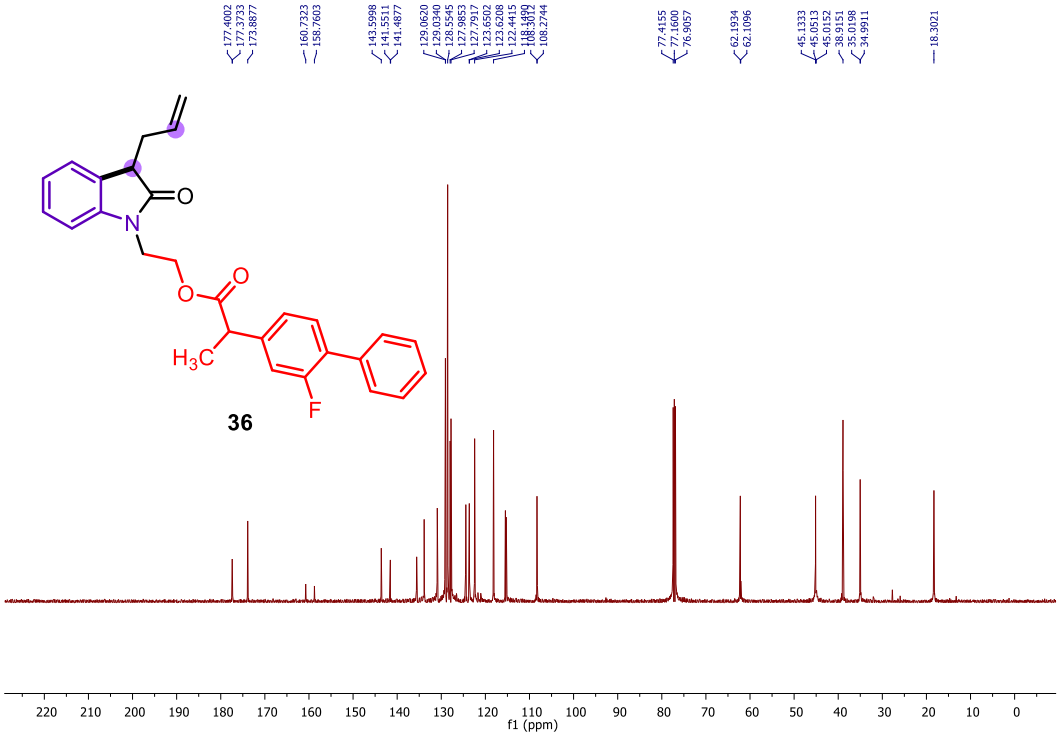


2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl) propanoate (**36**)

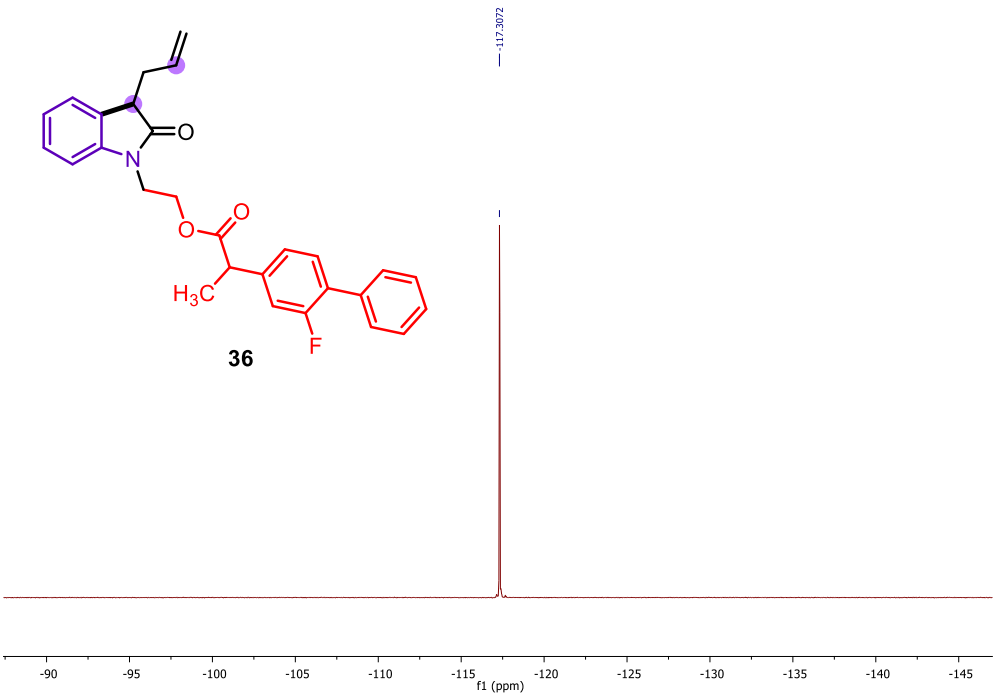
^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)



^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$, 24 °C)

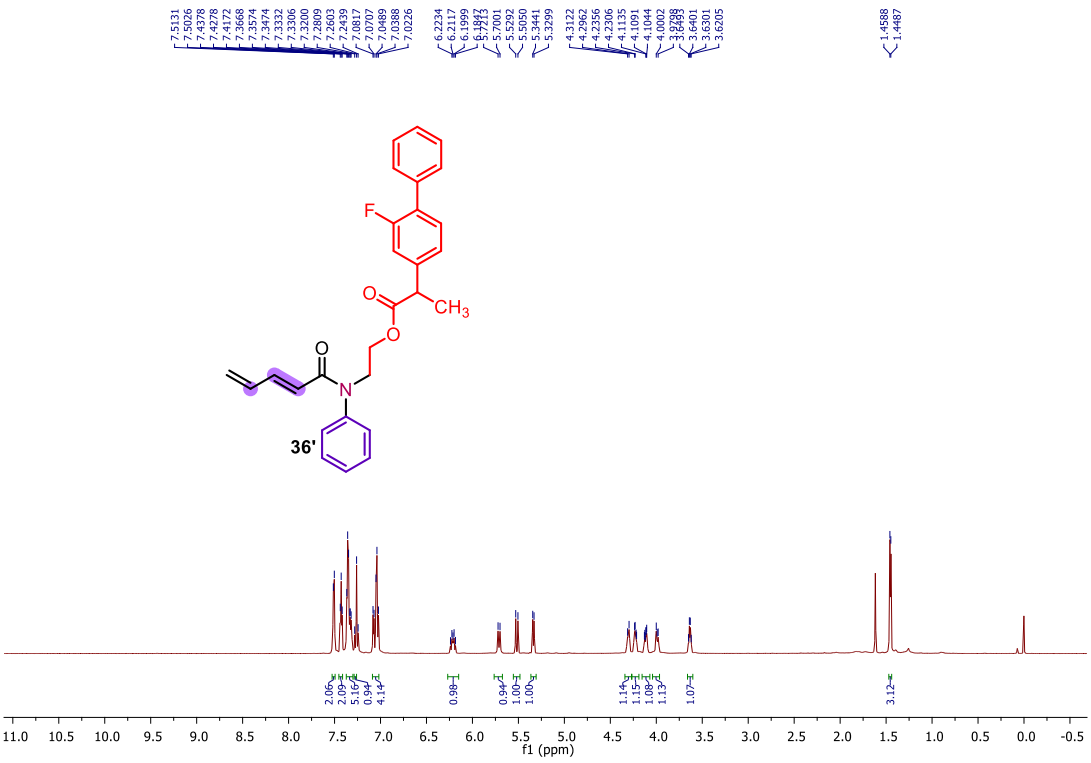


^{19}F NMR (471 MHz, $CDCl_3$, 24 °C)

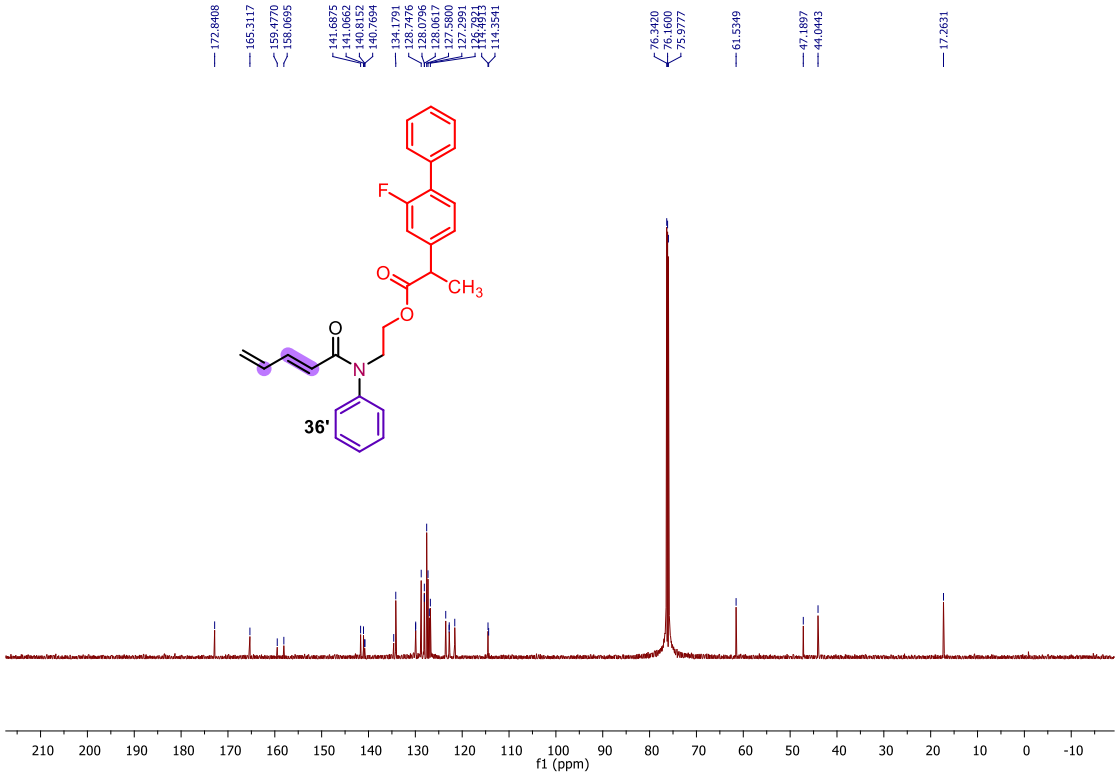


(*E*)-2-(*N*-phenylpenta-2,4-dienamido)ethyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (**36'**)

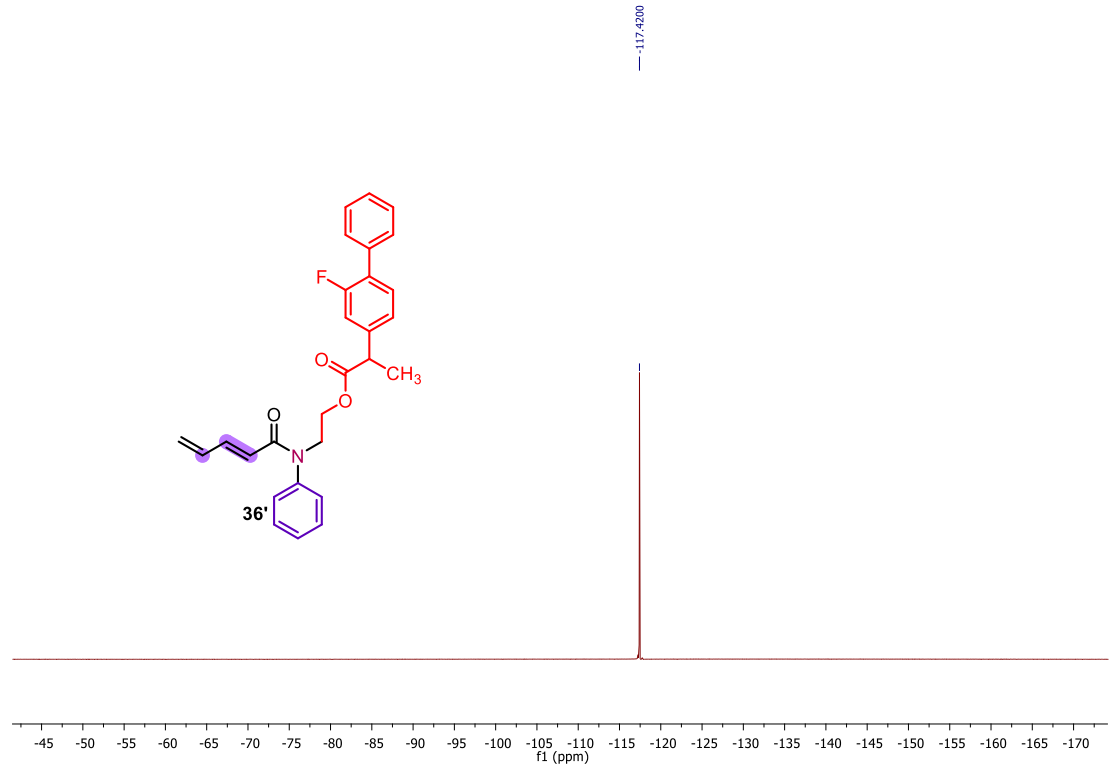
^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)



$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

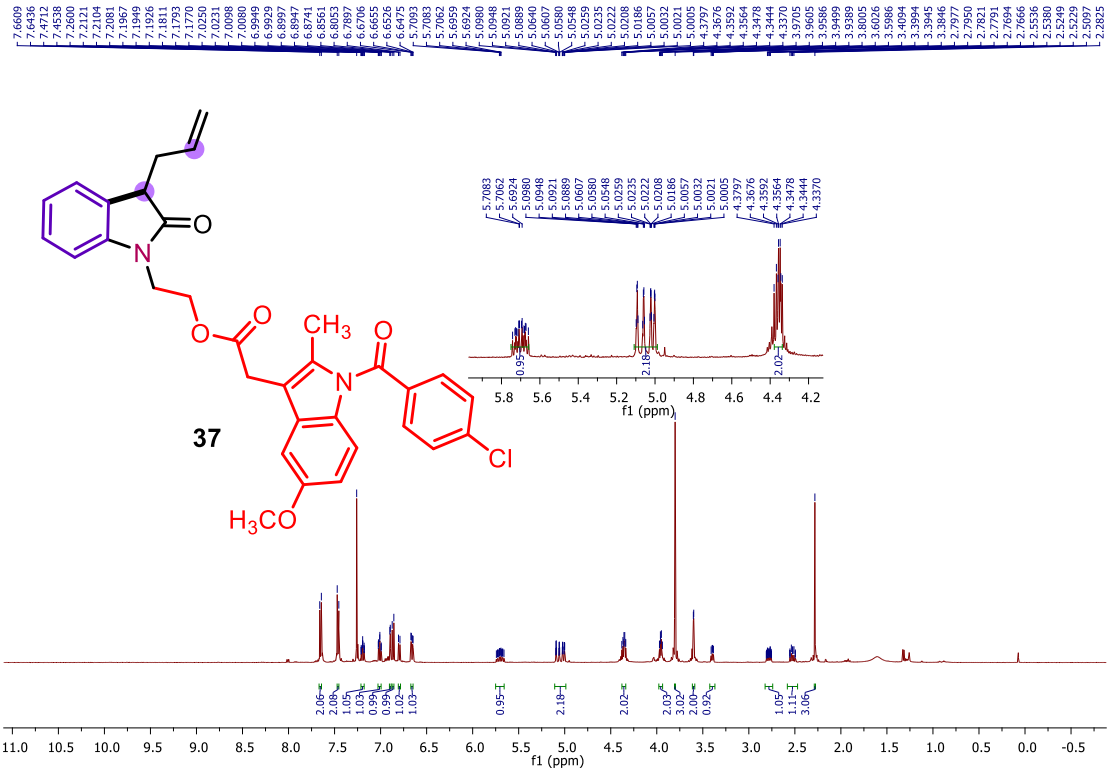


^{19}F NMR (471 MHz, $CDCl_3$, 24 °C)

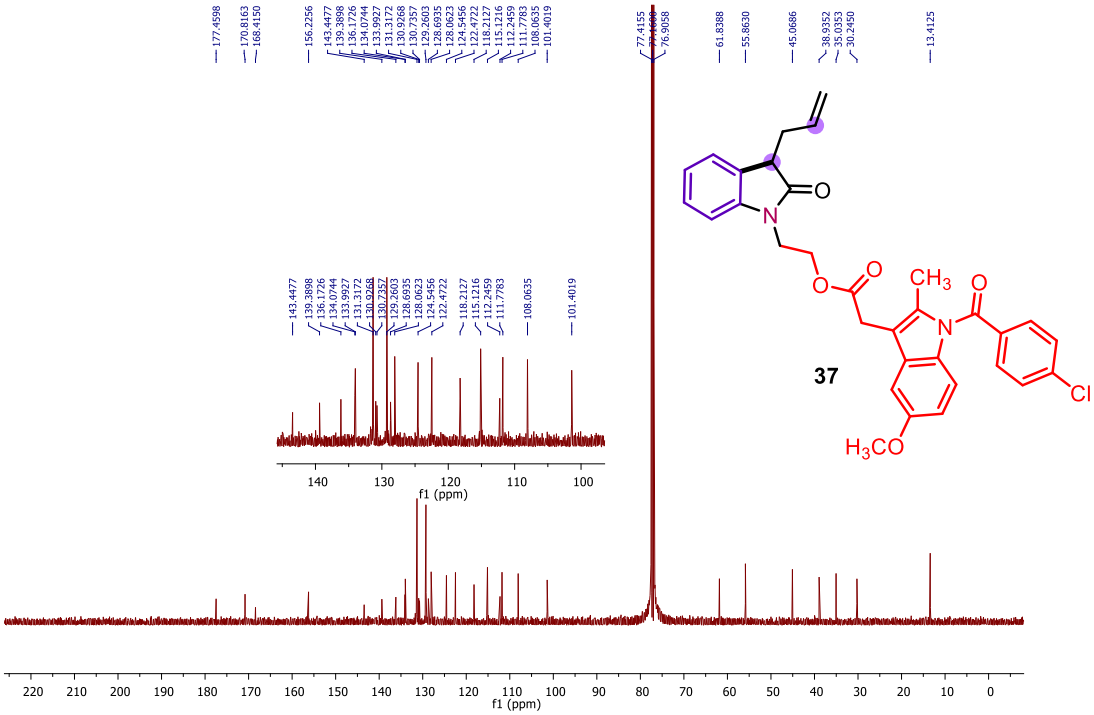


2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl) propanoate (**37**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

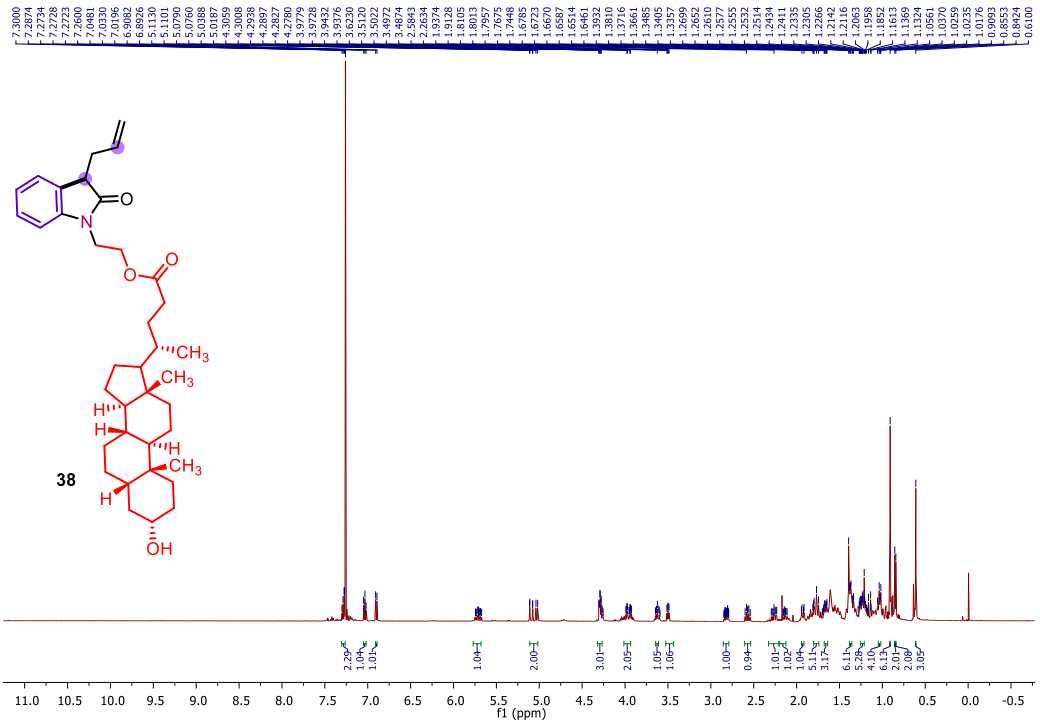


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

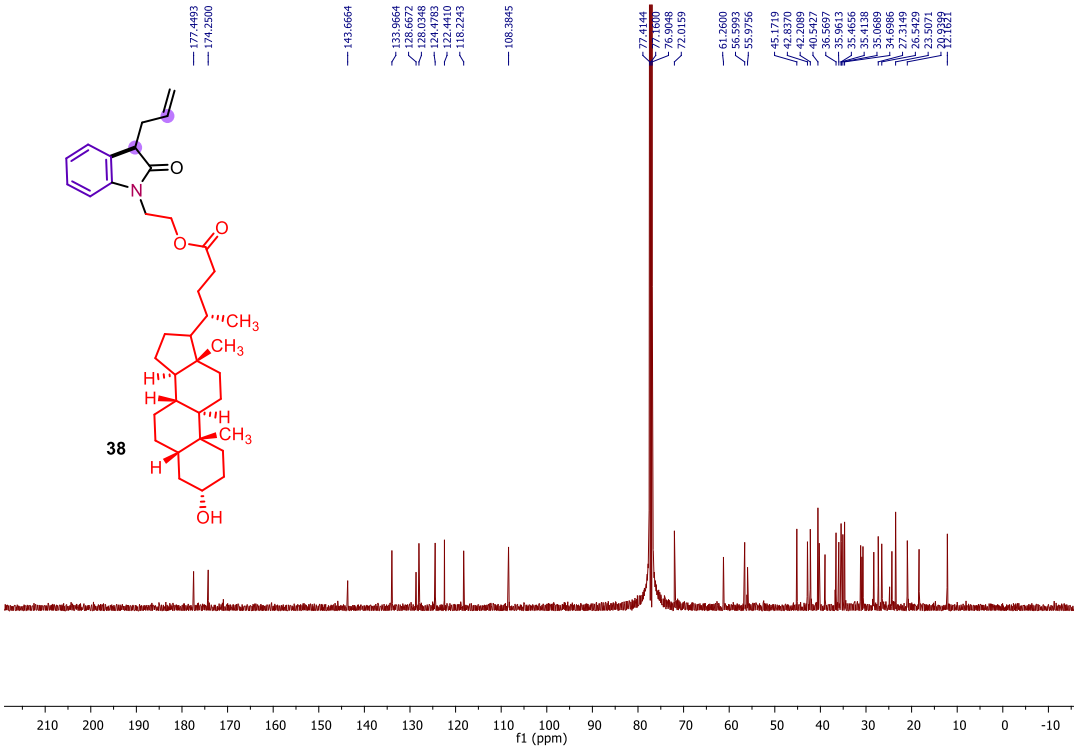


2-(3-Allyl-2-oxoindolin-1-yl) ethyl 3-hydroxy-10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)pentanoate (**38**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

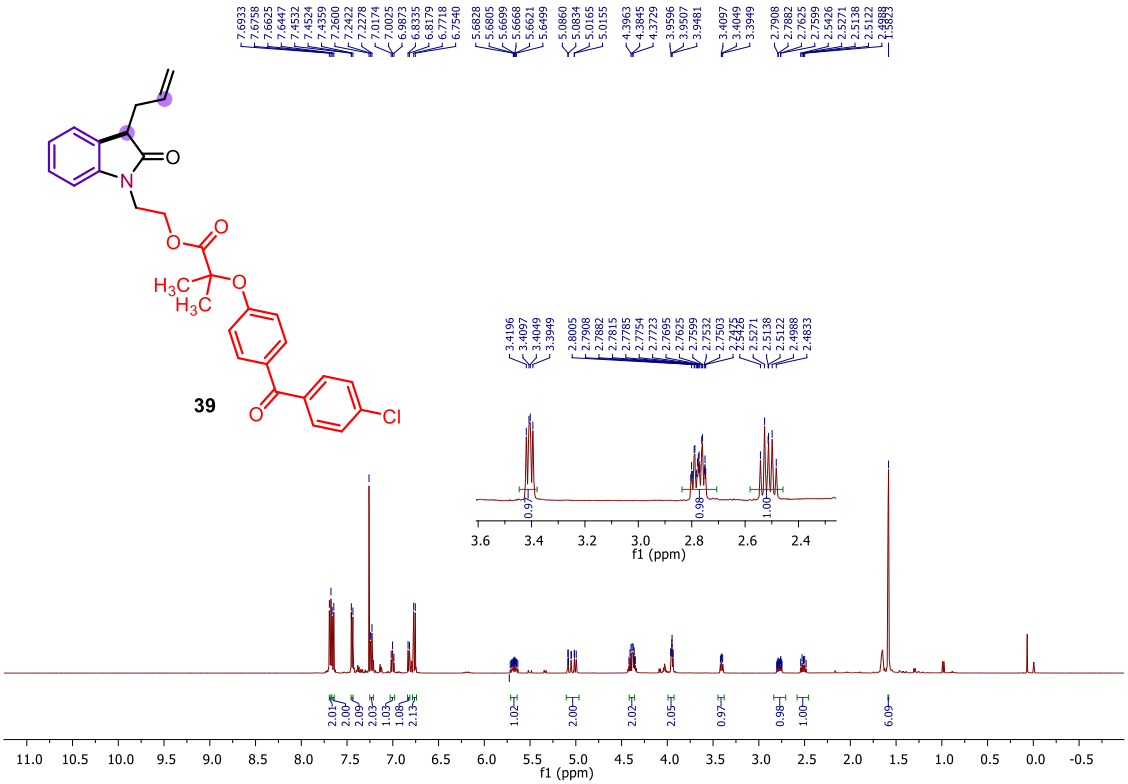


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

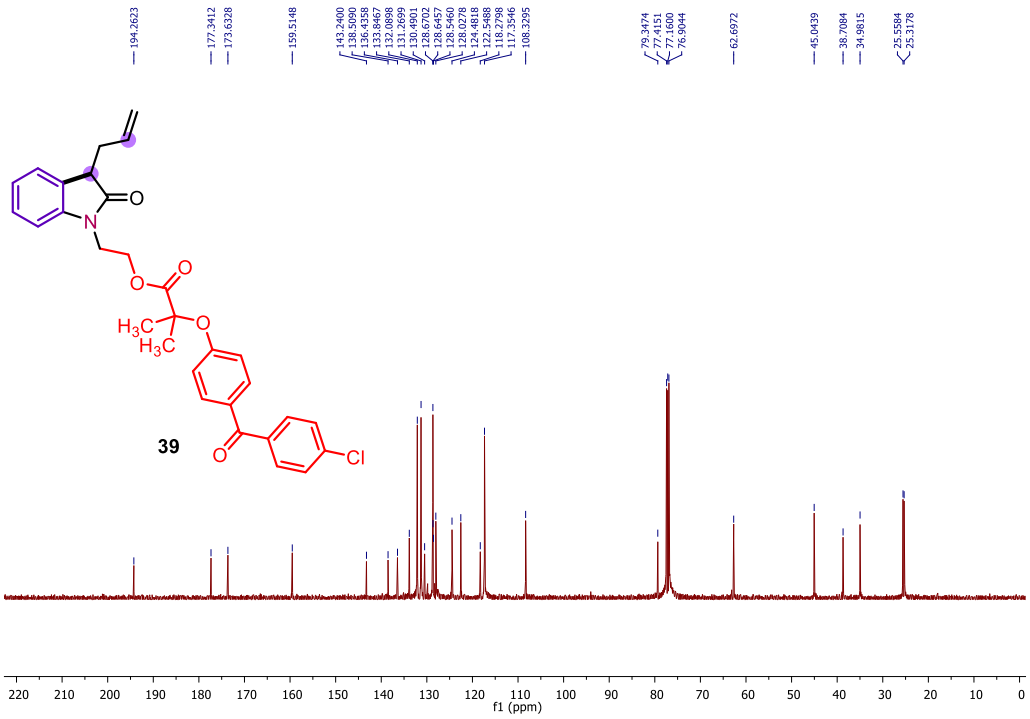


2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl) propanoate (**39**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

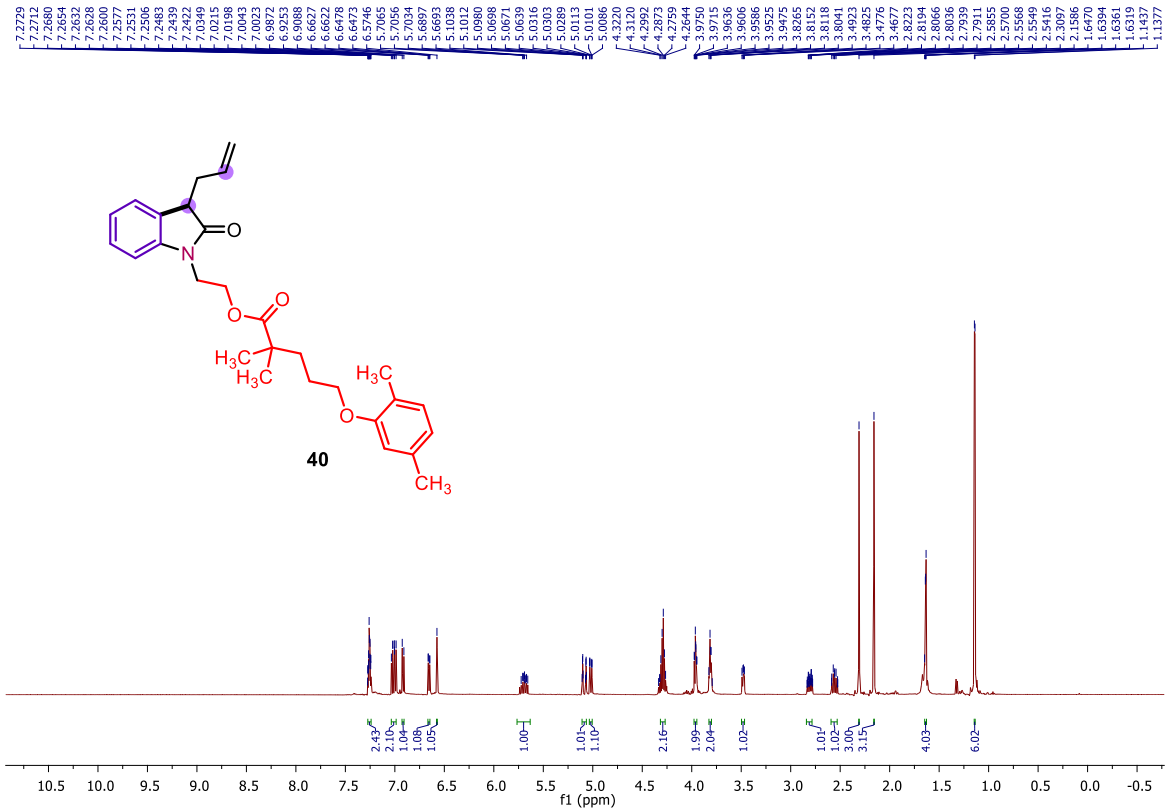


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

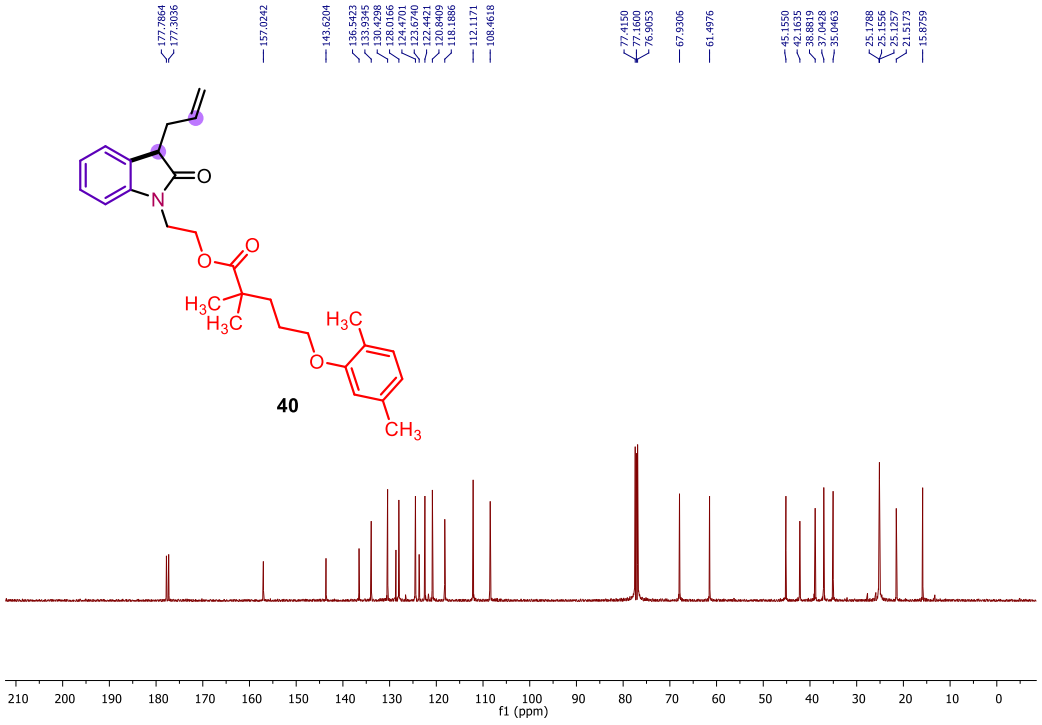


2-(3-Allyl-2-oxoindolin-1-yl)ethyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (**40**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

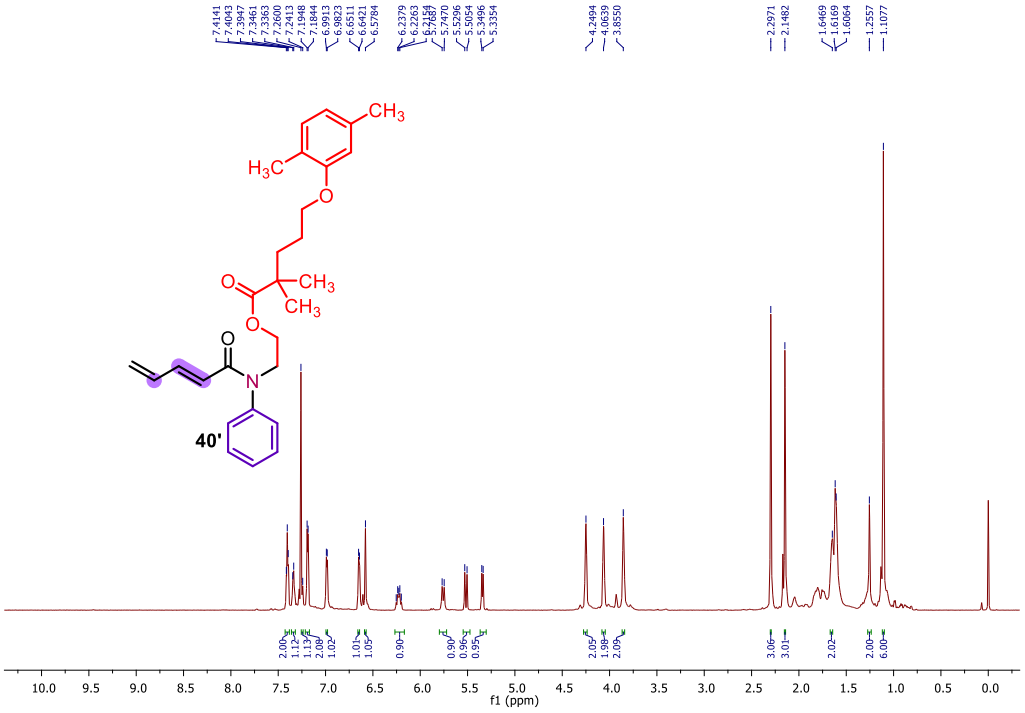


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

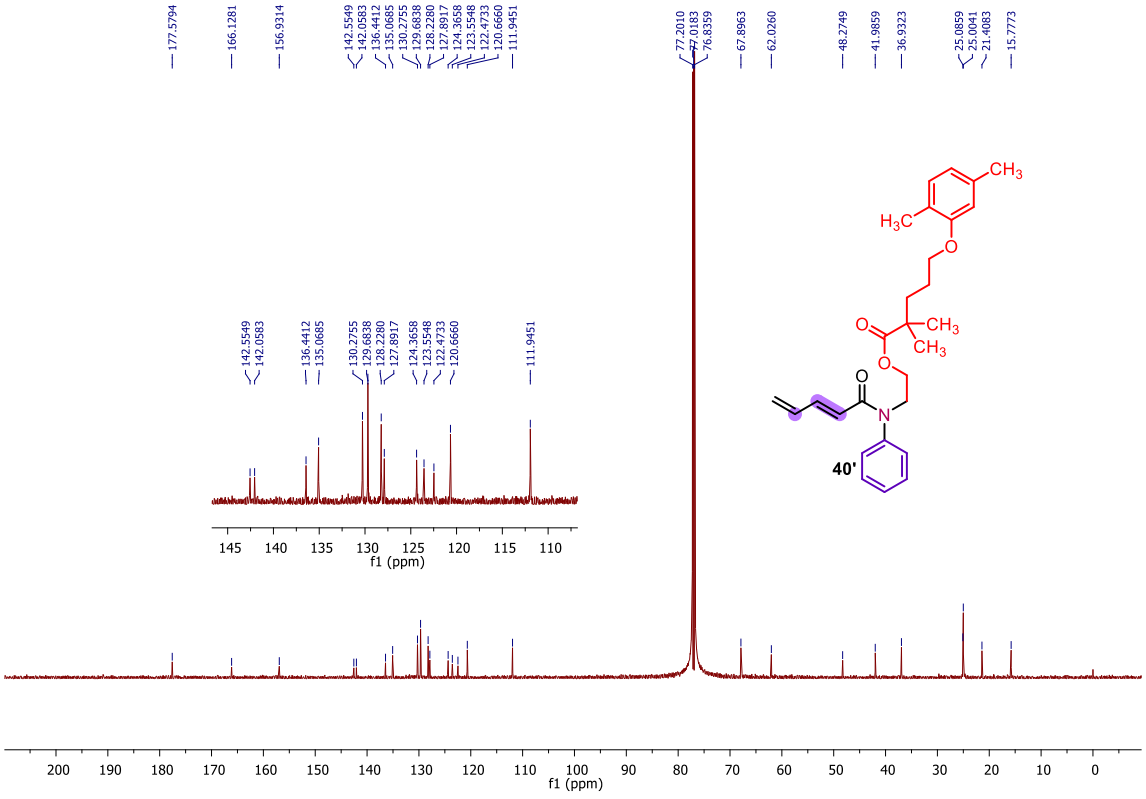


(*E*)-2-(*N*-phenylpenta-2,4-dienamido)ethyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (**40'**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

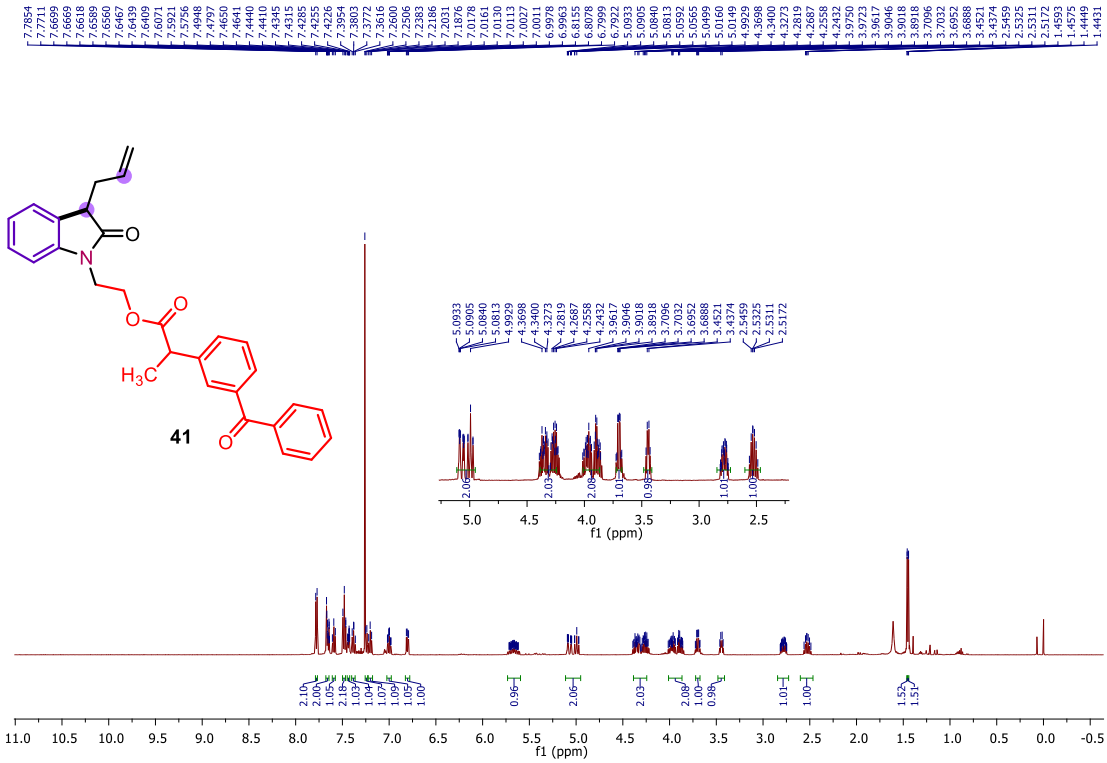


^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$, 24 °C)

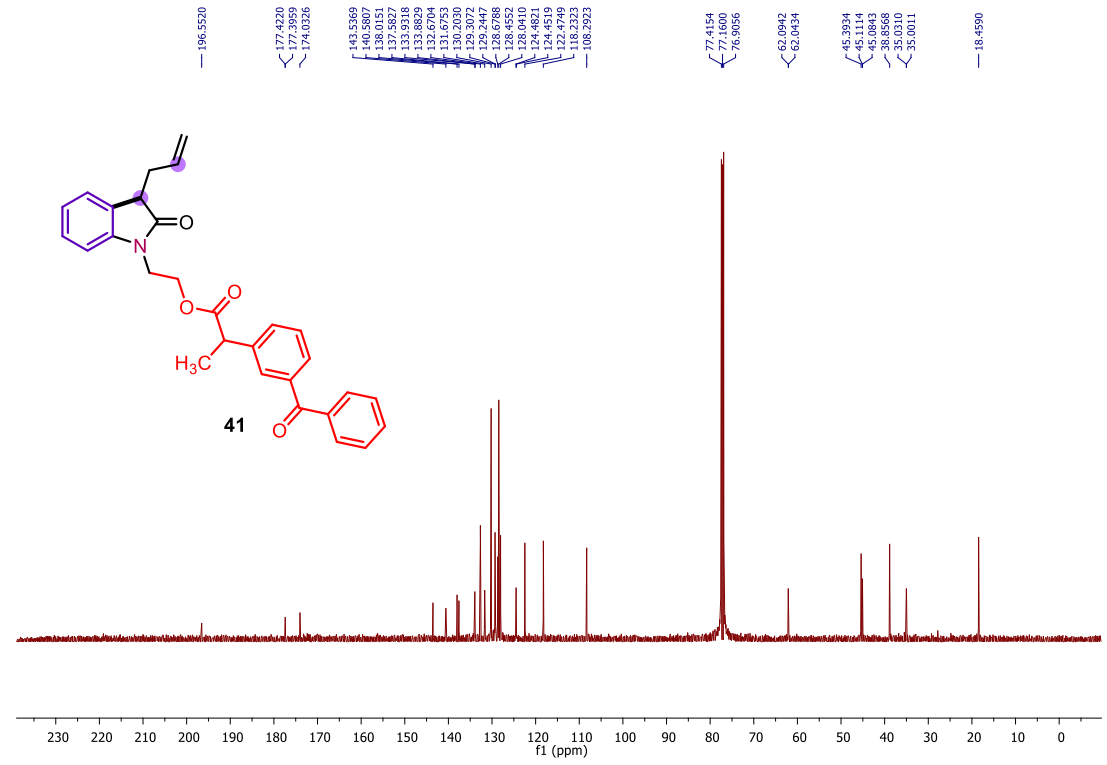


2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(3-benzoylphenyl) propanoate (**41**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

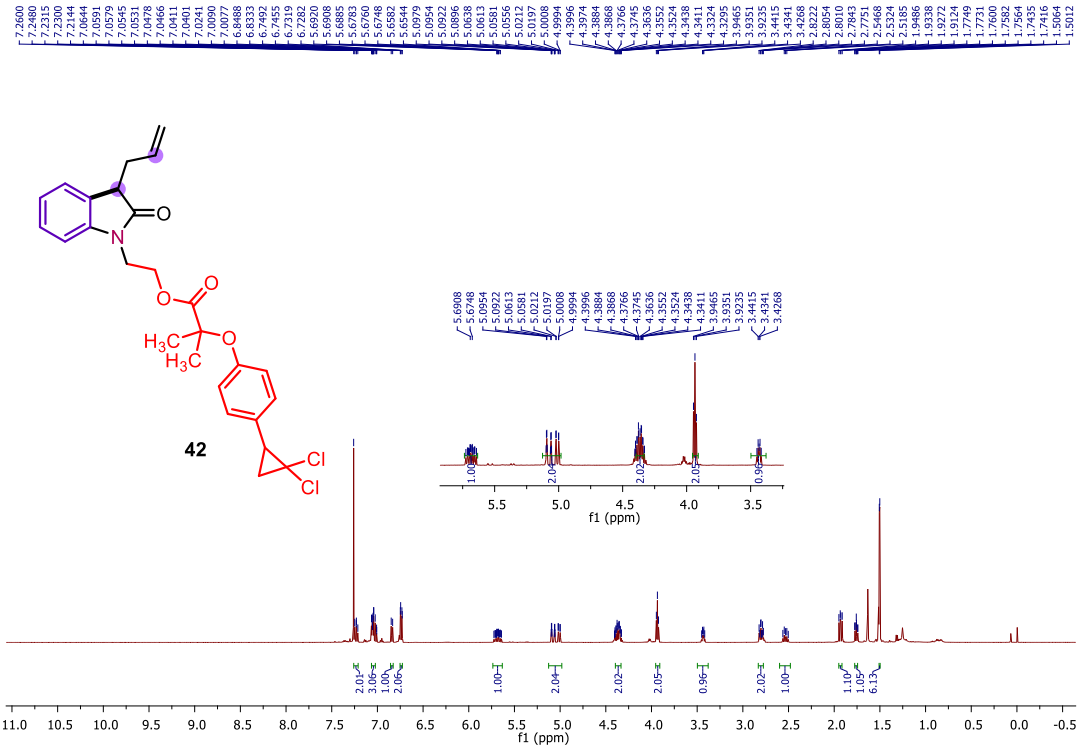


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

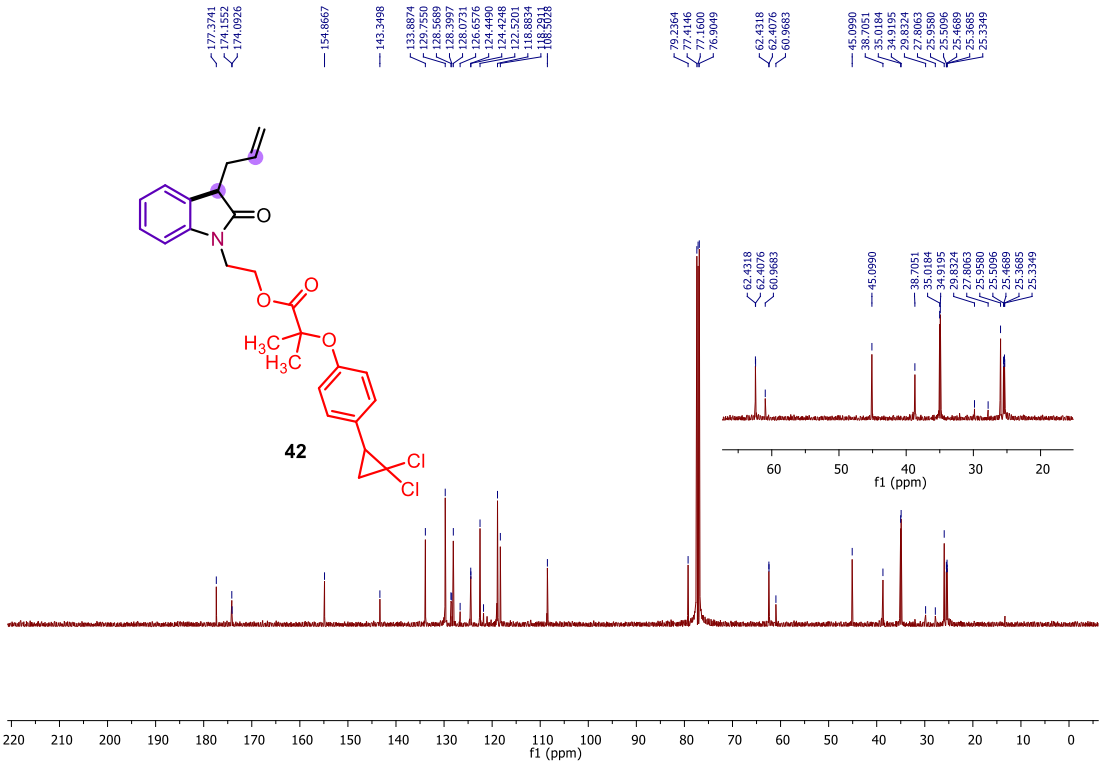


2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-(4-(2,2-dichlorocyclopropyl) phenoxy)-2-methylpropanoate (**42**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

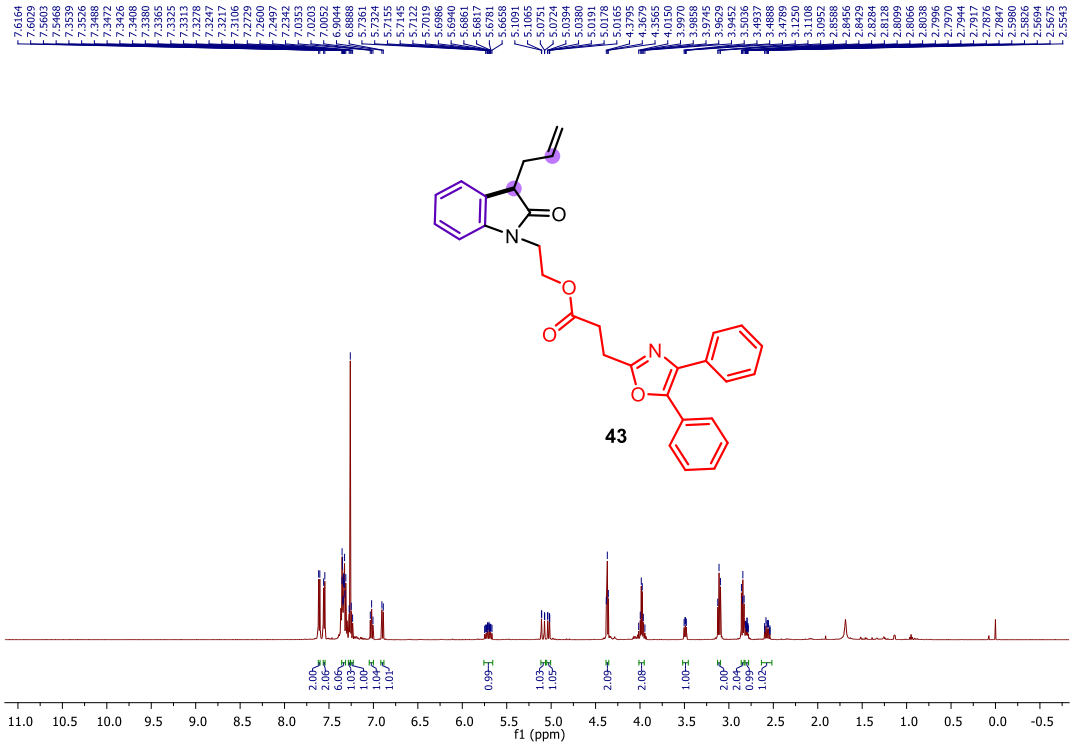


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

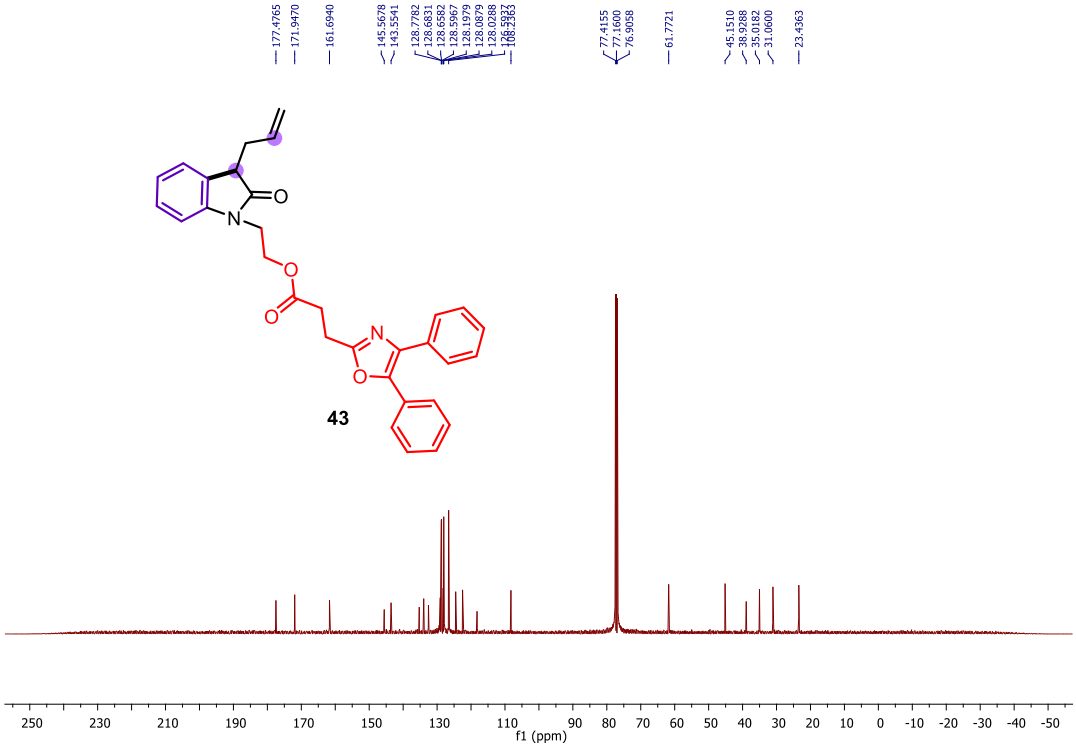


2-(3-Allyl-2-oxoindolin-1-yl) ethyl 3-(4,5-diphenyloxazol-2-yl) propanoate (**43**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

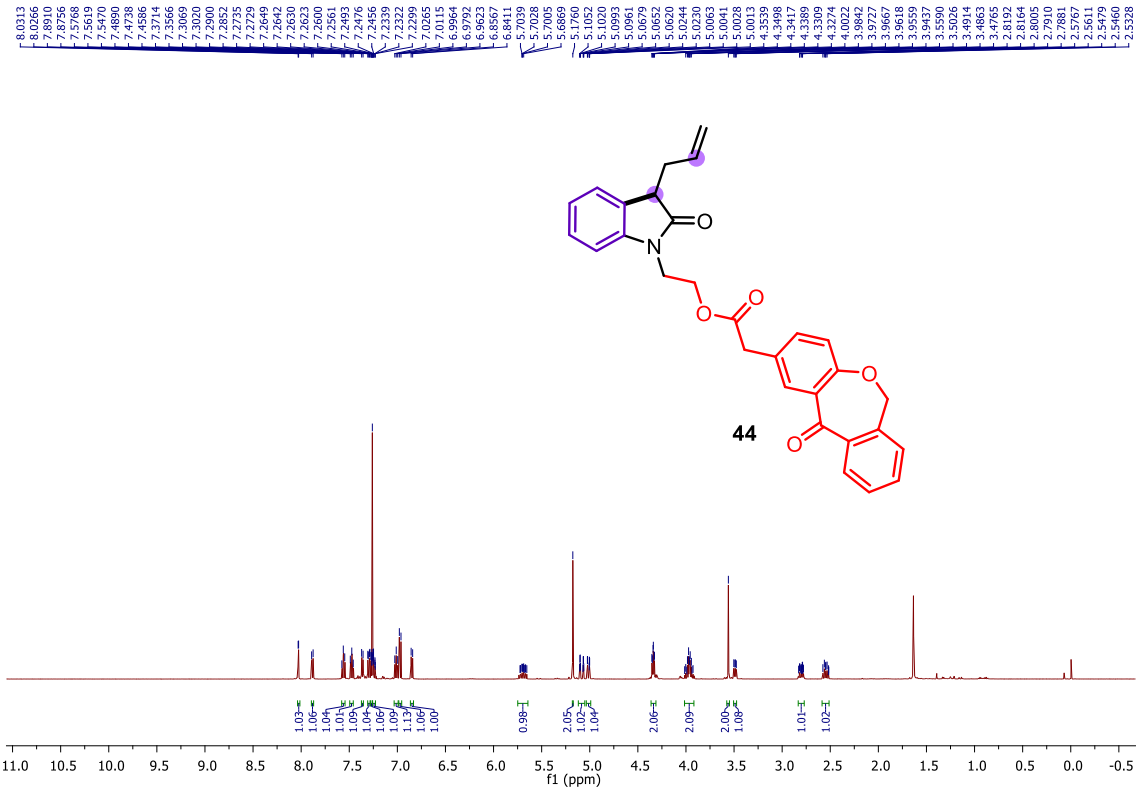


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

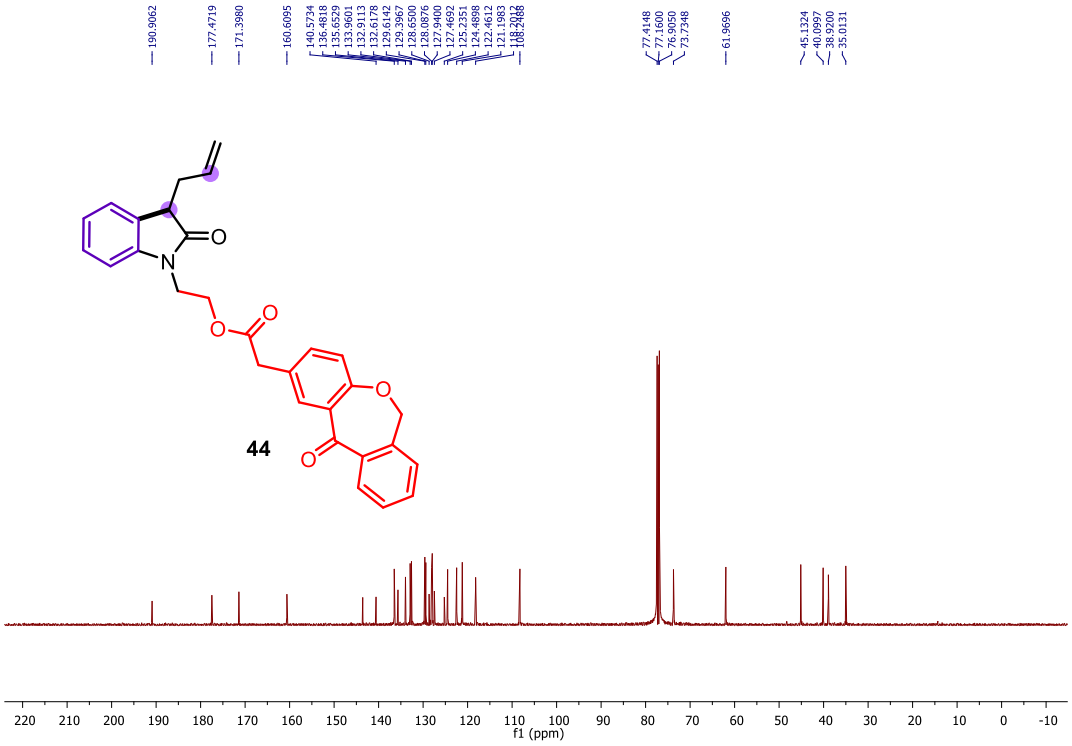


2-(3-Allyl-2-oxoindolin-1-yl)ethyl 2-(11-oxo-6,11-dihydrodibenzo[b,e]oxepin-2-yl)acetate (**44**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

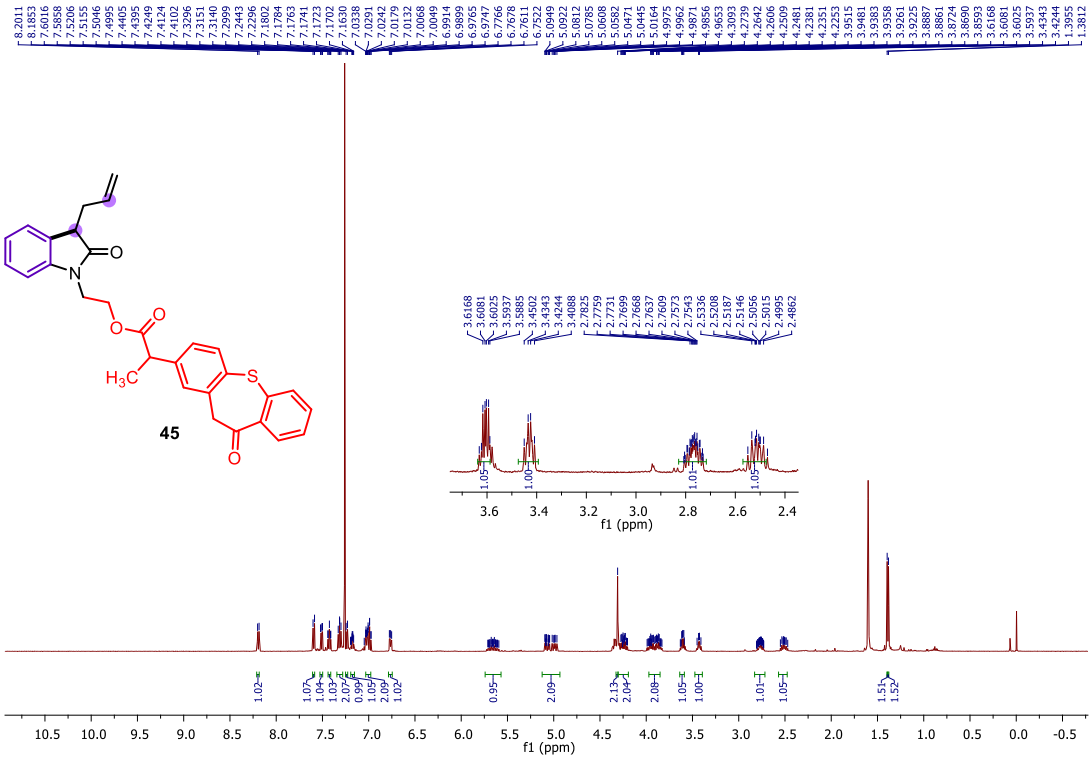


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

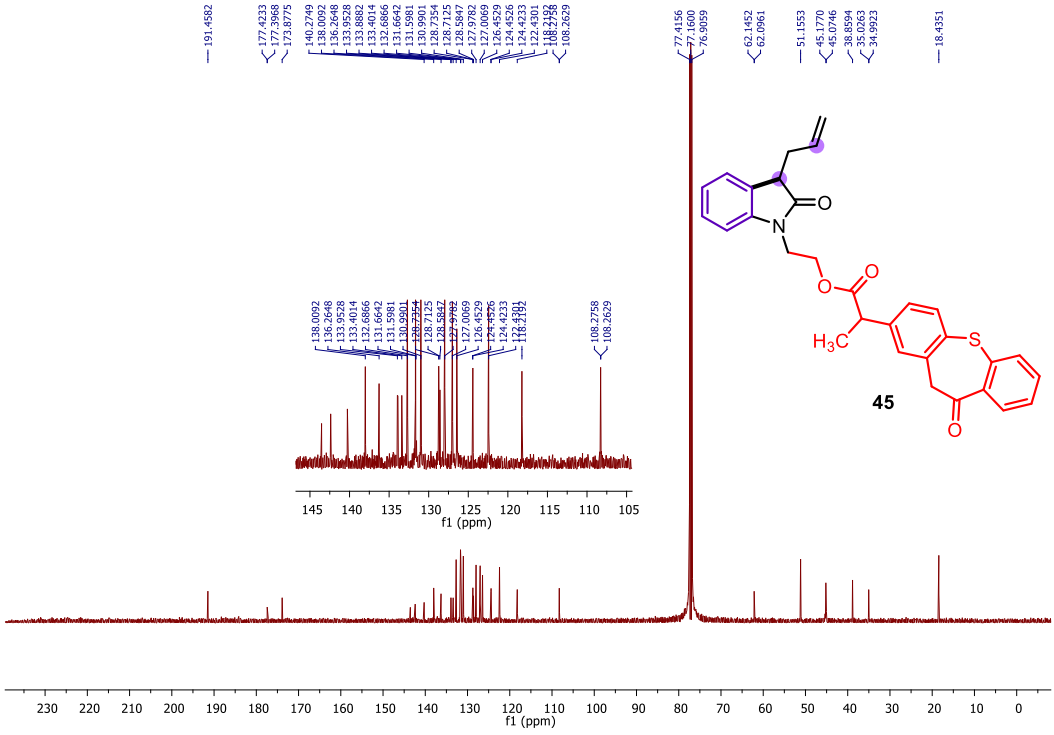


2-(3-Allyl-2-oxoindolin-1-yl)ethyl 2-(10-oxo-10,11-dihydrodibenzo[b,f]thiepin-2-yl)propanoate (**45**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

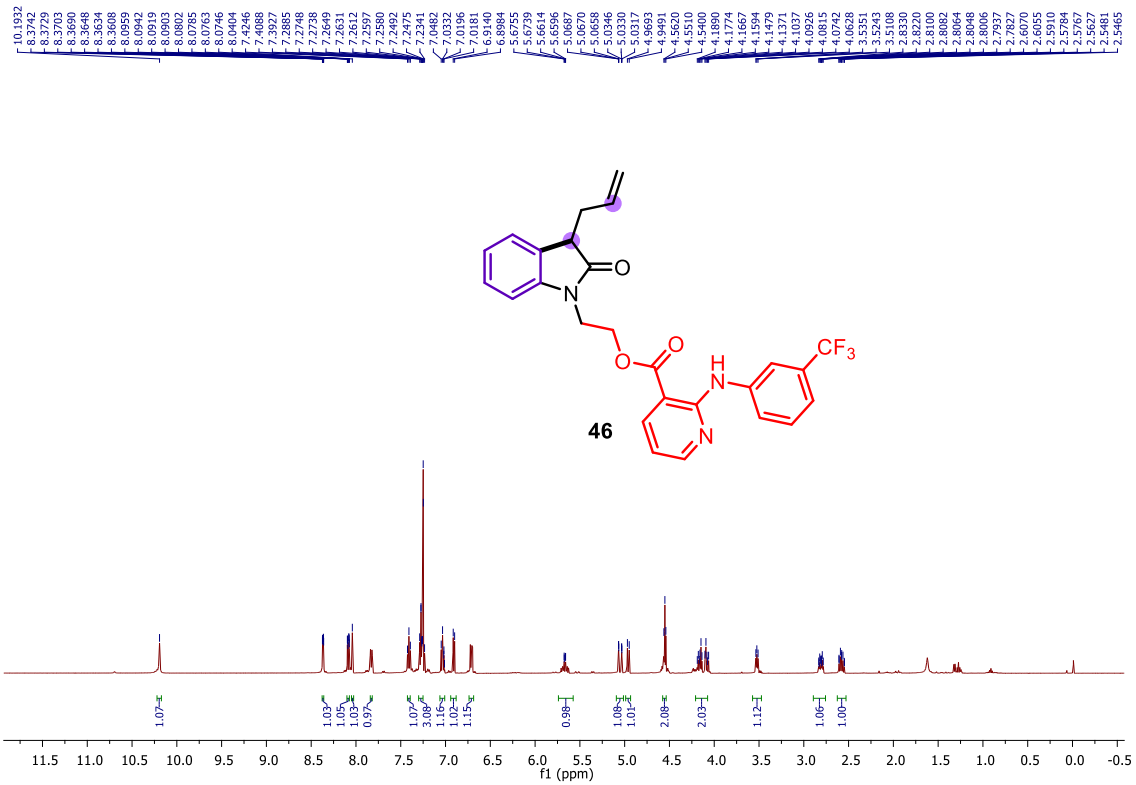


^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

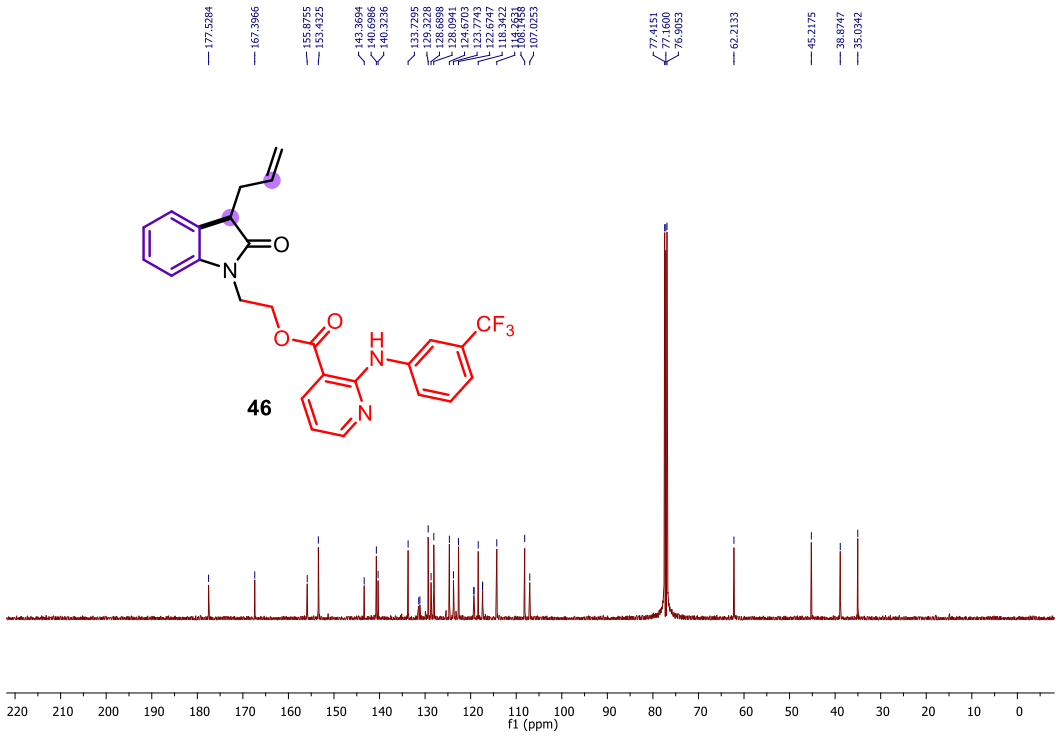


2-(3-Allyl-2-oxoindolin-1-yl) ethyl 2-((3-(trifluoromethyl) phenyl) amino) nicotinate (**46**)

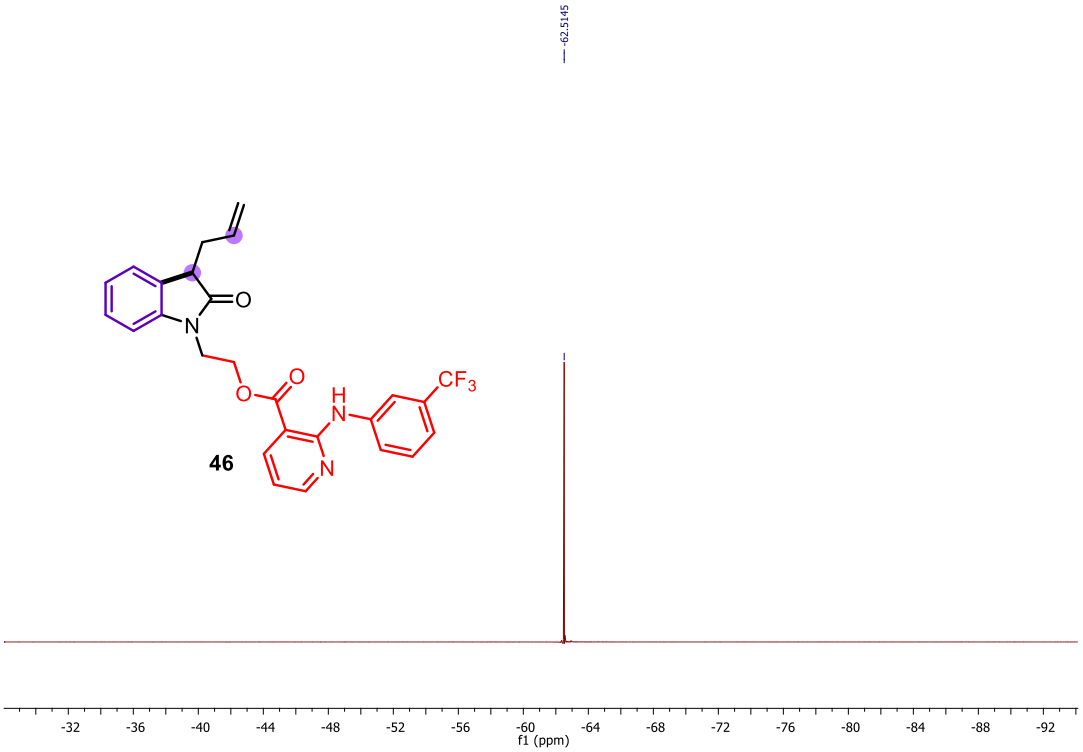
^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)



^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 24 °C)

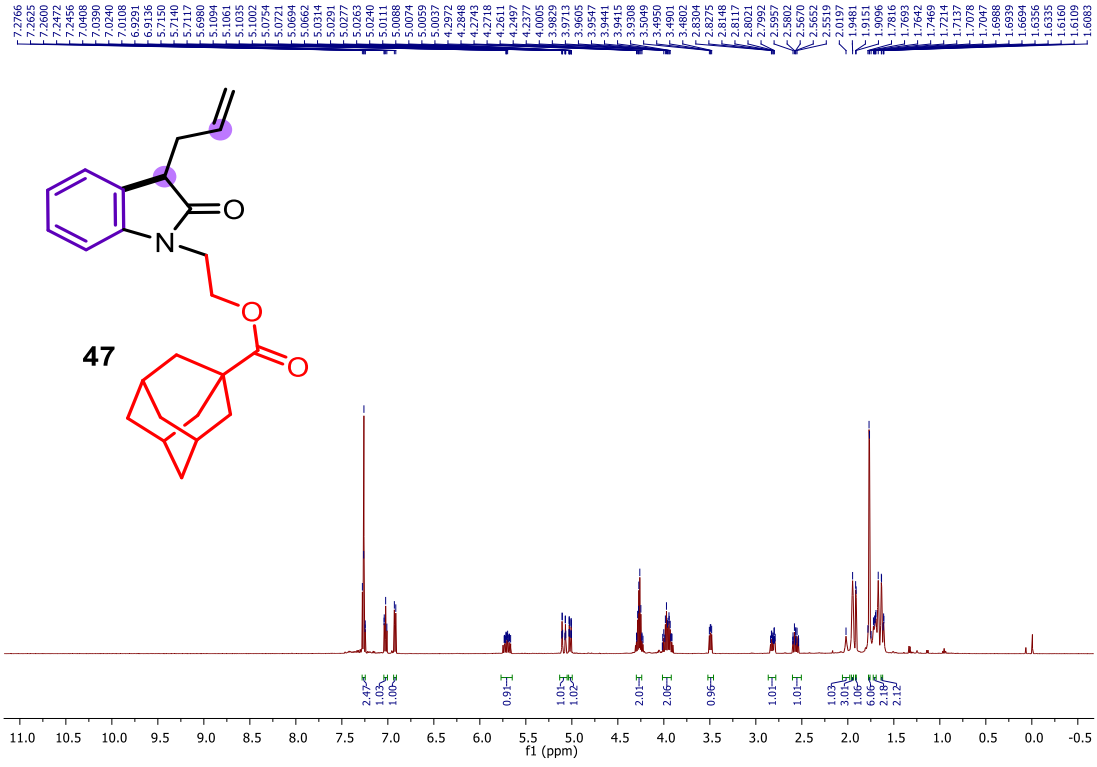


^{19}F NMR (471 MHz, $CDCl_3$, 24 °C)

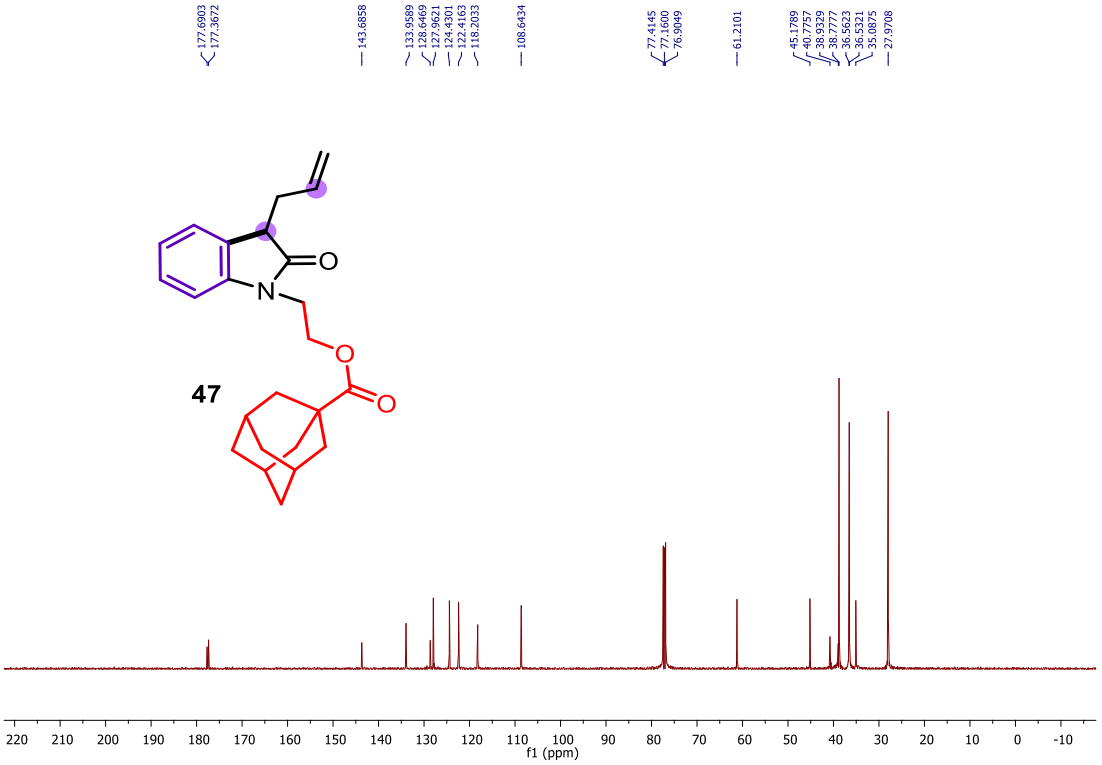


2-(3-Allyl-2-oxoindolin-1-yl) ethyl (1s,3s)-adamantane-1-carboxylate (**47**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

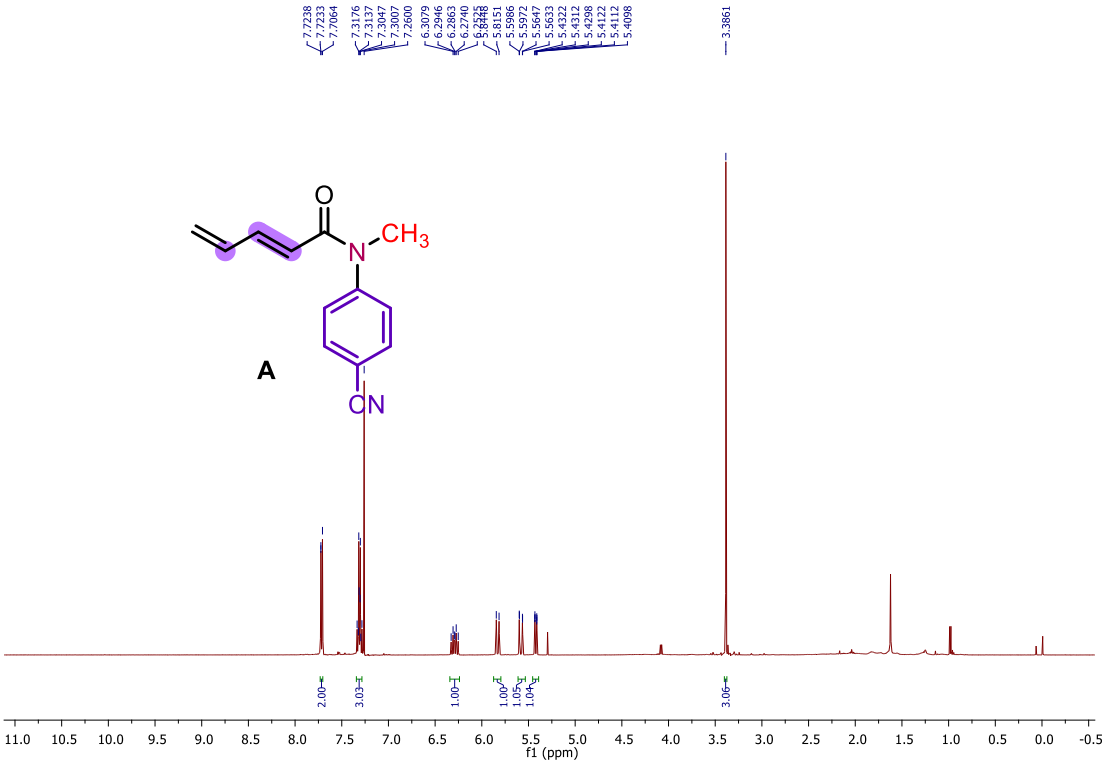


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

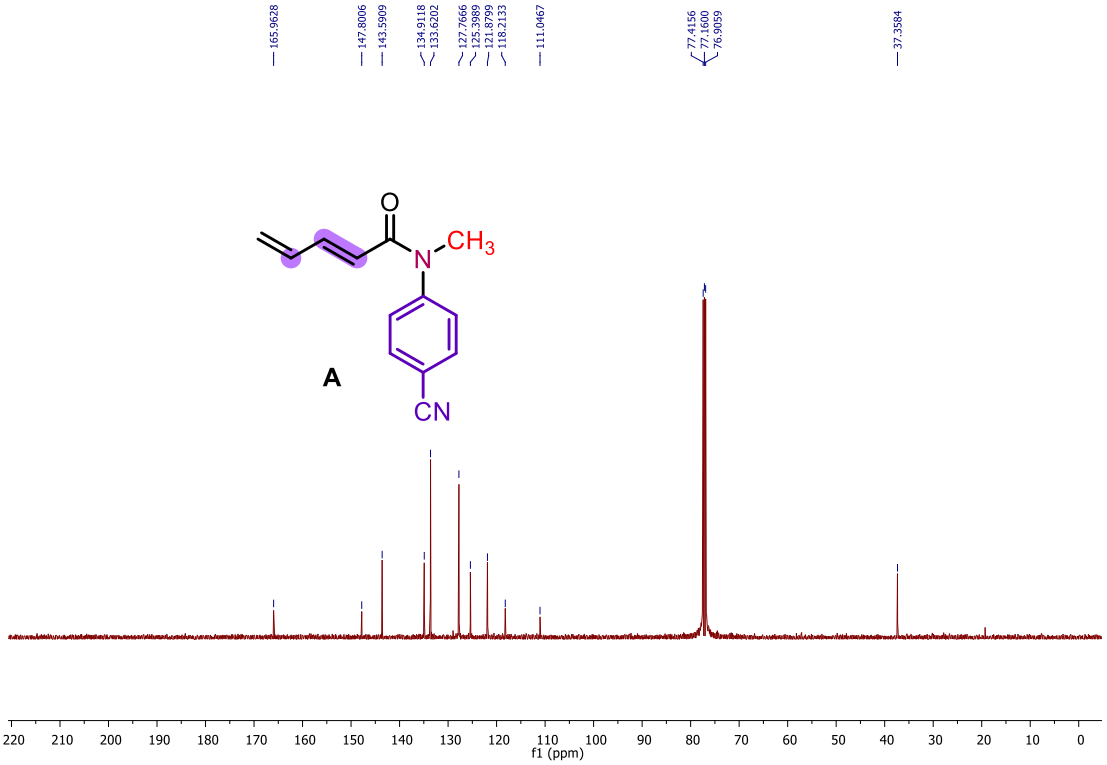


(*E*)-*N*-(4-cyanophenyl)-*N*-methylpenta-2,4-dienamide (**A**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

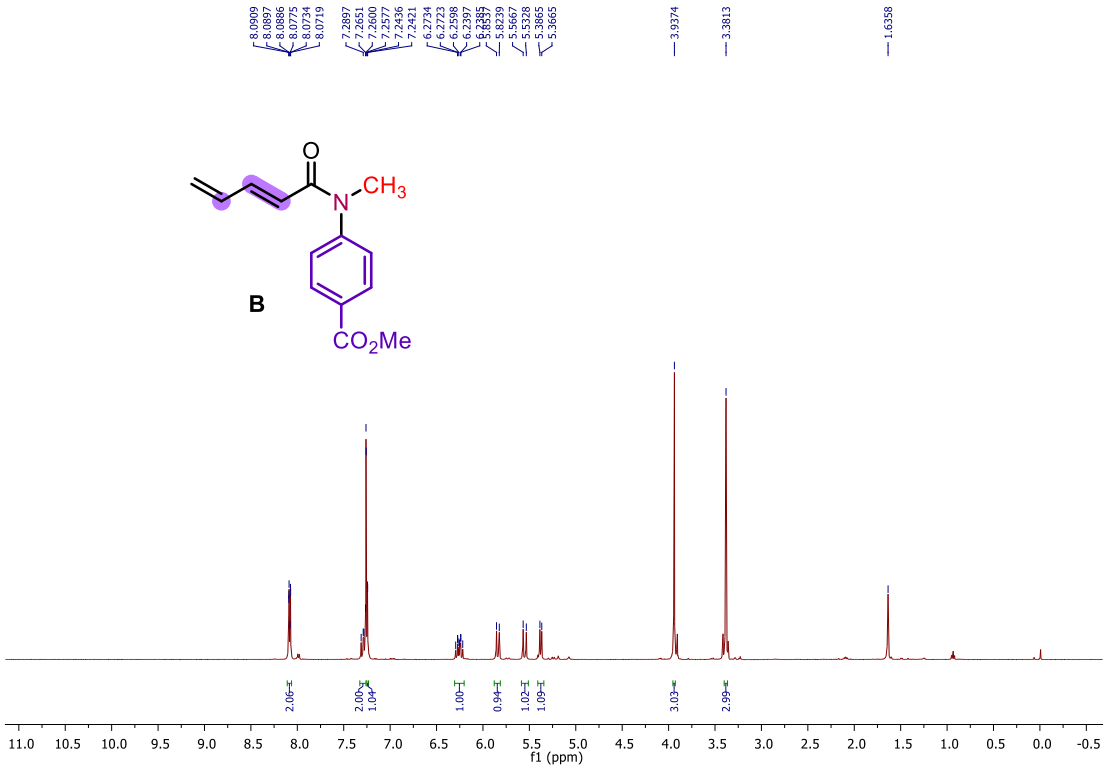


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

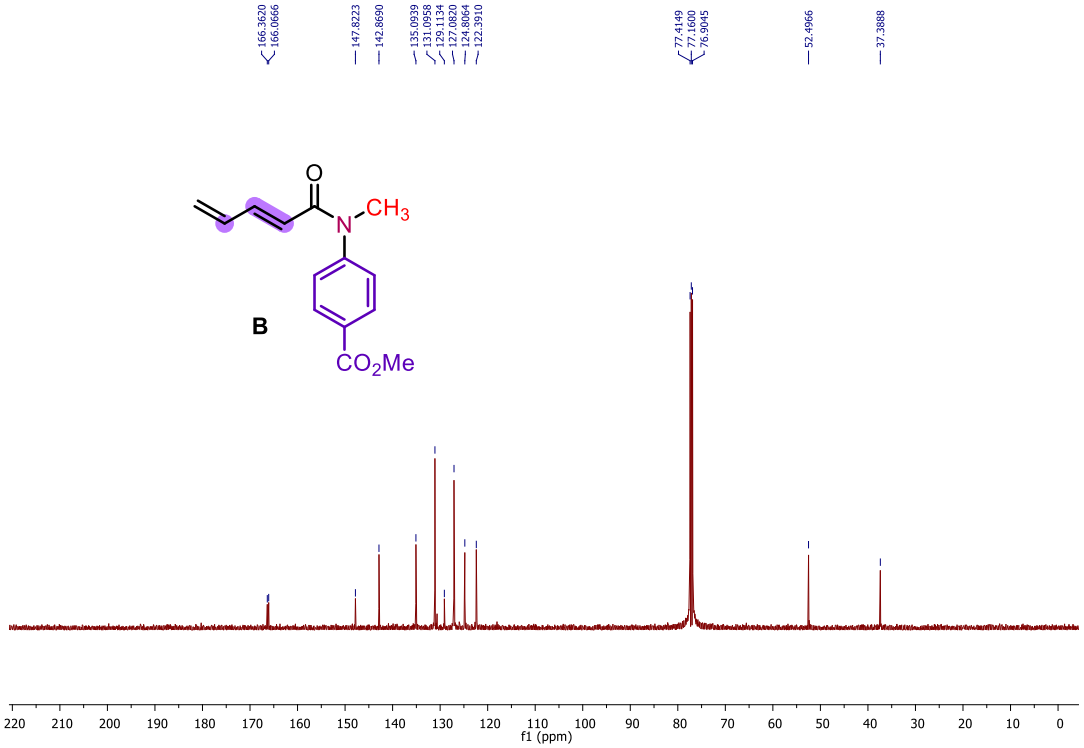


Methyl (*E*)-4-(*N*-methylpenta-2,4-dienamido)benzoate (**B**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

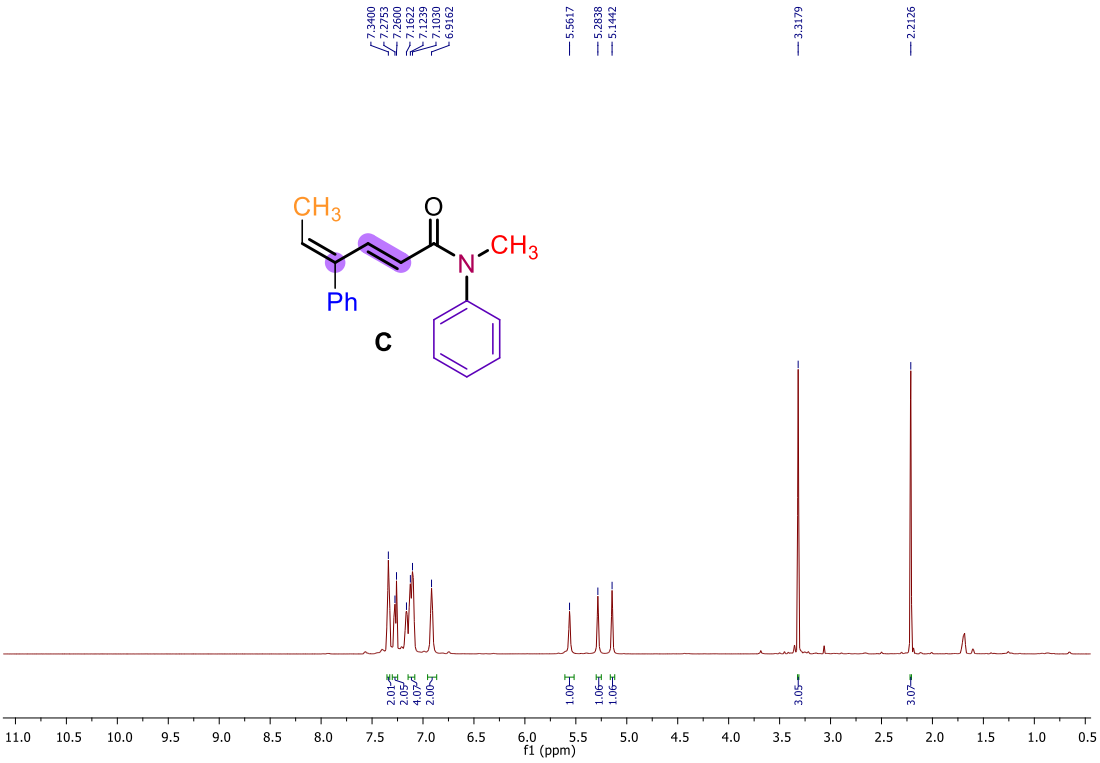


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

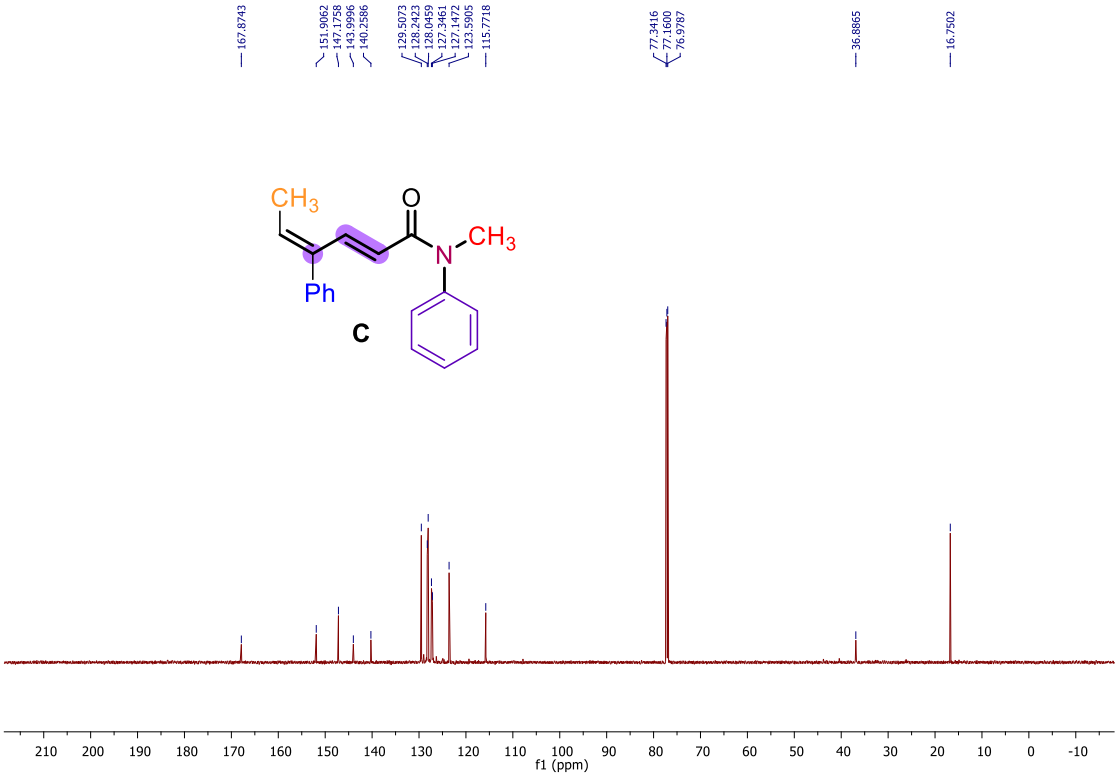


(2*E*,4*E*)-*N*-Methyl-*N*,4-diphenylhexa-2,4-dienamide (**C**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

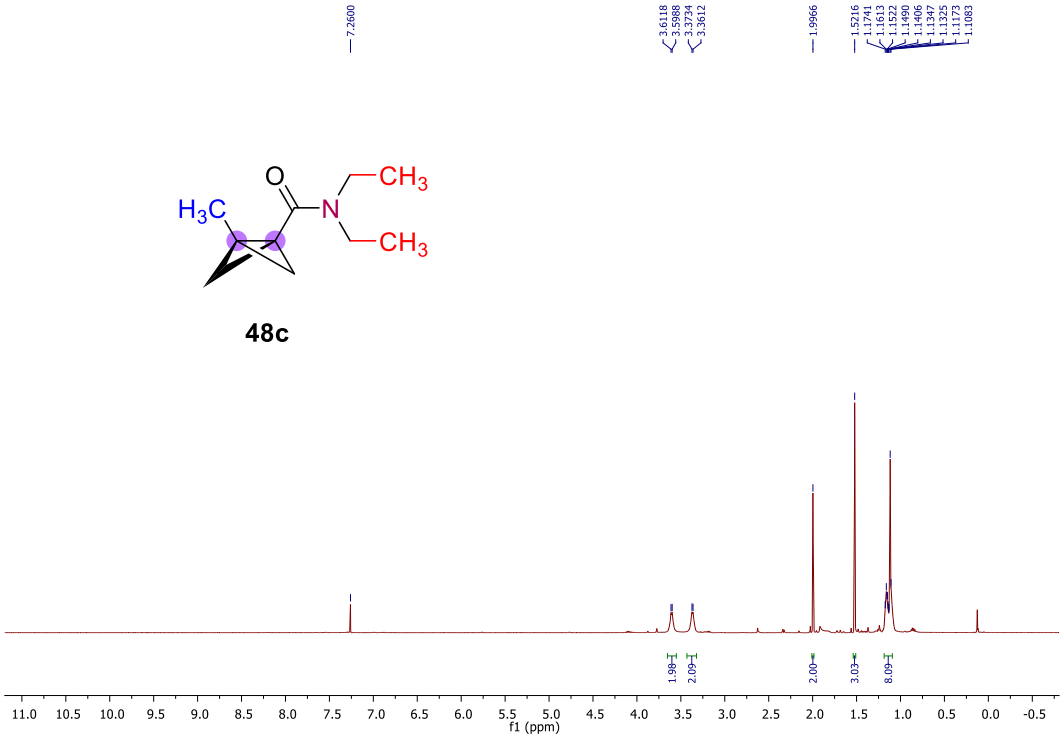


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

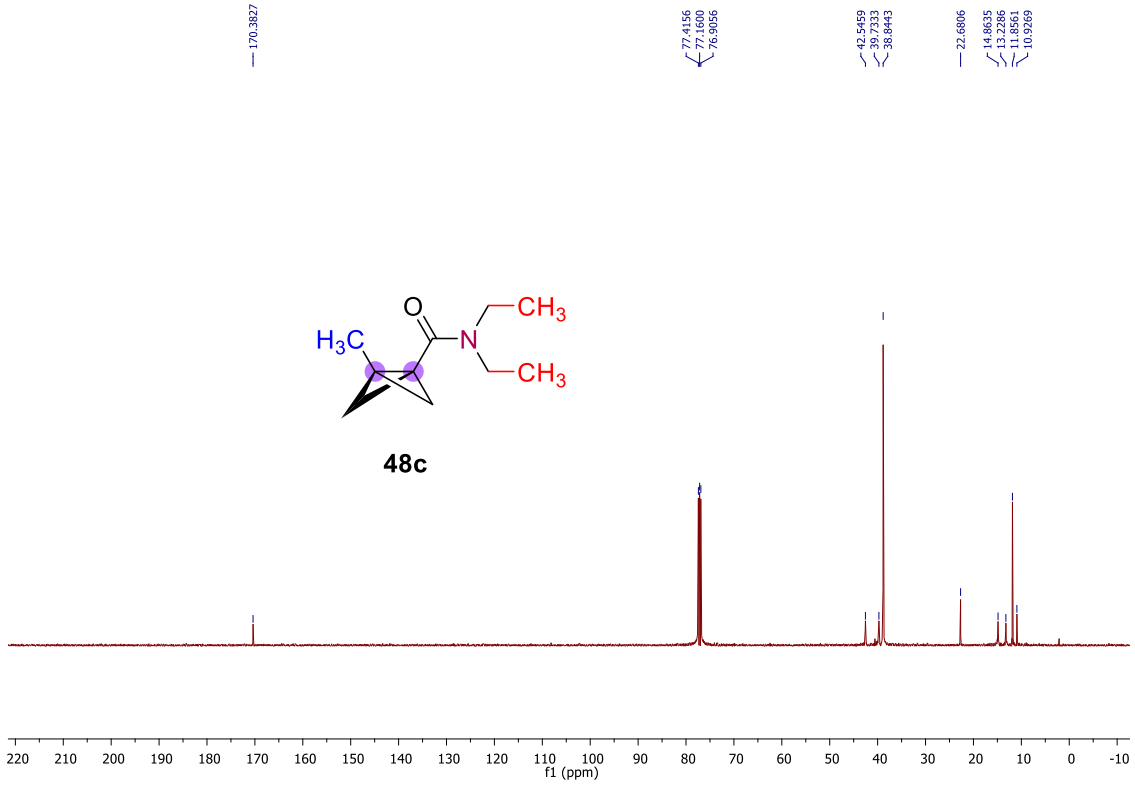


N, *N*-Diethyl-3-methylbicyclo[1.1.0]butane-1-carboxamide (**48c**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

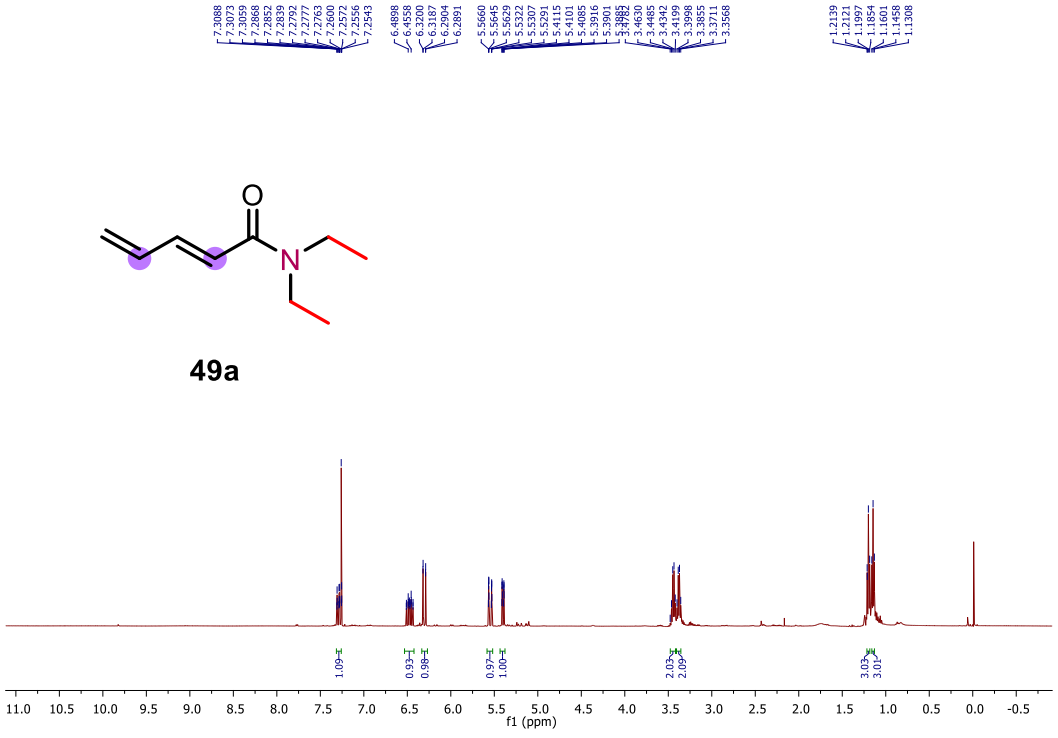


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

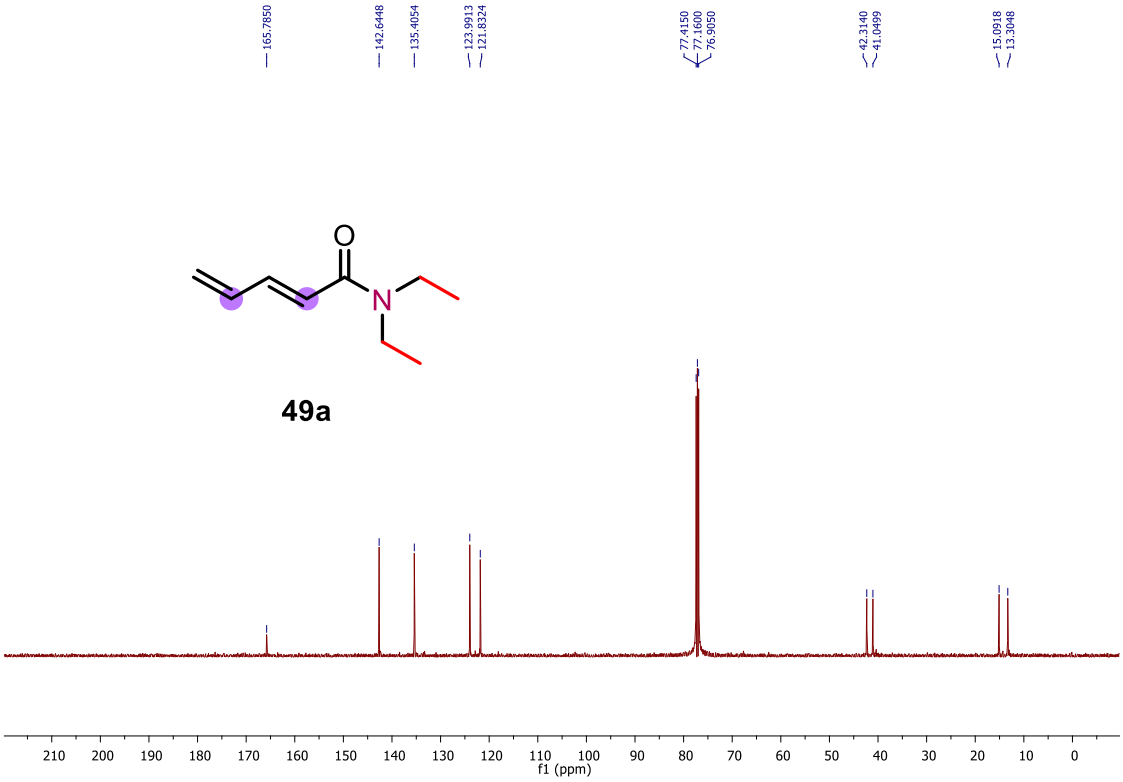


(*E*)-*N*,*N*-Diethylpenta-2,4-dienamide (**49a**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

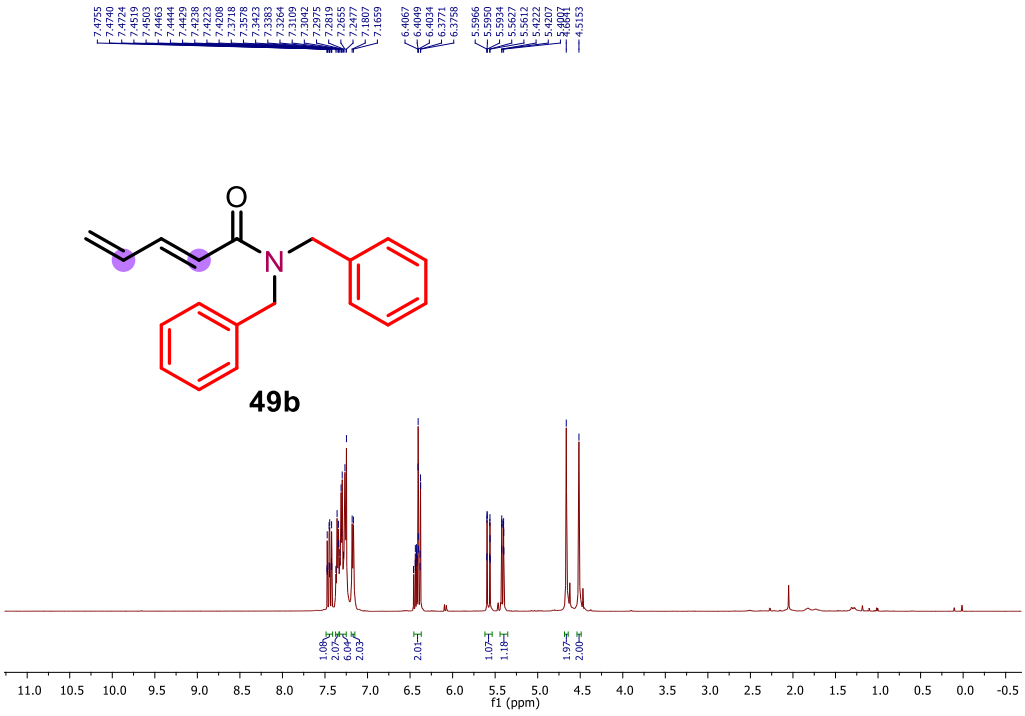


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

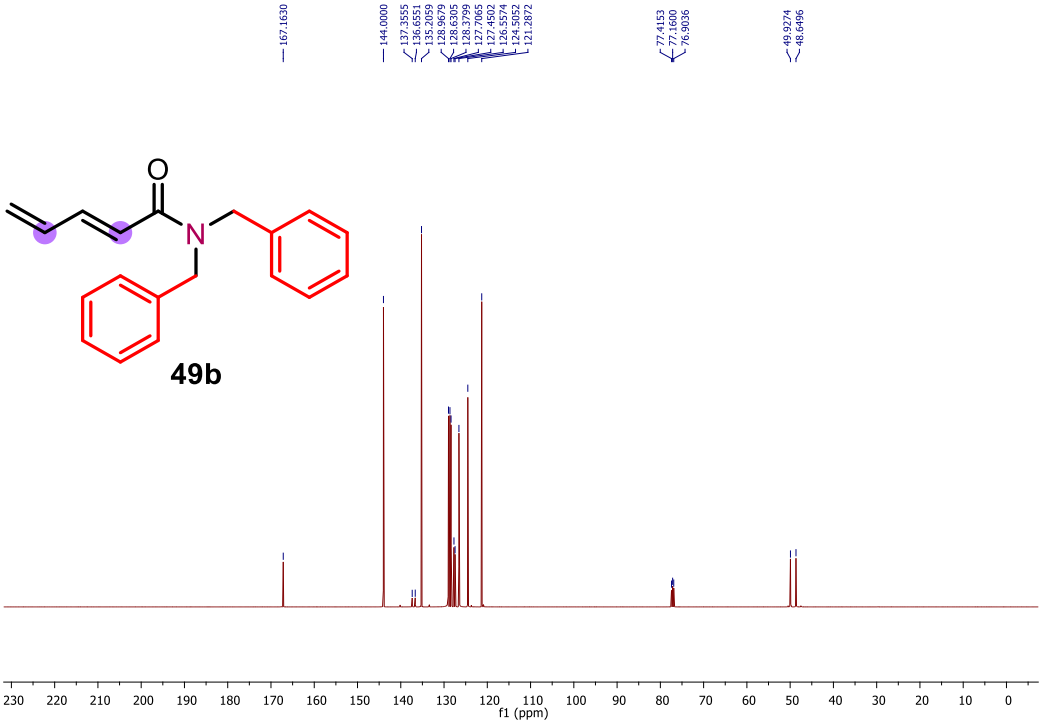


(*E*)-*N*,*N*-Dibenzylpenta-2,4-dienamide (**49b**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

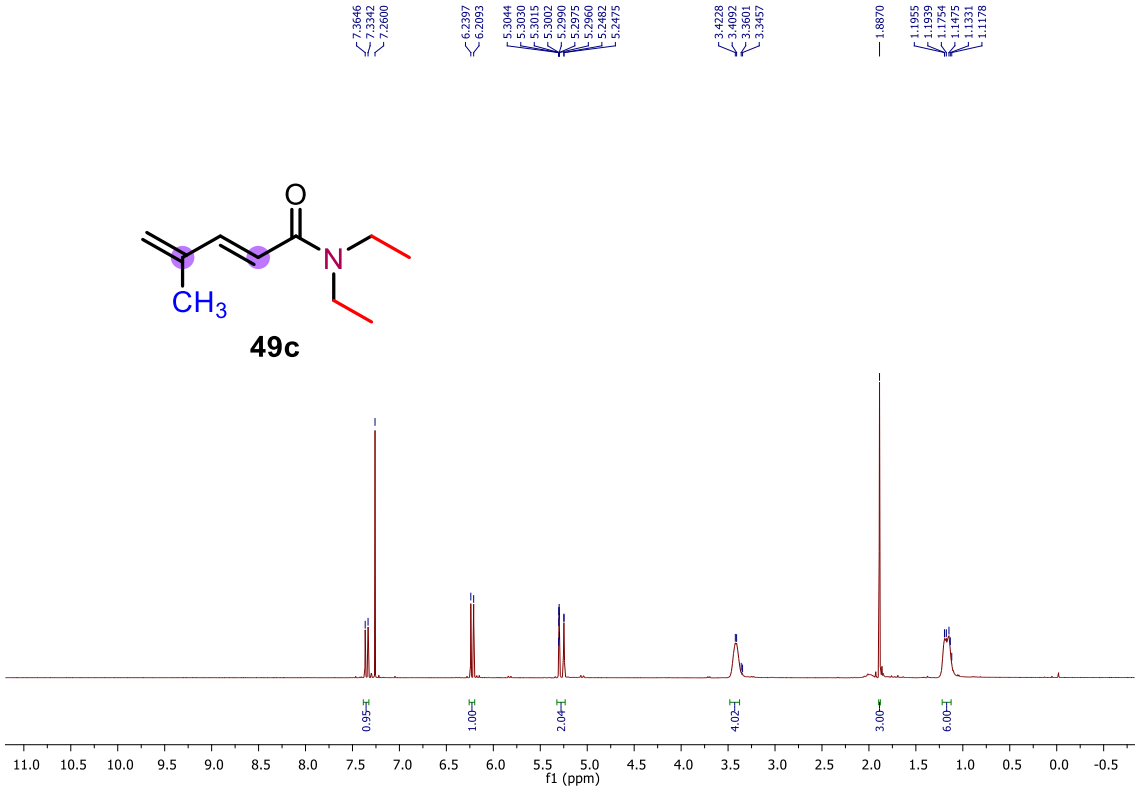


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

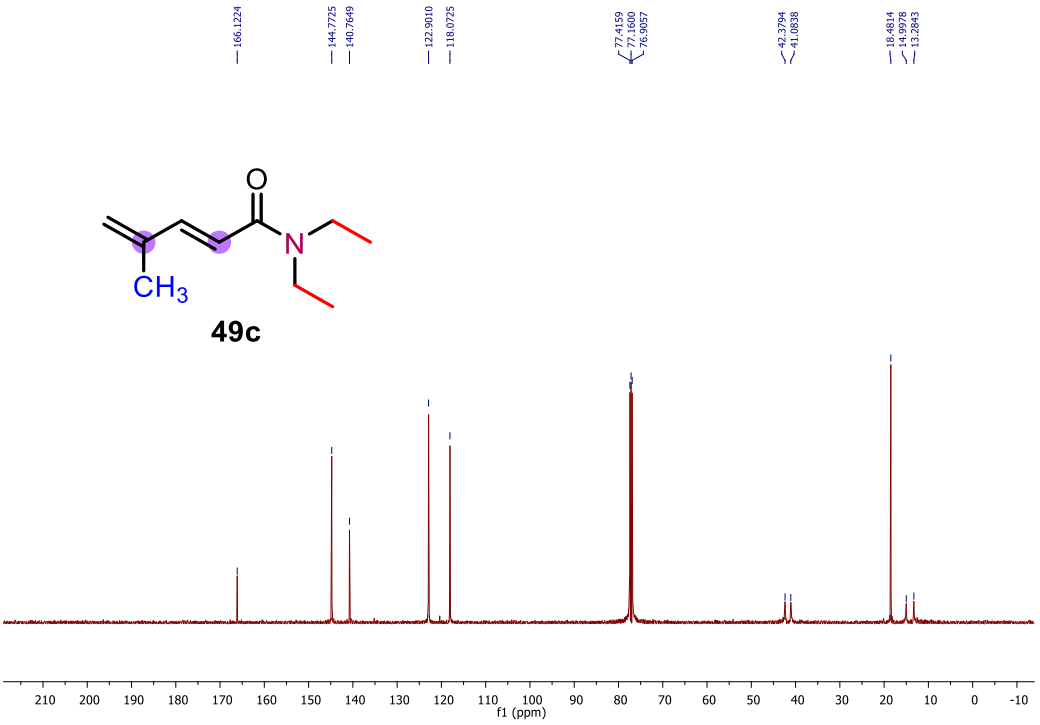


(*E*)-*N*,*N*-Diethyl-4-methylpenta-2,4-dienamide (**49c**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

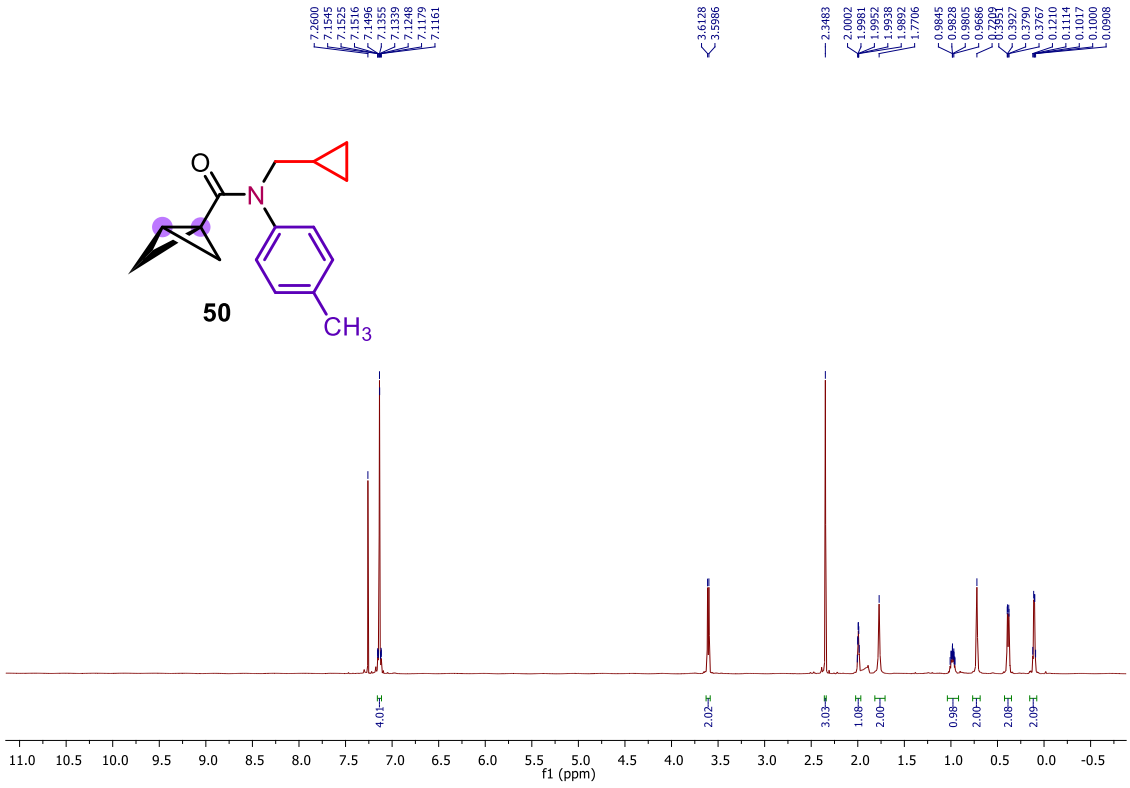


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

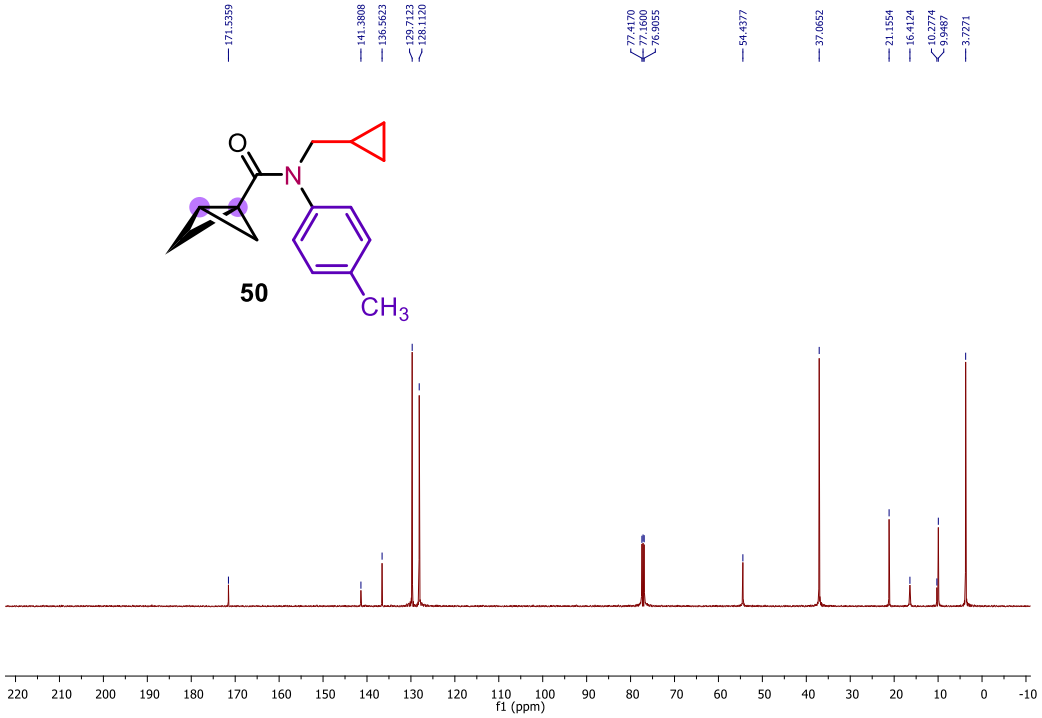


N-(Cyclopropylmethyl)-*N*-(p-tolyl)bicyclo[1.1.0]butane-1-carboxamide (**50**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

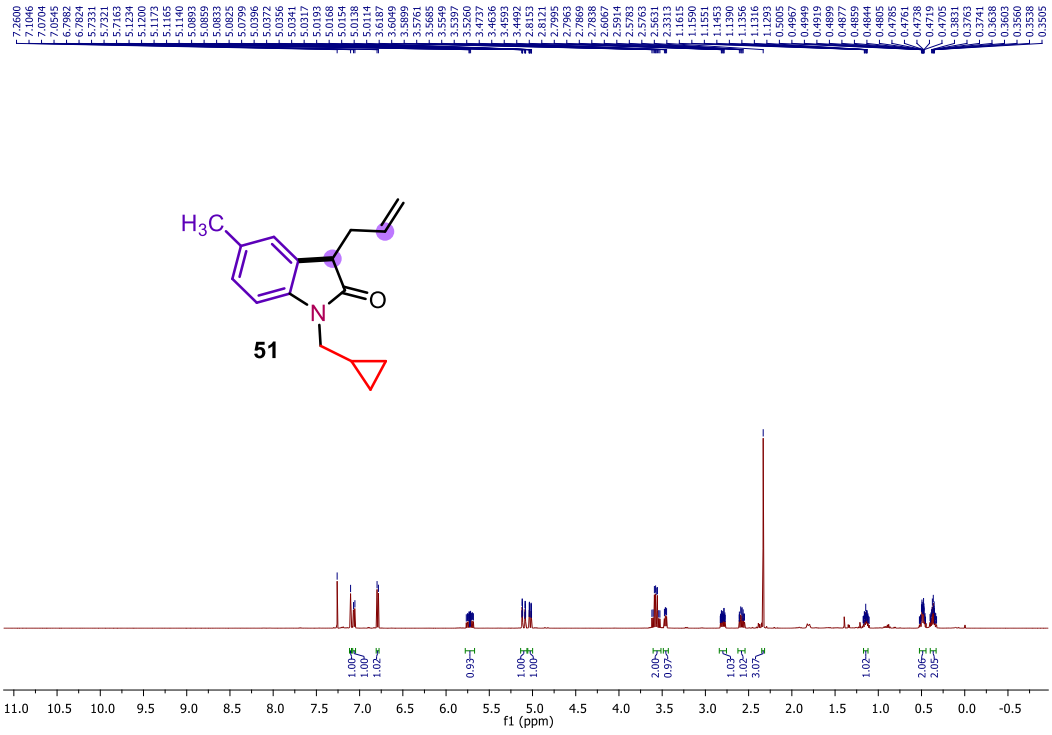


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

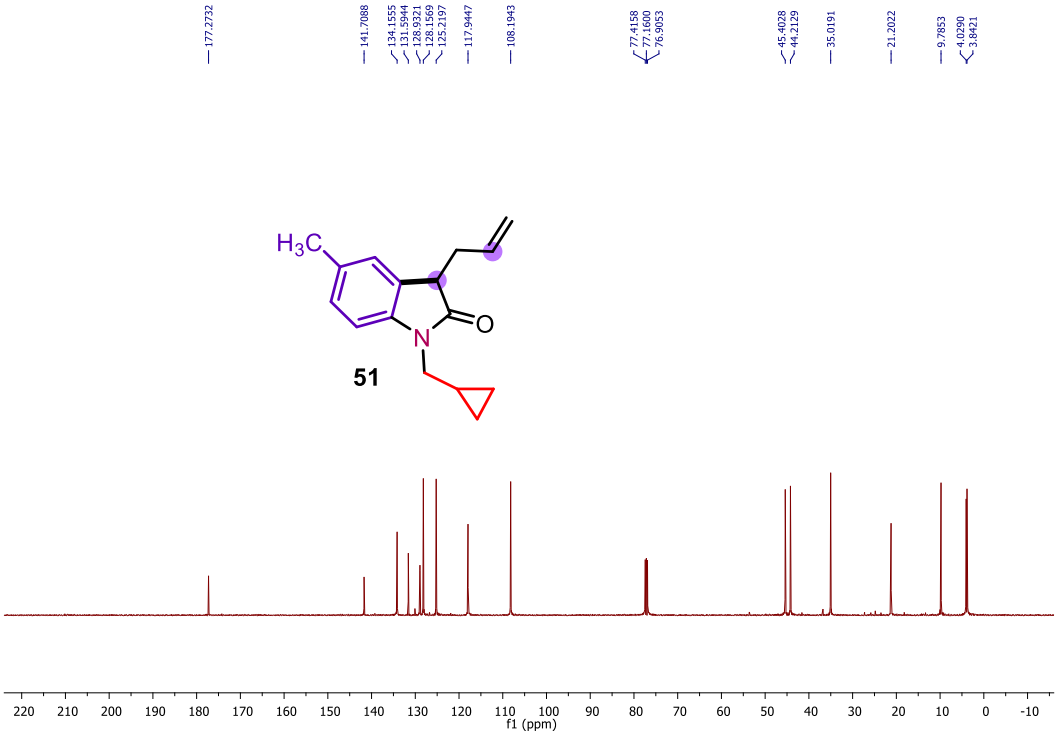


3-Allyl-1-(cyclopropylmethyl)-5-methylindolin-2-one (**51**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

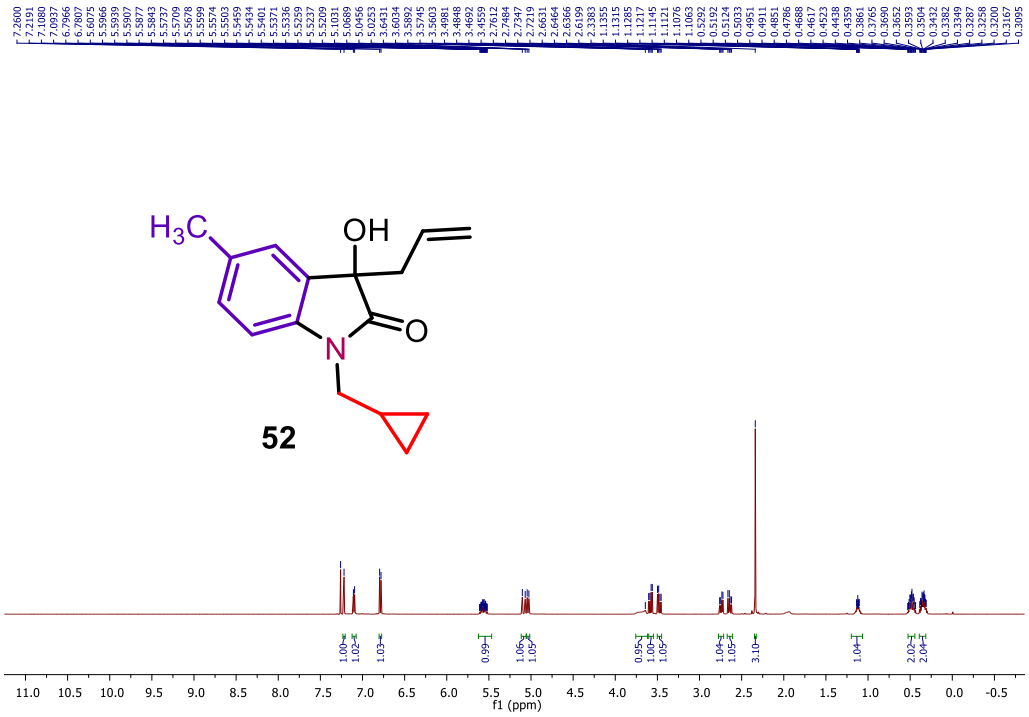


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

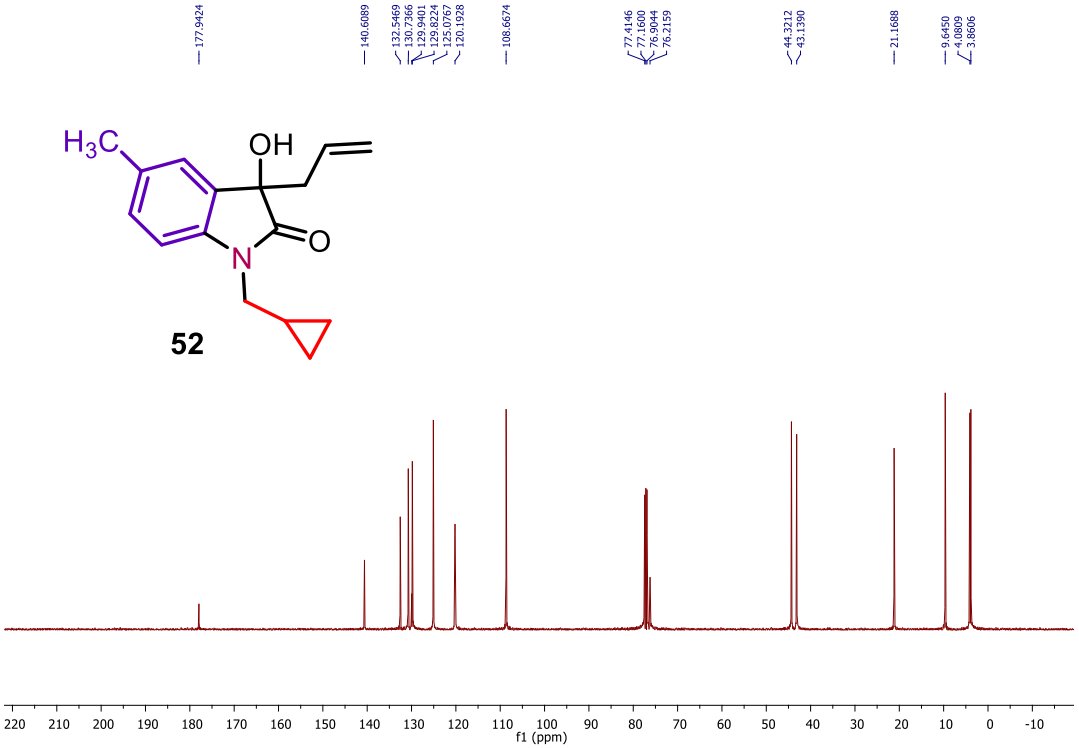


3-Allyl-1-(cyclopropylmethyl)-3-hydroxy-5-methylindolin-2-one (**52**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

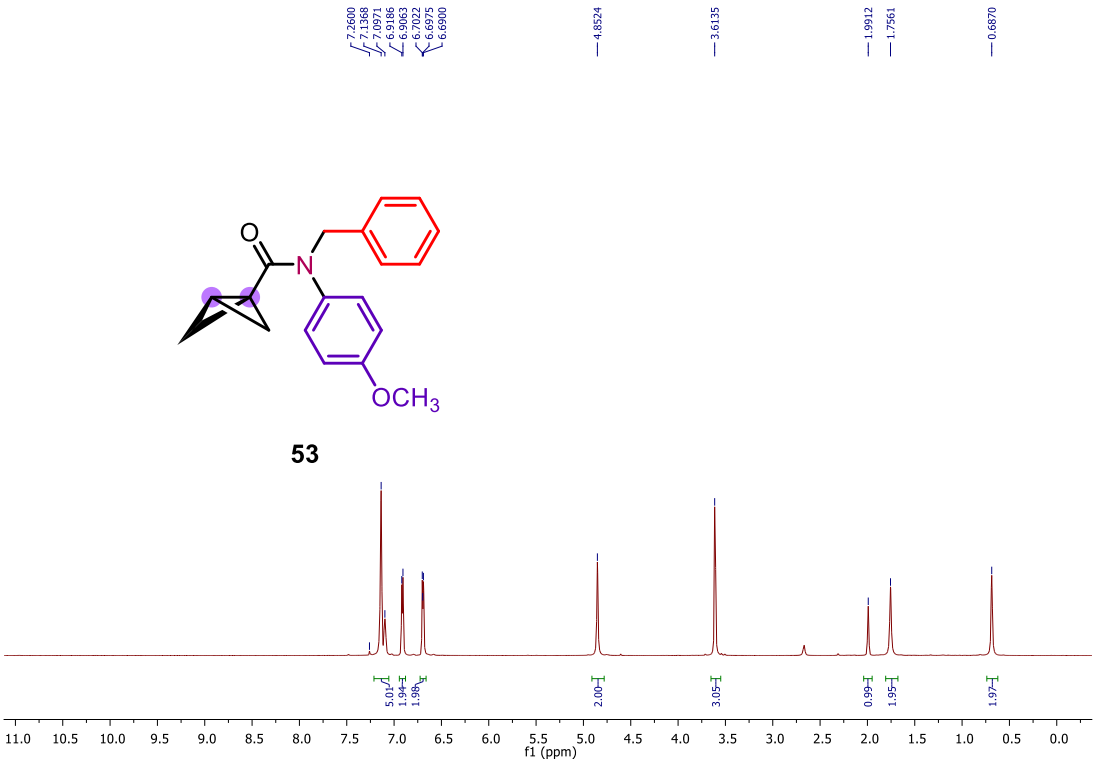


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

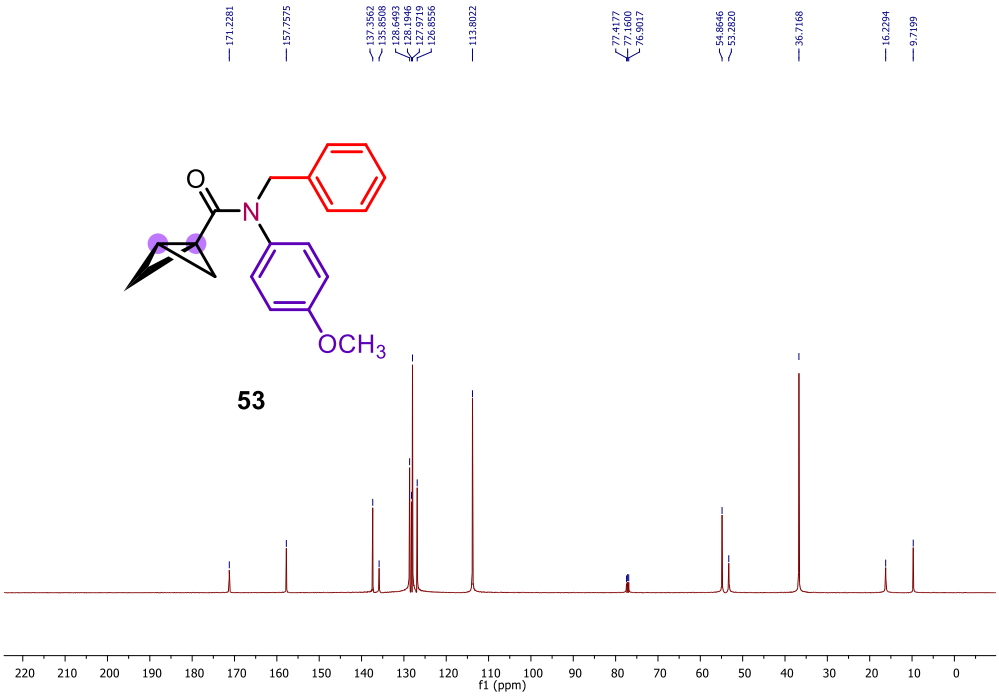


N-Benzyl-*N*-(4-methoxyphenyl)bicyclo[1.1.0]butane-1-carboxamide (**53**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

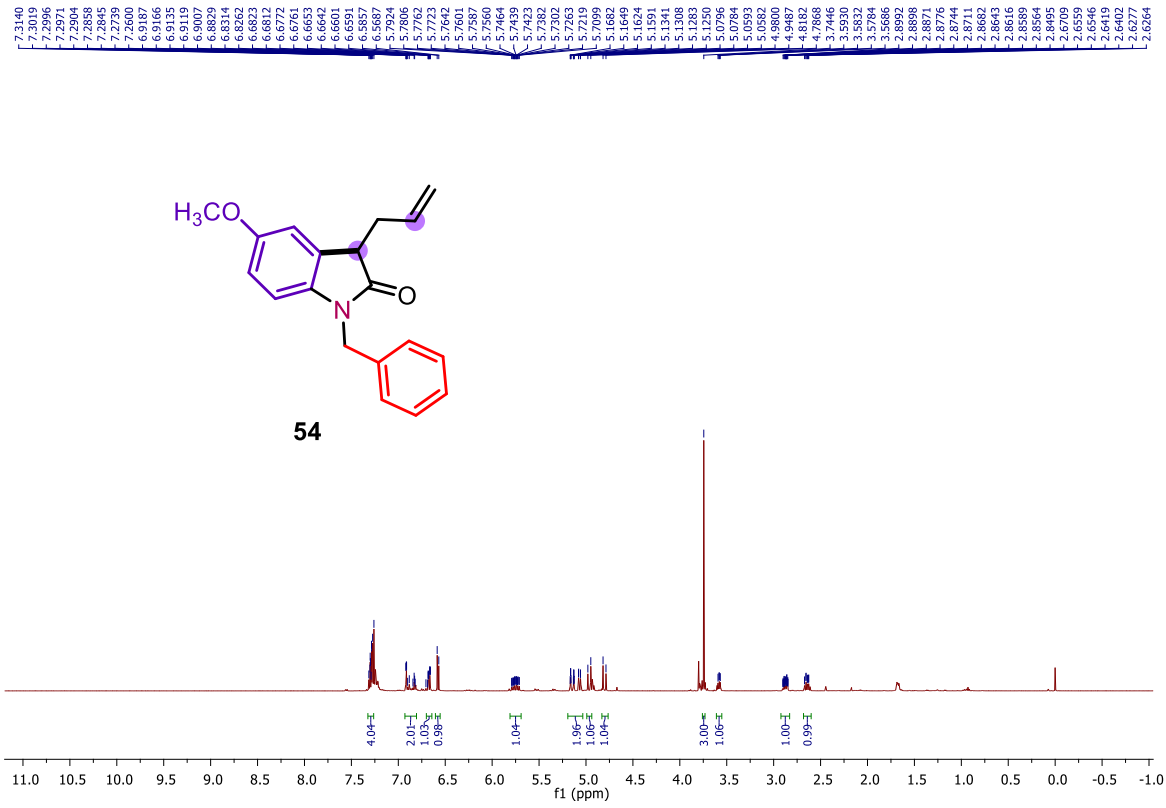


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

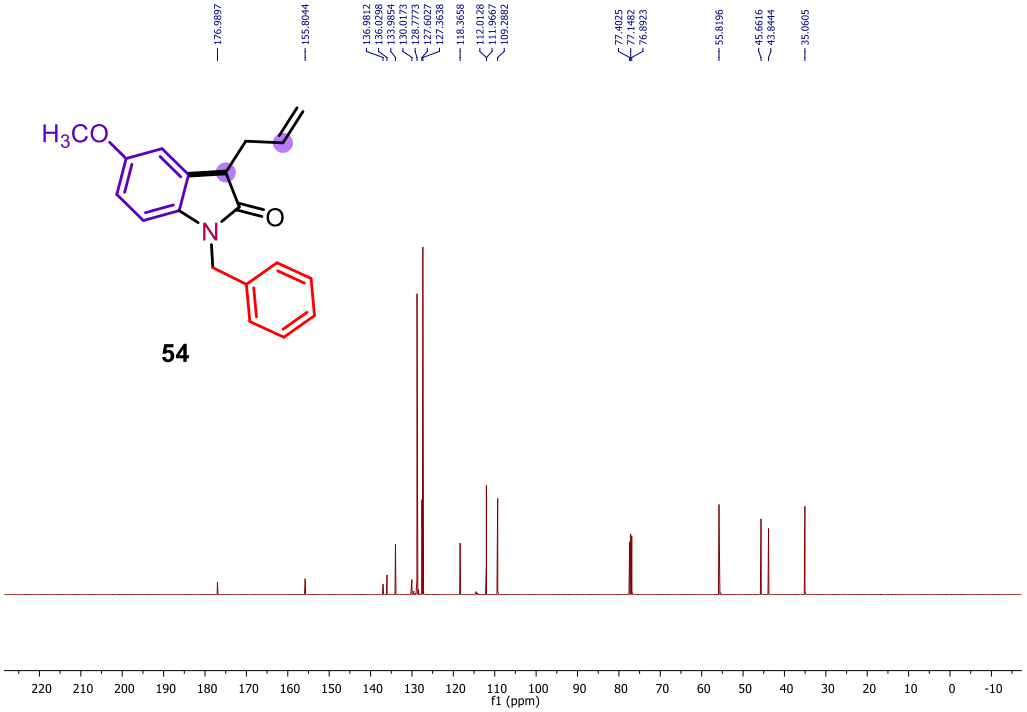


3-Allyl-1-benzyl-5-methoxyindolin-2-one (**54**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

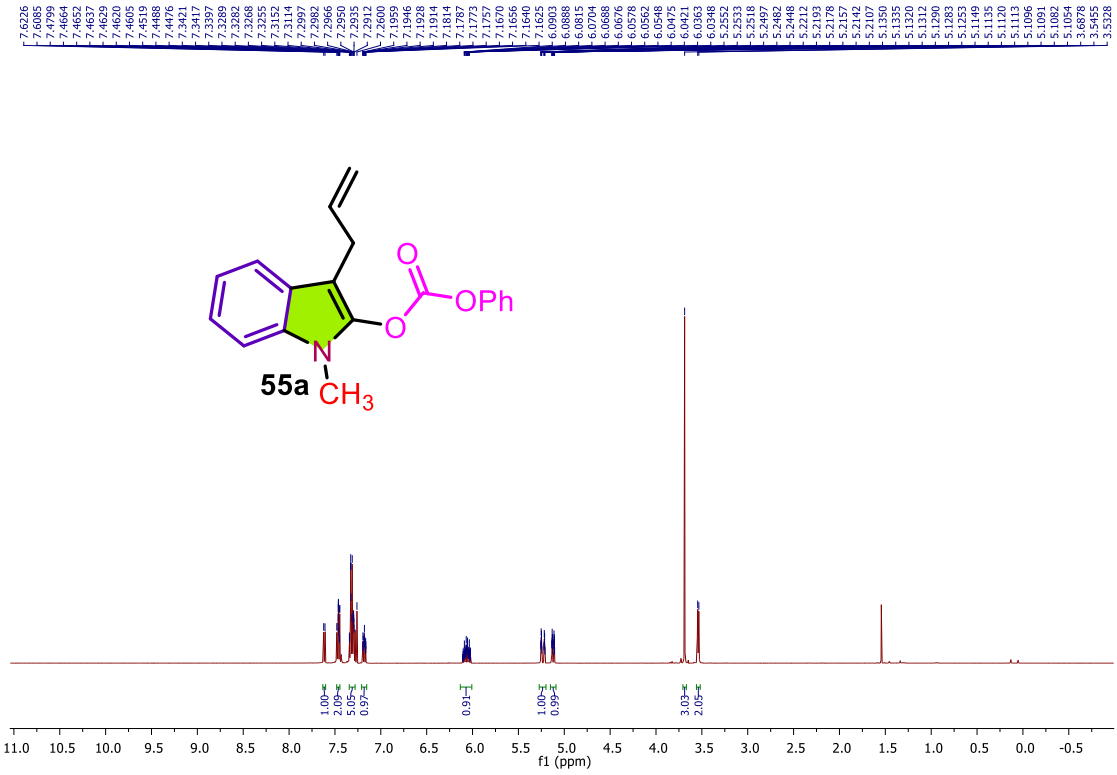


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

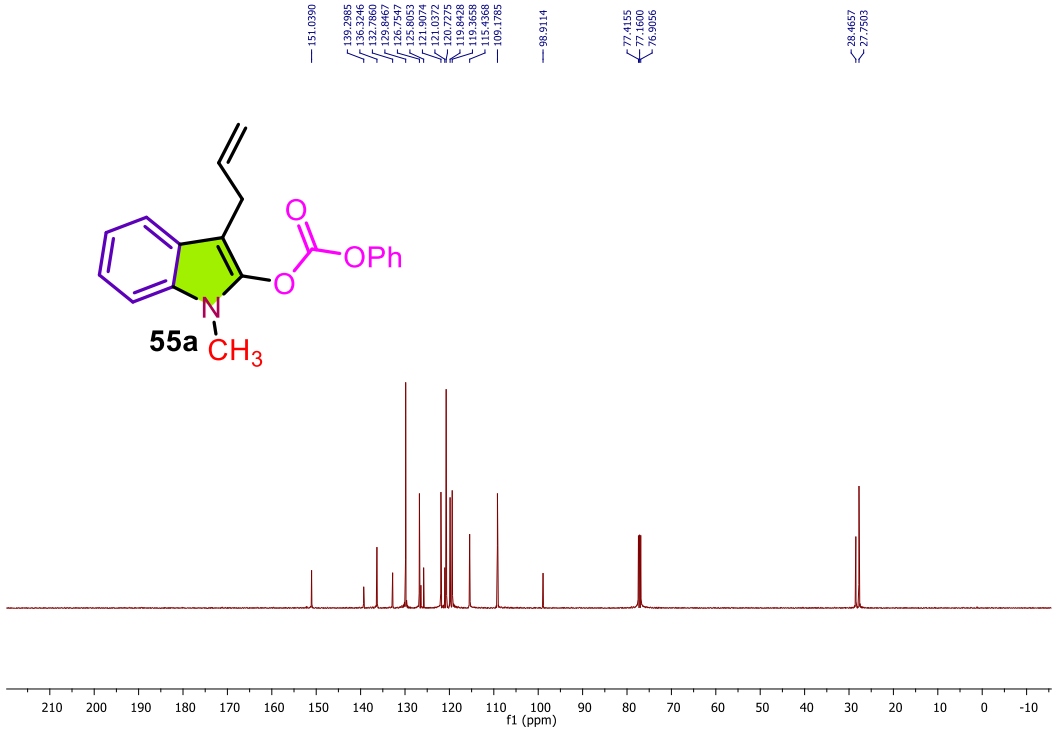


3-Allyl-1-methyl-1H-indol-2-yl phenyl carbonate (**55a**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

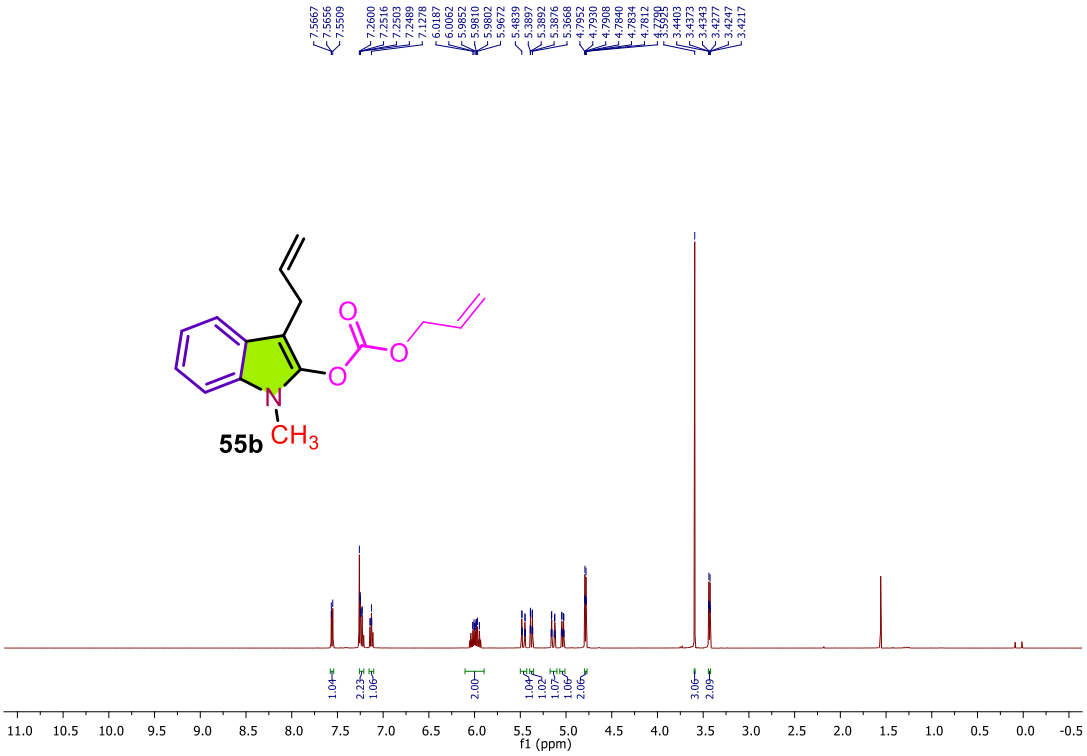


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

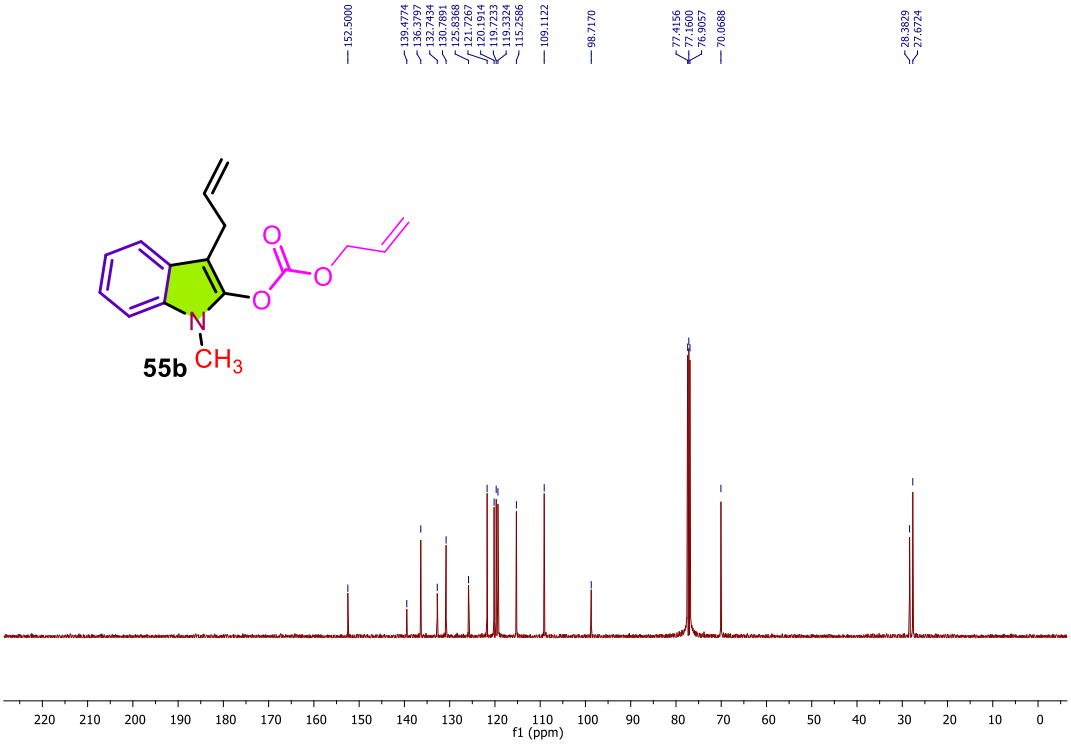


Allyl (3-allyl-1-methyl-1H-indol-2-yl) carbonate (**55b**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

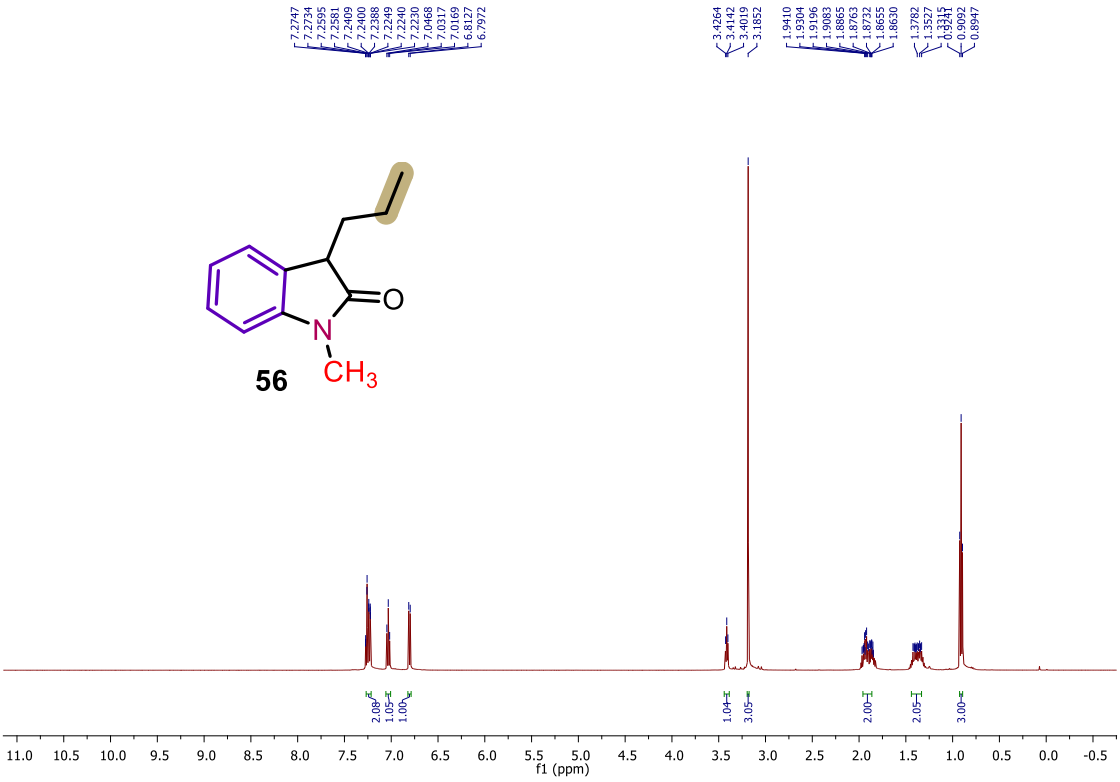


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

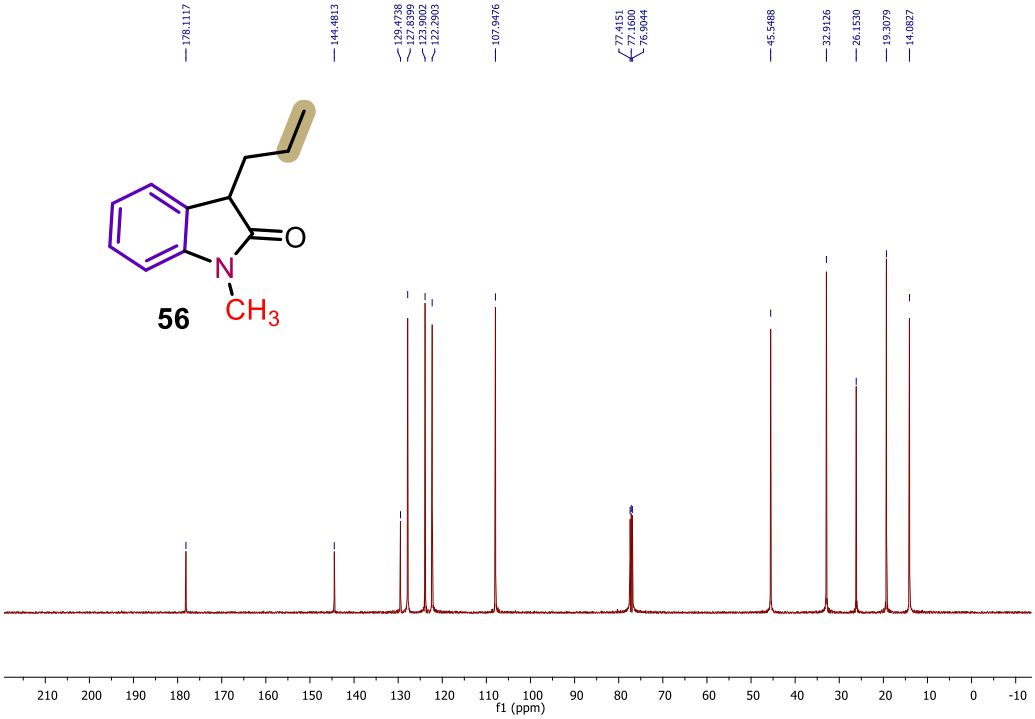


1-Methyl-3-propylindolin-2-one (**56**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

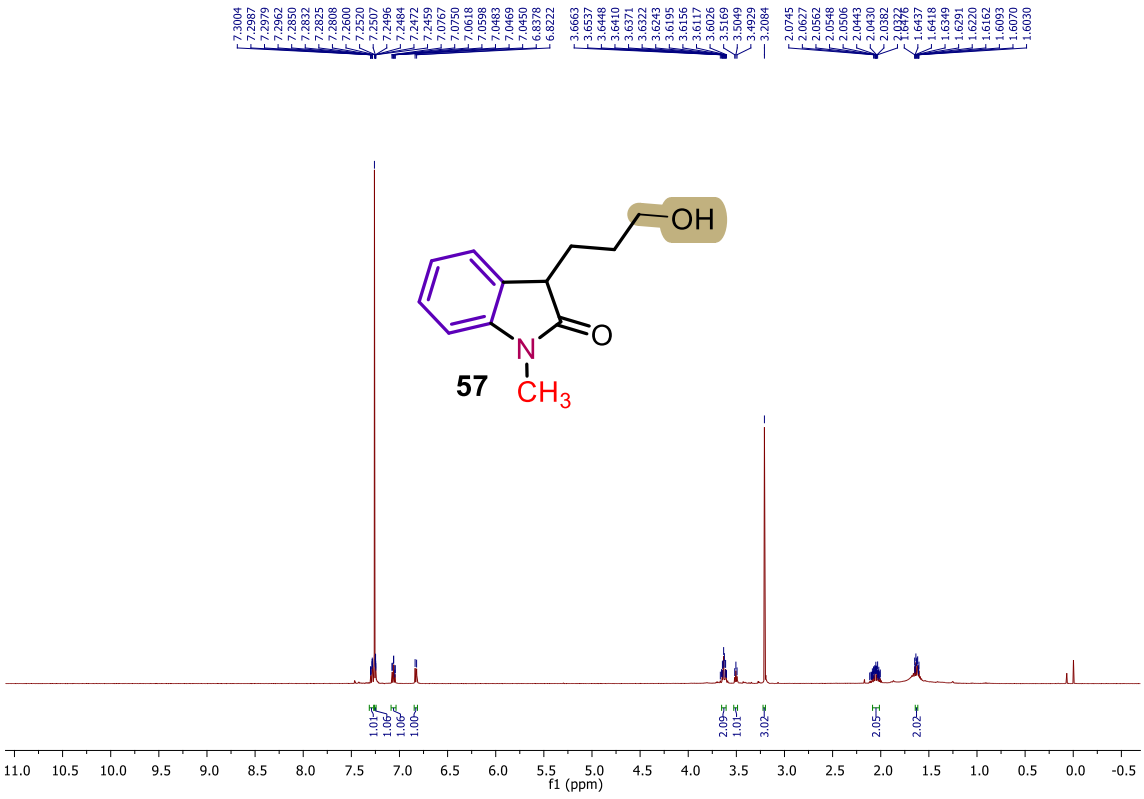


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

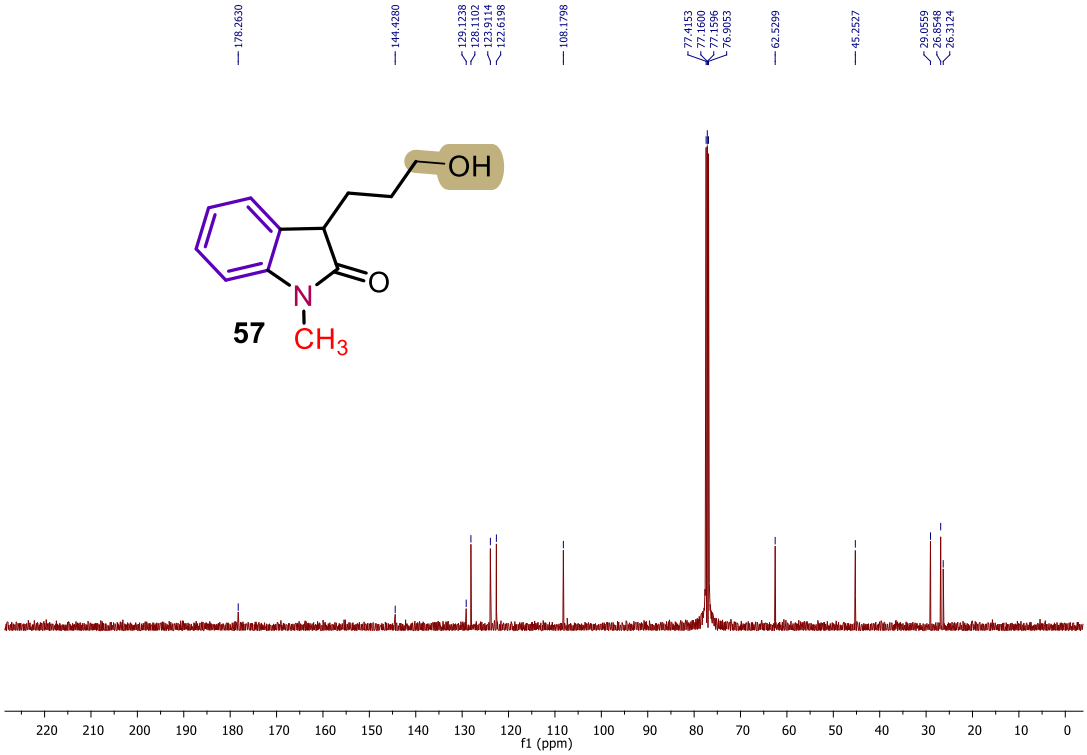


3-(3-Hydroxypropyl)-1-methylindolin-2-one (**57**).

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

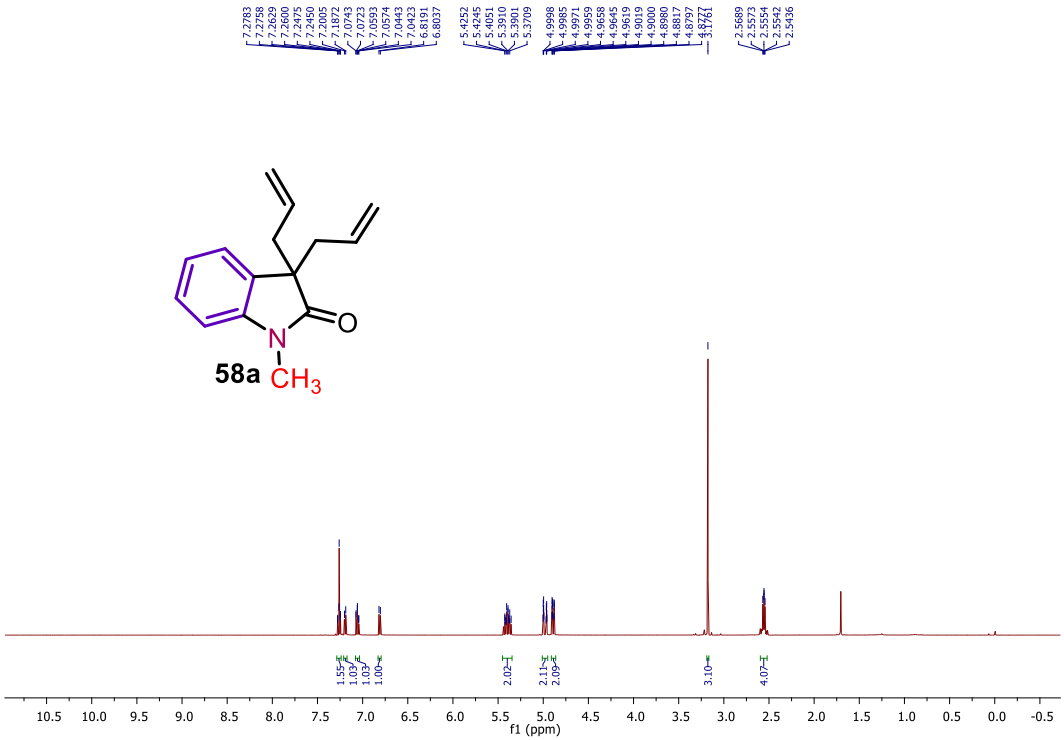


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

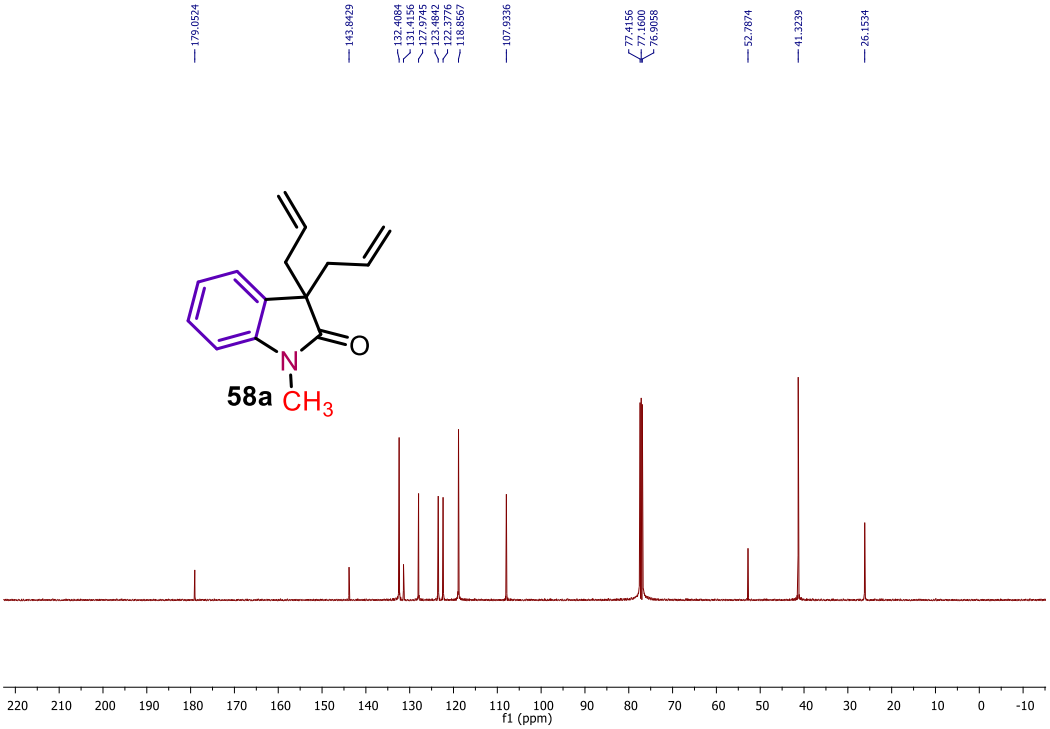


3,3-Diallyl-1-methylindolin-2-one (**58a**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

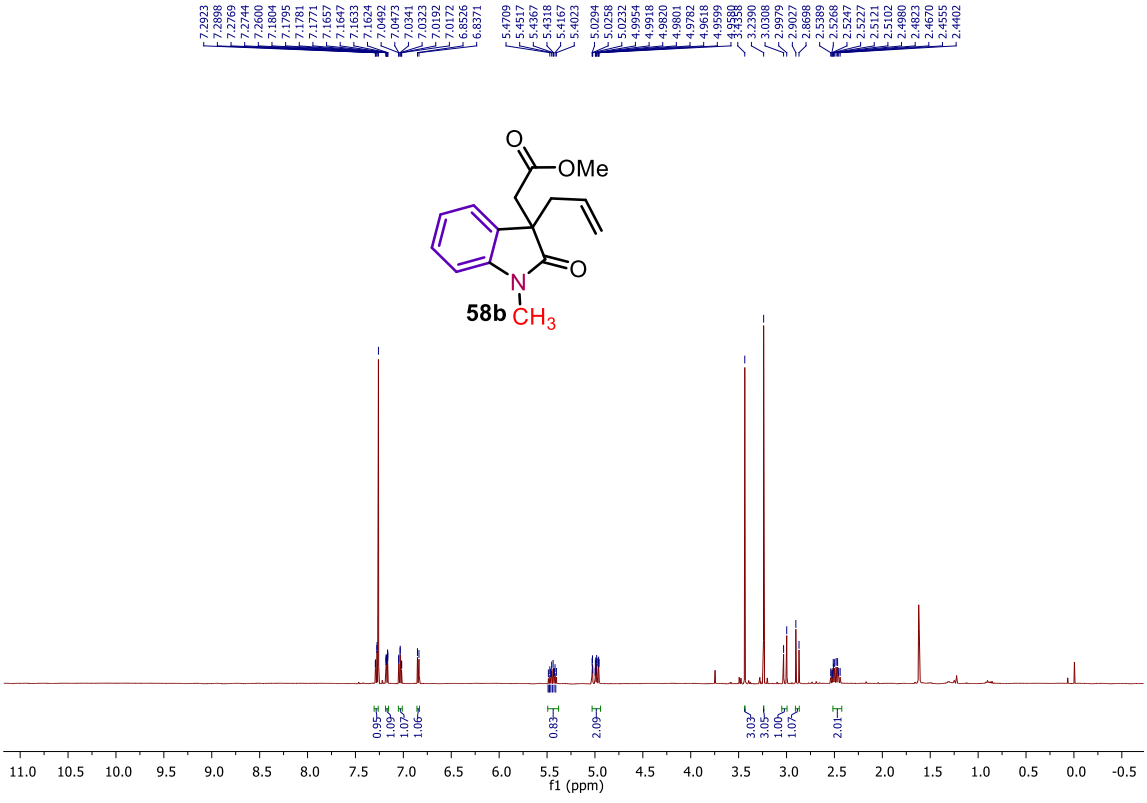


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

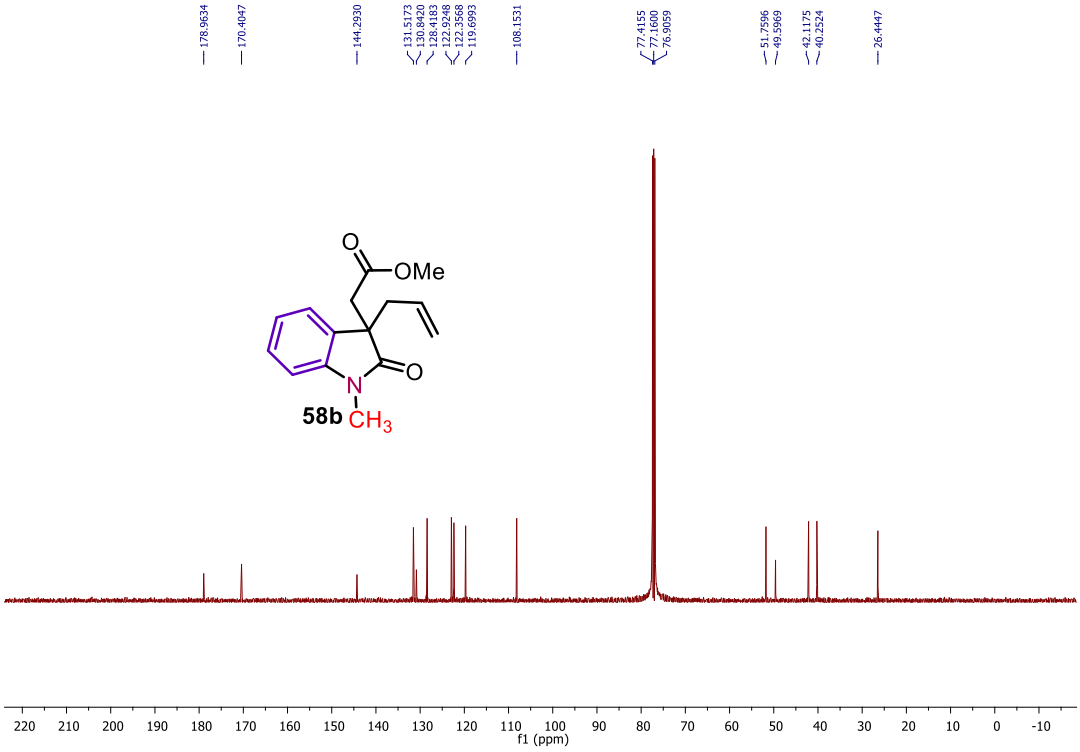


Methyl 2-(3-allyl-1-methyl-2-oxoindolin-3-yl)acetate (**58b**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

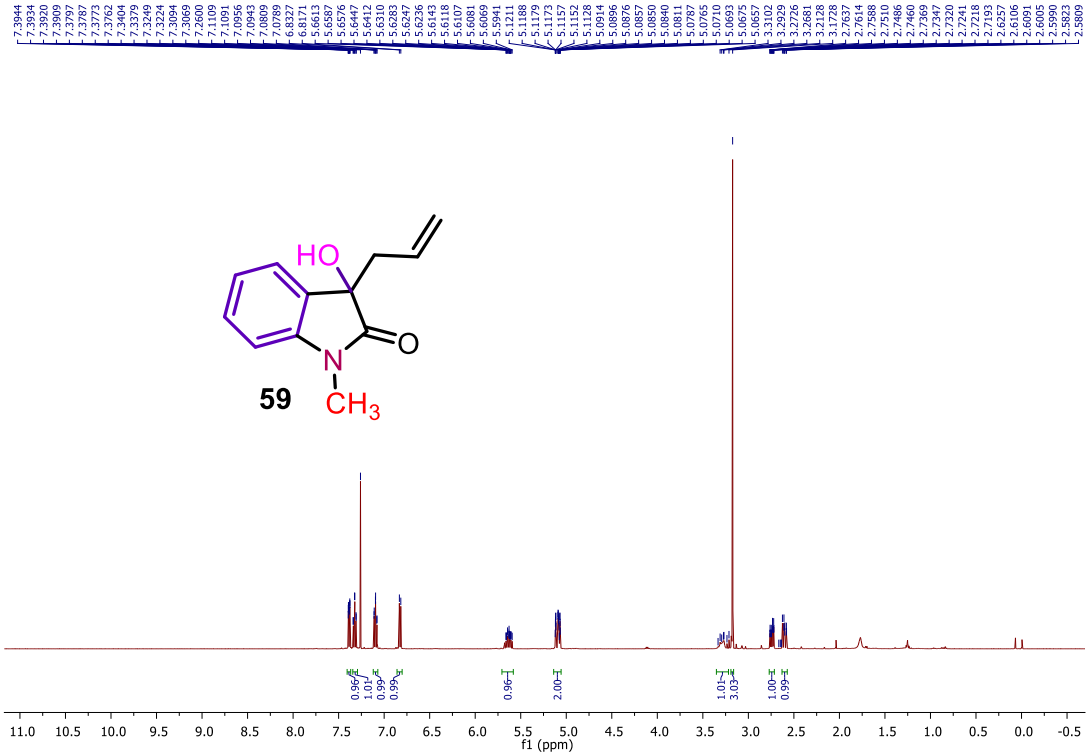


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

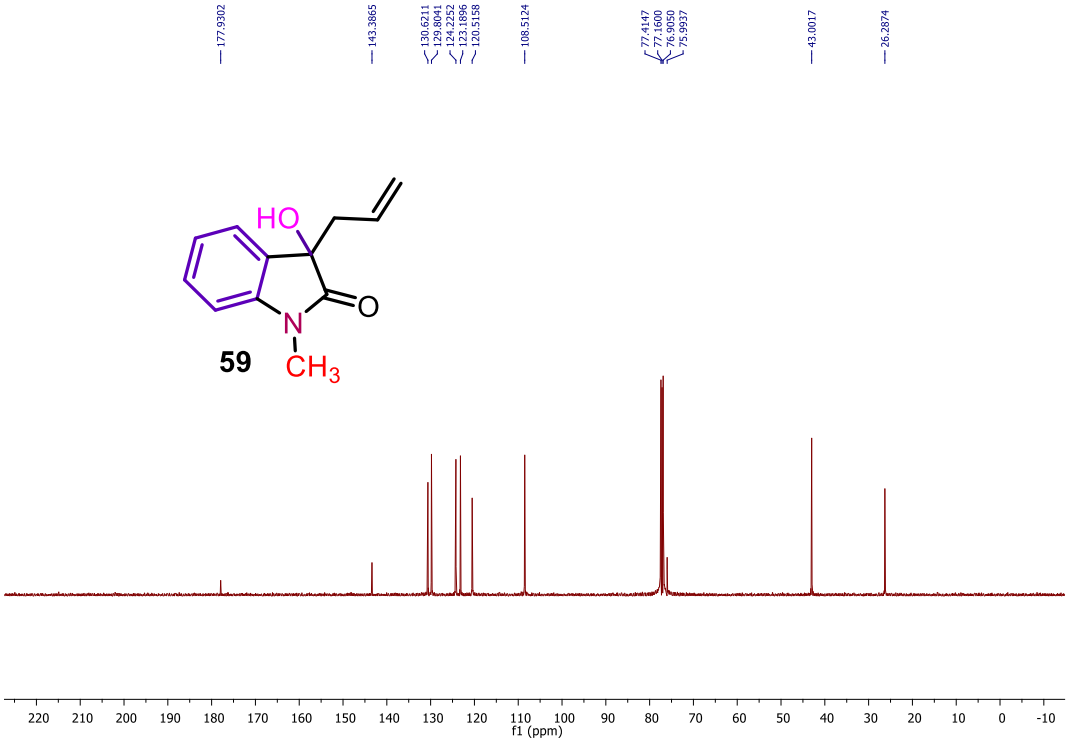


3-Allyl-3-hydroxy-1-methylindolin-2-one (**59**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

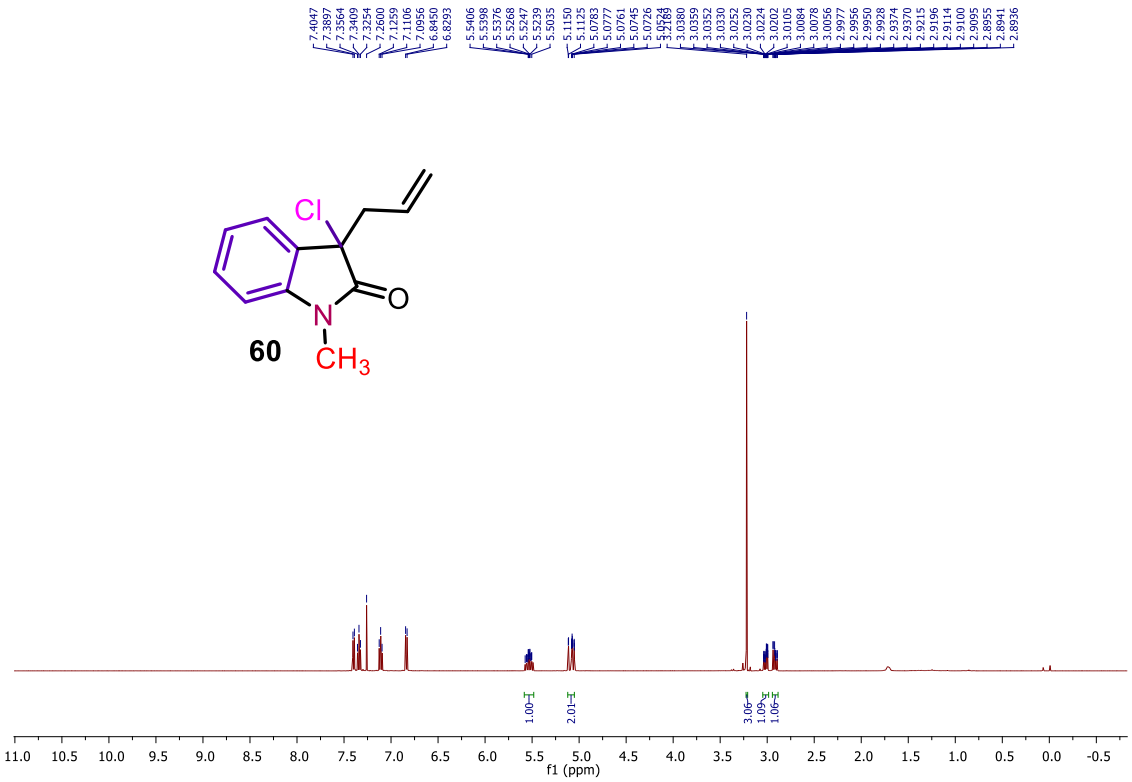


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

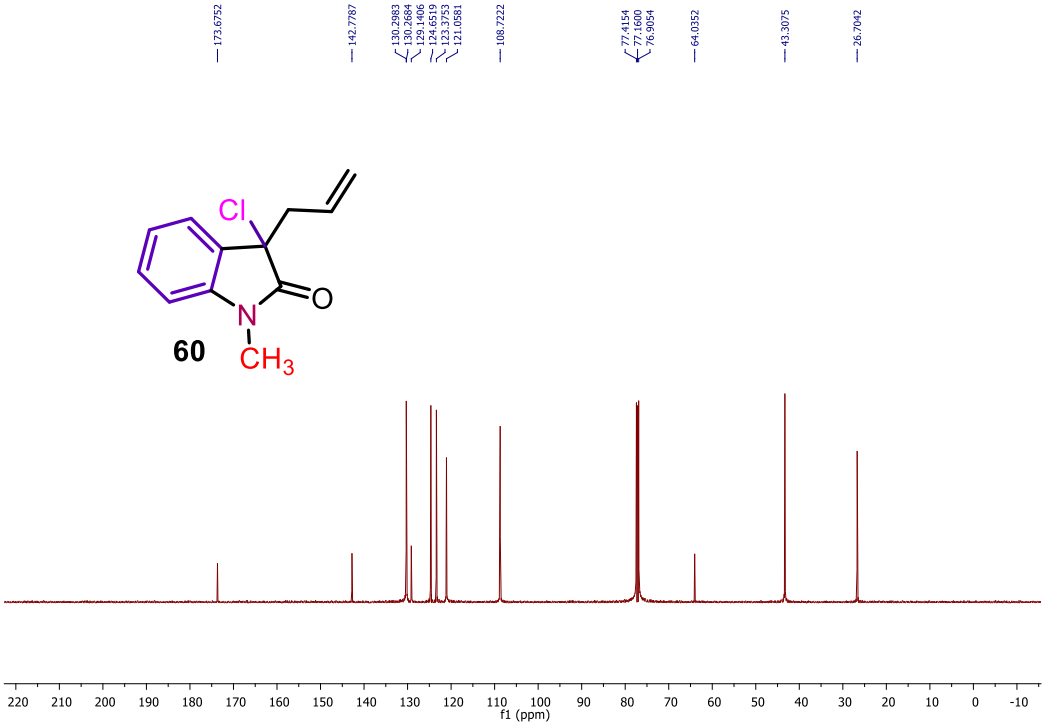


3-Allyl-3-chloro-1-methylindolin-2-one (**60**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

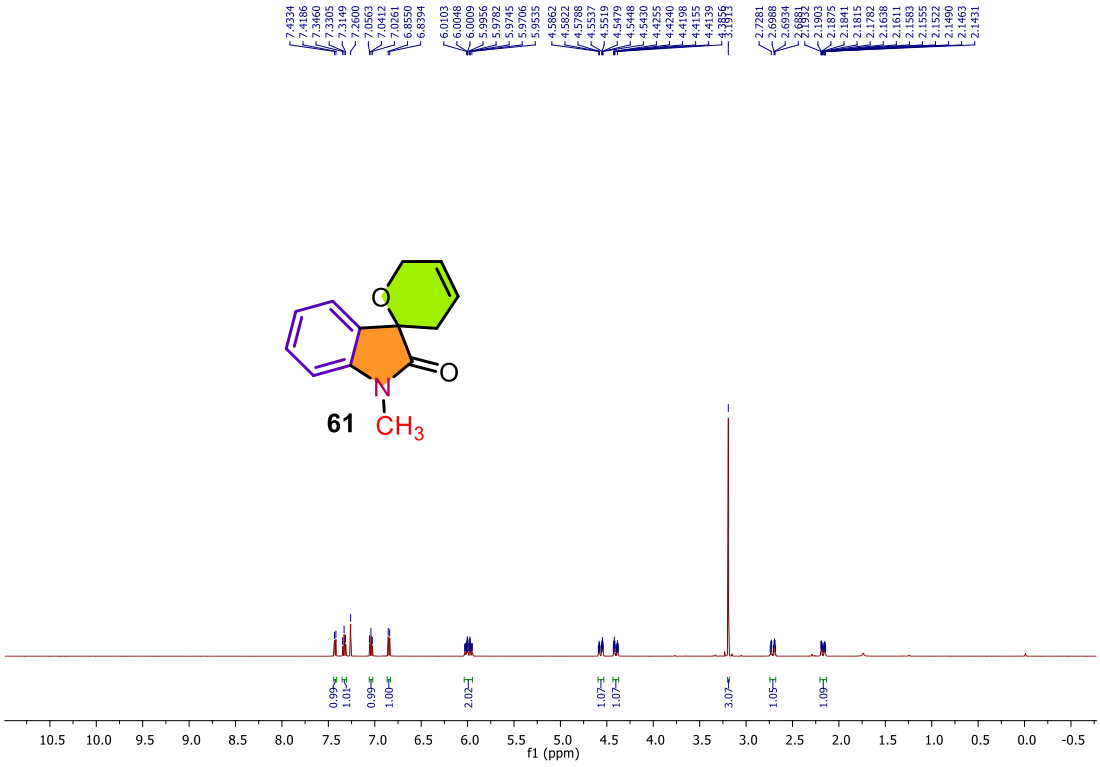


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

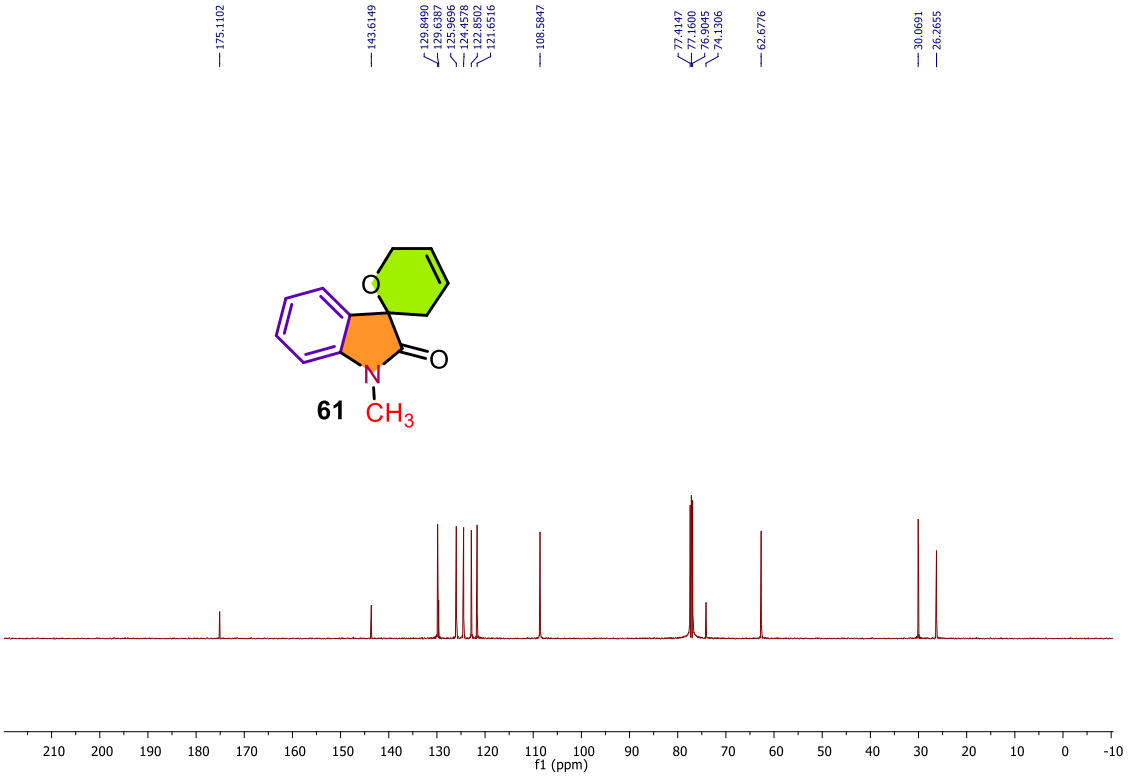


1-Methyl-3',4'-dihydrospiro[indoline-3,2'-pyran]-2-one (**61**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

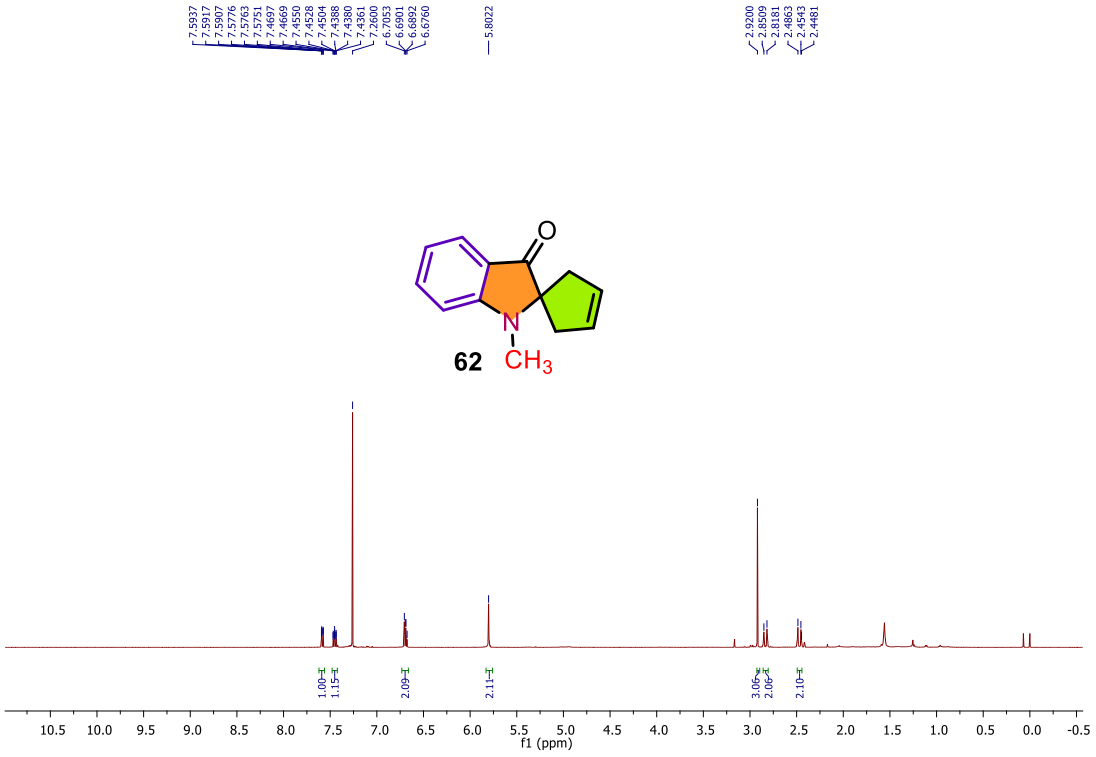


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

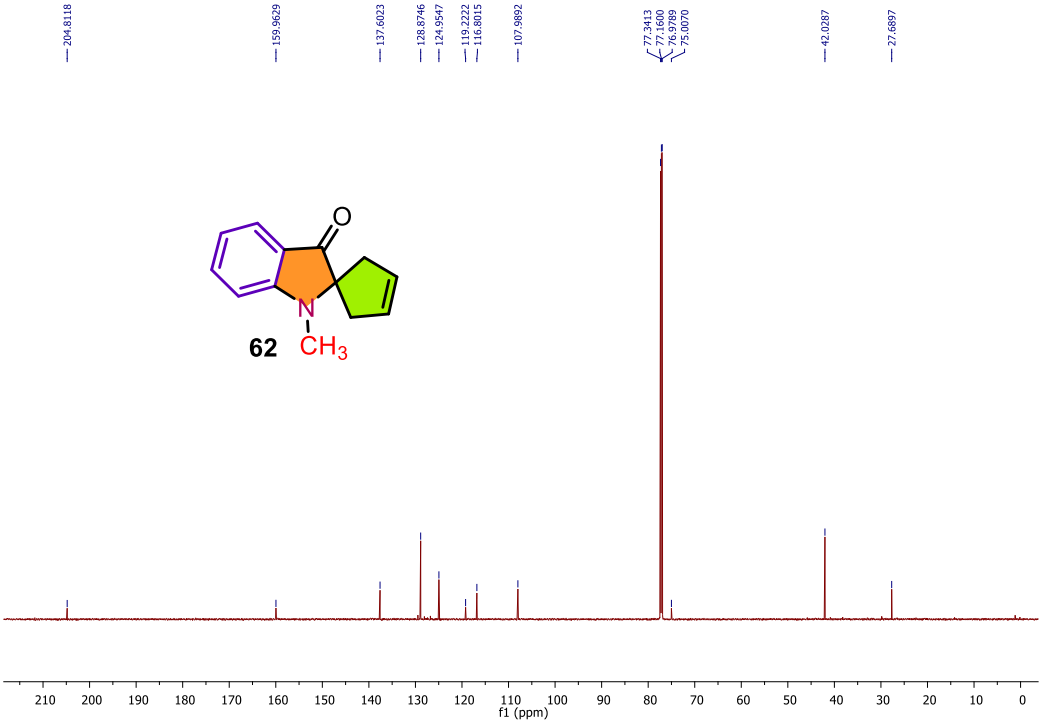


1'-Methylspiro[cyclopentane-1,2'-indolin]-3-en-3'-one (**62**).

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

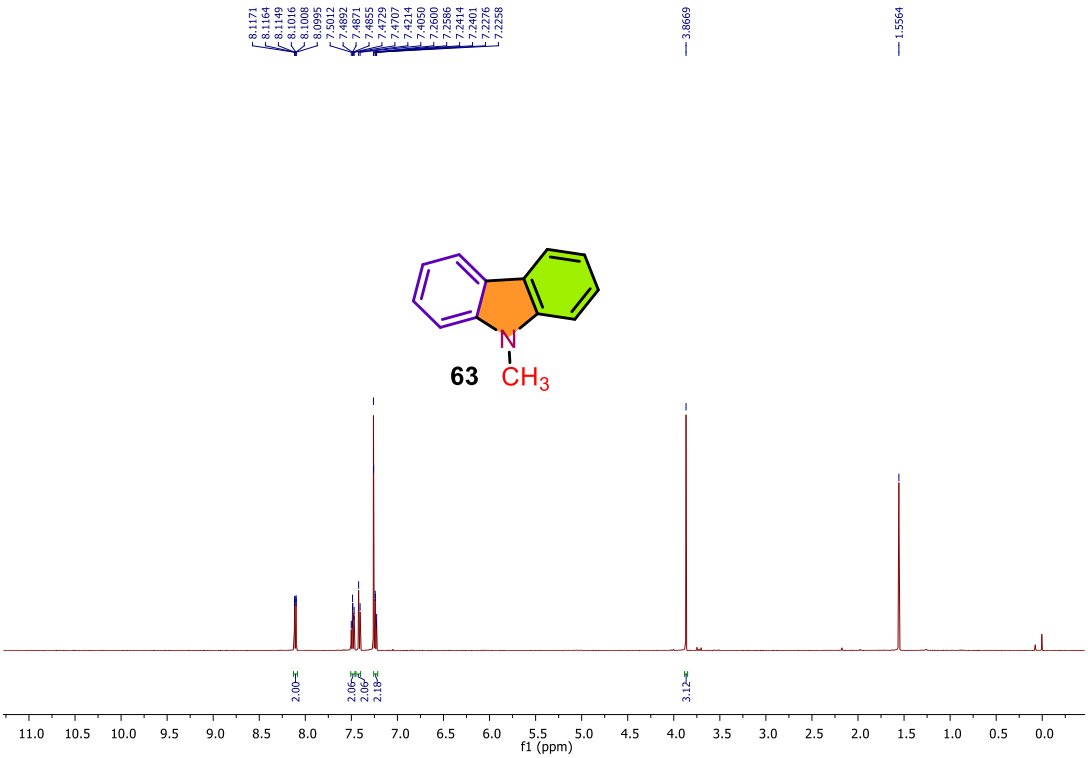


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

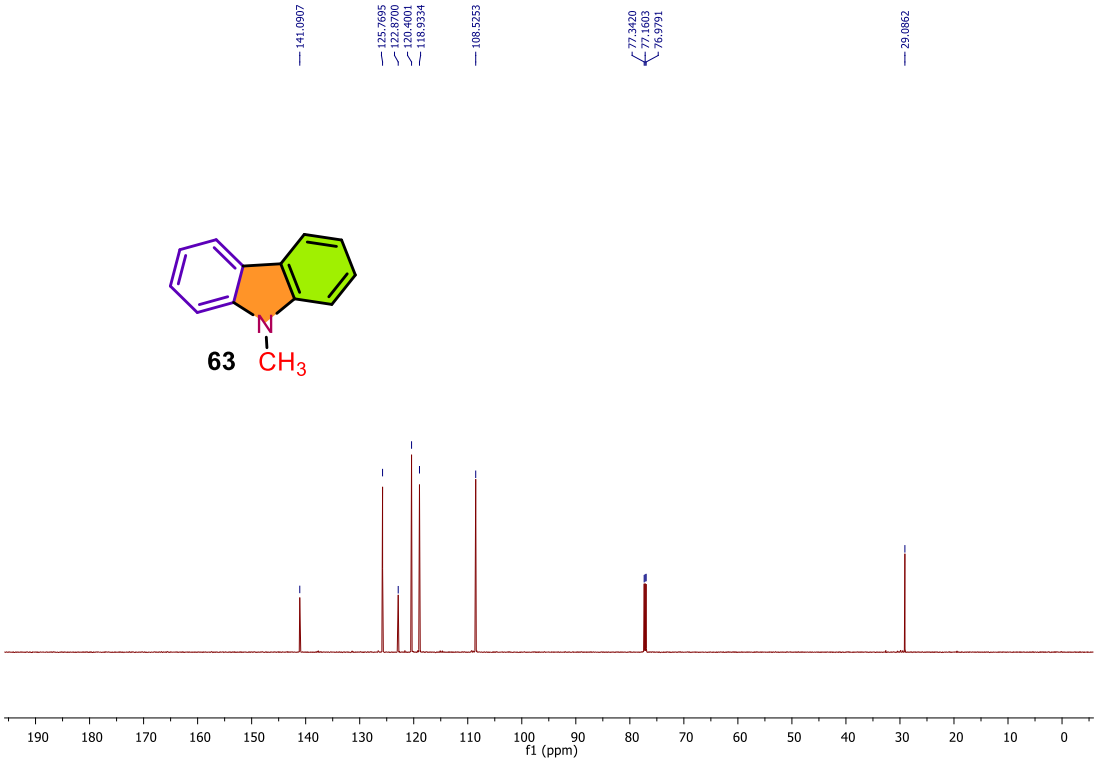


9-Methyl-9H-carbazole (**63**)

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

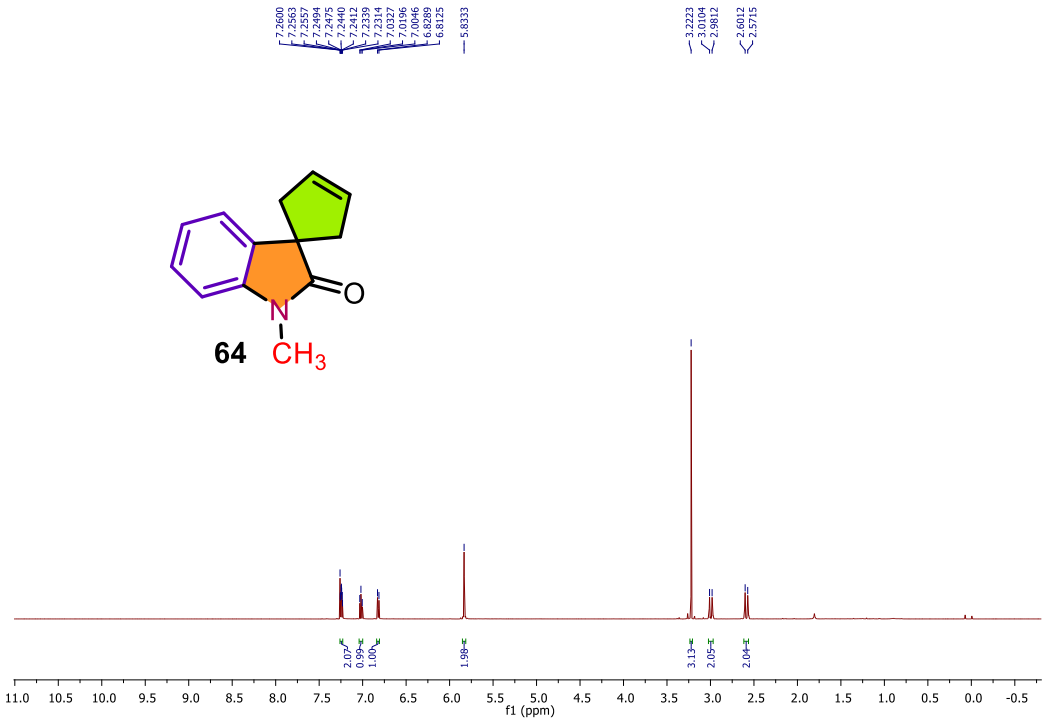


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

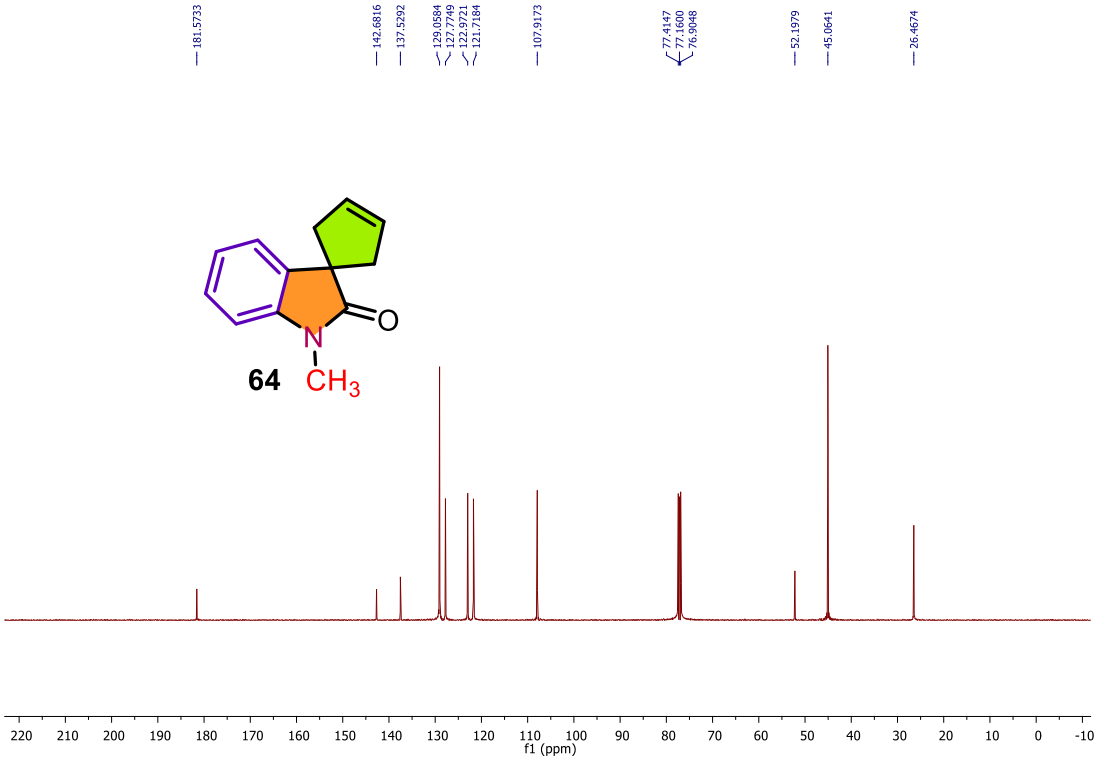


1'-Methylspiro[cyclopentane-1,3'-indolin]-3-en-2'-one (**64**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

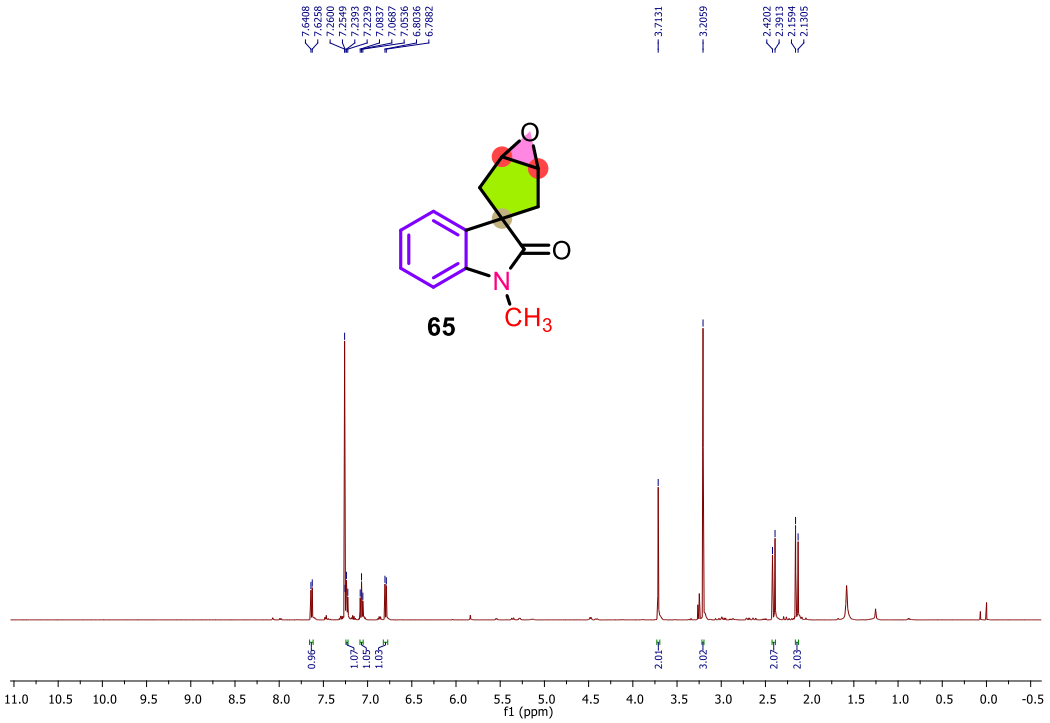


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

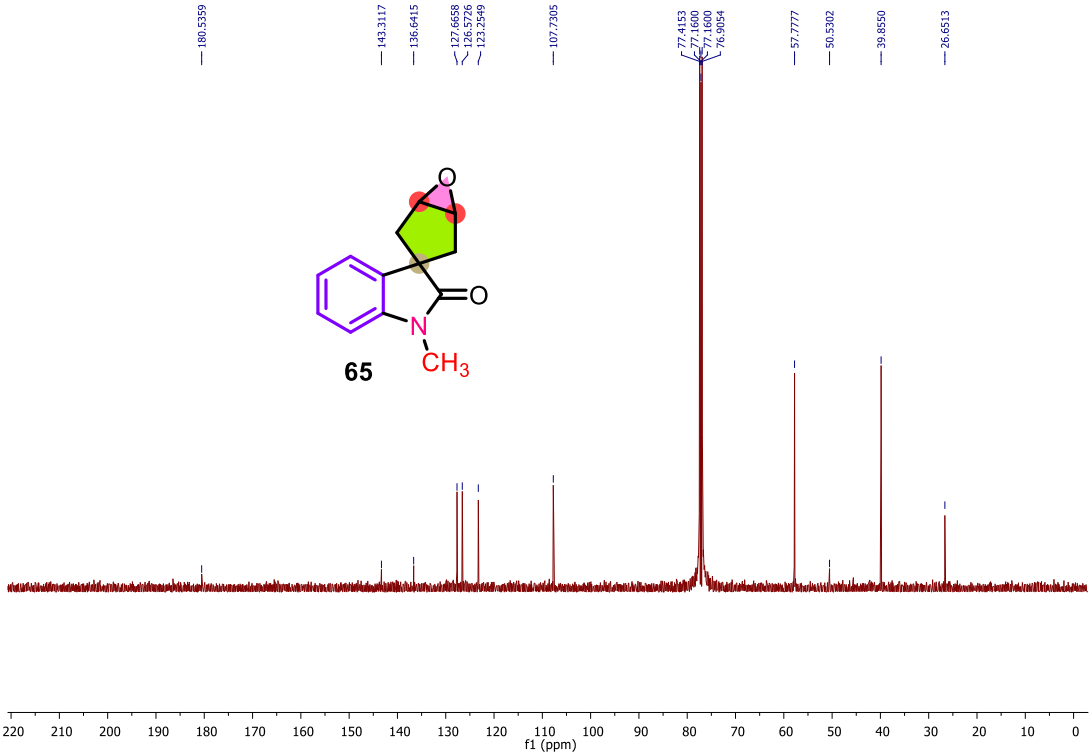


1'-Methyl-6-oxaspiro[bicyclo[3.1.0]hexane-3,3'-indolin]-2'-one (**65**).

^{1}H NMR (700 MHz, $CDCl_3$, 24 °C)

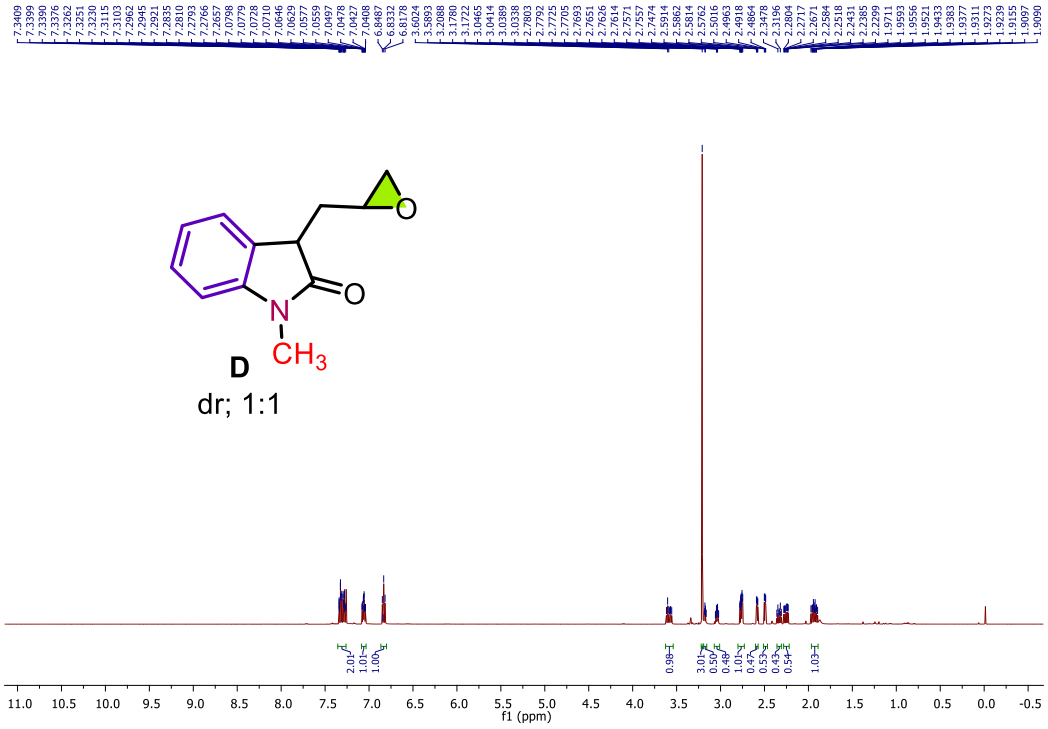


$^{13}C\{^{1}H\}$ NMR (176 MHz, $CDCl_3$, 24 °C)

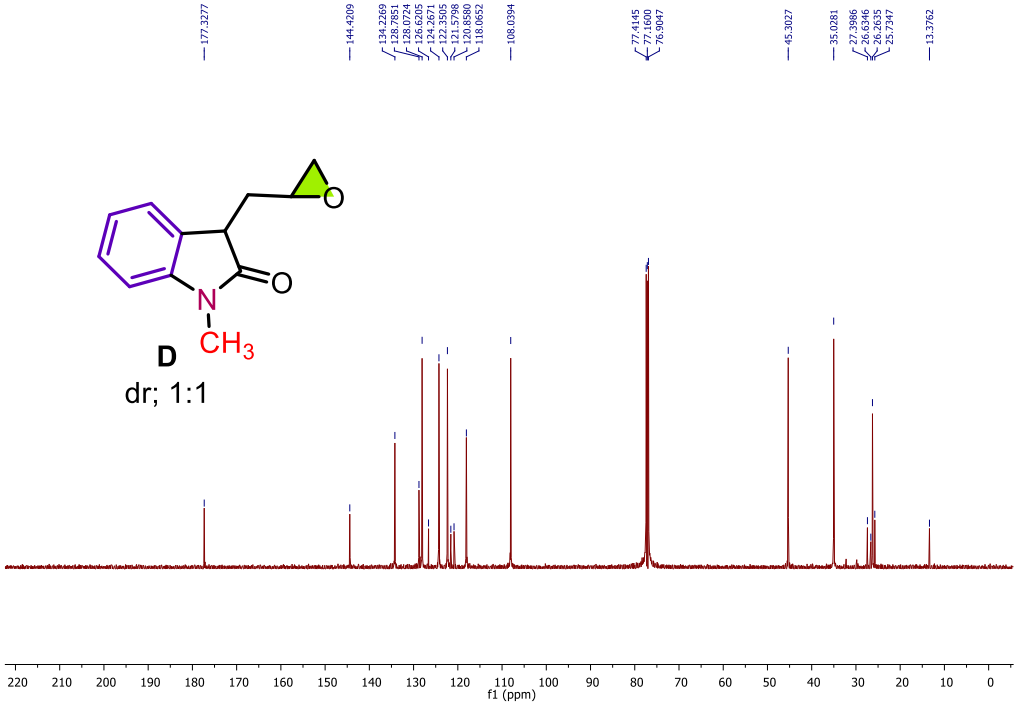


1-Methyl-3-(oxiran-2-ylmethyl)indolin-2-one (**D**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

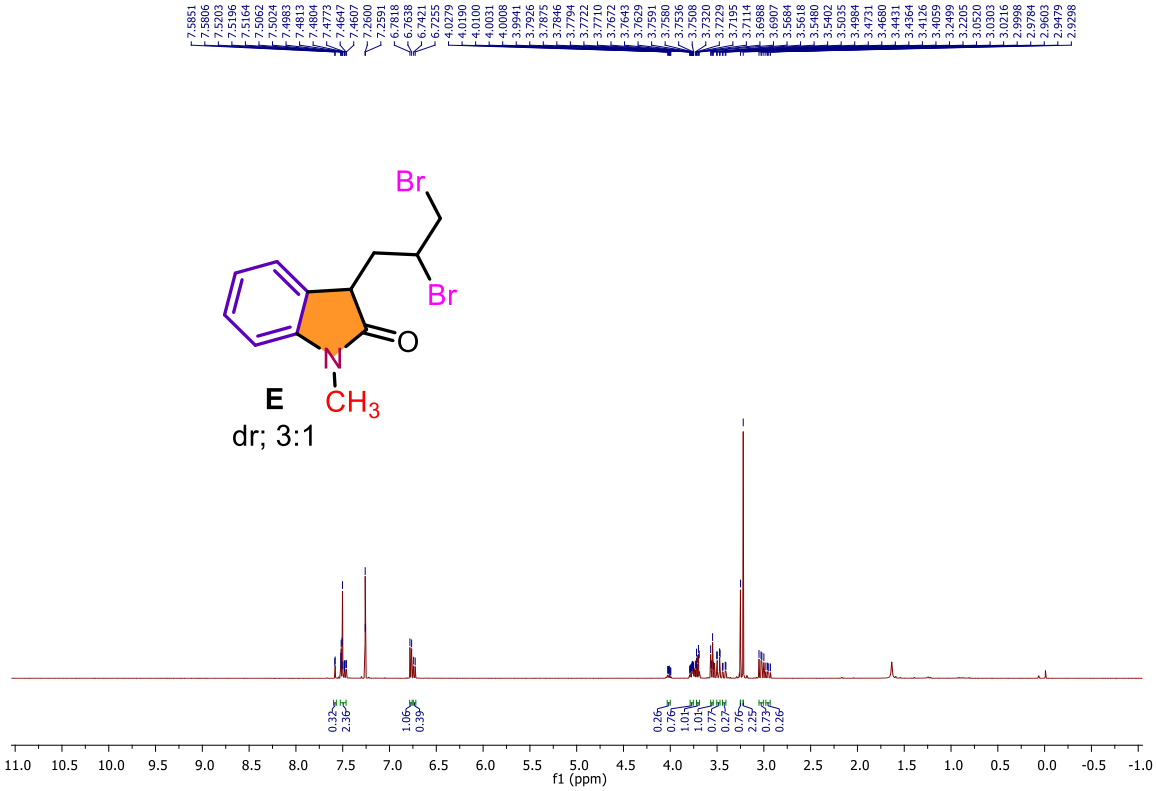


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)

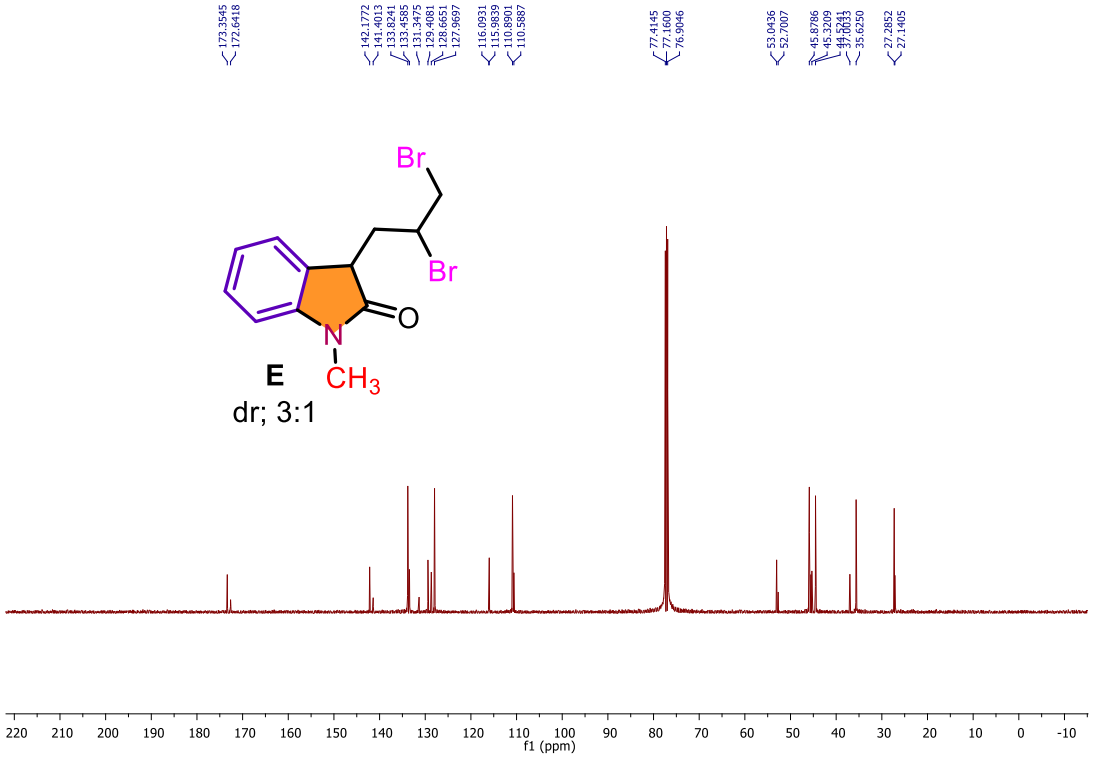


3-(2,3-dibromopropyl)-1-methylindolin-2-one (**E**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)

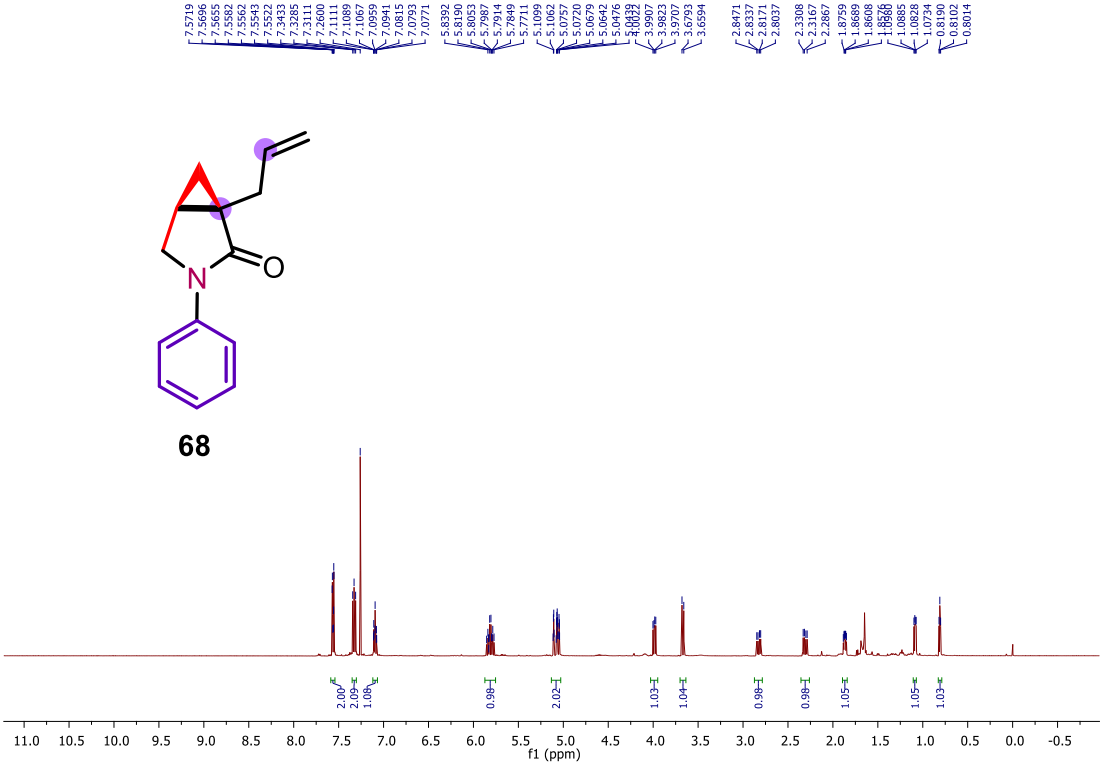


$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)



1-Allyl-3-phenyl-3-azabicyclo[3.1.0]hexan-2-one (**68**)

^{1}H NMR (500 MHz, $CDCl_3$, 24 °C)



$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 24 °C)