Supporting Information

Selective Ring Expansion and C−H Functionalization of Azulenes

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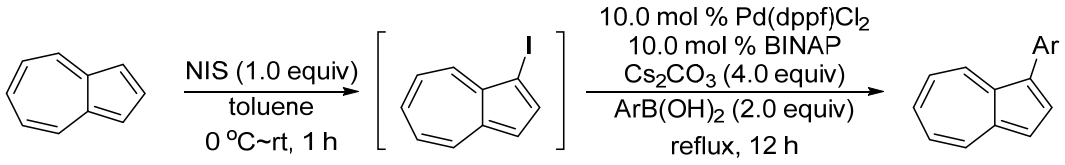
General Information

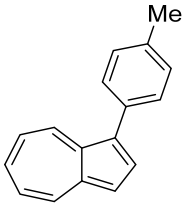
Reactions were carried out in oven-dried glassware under nitrogen atmosphere. $Cu(hfacac)_2$ and AgOTf were purchased and was used as received. Commercial available reagents were used without purification. 1,4-Dioxane, DCE, DCM, EtOAc, hexane, and toluene were dried with CaH_2. All reaction mixtures were stirred magnetically and were monitored by thin-layer chromatography using silica gel pre-coated glass plates, which were visualized with UV light and then developed using either iodine or a solution of anisaldehyde. Flash column chromatography was carried out using silica gel (230-400 mesh). ^1H NMR (400 MHz) and $^{13}C\{^1H\}$ NMR (100 MHz) spectra were recorded on NMR spectrometer. Deuterated chloroform and benzene were used as the solvents, and chemical shift values (δ) are reported in parts per million relative to the residual signals of these solvent [δ 7.26 for ^1H (chloroform-*d*), δ 7.16 for ^1H (benzene-d_6), δ 77.2 for $^{13}C\{^1H\}$ (chloroform-*d*) and δ 128.1 for $^{13}C\{^1H\}$ (benzene-d_6). Infrared spectra were recorded on FT-IR spectrometer as either a thin neat pressed between two sodium chloride plates or as a solid suspended in a potassium bromide disk. High resolution mass spectra (HRMS) were obtained by fast atom bombardment (FAB) using a double focusing magnetic sector mass spectrometer and electron impact (EI) ionization technique (magnetic sector – electric sector double focusing mass analyzer) from the KBSI (Korea Basic Science Institute Daegu Center). Melting points were determined in open capillar tube.

Experimental Section

A. Substrate preparation[1]



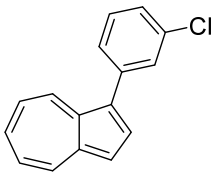
General procedure for the preparation of azulene derivatives: Azulene (256.0 mg, 2.0 mmol) and toluene (5.0 mL) were added to a 25 mL round-bottom flask with a stirring bar. The mixture was stirred at 0 °C for 10 min. After *N*-iodosuccinimide (450.0 mg, 2.0 mmol) was added in 5-portion to the mixture and then, the mixture was stirred at room temperature for 1 h. Completion of the reaction was indicated by the TLC. The residue was passed through a pad of Cellite to remove succinimide and eluted with toluene (5.0 mL) to a 25 mL round-bottom flask with a stirring bar, arylboronic acid (4.0 mmol), $Pd(dppf)Cl_2$ (14.6 mg, 0.02 mmol), BINAP (12.5 mg, 0.02 mmol), and Cs_2CO_3 (2.61 g, 8.0 mmol). The mixture was stirred at reflux for 12 h. The mixture was extracted with dichloromethane and was washed with H_2O. The solution was removed under reduced pressure and the residue was purified by column chromatography using hexane to give **1t-1v**.



1t

1-(*p*-Tolyl)azulene (1t)

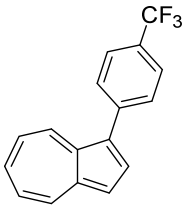
Blue solid; m.p. 38−40 °C; R_f = 0.3 (hexane); ^1H NMR (400 MHz, C_6D_6) δ 8.51 (d, J = 9.8 Hz, 1H), 8.02 (d, J = 3.9 Hz, 1H), 7.98 (d, J = 9.4 Hz, 1H), 7.51 (dd, J = 6.4 Hz, 1.6 Hz, 2H), 7.35 (d, J = 3.9 Hz, 1H), 7.17−7.13 (m, 3H), 6.72 (t, J = 9.8 Hz, 2H), 2.22 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, C_6D_6) δ 142.1, 137.9, 137.5, 137.2, 135.8, 135.7, 135.1, 132.0, 130.0, 129.6, 123.0, 122.8, 118.0, 21.1; IR (neat) 3023, 2917, 1569, 1524, 1493, 1392, 821 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{17}H_{14}$ 218.1096; Found 218.1094.



1u

1-(3-Chlorophenyl)azulene (1u)

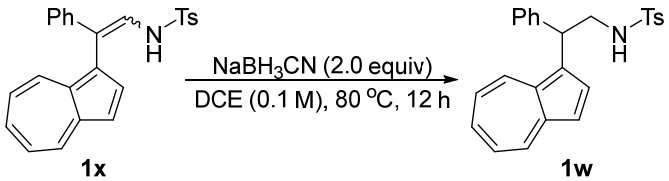
Blue oil; R_f = 0.3 (EtOAc:hexane = 1:50) ^{1}H NMR (400 MHz, C_6D_6) δ 8.30 (d, J = 9.8 Hz, 1H), 7.93 (d, J = 9.4 Hz, 1H), 7.79 (d, J = 3.9 Hz, 1H), 7.60 (t, J = 1.8 Hz, 1H), 7.27−7.24 (m, 2H), 6.96 (t, J = 7.8 Hz, 1H), 6.71 (t, J = 9.7 Hz, 1H), 6.65 (t, J = 9.8 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 142.2, 139.9, 138.0, 137.44, 137.41, 135.8, 135.4, 134.8, 130.02, 130.00, 129.9, 126.3, 123.7, 123.3, 118.0; IR (neat) 3060, 3024, 1592, 1575, 1561, 1475, 1394, 778 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{16}H_{11}Cl$ 238.0549; Found 238.0546.



1v

1-(4-(Trifluoromethyl)phenyl)azulene (1v)

Blue solid; m.p. 45-47 ºC; R_f = 0.3 (EtOAc:hexane = 1:50); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, J = 9.8 Hz, 1H), 8.39 (d, J = 9.5 Hz, 1H), 8.02 (d, J = 3.9 Hz, 1H), 7.75−7.70 (m, 4H), 7.64 (t, J = 9.8 Hz, 1H), 7.45 (d, J = 3.9 Hz, 1H), 7.212 (t, J = 9.7 Hz, 1H), 7.206 (t, J = 9.8 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 142.1, 141.2, 138.6, 137.7, 137.2, 135.5, 135.4, 129.8, 129.5, 128.3, 127.9, 125.6 (q, J = 3.8 Hz), 124.0, 123.8, 117.8; IR (neat) 2967, 1614, 1570, 1429, 1362, 1324, 1163, 1120, 1065, 1015, 845, 741 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{17}H_{11}F_3$ 272.0813; Found 272.0811.

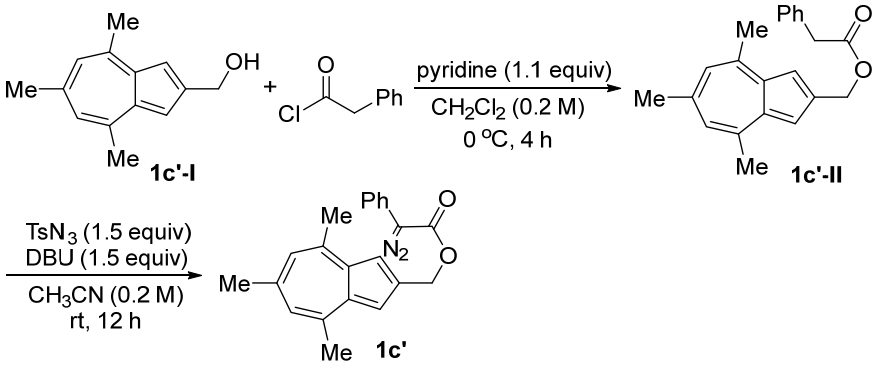


1x **1w**

_N_-(2-(Azulen-1-yl)-2-phenylethyl)-4-methylbenzenesulfonamide (1w)

A mixture of _N_-(2-(azulen-1-yl)-2-phenylvinyl)-tolylsulfonamide (**1x**)[2-3] (79.9 mg, 0.2 mmol) and $NaBH_3CN$ (25.1 mg, 0.4 mmol) in dichloroethane (2.0 mL) was stirred at 80 ºC for 12 h under a nitrogen atmosphere. The resulting mixture was diluted with CH_2Cl_2 after cooling to room temperature and filtered through a pad of Celite. The filtrate was concentrated under reduced pressure, and the residue was purified via silica gel flash column chromatography to give the _N_-(2-(azulen-1-yl)-2-phenylethyl)-4-methyl-benzenesulfonamide (45.8 mg, 57%). R_f = 0.2 (EtOAc:hexane = 1:5); Blue solid, m.p. 57-61 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J = 9.4 Hz, 1H), 8.11 (d, J = 9.7 Hz, 1H), 7.67 (d, J = 3.9 Hz, 1H), 7.66-7.63 (m, 2H), 7.56 (t, J = 9.9 Hz, 1H), 7.32 (d, J = 3.9 Hz, 1H), 7.28-7.26 (m, 2H), 7.25-7.21 (m, 2H), 7.18-7.10 (m, 4H), 7.07 (t, J = 10.0 Hz, 1H), 4.72 (t, J = 7.9 Hz, 1H), 4.40 (t, J = 6.2 Hz, 1H), 3.75-3.60 (m, 2H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6, 142.0, 141.0, 138.2, 137.3, 137.0, 136.3, 134.7, 133.6, 129.9, 128.9, 127.9, 127.3, 127.0, 123.2, 122.7, 117.4, 48.4, 43.4, 21.7; IR (film) : 3289, 3026, 1576, 1396, 1328, 1160, 1092, 739 cm^{-1}; HRMS (EI) _m/z_: [M^+] Calcd for $C_{25}H_{23}NO_2S$: 401.1449; Found 401.1448.

Preparation of diazo compound for intramolecular ring expansion reaction



(4,6,8-Trimethylazulen-2-yl)methyl 2-phenylacetate (1c'-II)

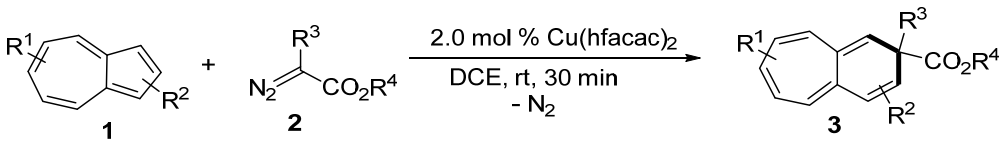
4,6,8-Trimethylazulene-2-methanol (**1c'-I**)[4] (332.2 mg, 1.7 mmol) and dichloromethane (8.3 mL) were added to a 25 mL round-bottom flask equipped with a stirring bar. After phenylacetyl chloride (247.3 μL, 1.9 mmol) and pyridine (153.7 μL, 1.9 mmol) were added to the mixture at 0 ºC for 10 min. The mixture was stirred at 0 ºC for 4 h. Completion of the reaction was indicated by the TLC. The mixture was

extracted with dichloromethane and was washed with H_2O. The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The filtrate was concentrated under reduced pressure and the residue was purified by Silica gel fresh column chromatography (EtOAc:hexane) to give **1c'-II** (382.0 mg, 72%) as violet oil. R_f = 0.2 (EtOAc:hexane = 1:3); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36−7.27 (m, 5H), 7.20 (s, 2H), 7.07 (s, 2H), 5.49 (s, 2H), 3.73 (s, 2H), 2.82 (s, 6H), 2.62 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 171.6, 146.4, 145.8, 141.6, 136.2, 134.2, 129.4, 128.6, 127.7, 127.1, 114.5, 63.3, 41.5, 28.8, 25.1; IR (neat) 3087, 3060, 3030, 2999, 2947, 2918, 1736, 1577, 1453, 1332, 1241, 1146 cm^{-1}; HRMS (EI) Calcd for *m/z*: [M^+] $C_{22}H_{22}O_2$ 318.1620; Found 316.1621.

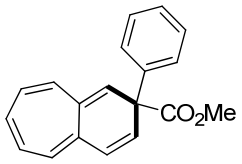
(4,6,8-Trimethylazulen-2-yl)methyl 2-diazo-2-phenylacetate (1c')

(4,6,8-Trimethylazulen-2-yl)methyl 2-phenylacetate **1c'-II** (382.0 mg, 1.2 mmol) and acetonitrile (6.0 mL) were added to a 25 mL round-bottom flask equipped with a stirring bar. After tosyl azide (236.7 mg, 1.2 mmol) and DBU (269.2 μL, 1.8 mmol) were added to the mixture at 0 °C, the mixture was stirred at room temperature for 12 h. Completion of the reaction was indicated by the TLC. The mixture was extracted with dichloromethane and was washed with H_2O. The organic layer was dried over $MgSO_4$ and concentrated *in vacuo*. The filtrate was concentrated under reduced pressure and the residue was purified by Silica gel fresh column chromatography to give **1c'** (70.3 mg, 17%) as violet solid. m.p. 80-82 °C; R_f = 0.3 (EtOAc:hexane = 1:20); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 8.1 Hz, 2H), 7.39 (t, J = 7.6 Hz, 2H), 7.30 (s, 2H), 7.18 (t, J = 7.0 Hz, 1H), 7.08 (s, 2H), 5.67 (s, 2H), 2.86 (s, 6H), 2.62 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 165.3, 146.5, 146.0, 141.5, 136.3, 128.9, 127.8, 125.8, 125.7, 124.1, 114.6, 63.3, 28.8, 25.1; IR (neat) 3058, 3024, 3000, 2951, 2920, 2086, 1703, 1577, 1498, 1448, 1330, 1243, 1149, 1014 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{22}H_{20}N_2O_2$ 344.1525; Found 344.1525.

B. Ring expansion of azulenes with alkyl and aryl diazo esters



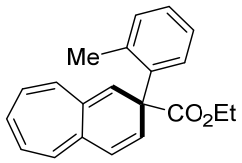
$Cu(hfacac)_2$ (1.9 mg, 2.0 mol %), azulene derivatives (0.2 mmol) and DCE (3.0 mL) were added to a test tube equipped with a stirring bar. To the solution was added aryl diazoacetate derivatives (0.2 mmol) in DCE (1.0 mL). The mixture was stirred at room temperature for 30 min. The residue was passed through a pad of Cellite to remove $Cu(hfacac)_2$ and eluted with CH_2Cl_2. The filtrate was concentrated under reduced pressure and the residue was purified by Silica gel fresh column chromatography (EtOAc:hexane) to give **3**.



3a

Methyl 2-phenyl-2*H*-benzo[7]annulene-2-carboxylate (3a)

Yield (51.4 mg, 93%); Red solid; m.p. 99−101 ºC; R_f = 0.7 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, C_6D_6) δ 7.37−7.32 (m, 2H), 7.24−7.18 (m, 3H), 6.10 (d, J = 9.8 Hz, 1H), 6.05−6.00 (m, 2H), 5.66−5.62 (m, 2H), 5.58−5.56 (m, 1H), 5.53−5.48 (m, 1H), 5.44 (s, 1H), 3.75 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.0, 145.0, 139.7, 136.7, 136.3, 130.8, 130.0, 129.5, 129.3, 128.8, 126.8, 126.6, 126.4, 121.9, 56.5, 52.6; IR (neat) 3025, 2950, 1730, 1431, 1217 cm^{-1}; HRMS (FAB) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{17}O_2$ 277.1229; Found 277.1227.

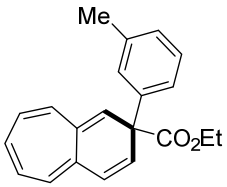


3b

Ethyl 2-(*o*-tolyl)-2*H*-benzo[7]annulene-2-carboxylate (3b)

The compound **3b** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3b** (50.3 mg, 82%) as a red

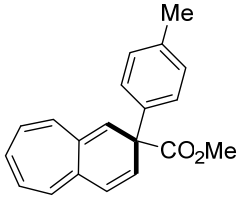
solid. m.p. 114−116 °C; R_f = 0.5 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, C_6D_6) δ 7.39 (d, J = 7.6 Hz, 1H), 7.11−7.07 (m, 1H), 7.00−6.98 (m, 2H), 6.00 (ddd, J = 9.7 Hz, 2.2 Hz, 0.5 Hz, 1H), 5.84 (d, J = 8.9 Hz, 1H), 5.78 (d, J = 12.2 Hz, 1H), 5.47 (d, J = 0.5 Hz, 1H), 5.36−5.29 (m, 2H), 5.20−5.14 (m, 2H), 3.94 (qd, J = 7.1 Hz, 1.2 Hz, 2H), 2.28 (s, 3H), 0.86 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 172.2, 143.4, 139.9, 137.9, 137.0, 134.7, 132.2, 130.9, 130.72, 130.70, 130.2, 129.7, 129.3, 126.9, 126.7, 126.6, 122.6, 61.2, 57.6, 20.3, 13.8; IR (neat) 3024, 2979, 1726, 1578, 1458, 1210, 1029, 859 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd $C_{21}H_{20}O_2$ 304.1463; Found 304.1465.



3c

Ethyl 2-(*m*-tolyl)-2*H*-benzo[7]annulene-2-carboxylate (3c)

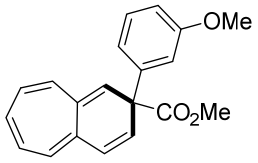
The compound **3c** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3c** (46.2 mg, 76%) as a red oil. R_f = 0.7 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, C_6D_6) δ 7.27 (s, 1H), 7.22 (d, J = 8.0 Hz, 1H), 7.10 (t, J = 7.6 Hz, 1H), 6.84 (d, J = 7.5 Hz, 1H), 6.25 (dd, J = 9.7 Hz, 2.0 Hz, 1H), 5.88 (d, J = 10.0 Hz, 1H), 5.85 (d, J = 12.7 Hz, 1H), 5.74 (s, 1H), 5.36−5.30 (m, 2H), 5.23−5.14 (m, 2H), 3.99−3.91 (m, 2H), 2.05 (s, 3H), 0.86 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 172.2, 145.8, 140.1, 138.5, 136.9, 136.8, 131.9, 130.7, 129.9, 129.5, 129.3, 128.9, 127.6, 126.5, 123.8, 123.2, 61.1, 56.8, 21.3, 13.9; IR (neat) 3024, 2980, 1727, 1445, 1213, 1033 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd $C_{21}H_{20}O_2$ 304.1463; Found 304.1462.



3d

Methyl 2-(*p*-tolyl)-2*H*-benzo[7]annulene-2-carboxylate (3d)

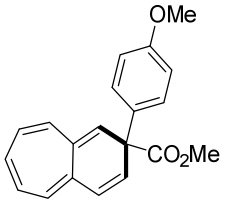
The compound **3d** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3d** (41.4 mg, 70%) as a red oil. R_f = 0.7 (EtOAc:hexane = 1:7); ^{1}H NMR (400 MHz, C_6D_6) δ 7.26 (d, J = 8.1 Hz, 2H), 6.98 (d, J = 8.1 Hz, 2H), 6.21 (dd, J = 9.7 Hz, 2.1 Hz, 1H), 5.85 (d, J = 9.8 Hz, 1H), 5.83 (d, J = 12.1 Hz, 1H), 5.69 (s, 1H), 5.35−5.30 (m, 2H), 5.22−5.15 (m, 2H), 3.28 (s, 3H), 2.04 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 172.7, 143.0, 140.0, 136.83, 136.80, 136.3, 131.9, 130.7, 129.8, 129.6, 129.5, 129.3, 126.7, 126.5, 123.1, 56.6, 51.7, 20.7; IR (neat) 3026, 2923, 1733, 1510, 1434, 1243, 1022 cm^{-1}; HRMS (FAB) *m/z*: [M + H]$^+$ Calcd $C_{20}H_{19}O_2$ 291.1385; Found 291.1381.



3e

Methyl 2-(3-methoxyphenyl)-2*H*-benzo[7]annulene-2-carboxylate (3e)

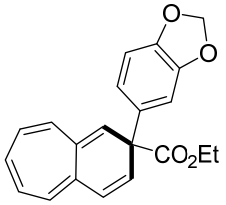
The compound **3e** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3e** (44.0 mg, 71%) as a red solid. m.p. 110−112 ºC; R_f = 0.3 (EtOAc:hexane = 1:7); ^{1}H NMR (400 MHz, C_6D_6) δ 7.29−7.25 (m, 1H), 6.79−6.75 (m, 3H), 6.10 (d, J = 9.8 Hz, 1H), 6.04 (d, J = 9.1 Hz, 1H), 6.02−6.00 (m, 1H), 5.66−5.64 (m, 2H), 5.59−5.56 (m 1H), 5.53−5.48 (m, 1H), 5.43 (s, 1H), 3.80 (s, 3H), 3.75 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 172.9, 159.9, 146.5, 139.7, 136.7, 136.3, 130.8, 130.6, 130.1, 129.8, 129.44, 129.40, 126.6, 121.7, 118.6, 113.0, 111.7, 56.4, 55.3, 52.6; IR (neat) 3027, 2979, 2933, 2899, 2869, 1727, 1487, 1212 cm^{-1}; HRMS (FAB) *m/z*: [M + H]$^+$ Calcd for $C_{20}H_{19}O_3$ 307.1334; Found 307.1335.



3f

Methyl 2-(4-methoxyphenyl)-2*H*-benzo[7]annulene-2-carboxylate (3f)

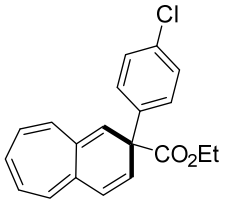
The compound **3f** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3f** (45.2 mg, 73%) as a red solid. m.p. 115−117 ºC; R_f = 0.2 (EtOAc:hexane = 1:20); ^{1}H NMR (400 MHz, C_6D_6) δ 7.25−7.21 (m, 2H), 6.76−6.73 (m, 2H), 6.20 (ddd, J = 9.8 Hz, 2.2 Hz, 0.5 Hz, 1H), 5.87−5.84 (m, 2H), 5.68 (d, J = 0.6 Hz, 1H), 5.39−5.31 (m, 2H), 5.24−5.16 (m, 2H), 3.30 (s, 3H), 3.25 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 172.7, 158.8, 140.0, 138.1, 136.8, 136.6, 132.0, 130.7, 129.6, 129.5, 129.3, 126.5, 123.2, 114.4, 56.1, 54.7, 51.8; IR (neat) 3003, 2952, 2837, 1731, 1607, 1509, 1252, 1182, 1033 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{20}H_{18}O_3$ 306.1256; Found 306.1253.



3g

Ethyl 2-(benzo[d][1,3]dioxol-5-yl)-2*H*-benzo[7]annulene-2-carboxylate (3g)

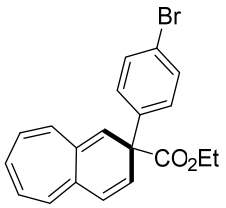
The compound **3g** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3g** (60.1 mg, 91%) as a red solid. m.p. 117−119 ºC; R_f = 0.3 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, C_6D_6) δ 7.01 (d, J = 1.9 Hz, 1H), 6.78 (d, J = 1.9 Hz, 1H), 6.76 (d, J = 1.9 Hz, 1H), 6.62 (d, J = 8.1 Hz, 1H), 6.18 (ddd, J = 9.8 Hz, 2.2 Hz, 0.5 Hz, 1H), 5.85−5.81 (m, 2H), 5.67 (d, J = 0.6 Hz, 1H), 5.37−5.30 (m, 2H), 5.24 (s, 2H), 5.23−5.15 (m, 2H), 3.94−3.86 (m, 2H), 0.84 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 172.1, 148.5, 146.7, 140.1, 140.0, 136.72, 136.70, 131.7, 130.7, 129.8, 129.5, 129.4, 126.5, 123.0, 120.3, 108.5, 107.5, 101.0, 61.1, 56.3, 13.8; IR (neat) 2981, 2899, 1726, 1504, 1487, 1240, 1038 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{21}H_{18}O_4$ 334.1205; Found 334.1203.



3h

Ethyl 2-(4-chlorophenyl)-2*H*-benzo[7]annulene-2-carboxylate (3h)

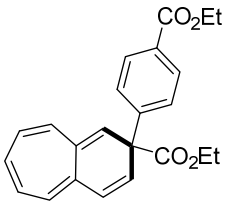
The compound **3h** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3h** (64.5 mg, 99%) as a red solid. m.p. 87−89 ºC; R_f = 0.6 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, C_6D_6) δ 7.11−7.06 (m, 4H), 6.06 (ddd, J = 9.8 Hz, 2.2 Hz, 0.6 Hz, 1H), 5.84−5.81 (m, 2H), 5.56 (d, J = 0.6 Hz, 1H), 5.38−5.31 (m, 2H), 5.23−5.17 (m, 2H), 3.95−3.83 (m, 2H), 0.83 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 171.7, 144.1, 139.9, 137.1, 136.5, 132.8, 131.1, 130.9, 130.2, 129.7, 129.5, 129.0, 128.3, 126.8, 122.2, 61.2, 56.3, 13.8; IR (neat) 3027, 2980, 1727, 1579, 1490, 1213, 1093, 1030 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{20}H_{17}ClO_2$ 324.0917; Found 324.0914.



3i

Ethyl 2-(4-bromophenyl)-2*H*-benzo[7]annulene-2-carboxylate (3i)

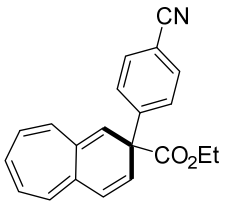
The compound **3i** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3i** (65.1 mg, 91%) as a red solid. m.p. 105−107 ºC; R_f = 0.7 (EtOAc:hexane = 1:7); ^{1}H NMR (400 MHz, C_6D_6) δ 7.47−7.44 (m, 2H), 7.10−7.06 (m, 2H), 6.10 (d, J = 9.8 Hz, 1H), 6.04 (d, J = 12.2 Hz, 1H), 5.97 (ddd, J = 9.7 Hz, 2.2 Hz, 6.5 Hz, 1H), 5.68−5.64 (m, 2H), 5.60−5.58 (m, 1H), 5.55−5.50 (m, 1H), 5.39 (s, 1H), 4.21 (q, J = 7.1 Hz, 2H), 1.25 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 172.1, 144.1, 139.6, 136.9, 136.1, 131.8, 130.9, 130.3, 130.2, 129.6, 129.5, 128.3, 126.7, 121.3, 120.9, 61.6, 56.0, 14.0; IR (neat) 3024, 2979, 2932, 2899, 1727, 1487, 1212, 1030 cm^{-1}; HRMS (FAB) *m/z*: [M + H]$^+$ Calcd for $C_{20}H_{18}O_2Br$ 369.0490; Found 369.0488.



3j

Ethyl 2-(4-(ethoxycarbonyl)phenyl)-2*H*-benzo[7]annulene-2-carboxylate (3j)

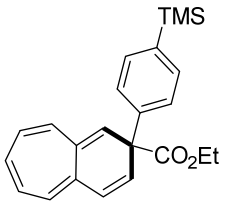
The compound **3j** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3j** (65.3 mg, 90%) as a red solid. m.p. 108−110 ºC; R_f = 0.6 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, C_6D_6) δ 8.15−8.13 (m, 2H), 7.34−7.32 (m, 2H), 6.10 (dd, J = 9.8 Hz, 1.7 Hz, 1H), 5.84 (d, J = 9.6 Hz, 1H), 5.82 (d, J = 11.7 Hz, 1H), 5.60 (d, J = 0.5 Hz, 1H), 5.38−5.31 (m, 2H), 5.22−5.16 (m, 2H), 4.09 (q, J = 7.1 Hz, 2H), 3.94−3.86 (m, 2H), 0.99 (t, J = 7.1 Hz, 3H), 0.83 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 171.6, 165.8, 149.8, 139.9, 137.3, 136.5, 130.93, 130.90, 130.5, 130.4, 129.8, 129.54, 129.50, 126.9, 126.8, 122.0, 61.3, 60.7, 56.9, 14.1, 13.8; IR (neat) 2981, 2939, 1718, 1607, 1367, 1278, 1214, 1107, 1021 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{23}H_{22}O_4$ 362.1518; Found 362.1514.



3k

Ethyl 2-(4-cyanophenyl)-2*H*-benzo[7]annulene-2-carboxylate (3k)

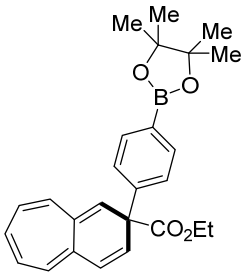
$Cu(hfacac)_2$ (1.9 mg, 2.0 mol %), azulene (25.6 mg, 0.2 mmol) and DCE (3.0 mL) were added to an oven-dried test tube equipped with a stirring bar. To the solution was added ethyl 2-(4-cyanophenyl)-2-diazoacetate (64.6 mg, 0.3 mmol) in DCE (1.0 mL). The mixture was stirred at room temperature for 30 min. The residue was passed through a pad of Cellite and eluted with CH_2Cl_2 to remove $Cu(hfacac)_2$. The filtrate was concentrated under reduced pressure and the residue was purified by Silica gel fresh column chromatography to give **3k** (51.5 mg, 81%) as a red oil. R_f = 0.5 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, C_6D_6) δ 7.05−6.99 (m, 4H), 5.92 (ddd, J = 9.8 Hz, 2.2 Hz, 0.6 Hz, 1H), 5.83 (d, J = 5.8 Hz, 1H), 5,80 (d, J = 9.6 Hz, 1H), 5.42 (d, J = 0.6 Hz, 1H), 5.36−5.34 (m, 2H), 5.24−5.19 (m, 2H), 3.90−3.84 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 171.2, 149.3, 139.6, 137.6, 136.2, 132.4, 131.2, 130.8, 130.13, 130.10, 129.6, 127.3, 127.1, 121.1, 118.5, 111.1, 61.4, 56.8, 13.8; IR (neat) 3031, 2981, 2228, 1728, 1499, 1215, 1029 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{21}H_{17}NO_2$ 315.1259; Found 315.1258.



3l

Ethyl 2-(4-(trimethylsilyl)phenyl)-2*H*-benzo[7]annulene-2-carboxylate (3l)

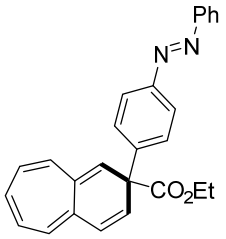
The compound **3l** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3l** (70.1 mg, 97%) as a red oil. R_f = 0.5 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, C_6D_6) δ 7.45−7.39 (m, 4H), 6.27 (dt, J = 9.7 Hz, 1.0 Hz, 1H), 5.90 (d, J = 10.2 Hz, 1H), 5.87 (d, J = 12.8 Hz, 1H), 5.75 (s, 1H), 5.39−5.32 (m, 2H), 5.25−5.17 (m, 2H), 4.00−3.94 (m, 2H), 0.88 (t, J = 7.1 Hz, 3H), 0.19 (s, 9H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.3, 147.5, 141.3, 139.7, 138.14, 138.11, 135.4, 133.0, 132.0, 131.3, 130.8, 130.6, 127.8, 127.5, 124.3, 62.4, 58.2, 15.2, 0.004; IR (neat) 3020, 2955, 2898, 1730, 1249, 1211, 1108, 1031, 842 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{23}H_{26}O_2Si$ 362.1702; Found 362.1703.



3m

Ethyl 2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-2*H*-benzo[7]-annulene- 2-carboxylate (3m)

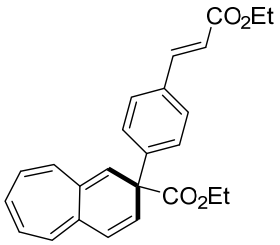
The compound **3m** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3m** (64.2 mg, 77%) as a red oil. R_f = 0.6 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, C_6D_6) δ 8.17 (d, J = 8.2 Hz, 2H), 7.45−7.43 (m, 2H), 6.16 (dd, J = 9.7 Hz, 1.8 Hz, 1H), 5.83 (d, J = 9.8 Hz, 1H), 5.79 (d, J = 12.2 Hz, 1H), 5.66 (s, 1H), 5.36−7.29 (m, 2H), 5.19−5.13 (m, 2H), 3.93−3.85 (m, 2H), 1.10 (s, 12H), 0.82 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 171.9, 148.7, 140.1, 137.0, 136.8, 135.9, 135.1, 131.4, 130.7, 130.2, 129.5, 129.4, 126.5, 126.3, 122.8, 83.6, 61.1, 57.1, 24.8, 13.8; IR (neat) 2979, 1730, 1607, 1362, 1212, 1145, 1091 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{26}H_{29}O_4B$ 416.2159; Found 416.2159.



3n

(*E*)-Ethyl 2-(4-(phenyldiazenyl)phenyl)-2*H*-benzo[7]annulene-2-carboxylate (3n)

The compound **3n** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3n** (60.2 mg, 76%) as a red solid. m.p. 67−69 ºC; R_f = 0.6 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, C_6D_6) δ 8.05−8.02 (m, 2H), 8.01−7.98 (m, 2H), 7.46−7.43 (m, 2H), 7.18−7.13 (m, 4H), 7.10−7.06 (m, 1H), 6.16 (dd, J = 9.7 Hz, 1.8 Hz, 1H), 5.87 (d, J = 9.6 Hz, 1H), 5.85 (d, J = 12.2 Hz, 1H), 5.66 (d, J = 0.4 Hz, 1H), 5.39−5.32 (m, 2H), 5.24−5.17 (m, 2H), 3.97−3.89 (m, 2H), 0.86 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 171.8, 153.1, 151.6, 148.1, 140.0, 137.2, 136.6, 131.1, 131.0, 130.9, 130.4, 129.7, 129.6, 129.3, 129.1, 126.8, 123.7, 123.2, 122.3, 61.3, 56.9, 13.9; IR (neat) 2980, 1728, 1213, 1029 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{26}H_{22}N_2O_2$ 394.1681; Found 394.1682.

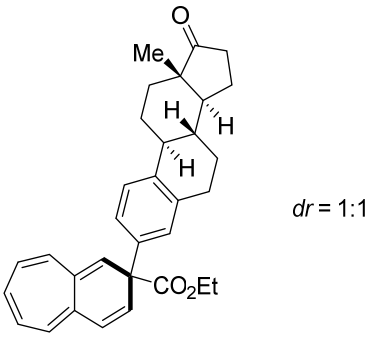


3o

(*E*)-Ethyl 2-(4-(3-ethoxy-3-oxoprop-1-en-1-yl)phenyl)-2*H*-benzo[7]annulene-2-carboxylate (3o)

The compound **3o** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3o** (67.1 mg, 86%) as a red solid. m.p. 138−140 ºC; R_f = 0.6 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, C_6D_6) δ 7.81 (d, J = 16.0 Hz, 1H), 7.22−7.21 (m, 2H), 7.15−7.11 (m, 2H), 6.45 (d, J = 16.0 Hz, 1H), 6.12 (ddd, J = 9.8 Hz, 2.2 Hz, 0.6 Hz, 1H), 5.87−5.82 (m, 2H), 5.61 (q, J = 0.7 Hz, 1H), 5.38−5.31 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 171.7, 166.3, 147.2, 143.9, 139.9, 137.1, 136.6, 133.2, 131.1, 130.9, 130.3, 129.7, 129.5, 128.6,

127.3, 126.8, 122.3, 118.9, 61.2, 60.2, 56.8, 14.2, 13.8; IR (neat) 3027, 2980, 2936, 1713, 1636, 1312, 1256, 1210, 1176, 1031 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{25}H_{24}O_4$ 388.1675; Found 388.1671.

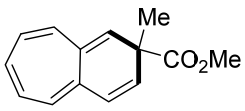


dr = 1:1

3p

Ethyl 2-((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a]-phenanthren-3-yl)-2*H*-benzo[7]annulene-2-carboxylate (3p)

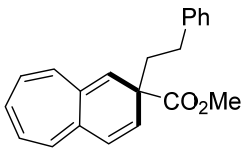
The compound **3p** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3p** (48.3 mg, 51%) as mixture (*dr* = 1:1) of diastereomer. Red solid. m.p. 107−109 °C; R_f = 0.3 (MeOH:$CHCl_3$ = 1:30); ^{1}H NMR (400 MHz, C_6D_6) δ 7.29 (dd, *J* = 8.1 Hz, 1.4 Hz, 1H), 7.24 (t, *J* = 2.0 Hz, 1H), 7.15-7.14 (m, 1H), 6.37-6.33 (m, 1H), 5.93 (d, *J* = 9.7 Hz, 1H), 5.90 (d, *J* = 12.2 Hz, 1H), 5.83 (t, *J* = 0.6 Hz, 1H), 5.37-5.31 (m, 2H), 5.26-5.15 (m, 2H), 4.04-3.96 (m, 2H), 2.64 (m, 2H), 2.13-2.10 (m, 2H), 1.95-1.89 (m, 2H), 1.76 (dt, *J* = 18.4 Hz, 9.2 Hz, 1H), 1.57-1.52 (m, 1H), 1.44-1.12 (m, 5H), 1.07-0.94 (m, 2H), 0.89 (td, *J* = 10.7 Hz, 0.7 Hz, 3H), 0.58 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 217.6, 172.3, 143.4, 140.1, 138.5, 137.1, 136.9, 136.8, 136.7, 132.0, 131.9, 130.7, 130.0, 129.9, 129.5, 129.3, 127.45, 127.41, 126.6, 126.2, 124.1, 124.0, 123.33, 123.30, 61.1, 56.5, 50.1, 47.5, 44.3, 38.1, 35.4, 32.0, 29.7, 26.5, 25.8, 21.3, 13.9, 13.5; IR (neat) 3053, 2930, 2860, 1731, 1581, 1454, 1261, 1216, 1032 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{32}H_{34}O_3$ 466.2508; Found 466.2510.



3q

Methyl 2-methyl-2*H*-benzo[7]annulene-2-carboxylate (3q)

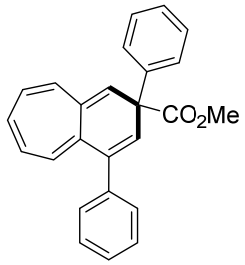
The compound **3q** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3q** (36.2 mg, 84%) as a red solid. m.p. 57−59 ºC; R_f = 0.4 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, C_6D_6) δ 5.75−5.69 (m, 3H), 5.31−5.25 (m, 2H), 5.18 (s, 1H), 5.16−5.09 (m, 2H), 3.26 (s, 3H), 1.32 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.5, 139.8, 137.5, 136.9, 132.7, 130.4, 130.3, 129.7, 128.5, 126.6, 124.4, 51.7, 48.2, 29.7; IR (neat) 3025, 2951, 1729, 1582, 1450, 1220, 1124 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{14}H_{14}O_2$ 214.0994; Found 214.0995.



3r

Methyl 2-phenethyl-2*H*-benzo[7]annulene-2-carboxylate (3r)

The compound **3r** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3r** (53.1 mg, 87%) as a red oil. R_f = 0.6 (Et_2O:CH_2Cl_2:hexane = 1:2:5); ^{1}H NMR (400 MHz, C_6D_6) δ 7.13−7.11 (m, 2H), 7.07−7.03 (m, 1H), 7.01−6.99 (m, 2H), 5.85 (d, J = 9.9 Hz, 1H), 5.79−5.75 (m, 2H), 5.32−5.27 (m, 2H), 5.23 (s, 1H), 5.18−5.13 (m, 2H), 3.27 (s, 3H), 2.67−2.50 (m, 2H), 2.07−1.94 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.1, 142.0, 139.9, 138.3, 137.6, 131.8, 131.3, 130.5, 129.7, 128.8, 128.6, 128.5, 126.5, 126.0, 122.8, 52.6, 51.7, 44.0, 31.6; IR (neat) 3026, 2950, 1729, 1455, 1218, 1053 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{21}H_{20}O_2$ 304.1463; Found 304.1465.

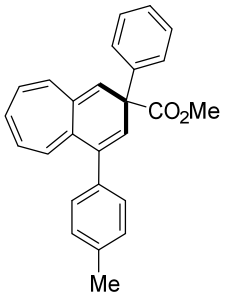


3s

Methyl 2,4-diphenyl-2*H*-benzo[7]annulene-2-carboxylate (3s)

The compound **3s** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3s** (50.4 mg, 70%) as a red

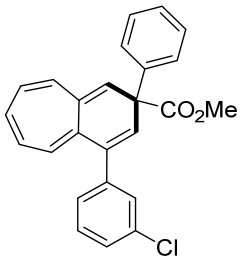
solid. m.p. 61−63 ºC; R_f = 0.3 (EtOAc:hexane = 1:20); ^{1}H NMR (400 MHz, C_6D_6) δ 7.43−7.41 (m, 2H), 7.19−7.17 (m, 2H), 7.14−7.11 (m, 2H), 7.05−7.02 (m, 3H), 7.02−7.97 (m, 1H), 6.44 (dd, J = 2.2 Hz, 0.6 Hz, 1H), 6.00 (dd, J = 12.0 Hz, 0.7 Hz, 1H), 5.91 (q, J = 0.7 Hz, 1H), 5.79 (d, J = 8.3 Hz, 1H), 5.41 (dd, J = 11.1 Hz, 7.4 Hz, 1H), 5.33−5.22 (m, 2H), 3.25 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 172.6, 145.4, 140.9, 140.3, 139.8, 137.7, 137.4, 133.0, 131.0, 129.7, 129.6, 129.2, 129.1, 128.3, 127.4, 126.9, 126.8, 126.7, 124.2, 56.8, 51.9; IR (neat) 3057, 3027, 2952, 1732, 1598, 1491, 1445, 1223, 1029 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{25}H_{20}O_2$ 352.1463; Found 352.1461.



3t

Methyl 2-phenyl-4-(*p*-tolyl)-2*H*-benzo[7]annulene-2-carboxylate (3t)

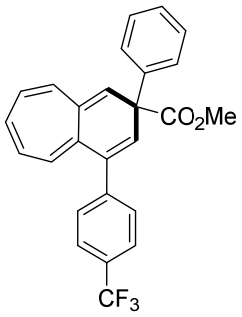
The compound **3t** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3t** (68.0 mg, 93%) as a red solid. m.p. 56−58 ºC; R_f = 0.2 (EtOAc:hexane = 1:40); ^{1}H NMR (400 MHz, C_6D_6) δ 7.45−7.42 (m, 2H), 7.15−7.11 (m, 4H), 7.01−6.97 (m, 1H), 6.88 (d, J = 7.7 Hz, 2H), 6.49 (d, J = 1.6 Hz, 1H), 6.01 (d, J = 12.7 Hz, 1H), 5.93 (s, 1H), 5.88 (d, J = 8.2 Hz, 1H), 5.43 (dd, J = 11.3 Hz, 7.1 Hz, 1H), 5.34−5.28 (m, 2H), 3.25 (s, 3H), 2.07 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 172.7, 145.5, 140.3, 139.8, 138.0, 137.7, 137.6, 136.9, 132.7, 131.0, 129.6, 129.5, 129.2, 129.1, 129.0, 126.9, 126.8, 126.7, 124.3, 56.8, 51.9, 20.9; IR (neat) 3025, 2951, 2921, 1732, 1585, 1491, 1434, 1221, 1032 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{26}H_{22}O_2$ 366.1620; Found 366.1622.



3u

Methyl 4-(3-chlorophenyl)-2-phenyl-2*H*-benzo[7]annulene-2-carboxylate (3u)

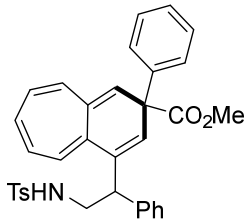
The compound **3u** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3u** (59.4mg, 76%) as a red solid. m.p. 51−53 ºC; R_f = 0.4 (EtOAc:hexane = 1:15); ^{1}H NMR (400 MHz, C_6D_6) δ 7.38−7.35 (m, 2H), 7.22 (t, J = 1.8 Hz, 1H), 7.14−7.10 (m, 2H), 7.01−6.97 (m, 2H), 6.85 (dt, J = 7.7 Hz, 1.3 Hz, 1H), 6.70 (t, J = 7.8 Hz, 1H), 6.33 (dd, J = 2.1 Hz, 0.6 Hz, 1H), 5.96 (dd, J = 12.0 Hz, 0.7 Hz, 1H), 5.86 (q, J = 0.7 Hz, 1H), 5.59 (d, J = 8.3 Hz, 1H), 5.39 (dd, J = 11.2 Hz, 7.3 Hz, 1H), 5.29 (ddd, J = 7.4 Hz, 12.0 Hz, 0.7 Hz, 1H), 5.20 (ddt, J = 8.4 Hz, 11.2 Hz, 1.0 Hz, 1H), 3.25 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 172.4, 145.1, 142.7, 139.8, 139.0, 137.6, 136.9, 134.3, 133.4, 131.2, 129.63, 129.60, 129.1, 128.0, 127.83, 127.80, 127.1, 126.9, 126.7, 124.1, 56.7, 51.9; IR (neat) 3060, 3027, 2951, 1732, 1593, 1433, 1223, 1032 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{25}H_{19}ClO_2$ 386.1074; Found 386.1074.



3v

Methyl 2-phenyl-4-(4-(trifluoromethyl)phenyl)-2*H*-benzo[7]annulene-2-carboxylate (3v)

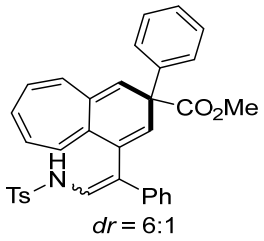
The compound **3v** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3v** (72.1 mg, 85%) as a red solid. m.p. 27−29 ºC; R_f = 0.4 (EtOAc:hexane = 1:7); ^{1}H NMR (400 MHz, C_6D_6) δ 7.41−7.38 (m, 2H), 7.20 (d, J = 8.0 Hz, 2H), 7.03−6.99 (m, 1H), 6.91 (d, J = 8.0 Hz, 2H), 6.31 (d, J = 2.0 Hz, 1H), 5.98 (d, J = 12.0 Hz, 1H), 5.87 (s, 1H), 5.43 (dd, J = 11.1 Hz, 7.4 Hz, 1H), 5.33−5.24 (m, 2H), 3.28 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 172.4, 145.1, 144.3, 139.8, 138.9, 137.6, 136.8, 133.8, 131.4, 129.9, 129.5, 129.1, 129.0, 128.0, 127.8, 127.2, 126.9, 126.7, 125.2 (J_{CF} = 3.8 Hz), 124.0, 56.7, 52.0; IR (neat) 3058, 3030, 2953, 1733, 1615, 1435, 1325, 1223, 1167, 1124, 1065 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{26}H_{19}F_3O_2$ 420.1337; Found 420.1335.



3w

Methyl 4-(2-(4-methylphenylsulfonamido)-1-phenylethyl)-2-phenyl-2*H*-benzo[7]annulene-2-carboxylate (3w)

The compound **3w** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3w** (97.2 mg, 88%) as a red solid. m.p. 59−61 ºC; R_f = 0.4 (acetone/hexane = 1:3); ^{1}H NMR (400 MHz, C_6D_6) δ 7.90 (d, J = 8.2 Hz, 2H), 7.24−7.22 (m, 2H), 7.00−6.95 (m, 1H), 6.91−6.85 (m, 3H), 6.82−6.79 (m, 4H), 6.02 (d, J = 1.5 Hz, 1H), 5.82 (d, J = 12.7 Hz, 1H), 5.75 (dd, J = 9.8 Hz, 3.0 Hz, 1H), 5.65 (d, J = 8.5 Hz, 1H), 5.59 (s, 1H), 5.33−5.29 (m, 2H), 5.22−5.14 (m, 2H), 3.89 (dd, J = 10.3 Hz, 5.5 Hz, 1H), 3.58 (dq, J = 13.5 Hz, 5.1 Hz, 1H), 3.39 (s, 3H), 3.15 (ddd, J = 13.3 Hz, 10.3 Hz, 3.1 Hz, 1H), 1.89 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 173.5, 144.7, 142.6, 140.5, 139.7, 138.9, 138.8, 135.4, 133.2, 132.5, 131.2, 129.7, 129.1, 129.04, 129.00, 127.8, 127.6, 127.4, 127.1, 126.81, 126.80, 126.4, 122.1, 56.5, 52.5, 48.1, 46.4, 21.1; IR (neat) 3060, 3028, 2952, 2926, 1731, 1433, 1331, 1231, 1150, 1392 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{34}H_{31}NO_4S$ 549.1974; Found 549.1974.

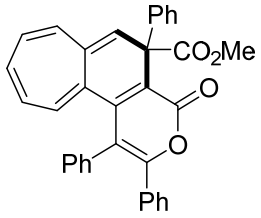


3x

Methyl 4-(2-(4-methylphenylsulfonamido)-1-phenylvinyl)-2-phenyl-2*H*-benzo[7]-annulene-2-carboxylate (3x)

Cu(hfacac)$_2$ (1.9 mg, 4.0 mol %), *N*-(2-(azulen-1-yl)-2-phenylvinyl)-4-methylbenzenesulfonamide (79.9 mg, 0.2 mmol), and DCE (3.0 mL) were added to a test tube equipped with a stirring bar. To the solution was added methyl 2-diazo-2-phenylacetate (35.2 mg, 0.2 mmol) in DCE (1.0 mL). The mixture was stirred at room temperature for 30 min. The residue was passed through a pad of Cellite to remove Cu(hfacac)$_2$ and eluted with CH_2Cl_2. The filtrate was concentrated under reduced pressure and the

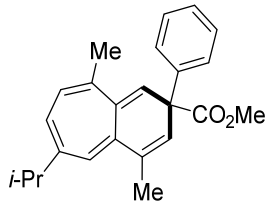
residue was purified by Silica gel fresh column chromatography (EtOAc:hexanes) to give **3x** (69.2 mg, 63%) as a red solid. m.p. 85−88 ºC; R_f = 0.5 (EtOAc:hexane = 1:7); ^{1}H NMR (400 MHz, C_6D_6) δ 8.33 (d, J = 11.7 Hz, 1H), 7.76 (d, J = 8.2 Hz, 2H), 7.18 (d, J = 11.7 Hz, 1H), 6.98−6.96 (m, 6H), 6.92−6.81 (m, 2H), 6.78−6.69 (m, 3H), 6.51 (d, J = 8.1 Hz, 1H), 5.74 (d, J = 11.8 Hz, 1H), 5.59 (d, J = 8.4 Hz, 1H), 5.50 (s, J = 1.6 Hz, 1H), 5.42 (s, 1H), 5.18−5.08 (m, 2H), 4.94−4.89 (m, 1H), 3.19 (s, 3H), 1.65 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 174.3, 144.4, 142.9, 139.1, 138.9, 138.4, 137.4, 137.2, 134.2, 133.9, 131.4, 129.7, 129.5, 128.88, 128.85, 128.7, 127.3, 127.12, 127.10, 127.0, 126.9, 125.1, 124.9, 122.8, 122.2, 56.8, 52.8, 21.0; IR (neat) 3028, 2951, 1732, 1706, 1632, 1597, 1407, 1339, 1224, 1166 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{34}H_{29}NO_4S$ 547.1817; Found 547.1816.



3y

Methyl 4-oxo-1,2,5-triphenyl-4,5-dihydrocyclohepta[*f*]isochromene-5-carboxylate (3y)

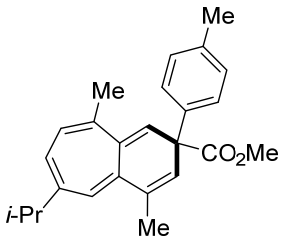
$Cu(hfacac)_2$ (1.9 mg, 2.0 mol %), methyl 3,4-diphenylazulenolactone (69.7 mg, 0.2 mmol), and 1,4-dioxane (3.0 mL) were added to a test tube equipped with a stirring bar. To the solution was added methyl 2-diazo-2-phenylacetate (35.3mg, 0.2 mmol) in 1,4-dioxane (1.0 mL). The mixture was stirred at 40 ºC for 3 h. The residue was passed through a pad of Cellite to remove $Cu(hfacac)_2$ and eluted with CH_2Cl_2. The filtrate was concentrated under reduced pressure and the residue was purified by Silica gel fresh column chromatography to give to give **3y** (94.3 mg, 95%) as a brown solid. m.p. 233−235 ºC; R_f = 0.3 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 7.2 Hz, 2H), 7.33-7.29 (m, 2H), 7.26-7.19 (m, 2H), 7.16-7.11 (m, 5H), 6.28 (d, J = 11.1 Hz, 1H), 6.01-5.92 (m, 2H), 5.61 (s, 1H), 5.56-5.51 (m, 1H), 5.39 (d, J = 7.8 Hz, 1H) 3.82 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 172.4, 159.8, 157.1, 146.6, 139.0, 137.6, 135.2, 135.0, 134.4, 133.3, 133.0, 131.84, 131.83, 130.1, 129.5, 129.3, 129.0, 128.72, 128.71, 128.6, 128.4, 128.1, 127.9, 127.7, 127.4, 116.6, 55.8, 53.1; IR (neat): 3059, 2925, 2854, 1711, 1487, 1232, 786, 697 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{34}H_{24}O_4$ 496.1675; Found 496.1675.



3z

Methyl 6-isopropyl-4,9-dimethyl-2-phenyl-2H-benzo[7]annulene-2-carboxylate (3z)

The compound **3z** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3z** (54.3 mg, 71%) as a red solid. m.p. 85−88 ºC; R_f = 0.5 (EtOAc:hexane = 1:40); ^{1}H NMR (400 MHz, C_6D_6) δ 7.44−7.42 (m, 2H), 7.14−7.09 (m, 2H), 7.00−6.96 (m, 1H), 6.43 (t, J = 0.9 Hz, 1H), 6.18 (t, J = 1.5 Hz, 1H), 6.11 (s, 1H), 5.86 (d, J = 8.1 Hz, 1H), 5.66 (d, J = 8.0 Hz, 1H), 3.29 (s, 3H), 2.12 (quintet, J = 6.8 Hz, 1H), 1.89 (d, J = 0.6 Hz, 3H), 1.86 (d, J = 1.2 Hz, 3H), 0.93 (d, J = 6.8 Hz, 6H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 173.1, 146.4, 145.4, 139.8, 138.0, 136.2, 133.4, 132.0, 128.9, 127.6, 126.8, 126.7, 126.1, 124.5, 122.7, 56.4, 51.8, 37.0, 26.6, 22.5, 22.4, 21.0 cm^{-1}; IR (neat) 3058, 2958, 2870, 1732, 1238 cm^{-1}; HRMS (FAB) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{27}O_2$ 347.2011; Found 347.2013.

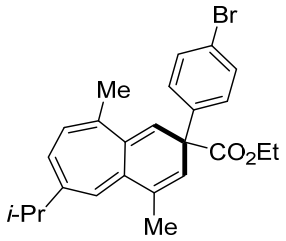


3a'

Methyl 6-isopropyl-4,9-dimethyl-2-(*p*-tolyl)-2*H*-benzo[7]annulene-2-carboxylate (3a')

The compound **3a'** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3a'** (61.1 mg, 85%) as a aurore solid. m.p. 83−86 ºC; R_f = 0.6 (EtOAc:hexane = 1:40); ^{1}H NMR (400 MHz, C_6D_6) δ 7.39−7.36 (m, 2H), 6.98−6.96 (m, 2H), 6.47 (s, 1H), 6.22 (t, J = 1.4 Hz, 1H), 6.12 (s, 1H), 5.86 (d, J = 8.0 Hz, 1H), 5.66 (d, J = 8.0 Hz, 1H), 3.31 (s, 3H), 2.12 (quintet, J = 6.8 Hz, 1H), 2.03 (s, 3H), 1.91 (s, 3H), 1.88 (d, J = 1.2 Hz, 3H), 0.94 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, C_6D_6) δ 173.3, 146.4, 142.6, 139.9, 137.8, 136.3, 136.2, 133.3, 132.3, 129.6, 127.5, 126.6, 126.0, 124.4, 123.0, 56.1, 51.8, 37.0, 26.6, 22.5, 22.4, 21.0,

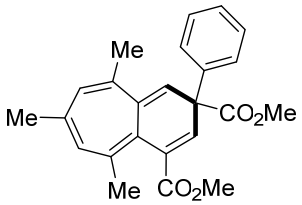
20.7; IR (neat) 3055, 2960, 2929, 2872, 1734, 1511, 1436, 1243, 1038 cm^{-1}; HRMS (FAB) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{29}O_2$ 361.2168; Found 361.2169.



3b'

Ethyl 2-(4-bromophenyl)-6-isopropyl-4,9-dimethyl-2*H*-benzo[7]annulene-2-carboxylate (3b')

The compound **3b'** was prepared according to the same procedure as that of the synthesis of **3a**. The crude residue was purified by Silica gel column chromatography to give **3b'** (60.1 mg, 68%) as a aurore solid. m.p. 62−65 °C; R_f = 0.4 (EtOAc:hexane = 1:3); ^{1}H NMR (400 MHz, C_6D_6) δ 7.23−7.20 (m, 2H), 7.14−7.12 (m, 2H), 6.35 (s, 1H), 6.12−6.10 (m, 2H), 5.88 (d, J = 8.0 Hz, 1H), 5.67 (d, J = 8.0 Hz, 1H), 3.95−3.87 (m, 2H), 2.12 (quintet, J = 6.8 Hz, 1H), 1.91 (s, 3H), 1.87 (d, J = 1.1 Hz, 3H), 0.93 (d, J = 6.8 Hz, 6H), 0.84 (t, J = 7.1 Hz, 4H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 172.2, 146.5, 144.2, 139.7, 138.3, 136.0, 133.9, 131.9, 131.4, 128.6, 126.3, 124.6, 122.1, 121.0, 61.2, 55.8, 37.0, 26.6, 22.5, 22.4, 21.0, 13.9; IR (neat) 3055, 2963, 2936, 2869, 1730, 1488, 1385, 1237, 1010cm^{-1}; HRMS (FAB) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{28}O_2Br$ 439.1273; Found 439.1270.

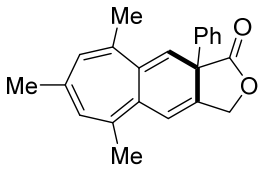


3c'

Dimethyl 5,7,9-trimethyl-2-phenyl-2*H*-benzo[7]annulene-2,4-dicarboxylate (3c')

$Cu(hfacac)_2$ (1.9 mg, 2.0 mol %), methyl 4,6,8-trimethylazulene-1-carboxylate (75.3 mg, 0.2 mmol), and 1,4-dioxane (3.0 mL) were added to a test tube equipped with a stirring bar. To the solution was added methyl 2-diazo-2-phenylacetate (35.3mg, 0.2 mmol) in 1,4-dioxane (1.0 mL). The mixture was stirred at

room temperature for 30 min. The residue was passed through a pad of Cellite to remove $Cu(hfacac)_2$ and eluted with CH_2Cl_2. The filtrate was concentrated under reduced pressure and the residue was purified by Silica gel fresh column chromatography to give to give **3c'** (66.4 mg, 88%) as a pale orange solid. m.p. 109−111 ºC; R_f = 0.2 (EtOAc:hexanes = 1:15); ^{1}H NMR (400 MHz, C_6D_6) δ 8.06 (d, J = 1.5 Hz, 1H), 7.48−7.46 (m, 2H), 7.04−7.00 (m, 2H), 6.93−6.89 (m, 1H), 6.60 (d, J = 1.4 Hz, 1H), 5.79 (s, 1H), 5.62 (s, 1H), 3.34 (s, 3H), 3.19 (s, 3H), 1.96 (s, 3H), 1.73 (s, 3H), 1.63 (d, J = 0.8 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 172.4, 167.0, 145.0, 142.1, 141.7, 140.4, 138.6, 135.0, 134.0, 130.4, 129.2, 128.9, 127.3, 126.9, 124.7, 124.5, 56.5, 52.3, 51.5, 26.0, 25.7, 24.5; IR (neat) 3059, 2978, 2951, 2917, 2845, 1732, 1579, 1435, 1270, 1235, 1193, 1093 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{24}H_{24}O_4$ 376.1675; Found 376.1674.



3d'

5,7,9-Trimethyl-10a-phenyl-3,10a-dihydro-1*H*-cyclohepta[f]isobenzofuran-1-one (3d')

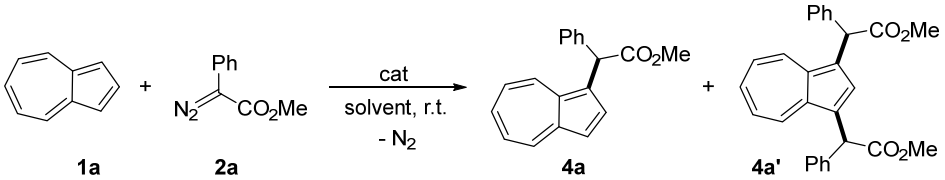
$Cu(hfacac)_2$ (1.9 mg, 2.0 mol %), **1c'** (68.9 mg, 0.2 mmol), and DCE (4.0 mL) were added to a test tube equipped with a stirring bar. The mixture was stirred at 40 ºC for 30 min. The residue was passed through a pad of Cellite to remove $Cu(hfacac)_2$ and eluted with CH_2Cl_2. The filtrate was concentrated under reduced pressure and the residue was purified by Silica gel fresh column chromatography to give **3d'** (60.3 mg, 95%) as an orange solid. m.p. 139−141 ºC; R_f = 0.2 (EtOAc:hexane = 1:20); ^{1}H NMR (400 MHz, C_6D_6) δ 7.52−7.50 (m, 2H), 7.04−7.00 (m, 2H), 6.93−6.89 (m, 1H), 6.43 (s, 1H), 6.22 (s, 1H), 5.71 (s, 1H), 5.69 (s, 1H), 4.32 (dd, J = 2.1 Hz, 12.3 Hz, 1H), 4.17 (d, J = 12.4 Hz, 1H), 1.82 (s, 3H), 1.72 (s, 3H), 1.60 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 175.6, 141.6, 139.5, 138.7, 138.6, 138.2, 133.8, 130.7, 129.8, 129.3, 128.2, 127.7, 126.1, 123.5, 123.1, 68.4, 53.7, 26.3, 25.6, 22.8; IR (neat) 3058, 3024, 2972, 2934, 2884, 1773, 1577, 1446, 1372, 1140, 999 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{22}H_{20}O_2$ 316.1463; Found 316.1461.

C. C-H Functionalization of azulenes with alkyl and aryl diazo esters

Screening of reactions conditions

Screening experiments for optimization were carried out using azulene (**1a**) and methyl 2-diazo-2-phenylacetate (**2a**). The conditions for each trial are specified in the footnote. All yields were determined by analysis of the crude ^{1}H NMR spectrum using CH_2Br_2 as the internal standard after filtration of the reaction mixture through a pad of silica gel unless otherwise noted.

Table S1. Optimization of C-H Functionalization

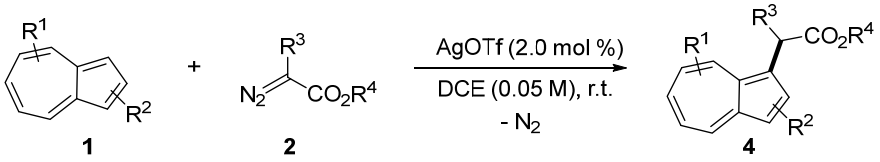


1a **2a** **4a** **4a'**

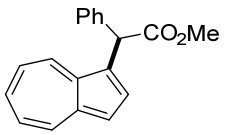
Entry	Catalyst (mol %)	Solvent	Azulene (equiv)	Time (h)	Conv. (%)	Yield (%)	
						4a	**4a'**
1	(IPr)AuCl (2)/$AgBF_4$ (2)	DCE	1	4	100	24	0
2	(IPr)AuCl (2)/$AgNTf_2$ (2)	DCE	1	4	100	42	0
3	(IPr)AuCl (2)/AgOTf (2)	DCE	1	1	100	40	21
4	(IPr)AuCl (2)/$AgPF_6$ (2)	DCE	1	20	85	14	0
5	(IPr)AuCl (2)/$AgSbF_6$ (2)	DCE	1	20	80	13	0
7	(IPr)AuCl (2)/AgOTf (2)	DCE	1.5	1	100	31	5
8	(IPr)AuCl (2)	DCE	1.5	1	0	0	0
9	AgOTf (2)	DCE	1.5	1	100	50	8
10	AgOTf (2)	DCE	1.5	1	100	62	16
11[a]	AgOTf (2)	DCE	1.5	1	100	59	14
12[b]	AgOTf (2)	DCE	1.5	1	100	57	15
13	AgOTf (2)	DCM	1.5	3	100	60	7
14	AgOTf (2)	toluene	1.5	3	80	0	0
15	AgOTf (2)	MeCN	1.5	3	100	51	8
16	AgOTf (2)	$CHCl_3$	1.5	3	50	33	0
17[c]	AgOTf (2)	DCE	2	1	100	74	5
18	AgOTf (5)	DCE	2	1	100	61	10

Conversions and yields were determined by ^{1}H NMR intergration methods with CH_2Br_2 as an internal standard. Entries 1-9 and 10-18 were conducted in 0.1 M and 0.05 M solutions, respectively. [a]Reaction temperature: 0 °C. [b]Methyl phenyl diazoacetate was added dropwise. [c]Isolated yield.

General procedure



AgOTf (2.0 mol %), azulene derivatives **1** (0.2 mmol), and DCE (3.0 mL) were added to a test tube equipped with a stirring bar. To the solution was added aryl diazoacetate derivatives **2** (0.3 mmol) in DCE (1.0 mL). The mixture was stirred at room temperature. Completion of the reaction was indicated by the TLC. The residue was passed through a pad of Cellite to remove AgOTf and eluted with CH_2Cl_2. The filtrate was concentrated under reduced pressure and the residue was purified by Silica gel fresh column chromatography to give **4**.

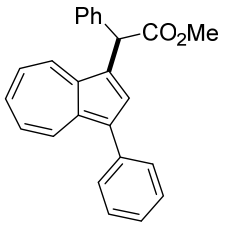


4a

Methyl 2-(azulen-1-yl)-2-phenylacetate (4a)

AgOTf (1.0 mg, 2.0 mol %), azulene **1a** (25.6 mg, 0.2 mmol), and DCE (3.0 mL) were added to a test tube equipped with a stirring bar. To the solution was added methyl phenyl diazoacetate **2a** (0.3 mmol) in DCE (1.0 mL). The mixture was stirred at room temperature. Completion of the reaction was indicated by the TLC. The residue was passed through a pad of Cellite to remove AgOTf and eluted with CH_2Cl_2. The filtrate was concentrated under reduced pressure and the residue was purified by Silica gel fresh column chromatography to give **4a** (41.1 mg, 74%).

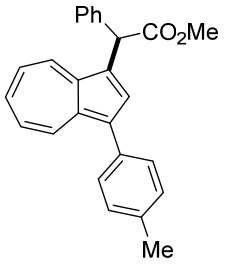
Blue oil; R_f = 0.3 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, J = 5.4 Hz, 1H), 8.30 (d, J = 5.7 Hz, 1H), 7.99 (d, J = 3.9 Hz, 1H), 7.58 (t, J = 9.9 Hz, 1H), 7.38 (d, J = 4.0 Hz, 1H), 7.36−7.34 (m, 2H), 7.32−7.27 (m, 2H), 7.25−7.22 (m, 1H), 7.149 (t, J = 9.8 Hz, 1H), 7.146 (t, J = 10.0 Hz, 1H), 5.71 (s, 1H), 3.75 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.5, 14101, 139.4, 137.8, 137.2, 137.1, 135.8, 133.2, 128.6, 128.4, 127.1, 125.7, 123.2, 122.7, 117.2, 52.4, 50.1; IR (neat) 3027, 2950, 1737, 1577, 1496, 1454, 1433, 1396, 1309, 1193, 1153 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{19}H_{16}O_2$ 276.1150; Found 276.1149.



4b

Methyl 2-phenyl-2-(3-phenylazulen-1-yl)acetate (4b)

The compound **4b** was prepared according to the same procedure as that of the synthesis of **4a**. The crude residue was purified by Silica gel column chromatography to give **4b** (56.0 mg, 80%) as a blue oil. R_f = 0.5 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 9.4 Hz, 1H), 8.29 (d, J = 9.4 Hz, 1H), 8.09 (s, 1H), 7.598 (d, J = 8.2 Hz, 1H), 7.595 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 9.8 Hz, 1H), 7.47 (t, J = 7.7 Hz, 2H), 7.39 (d, J = 7.2 Hz, 2H), 7.35−7.29 (m, 3H), 7.24 (t, J = 7.2 Hz, 1H), 7.11 (t, J = 9.9 Hz, 2H), 5.72 (s, 1H), 3.76 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.4, 139.2, 138.6, 137.4, 137.17, 137.09, 136.1, 135.9, 133.6, 130.2, 129.8, 128.6, 128.4, 127.2, 126.4, 125.1, 123.7, 122.8, 52.4, 50.0; IR (neat) 3026, 2949, 1736, 1570, 1493, 1430, 1153 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{25}H_{20}O_2$ 352.1463; Found 352.1461.

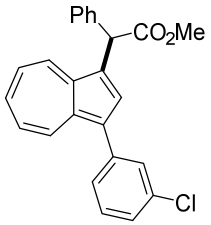


4c

Methyl 2-phenyl-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4c)

The compound **4c** was prepared according to the same procedure as that of the synthesis of **4a**. The crude residue was purified by Silica gel column chromatography to give **4c** (63.4 mg, 86%) as a blue solid. m.p. 39−41 °C; R_f = 0.3 (EtOAc:pentane = 1:5); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 9.7 Hz, 1H), 8.28 (d, J = 9.6 Hz, 1H), 8.07 (s, 1H), 7.55 (t, J = 9.8 Hz, 1H), 7.49 (d, J = 8.0 Hz, 2H), 7.39 (d, J = 7.5 Hz, 2H), 7.33−7.22 (m, 5H), 7.09 (t, J = 9.8 Hz, 2H), 5.72 (s, 1H), 3.76 (s, 3H), 2.42 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.4, 139.2, 138.5, 137.3, 137.1, 136.15, 136.11, 136.0, 134.2, 133.6, 130.3, 129.7, 129.4, 128.6, 128.5, 127.2, 125.0, 123.5, 122.7, 52.4, 50.0, 21.2; IR (neat) 3026, 2948, 2921,

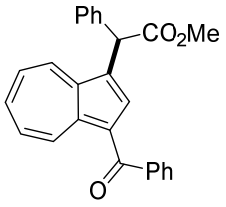
1737, 1571, 1432, 1194, 1154 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{26}H_{22}O_2$ 366.1620; Found 366.1620.



4d

Methyl 2-(3-(3-chlorophenyl)azulen-1-yl)-2-phenylacetate (4d)

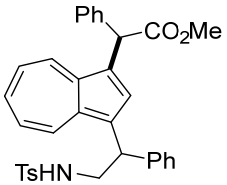
AgOTf (1.0 mg, 2.0 mol %), 1-(3-chlorophenyl)azulene (47.7 mg, 0.2 mmol) and DCE (3.0 mL) were added to a test tube equipped with a stirring bar. To the solution was added methyl 2-diazo-2-phenylacetate (52.9 mg, 0.3 mmol) in DCE (1.0 mL). The mixture was stirred at 50 ºC for 1 h. Completion of the reaction was indicated by the TLC. The residue was passed through a pad of Cellite to remove AgOTf and eluted with CH_2Cl_2. The filtrate was concentrated under reduced pressure and the residue was purified by Silica gel fresh column chromatography to give **4d** (55.2 mg, 72%) as a green oil. R_f = 0.4 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 9.4 Hz, 1H), 8.31 (d, J = 9.4 Hz, 1H), 8.06 (s, 1H), 7.61 (t, J = 9.6 Hz, 1H), 7.57 (t, J = 1.8 Hz, 1H), 7.47 (td, J = 7.6 Hz, 1.3 Hz, 1H), 7.42−7.38 (m, 3H), 7.34−7.27 (m, 4H), 7.17 (dd, J = 9.8 Hz, 3.5 Hz, 1H), 7.15 (dd, J = 9.6 Hz, 3.6 Hz, 1H), 5.71 (s, 1H), 3.77 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.3, 139.0, 138.9, 138.8, 137.3, 137.2, 136.2, 135.7, 134.4, 133.8, 129.8, 129.6, 128.6, 128.5, 128.3, 127.9, 127.2, 126.3, 125.3, 124.1, 123.3, 52.5, 49.9; IR (neat) 3025, 2949, 2850, 1735, 1591, 1432, 1154, 727 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{25}H_{19}ClO_2$ 386.1074; Found 386.1071.



4e

Methyl 2-(3-benzoylazulen-1-yl)-2-phenylacetate (4e)

AgOTf (1.0 mg, 2.0 mol %), azulen-1-yl(phenyl)methanone (46.5 mg, 0.2 mmol) and DCE (3.0 mL) were added to a test tube equipped with a stirring bar. To the solution was added methyl 2-diazo-2-phenylacetate (105.7 mg, 0.6 mmol) in DCE (1.0 mL). The mixture was stirred at 70 ºC for 15 h. Completion of the reaction was indicated by the TLC. The residue was passed through a pad of Cellite to remove AgOTf and eluted with CH_2Cl_2. The filtrate was concentrated under reduced pressure and the residue was purified by Silica gel fresh column chromatography to give **4e** (47.1 mg, 61%) as a purple solid. m.p. 48−50 ºC; R_f = 0.3 (EtOAc:hexane = 1:3); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.71 (dd, J = 9.9 Hz, 0.7 Hz, 1H), 8.45 (d, J = 9.7 Hz, 1H), 7.87 (m, 3H), 7.62 (t, J = 9.8 Hz, 1H), 7.58−7.54 (m, 1H), 7.51−7.46 (m, 3H), 7.33−7.23 (m, 5H), 5.65 (s, 1H), 3.19 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.7, 173.0, 142.6, 142.3, 141.1, 141.0, 140.0, 139.4, 138.6, 135.2, 131.4, 129.7, 129.4, 128.7, 128.3, 128.2, 127.41, 127.40, 125.3, 123.7, 52.5, 49.9; IR (neat) 3058, 3028, 2950, 1736, 1594, 1424, 1396, 1239, 1155 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{26}H_{20}O_3$ 380.1412; Found 380.1410.



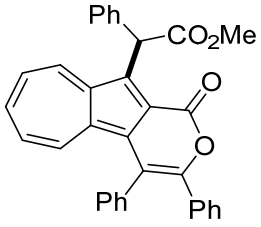
dr =1.5 : 1

4f

Methyl 2-(3-(2-(4-methylphenylsulfonamido)-1-phenylethyl)azulen-1-yl)-2-phenyl-acetate (4f)

The compound **4f** was prepared according to the same procedure as that of the synthesis of **4a**. The crude residue was purified by Silica gel column chromatography to give **4f-1** (53.4 mg, 48.6%) and **4f-2** (35.6 mg, 32.4%) as a blue solid. Major isomer; m.p. 69−71 ºC; R_f = 0.2 (EtOAc:hexane = 1:3); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, J = 9.7 Hz, 1H), 8.09 (d, J = 9.6 Hz, 1H), 7.84 (s, 1H), 7.62 (d, J = 8.3 Hz, 2H), 7.54 (t, J = 9.8 Hz, 1H), 7.35−7.11 (m, 12H), 7.09 (t, J = 9.6 Hz, 1H), 7.04 (t, J = 9.7 Hz, 1H), 5.66 (s, 1H), 4.72 (t, J = 7.8 Hz, 1H), 4.35 (s, 1H), 3.71 (s, 3H), 3.71−3.56 (m, 2H), 2.42 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 172.2, 142.4, 140.6, 138.2, 137.4, 136.2, 135.8, 135.4, 133.7, 132.8, 132.6, 128.8, 127.8, 127.6, 127.2, 126.8, 126.2, 126.0, 125.9, 123.8, 121.9, 51.3, 48.8, 47.3, 42.4, 20.5; IR (neat) 3060, 3027, 2951, 2924, 1735, 1710, 1645, 1431, 1329, 1159 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{34}H_{31}NO_4S$ 549.1974; Found 549.1976.

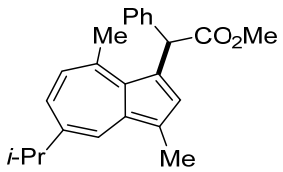
Minor isomer; m.p. 67−69 ºC; R_f = 0.15 (EtOAc:hexane = 1:3); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, J = 9.6 Hz, 1H), 8.09 (d, J = 9.6 Hz, 1H), 7.86 (s, 1H), 7.67 (dd, J = 6.6 Hz, 1.7 Hz, 2H), 7.56 (t, J = 9.8 Hz, 1H), 7.33−7.10 (m, 13H), 7.05 (t, J = 9.4 Hz, 1H), 5.67 (s, 1H), 4.72 (t, J = 7.9 Hz, 1H), 4.40 (t, J = 5.9 Hz, 1H), 3.74 (s, 3H), 3.72−3.59 (m, 2H), 2.44 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.4, 143.5, 141.7, 139.2, 138.5, 137.3, 137.0, 136.5, 134.7, 133.9, 133.6, 129.8, 128.8, 128.6, 128.2, 127.8, 127.2, 126.95, 126.92, 124.8, 123.0, 52.5, 49.8, 48.4, 43.4, 21.6; IR (neat) 3060, 3028, 2926, 2853, 1712, 1587, 1490, 1432, 1261, 1212, 1153 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{34}H_{31}NO_4S$ 549.1974; Found 549.1977.



4g

Methyl -2-(1-oxo-3,4-diphenyl-1*H*-azuleno[2,1-*c*]pyran-10-yl)-2-phenylacetate (4g)

The compound **4g** was prepared according to the same procedure as that of the synthesis of **4d**. The crude residue was purified by Silica gel column chromatography to give **4g** (69.5 mg, 70%) as a blue solid. m.p. 195−197 ºC; R_f = 0.3 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, J = 10.4 Hz, 1H), 7.58 (d, J = 9.5 Hz, 1H), 7.50-7.45 (m, 4H), 7.41-7.39 (m, 4H), 7.36-7.33 (m, 2H), 7.30-7.26 (m, 2H), 7.23-7.15 (m, 4H), 6.98 (t, J = 9.8 Hz, 1H), 6.93 (s, 1H), 6.69 (t, J = 9.9 Hz, 1H), 3.77 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.6, 161.4, 149.6, 143.0, 141.8, 140.4, 138.7, 137.0, 136.7, 135.9, 133.6, 131.4, 130.3, 129.44, 129.40, 128.9, 128.53, 128.49, 128.4, 127.9, 127.0, 125.4, 125.1, 124.8, 124.6, 116.6, 52.6, 48.1; IR (neat): 3059, 2924, 2283, 1716, 1495, 1199, 699 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{34}H_{24}O_4$ 496.1675; Found 496.1673.

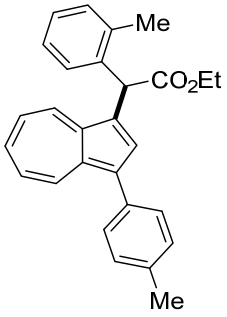


4h

Methyl 2-phenyl-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4h)

The compound **4h** was prepared according to the same procedure as that of the synthesis of **4d**. The crude residue was purified by Silica gel column chromatography to give **4h** (52.2 mg, 74%) as a blue oil.

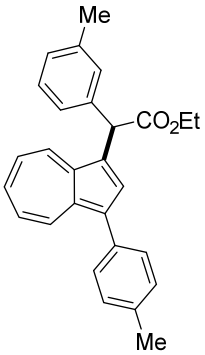
R_f = 0.2 (EtOAc:hexane = 1:20); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 2.1 Hz, 1H), 7.61 (s, 1H), 7.31−7.27 (m, 3H), 7.24−7.20 (m, 1H), 7.18−7.16 (m, 2H), 6.87 (d, J = 10.8 Hz, 1H), 6.10 (s, 1H), 3.74 (s, 3H), 3.03 (sextet, J = 6.9 Hz, 1H), 2.91 (s, 3H), 2.61 (s, 3H), 1.33 (dd, J = 6.9 Hz, 0.7 Hz, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 174.4, 144.7, 140.8, 140.1, 138.8, 138.2, 134.9, 134.0, 132.9, 128.8, 128.5, 127.4, 126.8, 124.7, 122.5, 52.3, 52.0, 37.7, 27.4, 24.6, 13.1; IR (neat) 2957, 2929, 2869, 1739, 1545, 1450, 1159 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{24}H_{26}O_2$ 346.1933; Found 346.1933.



4i

Ethyl 2-(*o*-tolyl)-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4i)

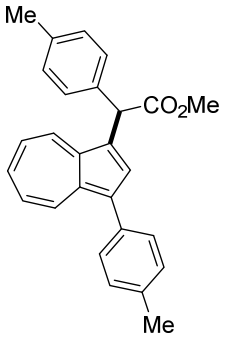
The compound **4i** was prepared according to the same procedure as that of the synthesis of **4a**. The crude residue was purified by Silica gel column chromatography to give **4i** (55.3 mg, 70%) as a blue oil. R_f = 0.2 (EtOAc:hexane = 1:20); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 9.6 Hz, 1H), 8.20 (d, J = 9.6 Hz, 1H), 7.91 (s, 1H), 7.55 (t, J = 9.8 Hz, 1H), 7.48 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 7.9 Hz, 2H), 7.25−7.13 (m, 4H), 7.09 (t, J = 9.7 Hz, 1H), 7.08 (J = 9.7 Hz, 1H), 5.82 (s, 1H), 4.30−4.18 (m, 2H), 2.42 (s, 3H), 2.39 (s, 3H), 1.26 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.0, 138.4, 137.9, 137.7, 137.2, 136.12, 136.10, 136.02, 136.00, 134.2, 133.4, 130.5, 130.2, 129.7, 129.3, 128.3, 127.1, 126.3, 124.9, 123.4, 122.5, 61.2, 47.1, 21.2, 19.9, 14.3; IR (neat) 3021, 2978, 2924, 1734, 1572, 1461, 1367, 1155, 1031 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{28}H_{26}O_2$ 394.1933; Found 394.1931.



4j

Ethyl 2-(*m*-tolyl)-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4j)

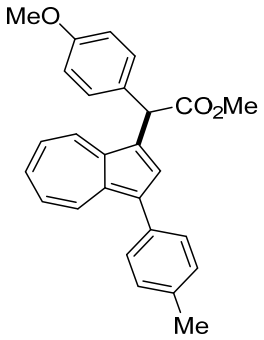
The compound **4j** was prepared according to the same procedure as that of the synthesis of **4d**. The crude residue was purified by Silica gel column chromatography to give **4j** (57.0 mg, 72%) as a blue oil. R_f = 0.5 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 9.8 Hz, 1H), 8.29 (d, J = 9.7 Hz, 1H), 8.09 (s, 1H), 7.55−7.48 (m, 3H), 7.28 (d, J = 8.0 Hz, 2H), 7.24−7.19 (m, 3H), 7.10−7.04 (m, 3H), 5.65 (s, 1H), 4.22 (q, J = 7.1 Hz, 2H), 2.42 (s, 3H), 2.30 (s, 3H), 1.26 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.0, 139.3, 138.4, 138.2, 137.4, 137.1, 136.1, 135.9, 134.3, 133.6, 130.3, 129.7, 129.5, 129.4, 129.2, 128.5, 127.9, 125.5, 125.4, 123.4, 122.6, 61.2, 50.1, 21.5, 21.2, 14.3; IR (neat) 3021, 2979, 2921, 2860, 1733, 1571, 1429, 1367, 1156, 1032 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{28}H_{26}O_2$ 394.1933; Found 394.1935.



4k

Methyl 2-(*p*-tolyl)-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4k)

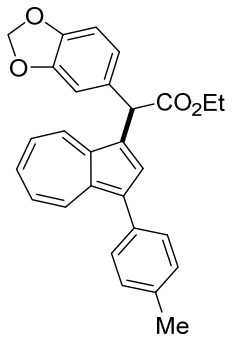
The compound **4k** was prepared according to the same procedure as that of the synthesis of **4d**. The crude residue was purified by Silica gel column chromatography to give **4k** (50.1 mg, 70%) as a blue oil. R_f = 0.5 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 9.4 Hz, 1H), 8.27 (d, J = 9.4 Hz, 1H), 8.06 (s, 1H), 7.55 (t, J = 9.8 Hz, 1H), 7.49 (d, J = 8.0 Hz, 2H), 7.29−7.26 (m, 4H), 7.12−7.06 (m, 4H), 5.67 (s, 1H), 3.75 (s, 3H), 2.42 (s, 3H), 2.30 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.5, 138.4, 137.3, 137.0, 136.8, 136.2, 136.1, 136.0, 135.9, 134.1, 133.5, 130.2, 129.7, 129.34, 129.30, 129.3, 125.2, 123.4, 122.6, 52.4, 49.6, 21.2, 21.0; IR (neat) 3021, 2948, 2919, 1737, 1569, 1509, 1431, 1191, 1154 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{27}H_{24}O_2$ 380.1776; Found 380.1776.



4l

Methyl 2-(4-methoxyphenyl)-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4l)

The compound **4l** was prepared according to the same procedure as that of the synthesis of **4a**. The crude residue was purified by Silica gel column chromatography to give **4l** (65.2 mg, 82%) as a green oil. R_f = 0.2 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 9.5 Hz, 1H), 8.26 (d, J = 9.4 Hz, 1H), 8.05 (s, 1H), 7.55 (t, J = 9.8 Hz, 1H), 7.49 (d, J = 8.0 Hz, 2H), 7.32−7.28 (m, 4H), 7.08 (t, J = 9.8 Hz, 2H), 6.84 (d, J = 8.8 Hz, 2H), 5.66 (s, 1H), 3.77 (s, 3H), 3.75 (s, 3H), 2.43 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.6, 158.6, 138.5, 137.2, 136.9, 136.1, 136.0, 135.9, 134.1, 133.5, 131.3, 130.2, 129.7, 129.4, 129.3, 125.3, 123.4, 122.6, 113.9, 55.2, 52.4, 49.2, 21.2; IR (neat) 3020, 2949, 2927, 1736, 1570, 1509, 1251, 1155 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{27}H_{24}O_3$ 396.1725; Found 396.1722.

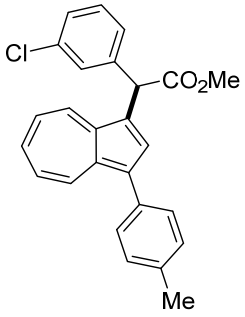


4m

Ethyl 2-(benzo[d][1,3]dioxol-5-yl)-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4m)

The compound **4m** was prepared according to the same procedure as that of the synthesis of **4a**. The crude residue was purified by Silica gel column chromatography to give **4m** (61.1 mg, 72%) as a blue solid. m.p. 51−53 ºC; R_f = 0.6 (EtOAc:hexane = 1:4); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 9.8 Hz, 1H), 8.25 (d, J = 9.7 Hz, 1H), 8.09 (s, 1H), 7.54 (t, J = 9.8 Hz, 1H), 7.49 (d, J = 7.9 Hz, 2H), 7.29 (d, J =

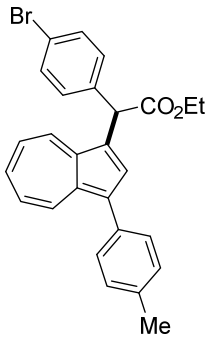
8.1 Hz, 2H), 7.08 (t, J = 9.9 Hz, 2H), 6.88−6.84 (m, 2H), 6.73 (d, J = 8.0 Hz, 1H), 5.93−5.89 (m, 2H), 5.60 (s, 1H), 4.22 (q, J = 7.1 Hz, 2H), 2.42 (s, 3H), 1.26 (t, J = 7.1 Hz, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 172.9, 147.8, 146.7, 138.5, 137.1, 137.0, 136.14, 136.10, 136.0, 134.2, 133.6, 133.3, 130.2, 129.7, 129.4, 125.2, 123.4, 122.6, 121.6, 109.1, 108.2, 101.0, 61.3, 49.8, 21.2, 14.2; IR (neat) 3024, 2980, 1731, 1502, 1488, 1248, 1154, 1038 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{28}H_{24}O_4$ 424.1675; Found 424.1672.



4n

Methyl 2-(3-chlorophenyl)-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4n)

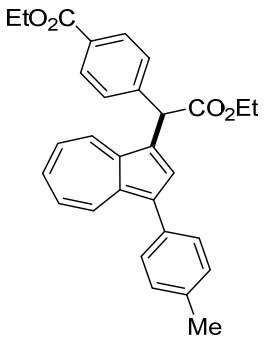
The compound **4n** was prepared according to the same procedure as that of the synthesis of **4d**. The crude residue was purified by Silica gel column chromatography to give **4n** (57.0 mg, 71%) as a green oil. R_f = 0.5 (EtOAc:hexane = 1:5); ^1H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 9.6 Hz, 1H), 8.24 (d, J = 9.6 Hz, 1H), 8.04 (s, 1H), 7.57 (t, J = 9.8 Hz, 1H), 7.49 (d, J = 8.0 Hz, 2H), 7.37 (s, 1H), 7.30 (d, J = 8.0 Hz, 2H), 7.29−7.22 (m, 3H), 7.11 (t, J = 9.8 Hz, 2H), 5.67 (s, 1H), 3.77 (s, 3H), 2.43 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 172.8, 141.1, 138.7, 137.08, 137.04, 136.2, 136.19, 136.16, 134.4, 134.0, 133.5, 130.4, 129.8, 129.7, 129.4, 128.6, 127.4, 126.6, 124.0, 123.7, 122.8, 52.5, 49.6, 21.2; IR (neat) 3021, 2949, 2919, 1737, 1571, 1430, 1193, 1157 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{26}H_{21}ClO_2$ 400.1230; Found 400.1230.



4o

Ethyl 2-(4-bromophenyl)-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4o)

The compound **4o** was prepared according to the same procedure as that of the synthesis of **4e** with diazo compound (1.5 equiv) at 70 °C. The crude residue was purified by Silica gel column chromatography to give **4o** (60.5 mg, 65%) as a blue oil. R_f = 0.4 (EtOAc:hexane = 1:5); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 9.6 Hz, 1H), 8.23 (d, J = 9.6 Hz, 1H), 8.04 (s, 1H), 7.56 (t, J = 9.8 Hz, 1H), 7.48 (d, J = 8.0 Hz, 2H), 7.42 (d, J = 8.4 Hz, 2H), 7.31−7.25 (m, 4H), 7.11 (dd, J = 9.7 Hz, 3.7 Hz, 1H), 7.09 (dd, J = 9.7 Hz,, 3.6 Hz, 1H), 5.63 (s, 1H), 4.21 (qd, J = 11.8 Hz, 1.6 Hz, 2H), 2.43 (s, 3H), 1.26 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 172.4, 138.6, 138.4, 137.06, 137.02, 136.2, 136.1, 134.0, 133.5, 131.6, 130.3, 130.2, 129.6, 129.4, 124.4, 123.6, 122.7, 121.1, 61.4, 49.6, 21.2, 14.2; IR (neat) 3021, 2978, 2922, 1732, 1571, 1486, 1367, 1154, 1010 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{27}H_{23}BrO_2$ 458.0881; Found 458.0883.

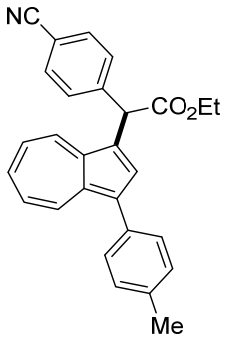


4p

Ethyl 4-(2-ethoxy-2-oxo-1-(3-(*p*-tolyl)azulen-1-yl)ethyl)benzoate (4p)

The compound **4p** was prepared according to the same procedure as that of the synthesis of **4d**. The crude residue was purified by Silica gel column chromatography to give **4p** (66.3 mg, 73%) as a blue oil. R_f = 0.4 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 9.6 Hz, 1H), 8.25 (d, J = 9.6

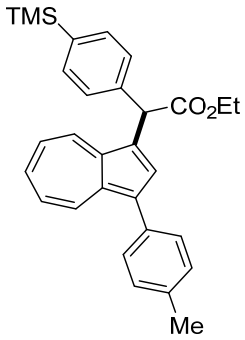
Hz, 1H), 8.05 (s, 1H), 8.00−7.97 (m, 2H), 7.55 (t, J = 9.8 Hz, 1H), 7.48 (d, J = 7.8 Hz, 2H), 7.46 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 7.8 Hz, 2H), 7.10 (t, J = 9.7 Hz, 1H), 7.09 (t, J = 9.7 Hz, 1H), 5.74 (s, 1H), 4.34 (q, J = 7.1 Hz, 2H), 4.24 (qd, J = 7.1 Hz, 1.4 Hz, 2H), 2.42 (s, 3H), 1.36 (t, J = 7.1 Hz, 3H), 1.26 (t, J = 7.1 Hz, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 172.3, 166.4, 144.4, 138.6, 137.2, 137.1, 136.22, 136.13, 134.0, 133.6, 130.4, 129.8, 129.7, 129.4, 124.4, 123.6, 122.8, 61.5, 60.9, 50.2, 21.2, 14.3, 14.2; IR (neat) 2980, 1716, 1572, 1366, 1277, 1155, 1106, 1022 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{30}H_{28}O_4$ 452.1988; Found 452.1986.



4q

Ethyl 2-(4-cyanophenyl)-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4q)

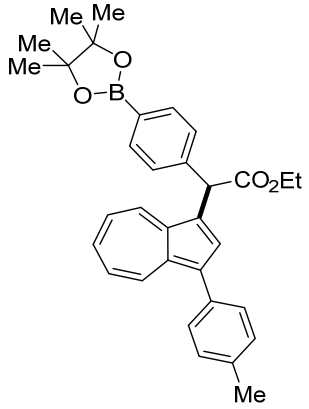
The compound **4q** was prepared according to the same procedure as that of the synthesis of **4d**. The crude residue was purified by Silica gel column chromatography to give **4q** (72.1 mg, 91%) as a blue solid. m.p. 62−64 °C; R_f = 0.5 (EtOAc:hexane = 1:4); ^1H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, J = 9.4 Hz, 1H), 8.22 (d, J = 9.5 Hz, 1H), 8.03 (s, 1H), 7.61−7.56 (m, 3H), 7.50−7.47 (m, 4H), 7.30 (d, J = 7.8 Hz, 2H), 7.13 (t, J = 9.6 Hz, 1H), 7.11 (t, J = 9.5 Hz, 1H), 5.72 (s, 1H), 4.30−4.19 (m, 2H), 2.43 (s, 3H), 1.26 (t, J = 7.1 Hz, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 171.9, 144.7, 138.9, 137.1, 136.9, 136.4, 136.3, 136.2, 133.9, 133.5, 132.4, 130.6, 129.7, 129.5, 129.3, 123.9, 123.5, 122.9, 118.8, 111.0, 61.7, 50.1, 21.2, 14.2; IR (neat) 2979, 2921, 2227, 1732, 1572, 1572, 1505, 1368, 1308, 1156, 1030 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{28}H_{23}NO_2$ 405.1729; Found 405.1728.



4r

Ethyl 2-(3-(*p*-tolyl)azulen-1-yl)-2-(4-(trimethylsilyl)phenyl)acetate (4r)

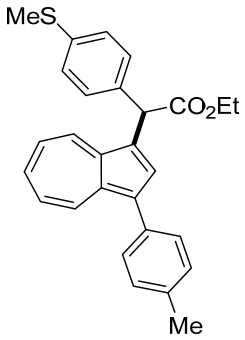
The compound **4r** was prepared according to the same procedure as that of the synthesis of **4d** The crude residue was purified by Silica gel column chromatography to give **4r** (68.2 mg, 75%) as a blue solid. m.p. 62−64 ºC; R_f = 0.3 (EtOAc:hexane = 1:20); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, J = 9.6 Hz, 1H), 8.30 (d, J = 9.6 Hz, 1H), 8.11 (s, 1H), 7.52 (t, J = 9.9 Hz, 1H), 7.49 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 8.2 Hz, 2H), 7.39 (d, J = 7.8 Hz, 2H), 7.28 (d, J = 7.8 Hz, 2H), 7.07 (t, J = 9.7 Hz, 1H), 7.06 (t, J = 9.6 Hz, 1H), 5.68 (s, 1H), 4.22 (q, J = 7.1 Hz, 2H), 2.42 (s, 3H), 1.26 (t, J = 7.1 Hz, 3H), 0.22 (s, 9H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 174.0, 141.0, 140.1, 139.6, 138.5, 138.2, 137.2, 137.0, 135.3, 134.73, 134.70, 131.4, 130.5, 128.9, 126.3, 124.5, 123.7, 62.4, 51.2, 22.3, 15.4, 0.004; IR (neat) 3019, 2954, 1735, 1572, 1506, 1367, 1248, 1152, 1110, 1032, 839, 741 cm^{-1}; HRMS (EI) *m/z*: [M^+] Calcd for $C_{30}H_{32}O_2Si$ 452.2172; Found 452.2170.



4s

Ethyl 2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4s)

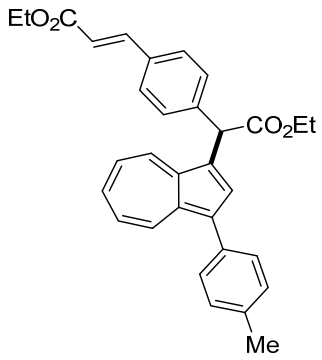
The compound **4s** was prepared according to the same procedure as that of the synthesis of **4d**. The crude residue was purified by Silica gel column chromatography to give **4s** (50.1 mg, 50%) as a blue oil. R_f = 0.2 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 9.5 Hz, 1H), 8.26 (d, J = 9.6 Hz, 1H), 8.04 (s, 1H), 7.75 (d, J = 8.1 Hz, 2H), 7.54 (t, J = 9.7 Hz, 1H), 7.47 (d, J = 8.0 Hz, 2H), 7.40 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 7.8 Hz, 2H), 7.07 (t, J = 10.1 Hz, 2H), 5.69 (s, 1H), 4.22 (q, J = 7.1 Hz, 2H), 2.42 (s, 3H), 1.31 (s, 12H), 1.25 (t, J = 7.0 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 172.6, 142.43, 140.2, 138.4, 137.4, 137.1, 136.0, 135.9, 135.0, 134.1, 133.5, 130.2, 129.7, 129.3, 127.8, 123.4, 122.6, 83.7, 61.2, 50.4, 24.8, 21.2, 14.2; IR (neat) 3025, 2948, 1730, 1610, 1427, 1320, 1160, 1043, 861, 740 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{33}H_{35}BO_4$ 506.2628; Found 506.2631.



4t

Ethyl 2-(4-(methylthio)phenyl)-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4t)

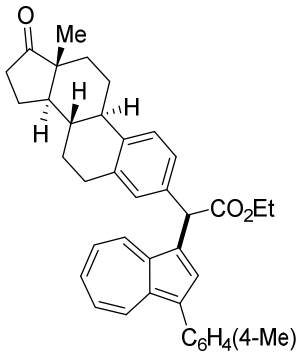
The compound **4t** was prepared according to the same procedure as that of the synthesis of **4d**. The crude residue was purified by Silica gel column chromatography to give **4t** (63.1 mg, 74%) as a blue oil. R_f = 0.2 (EtOAc:hexane = 1:20); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 9.7 Hz, 1H), 8.25 (d, J = 9.7 Hz, 1H), 8.07 (s, 1H), 7.53 (t, J = 9.8 Hz, 1H), 7.49 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.4Hz, 2H), 7.29 (d, J = 8.7 Hz, 2H), 7.19 (d, J = 8.4 Hz, 2H), 7.07 (t J = 9.8 Hz, 2H), 5.64 (s, 1H), 4.22 (q, J = 7.1 Hz, 2H), 2.43 (s, 3H), 2.42 (s, 3H), 1.25 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 172.8, 138.5, 137.25, 137.20, 137.1, 136.3, 136.1, 136.0, 134.2, 133.6, 130.3, 129.7, 129.4, 128.9, 126.8, 125.1, 123.5, 122.7, 61.3, 49.7, 21.2, 15.9, 14.3; IR (neat) 3020, 2979, 2919, 1732, 1572, 1493, 1428, 1367, 1313, 1153 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{28}H_{26}O_2S$ 426.1654; Found 426.1655.



4u

Ethyl 3-(4-(2-ethoxy-2-oxo-1-(3-(*p*-tolyl)azulen-1-yl)ethyl)phenyl)acrylate (4u)

The compound **4u** was prepared according to the same procedure as that of the synthesis of **4a**. The crude residue was purified by Silica gel column chromatography to give **4u** (74.5 mg, 74%) as a blue oil. R_f = 0.4 (EtOAc:hexane = 1:10); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 9.6 Hz, 1H), 8.26 (d, J = 9.6 Hz, 1H), 8.07 (s, 1H), 7.64 (d, J = 16.0 Hz, 1H), 7.56 (t, J = 9.8 Hz, 1H), 7.50-7.45 (m, 4H), 7.40 (d, J = 8.3 Hz, 2H), 7.29 (d, J = 7.9 Hz, 2H), 7.08 (td, J = 14.8, 1.2 Hz, 2H), 6.38 (d, J = 16.0 Hz, 1H), 5.69 (s, 1H), 4.27-4.22 (m, 4H), 2.43 (s, 3H), 1.32 (t, J = 7.1 Hz, 3H), 1.26 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.5, 167.0, 144.1, 141.6, 138.6, 137.1, 137.0, 136.2, 136.12, 136.09, 134.0, 133.5, 133.3, 130.3, 129.6, 129.3, 128.9, 128.2, 124.5, 123.5, 122.7, 118.1, 61.4, 60.5, 50.0, 21.2, 14.3, 14.2; IR (neat) 3027, 2947, 2846, 1734, 1598, 1428, 1151, 831, 727 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{32}H_{30}O_4$ 478.2144; Found 478.2146.



4v

Ethyl 2-((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a]-phenanthren-3-yl)-2-(3-(*p*-tolyl)azulen-1-yl)acetate (4v)

The compound **4v** was prepared according to the same procedure as that of the synthesis of **4a**. The crude residue was purified by Silica gel column chromatography to give **4v** (44.7 mg, 48%) as a blue solid. m.p. 166−168 ºC; R_f = 0.2 (EtOAc:hexane = 1:20); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 9.8 Hz, 1H), 8.31 (d, J = 9.7 Hz, 9.7 Hz, 1H), 8.10 (d, J = 1.4 Hz, 1H), 7.55 (t, J = 9.8 Hz, 1H), 7.50 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 7.8 Hz, 2H), 7.24−7.18 (m, 3H), 5.63 (s, 1H), 4.22 (q, J = 7.1 Hz, 2H), 2.86 (dd, J = 3.4 Hz, 8.1 Hz, 2H), 2.49 (dd, J = 18.9 Hz, 8.5 Hz, 1H), 2.43 (s, 3H), 2.42−2.36 (m ,1H), 2.29−2.24 (m, 1H), 2.17−1.93 (m, 4H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 173.0, 138.6, 138.4, 137.4, 137.1, 136.8, 136.7, 136.11, 136.10, 135.9, 134.2, 133.5, 130.2, 129.7, 129.3, 128.9, 125.8, 125.6, 125.4, 123.3, 122.6, 61.2, 50.5, 49.6, 48.0, 44.3, 38.0, 35.9, 31.6, 29.5, 26.5, 25.6, 21.6, 21.2, 14.3, 13.8; IR (neat) 2981, 2931, 1734, 1644, 1369, 1154 cm^{-1}; HRMS (EI) *m/z*: [M$^+$] Calcd for $C_{39}H_{40}O_3$ 556.2977; Found 556.2979.

D. X-ray crystallographic data of 3o, 3y, and 4g

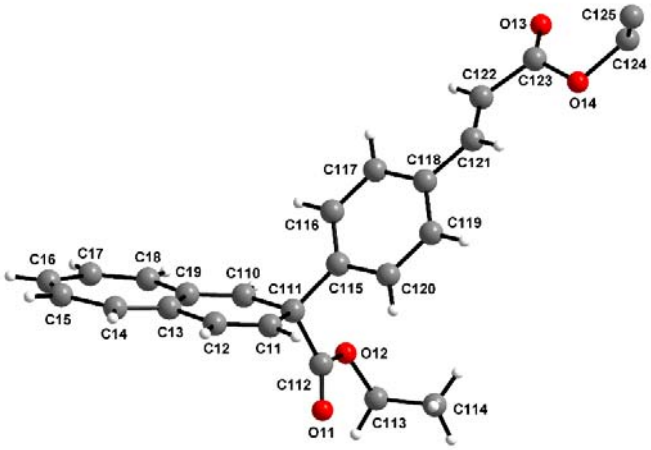


Table S2. Crystal data and structure refinement for 3o.

Empirical formula	$C_{25}H_{19}O_4$	
Formula weight	383.40	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.3196(4) Å	α= 89.980(3) °.
	b = 11.5152(6) Å	β= 89.980(3)°.
	c = 44.227(2) Å	γ = 89.990(3)°.
Volume	4237.0(4) $Å^3$	
Z	8	
Density (calculated)	1.202 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	1608	
Crystal size	0.360 x 0.240 x 0.100 mm^3	
θ range for data collection	1.381 to 28.271°.	
Index ranges	$-11 \le h \le 11$, $-15 \le k \le 15$, $-58 \le l \le 58$	
Reflections collected	89703	
Independent reflections	20228 [R(int) = 0.2026]	
Completeness to theta = 25.242°	98.8 %	
Absorption correction	multi-scan	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	20228 / 35 / 1034
Goodness-of-fit on F^2	0.938
Final R indices [I>2sigma(I)]	$R_1 = 0.1238$, $wR_2 = 0.2949$
R indices (all data)	$R_1 = 0.3406$, $wR_2 = 0.3639$
Extinction coefficient	0.026(2)
Largest diff. peak and hole	0.587 and -0.426 e·$Å^{-3}$

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 3o. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(11)	-795(6)	8527(5)	6646(1)	61(2)
C(12)	-1044(6)	7986(5)	6907(1)	58(2)
C(13)	-403(6)	8337(4)	7193(1)	55(2)
C(14)	-778(6)	7681(5)	7438(1)	58(2)
C(15)	-347(8)	7820(6)	7753(2)	76(2)
C(16)	495(7)	8652(6)	7893(2)	71(2)
C(17)	1238(7)	9628(5)	7747(1)	64(2)
C(18)	1279(6)	9948(5)	7452(1)	60(2)
C(19)	569(5)	9429(4)	7188(1)	45(1)
C(110)	843(6)	9974(4)	6920(1)	53(1)
C(111)	215(6)	9596(4)	6613(1)	52(1)
C(112)	-854(7)	10596(5)	6502(1)	54(1)
C(113)	-834(7)	12579(5)	6332(2)	75(2)
C(114)	-1035(10)	12500(7)	6003(2)	124(3)
C(115)	1545(6)	9403(4)	6381(1)	51(1)
C(116)	3135(6)	9438(4)	6449(1)	56(2)
C(117)	4307(7)	9267(5)	6227(2)	64(2)
C(118)	3882(8)	9045(5)	5931(2)	71(2)
C(119)	2300(8)	8989(6)	5860(1)	79(2)
C(120)	1117(7)	9167(5)	6082(1)	71(2)
C(121)	5092(9)	8905(6)	5687(2)	88(2)
C(122)	6506(11)	9197(8)	5688(2)	121(3)
C(123)	7629(8)	9106(8)	5413(2)	125(3)
C(124)	8080(30)	8748(14)	4891(6)	155(8)
C(126)	8470(20)	8110(20)	4985(4)	160(8)
C(125)	8106(17)	7475(12)	4785(4)	99(4)
C(127)	7640(40)	8720(30)	4736(7)	249(19)
C(21)	5789(7)	3520(5)	3354(1)	65(2)
C(22)	6046(6)	2976(5)	3093(1)	59(2)
C(23)	5401(6)	3345(4)	2801(1)	52(1)
C(24)	5759(6)	2701(5)	2559(1)	63(2)
C(25)	5365(7)	2810(5)	2243(2)	73(2)
C(26)	4500(7)	3656(6)	2110(1)	70(2)
C(27)	3768(6)	4639(5)	2253(1)	65(2)

C(28)	3740(6)	4953(5)	2546(1)	55(1)
C(29)	4415(6)	4421(4)	2815(1)	50(1)
C(210)	4150(6)	4967(4)	3082(1)	52(1)
C(211)	4797(6)	4612(4)	3385(1)	50(1)
C(212)	5850(7)	5588(5)	3503(1)	55(1)
C(213)	5830(8)	7581(5)	3669(2)	75(2)
C(214)	6059(10)	7499(6)	3996(2)	114(3)
C(215)	3472(6)	4398(4)	3621(1)	48(1)
C(216)	1866(7)	4432(4)	3555(1)	60(2)
C(217)	675(6)	4280(5)	3772(2)	60(2)
C(218)	1111(7)	4042(5)	4071(2)	67(2)
C(219)	2719(8)	3972(6)	4139(2)	81(2)
C(220)	3892(7)	4164(5)	3915(1)	72(2)
C(221)	-96(8)	3915(6)	4320(2)	89(2)
C(222)	-1507(10)	4213(7)	4314(2)	109(3)
C(223)	-2630(9)	4117(8)	4586(2)	121(3)
C(224)	-2680(20)	3967(16)	5173(2)	135(7)
C(226)	-3322(14)	3525(13)	5029(3)	110(5)
C(225)	-3030(40)	2683(17)	5244(6)	171(12)
C(227)	-3240(40)	2333(16)	5153(7)	185(13)
C(31)	4169(6)	9976(4)	1918(1)	53(1)
C(32)	4416(6)	9416(4)	2183(1)	46(1)
C(33)	3738(6)	9946(5)	2456(1)	58(1)
C(34)	3766(7)	9640(5)	2748(1)	66(2)
C(35)	4507(6)	8650(6)	2892(1)	66(2)
C(36)	5356(7)	7818(5)	2757(2)	73(2)
C(37)	5754(6)	7705(5)	2442(2)	69(2)
C(38)	5408(6)	8356(5)	2194(1)	57(1)
C(39)	6025(6)	7981(5)	1905(1)	61(2)
C(310)	5812(6)	8518(5)	1650(1)	62(2)
C(311)	4797(6)	9604(4)	1615(1)	47(1)
C(312)	5878(7)	10593(5)	1497(1)	52(1)
C(313)	5857(8)	12584(5)	1336(2)	77(2)
C(314)	6051(10)	12511(7)	1004(2)	120(3)
C(315)	3470(6)	9392(4)	1381(1)	51(1)
C(316)	3896(7)	9154(5)	1079(1)	72(2)
C(317)	2734(8)	8977(5)	868(1)	74(2)
C(318)	1122(8)	9038(5)	933(2)	67(2)
C(319)	682(6)	9277(4)	1230(2)	61(2)
C(320)	1846(6)	9442(4)	1445(1)	55(1)
C(321)	-73(9)	8919(6)	674(2)	104(3)
C(322)	-1507(11)	9210(8)	674(2)	120(3)
C(323)	-2646(9)	9100(8)	422(2)	123(3)
C(324)	-2760(30)	8974(19)	-162(3)	168(9)
C(326)	-3308(14)	8453(14)	-35(3)	104(5)
C(325)	-3070(40)	7687(19)	-235(7)	180(12)
C(327)	-3210(40)	7244(17)	-148(8)	211(14)
C(41)	9152(6)	5024(4)	1920(1)	51(1)
C(42)	9420(6)	5579(4)	2189(1)	47(1)
C(43)	8733(6)	5059(5)	2457(1)	58(2)
C(44)	8785(6)	5373(5)	2748(1)	58(2)
C(45)	9492(7)	6347(6)	2888(1)	66(2)
C(46)	10344(7)	7183(6)	2750(2)	72(2)
C(47)	10756(6)	7314(5)	2439(2)	60(2)
C(48)	10400(6)	6655(5)	2197(1)	54(1)
C(49)	11035(6)	7013(5)	1909(1)	61(2)

C(410)	10820(6)	6484(5)	1651(1)	61(2)
C(411)	9792(6)	5407(4)	1613(1)	51(1)
C(412)	10864(8)	4407(5)	1502(1)	60(2)
C(413)	10858(8)	2429(5)	1336(2)	77(2)
C(414)	11039(10)	2499(7)	1002(2)	124(3)
C(415)	8458(6)	5608(4)	1382(1)	52(1)
C(416)	8886(7)	5851(5)	1075(2)	80(2)
C(417)	7725(8)	6009(5)	864(1)	74(2)
C(418)	6123(8)	5967(5)	929(2)	68(2)
C(419)	5697(7)	5734(5)	1230(2)	66(2)
C(420)	6862(6)	5548(4)	1445(1)	56(1)
C(421)	4904(9)	6090(6)	679(2)	97(2)
C(422)	3490(11)	5795(7)	674(2)	119(3)
C(423)	2368(9)	5894(8)	424(2)	118(3)
C(424)	2340(30)	6020(20)	-170(3)	178(9)
C(426)	1779(16)	6594(14)	-45(3)	123(6)
C(425)	1840(40)	7270(20)	-245(6)	191(12)
C(427)	1950(30)	7771(16)	-176(6)	166(10)
O(11)	-2269(5)	10538(4)	6461(1)	86(1)
O(12)	-12(4)	11563(3)	6448(1)	65(1)
O(13)	8935(10)	9632(9)	5442(2)	94(3)
O(13*)	9073(11)	8813(15)	5423(4)	180(6)
O(14)	6867(13)	8938(12)	5150(2)	112(4)
O(14*)	7143(15)	8324(10)	5202(3)	122(4)
O(21)	7264(5)	5527(4)	3540(1)	85(1)
O(22)	5014(4)	6546(3)	3550(1)	62(1)
O(23)	-3908(10)	4679(10)	4557(2)	104(3)
O(23*)	-4109(10)	3950(15)	4568(3)	159(5)
O(24)	-1922(10)	3958(12)	4855(2)	118(4)
O(24*)	-2108(13)	3320(9)	4790(2)	120(4)
O(31)	7262(5)	10538(4)	1464(1)	86(1)
O(32)	4995(4)	11540(3)	1453(1)	64(1)
O(33)	-3884(11)	9709(10)	448(2)	106(3)
O(33*)	-4134(10)	8987(14)	441(3)	141(5)
O(34)	-1965(10)	8897(11)	152(2)	109(4)
O(34*)	-2154(13)	8297(10)	216(2)	124(4)
O(41)	12264(5)	4459(4)	1460(1)	86(1)
O(42)	10002(4)	3438(3)	1448(1)	62(1)
O(43)	891(10)	6068(15)	442(3)	156(5)
O(43*)	1100(11)	5314(9)	444(2)	100(3)
O(44)	3034(10)	6087(11)	153(2)	108(4)
O(44*)	2854(14)	6703(10)	220(2)	132(5)

Table S4. Bond lengths [Å] and angles [°] for 3o.

C(11)-C(12)	1.328(7)
C(11)-C(111)	1.498(7)
C(12)-C(13)	1.432(7)
C(13)-C(14)	1.355(7)
C(13)-C(19)	1.494(7)
C(14)-C(15)	1.447(8)
C(15)-C(16)	1.339(8)
C(16)-C(17)	1.434(8)

C(17)-C(18)	1.357(7)
C(18)-C(19)	1.441(7)
C(19)-C(110)	1.358(7)
C(110)-C(111)	1.521(7)
C(111)-C(115)	1.524(7)
C(111)-C(112)	1.536(7)
C(112)-O(11)	1.193(6)
C(112)-O(12)	1.336(6)
C(113)-O(12)	1.451(6)
C(113)-C(114)	1.466(9)
C(115)-C(116)	1.357(7)
C(115)-C(120)	1.398(7)
C(116)-C(117)	1.397(7)
C(117)-C(118)	1.383(8)
C(118)-C(119)	1.354(8)
C(118)-C(121)	1.483(9)
C(119)-C(120)	1.406(7)
C(121)-C(122)	1.224(9)
C(122)-C(123)	1.535(10)
C(123)-O(13*)	1.249(2)
C(123)-O(13)	1.251(2)
C(123)-O(14)	1.341(2)
C(123)-O(14*)	1.358(2)
C(124)-C(127)	0.78(3)
C(124)-C(126)	0.91(3)
C(124)-C(125)	1.541(2)
C(124)-O(14)	1.541(2)
C(124)-O(14*)	1.66(2)
C(126)-C(125)	1.19(2)
C(126)-C(127)	1.480(2)
C(126)-O(14*)	1.482(2)
C(126)-O(14)	1.79(2)
C(125)-C(127)	1.50(3)
C(21)-C(22)	1.329(7)
C(21)-C(211)	1.511(7)
C(22)-C(23)	1.462(8)
C(23)-C(24)	1.336(7)
C(23)-C(29)	1.487(7)
C(24)-C(25)	1.442(8)
C(25)-C(26)	1.346(8)
C(26)-C(27)	1.432(8)
C(27)-C(28)	1.349(7)
C(28)-C(29)	1.448(7)
C(29)-C(210)	1.358(7)
C(210)-C(211)	1.501(7)
C(211)-C(212)	1.516(7)
C(211)-C(215)	1.537(7)
C(212)-O(21)	1.190(6)
C(212)-O(22)	1.321(6)
C(213)-C(214)	1.461(8)
C(213)-O(22)	1.468(6)
C(215)-C(216)	1.369(7)
C(215)-C(220)	1.371(7)
C(216)-C(217)	1.393(7)
C(217)-C(218)	1.399(8)
C(218)-C(219)	1.372(8)

C(218)-C(221)	1.495(8)
C(219)-C(220)	1.407(8)
C(221)-C(222)	1.224(9)
C(222)-C(223)	1.529(9)
C(223)-O(23*)	1.248(2)
C(223)-O(23)	1.252(2)
C(223)-O(24)	1.342(2)
C(223)-O(24*)	1.358(2)
C(224)-C(226)	0.98(2)
C(224)-C(225)	1.539(2)
C(224)-O(24)	1.541(2)
C(224)-O(24*)	1.913(12)
C(224)-C(227)	1.94(3)
C(226)-C(225)	1.38(3)
C(226)-C(227)	1.480(2)
C(226)-O(24*)	1.481(2)
C(226)-O(24)	1.482(2)
C(225)-C(227)	0.59(4)
C(31)-C(32)	1.356(7)
C(31)-C(311)	1.501(7)
C(32)-C(33)	1.465(7)
C(32)-C(38)	1.474(7)
C(33)-C(34)	1.336(7)
C(34)-C(35)	1.445(8)
C(35)-C(36)	1.332(8)
C(36)-C(37)	1.436(8)
C(37)-C(38)	1.359(8)
C(38)-C(39)	1.443(8)
C(39)-C(310)	1.301(7)
C(310)-C(311)	1.518(7)
C(311)-C(315)	1.532(7)
C(311)-C(312)	1.541(7)
C(312)-O(31)	1.162(6)
C(312)-O(32)	1.330(6)
C(313)-C(314)	1.476(9)
C(313)-O(32)	1.494(6)
C(315)-C(320)	1.382(7)
C(315)-C(316)	1.407(7)
C(316)-C(317)	1.360(7)
C(317)-C(318)	1.373(8)
C(318)-C(319)	1.392(8)
C(318)-C(321)	1.523(10)
C(319)-C(320)	1.370(7)
C(321)-C(322)	1.239(9)
C(322)-C(323)	1.470(10)
C(323)-O(33*)	1.248(2)
C(323)-O(33)	1.252(2)
C(323)-O(34)	1.341(2)
C(323)-O(34*)	1.359(2)
C(324)-C(326)	0.94(2)
C(324)-C(325)	1.539(2)
C(324)-O(34)	1.541(2)
C(324)-O(34*)	1.912(12)
C(324)-C(327)	2.03(3)
C(326)-C(325)	1.26(3)
C(326)-C(327)	1.480(2)

C(326)-O(34*)	1.481(2)
C(326)-O(34)	1.482(2)
C(325)-C(327)	0.65(4)
C(41)-C(42)	1.369(7)
C(41)-C(411)	1.524(7)
C(42)-C(43)	1.443(7)
C(42)-C(48)	1.485(7)
C(43)-C(44)	1.336(7)
C(44)-C(45)	1.412(8)
C(45)-C(46)	1.343(8)
C(46)-C(47)	1.422(8)
C(47)-C(48)	1.346(7)
C(48)-C(49)	1.438(7)
C(49)-C(410)	1.307(7)
C(410)-C(411)	1.516(7)
C(411)-C(415)	1.525(7)
C(411)-C(412)	1.538(7)
C(412)-O(41)	1.180(6)
C(412)-O(42)	1.347(7)
C(413)-O(42)	1.451(6)
C(413)-C(414)	1.488(9)
C(415)-C(420)	1.358(7)
C(415)-C(416)	1.432(8)
C(416)-C(417)	1.357(8)
C(417)-C(418)	1.364(8)
C(418)-C(419)	1.406(8)
C(418)-C(421)	1.506(9)
C(419)-C(420)	1.372(7)
C(421)-C(422)	1.225(9)
C(422)-C(423)	1.451(10)
C(423)-O(43)	1.248(2)
C(423)-O(43*)	1.251(2)
C(423)-O(44)	1.341(2)
C(423)-O(44*)	1.358(2)
C(424)-C(426)	0.98(3)
C(424)-C(425)	1.539(2)
C(424)-O(44)	1.541(2)
C(426)-C(425)	1.18(3)
C(426)-C(427)	1.480(2)
C(426)-O(44*)	1.481(2)
C(426)-O(44)	1.483(2)
C(425)-C(427)	0.66(4)
O(13)-O(13*)	0.954(16)
O(14)-O(14*)	0.778(15)
O(23)-O(23*)	0.857(16)
O(24)-O(24*)	0.806(15)
O(33)-O(33*)	0.857(15)
O(34)-O(34*)	0.764(15)
O(43)-O(43*)	0.885(15)
O(44)-O(44*)	0.784(15)

C(12)-C(11)-C(111)	123.9(5)
C(11)-C(12)-C(13)	125.3(5)
C(14)-C(13)-C(12)	117.5(5)
C(14)-C(13)-C(19)	127.3(6)
C(12)-C(13)-C(19)	115.1(5)

C(13)-C(14)-C(15)	130.5(6)
C(16)-C(15)-C(14)	130.9(6)
C(15)-C(16)-C(17)	125.3(6)
C(18)-C(17)-C(16)	130.9(6)
C(17)-C(18)-C(19)	131.1(6)
C(110)-C(19)-C(18)	116.5(5)
C(110)-C(19)-C(13)	119.6(5)
C(18)-C(19)-C(13)	123.9(5)
C(19)-C(110)-C(111)	126.0(5)
C(11)-C(111)-C(110)	109.9(5)
C(11)-C(111)-C(115)	110.7(4)
C(110)-C(111)-C(115)	113.1(4)
C(11)-C(111)-C(112)	108.8(4)
C(110)-C(111)-C(112)	105.7(4)
C(115)-C(111)-C(112)	108.4(4)
O(11)-C(112)-O(12)	122.5(5)
O(11)-C(112)-C(111)	125.3(5)
O(12)-C(112)-C(111)	112.2(5)
O(12)-C(113)-C(114)	110.9(5)
C(116)-C(115)-C(120)	117.6(5)
C(116)-C(115)-C(111)	123.7(5)
C(120)-C(115)-C(111)	118.7(5)
C(115)-C(116)-C(117)	121.4(5)
C(118)-C(117)-C(116)	120.9(5)
C(119)-C(118)-C(117)	118.5(6)
C(119)-C(118)-C(121)	119.1(7)
C(117)-C(118)-C(121)	122.4(6)
C(118)-C(119)-C(120)	120.7(6)
C(115)-C(120)-C(119)	120.8(6)
C(122)-C(121)-C(118)	128.4(8)
C(121)-C(122)-C(123)	124.4(8)
O(13*)-C(123)-O(13)	44.9(8)
O(13*)-C(123)-O(14)	116.5(11)
O(13)-C(123)-O(14)	124.7(9)
O(13*)-C(123)-O(14*)	97.5(12)
O(13)-C(123)-O(14*)	130.5(9)
O(14)-C(123)-O(14*)	33.5(7)
O(13*)-C(123)-C(122)	125.2(10)
O(13)-C(123)-C(122)	114.5(8)
O(14)-C(123)-C(122)	114.2(8)
O(14*)-C(123)-C(122)	114.0(8)
C(127)-C(124)-C(126)	122(3)
C(127)-C(124)-C(125)	72(3)
C(126)-C(124)-C(125)	50.3(15)
C(127)-C(124)-O(14)	111(4)
C(126)-C(124)-O(14)	90.4(17)
C(125)-C(124)-O(14)	111.8(12)
C(127)-C(124)-O(14*)	120(3)
C(126)-C(124)-O(14*)	62.9(12)
C(125)-C(124)-O(14*)	88.9(12)
O(14)-C(124)-O(14*)	27.9(6)
C(124)-C(126)-C(125)	94(2)
C(124)-C(126)-C(127)	26.5(18)
C(125)-C(126)-C(127)	67.3(18)
C(124)-C(126)-O(14*)	84.0(15)
C(125)-C(126)-O(14*)	113.6(17)

C(127)-C(126)-O(14*)	93.2(18)
C(124)-C(126)-O(14)	59.2(11)
C(125)-C(126)-O(14)	116.3(15)
C(127)-C(126)-O(14)	72.7(17)
O(14*)-C(126)-O(14)	25.3(7)
C(126)-C(125)-C(127)	65.7(12)
C(126)-C(125)-C(124)	36.0(14)
C(127)-C(125)-C(124)	29.7(13)
C(124)-C(127)-C(126)	31.2(17)
C(124)-C(127)-C(125)	78(2)
C(126)-C(127)-C(125)	47.0(12)
C(22)-C(21)-C(211)	124.0(5)
C(21)-C(22)-C(23)	124.8(5)
C(24)-C(23)-C(22)	117.8(5)
C(24)-C(23)-C(29)	128.1(6)
C(22)-C(23)-C(29)	114.1(5)
C(23)-C(24)-C(25)	132.7(6)
C(26)-C(25)-C(24)	127.4(6)
C(25)-C(26)-C(27)	127.3(6)
C(28)-C(27)-C(26)	130.2(6)
C(27)-C(28)-C(29)	132.0(5)
C(210)-C(29)-C(28)	117.0(5)
C(210)-C(29)-C(23)	120.7(5)
C(28)-C(29)-C(23)	122.2(5)
C(29)-C(210)-C(211)	126.5(5)
C(210)-C(211)-C(21)	109.9(4)
C(210)-C(211)-C(212)	108.2(4)
C(21)-C(211)-C(212)	109.4(4)
C(210)-C(211)-C(215)	113.1(4)
C(21)-C(211)-C(215)	108.7(4)
C(212)-C(211)-C(215)	107.5(4)
O(21)-C(212)-O(22)	123.1(5)
O(21)-C(212)-C(211)	125.2(5)
O(22)-C(212)-C(211)	111.7(5)
C(214)-C(213)-O(22)	111.1(5)
C(216)-C(215)-C(220)	117.3(5)
C(216)-C(215)-C(211)	123.3(5)
C(220)-C(215)-C(211)	119.4(5)
C(215)-C(216)-C(217)	122.8(5)
C(216)-C(217)-C(218)	119.6(5)
C(219)-C(218)-C(217)	118.0(5)
C(219)-C(218)-C(221)	119.3(6)
C(217)-C(218)-C(221)	122.6(6)
C(218)-C(219)-C(220)	121.0(6)
C(215)-C(220)-C(219)	121.3(6)
C(222)-C(221)-C(218)	126.9(7)
C(221)-C(222)-C(223)	123.2(8)
O(23*)-C(223)-O(23)	40.1(8)
O(23*)-C(223)-O(24)	118.0(10)
O(23)-C(223)-O(24)	122.3(9)
O(23*)-C(223)-O(24*)	104.7(12)
O(23)-C(223)-O(24*)	133.6(9)
O(24)-C(223)-O(24*)	34.7(7)
O(23*)-C(223)-C(222)	124.3(10)
O(23)-C(223)-C(222)	113.6(8)
O(24)-C(223)-C(222)	116.2(7)

O(24*)-C(223)-C(222)	112.2(7)
C(226)-C(224)-C(225)	61.8(17)
C(226)-C(224)-O(24)	67.9(4)
C(225)-C(224)-O(24)	105.0(15)
C(226)-C(224)-O(24*)	49.7(5)
C(225)-C(224)-O(24*)	81.6(13)
O(24)-C(224)-O(24*)	24.0(5)
C(226)-C(224)-C(227)	48.2(14)
C(225)-C(224)-C(227)	14.6(15)
O(24)-C(224)-C(227)	92.8(11)
O(24*)-C(224)-C(227)	68.9(10)
C(224)-C(226)-C(225)	79.6(15)
C(224)-C(226)-C(227)	102(2)
C(225)-C(226)-C(227)	23.7(18)
C(224)-C(226)-O(24*)	100.2(9)
C(225)-C(226)-O(24*)	105.2(16)
C(227)-C(226)-O(24*)	94.8(15)
C(224)-C(226)-O(24)	74.5(5)
C(225)-C(226)-O(24)	117.2(16)
C(227)-C(226)-O(24)	117.8(16)
O(24*)-C(226)-O(24)	31.6(6)
C(227)-C(225)-C(226)	88(3)
C(227)-C(225)-C(224)	125(4)
C(226)-C(225)-C(224)	38.6(9)
C(225)-C(227)-C(226)	69(3)
C(225)-C(227)-C(224)	41(3)
C(226)-C(227)-C(224)	29.4(9)
C(32)-C(31)-C(311)	125.8(5)
C(31)-C(32)-C(33)	117.2(5)
C(31)-C(32)-C(38)	120.4(5)
C(33)-C(32)-C(38)	122.3(5)
C(34)-C(33)-C(32)	132.6(5)
C(33)-C(34)-C(35)	129.9(6)
C(36)-C(35)-C(34)	126.5(6)
C(35)-C(36)-C(37)	128.5(6)
C(38)-C(37)-C(36)	133.1(6)
C(37)-C(38)-C(39)	118.3(5)
C(37)-C(38)-C(32)	127.0(6)
C(39)-C(38)-C(32)	114.7(5)
C(310)-C(39)-C(38)	125.4(5)
C(39)-C(310)-C(311)	123.7(5)
C(31)-C(311)-C(310)	109.8(5)
C(31)-C(311)-C(315)	113.4(4)
C(310)-C(311)-C(315)	109.8(4)
C(31)-C(311)-C(312)	107.1(4)
C(310)-C(311)-C(312)	108.5(4)
C(315)-C(311)-C(312)	108.1(4)
O(31)-C(312)-O(32)	125.0(5)
O(31)-C(312)-C(311)	125.5(5)
O(32)-C(312)-C(311)	109.4(4)
C(314)-C(313)-O(32)	110.6(5)
C(320)-C(315)-C(316)	116.7(5)
C(320)-C(315)-C(311)	124.0(5)
C(316)-C(315)-C(311)	119.3(5)
C(317)-C(316)-C(315)	120.1(5)
C(316)-C(317)-C(318)	123.0(6)

C(317)-C(318)-C(319)	117.6(6)
C(317)-C(318)-C(321)	118.5(6)
C(319)-C(318)-C(321)	123.8(6)
C(320)-C(319)-C(318)	119.8(5)
C(319)-C(320)-C(315)	122.9(5)
C(322)-C(321)-C(318)	127.1(8)
C(321)-C(322)-C(323)	126.6(9)
O(33*)-C(323)-O(33)	40.1(7)
O(33*)-C(323)-O(34)	117.5(9)
O(33)-C(323)-O(34)	121.8(9)
O(33*)-C(323)-O(34*)	105.8(11)
O(33)-C(323)-O(34*)	133.7(9)
O(34)-C(323)-O(34*)	32.8(7)
O(33*)-C(323)-C(322)	126.6(9)
O(33)-C(323)-C(322)	114.3(8)
O(34)-C(323)-C(322)	114.8(7)
O(34*)-C(323)-C(322)	111.9(7)
C(326)-C(324)-C(325)	55.1(17)
C(326)-C(324)-O(34)	68.6(4)
C(325)-C(324)-O(34)	102.0(15)
C(326)-C(324)-O(34*)	49.2(5)
C(325)-C(324)-O(34*)	80.6(14)
O(34)-C(324)-O(34*)	22.4(5)
C(326)-C(324)-C(327)	42.6(15)
C(325)-C(324)-C(327)	14.0(17)
O(34)-C(324)-C(327)	89.8(12)
O(34*)-C(324)-C(327)	67.8(11)
C(324)-C(326)-C(325)	87.5(17)
C(324)-C(326)-C(327)	112(2)
C(325)-C(326)-C(327)	26(2)
C(324)-C(326)-O(34*)	102.3(10)
C(325)-C(326)-O(34*)	110.0(18)
C(327)-C(326)-O(34*)	95.9(16)
C(324)-C(326)-O(34)	75.4(6)
C(325)-C(326)-O(34)	121.0(17)
C(327)-C(326)-O(34)	118.1(17)
O(34*)-C(326)-O(34)	29.9(6)
C(327)-C(325)-C(326)	96(4)
C(327)-C(325)-C(324)	131(4)
C(326)-C(325)-C(324)	37.4(11)
C(325)-C(327)-C(326)	58(3)
C(325)-C(327)-C(324)	35(3)
C(326)-C(327)-C(324)	25.3(10)
C(42)-C(41)-C(411)	125.6(5)
C(41)-C(42)-C(43)	117.0(5)
C(41)-C(42)-C(48)	120.0(5)
C(43)-C(42)-C(48)	123.0(5)
C(44)-C(43)-C(42)	131.6(5)
C(43)-C(44)-C(45)	130.8(6)
C(46)-C(45)-C(44)	126.0(6)
C(45)-C(46)-C(47)	130.0(6)
C(48)-C(47)-C(46)	130.9(6)
C(47)-C(48)-C(49)	117.5(5)
C(47)-C(48)-C(42)	127.7(5)
C(49)-C(48)-C(42)	114.8(5)
C(410)-C(49)-C(48)	126.1(5)

C(49)-C(410)-C(411)	123.8(5)
C(410)-C(411)-C(41)	109.5(5)
C(410)-C(411)-C(415)	111.2(4)
C(41)-C(411)-C(415)	112.7(4)
C(410)-C(411)-C(412)	108.7(5)
C(41)-C(411)-C(412)	105.8(4)
C(415)-C(411)-C(412)	108.7(4)
O(41)-C(412)-O(42)	122.7(5)
O(41)-C(412)-C(411)	125.7(6)
O(42)-C(412)-C(411)	111.5(5)
O(42)-C(413)-C(414)	110.3(5)
C(420)-C(415)-C(416)	116.4(5)
C(420)-C(415)-C(411)	124.6(5)
C(416)-C(415)-C(411)	118.9(5)
C(417)-C(416)-C(415)	120.3(6)
C(416)-C(417)-C(418)	123.0(6)
C(417)-C(418)-C(419)	117.0(6)
C(417)-C(418)-C(421)	120.0(6)
C(419)-C(418)-C(421)	122.9(6)
C(420)-C(419)-C(418)	120.5(5)
C(415)-C(420)-C(419)	122.9(6)
C(422)-C(421)-C(418)	129.4(8)
C(421)-C(422)-C(423)	127.7(9)
O(43)-C(423)-O(43*)	41.5(8)
O(43)-C(423)-O(44)	116.0(10)
O(43*)-C(423)-O(44)	119.9(9)
O(43)-C(423)-O(44*)	103.0(12)
O(43*)-C(423)-O(44*)	131.5(9)
O(44)-C(423)-O(44*)	33.7(7)
O(43)-C(423)-C(422)	126.7(10)
O(43*)-C(423)-C(422)	116.6(8)
O(44)-C(423)-C(422)	115.4(7)
O(44*)-C(423)-C(422)	111.6(7)
C(426)-C(424)-C(425)	50.2(17)
C(426)-C(424)-O(44)	67.9(4)
C(425)-C(424)-O(44)	104.7(16)
C(424)-C(426)-C(425)	90.3(18)
C(424)-C(426)-C(427)	111(2)
C(425)-C(426)-C(427)	25.6(19)
C(424)-C(426)-O(44*)	102.5(10)
C(425)-C(426)-O(44*)	121(2)
C(427)-C(426)-O(44*)	100.1(14)
C(424)-C(426)-O(44)	74.4(6)
C(425)-C(426)-O(44)	132(2)
C(427)-C(426)-O(44)	121.6(15)
O(44*)-C(426)-O(44)	30.7(6)
C(427)-C(425)-C(426)	103(4)
C(427)-C(425)-C(424)	133(4)
C(426)-C(425)-C(424)	39.5(12)
C(425)-C(427)-C(426)	51(3)
C(112)-O(12)-C(113)	119.2(4)
O(13*)-O(13)-C(123)	67.4(4)
O(13)-O(13*)-C(123)	67.7(4)
O(14*)-O(14)-C(123)	74.5(4)
O(14*)-O(14)-C(124)	84.2(17)
C(123)-O(14)-C(124)	110.9(14)

O(14*)-O(14)-C(126)	54.4(13)
C(123)-O(14)-C(126)	94.5(10)
C(124)-O(14)-C(126)	30.4(11)
O(14)-O(14*)-C(123)	72.0(4)
O(14)-O(14*)-C(126)	100.4(18)
C(123)-O(14*)-C(126)	109.6(13)
O(14)-O(14*)-C(124)	67.9(14)
C(123)-O(14*)-C(124)	103.7(10)
C(126)-O(14*)-C(124)	33.1(10)
C(212)-O(22)-C(213)	119.4(4)
O(23*)-O(23)-C(223)	69.7(4)
O(23)-O(23*)-C(223)	70.2(4)
O(24*)-O(24)-C(223)	73.7(4)
O(24*)-O(24)-C(226)	74.2(4)
C(223)-O(24)-C(226)	99.2(8)
O(24*)-O(24)-C(224)	104.8(10)
C(223)-O(24)-C(224)	129.0(10)
C(226)-O(24)-C(224)	37.6(8)
O(24)-O(24*)-C(223)	71.5(4)
O(24)-O(24*)-C(226)	74.3(4)
C(223)-O(24*)-C(226)	98.5(8)
O(24)-O(24*)-C(224)	51.2(7)
C(223)-O(24*)-C(224)	104.2(9)
C(226)-O(24*)-C(224)	30.1(7)
C(312)-O(32)-C(313)	116.4(4)
O(33*)-O(33)-C(323)	69.7(4)
O(33)-O(33*)-C(323)	70.2(4)
O(34*)-O(34)-C(323)	74.9(4)
O(34*)-O(34)-C(326)	74.9(4)
C(323)-O(34)-C(326)	103.8(8)
O(34*)-O(34)-C(324)	107.3(10)
C(323)-O(34)-C(324)	127.5(11)
C(326)-O(34)-C(324)	36.0(10)
O(34)-O(34*)-C(323)	72.3(4)
O(34)-O(34*)-C(326)	75.2(4)
C(323)-O(34*)-C(326)	103.0(8)
O(34)-O(34*)-C(324)	50.3(8)
C(323)-O(34*)-C(324)	103.1(10)
C(326)-O(34*)-C(324)	28.6(8)
C(412)-O(42)-C(413)	117.5(4)
O(43*)-O(43)-C(423)	69.4(4)
O(43)-O(43*)-C(423)	69.1(4)
O(44*)-O(44)-C(423)	74.4(4)
O(44*)-O(44)-C(426)	74.6(4)
C(423)-O(44)-C(426)	107.6(9)
O(44*)-O(44)-C(424)	109.1(11)
C(423)-O(44)-C(424)	131.6(12)
C(426)-O(44)-C(424)	37.7(10)
O(44)-O(44*)-C(423)	71.9(4)
O(44)-O(44*)-C(426)	74.8(4)
C(423)-O(44*)-C(426)	106.7(9)

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 3o. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(11)	61(4)	53(4)	69(4)	-6(3)	4(3)	-15(3)
C(12)	65(4)	44(3)	66(4)	-2(3)	0(3)	-18(3)
C(13)	50(3)	41(3)	75(4)	2(3)	8(3)	2(3)
C(14)	55(3)	43(3)	75(5)	10(3)	14(3)	8(3)
C(15)	83(5)	70(5)	76(5)	33(4)	6(4)	-7(4)
C(16)	59(4)	78(5)	76(5)	26(4)	-1(3)	5(3)
C(17)	80(4)	66(4)	45(4)	1(3)	-10(3)	11(3)
C(18)	63(4)	51(4)	67(5)	-3(3)	-6(3)	-2(3)
C(19)	38(3)	35(3)	63(4)	-2(3)	4(3)	1(2)
C(110)	62(3)	45(3)	51(4)	-2(3)	-9(3)	-12(3)
C(111)	50(3)	46(3)	60(4)	2(3)	6(3)	7(3)
C(112)	47(4)	57(4)	58(4)	-5(3)	4(3)	-3(3)
C(113)	80(4)	50(4)	96(5)	-2(3)	-11(4)	19(3)
C(114)	161(8)	112(7)	100(7)	31(5)	-41(6)	16(6)
C(115)	51(4)	47(3)	54(4)	-1(3)	-2(3)	3(2)
C(116)	55(4)	43(3)	72(4)	7(3)	-3(3)	-2(3)
C(117)	46(3)	56(4)	92(5)	9(3)	0(3)	-7(3)
C(118)	59(4)	64(4)	90(5)	-3(4)	13(4)	-3(3)
C(119)	75(5)	100(5)	62(4)	-8(4)	9(4)	-1(4)
C(120)	59(4)	94(5)	61(4)	-10(3)	15(3)	-2(3)
C(121)	77(5)	105(6)	82(5)	5(4)	22(4)	9(4)
C(122)	102(6)	169(9)	92(6)	8(5)	38(5)	1(6)
C(123)	74(5)	185(9)	115(7)	33(6)	31(5)	-10(5)
C(21)	79(4)	54(4)	61(4)	15(3)	0(3)	13(3)
C(22)	61(3)	39(3)	78(5)	12(3)	3(3)	8(3)
C(23)	46(3)	40(3)	72(4)	0(3)	3(3)	-5(2)
C(24)	66(4)	50(4)	73(5)	-5(3)	11(3)	4(3)
C(25)	82(4)	60(4)	76(5)	-16(4)	9(4)	4(3)
C(26)	66(4)	80(5)	64(4)	-8(4)	-3(3)	-4(3)
C(27)	60(4)	72(4)	62(4)	4(3)	-11(3)	5(3)
C(28)	53(3)	58(4)	53(4)	5(3)	-1(3)	3(3)
C(29)	45(3)	39(3)	65(4)	4(3)	-5(3)	3(2)
C(210)	57(3)	45(3)	55(4)	2(3)	-10(3)	10(2)
C(211)	46(3)	49(3)	56(4)	-1(3)	1(3)	5(3)
C(212)	61(4)	56(4)	49(4)	10(3)	-6(3)	5(3)
C(213)	88(4)	53(4)	83(5)	-1(3)	-17(4)	-8(3)
C(214)	171(8)	97(6)	75(6)	-15(4)	-19(5)	-16(5)
C(215)	45(3)	45(3)	54(4)	9(3)	5(3)	1(2)
C(216)	68(4)	41(3)	71(4)	6(3)	-2(3)	-2(3)
C(217)	42(3)	56(4)	83(5)	-5(3)	8(3)	1(3)
C(218)	62(4)	60(4)	79(5)	4(3)	20(4)	-3(3)
C(219)	72(5)	103(5)	67(4)	23(4)	7(4)	3(4)
C(220)	74(4)	87(5)	57(4)	21(3)	4(3)	4(3)
C(221)	73(5)	104(6)	90(5)	9(4)	19(4)	11(4)
C(222)	95(6)	140(7)	93(6)	24(5)	22(5)	7(5)
C(223)	93(6)	167(9)	103(7)	-10(6)	39(5)	20(5)
C(31)	52(3)	41(3)	67(4)	-9(3)	5(3)	2(2)
C(32)	49(3)	33(3)	56(4)	1(3)	-2(3)	5(2)

C(33)	56(3)	55(4)	61(4)	3(3)	-4(3)	-3(3)
C(34)	74(4)	61(4)	63(4)	-3(3)	6(3)	1(3)
C(35)	54(4)	84(5)	61(4)	12(4)	-1(3)	-9(3)
C(36)	83(4)	57(4)	80(5)	27(4)	-5(4)	4(3)
C(37)	56(4)	57(4)	95(5)	9(4)	-17(4)	2(3)
C(38)	60(3)	45(3)	65(4)	7(3)	-7(3)	-5(3)
C(39)	66(4)	41(3)	77(5)	-12(3)	-11(3)	29(3)
C(310)	68(4)	60(4)	59(4)	-10(3)	-3(3)	17(3)
C(311)	47(3)	36(3)	59(4)	-8(3)	-1(3)	3(2)
C(312)	41(3)	64(4)	52(4)	6(3)	-4(3)	5(3)
C(313)	82(4)	51(4)	97(5)	13(3)	23(4)	-10(3)
C(314)	181(8)	100(6)	80(6)	34(4)	30(5)	-22(5)
C(315)	68(4)	34(3)	53(4)	-5(2)	3(3)	4(2)
C(316)	57(4)	80(5)	78(5)	-12(4)	-13(4)	6(3)
C(317)	76(5)	92(5)	53(4)	-2(3)	-9(4)	3(4)
C(318)	66(4)	66(4)	70(5)	-2(3)	-22(4)	0(3)
C(319)	45(3)	51(4)	86(5)	8(3)	-12(3)	1(3)
C(320)	48(3)	58(4)	59(4)	0(3)	5(3)	0(3)
C(321)	70(5)	81(5)	163(9)	-14(5)	2(5)	4(4)
C(322)	110(7)	133(8)	116(7)	8(5)	-19(6)	-1(6)
C(323)	104(6)	180(9)	86(6)	10(6)	-22(5)	32(6)
C(41)	51(3)	39(3)	63(4)	13(3)	1(3)	-6(2)
C(42)	49(3)	30(3)	61(4)	6(3)	-3(3)	-4(2)
C(43)	53(3)	45(3)	76(5)	4(3)	-2(3)	-4(2)
C(44)	64(4)	64(4)	46(4)	1(3)	17(3)	2(3)
C(45)	61(4)	86(5)	53(4)	-18(4)	0(3)	9(3)
C(46)	70(4)	63(5)	83(5)	-24(4)	-1(4)	3(3)
C(47)	48(3)	46(4)	87(5)	-10(3)	-5(3)	2(3)
C(48)	56(3)	42(3)	64(4)	8(3)	-3(3)	7(3)
C(49)	69(4)	53(4)	62(4)	9(3)	-8(3)	-22(3)
C(410)	63(4)	52(4)	68(4)	15(3)	0(3)	-13(3)
C(411)	48(3)	48(3)	59(4)	13(3)	-7(3)	-2(3)
C(412)	57(4)	73(5)	50(4)	3(3)	-7(3)	0(3)
C(413)	87(4)	56(4)	88(5)	0(3)	23(4)	14(3)
C(414)	169(8)	93(6)	110(7)	-25(5)	32(6)	11(5)
C(415)	50(3)	48(3)	58(4)	9(3)	4(3)	-2(2)
C(416)	57(4)	89(5)	94(5)	20(4)	-11(4)	1(3)
C(417)	74(5)	87(5)	60(4)	16(3)	-14(4)	0(3)
C(418)	77(5)	64(4)	64(5)	5(3)	-16(4)	4(3)
C(419)	45(3)	60(4)	94(5)	-7(3)	-12(4)	-2(3)
C(420)	53(4)	56(4)	59(4)	-1(3)	4(3)	0(3)
C(421)	70(5)	88(6)	133(7)	9(5)	-9(5)	-7(4)
C(422)	99(7)	133(8)	124(7)	9(5)	-33(6)	-9(5)
C(423)	83(6)	171(9)	101(7)	-12(6)	-17(5)	-26(5)
O(11)	47(3)	88(3)	121(4)	9(3)	-9(2)	-2(2)
O(12)	54(2)	50(3)	91(3)	9(2)	-9(2)	3(2)
O(21)	52(3)	92(3)	110(4)	-3(3)	-5(2)	0(2)
O(22)	58(2)	46(2)	80(3)	-4(2)	-13(2)	3(2)
O(31)	47(3)	90(3)	120(4)	16(3)	2(2)	3(2)
O(32)	60(2)	49(2)	82(3)	9(2)	12(2)	-2(2)
O(41)	51(3)	99(4)	107(4)	-10(3)	5(2)	-9(2)
O(42)	53(2)	52(3)	82(3)	-3(2)	13(2)	-1(2)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 3o.

H(11)	-1277	8223	6474	73
H(12)	-1686	7326	6904	70
H(14)	-1416	7038	7396	69
H(15)	-717	7233	7879	91
H(16)	609	8592	8101	86
H(17)	1783	10125	7877	76
H(18)	1866	10620	7414	73
H(110)	1473	10641	6926	63
H(11A)	-220	13269	6381	91
H(11B)	-1880	12646	6427	91
H(11C)	-11	12597	5906	186
H(11D)	-1757	13098	5936	186
H(11E)	-1470	11753	5951	186
H(116)	3451	9579	6647	68
H(117)	5388	9303	6280	77
H(119)	1993	8831	5662	95
H(120)	36	9127	6029	86
H(121)	4729	8549	5511	106
H(122)	6929	9493	5866	145
H(21)	6248	3209	3528	78
H(22)	6682	2313	3097	71
H(24)	6387	2054	2603	76
H(25)	5753	2230	2116	87
H(26)	4362	3595	1902	84
H(27)	3227	5139	2123	78
H(28)	3184	5639	2584	66
H(210)	3504	5626	3077	63
H(21A)	6867	7664	3571	90
H(21B)	5196	8265	3622	90
H(21C)	5033	7533	4095	171
H(21D)	6716	8132	4063	171
H(21E)	6576	6777	4044	171
H(216)	1558	4562	3355	72
H(217)	-404	4337	3719	72
H(219)	3038	3796	4335	97
H(220)	4973	4132	3967	87
H(221)	264	3573	4498	107
H(222)	-1917	4513	4134	131
H(31)	3555	10650	1924	64
H(33)	3178	10631	2419	69
H(34)	3225	10141	2877	79
H(35)	4378	8587	3100	79
H(36)	5742	7234	2883	88
H(37)	6374	7053	2399	83
H(39)	6624	7300	1902	74
H(310)	6312	8218	1478	75
H(31A)	5255	13279	1387	92
H(31B)	6906	12639	1430	92
H(31C)	6568	11792	953	180
H(31D)	6696	13148	935	180
H(31E)	5014	12543	910	180

H(316)	4974	9118	1024	86
H(317)	3046	8806	671	89
H(319)	-399	9324	1282	73
H(320)	1528	9595	1643	66
H(321)	315	8592	496	125
H(322)	-1904	9530	852	143
H(41)	8525	4355	1926	61
H(43)	8148	4386	2420	70
H(44)	8271	4864	2879	69
H(45)	9356	6417	3096	80
H(46)	10722	7767	2876	87
H(47)	11378	7965	2397	73
H(49)	11657	7684	1907	74
H(410)	11328	6785	1481	73
H(41A)	10272	1730	1389	92
H(41B)	11911	2388	1429	92
H(41C)	9997	2473	909	186
H(41D)	11671	1855	932	186
H(41E)	11565	3212	949	186
H(416)	9963	5901	1021	96
H(417)	8036	6153	665	89
H(419)	4619	5707	1285	79
H(420)	6543	5372	1641	67
H(421)	5279	6441	503	116
H(422)	3088	5469	851	142

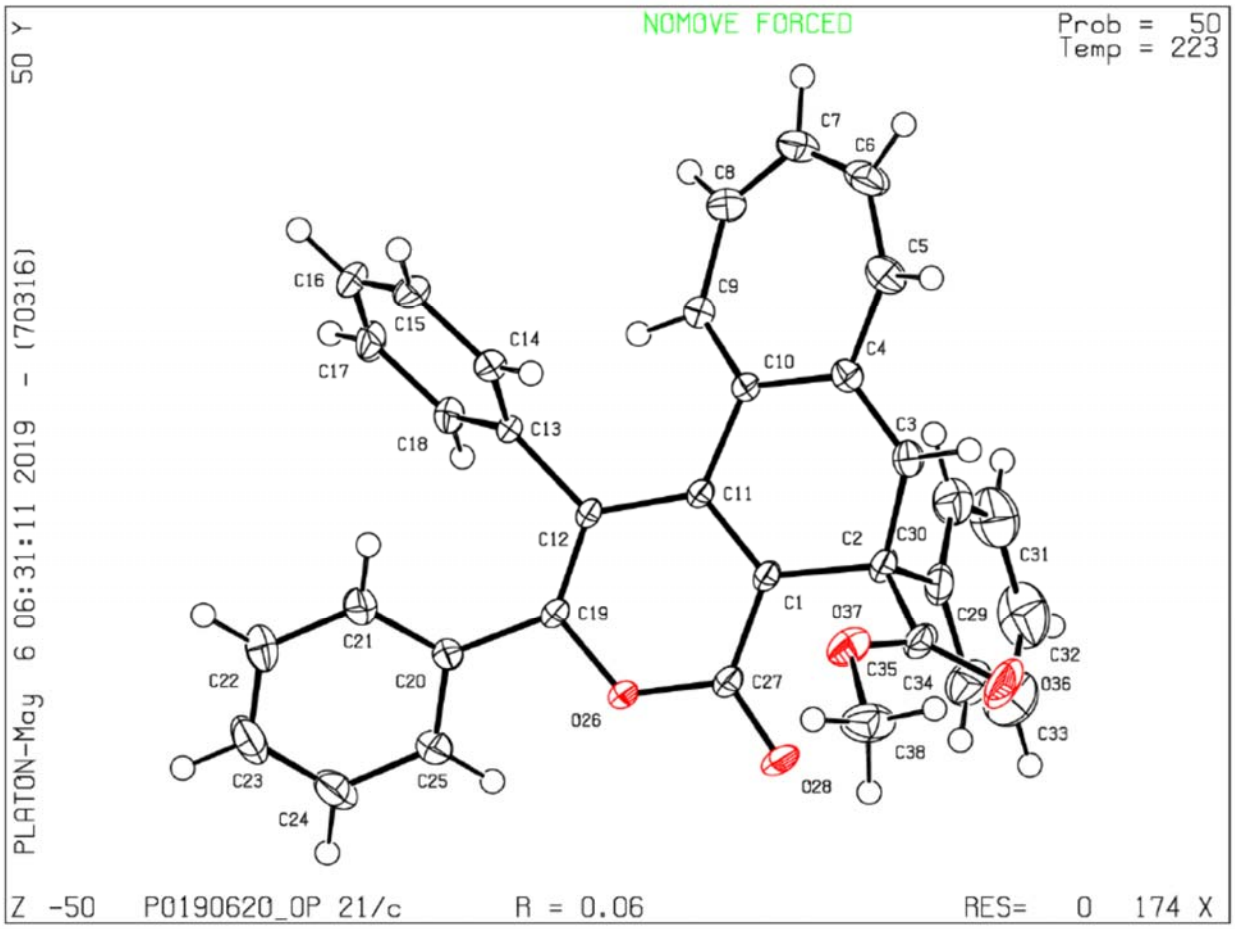


Table S7. Crystal data and structure refinement for 3y.

Empirical formula	$C_{34}H_{24}O_4$	
Formula weight	496.53	
Temperature	223(2) K	
Wavelength	0.730 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 6.0670(12) Å	α = 90°
	b = 22.895(5) Å	β = 90.85(3)°
	c = 17.994(4) Å	γ = 90°
Volume	2499.2(9) $Å^3$	
Z	4	
Density (calculated)	1.320 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	

F(000)	1040
Crystal size	0.102 x 0.052 x 0.048 mm^3
Theta range for data collection	1.478 to 29.998°.
Index ranges	–8<=h<=8, –31<=k<=31, –24<=l<=24
Reflections collected	23501
Independent reflections	6717 [R(int) = 0.0799]
Completeness to theta = 25.976°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.925
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6717 / 0 / 344
Goodness-of-fit on F^2	1.132
Final R indices [I>2sigma(I)]	R1 = 0.0614, wR2 = 0.1770
R indices (all data)	R1 = 0.0708, wR2 = 0.1842
Largest diff. peak and hole	0.568 and –0.308 e·$Å^{-3}$

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 3y. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6541(2)	7092(1)	2858(1)	17(1)
C(2)	7926(2)	7584(1)	3184(1)	20(1)
C(3)	9951(2)	7334(1)	3561(1)	24(1)
C(4)	10040(2)	6791(1)	3842(1)	20(1)
C(5)	12043(2)	6625(1)	4259(1)	27(1)
C(6)	12330(2)	6237(1)	4812(1)	31(1)
C(7)	10753(3)	5846(1)	5127(1)	33(1)
C(8)	8707(3)	5731(1)	4869(1)	30(1)
C(9)	7611(2)	5950(1)	4209(1)	22(1)
C(10)	8153(2)	6387(1)	3737(1)	17(1)
C(11)	6650(2)	6525(1)	3100(1)	16(1)
C(12)	5260(2)	6086(1)	2735(1)	16(1)
C(13)	5361(2)	5450(1)	2917(1)	17(1)
C(14)	7252(2)	5128(1)	2761(1)	22(1)
C(15)	7292(3)	4528(1)	2889(1)	32(1)

C(16)	5461(3)	4250(1)	3175(1)	36(1)
C(17)	3589(3)	4567(1)	3334(1)	31(1)
C(18)	3534(2)	5165(1)	3211(1)	23(1)
C(19)	3855(2)	6258(1)	2181(1)	18(1)
C(20)	2284(2)	5908(1)	1724(1)	19(1)
C(21)	2721(3)	5337(1)	1494(1)	27(1)
C(22)	1174(3)	5031(1)	1072(1)	36(1)
C(23)	-805(3)	5292(1)	867(1)	37(1)
C(24)	-1234(3)	5860(1)	1077(1)	32(1)
C(25)	286(2)	6168(1)	1507(1)	25(1)
O(26)	3711(2)	6832(1)	1968(1)	23(1)
C(27)	4984(2)	7262(1)	2279(1)	21(1)
O(28)	4714(2)	7753(1)	2040(1)	33(1)
C(29)	6520(2)	7936(1)	3743(1)	25(1)
C(30)	6419(3)	7753(1)	4478(1)	36(1)
C(31)	5030(4)	8028(1)	4977(1)	50(1)
C(32)	3745(4)	8492(1)	4751(1)	56(1)
C(33)	3827(4)	8676(1)	4025(1)	54(1)
C(34)	5201(3)	8404(1)	3521(1)	39(1)
C(35)	8810(2)	7969(1)	2551(1)	24(1)
O(36)	9128(2)	8486(1)	2590(1)	39(1)
O(37)	9332(2)	7636(1)	1970(1)	29(1)
C(38)	9977(3)	7942(1)	1308(1)	38(1)

Table S9. Bond lengths [Å] and angles [°] for 3y.

C(1)-C(11)	1.3694(16)
C(1)-C(27)	1.4490(17)
C(1)-C(2)	1.5192(17)
C(2)-C(3)	1.5077(19)
C(2)-C(35)	1.5427(19)
C(2)-C(29)	1.553(2)
C(3)-C(4)	1.3428(18)
C(3)-H(3)	0.9400

C(4)-C(5)	1.4688(18)
C(4)-C(10)	1.4821(17)
C(5)-C(6)	1.344(2)
C(5)-H(5)	0.9400
C(6)-C(7)	1.433(2)
C(6)-H(6)	0.9400
C(7)-C(8)	1.345(2)
C(7)-H(7)	0.9400
C(8)-C(9)	1.4423(19)
C(8)-H(8)	0.9400
C(9)-C(10)	1.3553(18)
C(9)-H(9)	0.9400
C(10)-C(11)	1.4883(16)
C(11)-C(12)	1.4625(16)
C(12)-C(19)	1.3611(17)
C(12)-C(13)	1.4916(16)
C(13)-C(14)	1.3961(19)
C(13)-C(18)	1.3969(19)
C(14)-C(15)	1.3927(19)
C(14)-H(14)	0.9400
C(15)-C(16)	1.386(3)
C(15)-H(15)	0.9400
C(16)-C(17)	1.381(3)
C(16)-H(16)	0.9400
C(17)-C(18)	1.3877(19)
C(17)-H(17)	0.9400
C(18)-H(18)	0.9400
C(19)-O(26)	1.3698(14)
C(19)-C(20)	1.4836(17)
C(20)-C(21)	1.3985(19)
C(20)-C(25)	1.4007(19)
C(21)-C(22)	1.388(2)
C(21)-H(21)	0.9400
C(22)-C(23)	1.385(3)
C(22)-H(22)	0.9400
C(23)-C(24)	1.381(2)

C(23)-H(23)	0.9400
C(24)-C(25)	1.3881(19)
C(24)-H(24)	0.9400
C(25)-H(25)	0.9400
O(26)-C(27)	1.3677(15)
C(27)-O(28)	1.2122(15)
C(29)-C(30)	1.390(2)
C(29)-C(34)	1.393(2)
C(30)-C(31)	1.391(3)
C(30)-H(30)	0.9400
C(31)-C(32)	1.376(3)
C(31)-H(31)	0.9400
C(32)-C(33)	1.375(3)
C(32)-H(32)	0.9400
C(33)-C(34)	1.389(3)
C(33)-H(33)	0.9400
C(34)-H(34)	0.9400
C(35)-O(36)	1.2000(17)
C(35)-O(37)	1.3372(19)
O(37)-C(38)	1.4409(18)
C(38)-H(38A)	0.9700
C(38)-H(38B)	0.9700
C(38)-H(38C)	0.9700

C(11)-C(1)-C(27)	120.83(11)
C(11)-C(1)-C(2)	123.77(11)
C(27)-C(1)-C(2)	115.35(10)
C(3)-C(2)-C(1)	109.56(10)
C(3)-C(2)-C(35)	105.05(11)
C(1)-C(2)-C(35)	109.60(11)
C(3)-C(2)-C(29)	110.92(11)
C(1)-C(2)-C(29)	109.19(10)
C(35)-C(2)-C(29)	112.44(11)
C(4)-C(3)-C(2)	123.28(12)
C(4)-C(3)-H(3)	118.4
C(2)-C(3)-H(3)	118.4

C(3)-C(4)-C(5)	117.35(12)
C(3)-C(4)-C(10)	120.25(11)
C(5)-C(4)-C(10)	122.38(12)
C(6)-C(5)-C(4)	130.28(14)
C(6)-C(5)-H(5)	114.9
C(4)-C(5)-H(5)	114.9
C(5)-C(6)-C(7)	128.73(14)
C(5)-C(6)-H(6)	115.6
C(7)-C(6)-H(6)	115.6
C(8)-C(7)-C(6)	127.19(14)
C(8)-C(7)-H(7)	116.4
C(6)-C(7)-H(7)	116.4
C(7)-C(8)-C(9)	128.90(15)
C(7)-C(8)-H(8)	115.6
C(9)-C(8)-H(8)	115.6
C(10)-C(9)-C(8)	131.25(13)
C(10)-C(9)-H(9)	114.4
C(8)-C(9)-H(9)	114.4
C(9)-C(10)-C(4)	125.08(11)
C(9)-C(10)-C(11)	119.24(11)
C(4)-C(10)-C(11)	115.35(10)
C(1)-C(11)-C(12)	118.93(11)
C(1)-C(11)-C(10)	118.24(11)
C(12)-C(11)-C(10)	122.81(10)
C(19)-C(12)-C(11)	118.69(11)
C(19)-C(12)-C(13)	117.88(10)
C(11)-C(12)-C(13)	123.39(10)
C(14)-C(13)-C(18)	119.21(12)
C(14)-C(13)-C(12)	120.16(11)
C(18)-C(13)-C(12)	120.56(11)
C(15)-C(14)-C(13)	120.02(14)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(16)-C(15)-C(14)	120.16(15)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9

C(17)-C(16)-C(15)	120.08(13)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	120.23(14)
C(16)-C(17)-H(17)	119.9
C(18)-C(17)-H(17)	119.9
C(17)-C(18)-C(13)	120.29(14)
C(17)-C(18)-H(18)	119.9
C(13)-C(18)-H(18)	119.9
C(12)-C(19)-O(26)	121.30(11)
C(12)-C(19)-C(20)	129.72(11)
O(26)-C(19)-C(20)	108.98(10)
C(21)-C(20)-C(25)	118.80(12)
C(21)-C(20)-C(19)	123.11(12)
C(25)-C(20)-C(19)	118.08(12)
C(22)-C(21)-C(20)	120.28(14)
C(22)-C(21)-H(21)	119.9
C(20)-C(21)-H(21)	119.9
C(23)-C(22)-C(21)	120.31(15)
C(23)-C(22)-H(22)	119.8
C(21)-C(22)-H(22)	119.8
C(24)-C(23)-C(22)	119.94(14)
C(24)-C(23)-H(23)	120.0
C(22)-C(23)-H(23)	120.0
C(23)-C(24)-C(25)	120.33(14)
C(23)-C(24)-H(24)	119.8
C(25)-C(24)-H(24)	119.8
C(24)-C(25)-C(20)	120.31(14)
C(24)-C(25)-H(25)	119.8
C(20)-C(25)-H(25)	119.8
C(27)-O(26)-C(19)	122.94(10)
O(28)-C(27)-O(26)	116.75(12)
O(28)-C(27)-C(1)	126.03(12)
O(26)-C(27)-C(1)	117.21(10)
C(30)-C(29)-C(34)	118.08(15)
C(30)-C(29)-C(2)	119.54(13)

C(34)-C(29)-C(2)	122.16(13)
C(29)-C(30)-C(31)	120.98(17)
C(29)-C(30)-H(30)	119.5
C(31)-C(30)-H(30)	119.5
C(32)-C(31)-C(30)	120.25(19)
C(32)-C(31)-H(31)	119.9
C(30)-C(31)-H(31)	119.9
C(33)-C(32)-C(31)	119.38(18)
C(33)-C(32)-H(32)	120.3
C(31)-C(32)-H(32)	120.3
C(32)-C(33)-C(34)	120.84(19)
C(32)-C(33)-H(33)	119.6
C(34)-C(33)-H(33)	119.6
C(33)-C(34)-C(29)	120.45(18)
C(33)-C(34)-H(34)	119.8
C(29)-C(34)-H(34)	119.8
O(36)-C(35)-O(37)	124.63(14)
O(36)-C(35)-C(2)	125.31(14)
O(37)-C(35)-C(2)	109.88(11)
C(35)-O(37)-C(38)	116.01(12)
O(37)-C(38)-H(38A)	109.5
O(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
O(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2$ x 10^3) for 3y. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(1)	10(1)	22(1)	1(1)	-2(1)	-2(1)
C(2)	22(1)	11(1)	28(1)	0(1)	-3(1)	-2(1)

C(3)	20(1)	20(1)	31(1)	2(1)	-6(1)	-7(1)
C(4)	18(1)	19(1)	22(1)	-1(1)	-3(1)	-1(1)
C(5)	18(1)	34(1)	30(1)	0(1)	-5(1)	0(1)
C(6)	25(1)	38(1)	29(1)	-2(1)	-10(1)	9(1)
C(7)	44(1)	29(1)	25(1)	3(1)	-14(1)	6(1)
C(8)	42(1)	24(1)	24(1)	7(1)	-9(1)	-3(1)
C(9)	26(1)	16(1)	22(1)	0(1)	-6(1)	-1(1)
C(10)	18(1)	13(1)	21(1)	-1(1)	-5(1)	2(1)
C(11)	16(1)	11(1)	20(1)	1(1)	-2(1)	-1(1)
C(12)	18(1)	9(1)	21(1)	0(1)	-2(1)	-1(1)
C(13)	22(1)	10(1)	19(1)	1(1)	-7(1)	-1(1)
C(14)	25(1)	17(1)	24(1)	-1(1)	-7(1)	3(1)
C(15)	42(1)	17(1)	35(1)	-4(1)	-15(1)	11(1)
C(16)	59(1)	12(1)	37(1)	2(1)	-20(1)	-4(1)
C(17)	44(1)	19(1)	29(1)	6(1)	-9(1)	-15(1)
C(18)	26(1)	18(1)	25(1)	1(1)	-5(1)	-6(1)
C(19)	20(1)	11(1)	23(1)	2(1)	-4(1)	0(1)
C(20)	22(1)	17(1)	19(1)	2(1)	-4(1)	-3(1)
C(21)	32(1)	22(1)	26(1)	-6(1)	-8(1)	2(1)
C(22)	48(1)	28(1)	32(1)	-10(1)	-11(1)	-5(1)
C(23)	39(1)	43(1)	28(1)	-6(1)	-11(1)	-14(1)
C(24)	26(1)	42(1)	28(1)	3(1)	-10(1)	-4(1)
C(25)	24(1)	24(1)	26(1)	2(1)	-6(1)	-1(1)
O(26)	26(1)	12(1)	30(1)	5(1)	-12(1)	-2(1)
C(27)	22(1)	13(1)	28(1)	3(1)	-5(1)	-2(1)
O(28)	36(1)	14(1)	48(1)	11(1)	-16(1)	-2(1)
C(29)	26(1)	17(1)	32(1)	-6(1)	-3(1)	-4(1)
C(30)	43(1)	32(1)	33(1)	-5(1)	-3(1)	-2(1)
C(31)	59(1)	56(1)	34(1)	-15(1)	5(1)	-2(1)
C(32)	53(1)	59(1)	56(1)	-29(1)	7(1)	7(1)
C(33)	57(1)	43(1)	63(1)	-16(1)	3(1)	20(1)
C(34)	45(1)	28(1)	44(1)	-4(1)	0(1)	10(1)
C(35)	23(1)	15(1)	36(1)	6(1)	-4(1)	-5(1)
O(36)	45(1)	16(1)	56(1)	7(1)	2(1)	-11(1)
O(37)	33(1)	22(1)	33(1)	8(1)	4(1)	-1(1)
C(38)	36(1)	43(1)	35(1)	18(1)	0(1)	-1(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 3y.

	x	y	z	U(eq)
H(3)	11215	7570	3602	29
H(5)	13329	6822	4117	33
H(6)	13759	6219	5021	37
H(7)	11196	5649	5562	40
H(8)	7878	5472	5158	36
H(9)	6289	5757	4085	26
H(14)	8498	5316	2569	27
H(15)	8564	4312	2782	38
H(16)	5493	3845	3260	43
H(17)	2349	4377	3526	37
H(18)	2262	5379	3326	28
H(21)	4068	5159	1625	32
H(22)	1470	4645	924	43
H(23)	-1853	5082	585	44
H(24)	-2563	6039	928	39
H(25)	-27	6553	1654	30
H(30)	7302	7439	4641	43
H(31)	4970	7896	5471	60
H(32)	2820	8681	5090	67
H(33)	2942	8991	3867	65
H(34)	5240	8536	3026	47
H(38A)	10361	7662	927	57
H(38B)	11241	8188	1421	57
H(38C)	8762	8183	1131	57

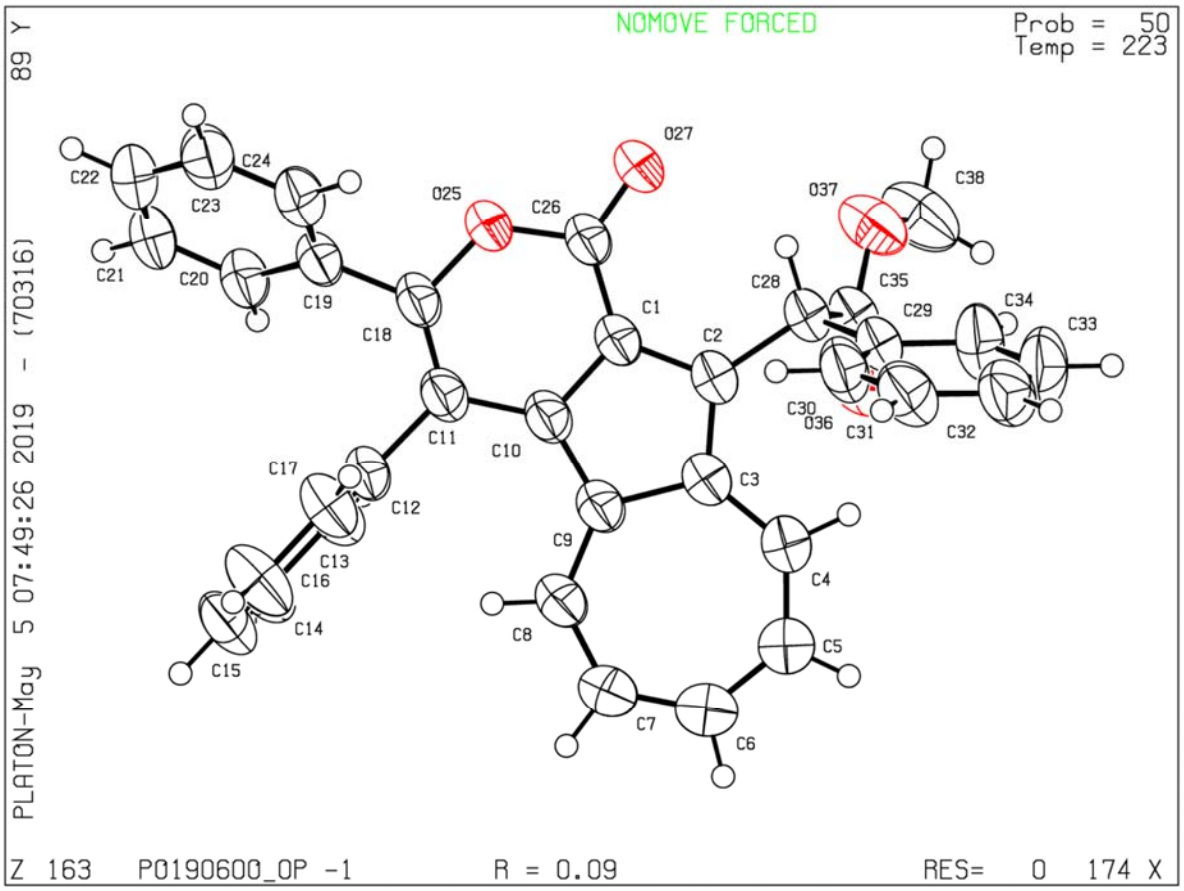


Table S12. Crystal data and structure refinement for 4g

Empirical formula	$C_{34}H_{24}O_4$	
Formula weight	496.53	
Temperature	223(2) K	
Wavelength	0.730 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 9.3460(19) Å	α = 95.94(3)°
	b = 10.173(2) Å	β = 102.85(3)°
	c = 14.036(3) Å	γ = 94.02(3)°
Volume	1288.1(5) $Å^3$	
Z	2	
Density (calculated)	1.280 Mg/m^3	
Absorption coefficient	0.087 mm^{-1}	

F(000)	520
Crystal size	0.082 x 0.032 x 0.017 mm^3
Theta range for data collection	1.540 to 29.999°.
Index ranges	–12<=h<=12, –13<=k<=13, –19<=l<=19
Reflections collected	13532
Independent reflections	6851 [R(int) = 0.0292]
Completeness to theta = 25.976°	99.8 %
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.917
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6851 / 0 / 344
Goodness-of-fit on F^2	1.107
Final R indices [I>2sigma(I)]	R1 = 0.0863, wR2 = 0.2796
R indices (all data)	R1 = 0.1267, wR2 = 0.3119
Largest diff. peak and hole	0.337 and –0.368 e·$Å^{-3}$

Table S13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 4g. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6713(3)	4473(2)	3192(2)	53(1)
C(2)	6269(3)	3392(3)	2447(2)	56(1)
C(3)	6263(3)	2241(3)	2912(2)	57(1)
C(4)	5957(3)	950(3)	2427(2)	67(1)
C(5)	5918(4)	-243(3)	2816(2)	73(1)
C(6)	6147(3)	-463(3)	3801(2)	72(1)
C(7)	6558(3)	416(3)	4638(2)	68(1)
C(8)	6819(3)	1787(3)	4722(2)	61(1)
C(9)	6699(3)	2630(3)	3996(2)	54(1)
C(10)	6974(3)	4034(2)	4132(2)	53(1)
C(11)	7442(3)	4984(3)	5007(2)	54(1)
C(12)	7773(3)	4567(3)	6017(2)	56(1)
C(13)	6648(3)	4272(3)	6486(2)	66(1)
C(14)	6965(4)	3862(3)	7422(2)	75(1)

C(15)	8394(4)	3745(4)	7885(2)	80(1)
C(16)	9525(4)	4033(4)	7425(2)	89(1)
C(17)	9205(3)	4446(3)	6493(2)	70(1)
C(18)	7678(3)	6270(3)	4880(2)	55(1)
C(19)	8183(3)	7412(3)	5638(2)	57(1)
C(20)	7481(3)	7683(3)	6409(2)	63(1)
C(21)	7959(4)	8777(3)	7098(2)	74(1)
C(22)	9139(4)	9615(3)	7027(2)	79(1)
C(23)	9843(4)	9362(3)	6268(2)	77(1)
C(24)	9362(3)	8277(3)	5570(2)	67(1)
O(25)	7459(2)	6678(2)	3945(1)	59(1)
C(26)	6938(3)	5855(2)	3082(2)	54(1)
O(27)	6734(2)	6378(2)	2329(1)	66(1)
C(28)	5895(3)	3506(3)	1349(2)	60(1)
C(29)	6827(3)	2685(3)	788(2)	61(1)
C(30)	8284(4)	2611(3)	1199(2)	73(1)
C(31)	9182(4)	1903(4)	699(2)	79(1)
C(32)	8596(4)	1251(4)	-221(2)	83(1)
C(33)	7142(5)	1321(4)	-646(2)	97(1)
C(34)	6249(4)	2039(4)	-148(2)	85(1)
C(35)	4251(3)	3202(3)	926(2)	65(1)
O(36)	3514(3)	2247(3)	1042(2)	97(1)
O(37)	3684(2)	4133(2)	411(2)	83(1)
C(38)	2129(4)	3917(5)	-49(3)	101(1)

Table S14. Bond lengths [Å] and angles [°] for 4g.

C(1)-C(2)	1.407(3)
C(1)-C(10)	1.411(3)
C(1)-C(26)	1.436(3)
C(2)-C(3)	1.398(4)
C(2)-C(28)	1.521(3)
C(3)-C(4)	1.395(4)
C(3)-C(9)	1.488(3)

C(4)-C(5)	1.383(4)
C(4)-H(4)	0.9400
C(5)-C(6)	1.396(4)
C(5)-H(5)	0.9400
C(6)-C(7)	1.364(4)
C(6)-H(6)	0.9400
C(7)-C(8)	1.388(4)
C(7)-H(7)	0.9400
C(8)-C(9)	1.389(3)
C(8)-H(8)	0.9400
C(9)-C(10)	1.419(4)
C(10)-C(11)	1.446(3)
C(11)-C(18)	1.348(4)
C(11)-C(12)	1.495(3)
C(12)-C(17)	1.376(4)
C(12)-C(13)	1.391(4)
C(13)-C(14)	1.395(4)
C(13)-H(13)	0.9400
C(14)-C(15)	1.368(4)
C(14)-H(14)	0.9400
C(15)-C(16)	1.386(5)
C(15)-H(15)	0.9400
C(16)-C(17)	1.391(4)
C(16)-H(16)	0.9400
C(17)-H(17)	0.9400
C(18)-O(25)	1.394(3)
C(18)-C(19)	1.465(3)
C(19)-C(24)	1.387(4)
C(19)-C(20)	1.400(3)
C(20)-C(21)	1.374(4)
C(20)-H(20)	0.9400
C(21)-C(22)	1.373(5)
C(21)-H(21)	0.9400
C(22)-C(23)	1.383(5)
C(22)-H(22)	0.9400
C(23)-C(24)	1.376(4)

C(23)-H(23)	0.9400
C(24)-H(24)	0.9400
O(25)-C(26)	1.370(3)
C(26)-O(27)	1.215(3)
C(28)-C(35)	1.516(4)
C(28)-C(29)	1.532(4)
C(28)-H(28)	0.9900
C(29)-C(30)	1.367(4)
C(29)-C(34)	1.380(4)
C(30)-C(31)	1.400(4)
C(30)-H(30)	0.9400
C(31)-C(32)	1.365(4)
C(31)-H(31)	0.9400
C(32)-C(33)	1.368(5)
C(32)-H(32)	0.9400
C(33)-C(34)	1.399(5)
C(33)-H(33)	0.9400
C(34)-H(34)	0.9400
C(35)-O(36)	1.198(4)
C(35)-O(37)	1.319(3)
O(37)-C(38)	1.444(4)
C(38)-H(38A)	0.9700
C(38)-H(38B)	0.9700
C(38)-H(38C)	0.9700

C(2)-C(1)-C(10)	110.7(2)
C(2)-C(1)-C(26)	128.0(2)
C(10)-C(1)-C(26)	121.2(2)
C(3)-C(2)-C(1)	107.1(2)
C(3)-C(2)-C(28)	128.1(2)
C(1)-C(2)-C(28)	124.8(2)
C(4)-C(3)-C(2)	124.9(2)
C(4)-C(3)-C(9)	126.5(2)
C(2)-C(3)-C(9)	108.5(2)
C(5)-C(4)-C(3)	129.3(3)
C(5)-C(4)-H(4)	115.3

C(3)-C(4)-H(4)	115.3
C(4)-C(5)-C(6)	128.8(3)
C(4)-C(5)-H(5)	115.6
C(6)-C(5)-H(5)	115.6
C(7)-C(6)-C(5)	130.0(3)
C(7)-C(6)-H(6)	115.0
C(5)-C(6)-H(6)	115.0
C(6)-C(7)-C(8)	128.3(3)
C(6)-C(7)-H(7)	115.8
C(8)-C(7)-H(7)	115.8
C(7)-C(8)-C(9)	130.0(3)
C(7)-C(8)-H(8)	115.0
C(9)-C(8)-H(8)	115.0
C(8)-C(9)-C(10)	127.3(2)
C(8)-C(9)-C(3)	126.9(2)
C(10)-C(9)-C(3)	105.8(2)
C(1)-C(10)-C(9)	107.8(2)
C(1)-C(10)-C(11)	120.1(2)
C(9)-C(10)-C(11)	132.1(2)
C(18)-C(11)-C(10)	117.4(2)
C(18)-C(11)-C(12)	120.3(2)
C(10)-C(11)-C(12)	122.2(2)
C(17)-C(12)-C(13)	118.8(2)
C(17)-C(12)-C(11)	120.2(2)
C(13)-C(12)-C(11)	120.9(2)
C(12)-C(13)-C(14)	120.6(3)
C(12)-C(13)-H(13)	119.7
C(14)-C(13)-H(13)	119.7
C(15)-C(14)-C(13)	119.9(3)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(14)-C(15)-C(16)	120.1(3)
C(14)-C(15)-H(15)	120.0
C(16)-C(15)-H(15)	120.0
C(15)-C(16)-C(17)	119.8(3)
C(15)-C(16)-H(16)	120.1

C(17)-C(16)-H(16)	120.1
C(12)-C(17)-C(16)	120.8(3)
C(12)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(11)-C(18)-O(25)	121.6(2)
C(11)-C(18)-C(19)	128.1(2)
O(25)-C(18)-C(19)	110.3(2)
C(24)-C(19)-C(20)	118.9(2)
C(24)-C(19)-C(18)	119.0(2)
C(20)-C(19)-C(18)	122.0(3)
C(21)-C(20)-C(19)	120.7(3)
C(21)-C(20)-H(20)	119.6
C(19)-C(20)-H(20)	119.6
C(22)-C(21)-C(20)	119.6(3)
C(22)-C(21)-H(21)	120.2
C(20)-C(21)-H(21)	120.2
C(21)-C(22)-C(23)	120.4(3)
C(21)-C(22)-H(22)	119.8
C(23)-C(22)-H(22)	119.8
C(24)-C(23)-C(22)	120.4(3)
C(24)-C(23)-H(23)	119.8
C(22)-C(23)-H(23)	119.8
C(23)-C(24)-C(19)	119.9(3)
C(23)-C(24)-H(24)	120.0
C(19)-C(24)-H(24)	120.0
C(26)-O(25)-C(18)	124.63(19)
O(27)-C(26)-O(25)	116.5(2)
O(27)-C(26)-C(1)	128.6(2)
O(25)-C(26)-C(1)	114.93(19)
C(35)-C(28)-C(2)	110.5(2)
C(35)-C(28)-C(29)	113.2(2)
C(2)-C(28)-C(29)	112.7(2)
C(35)-C(28)-H(28)	106.7
C(2)-C(28)-H(28)	106.7
C(29)-C(28)-H(28)	106.7
C(30)-C(29)-C(34)	118.1(3)

C(30)-C(29)-C(28)	120.1(2)
C(34)-C(29)-C(28)	121.8(3)
C(29)-C(30)-C(31)	121.8(3)
C(29)-C(30)-H(30)	119.1
C(31)-C(30)-H(30)	119.1
C(32)-C(31)-C(30)	119.7(3)
C(32)-C(31)-H(31)	120.1
C(30)-C(31)-H(31)	120.1
C(31)-C(32)-C(33)	119.3(3)
C(31)-C(32)-H(32)	120.4
C(33)-C(32)-H(32)	120.4
C(32)-C(33)-C(34)	120.9(3)
C(32)-C(33)-H(33)	119.6
C(34)-C(33)-H(33)	119.6
C(29)-C(34)-C(33)	120.2(3)
C(29)-C(34)-H(34)	119.9
C(33)-C(34)-H(34)	119.9
O(36)-C(35)-O(37)	122.2(3)
O(36)-C(35)-C(28)	125.4(3)
O(37)-C(35)-C(28)	112.4(3)
C(35)-O(37)-C(38)	116.6(3)
O(37)-C(38)-H(38A)	109.5
O(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
O(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S15. Anisotropic displacement parameters ($Å^2$ x 10^3) for 4g. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	67(1)	57(1)	36(1)	8(1)	14(1)	8(1)

C(2)	71(2)	60(1)	38(1)	6(1)	13(1)	6(1)
C(3)	70(2)	59(1)	42(1)	9(1)	13(1)	7(1)
C(4)	87(2)	63(2)	47(1)	4(1)	14(1)	4(1)
C(5)	95(2)	61(2)	61(2)	8(1)	16(1)	7(1)
C(6)	86(2)	62(2)	71(2)	18(1)	16(1)	10(1)
C(7)	86(2)	63(2)	58(2)	20(1)	17(1)	11(1)
C(8)	77(2)	65(2)	44(1)	13(1)	16(1)	11(1)
C(9)	66(1)	59(1)	40(1)	9(1)	15(1)	10(1)
C(10)	65(1)	60(1)	37(1)	8(1)	15(1)	11(1)
C(11)	64(1)	63(1)	38(1)	8(1)	15(1)	12(1)
C(12)	73(2)	61(1)	35(1)	4(1)	15(1)	12(1)
C(13)	73(2)	82(2)	49(1)	20(1)	20(1)	20(1)
C(14)	90(2)	95(2)	50(1)	22(1)	28(1)	16(2)
C(15)	98(2)	102(2)	43(1)	24(1)	14(1)	16(2)
C(16)	78(2)	136(3)	56(2)	36(2)	7(1)	16(2)
C(17)	70(2)	97(2)	46(1)	18(1)	15(1)	10(1)
C(18)	70(1)	64(2)	34(1)	6(1)	15(1)	11(1)
C(19)	72(2)	64(1)	35(1)	7(1)	11(1)	12(1)
C(20)	77(2)	71(2)	43(1)	4(1)	17(1)	9(1)
C(21)	103(2)	81(2)	39(1)	1(1)	22(1)	9(2)
C(22)	107(2)	78(2)	43(1)	-4(1)	10(1)	0(2)
C(23)	88(2)	83(2)	53(2)	3(1)	11(1)	-5(2)
C(24)	82(2)	75(2)	44(1)	5(1)	18(1)	5(1)
O(25)	84(1)	57(1)	36(1)	9(1)	15(1)	10(1)
C(26)	70(2)	59(1)	36(1)	8(1)	15(1)	10(1)
O(27)	99(1)	62(1)	38(1)	13(1)	16(1)	9(1)
C(28)	84(2)	60(1)	36(1)	6(1)	14(1)	3(1)
C(29)	85(2)	62(2)	37(1)	6(1)	15(1)	5(1)
C(30)	89(2)	89(2)	41(1)	2(1)	15(1)	10(2)
C(31)	89(2)	99(2)	57(2)	18(2)	22(1)	27(2)
C(32)	106(2)	92(2)	58(2)	8(2)	28(2)	30(2)
C(33)	120(3)	107(3)	56(2)	-20(2)	18(2)	19(2)
C(34)	93(2)	105(3)	49(2)	-13(2)	13(1)	14(2)
C(35)	84(2)	70(2)	40(1)	10(1)	13(1)	6(1)
O(36)	90(2)	89(2)	109(2)	34(2)	10(1)	0(1)
O(37)	84(1)	100(2)	67(1)	35(1)	8(1)	8(1)

C(38)	83(2)	136(3)	84(2)	47(2)	4(2)	8(2)

Table S16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 4g.

	x	y	z	U(eq)
H(4)	5746	881	1736	80
H(5)	5708	-1009	2354	87
H(6)	5993	-1356	3904	87
H(7)	6681	46	5234	82
H(8)	7125	2212	5371	73
H(13)	5665	4350	6170	79
H(14)	6198	3666	7734	90
H(15)	8608	3469	8516	96
H(16)	10506	3950	7742	107
H(17)	9975	4644	6184	84
H(20)	6673	7109	6458	76
H(21)	7482	8952	7613	89
H(22)	9470	10364	7497	94
H(23)	10656	9936	6229	92
H(24)	9831	8121	5047	80
H(28)	6142	4447	1278	72
H(30)	8694	3047	1835	88
H(31)	10185	1876	995	95
H(32)	9186	760	-558	99
H(33)	6736	882	-1282	116
H(34)	5253	2081	-451	101
H(38A)	1845	4639	-430	152
H(38B)	1570	3883	454	152
H(38C)	1929	3084	-481	152

Computational Sections

A. Computational methods

All calculations were performed at the density functional theory (DFT) level as implemented in the Jaguar 9.1.[5] Geometry optimizations were carried out with the Becke's three-parameter exchange functional (B3LYP)[6-7] and 6-31G** basis set[8]. Copper and silver were represented using the Los Alamos LACVP basis set[9-11], which contains effective core potentials. The energies of the optimized structures were reevaluated with a triple-ζ basis set cc-pVTZ(-f)[12] for the main group elemental and with LACV3P** for the copper and silver using Minnesota functional M06.[13] Vibrational frequency calculations are performed using the same level of theory used for geometry optimization. The zero-point energy (ZPE) values and entropy corrections obtained from the frequency calculations. Solvation energies were simulated by a self-consistent reaction field (SCRF)[14-16] approach with the dielectric constant ε = 10.125 (DCE) using the optimized gas phase structures.

The energy components have been computed with the following protocol. The free energy in solution phase G(sol) has been calculated as follows:

$$G(sol) = G(gas) + G(solv) \quad (1)$$

$$G(gas) = H(gas) - TS(gas) \quad (2)$$

$$H(gas) = E(SCF) + ZPE \quad (3)$$

$$\Delta E(SCF) = \sum E(SCF) \text{ for products } - \sum E(SCF) \text{ for reactants} \quad (4)$$

$$\Delta G(sol) = \sum G(sol) \text{ for products } - \sum G(sol) \text{ for reactants} \quad (5)$$

G(gas) is the free energy in gas phase; G(solv) is the free energy of solvation; H(gas) is the enthalpy in gas phase; T is the temperature (298.15K); S(gas) is the entropy in gas phase; E(SCF) is electronic energy as computed from the SCF procedure and ZPE is the zero point energy. The entropy we refer involves vibrational, rotational, and translational entropy of the solute(s) and the entropy of the solvent is implicitly included in the continuum solvation model.

B. Mechanistic details

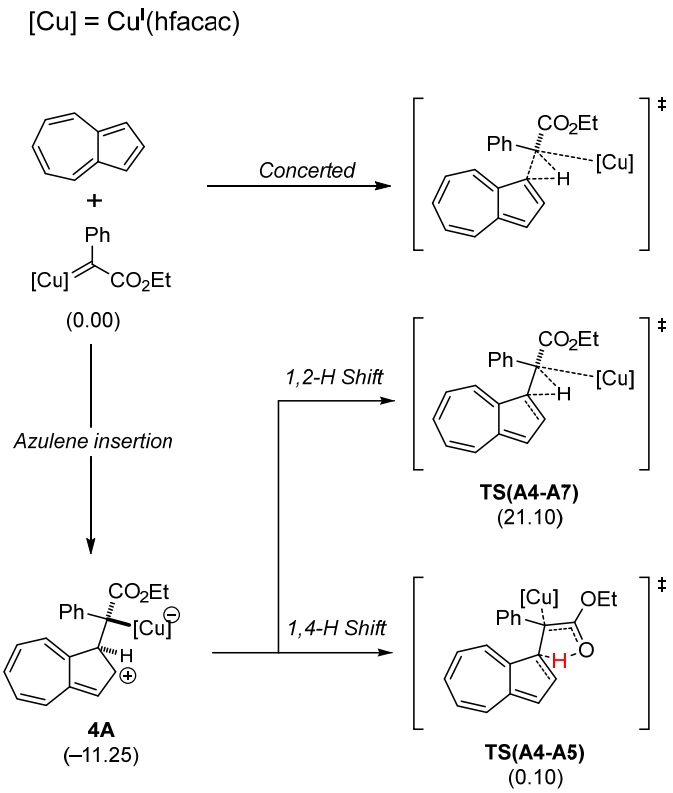


Fig. S1. Possible pathways for C–H insertion reaction. Numbers in parenthesis indicate a relative solvation phase free energy.

For the generation of the C–H insertion product, three possible pathways were considered. A C–H bond at the C3 position in azulene can be cleaved by the copper carbenoid species in a concerted manner. We tried to obtain the concerted transition state, but it seems to be located too high in energy that we were not able to find the transition state. Alternatively, C–C coupling between azulene and copper carbene species can occur first to form alkyl copper(I) intermediate **4A** with a negligible barrier. Next, this intermediate can undergo either 1,2-H shift traversing **TS(A4-A7)** or 1,4-H shift via **TS(A4-A5)**. The former pathway directly generates the C–H insertion product and the latter one first form enol intermediate followed by tautomerization to make the product. The calculated activation barrier for the 1,4-H shift, **TS(A4-A5)** is 21.0 kcal/mol lower than the barrier for the 1,2-H shift, **TS(A4-A7)**. Based on our computed results, we suggest the reaction affording the C–H insertion product would proceed *via* the 1,4-H shift followed by tautomerization in a stepwise fashion.

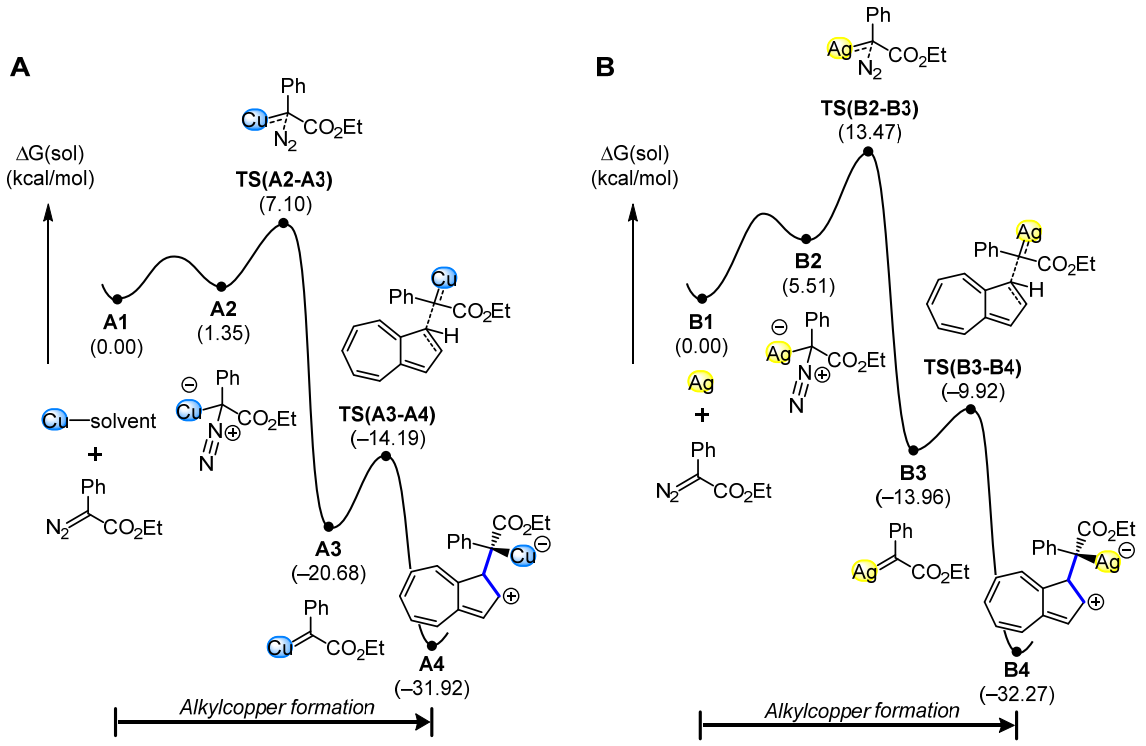


Fig. S2. Energy profiles of the formation of the metal alkyl intermediate with (**A**) Cu^{I}(hfacac) and (**B**) $Ag^{I}OTf$.

Fig. S2. shows the energy profile for the formation of the metal alkyl intermediate with Cu^{I}(hfacac) and $Ag^{I}OTf$. In the case of the copper(I) catalyst, one additional solvent coordinates the copper center, which is favored thermodynamically. As shown above, a dinitrogen extruding process is associated with a barrier of 7.1 kcal/mol for **TS(A2-A3)** and 13.5 kcal/mol for **TS(B2-B3)**. In both cases of copper and silver, after generation of the metal carbene intermediate **A3** and **B3**, the subsequent azulene insertion proceeds with a negligible barrier, giving the metal alkyl intermediate **A4** and **B4** which are located at –31.9 and –32.3 kcal/mol, respectively.

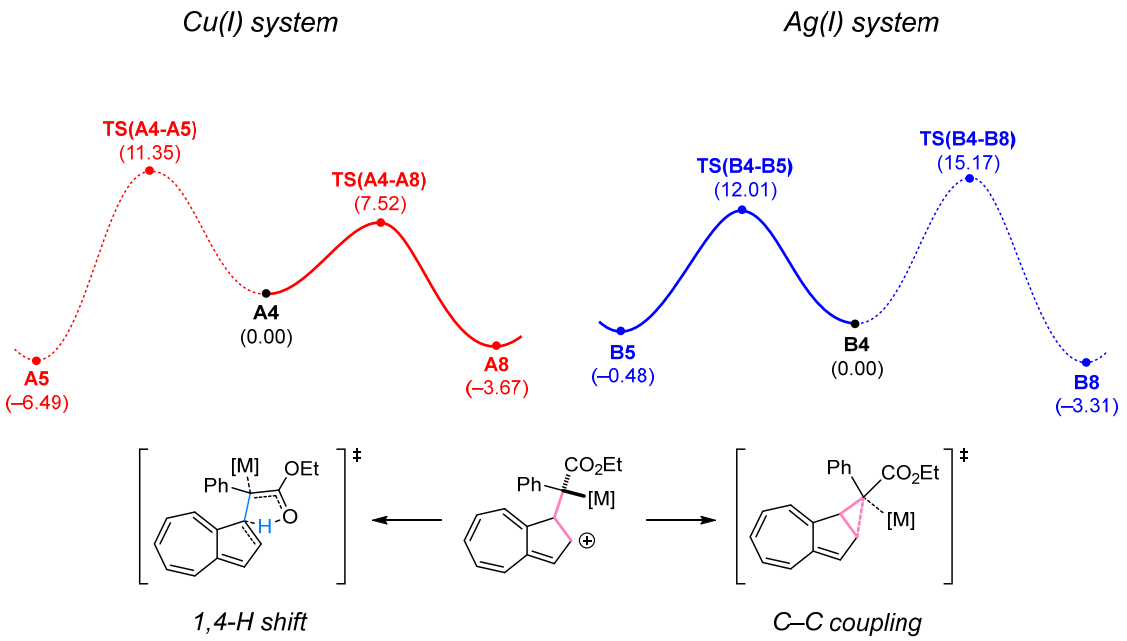


Fig. S3. Key steps for chemoselectivity in Cu^{I}(hfacac) and Ag^{I}OTf.

Simplified energy profiles in chemoselectivity determining steps of 1,4-H shift and C–C bond coupling are displayed in **Fig S3**. Since the free energy barrier for **TS(A4-A8)** is 3.8 kcal/mol lower than that for **TS(A4-A5)** in Cu(I) system, **A4** would be transformed into **A8** selectively. On the other hand, the barrier for **TS(B4-B8)** is 3.2 kcal/mol higher than that for **TS(B4-B5)** in Ag(I) system that **B4** would undergo 1,4-H shift process dominantly to form **B5**. Intriguingly, the barrier of cyclopropanation through C–C bond coupling is significantly different depending on catalyst whereas 1,4-H shift process is barely affected by changing the catalyst frame. Changing of the C–C bond coupling barrier with different catalyst is the reason for the chemoselectivity.

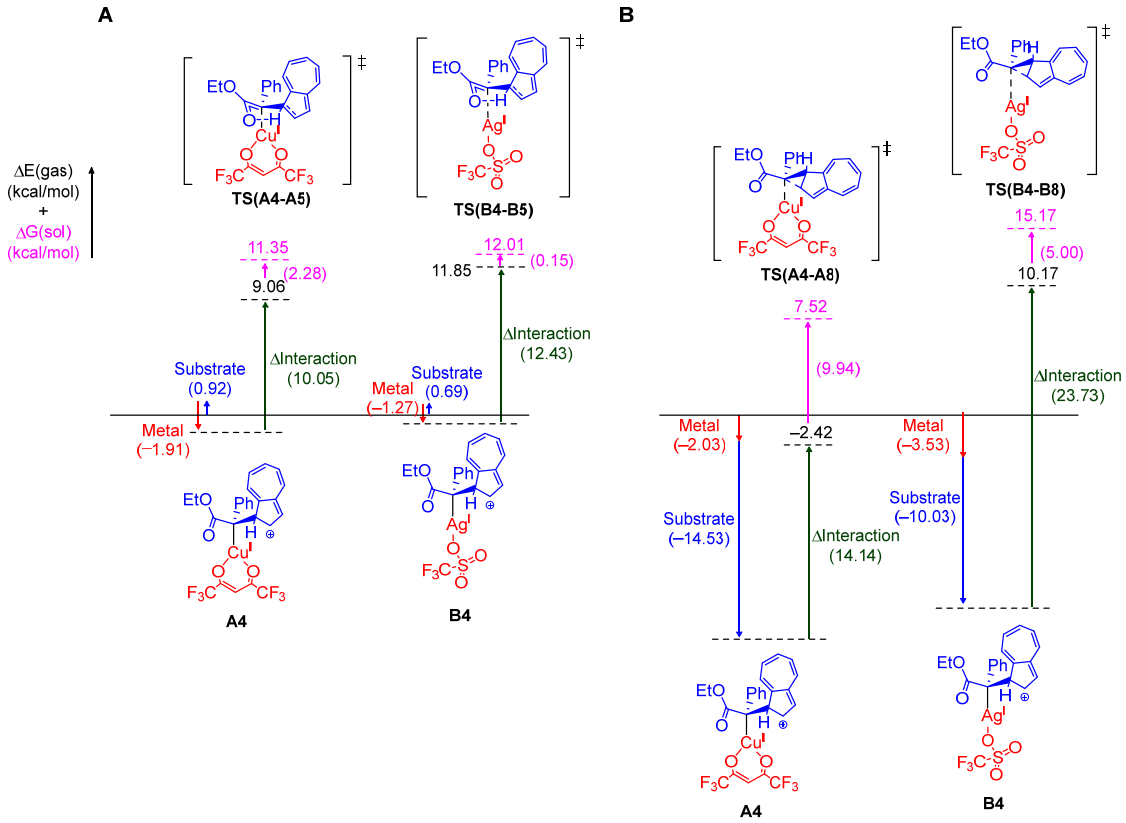


Fig. S4. Energy decomposition analysis of (**A**) 1,4-H shift and (**B**) cyclization

To better understand the chemoselectivity, we performed energy decomposition analysis by fragmentizing the transition states into a metal and substrate moiety denoted in red and blue, respectively. Fig. S4A and S4B show the energy decomposition analysis of 1,4-H shift and cyclization reaction, respectively. In the case of the 1,4-H shift, energy variance of metal and substrate moiety induced by structural change for transition state in Cu(I) system are -1.9 and 0.9 kcal/mol, respectively. Those in Ag(I) system are -1.3 and 0.7 kcal/mol, respectively. Interaction energy variance between metal and substrate moiety during the transformation of **X4** → **TS(X4-X5)** (X= A or B) in Cu(I) and Ag(I) system is 10.1 and 12.4 kcal/mol, respectively. Sum of variances of structural energy and interaction energy results in ΔE(gas) to be 9.1 kcal/mol in Cu(I) system and 11.9 kcal/mol in Ag(I) system, respectively. Adding the other energy components for free energy barrier renders the barrier for **TS(A4-A5)** and **TS(B4-B5)** to be 11.4 and 12.0 kcal/mol, respectively. These results show that there are no significant difference between each decomposed energy. On the contrary, in the case of cyclization reaction, the interaction energy variance in Cu(I) system is markedly different from that in Ag(I) system.

The interaction energy variance in Cu(I) system is 14.1 kcal/mol, whereas that in Ag(I) system 23.7 kcal/mol, making the much higher barrier for **TS(B4-B5)** than **TS(A4-A5)**. This higher interaction energy variance in Ag(I) system originates from a poor interaction between hard species of α-carbon and very soft species of silver metal at the transition state.

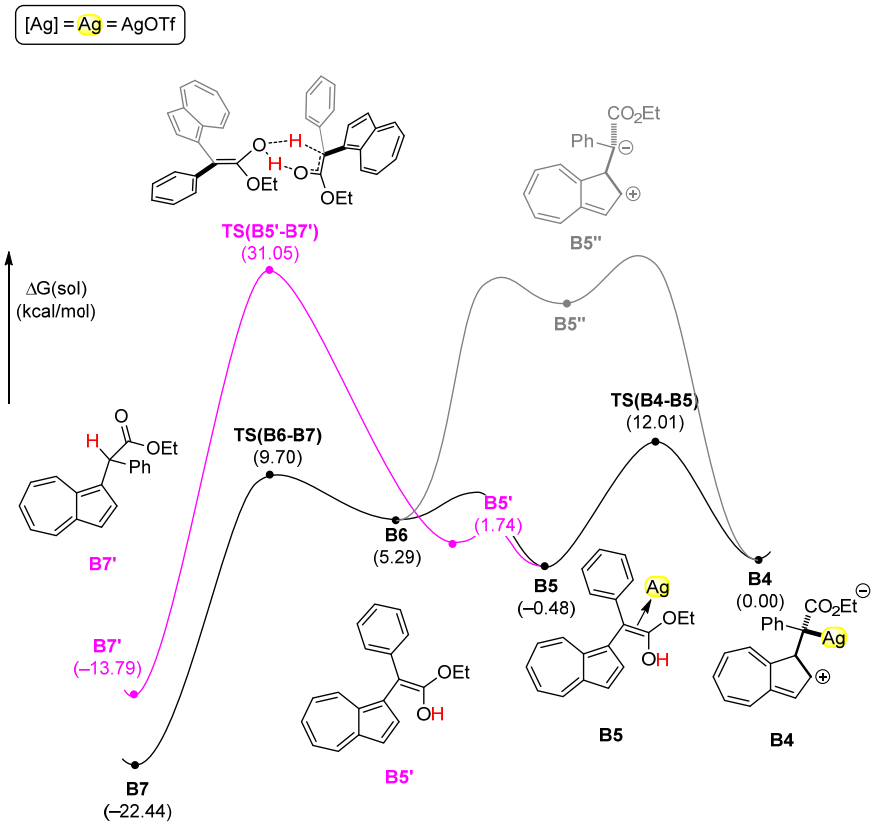


Fig. S5. Energy profiles of tautomerization with and without $Ag^{I}OTf$.

Since the ring-expansion reaction can occur without catalyst, tautomerization without catalyst is also considered as shown in Fig. S6. After silver catalyst dissociates from **B5**, enol intermediate **B5'** located at 1.7 kcal/mol can be generated. The formation of ylide species **B5''** from **B5** can be considered, but this is expected to have very high energy. Tautomerization can occur between two **B5'** traversing the **TS(B5'-B7')** with a barrier of 31.5 kcal/mol. This tautomerization without silver catalyst requires too much free energy that the reaction for C–H insertion product would not happen.

C. Energy components

	E(SCF) (eV)	***ZPE** (kcal/mol)	***S** (cal/mol·K)	**G(solv)** (kcal/mol)
azulene	-10493.618	91.85	81.88	-3.95
DCE	-27183.707	36.65	71.96	-3.47
N_2	-2979.521	3.52	45.78	0.00
Ethyl phenyl diazoacetate	-17599.215	117.17	116.69	-6.10
A1	-58117.997	78.86	162.41	-12.60
A2	-48533.648	159.05	203.37	-11.38
TS(A2-A3)	-48533.316	157.64	205.44	-11.26
A3	-45554.561	153.42	190.04	-11.61
TS(A3-A4)	-56048.499	245.85	228.90	-15.10
A4	-56049.150	246.62	227.86	-18.90
TS(A4-A8)	-56049.255	246.70	220.14	-11.34
A8	-56049.659	247.52	224.21	-12.82
TS(A4-A5)	-56048.757	244.29	224.66	-15.24
A5	-56049.806	247.24	229.80	-10.30
TS(A6-A7)	-112099.464	492.24	399.97	-14.90
A6	-112099.977	495.10	399.27	-16.71
TS(A4-A7)	-56047.849	243.38	227.42	-13.45
A7	-56050.429	247.68	229.07	-13.49
B1	-30128.897	17.62	99.98	-29.01
B2	-47728.901	134.79	185.91	-20.58
TS(B2-B3)	-47728.430	133.33	186.00	-21.99
B3	-44749.664	129.11	171.54	-21.21
TS(B3-B4)	-55243.801	221.76	208.17	-23.45
B4	-55244.638	223.04	208.11	-27.79
TS(B4-B8)	-55244.197	222.17	208.16	-21.55
B8	-55245.111	223.55	207.55	-20.87
TS(B4-B5)	-55244.124	220.25	206.02	-25.47
B5	-55244.980	223.04	210.21	-19.76
B6	-110490.653	446.91	375.90	-31.87
TS(B6-B7)	-110490.825	444.90	355.23	-27.65
B7	-55245.815	223.46	215.71	-21.24
B5'	-25114.736	204.82	146.93	-8.05
TS(B5'-B7')	-50228.770	406.23	246.11	-13.80
B7'	-25115.565	205.23	148.11	-4.52
C1	-25114.839	205.08	143.08	-8.44
TS(C1-C2)	-25113.931	203.51	143.49	-8.86
C2	-25114.939	205.34	144.54	-7.98

*ZPE and entropy are taken from optimized structures with B3LYP/LACVP** level of theory.

D. XYZ coordinates

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azulene

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C	4.700373650	5.496918201	-4.929765701
C	4.700373650	6.762944221	-4.337166786
C	4.700373650	7.091388226	-2.978455544
C	4.700373650	4.230892181	-4.337166786
C	4.700373650	6.247118950	-1.871900678
C	4.700373650	3.902447939	-2.978455544
C	4.700373650	4.746716976	-1.871900678
H	4.700373650	5.496918201	-6.018296719
H	4.700373650	7.604775906	-5.025189400
H	4.700373650	8.156770706	-2.750119686
H	4.700373650	3.389060020	-5.025189400
H	4.700373650	2.837064981	-2.750119686
C	4.700373650	6.646834850	-0.524572611
H	4.700373650	7.672832966	-0.178237617
C	4.700373650	5.496918201	0.281359375
H	4.700373650	5.496918201	1.365724325
C	4.700373650	4.347001076	-0.524572611
H	4.700373650	3.321002960	-0.178237617

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DCE

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C	-6.780385494	2.187914371	-0.150900185
H	-6.309628963	2.581785440	0.750021517
H	-6.300564289	2.618680477	-1.029889107
C	-6.740122795	0.669880390	-0.182215199
H	-7.220683575	0.239040464	0.696331084
H	-7.210130692	0.276101351	-1.083569884
Cl	-8.507629395	2.734161854	-0.148536250
Cl	-5.012882710	0.123608917	-0.183509186

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N_2

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N	-0.216015220	6.817907333	1.818212986
N	-0.293444067	7.804518223	1.326783895

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Ethyl phenyl diazoacetate

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C	0.232650340	4.114698887	1.681820512
C	0.125544816	2.784274578	2.124729156
C	0.409035653	4.353125572	0.305848271
H	-0.013006612	2.585133076	3.178594828
H	0.497154653	5.368555069	-0.069408789
C	0.193733081	1.734743118	1.209973931
C	0.475837499	3.296507120	-0.597237527
H	0.107732050	0.714440882	1.573351383
H	0.613047421	3.507775307	-1.653924704
C	0.369037181	1.978150249	-0.151779354
H	0.421262115	1.154015541	-0.856929243
C	0.164938122	5.242516994	2.635923862
O	-0.097011931	4.122368336	4.730332375
C	0.023278218	5.155584812	4.098282814
O	0.040639691	6.383479595	4.671595573
C	-0.052416705	7.853933811	6.550653458
H	-0.161546394	7.913933754	7.637979984
H	0.902435422	8.310714722	6.274924278
H	-0.858043313	8.433720589	6.091216564
C	-0.107366949	6.403632641	6.110716343
H	-1.057350397	5.928046703	6.373977661
H	0.694684982	5.807074547	6.556090355
N	0.260812491	6.465207100	2.152782917
N	0.337925762	7.510133743	1.706299901

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A1

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Cu	-2.913711786	0.015248353	-0.103235081
O	-1.572691321	-1.479306102	-0.146559894
O	-1.589062810	1.528224349	-0.124738567
C	-0.339054585	-1.212879419	-0.183284491
C	-0.352718294	1.276275396	-0.162873656
C	0.304630995	0.035357501	-0.194454089
H	1.383368611	0.041695297	-0.228707954
C	0.548607171	-2.475346327	-0.219058543
F	1.869459391	-2.200772285	-0.267128795
F	0.330205441	-3.228826761	0.875880539
F	0.250045419	-3.223722935	-1.298311114
C	0.521878302	2.548732042	-0.170579374
F	0.188626766	3.337259054	-1.211113691
F	0.324212044	3.255148649	0.960394025
F	1.844504833	2.289638042	-0.262643248
C	-6.219992638	0.371471077	0.627080202
H	-6.188002586	1.453475714	0.496505320
H	-7.098230839	0.092181884	1.213068366
C	-6.238522530	-0.364085883	-0.695662439
H	-6.172889709	-1.444758058	-0.566799164
H	-7.148139954	-0.108283944	-1.243246198
Cl	-4.777494907	-0.075101055	1.641265750
Cl	-4.852974415	0.118387863	-1.771005154

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A2

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Cu	-2.974498510	-0.282152891	-0.236866102
O	-1.550134063	-1.641373158	-0.182913795
O	-1.766360641	1.309223890	-0.524084628
C	-0.335680246	-1.314434886	-0.314527512
C	-0.516773999	1.147500396	-0.586417556
C	0.226101235	-0.042776171	-0.504406929
H	1.299863219	0.025902161	-0.588985264
C	0.620503724	-2.523034811	-0.235460639
F	1.913112879	-2.190915585	-0.435940683
F	0.532012224	-3.105091572	0.976696968
F	0.286093205	-3.442459345	-1.159251690
C	0.255346775	2.471031189	-0.769946337
F	-0.155572355	3.098750591	-1.887639880
F	0.018899463	3.290144205	0.274055332
F	1.590570569	2.300714493	-0.862810194
C	-5.496805191	-0.483662218	-1.316533089
C	-5.359350204	-1.824151278	-1.720828056
C	-6.042693138	0.448979706	-2.212926865
H	-4.949676991	-2.554903269	-1.034843683
H	-6.162465096	1.490525484	-1.926721215
C	-5.776868820	-2.213426828	-2.992287636
C	-6.448649406	0.048430335	-3.484768629

H	-5.670009613	-3.253628969	-3.287152767
H	-6.872586250	0.783036411	-4.163591862
C	-6.320667267	-1.283963203	-3.879965067
H	-6.641025066	-1.594053149	-4.870302677
C	-5.040358067	-0.081820332	0.061256897
O	-5.552799702	-2.132289648	1.206351995
C	-5.299695492	-0.949497461	1.267650962
O	-5.198099613	-0.241475597	2.408436060
C	-5.396070004	-0.000824329	4.784900665
H	-5.544682503	-0.534032822	5.729580879
H	-4.442969322	0.532874346	4.838406086
H	-6.200543404	0.732888877	4.675464630
C	-5.404118538	-0.993275940	3.638806343
H	-6.353328705	-1.530456305	3.560655594
H	-4.603209972	-1.734434962	3.724390745
N	-5.135486126	1.242114067	0.339626461
N	-5.209854603	2.347827435	0.556712210

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TS(A2-A3)

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Cu	-2.956444979	-0.496405631	-0.304075003
O	-1.320969701	-1.581369519	-0.145128489
O	-1.895200610	1.252891898	-0.498410314
C	-0.149170324	-1.109763026	-0.148402363
C	-0.636040270	1.288551450	-0.455756158
C	0.262787968	0.221887276	-0.295383722
H	1.320078969	0.437369436	-0.277314305
C	0.934627652	-2.186686516	0.058819074
F	2.189310551	-1.695685387	-0.020450504
F	0.794555068	-2.752593279	1.273250341
F	0.815449297	-3.156094551	-0.864928842
C	-0.054585703	2.710481167	-0.596039832
F	-0.441211998	3.256918907	-1.764610529
F	-0.510553181	3.498034239	0.396997690
F	1.293571830	2.741018772	-0.556026399
C	-5.693912029	-0.741948128	-1.458464980
C	-6.957303524	-1.362362385	-1.478468657
C	-5.147796631	-0.275060415	-2.669134855
H	-7.381804943	-1.747936964	-0.559236884
H	-4.171850681	0.204099402	-2.659432173
C	-7.640563965	-1.523670316	-2.680220127
C	-5.843759537	-0.417691261	-3.865321159
H	-8.607023239	-2.018850803	-2.686188936
H	-5.410236359	-0.050203502	-4.790365696
C	-7.090528011	-1.047474861	-3.872863770
H	-7.630583763	-1.171714902	-4.807075977
C	-4.909886360	-0.568129539	-0.210813805
O	-5.617267609	-2.495141268	0.977778375
C	-5.304394245	-1.321617961	1.019816995
O	-5.169054031	-0.610354662	2.155876398
C	-5.204986572	-0.373138875	4.538310528
H	-5.356001854	-0.895463228	5.488237381
H	-4.198497295	0.054990038	4.538629055
H	-5.930334091	0.443581492	4.477443695
C	-5.381388187	-1.347645640	3.390487194
H	-6.384129524	-1.784605026	3.367368460
H	-4.658820152	-2.168212891	3.429493427
N	-5.201463223	1.089560270	0.239348128
N	-5.122295380	2.197575092	0.286330074

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A3

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Cu	-0.072817266	0.047420457	-0.072471969
O	1.355311751	-0.629064620	-1.276468635
O	1.280083418	0.613467038	1.292316437
C	2.591061115	-0.619181037	-1.020532727
C	2.526257038	0.446076602	1.184816122
C	3.236188650	-0.130387455	0.123354807
H	4.310986996	-0.198783278	0.188019365
C	3.456616402	-1.225661516	-2.142698050
F	4.776527405	-1.188497901	-1.863122821
F	3.116725683	-2.509864569	-2.351102591
F	3.262644529	-0.552861273	-3.291597128
C	3.322815180	0.964703023	2.398704529
F	3.104762554	2.282045603	2.568331242
F	2.928104401	0.332329452	3.518279076
F	4.653424263	0.780675292	2.270248652
C	-2.744874716	1.321526170	-0.369903415
C	-4.166330338	1.321863770	-0.309551746
C	-2.092428207	2.522347212	-0.759571791
H	-4.683837414	0.406141996	-0.047350187
H	-1.007834435	2.525235653	-0.813666284
C	-4.886085510	2.465211868	-0.619065046
C	-2.816179752	3.667464733	-1.054735065
H	-5.970834255	2.452773094	-0.577070892
H	-2.302977085	4.579013824	-1.344130397
C	-4.213820457	3.638147354	-0.986063182
H	-4.783393383	4.532209873	-1.224135399
C	-1.944642305	0.182305738	-0.037030507
O	-3.354991198	-1.704870343	-0.356694251
C	-2.640163422	-1.057556033	0.388962835
O	-2.314617634	-1.416670084	1.640952229
C	-2.334628105	-2.902611017	3.515200615
H	-2.725085497	-3.846439362	3.908559322
H	-1.242299199	-2.956314325	3.510455370
H	-2.637051821	-2.096367836	4.189542770
C	-2.870495558	-2.672403336	2.115839958
H	-3.962908030	-2.602502584	2.096946001
H	-2.574672937	-3.465322495	1.422566533

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TS(A3-A4)

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Cu	-0.107678063	-0.122694366	-0.244422734
O	1.414640546	-1.143929005	-1.114500523
O	1.238299370	0.915405750	0.903172910
C	2.637699604	-0.978413939	-0.876321316
C	2.492639065	0.780745089	0.836909592
C	3.237345457	-0.086284399	0.029328981
H	4.313753605	-0.068474405	0.103382349
C	3.559580326	-1.885964990	-1.718136191
F	4.869859695	-1.721527576	-1.432180405
F	3.257343531	-3.181171417	-1.510617852
F	3.394979000	-1.629284739	-3.029321432
C	3.259798527	1.714122415	1.792967677
F	2.933533669	2.999883413	1.551857829
F	2.931366682	1.443377972	3.072276592
F	4.600504398	1.607860088	1.684755921
C	-2.646986485	0.840762198	-1.451488853
C	-3.915164232	0.628664911	-2.041844845
C	-1.933317304	1.993883848	-1.843615174

H	-4.482060909	-0.255974710	-1.779046297
H	-0.956584513	2.173576593	-1.402791739
C	-4.420917511	1.508739471	-2.991472483
C	-2.442532301	2.879858732	-2.790051699
H	-5.388603210	1.312254310	-3.445278645
H	-1.862244964	3.750299215	-3.082886219
C	-3.688949108	2.638721228	-3.369354486
H	-4.085833549	3.321270466	-4.116134644
C	-2.036984682	-0.080355346	-0.479461581
O	-2.940989971	-2.076367855	-1.420271754
C	-2.571052074	-1.466388583	-0.429225177
O	-2.485346556	-2.076637745	0.788890362
C	-2.579283953	-4.000458241	2.205479145
H	-2.776876688	-5.076418400	2.245149374
H	-1.555723906	-3.826901436	2.550336361
H	-3.265096664	-3.501998901	2.898211956
C	-2.765424013	-3.496483803	0.786565304
H	-3.785046577	-3.659538269	0.421622068
H	-2.084784269	-3.987513781	0.084632084
C	-6.984790325	1.516854405	0.919860303
C	-6.459157944	2.797500372	0.728436351
C	-5.130054474	3.217964649	0.817614675
C	-6.321967125	0.324859679	1.228999853
C	-3.993965864	2.461423635	1.103732347
C	-4.953243732	0.098108485	1.404254317
C	-3.906349897	1.012451887	1.335009933
H	-8.064799309	1.435838819	0.815847874
H	-7.183317184	3.573943615	0.493712842
H	-4.955862522	4.280690193	0.657475233
H	-6.958656311	-0.549615741	1.340169311
H	-4.659631252	-0.927565813	1.614896655
C	-2.673127174	2.984409571	1.246020198
H	-2.416597366	4.031602383	1.145310640
C	-1.805035591	1.951804519	1.521314859
H	-0.734786093	2.034656286	1.673661590
C	-2.512479544	0.700003147	1.485464454
H	-2.164017439	-0.208440453	1.953273535

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A4

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Cu	-0.335450649	-0.564995766	0.057928231
O	-0.134501740	-2.186356783	-1.096183181
O	1.758840322	-0.520869374	0.381608725
C	0.955371439	-2.685581446	-1.477631807
C	2.556947708	-1.283176780	-0.227718651
C	2.265643120	-2.325464010	-1.118386507
H	3.086001873	-2.875340462	-1.553668737
C	0.775193632	-3.842229843	-2.483553171
F	1.944481850	-4.383214951	-2.890817642
F	0.040451031	-4.830148697	-1.937508464
F	0.126527578	-3.407801628	-3.581141710
C	4.039693832	-0.977289796	0.062723428
F	4.344690800	0.272647500	-0.346687883
F	4.280634403	-1.037439823	1.388277054
F	4.897477627	-1.822789907	-0.545322299
C	-1.367369294	2.035605907	-0.439133525
C	-2.455791712	2.717365503	-1.018108845
C	-0.077624813	2.423171997	-0.853418767
H	-3.467675209	2.439310074	-0.743135691
H	0.787024617	1.900800228	-0.452574015
C	-2.265566826	3.724002838	-1.964535713
C	0.115391366	3.440721035	-1.787770748
H	-3.130307674	4.219617367	-2.399631739
H	1.125835180	3.705410242	-2.088772535
C	-0.978531182	4.098496914	-2.351424217
H	-0.830697536	4.881798744	-3.089964628
C	-1.542544007	0.981416821	0.632253170
O	-3.384746313	-0.070969194	1.777272105
C	-2.832289219	0.268787056	0.725636125
O	-3.381923914	-0.026746264	-0.483515322
C	-5.080023766	-0.932706118	-1.889294624
H	-5.984025955	-1.549689651	-1.924350500
H	-5.323719501	0.057610925	-2.286578178
H	-4.326054096	-1.386294007	-2.538723946
C	-4.573982239	-0.835728884	-0.461384147
H	-4.327384949	-1.821342826	-0.051662400
H	-5.311511517	-0.377734452	0.206311390
C	-3.086270809	5.513517857	3.179080009
C	-1.729206204	5.819403172	3.374794960
C	-0.618153930	4.998530865	3.237484694
C	-3.657184124	4.296685219	2.816478252
C	-0.572964907	3.651503325	2.829566002
C	-3.032086849	3.074263811	2.523885727
C	-1.673236489	2.789833307	2.495940447
H	-3.781004667	6.332174778	3.349636316
H	-1.521483421	6.841414452	3.683978319
H	0.343895733	5.452663898	3.465472698
H	-4.743199348	4.288463593	2.753830433
H	-3.682636499	2.235703707	2.286353588
C	0.641682863	2.889525652	2.700124025
H	1.627885222	3.287919521	2.906514406
C	0.350385159	1.632790923	2.270440102
H	1.072251320	0.854857087	2.043367624
C	-1.114814639	1.453901529	2.068721771
H	-1.524693727	0.668599784	2.724507332

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TS(A4-A8)

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Cu	-0.113090806	0.046602350	0.397067785
O	0.899984121	-1.025019526	-0.961077273
O	1.468483567	1.294732571	0.729339778
C	2.080479383	-0.761613607	-1.318554521
C	2.557121038	1.203324795	0.098507054
C	2.925815105	0.269263506	-0.880270600
H	3.911643744	0.342650414	-1.313289642
C	2.631479025	-1.748539567	-2.368135929
F	3.844146729	-1.398641229	-2.842714787
F	2.740406752	-2.979533195	-1.831883192
F	1.791427255	-1.832885861	-3.419394732
C	3.580601931	2.288574219	0.489932686
F	3.084922075	3.511139870	0.211687103
F	3.830205441	2.238735437	1.811727762
F	4.758837223	2.168668032	-0.155243218
C	-2.744333506	0.722564459	-0.538704336
C	-3.992156744	0.458505392	-1.129629135
C	-2.017721653	1.830361724	-0.995173216
H	-4.571943760	-0.396677852	-0.793380439
H	-1.059320092	2.075595379	-0.544141054
C	-4.482436657	1.260039926	-2.157997131
C	-2.513085365	2.640521765	-2.020190001
H	-5.442804337	1.026017427	-2.609620333
H	-1.927600145	3.490396261	-2.359369993

C	-3.745001554	2.358075857	-2.607678652
H	-4.127390862	2.984189749	-3.408747673
C	-2.284837961	-0.175948977	0.578956485
O	-2.089419603	-2.459040165	1.287239432
C	-2.160497189	-1.653906703	0.369773060
O	-2.118042469	-1.988847494	-0.931046188
C	-1.487911344	-3.464587212	-2.699920416
H	-1.294071078	-4.507287979	-2.972114086
H	-2.310939550	-3.095254183	-3.319439650
H	-0.593380034	-2.875689507	-2.915837765
C	-1.834470510	-3.379244089	-1.226348877
H	-1.009521246	-3.708831310	-0.589501798
H	-2.717283726	-3.975711107	-0.970151365
C	-5.195891380	4.045437813	2.681550264
C	-3.842170715	4.539868832	2.720933437
C	-2.665929079	3.864589691	2.607252598
C	-5.629281521	2.765851259	2.501169205
C	-2.448152781	2.448965549	2.420898438
C	-4.850654125	1.573164463	2.294392586
C	-3.497882605	1.440468788	2.237769127
H	-5.965161800	4.803605080	2.810068130
H	-3.757784128	5.615173340	2.864946842
H	-1.756517529	4.459294796	2.670492649
H	-6.706756592	2.615462542	2.499285460
H	-5.429393768	0.662105978	2.154356480
C	-1.210291624	1.848275423	2.365776300
H	-0.256994247	2.356705427	2.425873995
C	-1.348643899	0.422297716	2.140595913
H	-0.694547236	-0.344588667	2.554183722
C	-2.804321289	0.127028570	2.000651121
H	-3.212291002	-0.750980318	2.496304750

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A8

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Cu	1.803378344	-0.672159672	3.049252033
O	3.479326725	-1.074569583	1.988701701
O	2.058871746	-2.170705795	4.323821545
C	4.275688171	-1.986466169	2.336721420
C	3.077109814	-2.919191837	4.288497448
C	4.161637783	-2.896221399	3.401520491
H	4.951736450	-3.617888451	3.542235374
C	5.529220104	-2.070880175	1.441621661
F	6.405006886	-3.017017841	1.838786602
F	5.176393509	-2.347472429	0.172571272
F	6.175339699	-0.889603615	1.442243814
C	3.071074724	-3.992919922	5.394085884
F	2.974187851	-3.417923927	6.605982304
F	2.005282402	-4.807602406	5.240072250
F	4.175791264	-4.766094208	5.391849518
C	-1.644366741	-0.047073200	2.583621025
C	-1.058448911	0.082224920	1.306514621
C	-0.926670909	0.379566431	3.698317766
H	-1.612488389	-0.257081598	0.437035799
H	-1.364970922	0.287151843	4.687205315
C	0.200315624	0.644338906	1.143494010
C	0.354874909	0.952454388	3.558393240
H	0.626770794	0.754392922	0.151284844
H	0.847235382	1.383424759	4.426537991
C	0.923823297	1.108323216	2.267988682
H	1.832669854	1.688299417	2.128169298
C	-3.003622532	-0.666077137	2.732001543
O	-4.126053810	-2.775837898	2.966985464
C	-3.082589626	-2.162478447	2.833723783
O	-1.874627948	-2.753420115	2.757191181
C	-0.456764936	-4.680992126	2.651306868
H	-0.431554198	-5.775064945	2.684928179
H	-0.062879883	-4.360918999	1.681495667
H	0.197387055	-4.298153400	3.438133240
C	-1.882987380	-4.203283787	2.837026358
H	-2.294774055	-4.495208263	3.808085203
H	-2.555121660	-4.588761806	2.063991308
C	-4.227082253	4.055116653	-0.017180365
C	-3.961999416	4.420674801	1.355414510
C	-3.866636276	3.633659601	2.459003210
C	-4.426849365	2.817675591	-0.547605455
C	-4.016843796	2.198400259	2.571302891
C	-4.414053440	1.539494514	0.120239452
C	-4.212233067	1.269637465	1.436861396
H	-4.272969723	4.891112804	-0.711738944
H	-3.828255177	5.487708569	1.520792603
H	-3.670513630	4.142134190	3.401689053
H	-4.613014698	2.772473812	-1.618567705
H	-4.588509560	0.679304004	-0.524374545
C	-3.999600649	1.492608547	3.738739967
H	-3.889675140	1.928421259	4.725295544
C	-4.146312714	0.036483105	3.499636412
H	-4.719254971	-0.599546850	4.167096138
C	-4.253630638	-0.107734866	1.999276280
H	-4.885294437	-0.861376882	1.542639852

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TS(A4-A5)

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Cu	-0.122172333	-0.232004404	-0.195730284
O	-0.052448254	-1.615122199	-1.663272262
O	1.723939896	-0.738810599	0.506844103
C	0.935097456	-2.368716955	-1.857745409
C	2.427892923	-1.642232537	-0.025190830
C	2.137257576	-2.449902773	-1.132957697
H	2.876724243	-3.169599533	-1.449154496
C	0.756672919	-3.304908752	-3.071547270
F	1.803140998	-4.136613846	-3.264847517
F	-0.343896836	-4.066983700	-2.917079926
F	0.599481344	-2.582834482	-4.197367191
C	3.789376497	-1.834934831	0.670288622
F	4.500987053	-0.689585924	0.625428021
F	3.610777140	-2.152138233	1.969332337
F	4.544915199	-2.805319786	0.114417754
C	-1.439916372	2.143173933	-0.774571598
C	-2.333164454	2.051828861	-1.863889337
C	-0.484111875	3.181616068	-0.818557382
H	-3.076085567	1.266128302	-1.884295344
H	0.233058512	3.280233860	-0.008948341
C	-2.273089886	2.958397388	-2.921856880
C	-0.429566830	4.084275246	-1.877513885
H	-2.981177092	2.858775139	-3.741007090
H	0.322432369	4.869503975	-1.869274855
C	-1.327583909	3.983883619	-2.940557718
H	-1.287728667	4.686811924	-3.767776251
C	-1.465791702	1.234696269	0.416218549
O	-2.720472097	-0.012866111	1.952512383
C	-2.533958197	0.310900956	0.734002471
O	-3.323730946	-0.184415266	-0.221337318

C	-5.139920235	-1.485141635	-1.058423281
H	-5.886003971	-2.248750448	-0.816827297
H	-5.665837765	-0.588739395	-1.401731372
H	-4.516852856	-1.856575012	-1.876766205
C	-4.299588203	-1.183706403	0.167908624
H	-3.765883923	-2.068786383	0.527836323
H	-4.898883343	-0.790365338	0.994189322
C	-2.885493517	5.704656601	3.379795790
C	-1.706351399	5.646841049	4.139353275
C	-0.677871168	4.713446140	4.082711220
C	-3.337862968	4.828264713	2.397189856
C	-0.559309959	3.584190845	3.257390499
C	-2.744912148	3.646205902	1.928573728
C	-1.534932137	3.074804783	2.298373222
H	-3.533337116	6.553267479	3.588017464
H	-1.573629260	6.450421810	4.859905243
H	0.157396957	4.884185314	4.759963512
H	-4.287185192	5.088443279	1.935026407
H	-3.298148870	3.111072063	1.160992026
C	0.558470428	2.703828335	3.238404036
H	1.444220066	2.821864128	3.850578547
C	0.315283537	1.686871171	2.341292143
H	0.994755149	0.875822306	2.097304106
C	-1.019176245	1.806655288	1.770331502
H	-1.748606324	0.929542363	2.350700855

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Cu	-0.718201101	-0.782587707	0.440033138
O	-0.795530260	-2.808815002	0.397576749
O	0.787807584	-0.675048947	-0.864373684
C	-0.037035733	-3.493776560	-0.341456950
C	1.296901941	-1.698867917	-1.398218513
C	0.971716464	-3.052008390	-1.209514856
H	1.524606466	-3.791834593	-1.768120646
C	-0.321317583	-5.006504536	-0.262270451
F	0.576695025	-5.755930901	-0.932214618
F	-0.318407863	-5.414661407	1.021738529
F	-1.540579438	-5.273614883	-0.772798181
C	2.426432133	-1.361564279	-2.392954111
F	1.968112707	-0.540862143	-3.355313301
F	3.431415081	-0.729009449	-1.756369591
F	2.946802855	-2.451156855	-2.996722221
C	-2.920191765	0.905682981	0.233262956
C	-4.204775810	0.338218212	0.123300642
C	-2.511014223	1.801676750	-0.775647104
H	-4.562371731	-0.345449209	0.880791485
H	-1.529155493	2.259984732	-0.707332551
C	-5.031817436	0.653769910	-0.955850840
C	-3.340141773	2.111467838	-1.849229217
H	-6.020223618	0.205170453	-1.013499022
H	-2.991783142	2.803661585	-2.611026764
C	-4.609087944	1.537595510	-1.947878361
H	-5.258615971	1.778266430	-2.784729004
C	-1.973052621	0.662441492	1.376538873
O	-1.407440543	-0.441990018	3.441866159
C	-2.124964237	-0.382066935	2.301932812
O	-3.063292503	-1.319233894	2.206124306
C	-4.091681004	-3.438616276	2.568450689
H	-4.006448746	-4.408442497	3.068377733
H	-5.011465073	-2.954748392	2.911836863
H	-4.165056705	-3.611973524	1.491490722
C	-2.875832081	-2.593852520	2.892752886
H	-1.957009554	-3.046937943	2.512392282
H	-2.781906128	-2.404435396	3.965021133
C	-3.105945826	5.463756084	3.871905327
C	-1.759327888	5.851161003	3.890727520
C	-0.647498727	5.158166885	3.412571430
C	-3.689598322	4.295039654	3.380577803
C	-0.587279439	3.906200886	2.795730114
C	-3.071594954	3.193143129	2.774637222
C	-1.723604679	2.983179331	2.503229380
H	-3.800024986	6.183496952	4.302359104
H	-1.555869460	6.823414326	4.333065510
H	0.311391264	5.662070274	3.529601336
H	-4.770783901	4.230728149	3.477421761
H	-3.741692066	2.395430326	2.460601091
C	0.577528417	3.278131723	2.327954769
H	1.576916456	3.690120697	2.384307384
C	0.222762331	2.042557716	1.765884876
H	0.909504116	1.351073146	1.286789179
C	-1.170983076	1.833968997	1.867596388
H	-0.832721770	0.346310496	3.459080458

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TS(A6-A7)

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C	0.857578993	5.751628876	6.347418308
C	2.219135284	5.369556427	6.227357388
C	4.379863739	4.816106319	7.129346371
C	4.881399632	4.304234028	8.463655472
O	2.890705347	5.530443192	5.092190266
O	2.918464422	4.893634796	7.226157665
H	4.632287025	4.141333103	6.307200909
H	4.758140087	5.813912868	6.905140400
H	4.596230507	4.981020927	9.273924828
H	4.482313633	3.309860229	8.683555603
H	5.972890377	4.245401859	8.436088562
C	0.241980687	5.794604301	7.719470024
C	0.948371470	6.325736523	8.814268112
C	-1.075636029	5.367750168	7.935120106
C	0.373516470	6.399010181	10.079187393
C	-1.658096552	5.446793556	9.201054573
C	-0.935156047	5.952281952	10.280447960
H	1.959159136	6.696709156	8.678045273
H	-1.664624214	4.993523121	7.105058670
H	0.942903697	6.831980228	10.897320747
H	-2.688207626	5.128775597	9.328424454
H	-1.390497088	6.015904427	11.264978409
C	0.310028791	1.497554302	5.025421143
C	-0.357429534	0.920450866	3.929966927
C	0.404575229	2.836600542	5.382547379
C	-1.121834278	1.526850581	2.939138889
C	-0.148316830	3.963730097	4.753045082
C	-1.442731142	2.886289120	2.790894985
C	-1.045833945	3.963149786	3.571233034
H	-0.269483089	-0.161905050	3.854540825
H	0.823692799	0.798112214	5.680835724
H	0.982399464	3.042186022	6.281261921
H	-1.550648928	0.860163152	2.195266724
H	-2.108059883	3.128346920	1.964222431
C	0.002661838	5.305904388	5.182940483
H	2.467099428	6.278433800	4.612125874

C	-0.794105172	6.118571758	4.339111805
H	-0.834488928	7.197052002	4.389124870
C	-1.443920732	5.325940609	3.355289459
H	-1.867311001	5.695481777	2.424942017
H	1.150984406	7.114703655	5.806665897
C	1.389905214	9.929062843	6.207255363
C	1.999955297	9.064720154	5.276661873
C	1.833942294	11.361828804	6.366981030
C	-0.009572745	9.592236519	6.610175133
O	1.567698002	7.851315022	4.969306469
O	3.013766527	9.517394066	4.511521339
C	3.912405491	8.558785439	3.911683559
C	5.015683651	9.341403008	3.224488735
H	4.315271378	7.911878586	4.698885441
H	3.360812187	7.946840763	3.189366341
H	4.602169991	10.008864403	2.462917089
H	5.578494549	9.940690041	3.945468664
H	5.708990574	8.647913933	2.737399578
C	3.176897526	11.782198906	6.253286362
C	0.877519488	12.344220161	6.682618141
C	3.534881592	13.115514755	6.435290337
H	3.949327946	11.061491966	6.015079498
C	1.239053249	13.678761482	6.860244274
H	-0.162526116	12.057695389	6.788649082
C	2.569206953	14.076862335	6.737433434
H	4.579263687	13.401711464	6.339769840
H	0.470178515	14.409906387	7.096267700
H	2.850676298	15.116736412	6.877357960
C	-3.505697250	9.288954735	3.678079605
C	-2.174894571	9.664333344	3.450899363
C	-1.119690776	9.750741005	4.365497589
H	-1.925439715	9.912240028	2.421481371
C	-4.140798092	8.936732292	4.872002602
H	-4.140468597	9.275023460	2.793158770
C	-1.125027895	9.510838509	5.738342285
H	-0.158994317	10.047840118	3.946824789
C	-3.610193491	8.893260956	6.167518616
H	-5.192712784	8.673324585	4.787904739
C	-2.312190771	9.165523529	6.586163521
H	-4.301132202	8.590229034	6.951119900
C	-1.856693983	9.118096352	7.914239883
C	-0.483545989	9.379215240	7.924121380
H	0.143875197	9.397300720	8.807906151
H	-2.467515945	8.879749298	8.774770737
O	2.789824247	9.288789749	9.643156052
Cu	2.779839516	9.145781517	7.629862785
O	4.654610634	8.321321487	7.568659306
C	3.817103386	9.081322670	10.336585045
C	5.399064541	8.314394951	8.592148781
C	5.085825443	8.633966446	9.918486595
C	3.608718872	9.358788490	11.840868950
C	6.855609894	7.906858921	8.283123016
H	5.863977909	8.546852112	10.661532402
F	4.733901978	9.208103180	12.570056915
F	3.160225153	10.609669685	12.031205177
F	2.686020374	8.507486343	12.339375496
F	6.894755363	6.690256596	7.685662746
F	7.411898136	8.786835670	7.430474758
F	7.640142441	7.838456631	9.374884605
O	-4.602338791	4.075865746	3.699515343
Cu	-3.212469339	5.403186321	4.467683315
O	-4.263494968	5.705593586	6.126093864
C	-5.632941723	3.747206688	4.342670441
C	-5.358241558	5.126889706	6.377501011
C	-6.070192814	4.204533577	5.599806786
C	-6.494895458	2.683462381	3.626949072
C	-5.937522888	5.499917507	7.758553028
H	-6.994996548	3.810055494	5.992942333
F	-7.616494179	2.360259295	4.304869652
F	-6.865530014	3.121933699	2.407431364
F	-5.780758858	1.549767137	3.456093550
F	-5.134461880	5.039043427	8.742145538
F	-6.019492149	6.839396000	7.894001484
F	-7.168328762	4.994856834	7.974369526

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C	0.718905866	5.081579208	6.873501301
C	2.066991091	4.899711609	6.743842125
C	4.260643482	4.927888870	7.746049881
C	4.853206635	4.479822636	9.069128990
O	2.750001431	4.912077904	5.565630913
O	2.842520237	4.640657425	7.806006432
H	4.706953526	4.388968468	6.904948235
H	4.406750202	6.001620293	7.588201523
H	4.388454437	5.013600826	9.903332710
H	4.702092171	3.406953573	9.220320702
H	5.926188946	4.689469337	9.081397057
C	0.118385337	5.293971539	8.222210884
C	0.614077330	6.278065681	9.094579697
C	-0.996779442	4.544289112	8.629960060
C	0.021820115	6.504655361	10.335533142
C	-1.586710453	4.764992237	9.874927521
C	-1.081413269	5.744887352	10.731245041
H	1.467939734	6.878678799	8.792752266
H	-1.408156276	3.783859968	7.973108292
H	0.412985295	7.286890984	10.980030060
H	-2.438890696	4.160511971	10.171697617
H	-1.545499444	5.919581413	11.698262215
C	0.584995508	2.137216806	3.402631760
C	-0.133123398	2.164258957	2.193581343
C	0.545156837	3.040575266	4.459795952
C	-1.119236708	3.048949957	1.767470241
C	-0.234496668	4.197684288	4.607566357
C	-1.675276518	4.137319088	2.461800337
C	-1.328425050	4.643519878	3.706655025
H	0.109450594	1.365746140	1.494599700
H	1.275687456	1.305694103	3.519374371
H	1.212830067	2.826802254	5.289790630
H	-1.538498998	2.855266094	0.783114851
H	-2.490642786	4.654416084	1.957181215
C	-0.183912247	5.094725132	5.709899902
H	2.243889332	5.440252304	4.928166389
C	-1.239561081	6.032632351	5.533341885
H	-1.426633358	6.868723869	6.196989059
C	-1.948704243	5.774097443	4.331550598
H	-2.594490051	6.478239059	3.817015409
H	0.857546985	7.575137138	5.084909916
C	1.629029751	9.847895622	5.497992039
C	2.350300312	8.765141487	4.970502377
C	2.143721104	11.262716293	5.557002068
C	0.147414193	9.646758080	5.611354828
O	1.766363740	7.559576988	4.726912022

O	3.582955360	8.865114212	4.471582413
C	4.411616325	7.669877052	4.361874104
C	5.858830929	8.112879753	4.440718651
H	4.158305645	6.981813908	5.169671535
H	4.178327560	7.190268993	3.405162573
H	6.086576462	8.855051994	3.669215679
H	6.076885223	8.534930229	5.424758911
H	6.510747433	7.247424126	4.282282829
C	3.459329844	11.657141685	5.208310604
C	1.254471540	12.277076721	5.986009598
C	3.851253510	12.993227005	5.286194801
H	4.180938244	10.921689987	4.871925831
C	1.652057886	13.609367371	6.061307907
H	0.235061198	12.019019127	6.263787270
C	2.956011295	13.982182503	5.711691856
H	4.871740341	13.258677483	5.003627300
H	0.932724178	14.358138084	6.395949364
H	3.267256260	15.021259308	5.768073082
C	-2.663614273	9.500664711	2.008512497
C	-1.274176836	9.660115242	2.054284811
C	-0.434448987	9.703703880	3.171417475
H	-0.778990924	9.757077217	1.090891004
C	-3.583464861	9.367848396	3.054986715
H	-3.095232248	9.482966423	1.009132385
C	-0.765261173	9.610404015	4.522789478
H	0.625272870	9.831476212	2.957002401
C	-3.345946550	9.370469093	4.433231831
H	-4.623806000	9.259493828	2.757595301
C	-2.132954597	9.482662201	5.112104893
H	-4.226364136	9.269489288	5.066737175
C	-1.973482966	9.471908569	6.510044098
C	-0.609689891	9.571118355	6.804147720
H	-0.180853754	9.595060349	7.800404072
H	-2.777726173	9.388990402	7.229875565
O	2.098072529	9.674616814	9.129899025
Cu	2.559183359	9.119963646	7.253604412
O	4.417403698	8.482924461	7.757095337
C	2.963857412	9.735259056	10.042788506
C	4.926571369	8.781369209	8.876184464
C	4.315951824	9.351097107	9.999876976
C	2.425451279	10.329192162	11.361754417
C	6.435032845	8.471859932	8.953097343
H	4.918824673	9.512781143	10.880418777
F	3.362391472	10.411789894	12.327926636
F	1.940961123	11.565452576	11.153689384
F	1.417850614	9.567105293	11.835856438
F	6.662096024	7.160467148	8.725817680
F	7.091510296	9.165552139	7.999728680
F	6.987411976	8.782029152	10.140732765
O	-5.383673668	5.308955193	5.816963673
Cu	-3.429866314	4.927688122	5.602864742
O	-3.471178055	3.243654966	6.726531982
C	-6.132786751	4.572895527	6.519156456
C	-4.522546291	2.865301371	7.310446739
C	-5.811602592	3.419317961	7.250749588
C	-7.594413280	5.065291405	6.556456566
C	-4.310093403	1.630161881	8.209680557
H	-6.599576950	2.938000917	7.810097218
F	-8.405608177	4.275151730	7.290758133
F	-7.653626919	6.308371544	7.078378201
F	-8.100402832	5.120162964	5.306723118
F	-3.813265800	0.605987012	7.493034363
F	-3.419502258	1.918492675	9.184503555
F	-5.440613747	1.202509761	8.807053566

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TS(A4-A7)

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Cu	-0.096402369	-0.224414423	0.406345278
O	1.434663415	-1.252348781	-0.285604656
O	0.989293993	1.578045487	0.363825172
C	2.520580769	-0.742683649	-0.680683374
C	2.145059586	1.639183640	-0.134241149
C	2.936728716	0.595742464	-0.641137064
H	3.912335396	0.837882340	-1.034189939
C	3.479982376	-1.778884888	-1.301359177
F	4.659049511	-1.246569872	-1.687970757
F	3.743991375	-2.759848118	-0.419611663
F	2.912606955	-2.341478348	-2.386008263
C	2.707145691	3.074458361	-0.208872706
F	1.945605993	3.819109440	-1.045759916
F	2.673919678	3.659872293	1.007309556
F	3.980722904	3.127949476	-0.658265531
C	-2.664268494	0.525833547	-0.723216534
C	-4.023715973	0.373565555	-1.047096252
C	-1.850463271	1.249958396	-1.602770090
H	-4.675168991	-0.174456611	-0.371556401
H	-0.804177403	1.413069725	-1.359857798
C	-4.544432163	0.906129122	-2.223532438
C	-2.373882055	1.790555120	-2.781353235
H	-5.597050667	0.768082500	-2.456709623
H	-1.721995234	2.347847939	-3.448546648
C	-3.719654083	1.618408918	-3.099106073
H	-4.125538349	2.036896467	-4.015800476
C	-2.181969881	-0.047894202	0.600786686
O	-2.258777857	-2.051817417	1.954793692
C	-2.335063219	-1.505491138	0.858455837
O	-2.531543493	-2.195529699	-0.287355542
C	-2.845770121	-4.196766853	-1.547362566
H	-2.855182409	-5.290858746	-1.509480357
H	-3.825130224	-3.854882717	-1.895707726
H	-2.092835665	-3.883176327	-2.276134253
C	-2.533640146	-3.637052774	-0.171866089
H	-1.552085996	-3.960944414	0.189817458
H	-3.277660370	-3.933972836	0.573777080
C	-5.885281563	0.577867329	4.987134933
C	-5.341317654	-0.396300465	4.152424812
C	-4.324700832	-0.286427200	3.191095352
C	-5.555227280	1.935322285	5.089642048
C	-3.603114367	0.838098764	2.805099010
C	-4.605870724	2.648022890	4.362562180
C	-3.748333931	2.206079960	3.349273205
H	-6.672421455	0.236221164	5.656195164
H	-5.758221149	-1.394273877	4.264496326
H	-4.047938347	-1.212209463	2.702359200
H	-6.115878105	2.506689787	5.825257301
H	-4.525002480	3.708166122	4.598843575
C	-2.575282812	0.914865911	1.791362166
H	-1.439875364	0.350366741	1.751331687
C	-2.151547670	2.289611578	1.735545754
H	-1.365751743	2.642393827	1.077684045
C	-2.843348265	3.046246767	2.658864021
H	-2.709485531	4.103103638	2.850098133

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A7

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C	0.981426299	5.540881634	6.538434505
C	2.486932993	5.387676239	6.257246971
C	4.431103230	4.049672604	6.504055023
C	4.853905201	2.787554264	7.232007504
O	3.134641886	6.207858086	5.641890049
O	3.012924194	4.242078781	6.741427422
H	4.599379539	3.980581284	5.424666405
H	4.968039989	4.932052135	6.864851952
H	4.666080952	2.873512983	8.306356430
H	4.314561367	1.913412452	6.855120182
H	5.925259113	2.617500305	7.083696365
C	0.573130965	5.303185463	7.997410297
C	1.473573089	5.544186592	9.044710159
C	-0.743371665	4.946799755	8.316416740
C	1.073849559	5.411736488	10.374208450
C	-1.145690799	4.817973137	9.646728516
C	-0.237485170	5.045216560	10.680406570
H	2.497137547	5.837125778	8.828021049
H	-1.470554233	4.766427040	7.531267166
H	1.789849401	5.596278191	11.170714378
H	-2.174203396	4.545721531	9.862473488
H	-0.548381090	4.941158295	11.716285706
C	0.401138335	0.997976422	6.176068783
C	-0.216831222	0.214863449	5.201824188
C	0.510774672	2.391913652	6.250444889
C	-0.922131240	0.608978629	4.056648254
C	-0.003856643	3.360306740	5.388965607
C	-1.224536777	1.897878647	3.626879930
C	-0.873794854	3.124953270	4.205884933
H	-0.134797946	-0.860530674	5.348268032
H	0.887733936	0.450875312	6.980063438
H	1.095965862	2.769302845	7.082144260
H	-1.295588374	-0.197618142	3.430938959
H	-1.811303020	1.970739007	2.712105989
C	0.176496744	4.769835949	5.505791187
C	-0.533373058	5.379389286	4.464980125
H	-0.545554757	6.446969509	4.274085999
C	-1.200316548	4.405042648	3.663859367
H	-1.576897621	4.573144436	2.659414053
H	0.811929405	6.601097107	6.319222450
O	-4.677839756	5.287347317	3.884734869
Cu	-3.037192583	4.445025921	4.692750931
O	-3.858922482	4.123650074	6.480340004
C	-5.722173214	5.466802597	4.565345764
C	-5.038538933	4.495753288	6.741508961
C	-5.971235752	5.127430916	5.907274246
C	-6.848606586	6.155245781	3.767997265
C	-5.458724499	4.180233002	8.190587044
H	-6.939141750	5.368980408	6.319113255
F	-7.963345528	6.371671200	4.496744156
F	-6.425544739	7.345731258	3.304278135
F	-7.192811966	5.398935795	2.708195210
F	-5.404457569	2.854700089	8.413636208
F	-4.612731457	4.775423050	9.060464859
F	-6.705275059	4.597653866	8.490502357

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B1

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Ag	4.681376934	-1.474266410	-2.715120554
O	4.210812092	0.197821707	-4.279291153
S	5.418848515	1.019643426	-3.881602764
O	5.985451698	0.464963853	-2.592670441
O	5.296311855	2.467145681	-3.981706858
C	6.685886860	0.479886115	-5.135544777
F	6.838129997	-0.860672355	-5.054326534
F	7.863147259	1.054641604	-4.893591881
F	6.286770821	0.785915911	-6.368929386

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B2

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Ag	4.743606567	-1.710695267	-2.519830704
O	4.177431107	-0.181150973	-4.084354401
S	5.169365406	0.905857921	-3.702080488
O	5.781409264	0.575157702	-2.377187252
O	4.730947018	2.277096033	-3.937167406
C	6.562492847	0.575625598	-4.892684460
F	6.984181881	-0.699369669	-4.736691952
F	7.592918873	1.390371442	-4.651521206
F	6.165807724	0.735379815	-6.157000542
C	3.184109688	-4.671567440	-2.393893480
C	3.714169025	-4.237157822	-1.166894674
C	2.980114222	-4.442267895	0.009881845
C	5.055094719	-3.544812441	-1.143271804
H	3.736136675	-4.505828381	-3.316542864
C	1.946963310	-5.308367729	-2.442825079
H	3.366717577	-4.091993809	0.957975328
C	1.733109832	-5.064917564	-0.052521493
H	1.550881743	-5.636299133	-3.399078608
C	1.213713408	-5.502478600	-1.270757556
H	1.167276621	-5.207406998	0.863521576
H	0.241178453	-5.983875751	-1.309107780
C	5.582008362	-2.800537586	0.060357802
N	6.031219959	-4.224555969	-1.799286842
O	4.870321751	-2.371706009	0.941565216
O	6.914514065	-2.665849209	0.001883458
C	7.526845932	-1.871585727	1.063600063
C	9.023834229	-1.885504246	0.831676543
H	9.516764641	-1.297489405	1.612320185
H	9.419243813	-2.905044794	0.870447159
H	9.275308609	-1.446843863	-0.137951329
H	7.105950356	-0.863467038	1.015253067
H	7.248769760	-2.314133883	2.024379730
N	6.830352306	-4.786913395	-2.362963915

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TS(B2-B3)

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Ag	2.170630455	0.000088883	-0.132087052
C	0.015318239	-0.237548783	-0.153200522
C	-0.576182663	0.999463797	0.446407944
C	-1.043623686	2.248118639	2.412025452
C	-1.415780187	1.951950073	3.850837708
O	-0.818015218	1.949511766	-0.271428436
O	-0.692953587	0.980003536	1.779666901
H	-0.173304275	2.906617403	2.336424589
H	-1.866218090	2.697972059	1.850786448
H	-2.283069134	1.287070870	3.904691219
H	-0.583153486	1.487259269	4.386174679
H	-1.669892550	2.886904478	4.359728813

C	-0.633732796	-0.851193547	-1.325210810
C	0.093623474	-1.760668755	-2.118224859
C	-1.956529498	-0.532839358	-1.696429372
C	-0.478838414	-2.334661961	-3.248089314
C	-2.519300461	-1.093220115	-2.837450266
C	-1.785395503	-1.998122096	-3.610252619
H	1.116829634	-2.002104282	-1.842193842
H	-2.522920132	0.184266299	-1.112690806
H	0.095485322	-3.029830933	-3.852266073
H	-3.530795813	-0.825704634	-3.127027988
H	-2.229883432	-2.434532404	-4.500020027
O	4.343799114	0.105668813	-0.295613974
S	4.769881248	1.054213047	0.821290374
O	6.030881882	1.747717500	0.577726066
O	3.601476431	1.831717372	1.305240273
C	5.097346306	-0.153019309	2.201886654
F	5.421340942	0.489604831	3.327514887
F	6.082716942	-0.996152580	1.883491278
F	3.980654001	-0.880473614	2.438519001
N	-0.217201695	-1.444008708	1.157371521
N	-0.110619709	-2.328454494	1.818504810

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B3

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Ag	-0.581707716	1.978531718	6.739452362
C	0.272545487	2.750656366	4.992208004
C	0.897256553	1.789721131	4.060494423
C	2.680849075	0.256137699	3.716846228
C	3.906601667	-0.209414706	4.476796627
O	0.322256774	1.440949559	3.044502974
O	2.066758871	1.320225120	4.501734734
H	1.944248796	-0.541755438	3.586361170
H	2.929235220	0.651970685	2.727310419
H	4.621480942	0.607655585	4.609194756
H	3.630920410	-0.592303038	5.463406086
H	4.400011063	-1.012631297	3.920830250
C	0.254801989	4.126487255	4.663666725
C	-0.332262665	5.055452347	5.576910019
C	0.820564747	4.626190186	3.448615074
C	-0.334812790	6.412006378	5.289299488
C	0.798177838	5.978679657	3.168520451
C	0.224304944	6.869547844	4.090881348
H	-0.759669125	4.691116810	6.508859634
H	1.241285801	3.926791668	2.733973503
H	-0.774382591	7.114136219	5.989925861
H	1.219728827	6.354709148	2.241824389
H	0.212849110	7.932889938	3.866686821
O	-1.481171250	1.423027635	8.609691620
S	-1.883367181	2.699432373	9.346014023
O	-1.864202738	2.576720238	10.800012589
O	-1.252793670	3.891050816	8.725369453
C	-3.671313286	2.840080261	8.849769592
F	-4.219148636	3.934000015	9.389066696
F	-4.364659786	1.768355489	9.239123344
F	-3.757246494	2.940509319	7.507666588

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TS(B3-B4)

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Ag	1.870667100	1.169023871	5.642396927
C	0.362140357	2.512322664	4.965311050
C	-0.652685165	2.808405876	6.017225266
C	-2.544627190	1.864857197	7.108981609
C	-3.504350185	0.708551884	6.906064034
O	-0.638725698	3.704633713	6.845690727
O	-1.601189852	1.840796471	6.007090092
H	-1.988252044	1.779950023	8.047937393
H	-3.056980610	2.832075596	7.114080906
H	-4.044207096	0.808197498	5.959660053
H	-2.970646858	-0.245968431	6.899599075
H	-4.236356735	0.689445138	7.719759464
C	-0.035329089	2.498712301	3.575257540
C	-1.313190937	2.937689304	3.136067629
C	0.860101223	2.002976179	2.593673944
C	-1.684331179	2.838061333	1.803502321
C	0.488822192	1.916848421	1.255453348
C	-0.784663856	2.328052044	0.858280003
H	-2.021318197	3.324513912	3.860455751
H	1.843235731	1.666729689	2.908629179
H	-2.676125288	3.153964758	1.492650986
H	1.187543035	1.516942382	0.526642323
H	-1.081214428	2.247139692	-0.183984190
S	4.708320141	0.132139742	5.610531330
C	5.761888981	-0.060219537	7.130421162
O	3.356122494	-0.350963116	6.121847630
O	5.312469006	-0.729497433	4.591311455
O	4.687813759	1.595079541	5.355922222
F	7.007096767	0.362682551	6.877150059
F	5.808328152	-1.343091965	7.507017612
F	5.261661053	0.667048216	8.140912056
C	1.028933525	6.109221458	1.881167173
C	-0.111499280	6.894043922	1.709076047
C	-1.099079013	7.220529556	2.646604300
C	-1.208144307	6.841802120	3.986385584
C	-0.359937578	6.026844978	4.748855114
C	0.812383473	5.393607140	4.349826813
C	1.466417789	5.448249340	3.030368328
C	2.672028780	4.698266983	3.135518789
C	2.783308744	4.190071106	4.417721748
C	1.620242000	4.542355061	5.169200897
H	1.670910239	6.003900051	1.008511543
H	-0.246555716	7.317162991	0.716451287
H	-1.895496249	7.863443375	2.277478456
H	-2.074761868	7.233645439	4.513922215
H	-0.657986104	5.842875957	5.777691364
H	1.499901652	4.447088242	6.237891197
H	3.598345280	3.567559481	4.772810936
H	3.383502722	4.562121391	2.330650568

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B4

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Ag	-2.848693609	4.620157242	6.252839565
C	-1.357409835	5.795849800	5.091126919
C	-1.924180031	7.156152725	5.210373402
C	-3.774894476	8.574582100	4.744259834
C	-5.126779079	8.469323158	4.062930584
O	-1.445021749	8.068946838	5.887394428
O	-3.089808702	7.323538303	4.529687881
H	-3.872586012	8.748085022	5.820631981
H	-3.171833277	9.393077850	4.334539890
H	-5.014516830	8.287789345	2.989949465
H	-5.711614132	7.648901463	4.489265919

H	-5.686786175	9.399903297	4.199869156
C	-1.328700185	5.126960754	3.733120441
C	-1.415061474	5.854826927	2.531600952
C	-1.150720477	3.732840538	3.629714489
C	-1.338998795	5.220542431	1.290727496
C	-1.057576656	3.101118088	2.390019894
C	-1.151665211	3.840349436	1.209628701
H	-1.570625544	6.928217888	2.564586639
H	-1.122491956	3.124773264	4.530629158
H	-1.425914884	5.812285423	0.382813007
H	-0.934591234	2.021972418	2.352338791
H	-1.095865965	3.346077204	0.243840232
S	-3.086136341	1.839493155	7.500939846
C	-2.634643316	1.853824735	9.305389404
O	-3.949223042	3.085447550	7.394134045
O	-3.802667618	0.585357070	7.271931171
O	-1.773818254	2.018078089	6.822270870
F	-1.841072798	0.814015090	9.592858315
F	-3.724365234	1.789654970	10.075671196
F	-1.967092037	2.986662865	9.601402283
C	2.374859095	7.832117081	3.610560894
C	3.586745262	7.222476006	3.307560205
C	1.323137045	7.359980106	4.414257050
C	4.079165936	5.982563972	3.752002954
C	1.226462245	6.145611286	5.077161789
C	3.479126453	5.046860218	4.581496716
C	2.199235201	5.094012260	5.167662144
H	4.250837326	7.782303333	2.653782606
H	2.217707157	8.814483643	3.170959234
H	0.473252863	8.024737358	4.545382500
H	5.074883461	5.724695683	3.398119450
H	4.064696312	4.157624722	4.805144787
C	0.001666990	5.729990959	5.863534451
H	-0.125969291	6.452760220	6.687434673
C	0.405644268	4.397464752	6.407059669
H	-0.249275744	3.775738478	7.010699749
C	1.659738660	4.058090687	6.009006500
H	2.187413216	3.146056652	6.261938572

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TS(B4-B8)

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Ag	-2.043086529	4.690597534	6.474931717
C	-1.231668830	6.202996731	4.746829987
C	-2.603879213	6.787996292	4.680295467
C	-4.874497414	6.364007473	4.063298225
C	-5.697344780	5.110449314	3.829126120
O	-2.903792858	7.870277882	5.162708759
O	-3.476756334	5.969359875	4.054721832
H	-5.098520756	6.833196163	5.024601460
H	-5.022558689	7.113513470	3.276831150
H	-5.435468674	4.640110493	2.876137733
H	-5.533318996	4.389631271	4.635754108
H	-6.761044502	5.368906975	3.803349495
C	-0.782888889	5.194118023	3.726530552
C	-0.889492631	5.548761368	2.369562626
C	-0.220705509	3.949223518	4.040735245
C	-0.471242875	4.678665638	1.365696073
C	0.207945779	3.079547882	3.035307646
C	0.082858592	3.439834118	1.695015192
H	-1.326216340	6.506964684	2.100643158
H	-0.105949536	3.651404381	5.080423832
H	-0.581385672	4.968146324	0.324039578
H	0.631456494	2.116421223	3.305518389
H	0.408674031	2.760564804	0.912588656
S	-3.649351358	2.954319954	8.185815811
C	-3.371556997	1.176755786	7.708356857
O	-2.244922638	3.439998150	8.458099365
O	-4.568948269	2.936353683	9.320712090
O	-4.144762516	3.577198029	6.909656048
F	-4.520788193	0.605137944	7.333716393
F	-2.859004259	0.490298808	8.734576225
F	-2.505849361	1.114245296	6.678585052
C	3.161633015	7.469422817	3.253790140
C	4.182641029	6.735815525	3.788051844
C	1.814137340	7.605780125	3.726161957
C	4.175711155	5.911531448	4.964946747
C	1.234709501	7.037573814	4.821305275
C	3.166023731	5.662034512	5.848350048
C	1.821016312	6.171474934	5.843896866
H	5.131383896	6.771331310	3.257499933
H	3.387755394	8.022068024	2.344623804
H	1.172857285	8.243795395	3.121257544
H	5.121211052	5.417280674	5.177880287
H	3.400234699	4.996827602	6.677283764
C	-0.206394091	7.262059689	5.203173637
H	-0.590658009	8.277132988	5.107219219
C	-0.351505816	6.576317787	6.512746811
H	-1.103364944	6.900881767	7.223965645
C	0.872542560	5.903794289	6.820537567
H	1.027751565	5.271351814	7.686388016

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C	2.027175426	7.564746380	5.331480503
C	2.843536615	6.338421345	5.127009869
C	4.303812027	4.728306770	6.098708153
C	4.904731750	4.451786995	7.462190628
O	2.913126469	5.687243462	4.077606678
O	3.538200378	5.961756706	6.205315590
H	3.629283905	3.931325674	5.773131371
H	5.066350937	4.861062050	5.325923443
H	5.566972733	5.264510155	7.773838997
H	4.123479843	4.330253124	8.218112946
H	5.489359856	3.527525902	7.422452450
C	1.325005054	8.080383301	4.107100964
C	0.041314479	7.615772724	3.773842573
C	1.957608700	8.993724823	3.251454592
C	-0.601061821	8.056411743	2.608181000
C	1.317090273	9.436373711	2.093685865
C	0.039552502	8.969569206	1.770328045
H	-0.472731769	6.918181896	4.426748753
H	2.951014280	9.358109474	3.497959614
H	-1.582084060	7.664937973	2.356543779
H	1.817788601	10.144290924	1.439052343
H	-0.453257561	9.310367584	0.864370823
C	-2.237551689	8.817583084	7.555823326
C	-2.460946083	10.148247719	7.372375011
C	-1.023068666	8.073745728	7.337204456
C	-1.541371465	11.169090271	6.929087639
C	0.188334927	8.528846741	6.921279430
C	-0.222379193	11.071532249	6.615362167
C	0.636863112	9.908404350	6.644300461

H	-3.468586683	10.500938416	7.581329823
H	-3.084205866	8.223625183	7.892205715
H	-1.099120498	7.002607346	7.516880989
H	-1.977705598	12.161749840	6.839760780
H	0.271879047	11.991003036	6.306920052
C	1.371868134	7.643122673	6.746802330
H	1.466437817	6.750699997	7.354015350
C	2.539099932	8.540884018	6.434660912
H	3.535101175	8.343703270	6.816537857
C	1.979195356	9.911517143	6.393179893
H	2.566524506	10.790835381	6.158113956
O	-1.131796718	4.627845764	3.397904634
Ag	1.217691541	5.424488544	2.584142923
C	-2.109349012	2.777215958	1.765810609
S	-1.526294112	4.532495499	1.963018417
O	-2.643753529	5.375013828	1.522300363
O	-0.291538239	4.587210655	1.084892988
F	-2.437637091	2.530701876	0.493724525
F	-3.181353092	2.566509485	2.538663149
F	-1.142581105	1.925200939	2.134913206

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TS(B4-B5)

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Ag	-2.718749285	4.355007648	6.042196274
C	-1.300350428	5.717597961	4.930077553
C	-1.943342090	6.952126026	5.349130154
C	-3.762304544	8.481998444	5.416828632
C	-5.086587906	8.657264709	4.700500011
O	-1.402637720	7.634966373	6.276063442
O	-3.083336353	7.359195232	4.790830612
H	-3.897169113	8.255208015	6.478516102
H	-3.124100447	9.367044449	5.337067127
H	-4.935779095	8.872382164	3.638471603
H	-5.698625565	7.755230904	4.789235592
H	-5.636810303	9.492125511	5.145413876
C	-1.384362221	5.119211674	3.555506945
C	-2.288942337	5.547064781	2.562558889
C	-0.513831794	4.061043739	3.219957113
C	-2.314620733	4.941692829	1.305627584
C	-0.543473542	3.461441755	1.963950396
C	-1.445768952	3.896523714	0.991946161
H	-2.982510567	6.349564075	2.776595592
H	0.183091268	3.685916424	3.963257074
H	-3.027730942	5.295476437	0.565379441
H	0.138211936	2.642342567	1.750532508
H	-1.475469708	3.425061464	0.014218474
S	-3.515822172	1.834053040	7.421475887
C	-2.594877720	2.072246313	9.024125099
O	-4.172954559	3.194342613	7.249603748
O	-4.445667267	0.732901990	7.661624908
O	-2.425614595	1.646838903	6.432018280
F	-1.878735185	0.984550297	9.327070236
F	-3.427681446	2.335743904	10.033983231
F	-1.735027552	3.118628740	8.912754059
C	2.383571148	7.671781063	3.238083601
C	3.740925074	7.523725986	3.509509563
C	1.285615683	7.108024120	3.902841568
C	4.363443851	6.752874374	4.503438950
C	1.279129863	6.224962711	4.973947525
C	3.783748150	5.919385910	5.453272343
C	2.424582481	5.642017841	5.664306164
H	4.413425446	8.081865311	2.862021923
H	2.138038635	8.323112488	2.402590990
H	0.306914419	7.386613846	3.520699739
H	5.449441433	6.805676460	4.524021626
H	4.473891258	5.401283741	6.116172314
C	0.065199882	5.729430676	5.630042076
H	-0.314437747	6.760372639	6.303462982
C	0.545371115	4.754567146	6.600191593
H	-0.107972227	4.158452034	7.228872776
C	1.921153307	4.739964962	6.643285751
H	2.536052704	4.158292294	7.318795204

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Ag	-2.980279207	5.943822384	5.848526001
C	-0.789940178	6.778492928	5.581244946
C	-0.978148341	7.545338631	6.738336563
C	-2.196037531	9.138031006	8.047016144
C	-3.086796761	10.329290390	7.760955811
O	-0.436993986	7.204177380	7.916976452
O	-1.649207711	8.693706512	6.769614220
H	-2.758006811	8.306264877	8.486296654
H	-1.368005395	9.389883995	8.714540482
H	-2.518370152	11.143261909	7.301887512
H	-3.907010555	10.052574158	7.092914581
H	-3.514860630	10.695582390	8.699169159
C	-1.126636863	7.233114243	4.184542179
C	-1.459436774	8.556442261	3.834717751
C	-1.090926170	6.270314217	3.153906822
C	-1.757651329	8.888800621	2.512847900
C	-1.391453385	6.609306812	1.838094115
C	-1.730655670	7.922449112	1.507180810
H	-1.486959577	9.326597214	4.593970776
H	-0.834247887	5.244040489	3.395540953
H	-2.012216806	9.917201042	2.271147490
H	-1.367353678	5.839288712	1.072399616
H	-1.971530318	8.187171936	0.482005298
S	-5.111654282	3.968353271	5.529011250
C	-4.653981209	2.778648376	6.888299942
O	-5.097367287	5.295733929	6.268703461
O	-6.417420864	3.537989140	5.038074017
O	-3.943728209	3.891552925	4.606366158
F	-4.520133495	1.538532853	6.410630226
F	-5.572236538	2.775181055	7.856770515
F	-3.468321562	3.147827387	7.435827732
C	3.545258760	7.114466190	4.479767323
C	4.607563019	6.212502956	4.555373669
C	2.208802462	6.926034451	4.850866795
C	4.627151489	4.889412403	5.014611244
C	1.597961903	5.795004368	5.383994579
C	3.573869228	4.126101494	5.517714500
C	2.234490395	4.481850147	5.692895889
H	5.564465523	6.593654633	4.202918530
H	3.786204576	8.094959259	4.076268673
H	1.554538846	7.780364513	4.690914154
H	5.592571259	4.391051292	4.970367432
H	3.825366497	3.108706713	5.815092087
C	0.222468942	5.679815292	5.733892441
H	0.080828674	6.388660908	7.770244598
C	0.021950927	4.368386269	6.225524426
H	-0.935620964	3.969013691	6.548014164

C	1.226440191	3.650074959	6.207387924
H	1.361838222	2.624160290	6.525216103

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C	0.980188072	4.431901455	6.818547726
C	2.336611032	4.339323521	6.636898994
C	4.614537716	4.452000141	7.434576035
C	5.330566406	4.067896366	8.715441704
O	2.930839539	4.369186401	5.415709019
O	3.203973055	4.152414322	7.634944916
H	4.984334946	3.878089666	6.581071854
H	4.726553917	5.519445419	7.216743946
H	4.952082157	4.642007828	9.565035820
H	5.207818031	3.001488924	8.927298546
H	6.396999836	4.287065506	8.613241196
C	0.291054726	4.468758583	8.133072853
C	0.957622230	4.682348728	9.360595703
C	-1.109322667	4.313045502	8.183586121
C	0.253126830	4.723371983	10.561603546
C	-1.811538339	4.359675407	9.386393547
C	-1.134201884	4.562317848	10.588784218
H	2.031070948	4.803800583	9.376146317
H	-1.674608350	4.161706448	7.271150589
H	0.799560726	4.883489132	11.488220215
H	-2.891674519	4.246404648	9.365549088
H	-1.675576687	4.594707489	11.530401230
C	-0.271324784	0.661120236	4.799763203
C	-0.921382129	0.404107630	3.586447716
C	0.052747015	1.891651511	5.371341228
C	-1.443094492	1.299980402	2.648274899
C	-0.229257077	3.177796841	4.901166439
C	-1.492703676	2.695533752	2.705593348
C	-1.003460288	3.544338465	3.699207544
H	-1.036433816	-0.648378551	3.335571051
H	0.038225658	-0.215868726	5.362709045
H	0.599775493	1.861924887	6.312069416
H	-1.893437266	0.850467622	1.766978860
H	-1.991596818	3.187986851	1.871599317
C	0.163030207	4.381464958	5.565881252
H	2.273593187	4.686526775	4.778039932
C	-0.368983120	5.450933456	4.828360081
H	-0.242565095	6.498830795	5.069723606
C	-1.104812980	4.977216244	3.697501659
H	-1.311012268	5.563068867	2.804518700
Ag	-3.211366177	5.250627995	4.561266899
C	-6.598866940	3.816529751	6.574692249
F	-6.760139465	3.573933363	7.879186630
O	-4.266129971	5.040287971	6.948502064
O	-6.367264748	6.442965031	6.954040051
S	-5.589443684	5.361763000	6.338831425
O	-5.451076984	5.446877003	4.830617428
F	-5.969755650	2.770276070	6.017226219
F	-7.798889160	3.949366331	6.003840446
H	1.557721376	7.296964645	6.211915970
Ag	3.635675192	9.902104378	7.472183228
C	1.772344232	9.685831070	6.046672344
O	5.703615189	8.153952599	6.775964737
C	2.455280542	8.702198982	5.314365864
C	1.875384688	11.169613838	5.796880245
C	0.565442443	9.171285629	6.775361538
O	2.194272995	7.395706654	5.476771832
O	3.372064352	8.953338623	4.395678997
C	4.269074917	7.873258591	3.965289593
C	5.449005127	8.523880959	3.275918484
H	4.582567692	7.316637516	4.848118782
H	3.701270819	7.219630241	3.295677423
H	5.130276203	9.140435219	2.429865837
H	6.010588169	9.137912750	3.984110355
H	6.117309093	7.742457867	2.899735689
C	2.674336433	11.764105797	4.796643257
C	1.127660275	12.033334732	6.628345013
C	2.729763746	13.150982857	4.656690598
H	3.255514383	11.143635750	4.129460335
C	1.188648462	13.416046143	6.480113506
H	0.494174987	11.606566429	7.399285316
C	1.995046139	13.989317894	5.494942188
H	3.358171940	13.575451851	3.878188610
H	0.601348341	14.046663284	7.142178535
H	2.046230078	15.067905426	5.381202221
S	6.488400459	8.940478325	7.768628597
C	6.792851448	7.730543613	9.148638725
O	7.804018497	9.428002357	7.358084679
O	5.610923767	9.972856522	8.457880020
F	7.422369957	8.314574242	10.168231964
F	7.538094044	6.706354618	8.705976486
F	5.619808674	7.238129139	9.590144157
C	-3.610251904	9.163202286	4.910599232
C	-2.391535521	9.598210335	4.377424240
C	-1.124547958	9.587734222	4.971772194
H	-2.435133934	10.009374619	3.371206760
C	-3.892410278	8.598304749	6.161803722
H	-4.472321987	9.278956413	4.255411625
C	-0.752376080	9.139572144	6.238496780
H	-0.317403495	9.995637894	4.365086555
C	-3.009565353	8.316269875	7.209470749
H	-4.928762436	8.323830605	6.339688301
C	-1.633434534	8.545136452	7.286904335
H	-3.456829071	7.843505383	8.081692696
C	-0.814011574	8.241493225	8.388009071
C	0.498286337	8.623598099	8.079125404
H	1.350692630	8.515586853	8.745735168
H	-1.143832207	7.768785954	9.303886414

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TS(B6-B7)

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C	1.434018135	5.359901905	6.199109077
C	2.736988306	4.909326077	5.825631142
C	4.934957027	4.035928726	6.277373314
C	5.557383060	3.251367807	7.412471771
O	3.227984905	5.181263447	4.628319740
O	3.512916327	4.225876808	6.618191242
H	4.979332447	3.501191139	5.325668812
H	5.371897221	5.029301167	6.167962551
H	5.504714966	3.811875582	8.347865105
H	5.065248966	2.283472300	7.545866966
H	6.612508774	3.071909428	7.182458401
C	1.085340023	5.467237473	7.658181190
C	2.048771858	5.891161442	8.609582901
C	-0.225866780	5.269547939	8.110705376
C	1.688141704	6.128032207	9.942613602
C	-0.583264351	5.510504246	9.441568375

C	0.363732129	5.952679157	10.361960411
H	3.092759609	5.963290691	8.328999519
H	-0.999223053	4.927157879	7.434572697
H	2.458406448	6.424137115	10.650196075
H	-1.618523598	5.362918377	9.735774994
H	0.086073101	6.141774178	11.394732475
C	-0.031442903	1.141929150	5.840398788
C	-0.961629331	0.526672661	4.990665436
C	0.353451490	2.479462385	5.892345428
C	-1.756125450	1.084308505	3.988327503
C	-0.096043661	3.555506468	5.117388248
C	-1.844843984	2.422935486	3.589336157
C	-1.147922635	3.525150299	4.074471474
H	-1.082669377	-0.544937670	5.136754036
H	0.458971083	0.483635843	6.553299427
H	1.108412027	2.726041555	6.635913849
H	-2.404040575	0.391080946	3.457960606
H	-2.561014652	2.635140657	2.796390772
C	0.368346363	4.894834518	5.227983475
H	2.800992489	6.017434120	4.323604107
C	-0.351148605	5.671347618	4.295553207
H	-0.174469739	6.720851421	4.100379944
C	-1.295056701	4.865503311	3.603001356
H	-1.814152122	5.141068935	2.690662622
Ag	-2.872693300	5.844036579	5.101979733
C	-5.795918941	4.082237720	7.833149910
F	-5.542626858	3.257104397	8.855176926
O	-3.222144604	4.374227524	7.251393795
O	-4.262379169	6.009797096	8.858944893
S	-4.372983932	5.257116318	7.603383541
O	-4.794442177	6.068245888	6.397515297
F	-5.974040031	3.349851370	6.724156380
F	-6.920466900	4.757192612	8.088225365
H	1.616626740	6.728282928	5.597202778
Ag	2.161379814	8.444302559	8.091996193
C	1.245938420	9.466784477	6.090071201
O	4.567027092	7.171202660	6.840945721
C	2.126906633	8.767405510	5.236539841
C	1.525247455	10.891565323	6.504262924
C	-0.192948475	9.052837372	6.033586979
O	1.912276745	7.530367851	4.811131954
O	3.208418369	9.377722740	4.758020401
C	4.187510490	8.631407738	3.984344244
C	5.355585575	9.565344810	3.733786106
H	4.494646072	7.759024620	4.563501835
H	3.712582588	8.310642242	3.049998045
H	5.029359341	10.475363731	3.221274614
H	5.834940910	9.832048416	4.678732872
H	6.093758583	9.059084892	3.102674007
C	2.825540066	11.370152473	6.776926994
C	0.457625270	11.792246819	6.680776119
C	3.037424803	12.680281639	7.196610451
H	3.681347847	10.714558601	6.675439358
C	0.675195336	13.104193687	7.101667404
H	-0.557862997	11.462409973	6.492809296
C	1.965836644	13.560146332	7.361849308
H	4.052330017	13.009175301	7.403400421
H	-0.175166279	13.769996643	7.225862026
H	2.135470629	14.580680847	7.693310738
S	5.293333054	8.110457420	7.747388363
C	6.338911057	6.958526134	8.765464783
O	6.228685856	9.034564018	7.097264767
O	4.390116215	8.717482567	8.780151367
F	7.082056046	7.622608185	9.649108887
F	7.147297859	6.239499569	7.968172550
F	5.545380592	6.095098495	9.435277939
C	-2.781352758	9.587348938	2.297647238
C	-1.416618824	9.823102951	2.483880758
C	-0.646176040	9.655275345	3.641841888
H	-0.882176936	10.204141617	1.616978407
C	-3.746155739	9.128651619	3.202911139
H	-3.154834747	9.805053711	1.298261523
C	-1.033888459	9.189981461	4.894537449
H	0.401692212	9.936838150	3.554264307
C	-3.582271099	8.770000458	4.543756485
H	-4.758948803	9.048381805	2.815160036
C	-2.411210537	8.769316673	5.311245441
H	-4.478791237	8.450369835	5.074372292
C	-2.326717854	8.405945778	6.671832085
C	-1.000100374	8.589791298	7.090818882
H	-0.646217942	8.397486687	8.099413872
H	-3.151893854	8.068560600	7.285953045

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B7

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C	1.594494820	8.445208549	4.894057751
C	0.239602029	9.127655983	5.157327652
C	-1.926718235	9.568996429	4.260369301
C	-2.563032389	9.560475349	2.884433270
O	-0.009720814	9.759596825	6.161248684
O	-0.624267519	8.927404404	4.149006844
H	-2.520160437	9.006488800	4.989496708
H	-1.779215574	10.578447342	4.652847767
H	-1.945964456	10.114017487	2.169399977
H	-2.703840017	8.540319443	2.518316984
H	-3.543928623	10.044707298	2.936114550
C	2.250166893	9.034216881	3.644005299
C	3.324922085	9.920288086	3.796857357
C	1.795139790	8.743031502	2.349146366
C	3.943010092	10.497025490	2.684642315
C	2.414175034	9.317776680	1.239685178
C	3.490587950	10.194563866	1.400564432
H	3.681948900	10.160706520	4.795720577
H	0.953189909	8.073719978	2.206835032
H	4.775877476	11.180583954	2.825666189
H	2.051470757	9.080327034	0.243357539
H	3.969654322	10.638746262	0.532697082
C	4.435330868	5.180921555	3.307489157
C	4.379206657	3.779244423	3.361971378
C	3.526884794	6.121719837	3.783016920
C	3.403094769	2.956686020	3.916923046
C	2.303963900	5.924254894	4.446452141
C	2.214133024	3.332870007	4.555692196
C	1.710380435	4.606036186	4.793633938
H	5.224251747	3.263522625	2.910402060
H	5.318628311	5.592573643	2.825566053
H	3.810837507	7.157030106	3.624942780
H	3.582696676	1.887019157	3.846490383
H	1.592549443	2.514289379	4.915549755
C	1.432849884	6.930745125	4.936554909
C	0.369133890	6.283840656	5.603008270
H	-0.399094313	6.791065693	6.175888538
C	0.491092235	4.871644974	5.493583679

H	-0.037114698	4.140786648	6.096984863
Ag	-1.110869050	5.111327648	3.814743042
C	-1.869126797	6.166341782	0.247747302
F	-1.637267590	5.524754524	-0.898792982
O	-1.813017249	3.996009111	1.747122645
O	-4.042462349	4.709125519	0.775356889
S	-2.800650120	5.084372044	1.444265366
O	-2.929518938	5.992168427	2.647564888
F	-0.678579390	6.515588284	0.785499156
F	-2.554315567	7.285751820	-0.010230662
H	2.203974247	8.747310638	5.753674030

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B5'

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H	0.678784907	7.159441471	5.355304241
C	1.013375163	9.533903122	5.576511860
C	1.919024825	8.574509621	5.226519585
C	1.325542569	10.979972839	5.666639805
C	-0.347468525	9.055554390	5.939988136
O	1.622957706	7.252176762	5.140544891
O	3.201515198	8.842745781	4.925963402
C	4.133394718	7.751747131	4.788228035
C	5.496260643	8.366518974	4.528480053
H	4.132484913	7.153145313	5.706060410
H	3.820669889	7.102636337	3.963939905
H	5.487480640	8.957586288	3.608113766
H	5.790536404	9.019546509	5.354729176
H	6.246970177	7.576848030	4.424304485
C	2.344310522	11.605701447	4.917315006
C	0.559155881	11.800303459	6.520806789
C	2.587334633	12.972971916	5.033135414
H	2.946821690	11.015827179	4.239160061
C	0.803662956	13.166725159	6.631374359
H	-0.236762106	11.352172852	7.106664658
C	1.822205305	13.765907288	5.889231205
H	3.378738642	13.423530579	4.439114571
H	0.194257900	13.765708923	7.303431511
H	2.013519526	14.832035065	5.973457336
C	-4.165705204	10.188955307	3.698839664
C	-2.837596178	10.528827667	3.436862707
C	-1.684111357	10.163020134	4.141972065
H	-2.675356150	11.164047241	2.569276810
C	-4.701792240	9.395330429	4.720686436
H	-4.895252705	10.601914406	3.004178286
C	-1.565694928	9.371603966	5.278182030
H	-0.746318161	10.554174423	3.753541946
C	-4.032295704	8.733811378	5.751349449
H	-5.782935619	9.279372215	4.708418369
C	-2.666421652	8.698392868	6.031611443
H	-4.660977840	8.166085243	6.436789989
C	-2.064713240	8.006869316	7.094759464
C	-0.680687129	8.228873253	7.040195465
H	0.043994028	7.843009472	7.750029564
H	-2.591000080	7.414016724	7.832001209

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TS(B5'-B7')

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C	1.189185023	5.068337440	6.550560474
C	2.558329821	4.992899418	6.124753475
C	4.902254581	4.681951046	6.520418167
C	5.741292477	4.131660938	7.655889034
O	2.943904400	5.488157272	4.978748322
O	3.505596399	4.507337093	6.904130459
H	5.071033478	4.148291588	5.581363201
H	5.083400249	5.745630741	6.344419003
H	5.543042660	4.671449184	8.585929871
H	5.531315804	3.071193695	7.820347309
H	6.802306652	4.239999771	7.411174774
C	0.900786638	4.931242466	8.022205353
C	1.603856325	5.705046177	8.964923859
C	-0.119606018	4.094768524	8.500129700
C	1.318266749	5.627524376	10.325142860
C	-0.413266599	4.021406174	9.862401009
C	0.305115789	4.782223225	10.783965111
H	2.380692005	6.385610104	8.627009392
H	-0.691038191	3.500116587	7.796237946
H	1.878565550	6.239727497	11.027709961
H	-1.209957242	3.364295006	10.201935768
H	0.074181229	4.726865292	11.844027519
C	1.212005138	0.756430387	5.136379719
C	0.370187104	0.047422651	4.274618149
C	1.147782922	2.100468636	5.520636559
C	-0.765407324	0.479637444	3.582637548
C	0.232143670	3.080915213	5.148924351
C	-1.355111241	1.747186303	3.585031509
C	-0.958450019	2.901657343	4.255842209
H	0.633472145	-0.998491526	4.126605034
H	2.028317690	0.184516966	5.571332932
H	1.919254661	2.420180559	6.218135834
H	-1.261364102	-0.271107465	2.972007751
H	-2.256266117	1.851555109	2.981210709
C	0.215894863	4.430297852	5.585330009
H	2.259924412	6.221655369	4.736804485
C	-0.920586050	5.047742367	5.017742157
H	-1.192042112	6.083439350	5.174777508
C	-1.623816848	4.137225628	4.221867085
H	-2.527073383	4.343820095	3.661276579
H	1.064058304	6.404520988	6.050751686
C	0.729126036	9.552249908	5.609537125
C	1.556212902	8.491485596	5.394315243
C	1.235887766	10.948606491	5.732121468
C	-0.723080575	9.317392349	5.783720493
O	1.133548856	7.241236687	5.156805038
O	2.932386398	8.630426407	5.320966721
C	3.608564138	8.759405136	6.582103729
C	5.069359303	9.064747810	6.302094936
H	3.146064758	9.560834885	7.172415257
H	3.509207249	7.820838928	7.152754307
H	5.517512798	8.284020424	5.676858425
H	5.162720203	10.019985199	5.776211739
H	5.630613327	9.127939224	7.241316795
C	2.291997433	11.447922707	4.943365574
C	0.623647630	11.838360786	6.635682106
C	2.724126101	12.767245293	5.070404053
H	2.770951748	10.791581154	4.226028919
C	1.058566570	13.156688690	6.762660503
H	-0.204454631	11.483722687	7.241896629
C	2.114620924	13.631382942	5.982777119
H	3.536183119	13.125042915	4.442102432
H	0.567699969	13.815815926	7.474287033
H	2.451580524	14.659790993	6.077588081
C	-4.003523350	11.283009529	3.277513266

C	-2.613102913	11.393617630	3.181856394
C	-1.627223134	10.781917572	3.965309620
H	-2.246533632	12.044354439	2.391374111
C	-4.782540321	10.534022331	4.165230751
H	-4.564866066	11.866233826	2.549073696
C	-1.775228262	9.907419205	5.037734509
H	-0.599619031	11.023299217	3.701874733
C	-4.357316971	9.689084053	5.195519924
H	-5.859066963	10.614850044	4.033551693
C	-3.061775923	9.387516022	5.605351925
H	-5.148234844	9.193588257	5.758478165
C	-2.714520216	8.514828682	6.650116444
C	-1.318322778	8.477538109	6.751741409
H	-0.761667192	7.897417545	7.479319096
H	-3.417450428	7.975490093	7.272376060

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B7'

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C	1.283659458	8.335537910	4.758494377
C	0.210073382	9.119142532	5.522076130
C	-1.997631907	9.974216461	5.485001087
C	-3.189141035	9.998482704	4.547341824
O	0.389085561	9.634875298	6.604356766
O	-0.954269528	9.201413155	4.843789577
H	-2.238152504	9.512485504	6.448007107
H	-1.612629652	10.977869034	5.688606739
H	-2.922116995	10.453754425	3.589592457
H	-3.561391830	8.987603188	4.356887341
H	-3.999202967	10.583367348	4.994248867
C	1.582915664	9.012044907	3.414617777
C	2.493705750	10.075325012	3.376085758
C	0.960640848	8.614099503	2.226713657
C	2.781451941	10.726323128	2.175927162
C	1.246400714	9.263844490	1.026301622
C	2.157630205	10.321174622	0.995793581
H	2.981630087	10.394165993	4.294519901
H	0.259168774	7.786608696	2.244154215
H	3.495571375	11.545154572	2.163270235
H	0.758641720	8.940508842	0.110680223
H	2.382113457	10.822308540	0.058338586
C	4.370327473	5.090418816	4.371809483
C	4.273796558	3.699835300	4.286833763
C	3.345304251	6.037303925	4.488778591
C	3.138533115	2.881965399	4.292874336
C	1.969316006	5.843671322	4.553085327
C	1.796835899	3.258556366	4.381229877
C	1.243839622	4.532594204	4.493228436
H	5.222892761	3.173673153	4.200433254
H	5.378967285	5.495296955	4.340821266
H	3.679400444	7.072748184	4.527757645
H	3.324969292	1.814018488	4.209723949
H	1.074355125	2.443004370	4.355944633
C	0.982705832	6.853588581	4.667953014
C	-0.275554478	6.220736980	4.672100067
H	-1.221291065	6.742370129	4.742825985
C	-0.124140576	4.829425812	4.569754601
H	-0.924855292	4.100748539	4.556664467
H	2.167231798	8.462956429	5.390471935

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C1

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C	-1.667757988	-0.041352440	2.532296896
C	-1.107760787	0.124450304	1.261283517
C	-0.925882876	0.351902783	3.653270960
H	-1.678611517	-0.170071185	0.385629565
H	-1.356449485	0.229908302	4.643059731
C	0.168871909	0.668509364	1.110366464
C	0.350112110	0.893655956	3.507150173
H	0.588362157	0.792301476	0.115709223
H	0.914969504	1.192007184	4.386306286
C	0.901208222	1.053379059	2.233345985
H	1.895407796	1.477028966	2.118430138
C	-3.020083427	-0.671359003	2.692645073
O	-4.118966103	-2.802550077	2.896032810
C	-3.083723068	-2.167501926	2.793682098
O	-1.864203572	-2.740440607	2.772487640
C	-0.390654564	-4.617374897	2.794922829
H	-0.322987556	-5.707125187	2.874133825
H	0.052845333	-4.311120510	1.843142033
H	0.197873294	-4.174877167	3.603959084
C	-1.841508150	-4.181240082	2.880336523
H	-2.303348780	-4.472743988	3.829470634
H	-2.450371981	-4.606979370	2.076483727
C	-4.199338913	4.083764553	0.030652994
C	-3.928654432	4.424176693	1.408688068
C	-3.850798130	3.618150949	2.499188185
C	-4.422102451	2.858016729	-0.516830623
C	-4.027543068	2.184090853	2.589451075
C	-4.431860924	1.568572640	0.130360380
C	-4.234376907	1.274443746	1.441919327
H	-4.226068974	4.930450439	-0.651980221
H	-3.769633770	5.485328674	1.589591026
H	-3.639029741	4.106747627	3.448963404
H	-4.605101109	2.832120895	-1.589007616
H	-4.612054348	0.721663177	-0.529676914
C	-4.010996819	1.462133169	3.745710850
H	-3.883811951	1.883391380	4.736418247
C	-4.159252167	0.010903722	3.484896183
H	-4.723228455	-0.636328101	4.148852348
C	-4.280512810	-0.110692382	1.983538866
H	-4.916341305	-0.856578290	1.520610690

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TS(C1-C2)

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C	-2.578378439	-0.290122032	2.429020405
C	-1.865245700	-0.116702802	1.239678502
C	-2.217877150	0.465451419	3.549361229
H	-2.148973227	-0.688390315	0.360514194
H	-2.776118994	0.347427607	4.473751545
C	-0.808610857	0.792295694	1.169781089
C	-1.163246632	1.374454618	3.483776331
H	-0.266400725	0.919087470	0.236632049
H	-0.898179531	1.958275318	4.361220360
C	-0.454953164	1.541770339	2.291932583
H	0.361840338	2.256191254	2.237400293
C	-3.709849119	-1.305895686	2.503657818
O	-4.011747360	-3.673880339	2.911865950
C	-3.272232771	-2.709489584	2.919358253
O	-1.990116715	-2.760336161	3.315295935

C	-0.064957358	-3.897245646	4.153528214
H	0.335350156	-4.859140396	4.489280224
H	0.538052440	-3.546464920	3.311220169
H	0.035004422	-3.176783085	4.970333099
C	-1.517467380	-4.058200359	3.748725891
H	-2.144487858	-4.401904583	4.577492714
H	-1.642726660	-4.769732952	2.926470757
C	-6.195503235	2.167694092	-1.058869123
C	-6.089263916	2.782775164	0.200925499
C	-5.818190575	2.191951990	1.427570224
C	-6.032790661	0.828981757	-1.389925718
C	-5.474155903	0.864030659	1.743202448
C	-5.601703644	-0.231765807	-0.572140157
C	-5.197869778	-0.229097098	0.756828010
H	-6.478115559	2.825800896	-1.878506064
H	-6.302025795	3.848840714	0.225689456
H	-5.901407719	2.851677179	2.290568113
H	-6.222373486	0.567405939	-2.428298473
H	-5.500388622	-1.192785025	-1.076432705
C	-5.497543812	0.364521623	3.047168732
H	-6.013679981	0.887869596	3.846351862
C	-4.960877419	-0.922838807	3.247966766
H	-5.333953381	-1.599066496	4.012126923
C	-4.649249077	-1.397616744	1.328404784
H	-4.812649727	-2.373944044	0.885365248

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C2

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C	-1.821268916	-0.121904753	2.454286575
C	-0.594030142	-0.310738415	1.801369905
C	-1.940980792	0.935089469	3.364668608
H	-0.483456522	-1.117322803	1.083240867
H	-2.886789799	1.103676558	3.869149923
C	0.486918747	0.531163394	2.062431574
C	-0.857639492	1.775239468	3.626735449
H	1.429233432	0.369465590	1.546016812
H	-0.969426632	2.588705778	4.338524818
C	0.361044794	1.576381087	2.978505850
H	1.202926874	2.232330322	3.181436777
C	-3.042099476	-1.028295398	2.116724968
O	-2.115933418	-3.007842064	1.009015203
C	-2.503251314	-2.480016470	2.030160189
O	-2.479701042	-3.074656248	3.239457130
C	-0.431136757	-4.387707710	3.517464161
H	-0.055537947	-5.408069134	3.648721218
H	0.072435655	-3.944341898	2.654835701
H	-0.176075965	-3.808812618	4.409992695
C	-1.936833262	-4.416536331	3.303914070
H	-2.452308416	-4.877892971	4.149868965
H	-2.199080706	-4.946510315	2.385401011
C	-7.377218723	1.423008800	-0.785137057
C	-7.724554539	1.329900980	0.524607122
C	-6.999775410	0.706077933	1.600089788
C	-6.183274746	0.910395384	-1.411318541
C	-5.766761780	0.112245552	1.644679189
C	-5.118315697	0.285150737	-0.851975918
C	-4.806407452	-0.068861127	0.532442749
H	-8.074883461	1.929276824	-1.448515892
H	-8.677283287	1.768585443	0.813018680
H	-7.529591084	0.722750723	2.551320791
H	-6.132058620	1.054398894	-2.488653421
H	-4.330926418	-0.003553814	-1.546730161
C	-5.332225800	-0.411365151	2.933616638
H	-6.049520016	-0.359500915	3.749783516
C	-4.117668629	-0.931730688	3.169883966
H	-3.864910364	-1.294756770	4.160037041
C	-3.588811159	-0.623751521	0.767266572
H	-2.913375854	-0.782799304	-0.066629060

E. Vibrational frequencies

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azulene

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166.10 172.36 321.80 337.47 411.98 430.77
498.63 574.77 610.87 683.13 729.75 745.69
749.09 786.97 799.87 830.96 880.74 913.10
941.35 968.99 978.70 996.66 1008.95 1037.99
1070.59 1089.62 1194.51 1248.57 1249.26 1312.03
1326.45 1342.83 1432.21 1440.17 1498.22 1502.44
1551.73 1594.32 1650.05 1658.94 3147.89 3149.56
3157.83 3177.79 3186.73 3216.09 3234.88 3243.63

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DCE

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118.60 215.58 298.92 713.23 757.17 782.65
1015.79 1062.60 1148.17 1268.21 1301.12 1350.28
1504.60 1505.10 3111.78 3119.92 3171.15 3192.13

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N_2

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2460.76

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Ethyl phenyl diazoacetate

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26.72 33.51 72.55 97.74 104.32 148.05
149.65 221.03 261.86 301.98 307.58 334.42
398.25 413.80 495.16 504.93 553.74 556.49
634.81 679.98 708.05 730.48 775.53 814.25
822.35 858.27 883.73 926.85 979.75 1006.92
1008.45 1013.70 1059.48 1082.94 1118.95 1140.18
1185.06 1190.44 1202.00 1225.02 1293.67 1297.75
1348.48 1361.26 1377.72 1409.71 1440.28 1495.09
1499.75 1511.60 1532.85 1542.30 1631.92 1660.65
1785.85 2209.12 3057.35 3067.91 3108.88 3132.07
3140.50 3179.01 3186.42 3196.15 3208.02 3255.22

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A1

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10.67 15.33 21.61 25.22 35.16 54.57
80.61 82.33 89.47 97.87 113.93 152.84
154.52 168.21 177.51 253.84 256.14 260.65
265.63 312.78 348.93 376.20 418.16 469.24
495.77 505.35 519.05 577.29 582.81 636.88
658.72 669.48 737.89 745.29 790.93 817.54
842.91 893.41 957.77 959.87 1044.45 1113.93
1167.81 1179.29 1202.49 1206.69 1225.36 1229.18
1235.89 1281.75 1320.21 1351.97 1355.71 1475.77
1481.07 1552.18 1583.59 1684.80 3103.64 3108.22
3170.43 3182.23 3274.03

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A2

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5.93 14.13 15.10 28.63 29.19 31.00
34.00 47.90 60.09 75.37 86.26 89.28
94.99 98.69 111.61 128.52 142.78 152.46
159.72 167.11 201.23 220.65 253.28 256.27
260.68 267.09 282.41 313.31 328.41 348.34
367.06 377.01 398.84 412.29 470.95 472.16
498.78 503.86 505.03 518.89 544.57 561.34
580.11 585.43 631.56 669.49 671.61 704.32
737.17 738.60 745.57 773.14 791.00 812.29
817.10 818.35 843.88 850.76 875.71 923.88
959.27 975.37 992.59 1004.65 1012.71 1049.32
1068.97 1104.72 1116.20 1134.39 1148.67 1176.87
1184.23 1193.05 1204.68 1207.63 1219.57 1226.29
1229.24 1239.53 1280.69 1287.00 1300.83 1339.74
1358.56 1374.30 1406.19 1439.65 1490.81 1499.96
1510.97 1530.30 1535.97 1546.93 1582.69 1631.49
1653.25 1684.73 1806.99 2232.97 3055.83 3073.12
3117.03 3130.11 3142.78 3180.23 3188.86 3197.78
3209.59 3241.59 3274.86

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TS(A2-A3)

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-467.32 3.57 11.12 14.67 24.08 26.52
30.29 36.24 60.32 63.08 73.73 88.68
92.00 94.56 102.89 109.03 114.55 134.51
146.81 166.70 174.06 190.80 244.96 251.50
261.00 261.24 268.15 285.31 304.44 313.14
338.88 346.44 358.33 372.33 379.90 414.64
459.92 463.85 500.56 505.23 519.20 557.64
578.62 585.56 616.26 627.70 667.89 687.64
703.63 738.72 746.27 785.17 790.23 793.52
814.74 818.46 840.87 859.90 865.03 891.11
953.49 963.42 984.71 994.36 1012.09 1016.39
1053.08 1065.53 1118.63 1122.20 1139.64 1174.42
1183.80 1191.64 1205.56 1209.34 1210.55 1225.62
1229.73 1239.89 1279.74 1299.40 1316.41 1340.69
1362.83 1367.93 1407.61 1440.11 1487.44 1500.01
1510.41 1530.08 1531.87 1549.42 1585.17 1628.17
1650.63 1690.53 1782.14 2326.54 3057.23 3072.36
3114.59 3132.28 3142.01 3179.93 3190.15 3202.02
3212.35 3232.66 3276.46

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A3

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13.50 15.98 20.15 27.01 28.34 29.34
44.96 58.47 69.20 82.07 93.73 96.01
106.27 116.57 143.68 150.07 157.93 180.46
194.21 249.25 255.88 260.87 263.15 277.80
296.40 314.97 318.91 349.86 376.06 379.40
402.76 447.39 470.11 498.42 505.52 520.32
568.67 582.53 588.25 617.42 626.37 669.05
681.35 709.17 739.62 745.92 787.96 795.33
798.92 814.59 820.17 840.91 855.73 871.91
929.61 967.49 970.51 992.03 996.02 1013.07
1021.23 1049.38 1057.78 1122.26 1128.94 1138.77
1171.09 1181.87 1192.66 1210.10 1212.43 1214.24
1229.78 1239.41 1260.81 1277.65 1297.46 1339.59
1363.73 1371.24 1377.50 1409.48 1440.48 1481.91
1498.82 1509.75 1525.63 1529.55 1545.34 1585.25
1609.26 1645.53 1691.21 1756.87 3058.29 3067.14
3110.87 3133.03 3142.77 3190.55 3198.12 3206.64
3216.07 3229.53 3280.54

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TS(A3-A4)

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-246.60 9.41 10.94 18.64 21.84 25.60
28.91 31.72 46.82 54.59 61.00 67.58
71.12 79.26 88.19 90.63 97.95 110.24
111.30 123.14 128.23 141.31 164.67 175.11
191.36 204.69 213.93 246.93 252.58 260.37
265.14 270.47 303.45 312.31 316.39 332.50
342.10 346.81 365.07 387.71 411.70 415.40
415.77 451.37 459.62 486.95 504.96 508.04
518.71 537.61 575.59 581.49 586.97 602.64
608.57 629.09 665.88 685.46 693.38 702.46
737.42 738.48 744.76 760.03 762.14 779.61
787.93 792.70 814.08 816.36 825.42 833.69
841.90 853.53 868.50 890.42 897.85 909.49
931.88 946.35 963.89 971.85 976.73 982.65
986.69 994.28 999.40 1014.91 1017.83 1028.03
1056.09 1066.35 1070.24 1077.74 1115.69 1118.23
1122.86 1138.62 1173.05 1184.55 1187.82 1191.32
1193.99 1201.01 1209.49 1216.77 1225.57 1236.42
1255.18 1260.92 1278.35 1281.67 1295.53 1309.61
1325.50 1333.14 1361.64 1363.62 1380.88 1402.05
1420.04 1431.79 1437.37 1472.29 1482.06 1491.45

1499.84 1510.03 1527.74 1532.09 1552.34 1560.10
1585.78 1592.06 1619.77 1632.17 1646.07 1648.57
1694.08 1735.82 3052.34 3063.49 3104.88 3126.72
3135.38 3161.18 3167.12 3176.41 3178.21 3183.52
3187.78 3192.84 3194.17 3204.10 3231.34 3233.81
3246.80 3275.66 3276.59

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A4

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12.30 14.09 21.47 22.52 27.70 28.95
38.81 41.12 52.39 60.73 63.57 73.87
82.26 83.32 88.22 100.66 109.48 116.52
122.03 130.11 147.48 157.59 177.37 190.98
197.36 225.31 237.34 247.16 255.87 261.64
267.85 292.53 304.18 310.80 321.46 339.93
361.95 369.44 386.51 401.18 415.81 423.65
432.60 453.22 483.72 499.19 504.12 516.42
517.35 570.70 573.87 582.87 590.25 621.47
630.04 664.68 670.20 687.41 713.35 724.36
735.02 744.26 754.58 767.20 774.67 790.28
790.91 797.43 813.64 814.50 828.92 831.56
857.34 863.60 889.24 906.65 915.65 930.44
954.69 962.17 972.73 974.67 987.39 993.66
1000.68 1005.20 1009.84 1039.03 1051.82 1055.67
1059.10 1065.48 1087.75 1114.19 1115.68 1121.40
1140.06 1140.41 1161.61 1173.77 1185.32 1186.37
1195.50 1206.28 1216.76 1223.18 1234.36 1236.12
1236.81 1255.90 1264.21 1277.83 1284.22 1293.94
1300.74 1325.20 1350.04 1358.07 1367.16 1402.76
1417.10 1436.97 1452.23 1471.59 1481.36 1485.45
1499.11 1511.26 1532.12 1533.51 1555.44 1568.78
1583.54 1600.19 1624.03 1625.66 1642.13 1651.51
1683.49 1693.75 3001.28 3052.71 3054.97 3094.42
3124.63 3137.68 3168.04 3168.76 3174.02 3175.97
3183.21 3187.52 3189.83 3196.61 3198.20 3207.82
3223.24 3240.80 3274.05

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TS(A4-A8)

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-105.32 12.00 17.99 20.56 26.19 30.17
40.04 52.06 57.54 61.04 68.88 71.74
75.95 80.44 85.78 94.07 106.63 108.12
134.32 141.69 145.29 158.73 177.19 192.78
203.94 215.48 231.00 252.97 256.57 262.36
274.92 287.45 312.90 331.09 338.09 347.13
361.53 371.21 374.31 406.57 415.53 433.71
462.59 466.51 492.31 495.57 505.61 515.50
519.31 556.21 578.50 584.02 592.87 597.56
634.34 665.24 667.01 668.42 711.59 733.65
738.01 745.75 746.11 770.98 780.68 787.77
792.67 810.38 814.69 817.89 824.01 829.79
840.76 854.57 877.38 883.66 901.15 919.99
933.54 943.34 943.51 963.03 969.55 975.17
997.72 1007.55 1013.65 1017.46 1023.01 1037.17
1052.44 1066.87 1068.58 1090.35 1114.30 1119.61
1140.80 1147.97 1175.45 1176.27 1185.85 1188.56
1200.45 1204.97 1216.73 1228.22 1232.79 1240.92
1261.13 1264.48 1277.63 1279.98 1298.22 1302.63
1306.74 1332.41 1337.08 1351.32 1361.43 1363.78
1404.84 1437.08 1439.11 1454.25 1482.31 1497.87
1499.77 1513.94 1531.00 1537.29 1550.11 1569.65
1586.01 1597.38 1631.85 1654.21 1655.59 1691.13
1699.46 1751.95 3057.10 3061.09 3114.36 3129.41
3153.56 3155.33 3155.40 3159.43 3164.56 3168.75
3172.10 3177.19 3177.60 3188.11 3188.58 3195.88
3207.02 3251.86 3275.52

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A8

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9.77 13.23 21.24 24.83 26.39 31.71
44.79 47.00 50.64 59.06 70.02 79.46
86.18 89.82 102.28 104.85 109.30 133.48
141.58 155.20 161.86 165.59 182.25 210.49
217.51 239.54 254.54 256.56 262.46 274.38
276.46 309.03 313.69 326.64 349.93 358.10
369.72 377.58 380.83 409.75 422.65 430.71
469.06 479.28 500.17 503.38 505.26 519.02
554.55 572.86 579.57 584.37 596.56 623.68
652.89 667.80 669.46 709.80 724.14 736.96
737.88 746.75 758.40 772.12 786.49 791.58
792.99 801.72 817.80 818.13 819.69 841.94
855.42 865.26 868.80 876.70 896.00 911.89
922.09 935.95 945.39 961.89 963.79 966.78
982.32 1001.62 1003.96 1015.40 1018.92 1023.95
1036.46 1059.15 1088.18 1090.74 1104.40 1118.40
1140.98 1145.03 1168.85 1174.71 1175.31 1185.78
1199.70 1202.15 1209.09 1230.27 1231.14 1241.11
1263.81 1272.23 1280.77 1284.85 1299.14 1321.58
1330.15 1337.85 1345.59 1356.32 1361.67 1362.78
1406.46 1433.00 1440.47 1451.49 1467.85 1499.62
1499.66 1512.91 1520.00 1531.32 1550.57 1585.49
1591.87 1593.23 1619.77 1643.15 1662.06 1690.00
1706.33 1785.73 3057.13 3067.39 3109.31 3126.72
3150.68 3153.25 3153.71 3163.35 3174.14 3180.33
3185.85 3192.12 3192.16 3200.44 3207.77 3207.99
3215.39 3221.01 3275.09

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TS(A4-A5)

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-965.71 9.08 19.41 19.69 28.72 29.86
34.14 38.22 46.95 49.78 59.12 62.91
70.13 86.56 87.83 97.12 99.52 116.93
129.97 135.41 140.13 146.30 157.16 181.39
185.74 213.07 226.78 251.79 253.80 259.88
267.18 288.61 302.20 312.07 319.72 335.83
344.04 366.63 379.15 406.99 415.94 417.42
430.15 461.36 486.27 491.84 504.44 518.00
521.04 546.98 574.89 576.11 582.34 598.01
629.81 666.51 668.29 680.67 693.64 710.62
731.18 736.38 743.65 755.14 764.32 774.30
785.66 790.51 793.23 815.34 816.35 833.83
834.68 850.18 854.45 894.07 902.54 915.88
921.41 961.75 971.34 972.25 985.94 990.78
991.82 1002.93 1017.81 1021.51 1023.17 1034.15
1064.01 1067.74 1078.89 1108.50 1117.71 1123.04
1138.26 1153.02 1175.36 1182.73 1187.65 1197.20
1202.93 1205.42 1220.34 1224.66 1235.99 1251.54
1260.71 1272.64 1279.56 1296.69 1297.67 1318.00
1326.45 1346.57 1354.78 1359.73 1373.64 1419.08
1427.66 1435.89 1446.46 1467.45 1487.96 1488.81
1499.16 1511.75 1529.12 1534.38 1555.60 1562.75
1584.41 1587.98 1596.06 1622.59 1636.36 1647.63
1654.25 1691.80 1719.62 3055.52 3068.87 3111.87
3129.79 3142.04 3162.30 3169.97 3170.76 3177.68
3180.94 3189.90 3191.57 3196.56 3201.73 3217.95
3240.83 3252.69 3274.31

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A5

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4.57 14.75 17.83 24.56 25.16 26.75
35.18 37.80 46.80 56.04 62.56 83.34
85.41 89.28 97.10 97.55 117.57 124.12
133.20 140.74 152.39 163.44 171.49 182.05
208.08 224.16 251.16 255.71 261.44 267.15
288.70 302.40 312.85 320.74 329.38 347.47
369.76 373.07 374.08 406.90 416.02 424.84
452.59 467.80 486.30 497.95 504.96 518.70
519.85 559.43 563.86 579.35 584.03 591.82
618.60 633.28 646.09 668.60 671.98 696.57
708.41 715.09 738.09 741.19 745.64 764.47

769.22 783.98 791.61 799.80 818.21 828.43
830.50 840.67 860.37 879.93 885.70 914.61
931.39 936.52 961.50 969.39 979.79 986.19
993.07 999.80 1004.96 1012.64 1017.15 1024.53
1053.57 1063.68 1074.46 1083.18 1117.85 1124.21
1134.08 1175.50 1183.25 1189.19 1197.79 1200.75
1207.87 1208.30 1218.75 1228.97 1240.95 1249.08
1253.21 1257.98 1280.35 1310.41 1326.69 1331.27
1334.29 1359.87 1362.01 1369.03 1387.34 1422.53
1434.82 1437.62 1442.69 1468.96 1486.33 1498.12
1500.89 1511.03 1521.28 1533.89 1551.48 1554.63
1583.20 1586.55 1593.68 1627.89 1642.58 1651.50
1655.54 1690.03 3056.45 3081.88 3125.90 3135.92
3152.08 3152.08 3158.51 3169.64 3176.98 3181.32
3185.20 3188.56 3198.69 3206.41 3206.93 3244.17
3254.37 3273.73 3657.26

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TS(A6-A7)

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-1230.28 4.12 11.73 14.12 15.47 19.49
20.78 22.64 24.09 26.12 27.48 30.17
30.76 33.38 35.73 37.31 40.93 42.07
44.16 47.76 52.32 56.47 58.61 62.61
67.24 68.74 75.98 79.56 82.45 84.99
88.16 90.04 92.38 92.91 99.11 100.53
101.58 112.09 114.43 119.20 122.92 131.68
136.75 141.86 145.33 146.37 148.37 156.29
159.85 162.18 184.18 187.29 191.53 192.06
203.50 215.88 229.34 247.90 251.90 253.03
253.13 260.78 261.56 263.21 265.71 267.61
273.55 287.32 291.30 301.76 311.56 312.10
312.31 323.06 326.15 334.40 339.57 344.41
345.95 363.08 367.91 373.08 375.78 387.45
399.38 414.86 417.38 418.71 422.50 433.53
448.95 458.30 459.59 460.47 477.50 480.79
488.35 493.97 499.33 505.29 505.56 518.76
519.16 527.22 532.51 566.62 574.20 575.67
581.52 582.14 582.84 594.01 596.94 621.64
627.93 635.66 636.93 643.07 667.29 667.86
669.46 672.11 679.20 681.89 702.91 708.80
714.12 728.41 732.80 735.87 737.37 744.35
744.66 746.07 746.71 755.31 763.25 772.32
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802.40 813.72 815.78 817.36 828.86 837.53
838.27 839.05 839.54 847.73 852.82 867.58
877.17 882.66 888.67 891.29 915.00 918.57
924.56 925.94 939.58 950.51 960.20 961.05
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1012.23 1012.96 1018.50 1021.75 1024.63 1037.25
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A6

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161.81 164.33 182.44 183.99 190.38 196.58
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481.81 494.43 495.52 504.92 505.33 518.44
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1014.88 1017.30 1017.68 1018.25 1025.51 1033.63
1057.65 1058.51 1060.01 1063.70 1070.28 1078.08
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1186.55 1188.96 1190.27 1191.90 1194.58 1195.10
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1333.89 1334.89 1347.93 1357.94 1358.79 1359.15
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1626.14 1630.01 1640.18 1648.97 1649.77 1650.97
1652.77 1666.73 1685.94 1686.92 3056.31 3059.44
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TS(A4-A7)

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343.26 362.30 368.89 391.86 412.35 415.77

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839.57 839.94 856.06 874.42 893.30 907.74
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991.45 996.80 998.71 1014.94 1016.97 1027.76
1054.97 1059.80 1076.14 1097.07 1111.04 1115.61
1122.92 1139.24 1160.02 1174.91 1184.74 1185.91
1187.77 1208.32 1215.02 1216.56 1221.81 1227.48
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A7

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B1

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B2

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TS(B2-B3)

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B3

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TS(B3-B4)

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221.76 253.77 267.88 286.43 307.88 325.79
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413.78 419.03 463.73 493.05 505.09 517.03
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620.33 623.62 684.54 688.44 694.49 738.46
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986.72 989.44 1001.33 1007.79 1011.98 1017.60
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B4

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TS(B4-B8)

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B8

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TS(B4-B5)

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415.03 431.26 487.12 490.85 518.08 520.85
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1347.22 1352.24 1372.81 1418.03 1428.07 1438.66
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1528.65 1536.14 1564.61 1590.26 1606.71 1625.08
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B5

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266.21 289.29 297.93 302.04 319.59 326.65
329.21 353.34 364.50 377.14 406.07 414.58
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B6

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TS(B6-B7)

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B7

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B5'

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TS(B5'-B7')

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300.72 308.70 320.70 328.34 329.89 358.25
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B7'

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C1

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380.88 408.91 418.78 431.45 476.07 502.55
552.71 572.28 596.64 631.95 654.42 671.60
713.45 726.02 737.84 751.58 769.52 785.79
789.90 800.06 812.81 815.74 855.96 864.42
869.11 876.64 897.61 914.81 927.79 932.75
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1101.39 1107.95 1141.12 1146.69 1165.68 1184.64
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TS(C1-C2)

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C2

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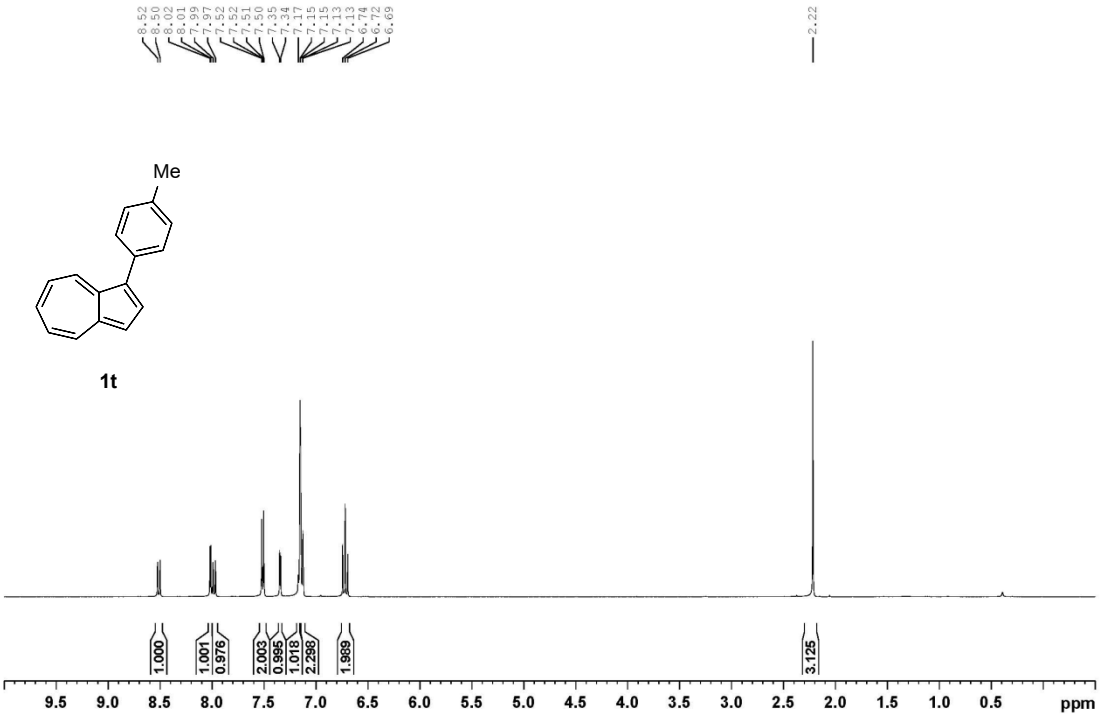
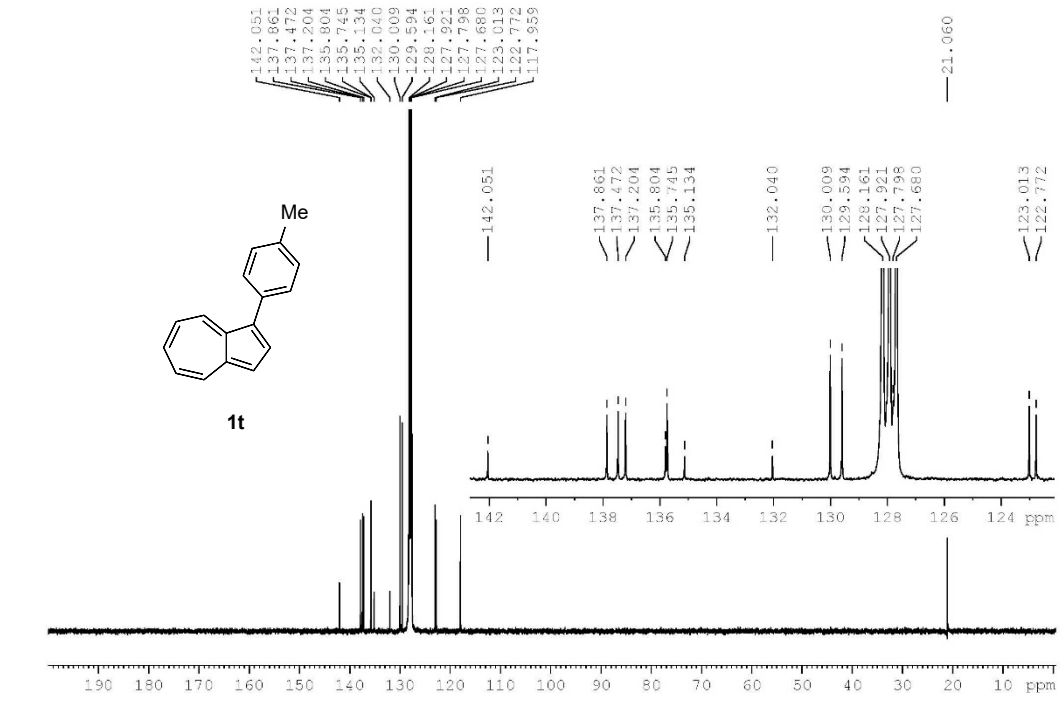
^{1}H and ^{13}C NMR spectra

^{1}H NMR (400 MHZ, C_6D_6)



^{13}C{^{1}H}NMR (100 MHz, C_6D_6)



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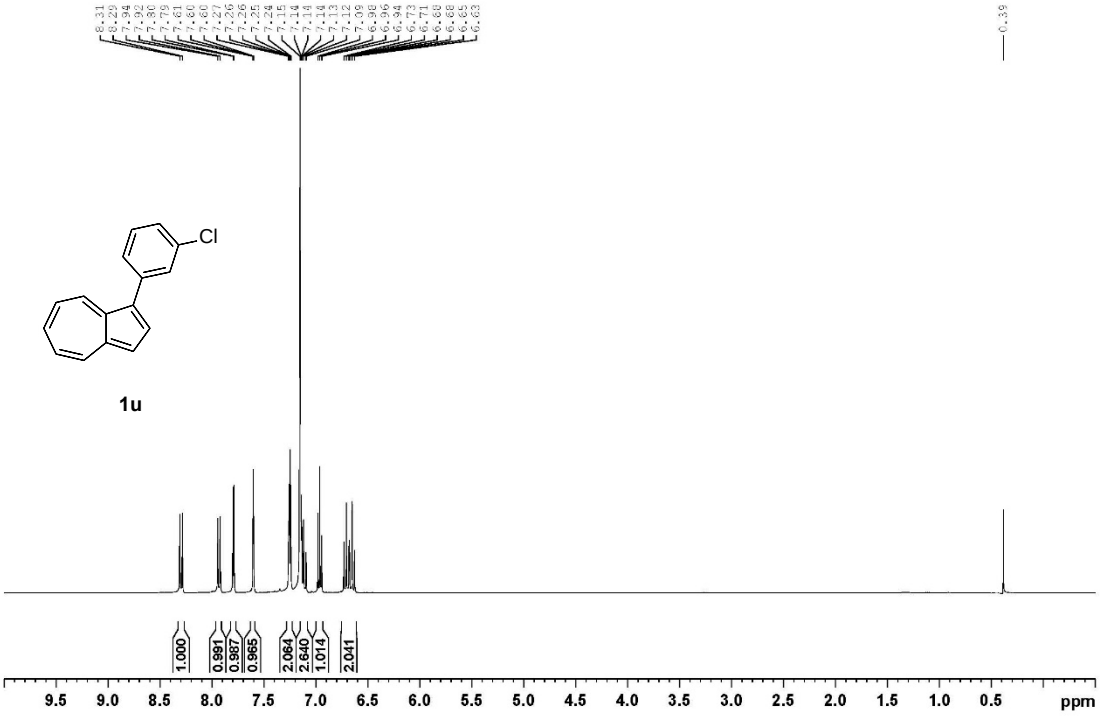

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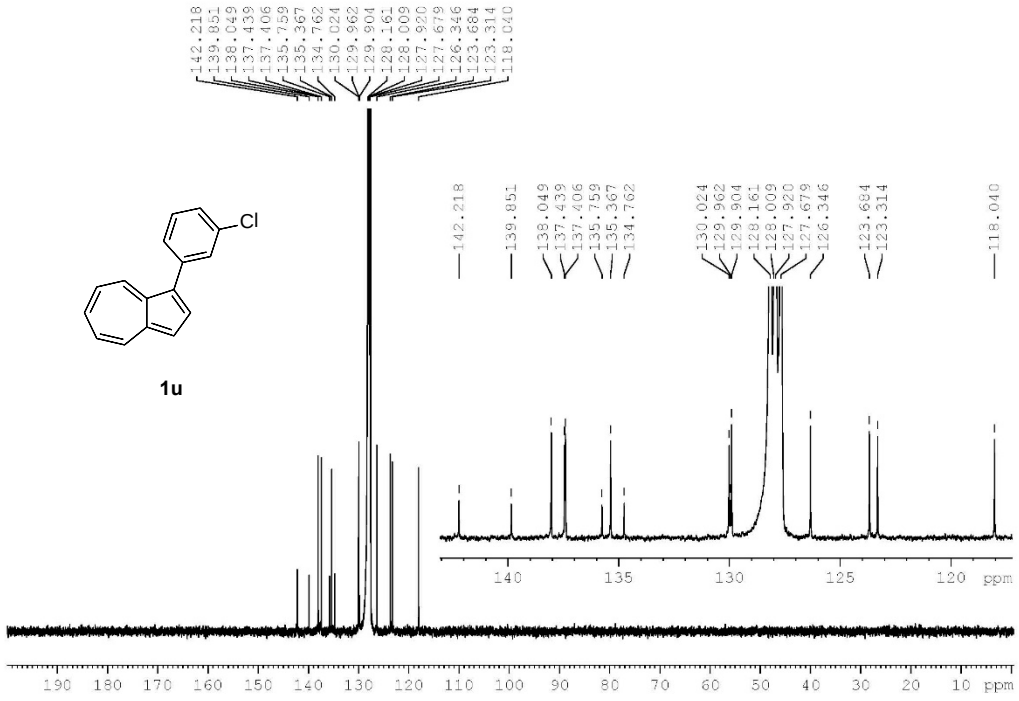
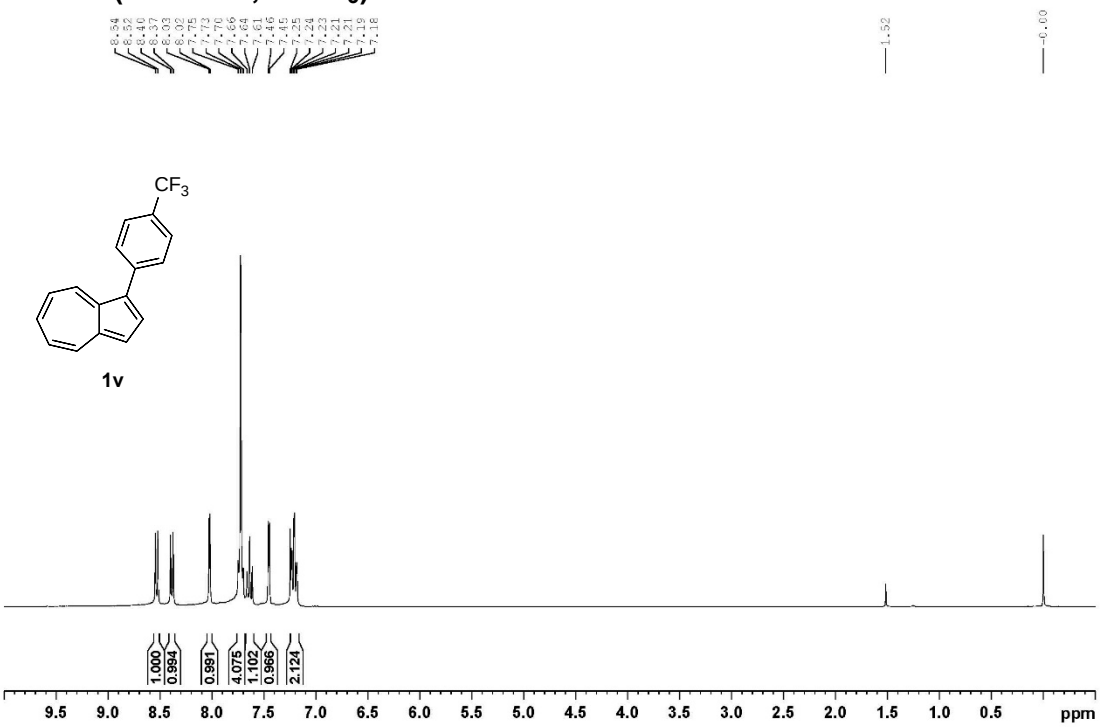
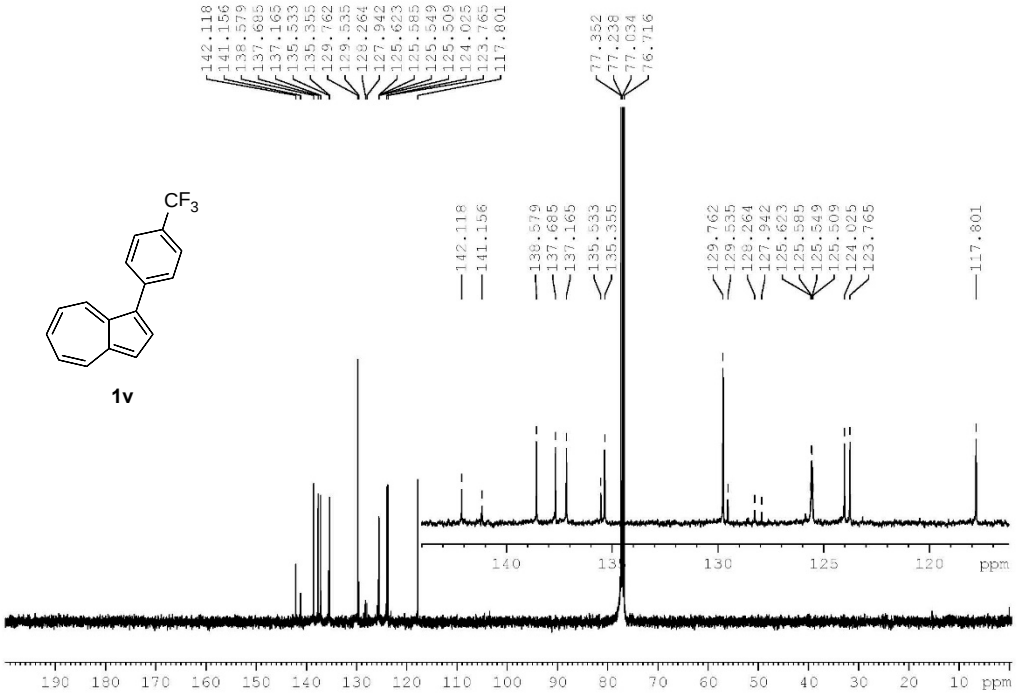


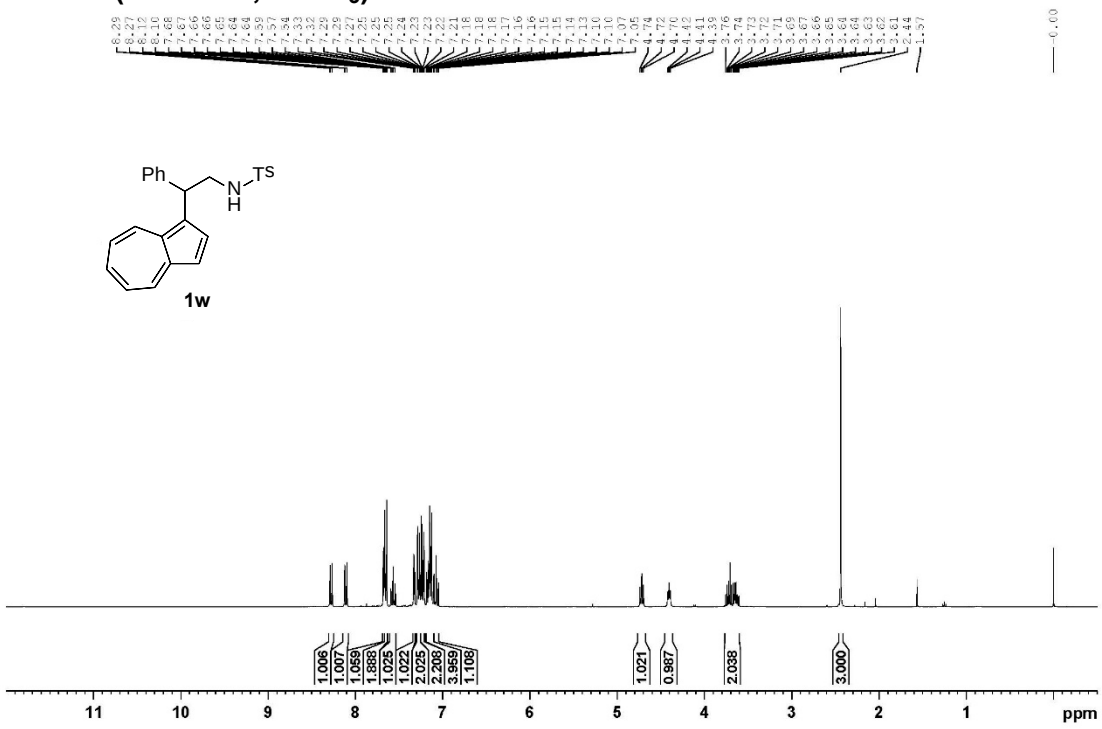
^{1}H NMR (400 MHz, $CDCl_3$)



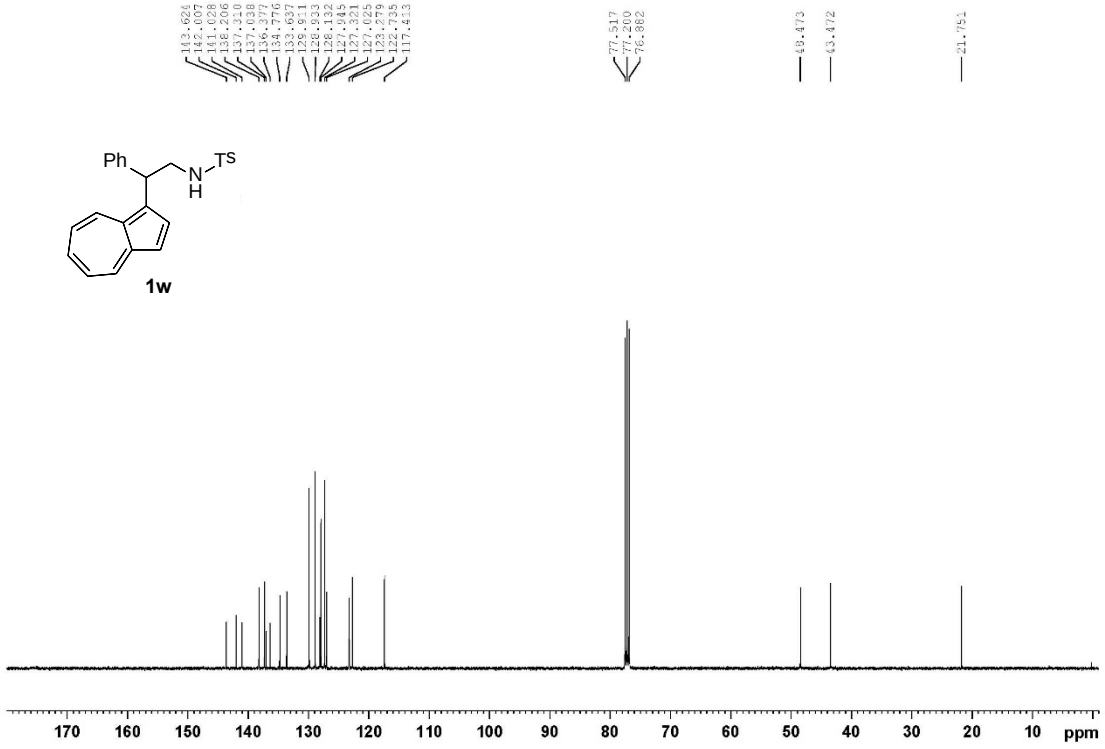
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



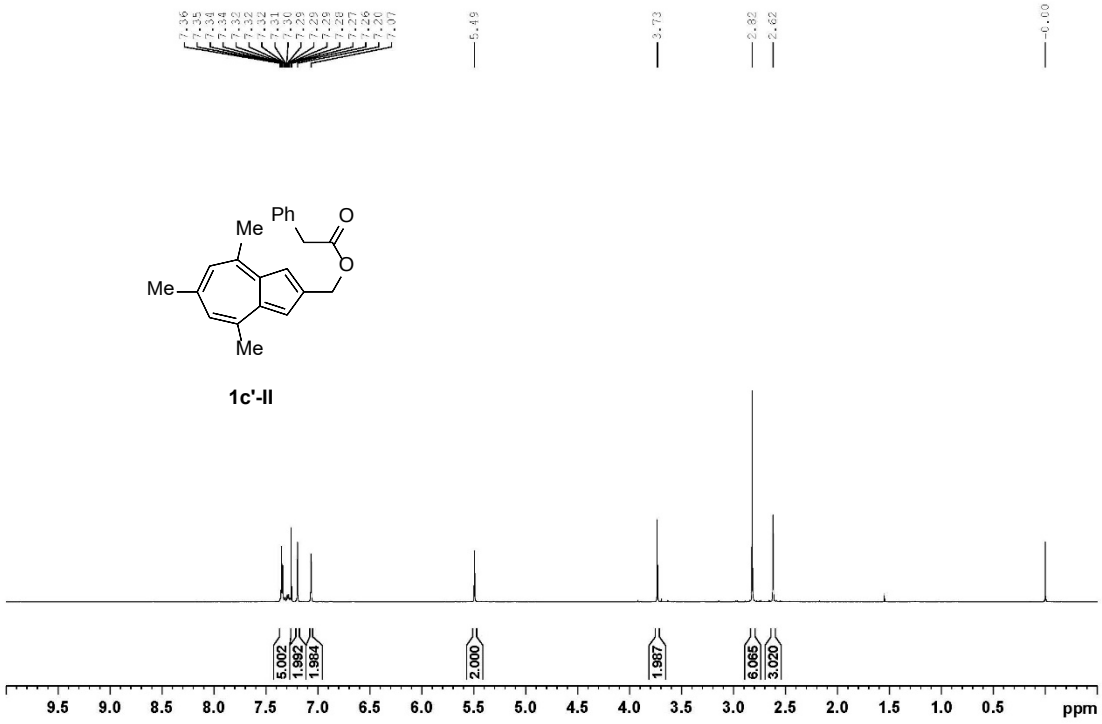
^{1}H NMR (400 MHz, $CDCl_3$)



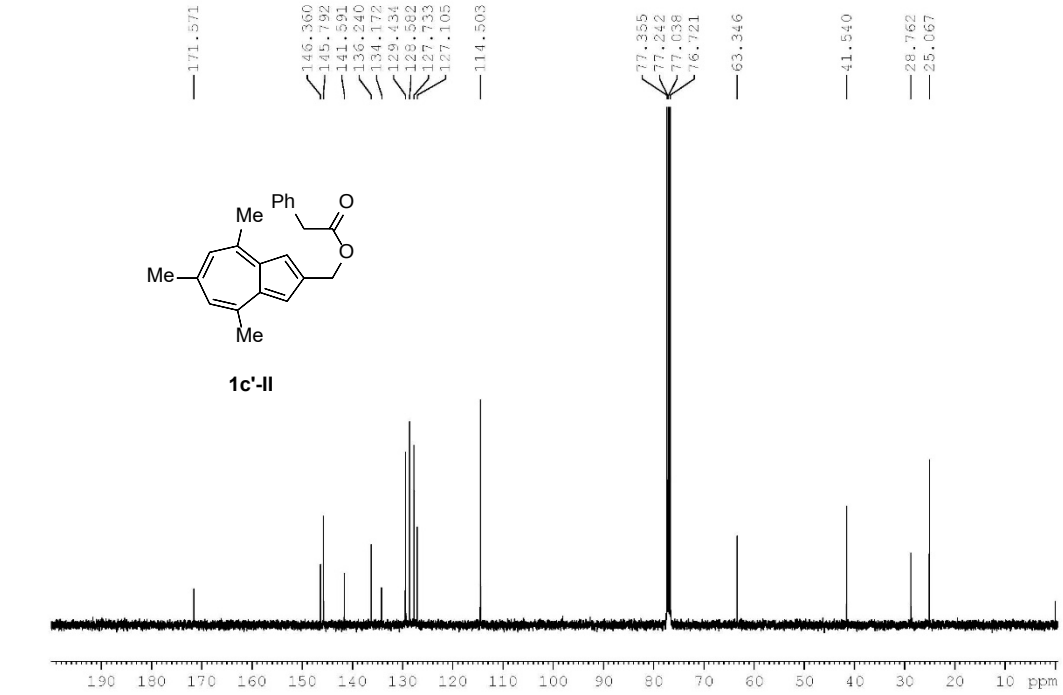
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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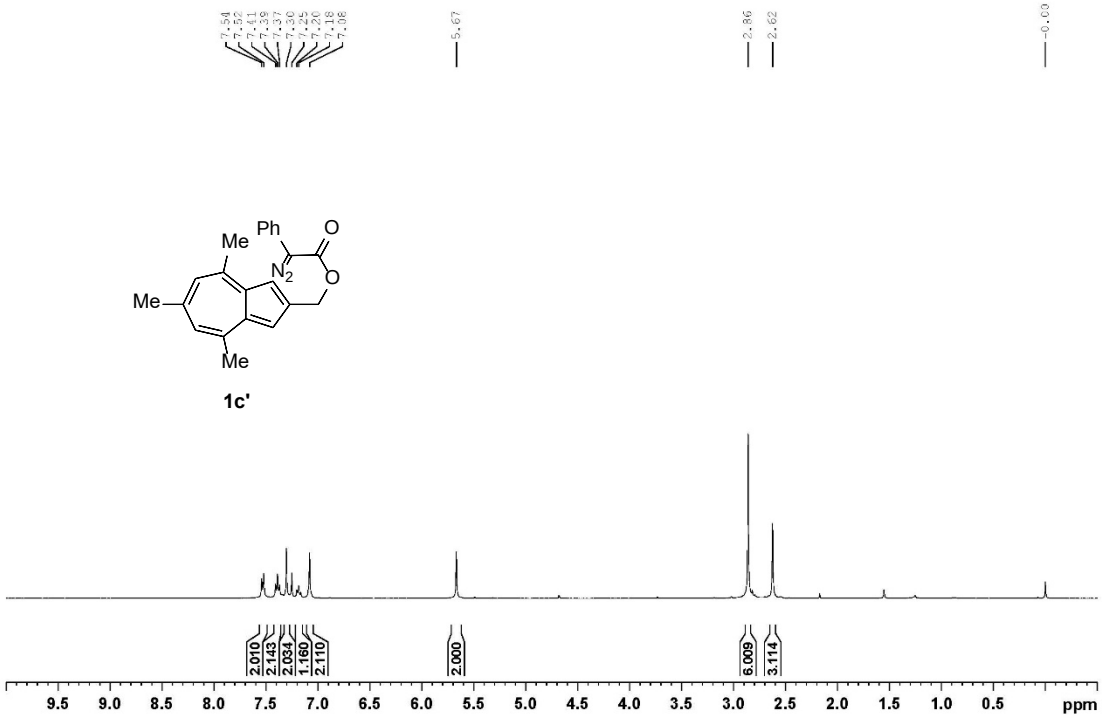
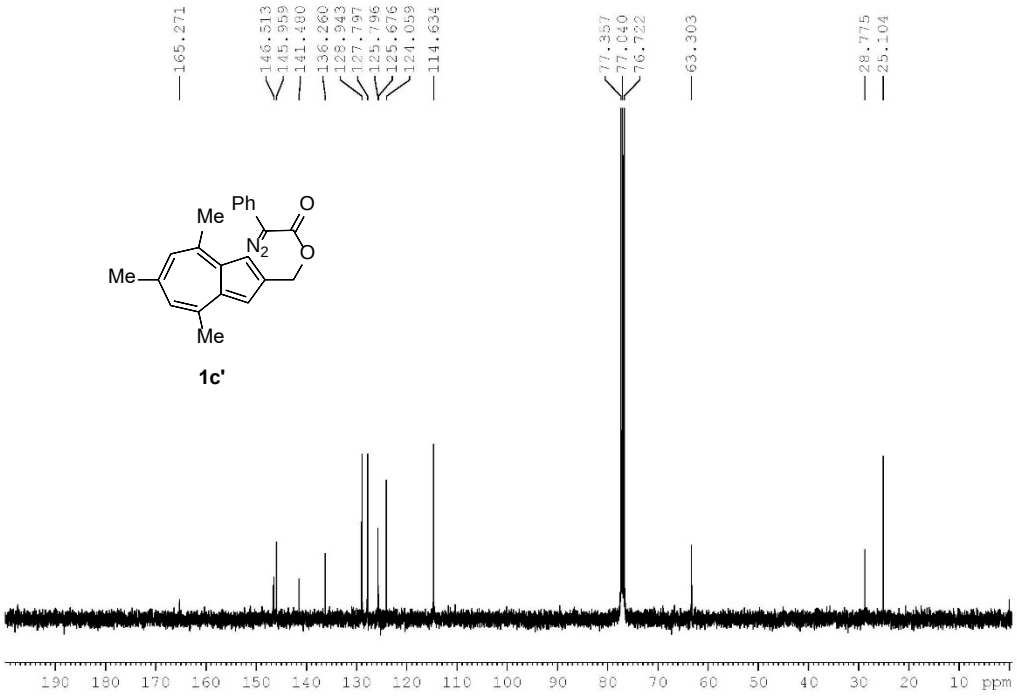


1c'

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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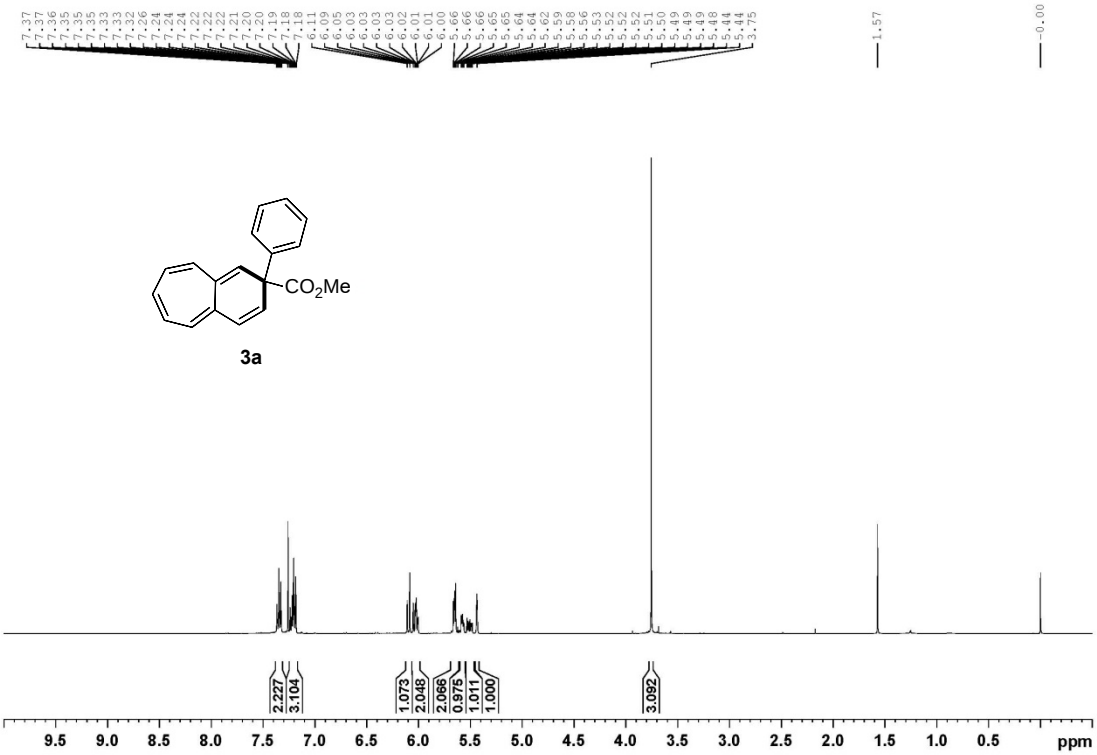
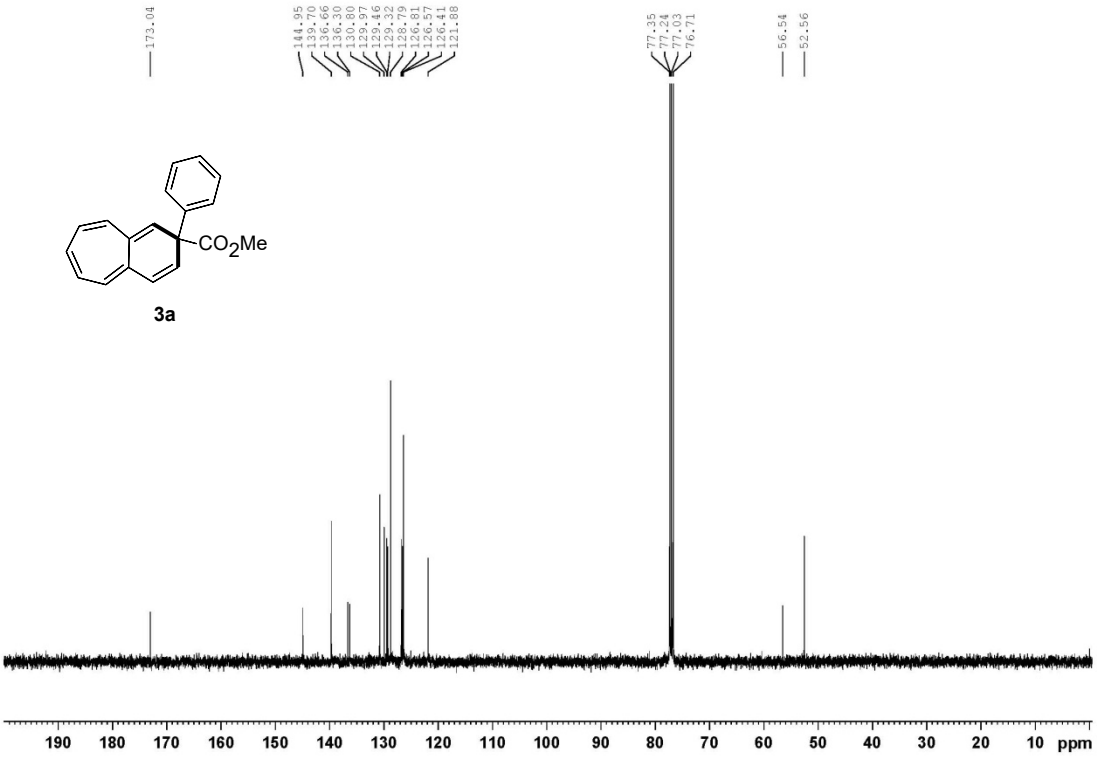
^{1}H NMR (400 MHZ, C_6D_6)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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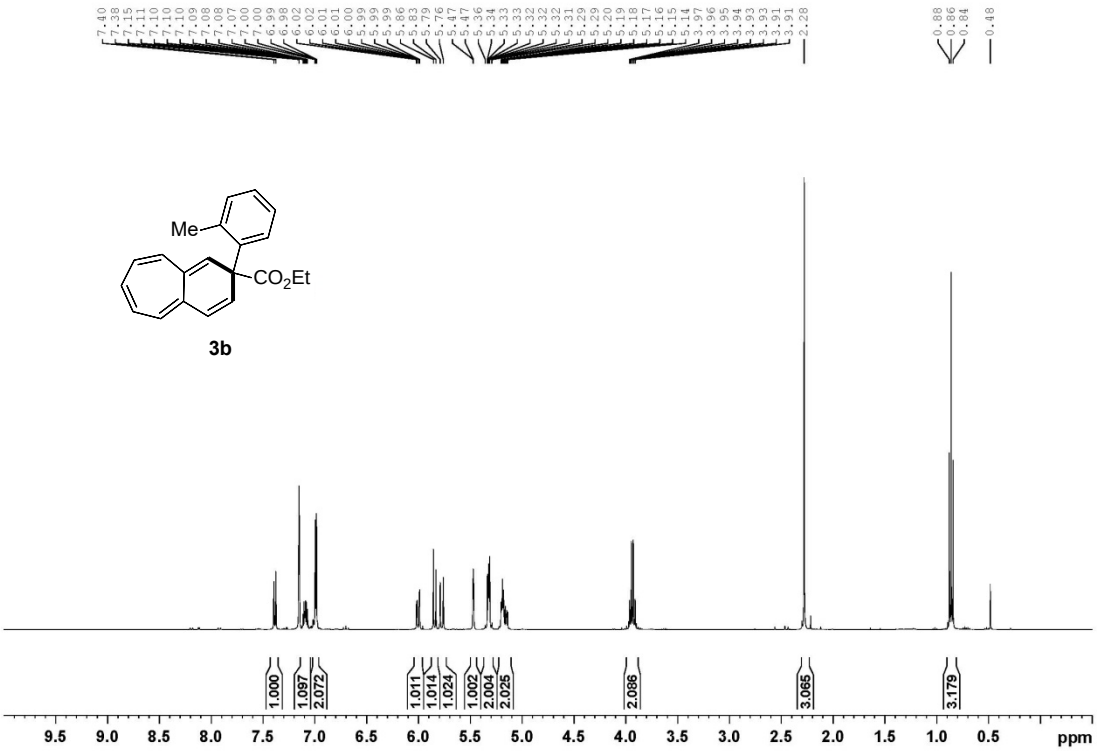
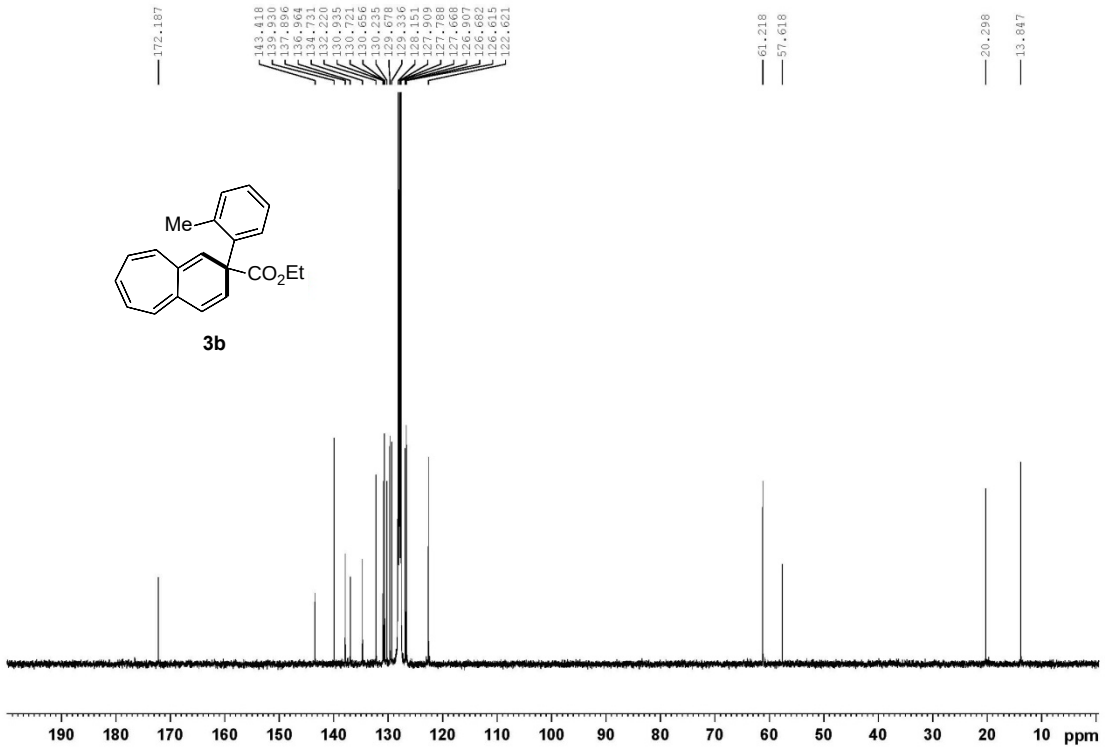


^{13}C{^{1}H}NMR (100 MHz, C_6D_6)



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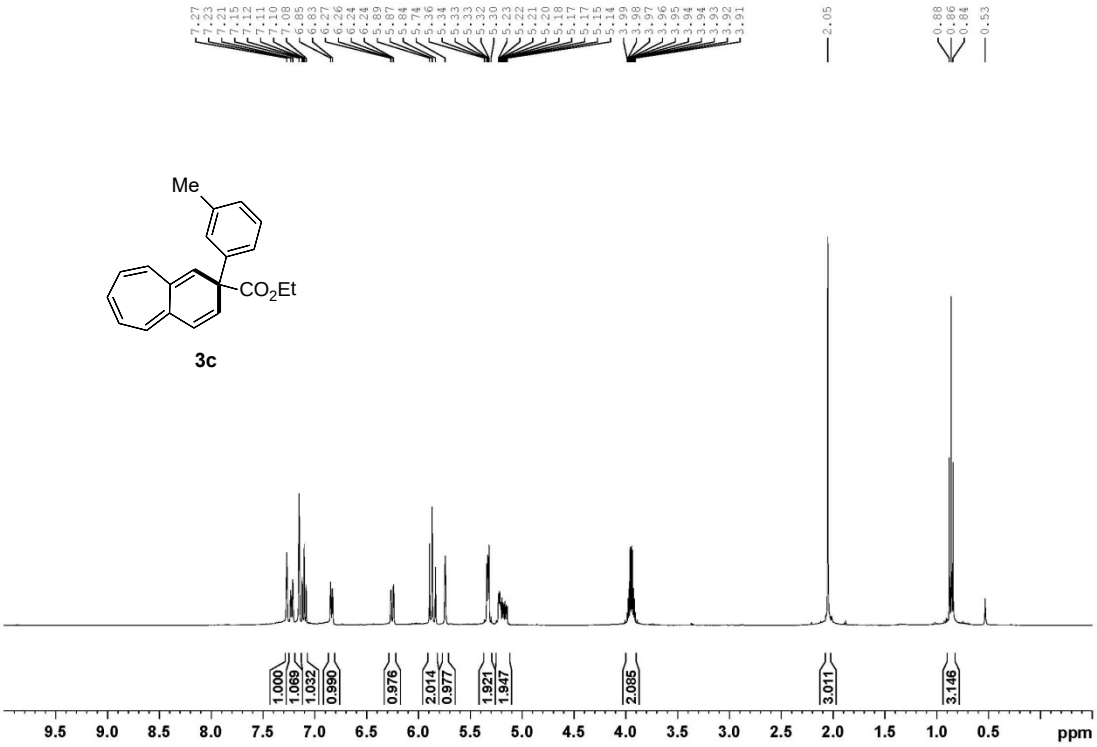

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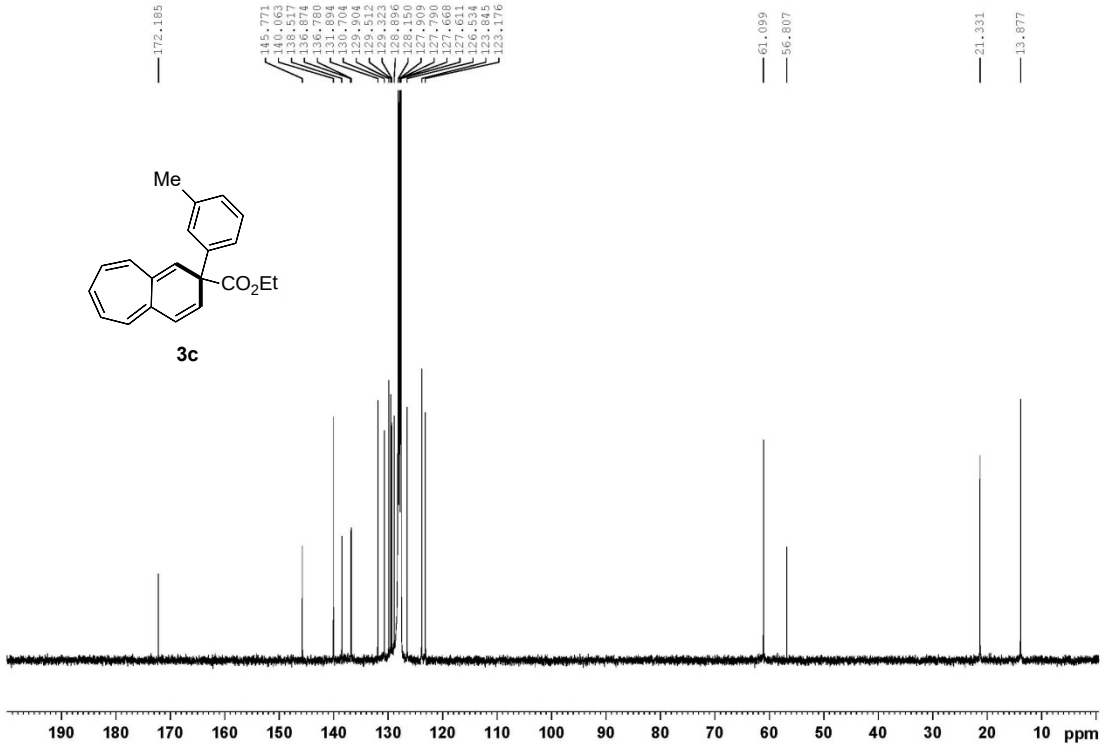

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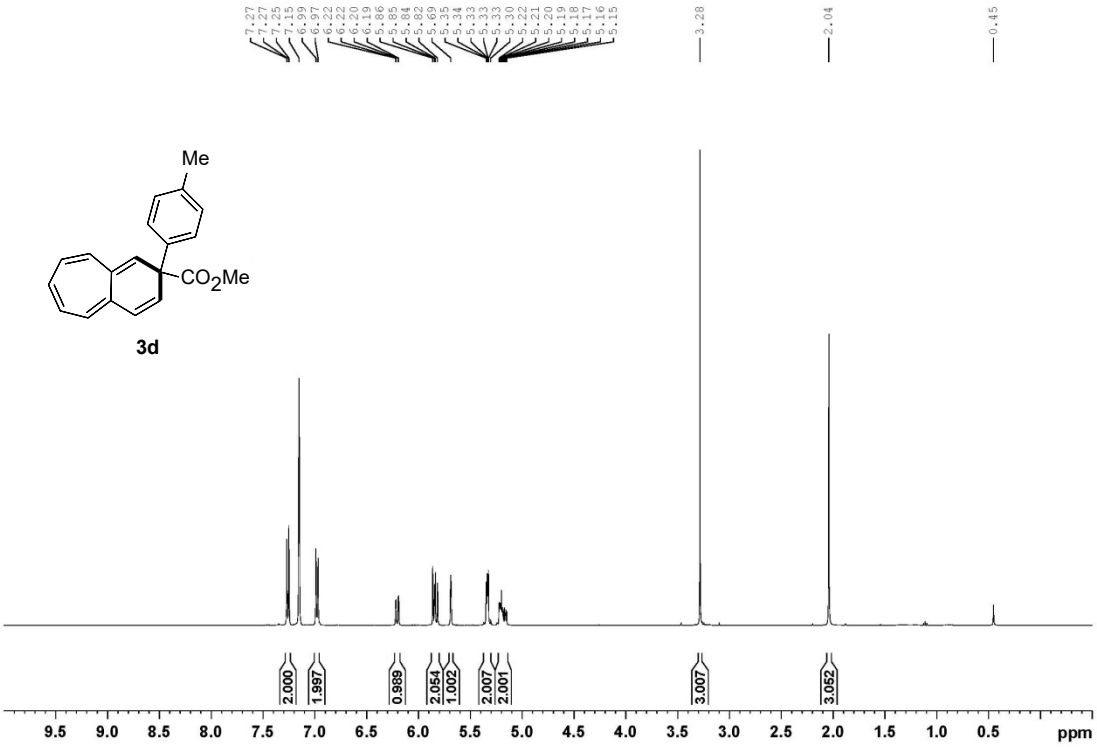

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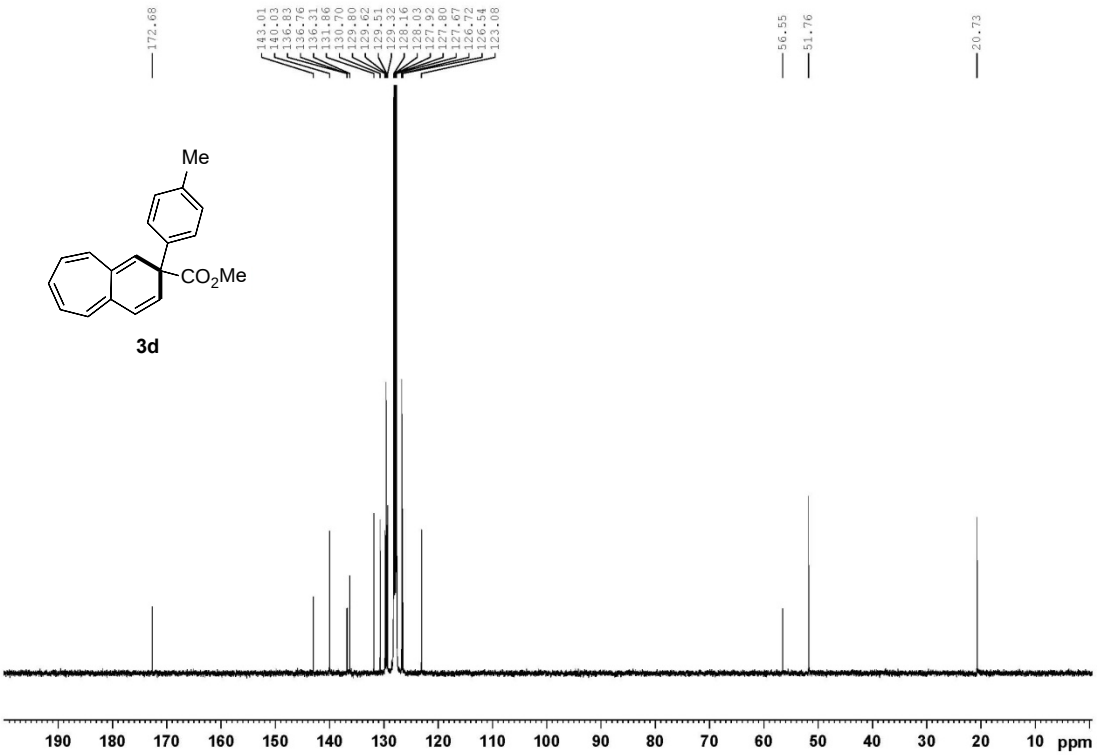

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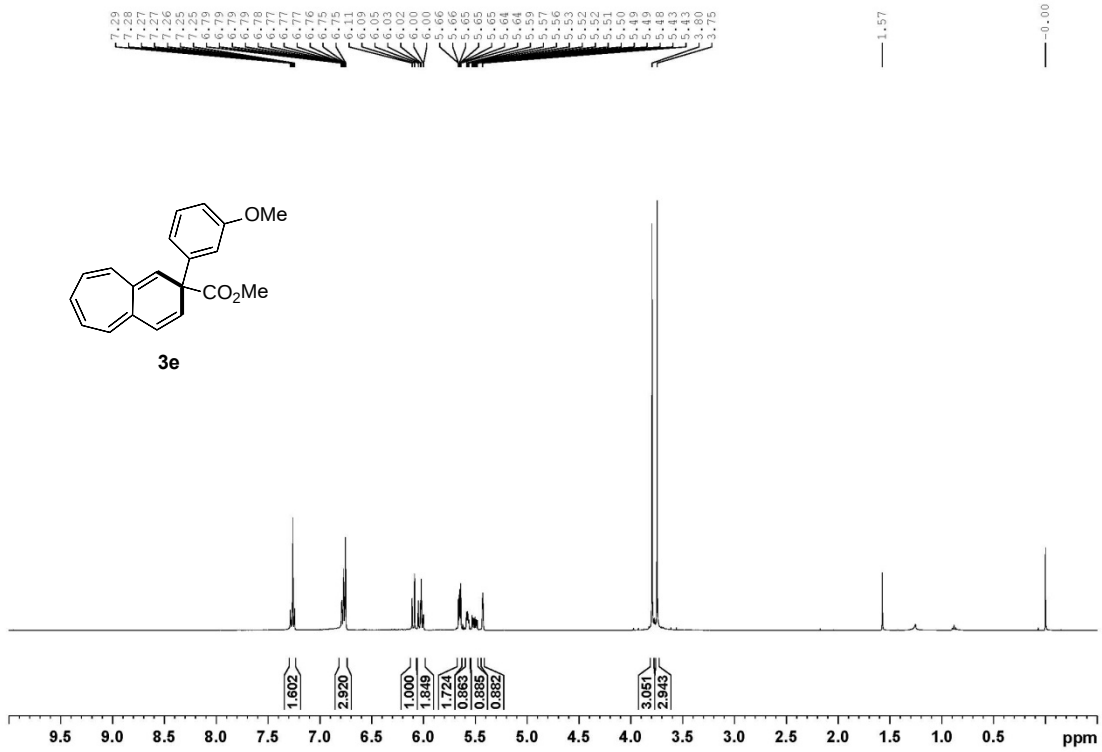
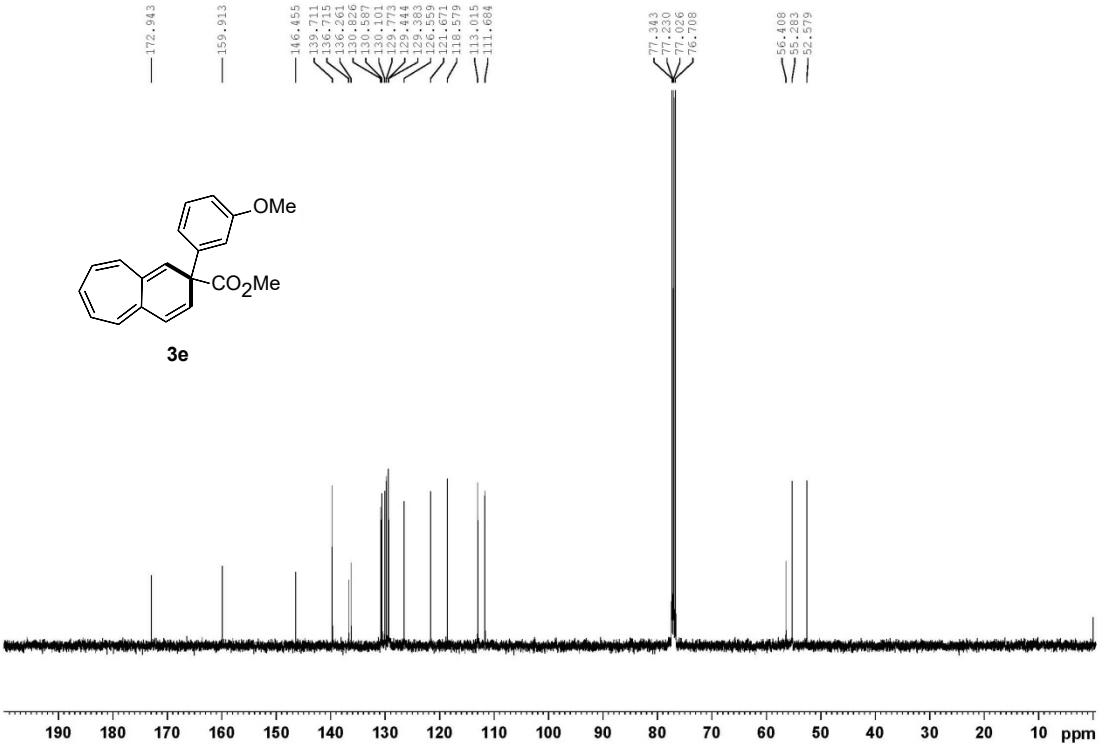


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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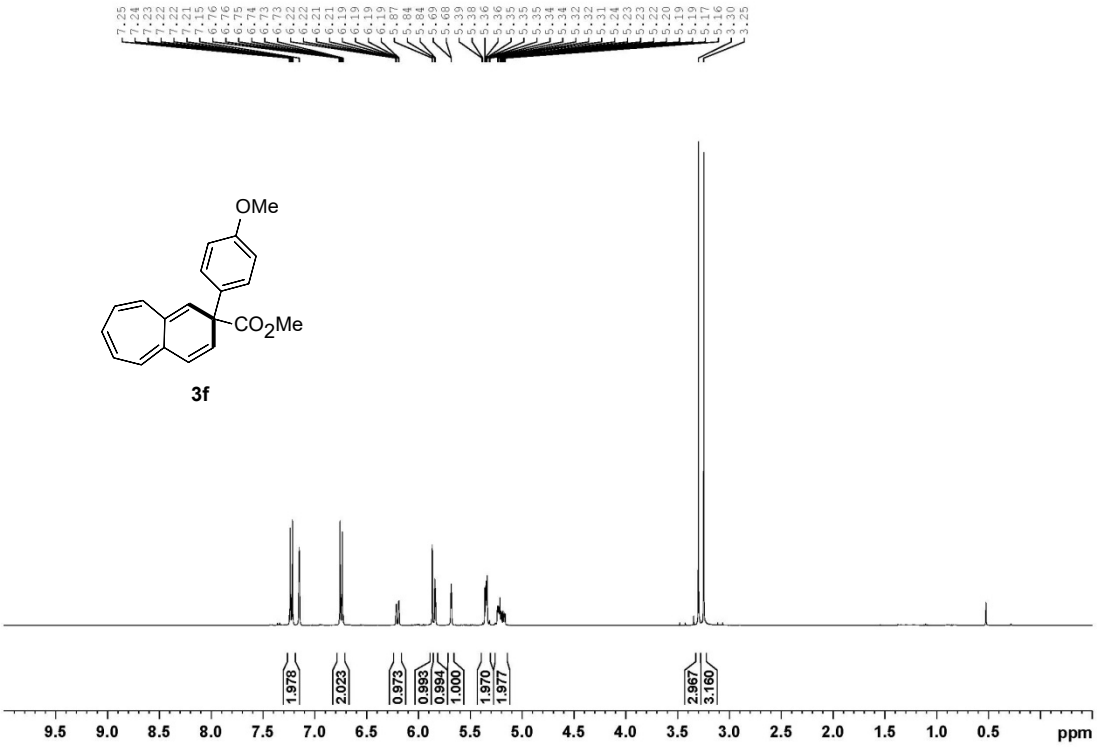

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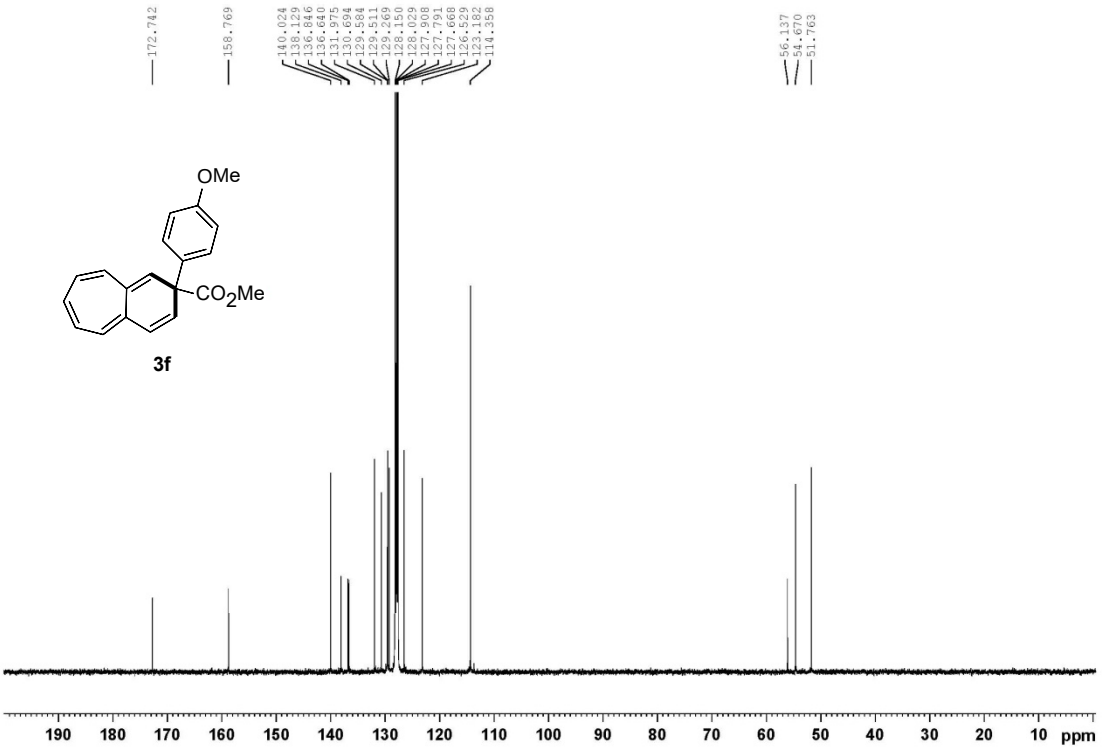

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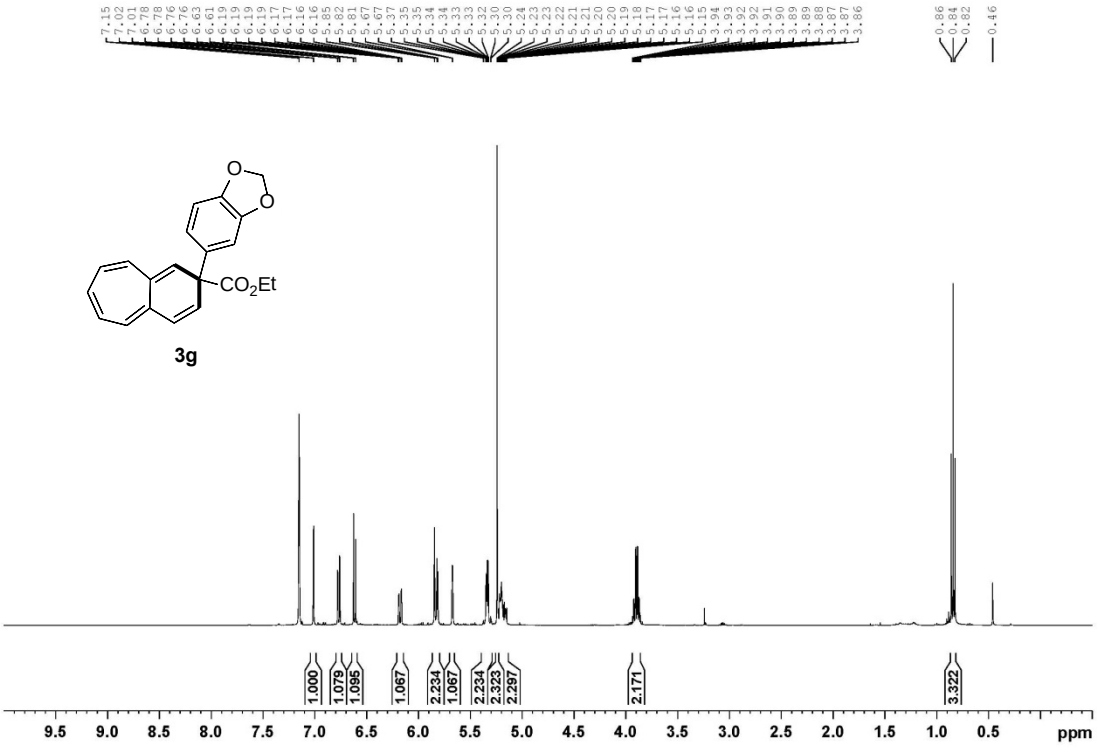

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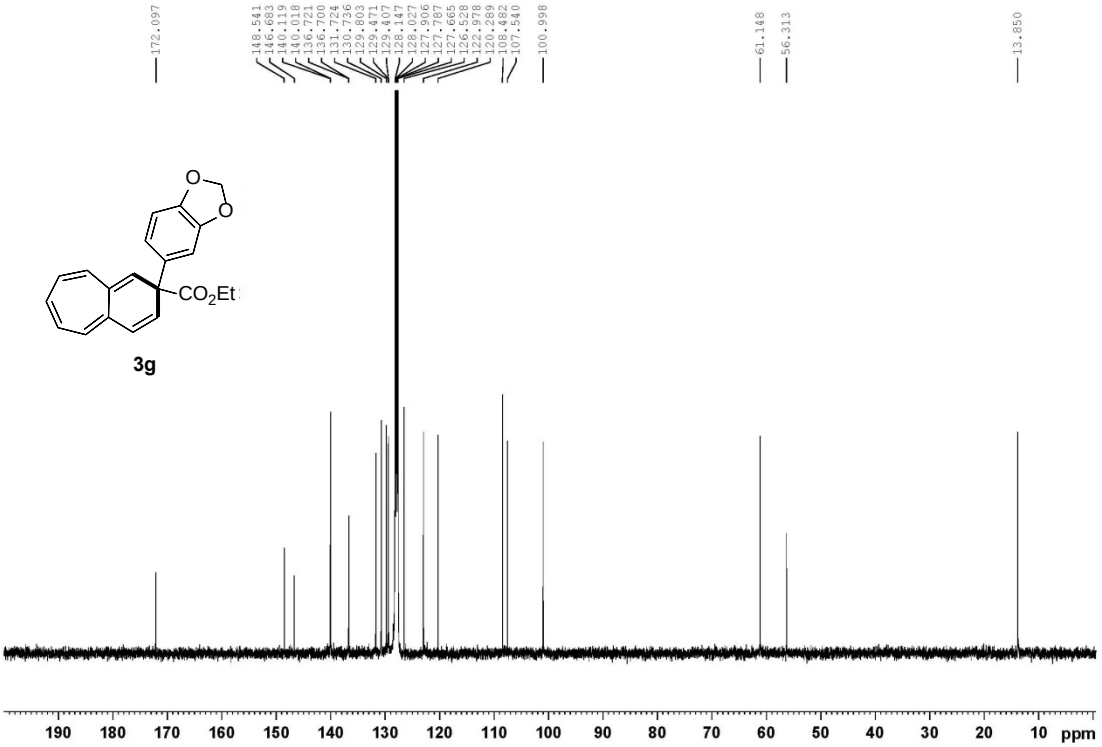

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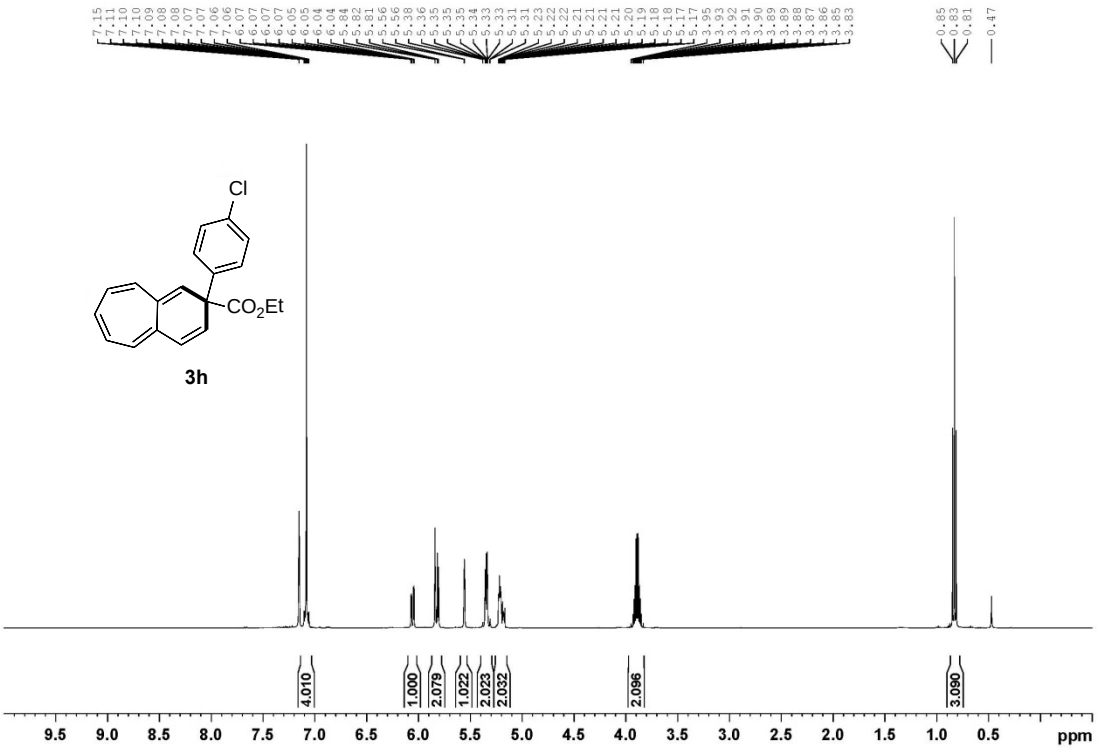

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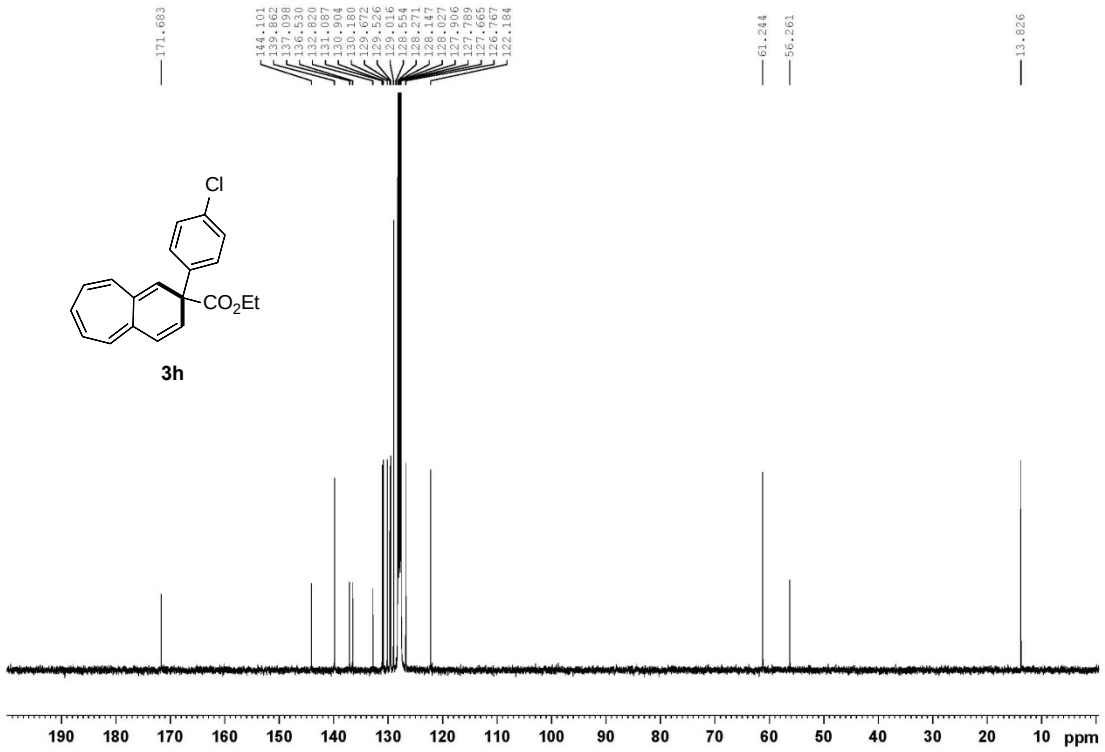

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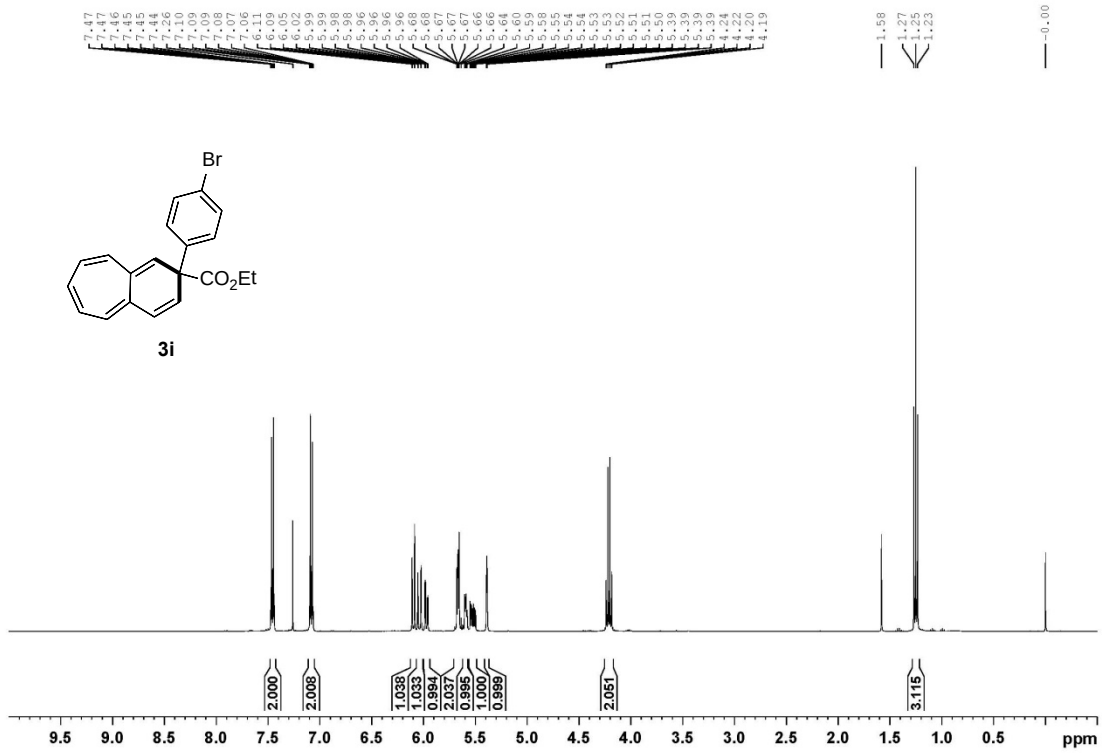

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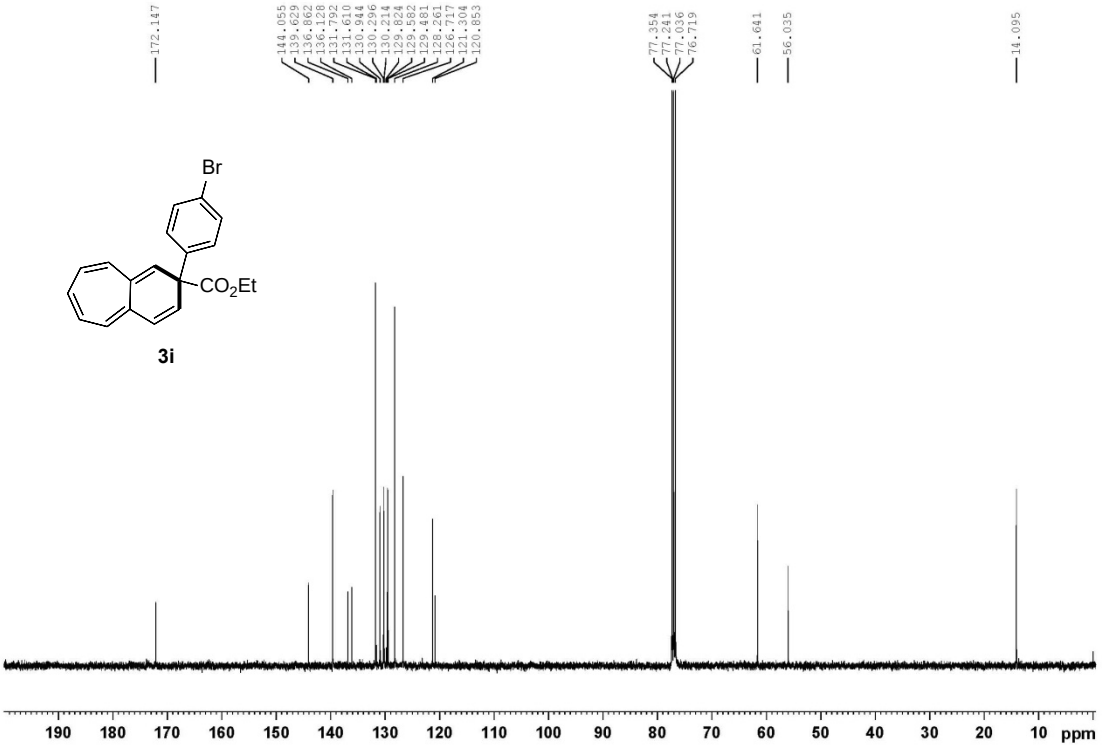

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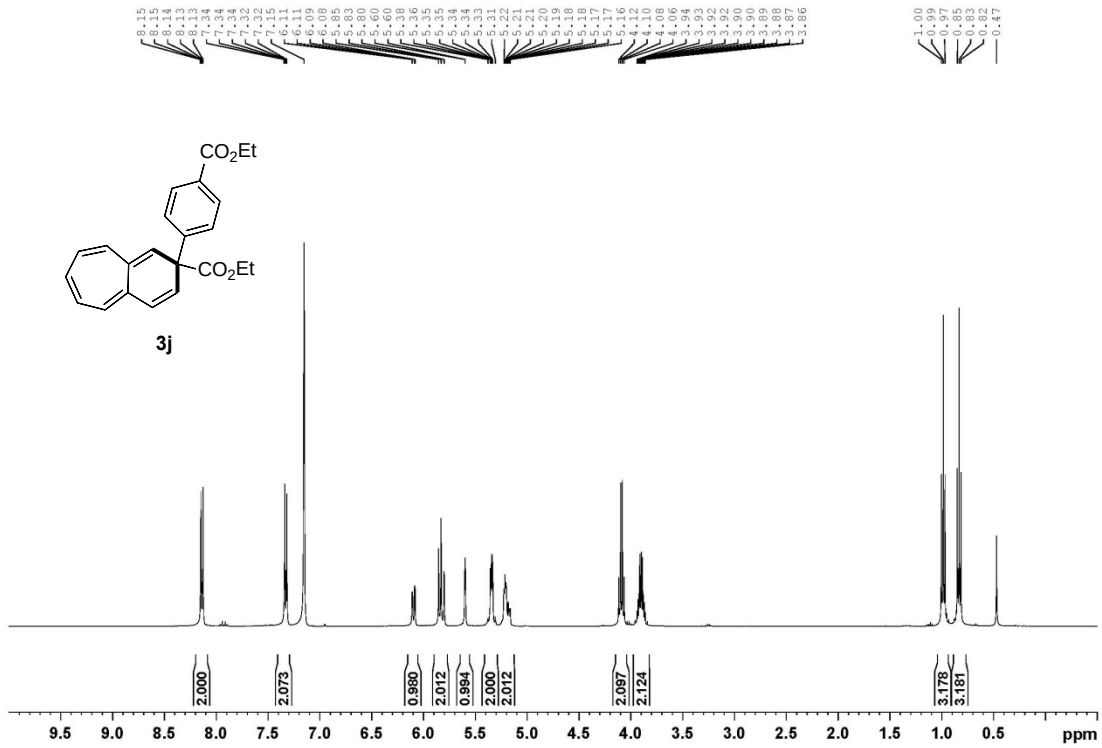

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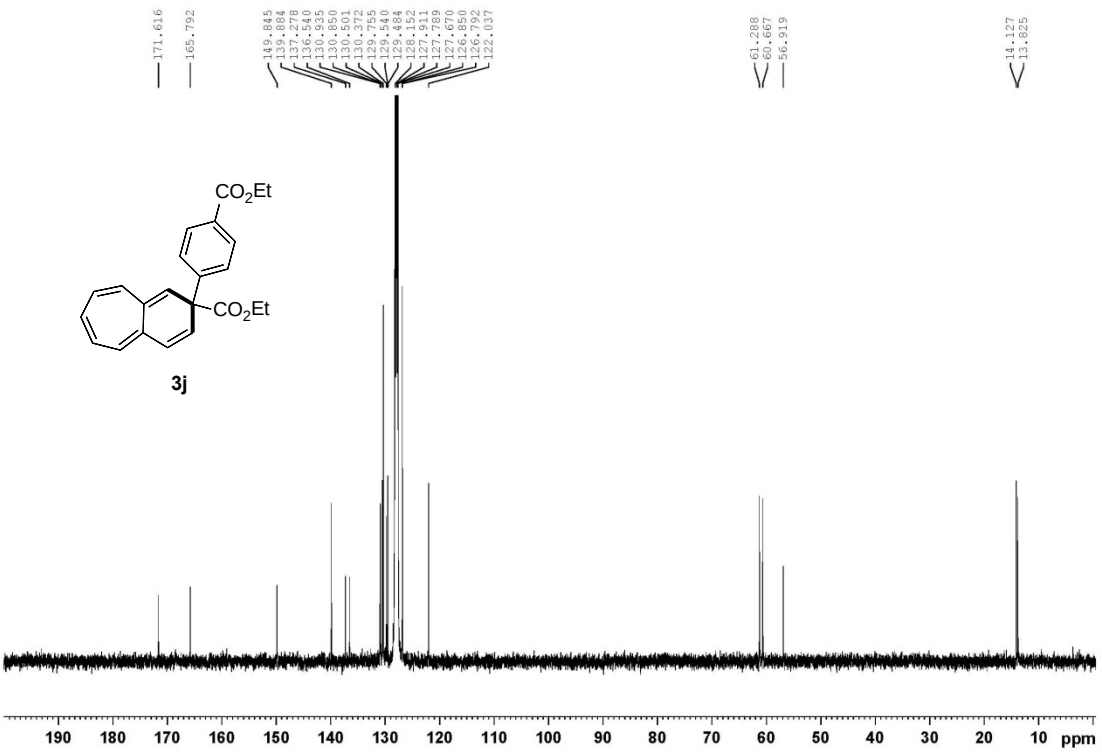

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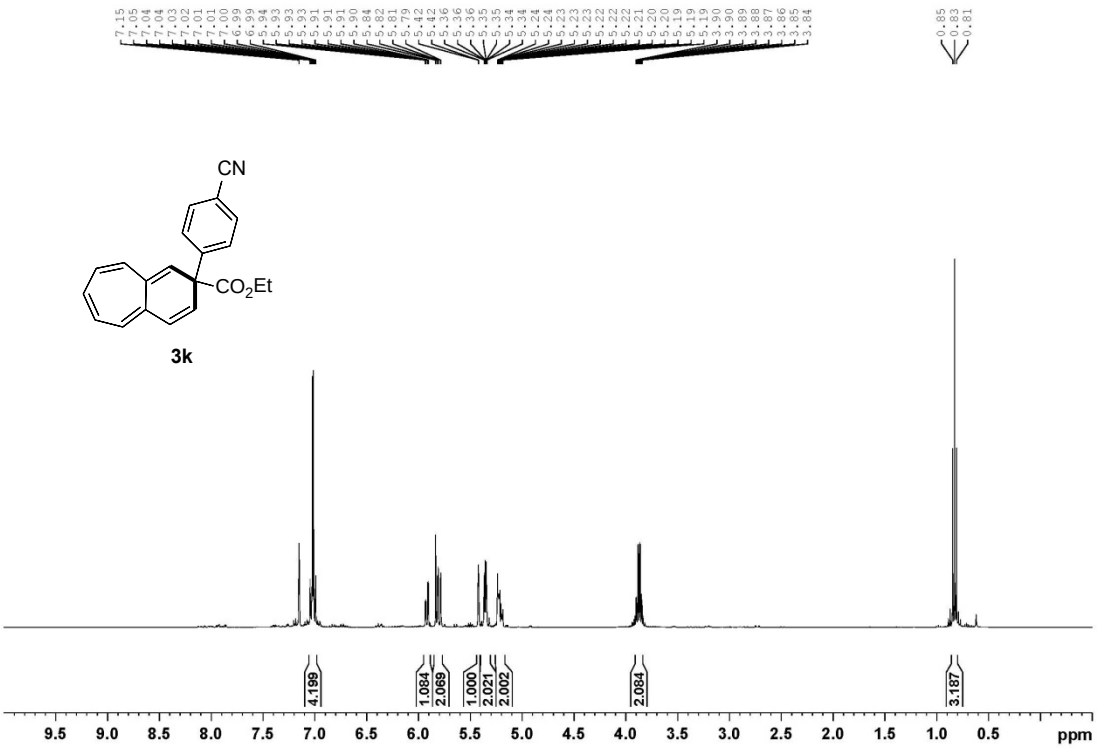

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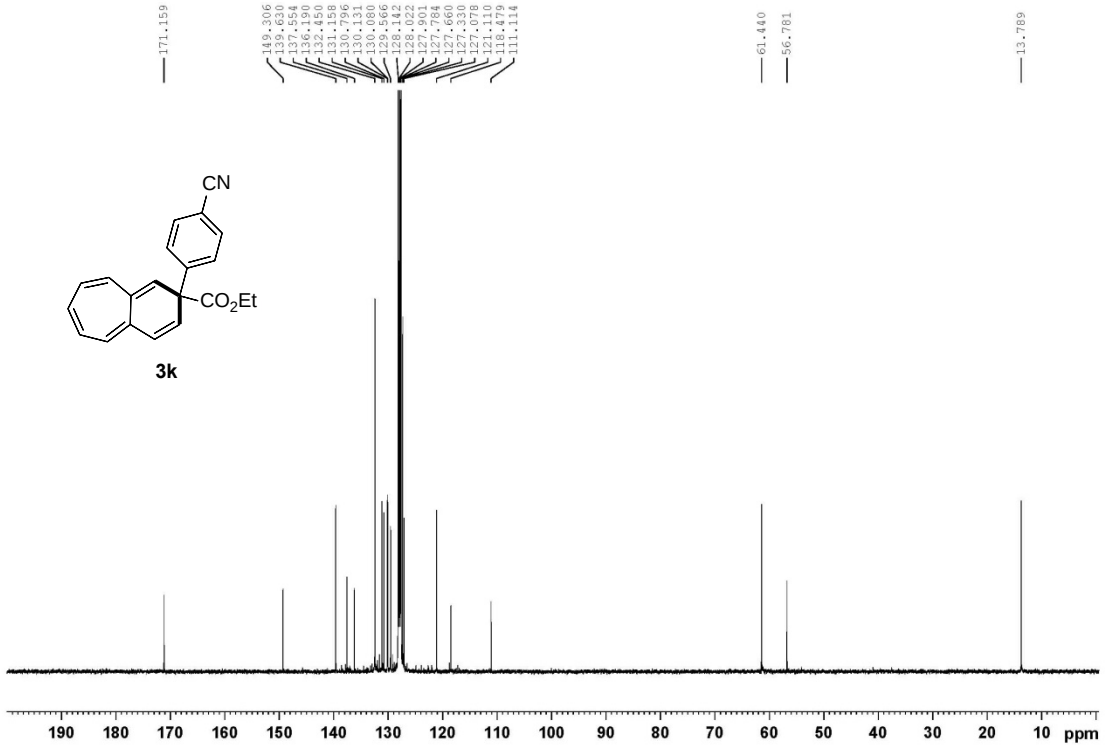

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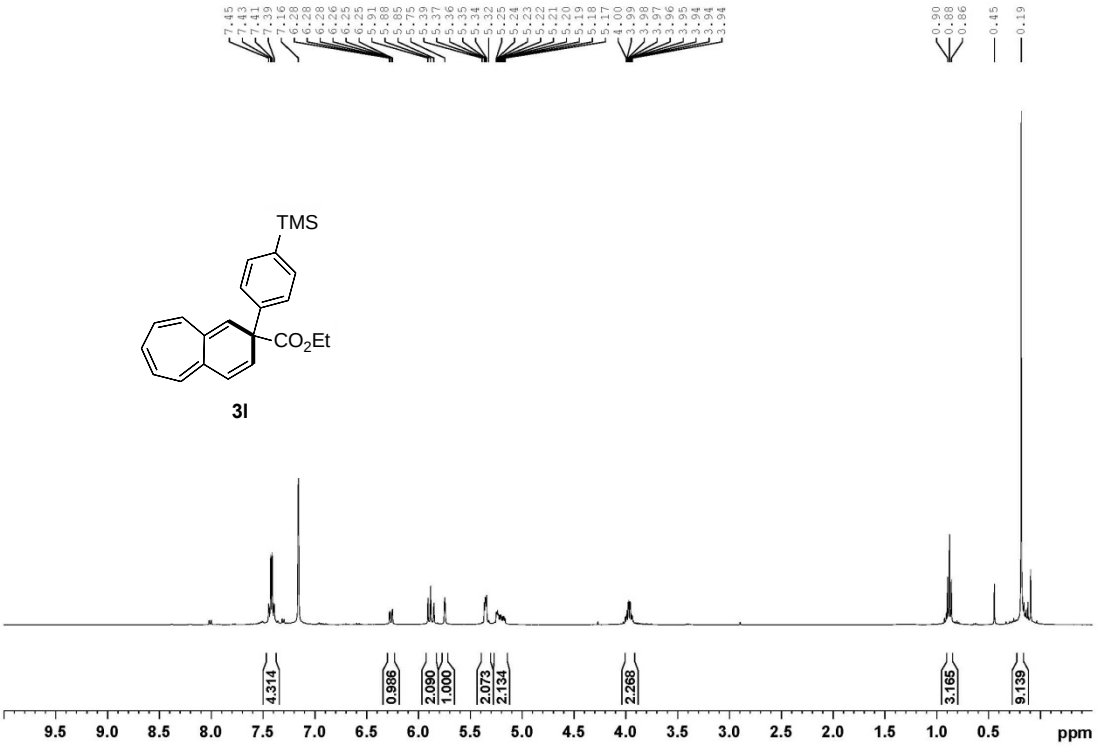

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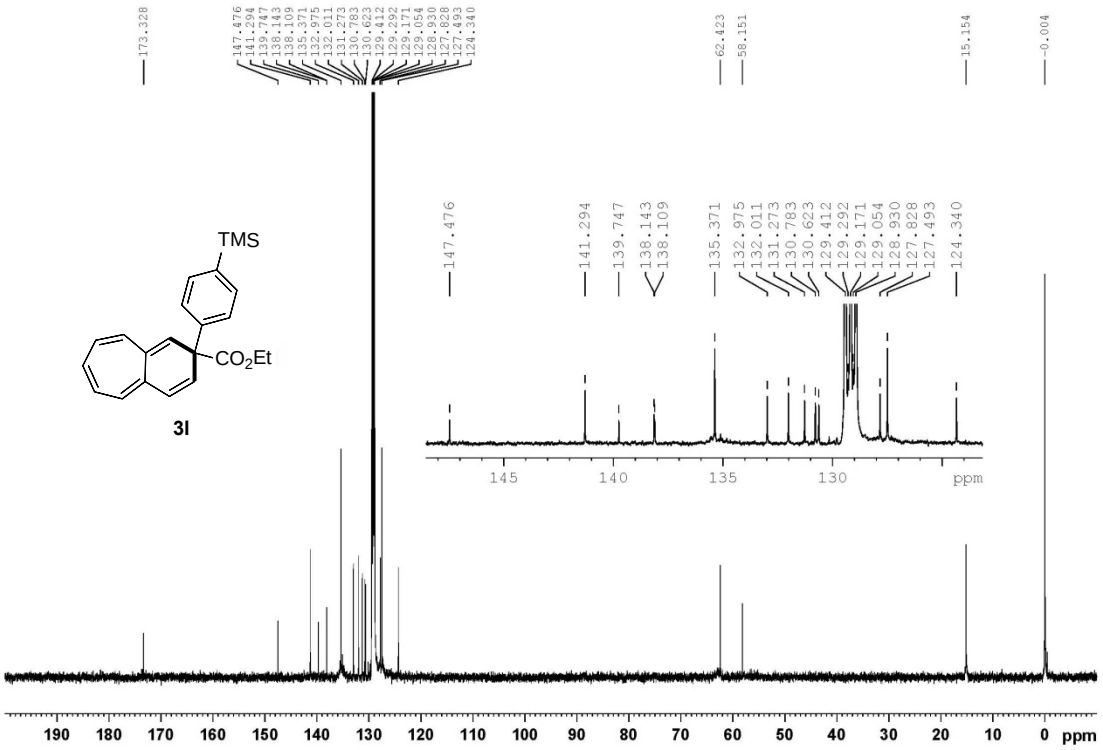

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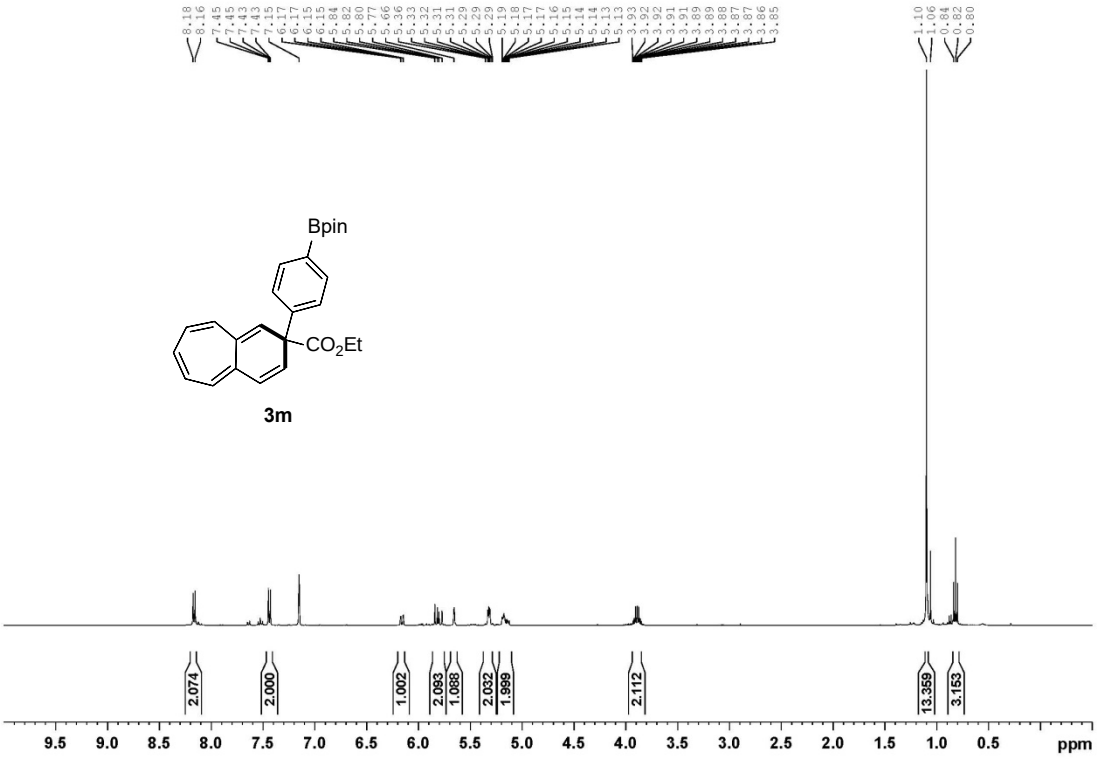
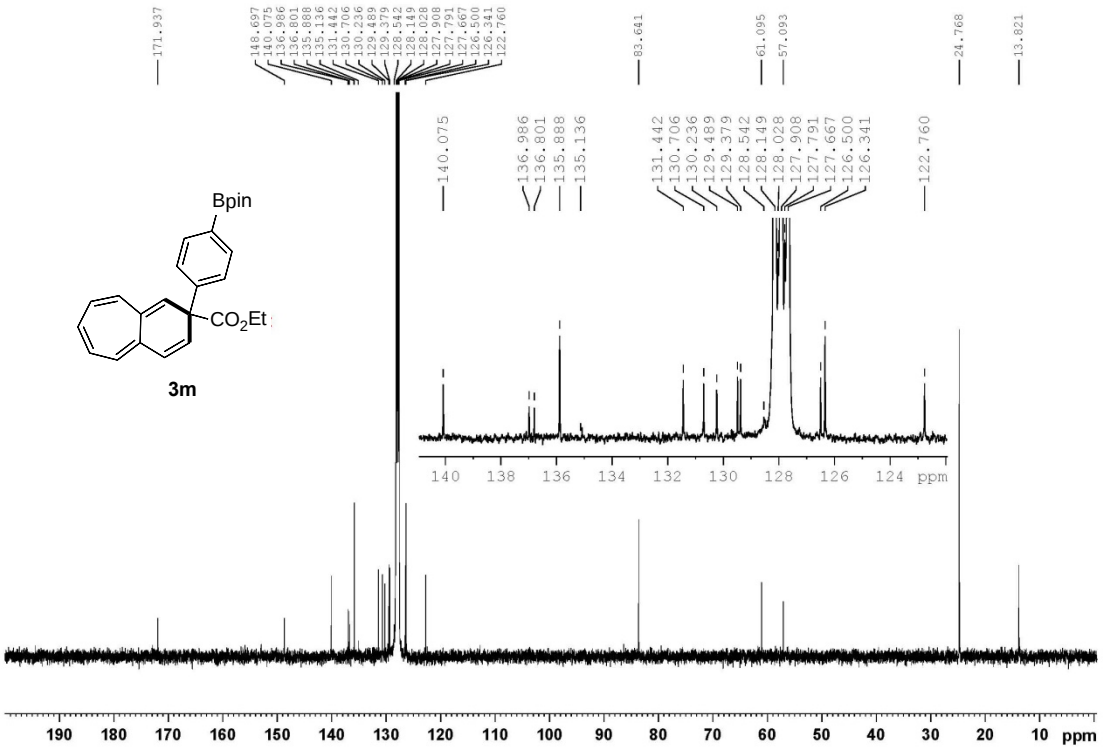


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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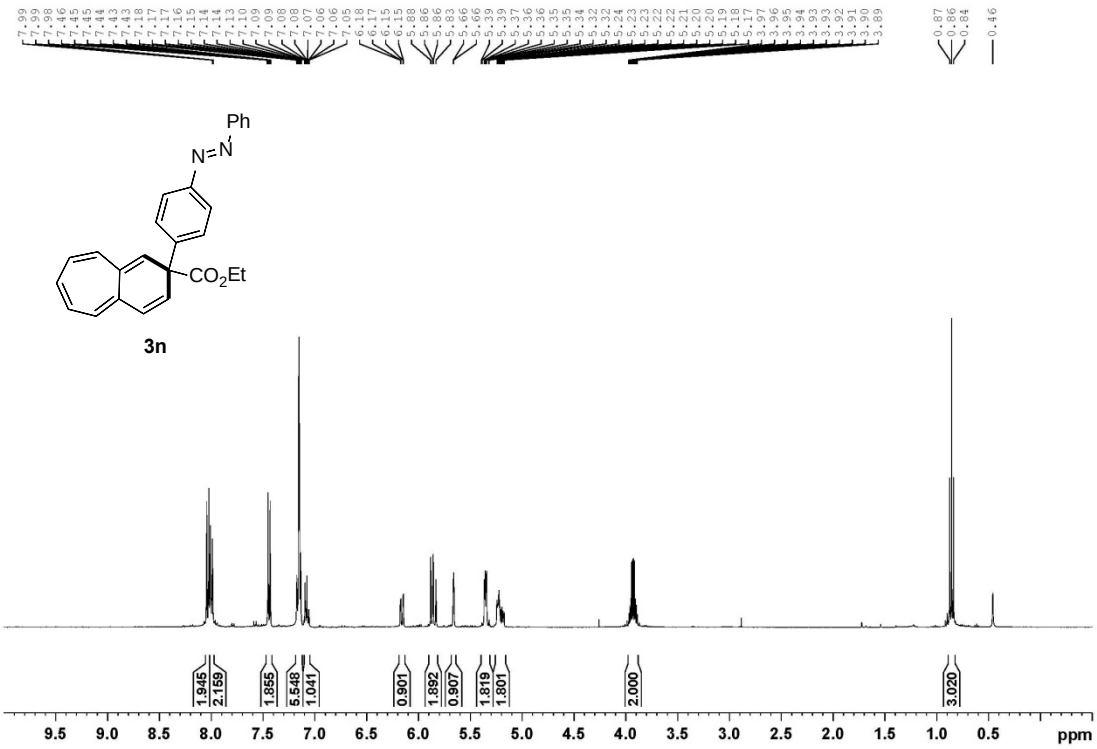
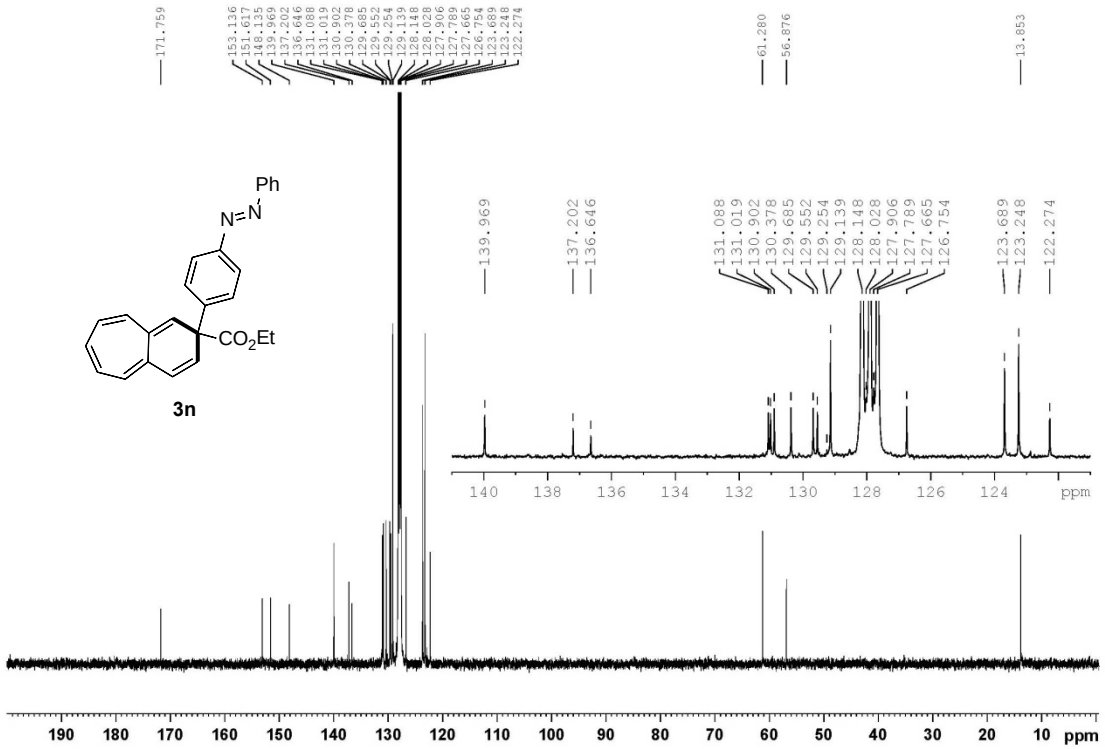


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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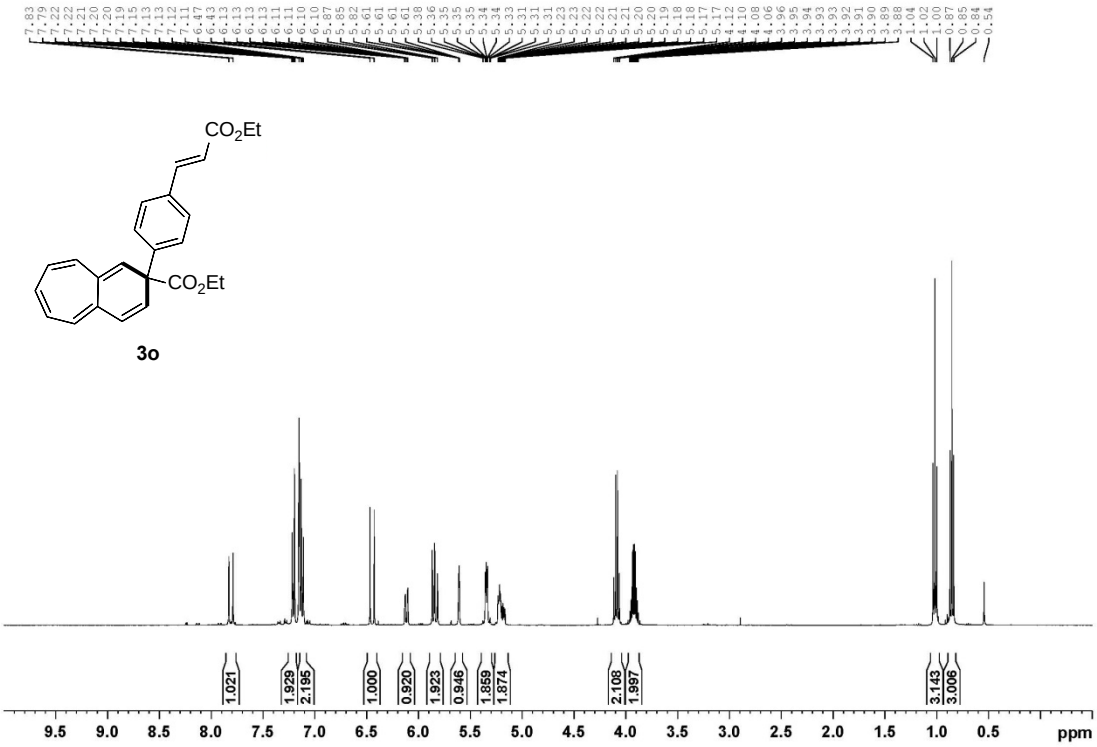
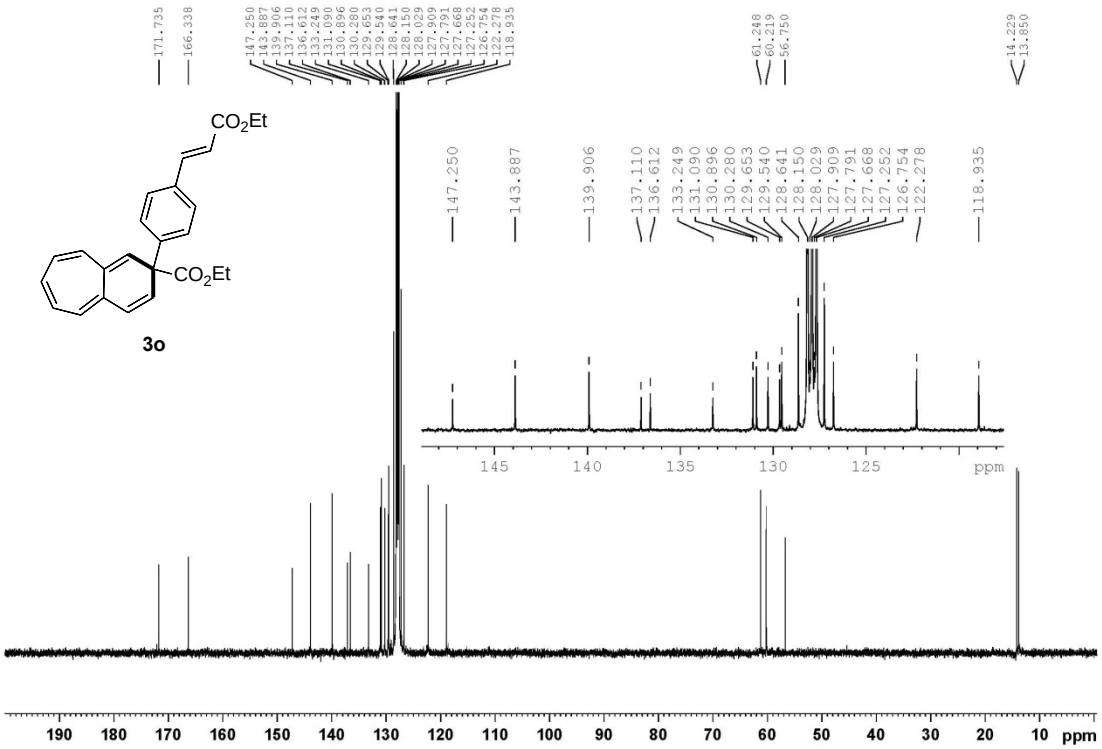


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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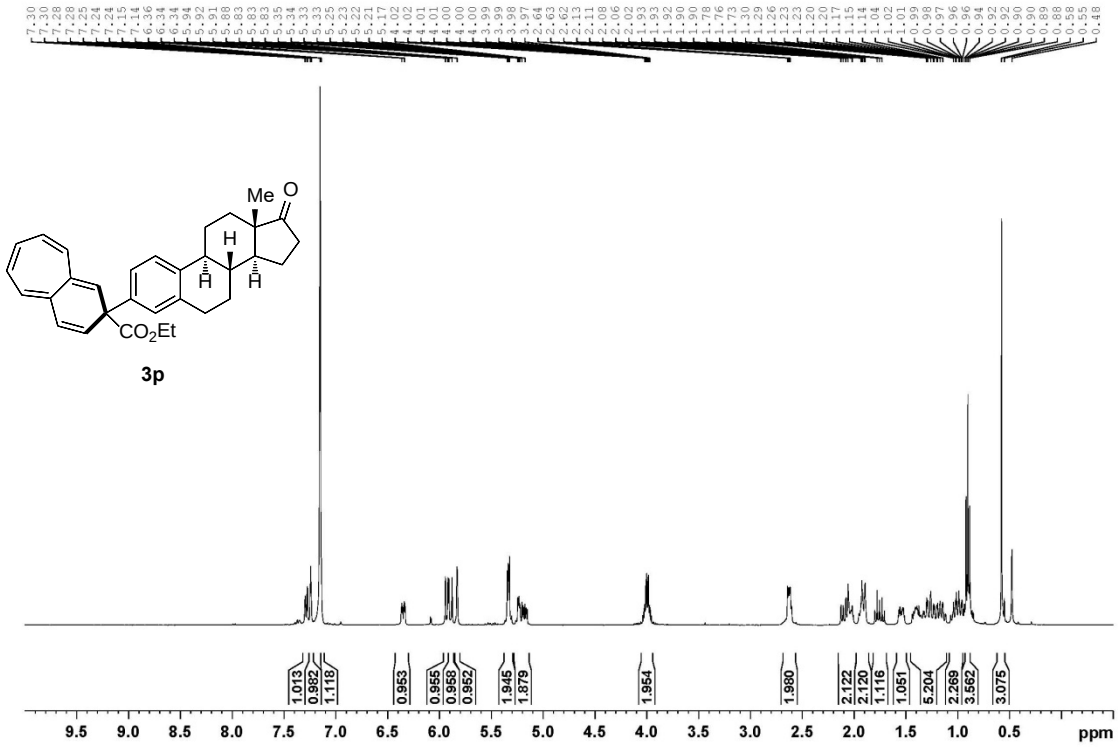
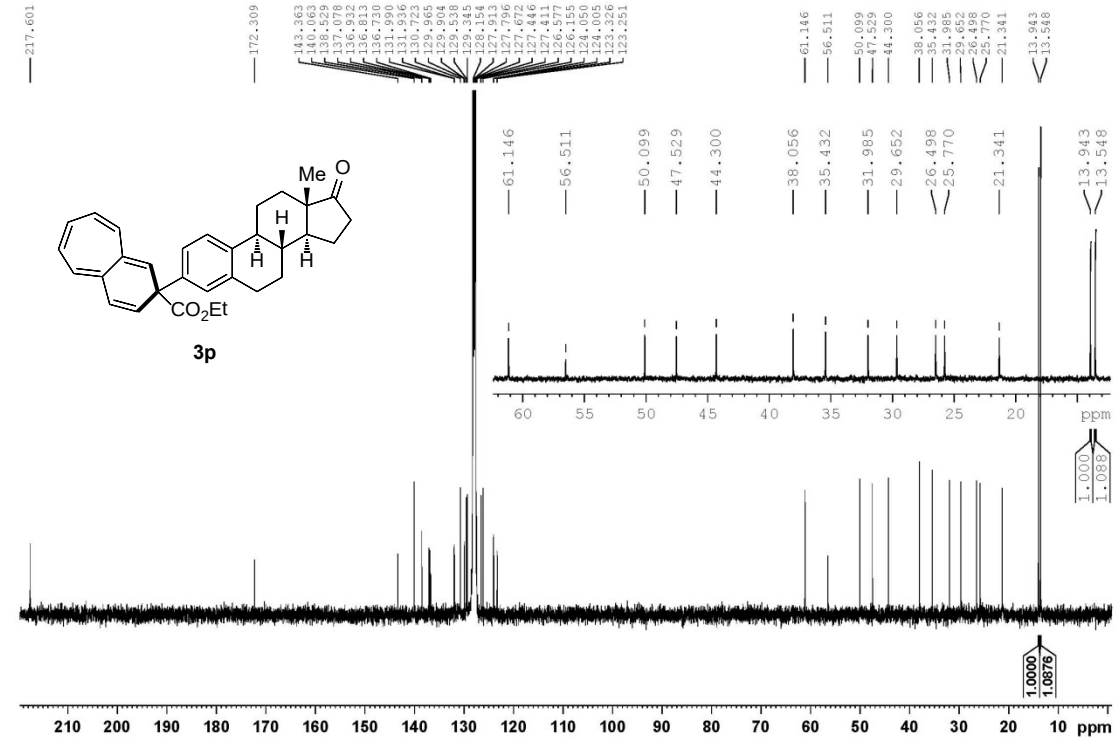


^{13}C{^{1}H}NMR (100 MHz, C_6D_6)



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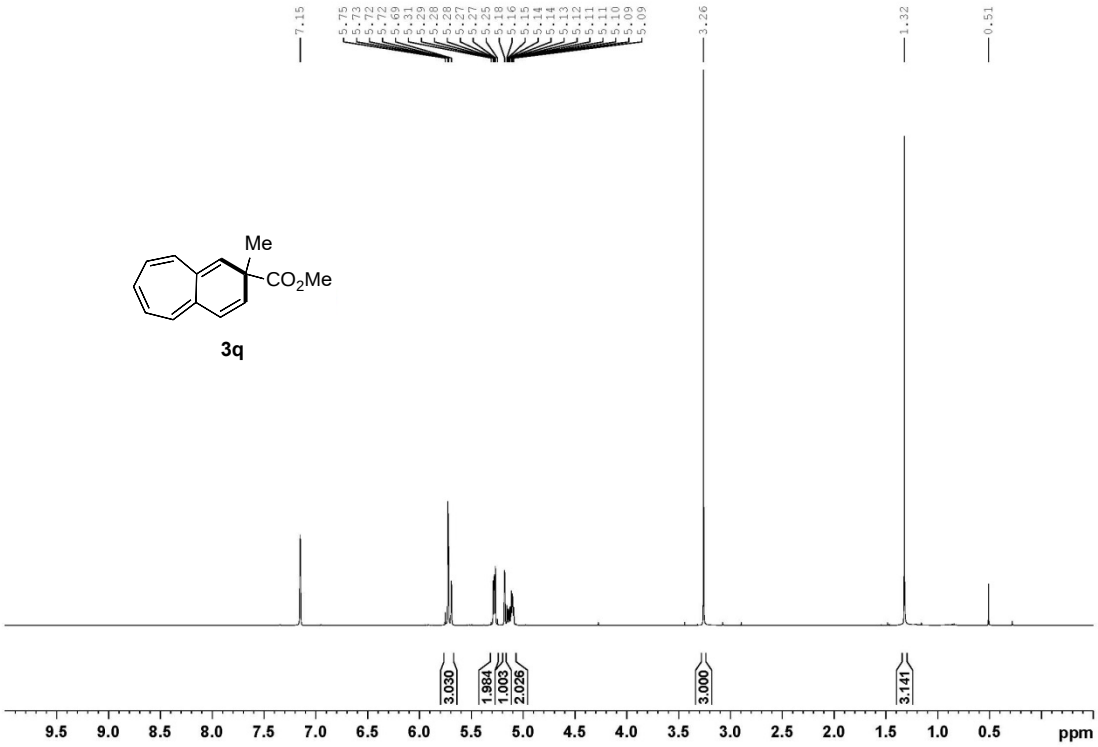
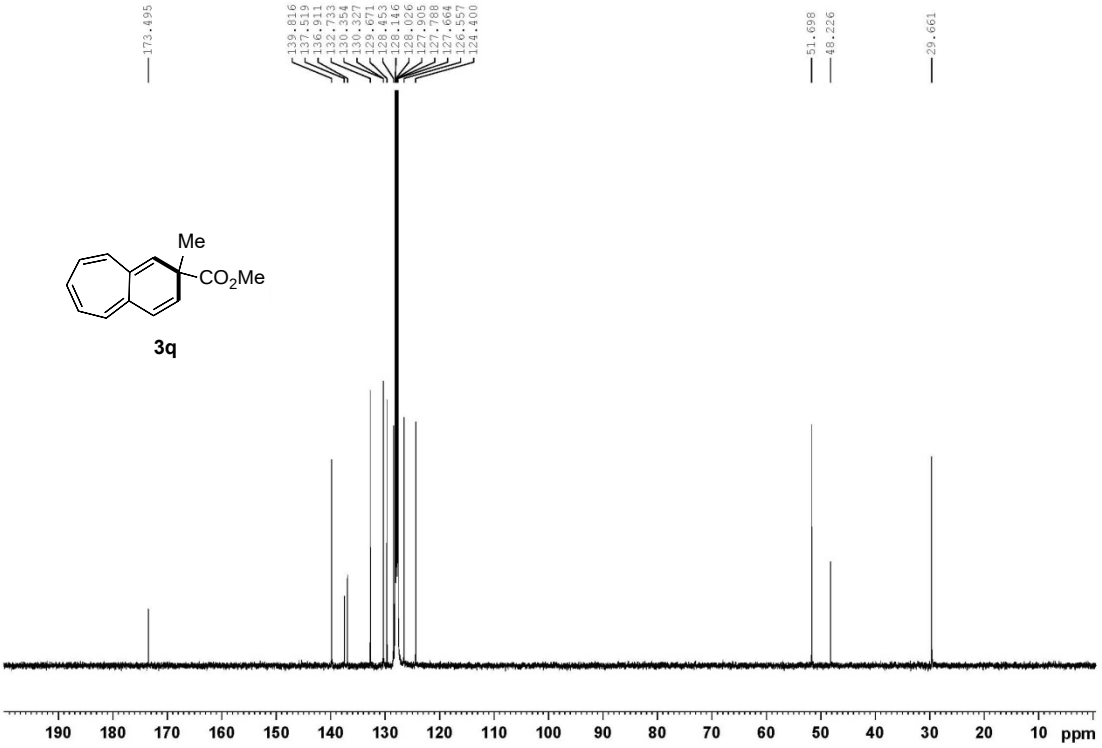


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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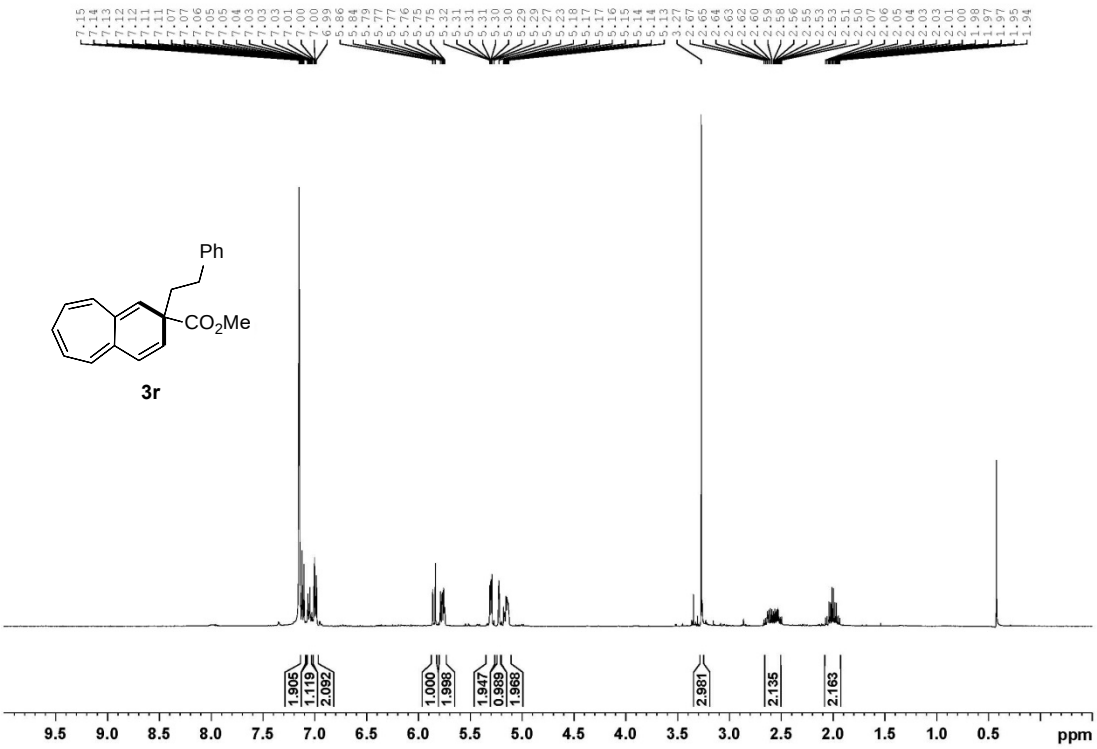
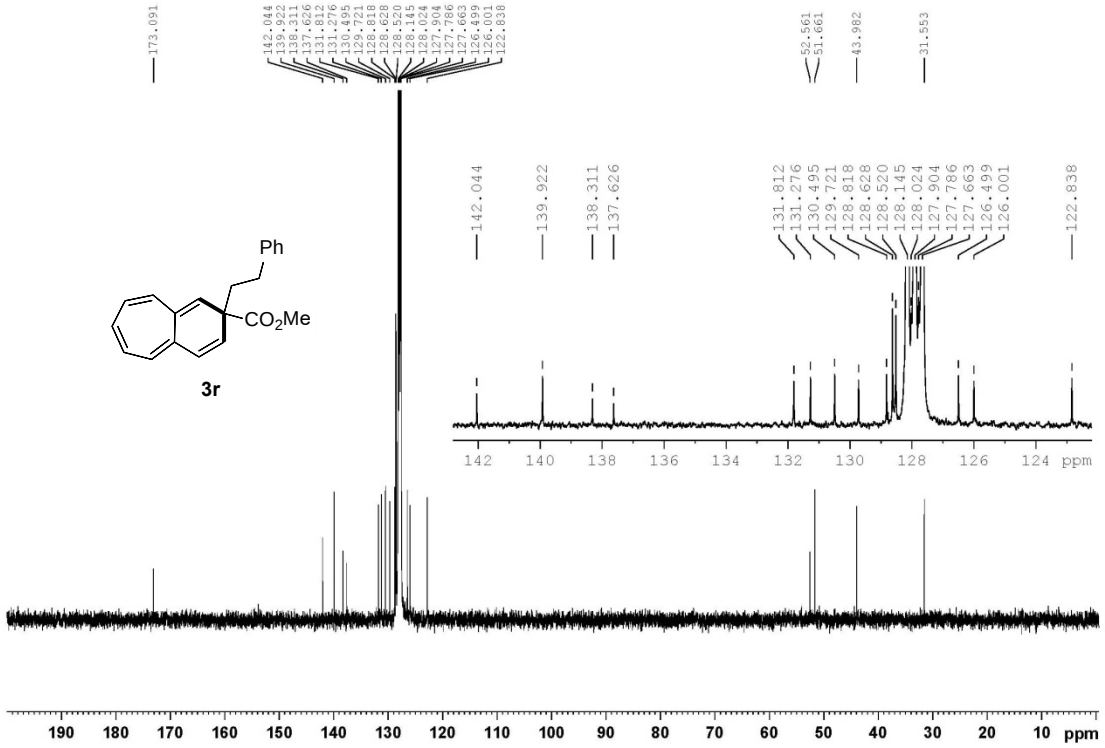


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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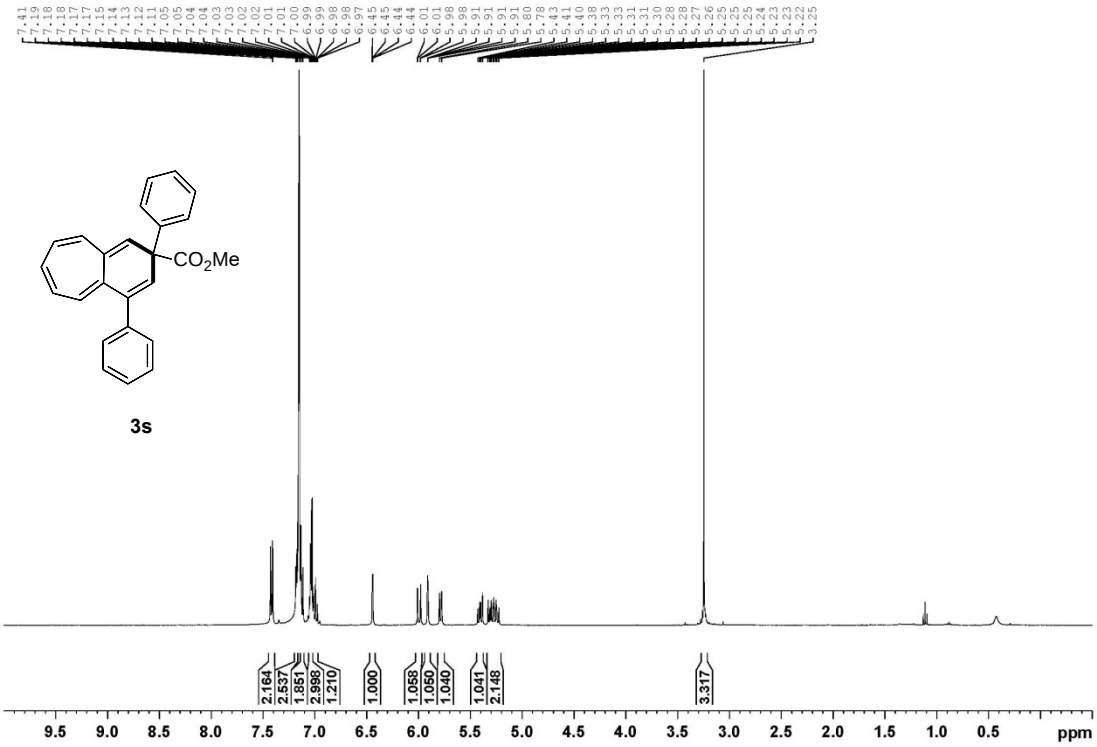

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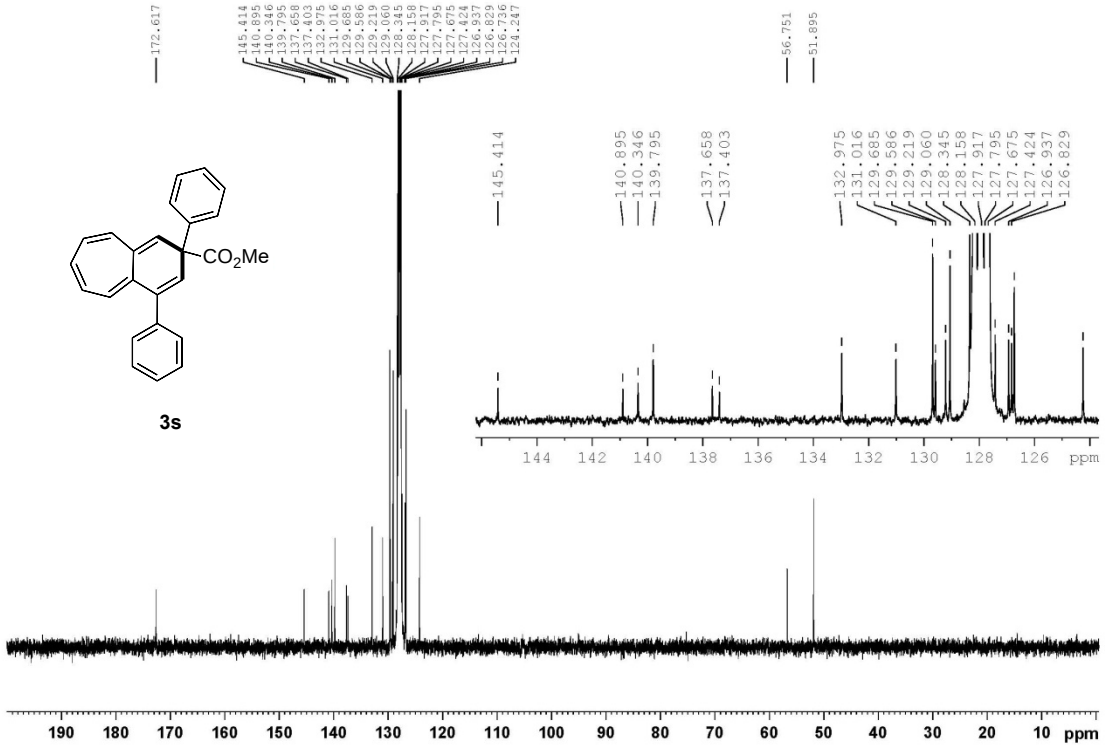

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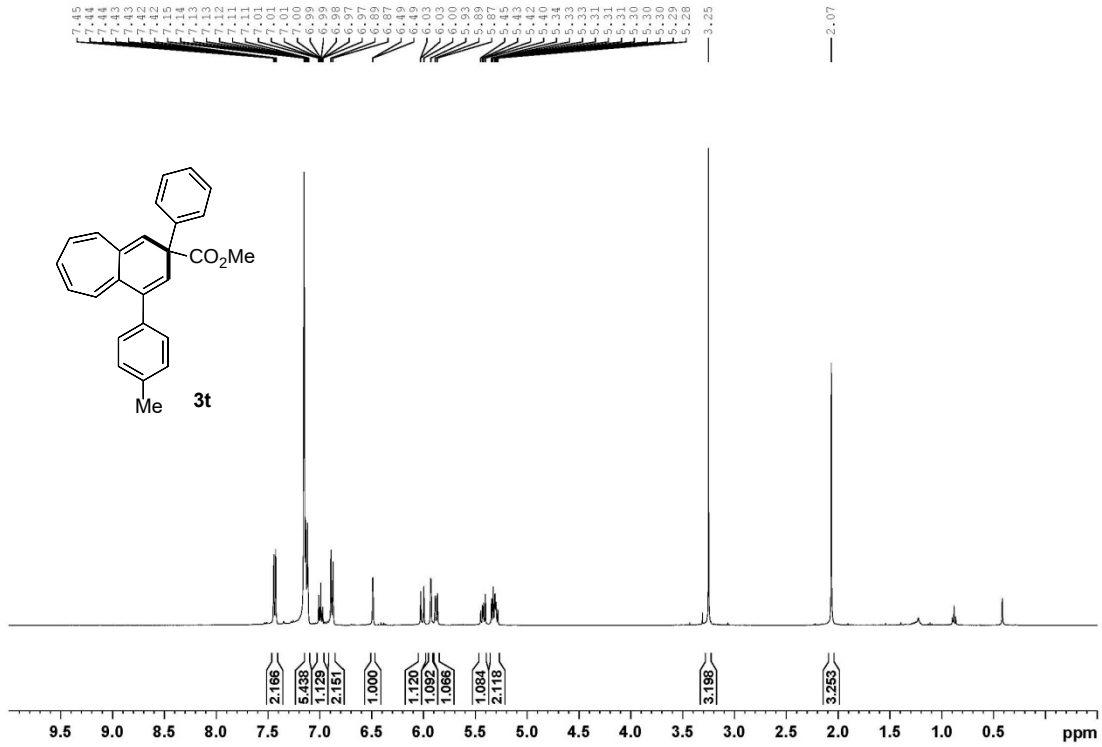
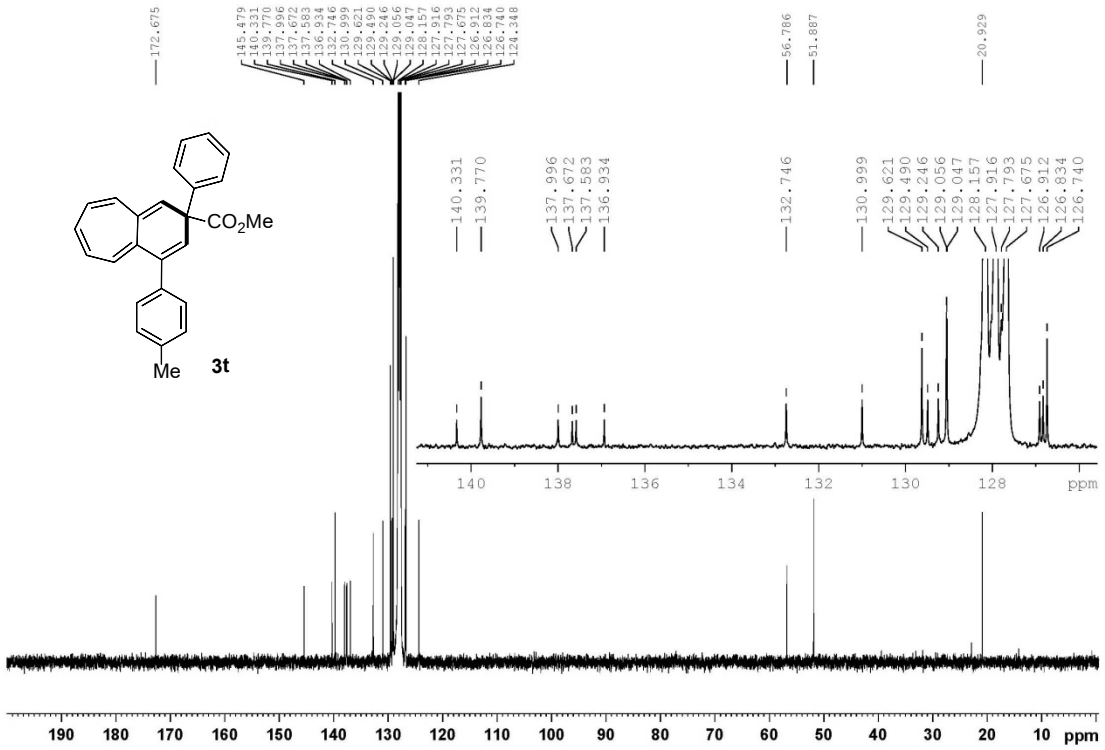


^{13}C{^{1}H}NMR (100 MHz, C_6D_6)



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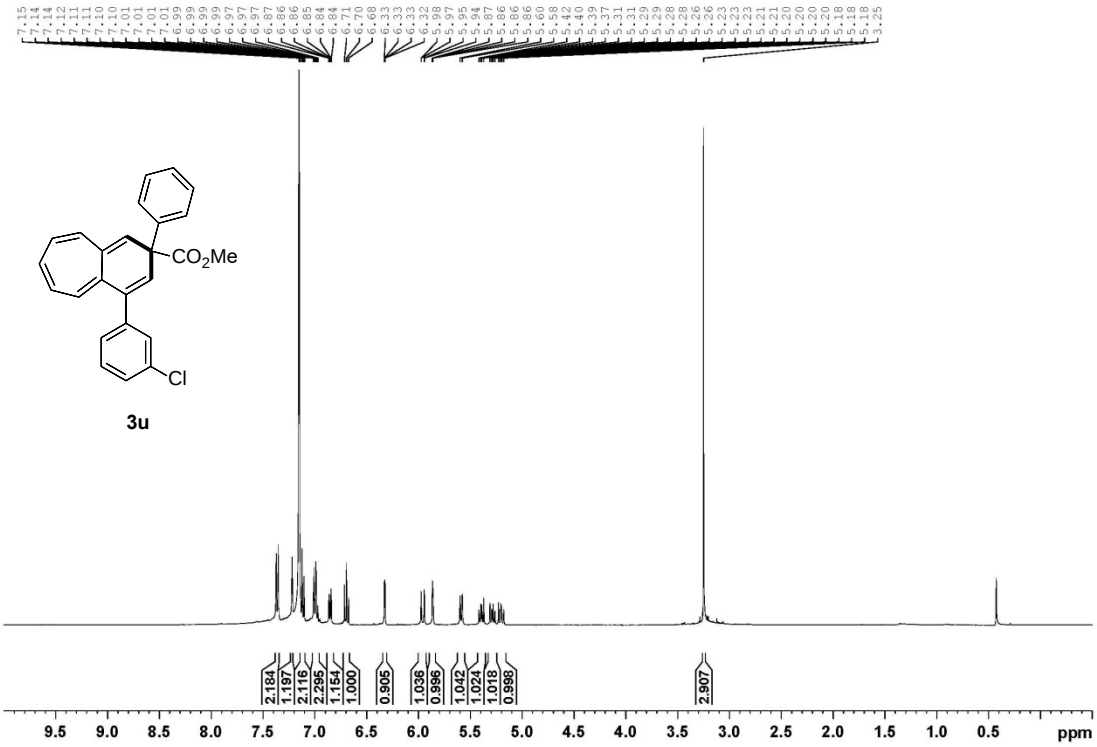

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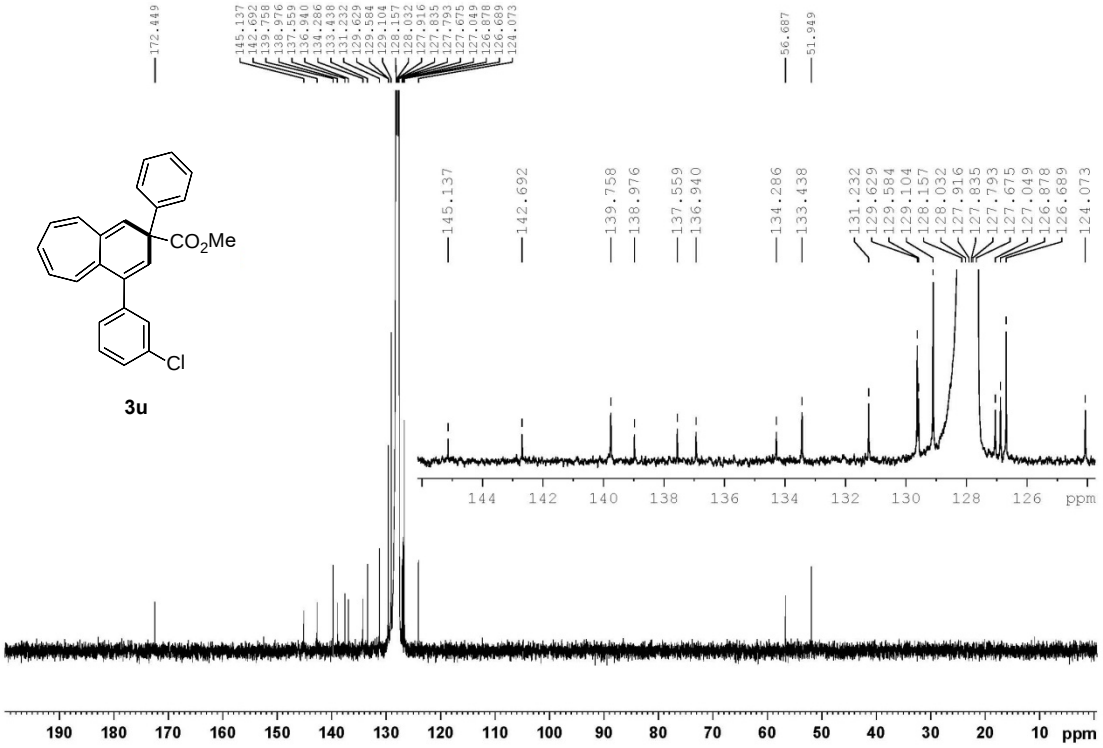

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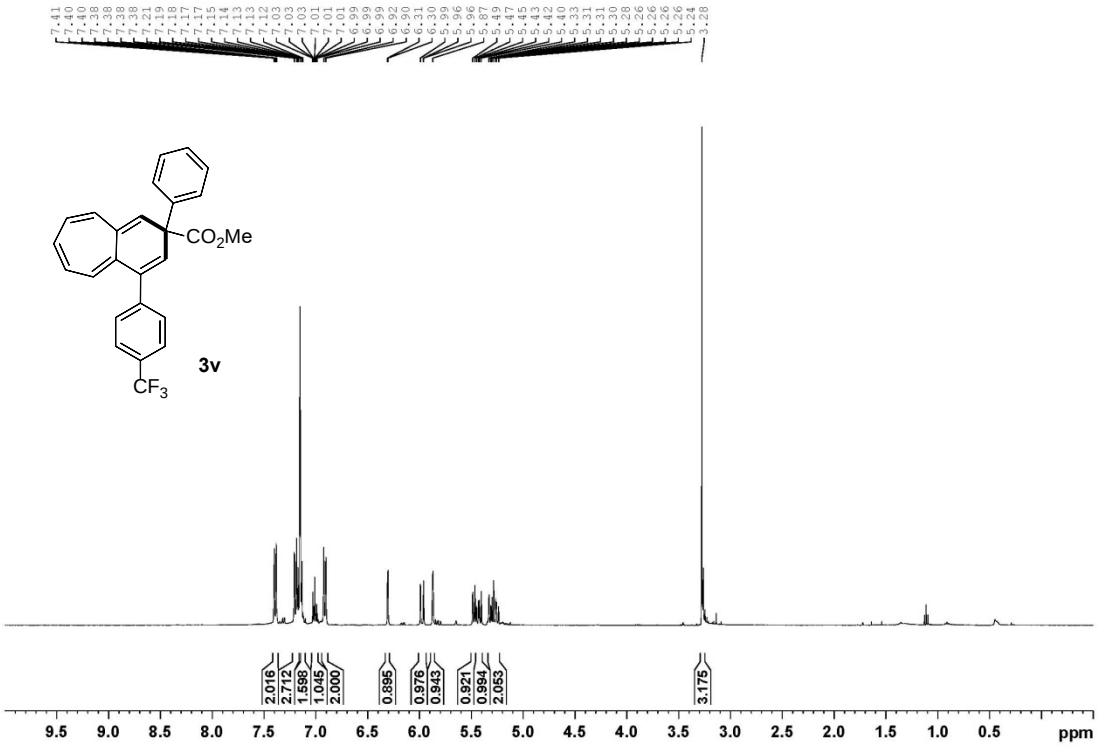
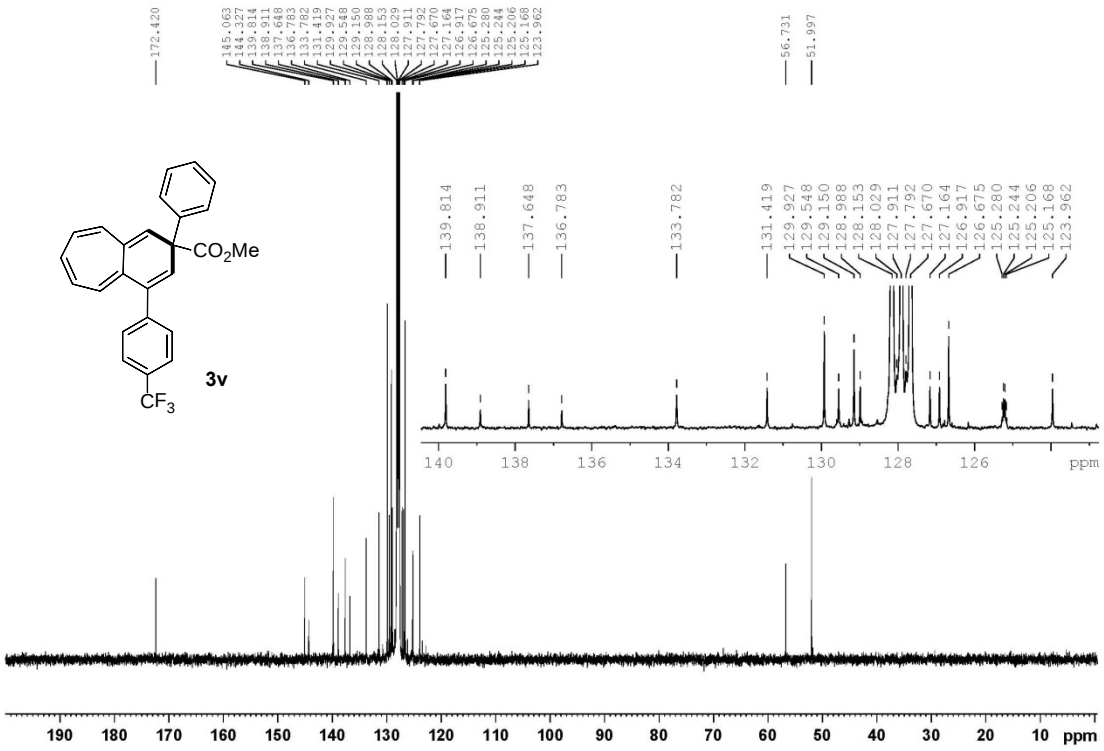


^{13}C{^{1}H}NMR (100 MHz, C_6D_6)



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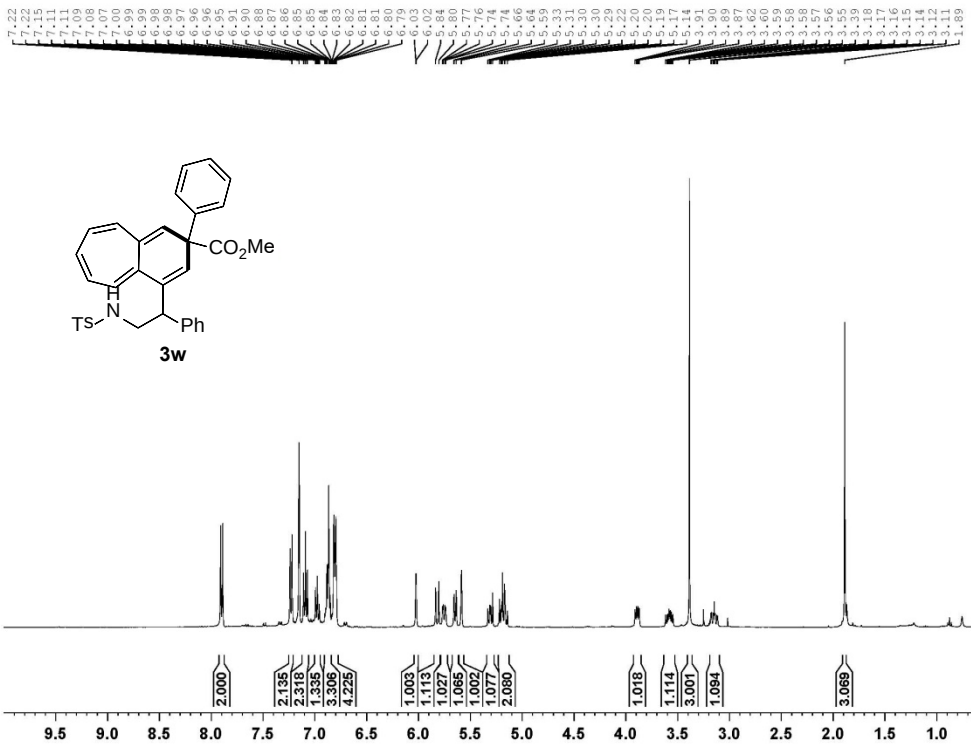
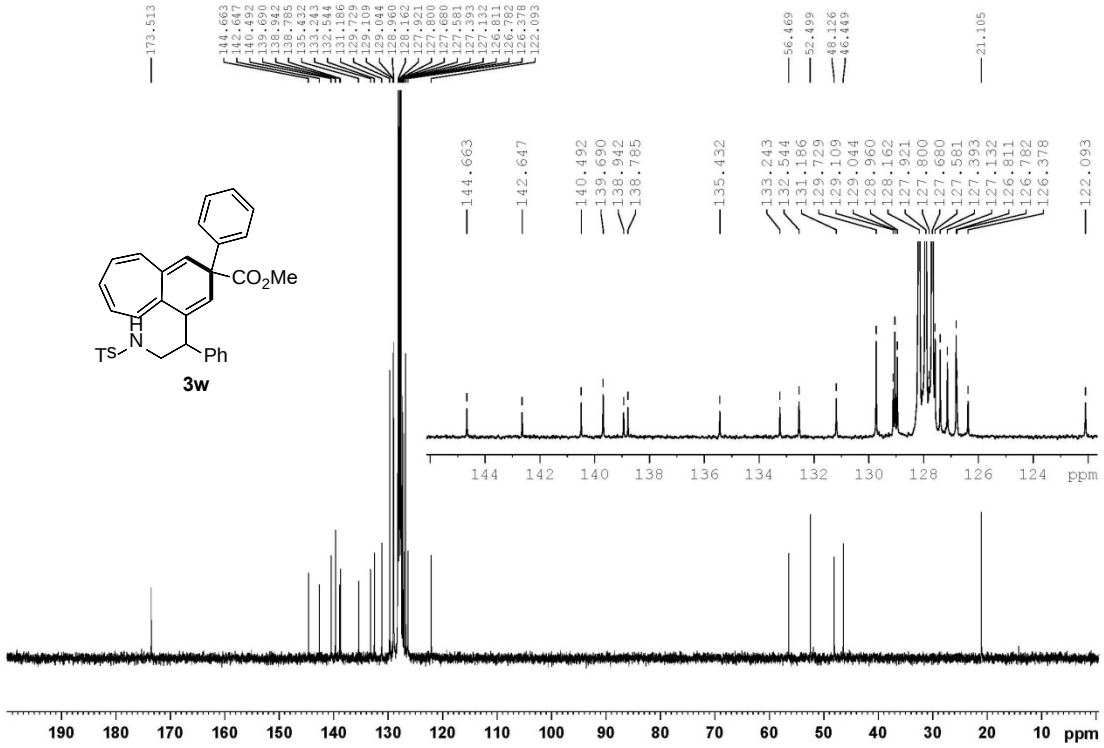
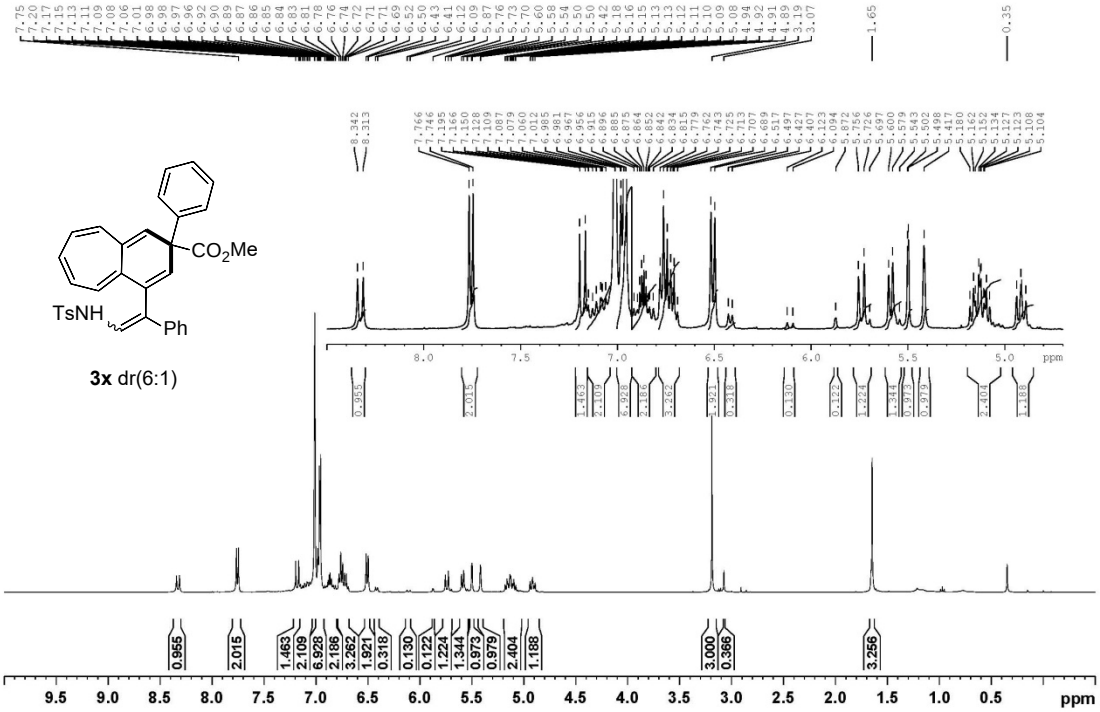


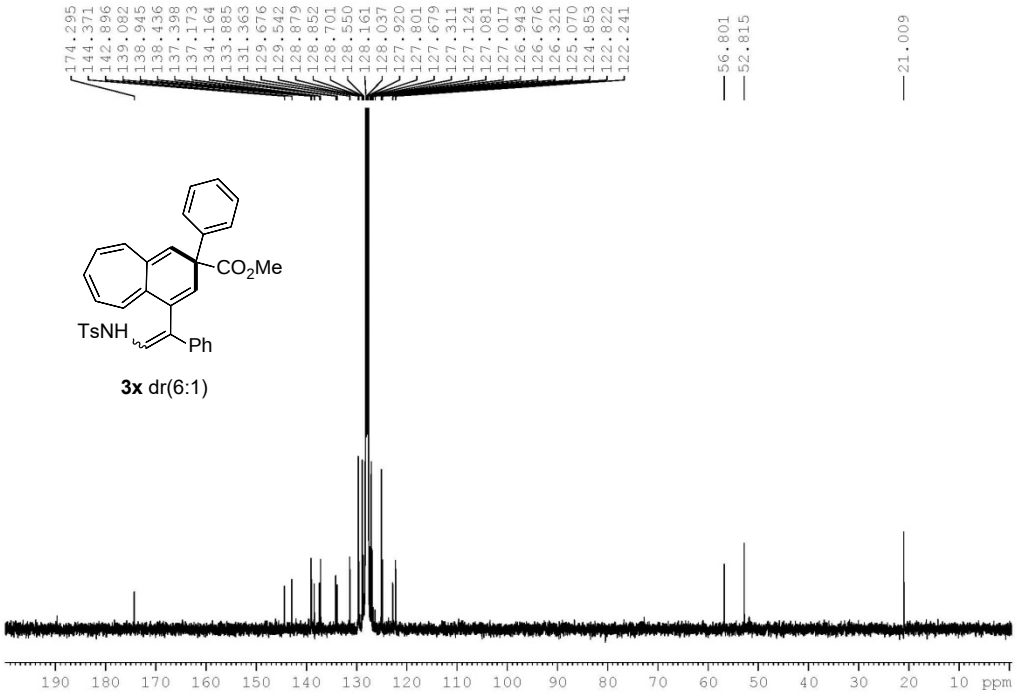
^{13}C{^{1}H}NMR (100 MHz, C_6D_6)



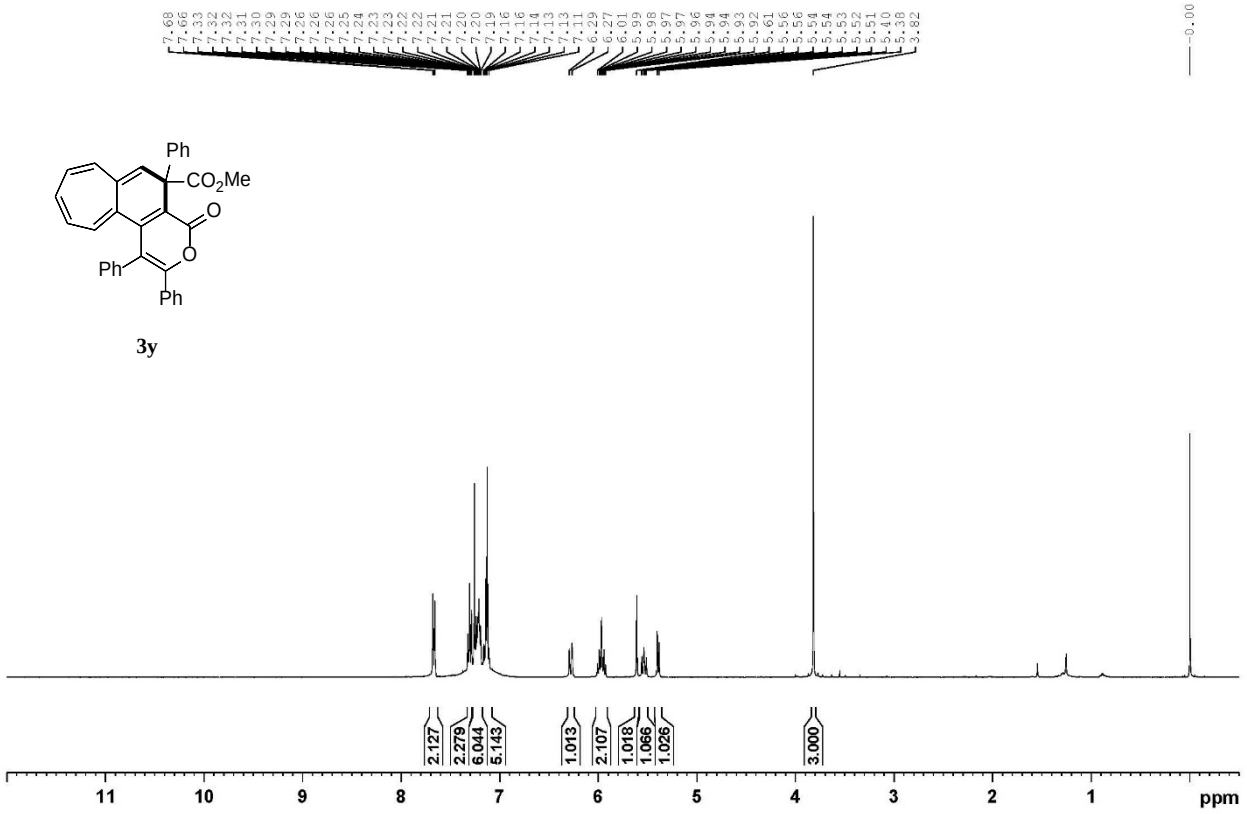
^{1}H NMR (400 MHZ, C_6D_6)



^{13}C{^{1}H}NMR (100 MHz, C_6D_6)

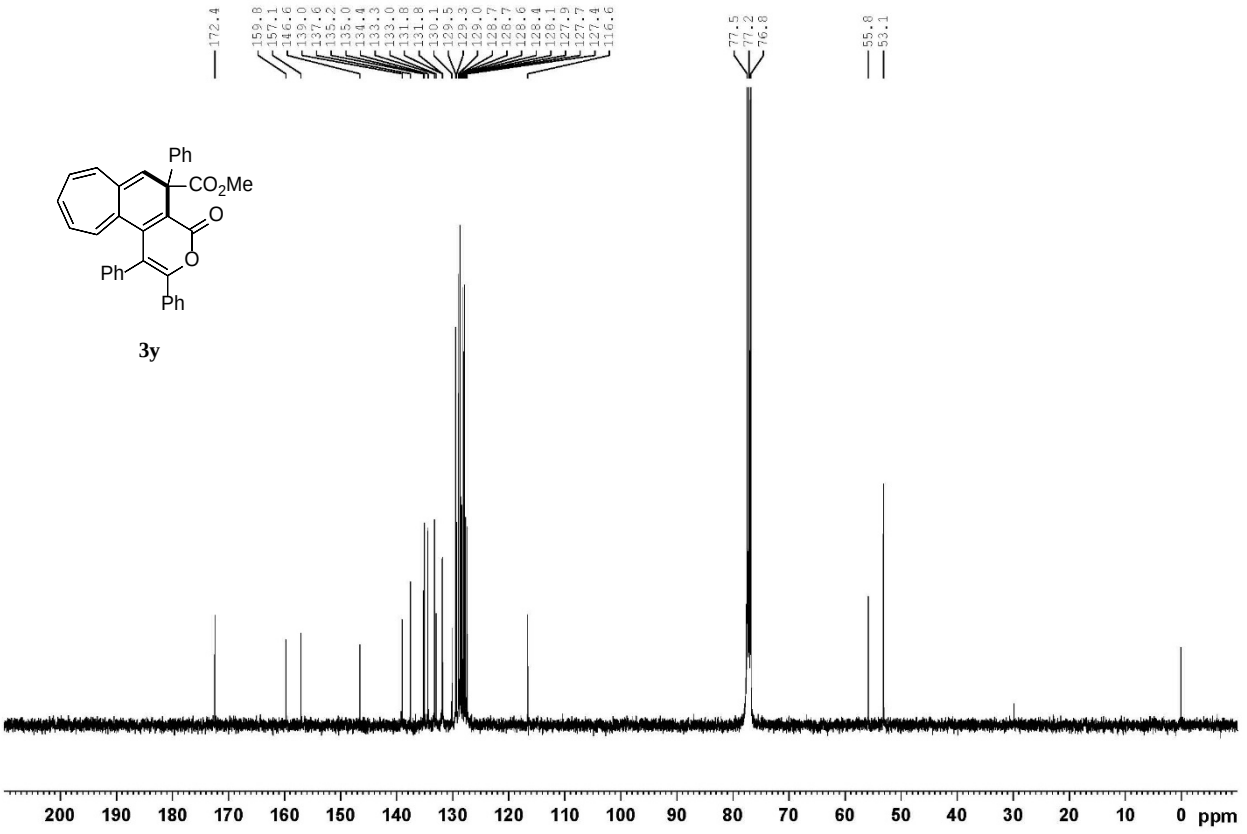


^{1}H NMR (400 MHz, $CDCl_3$)



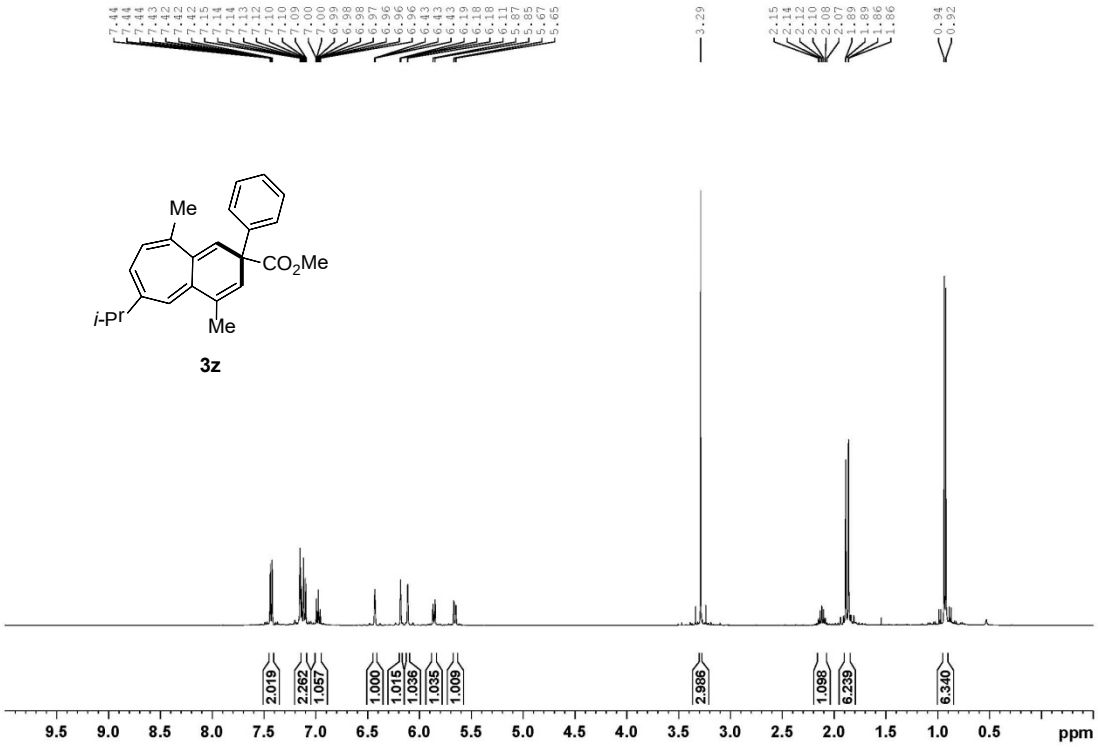
3y

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)

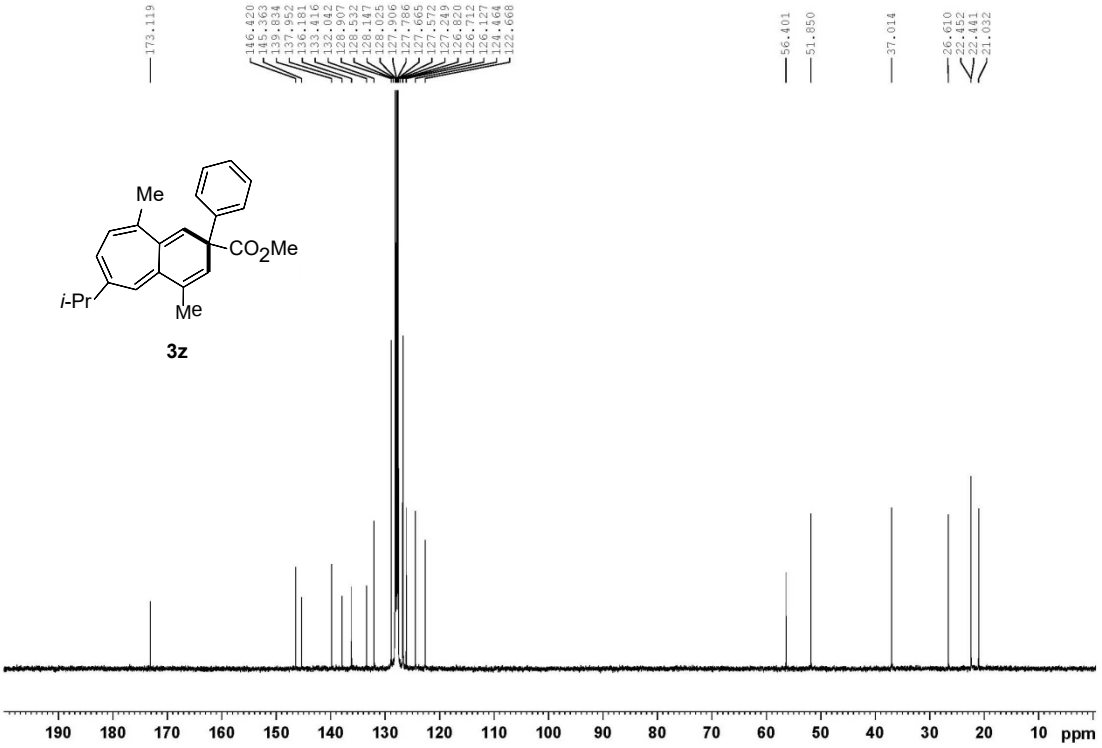


3y

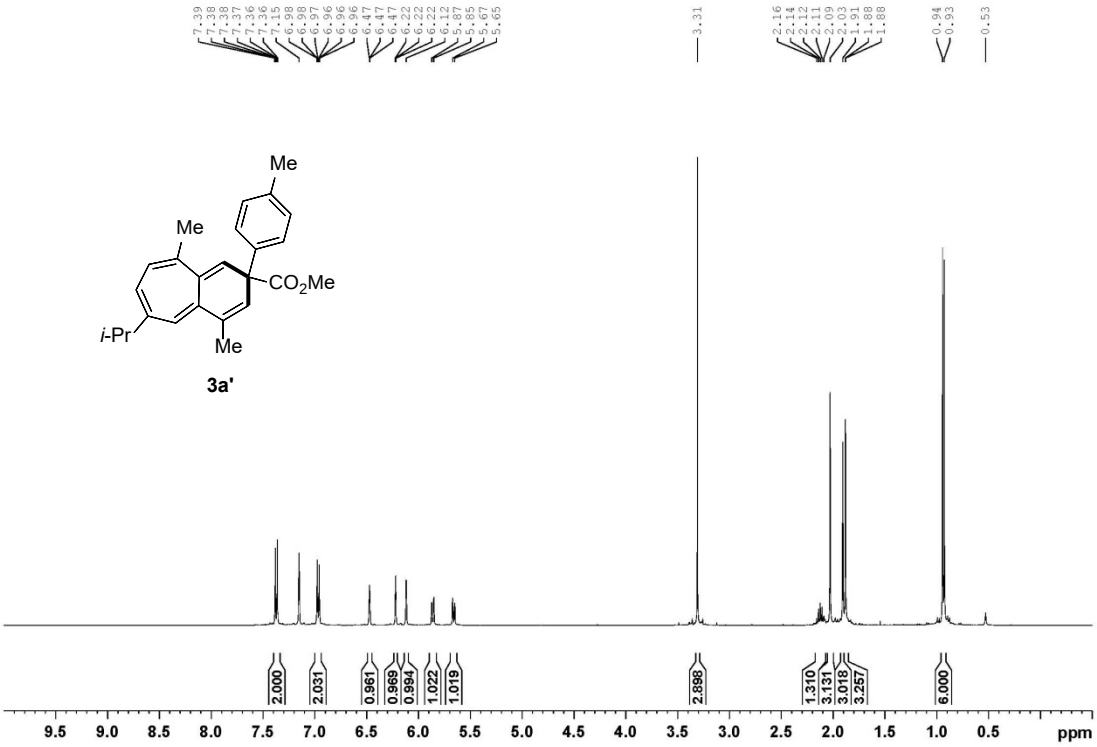
^{1}H NMR (400 MHZ, C_6D_6)



^{13}C{^{1}H}NMR (100 MHz, C_6D_6)



^{1}H NMR (400 MHZ, C_6D_6)



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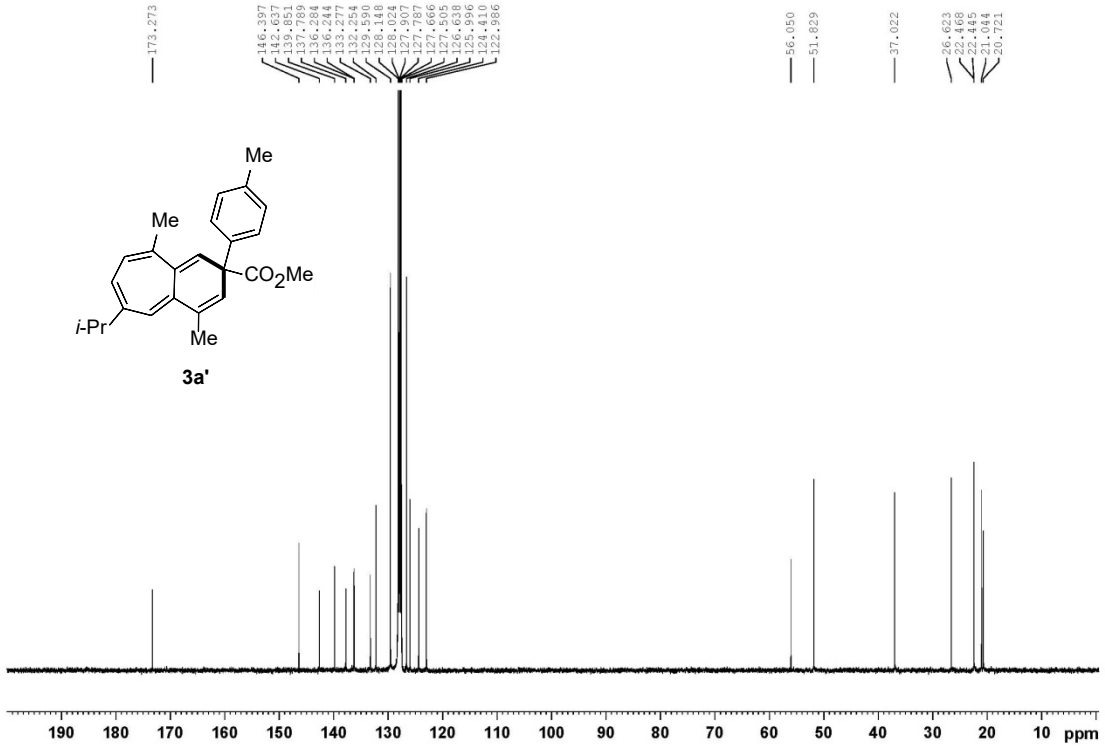
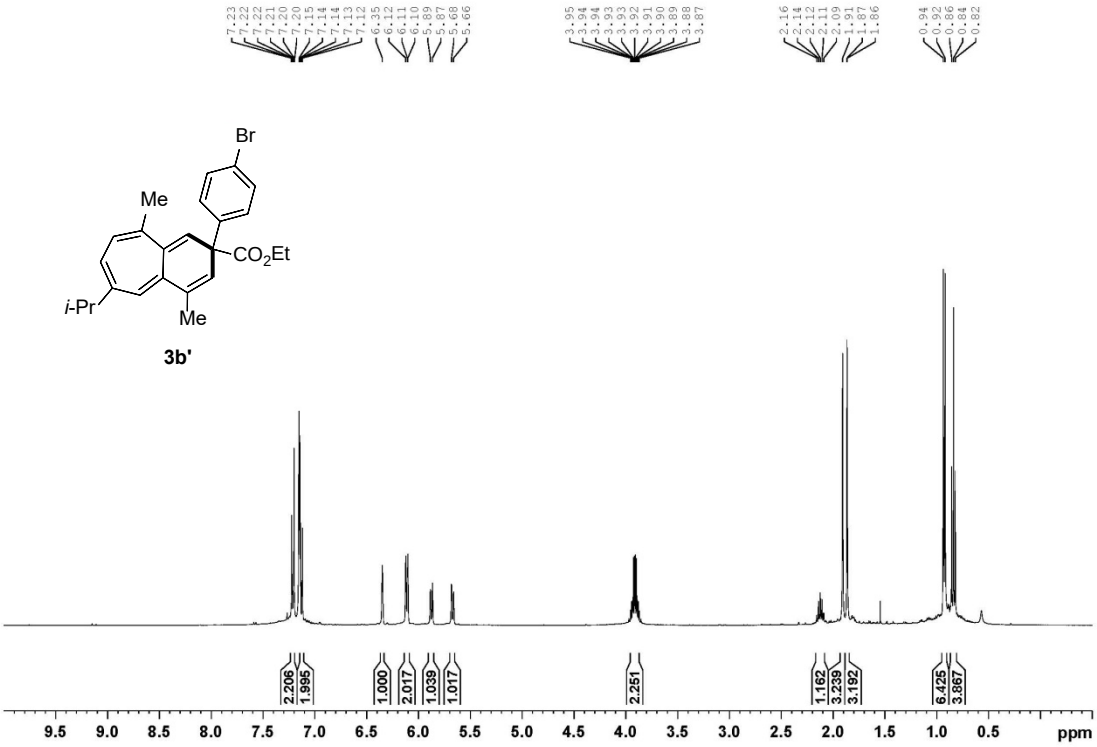
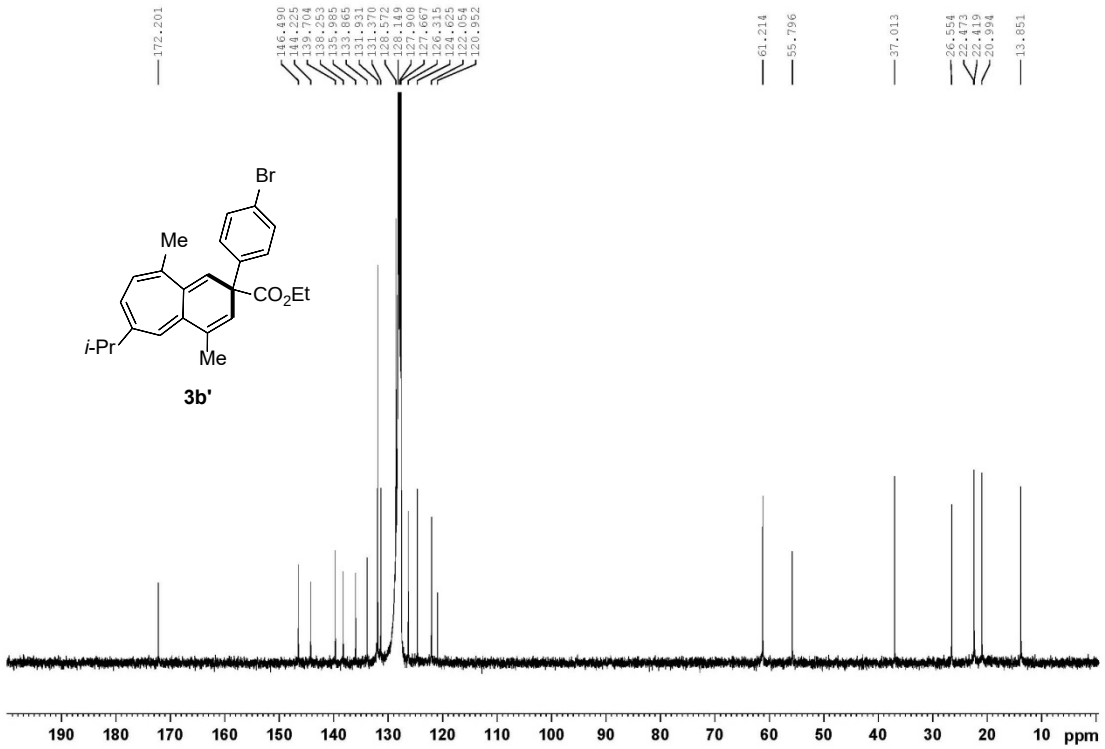


^{1}H NMR (400 MHZ, C_6D_6)



^{13}C{^{1}H}NMR (100 MHz, C_6D_6)



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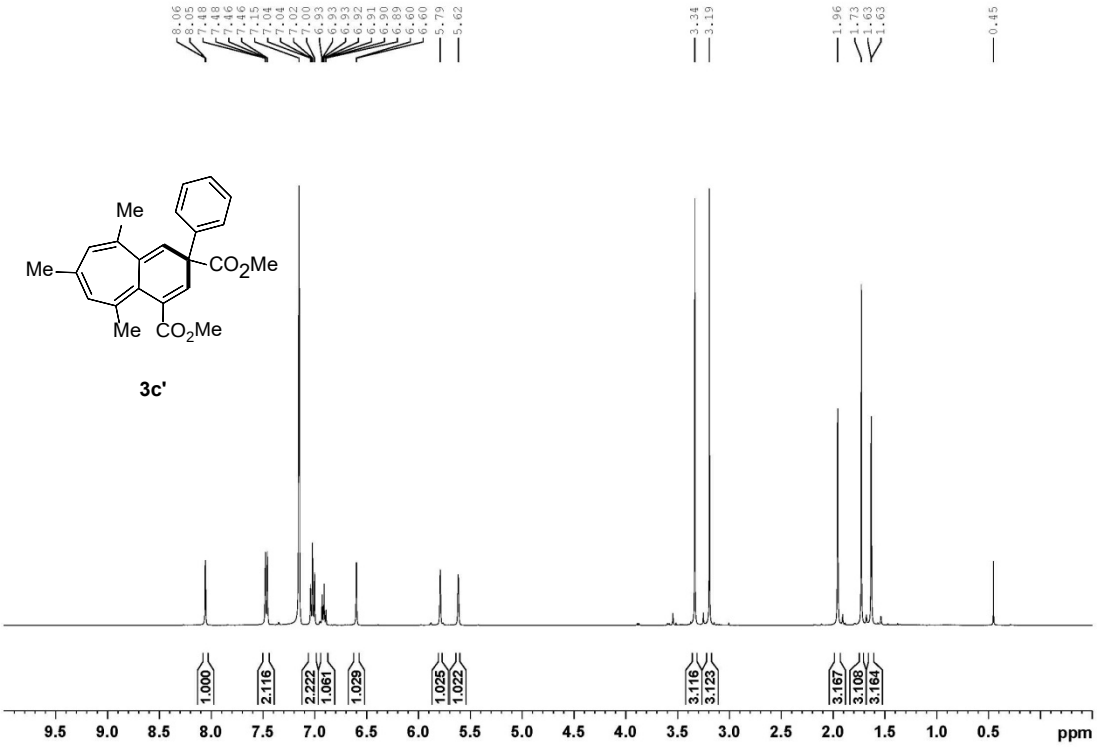
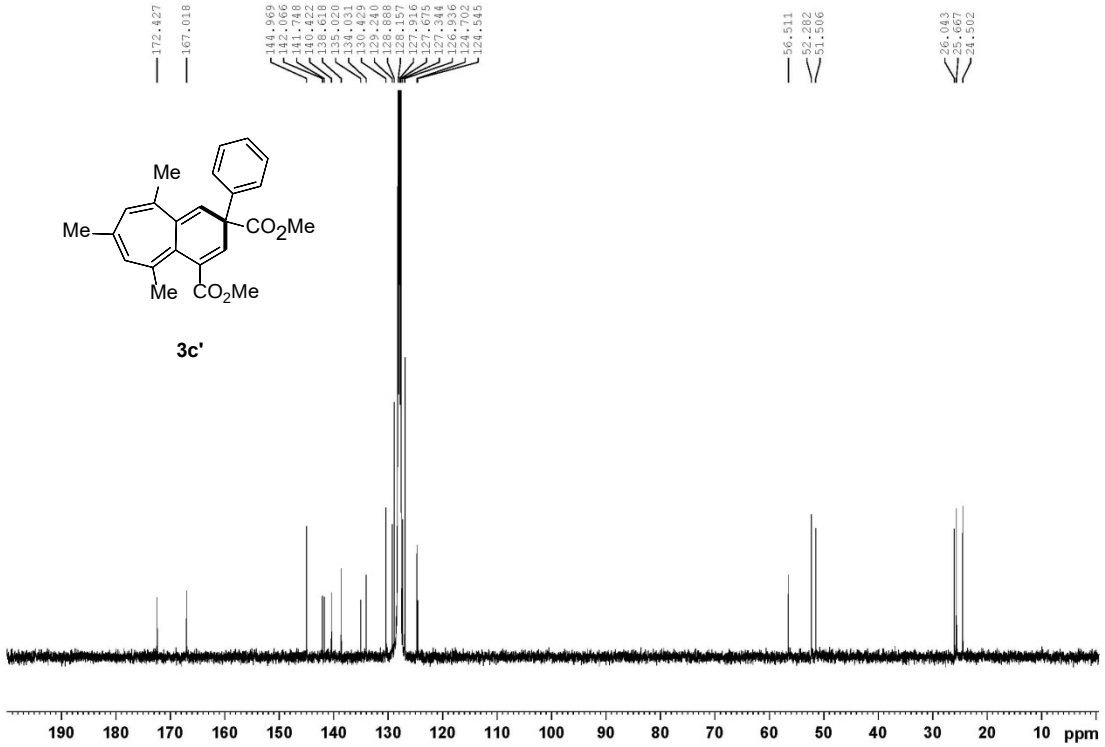


^{13}C{^{1}H}NMR (100 MHz, C_6D_6)



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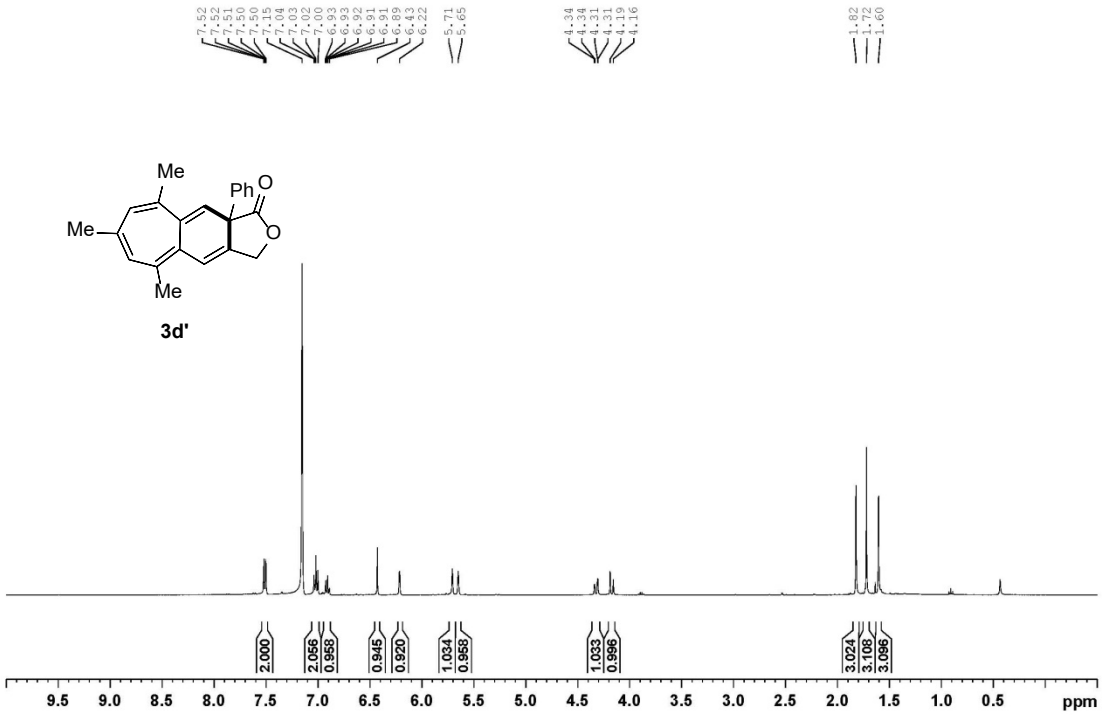
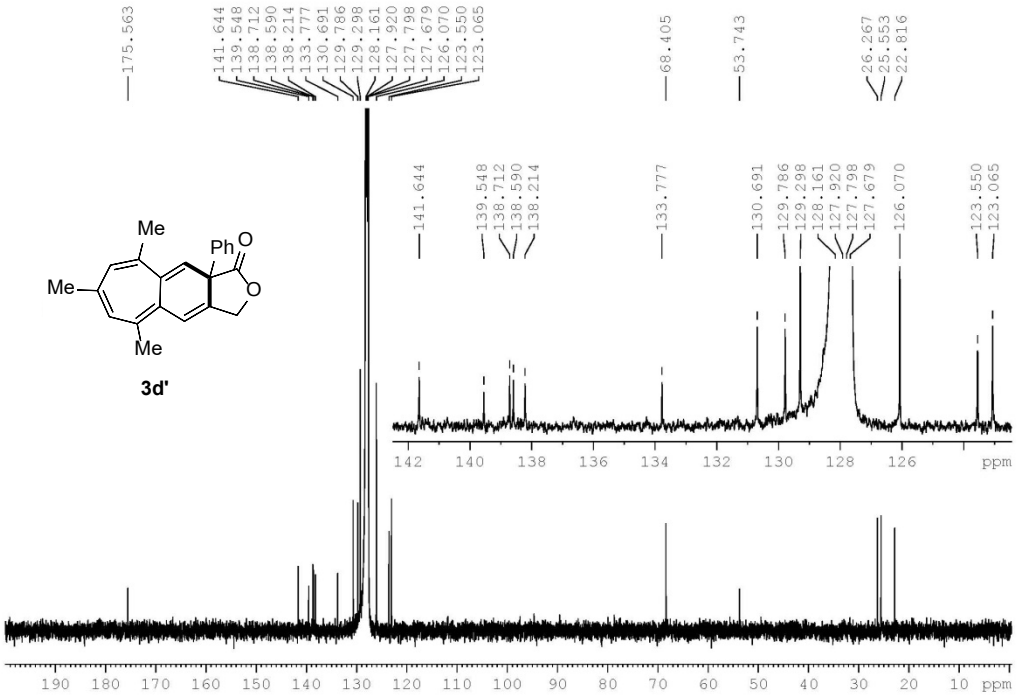
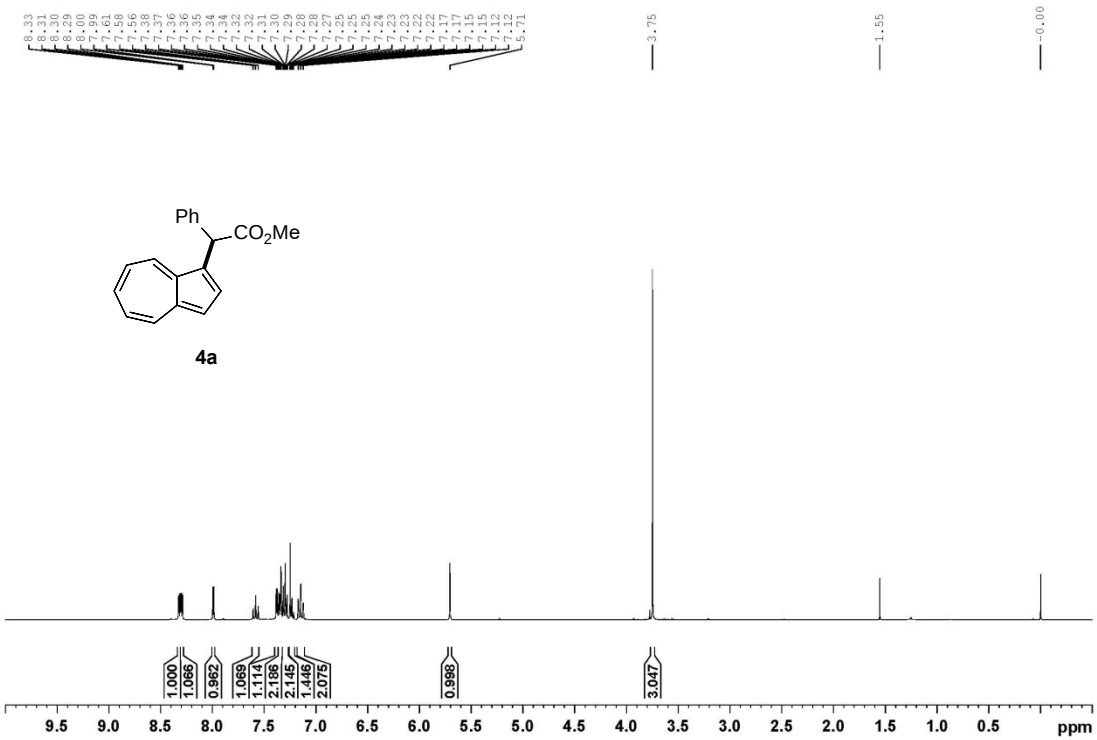


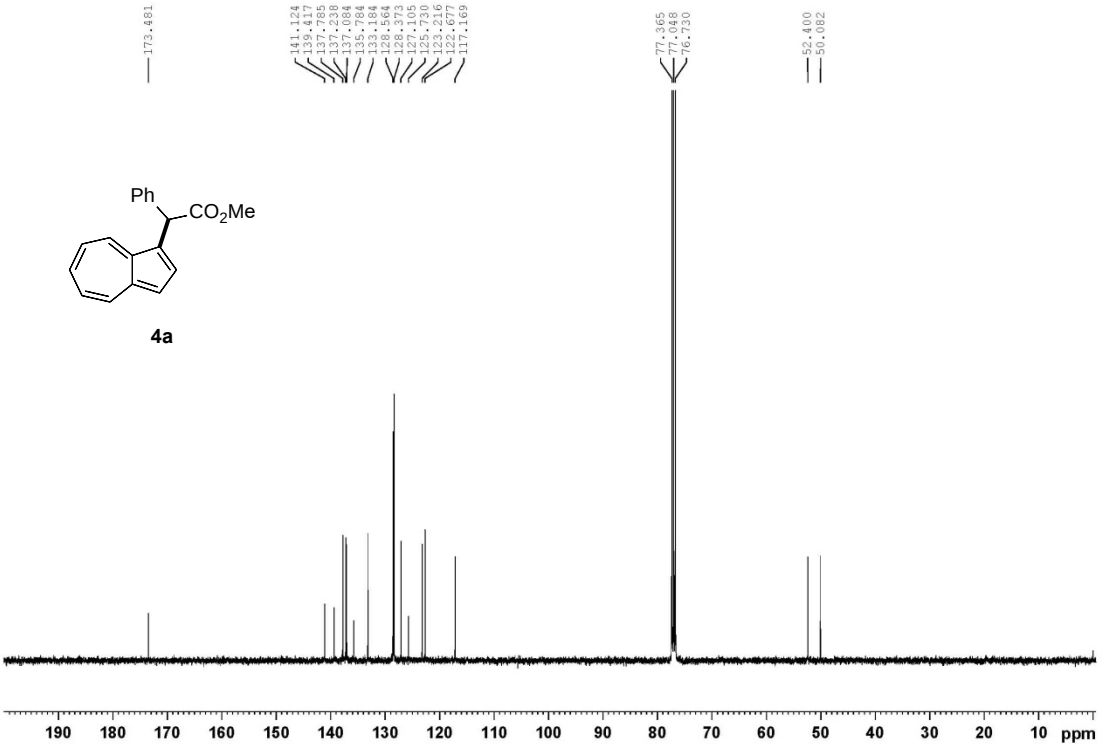
^{13}C{^{1}H}NMR (100 MHz, C_6D_6)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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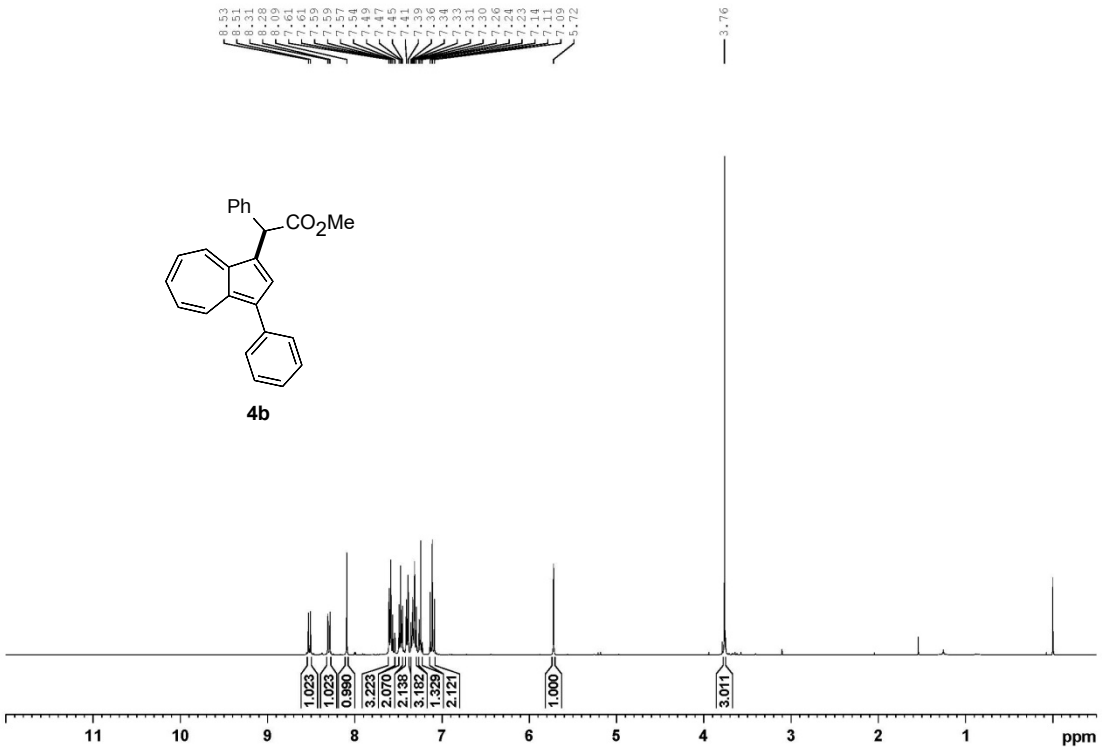
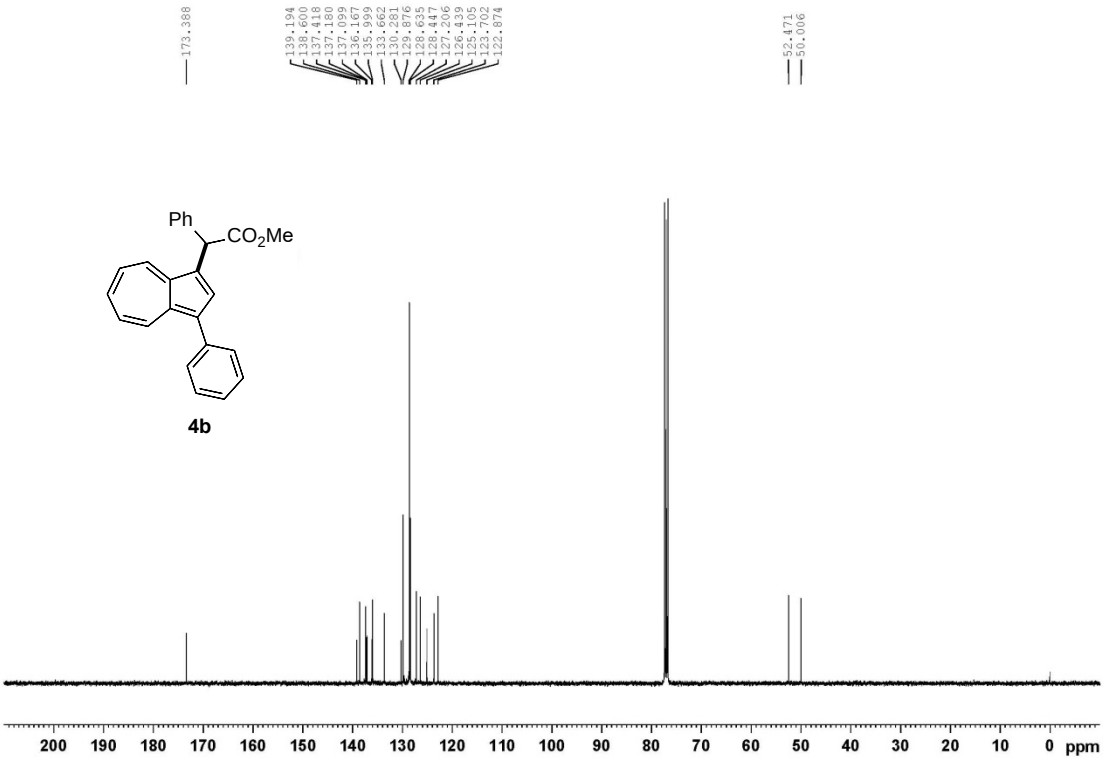


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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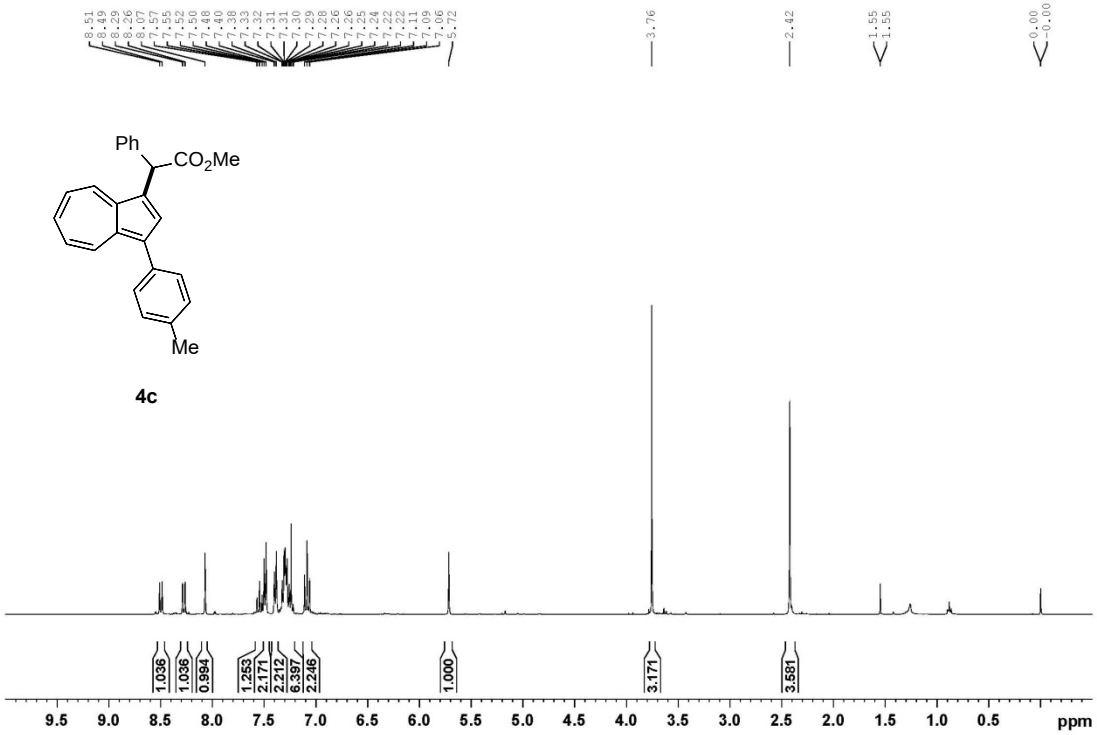

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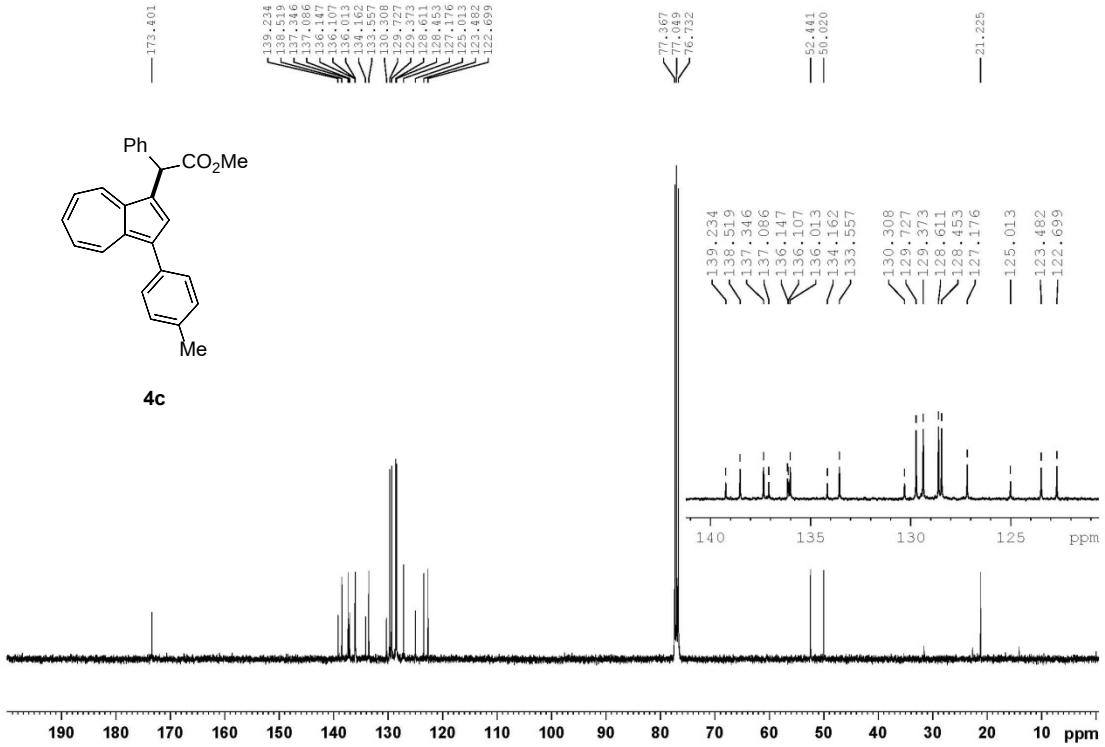

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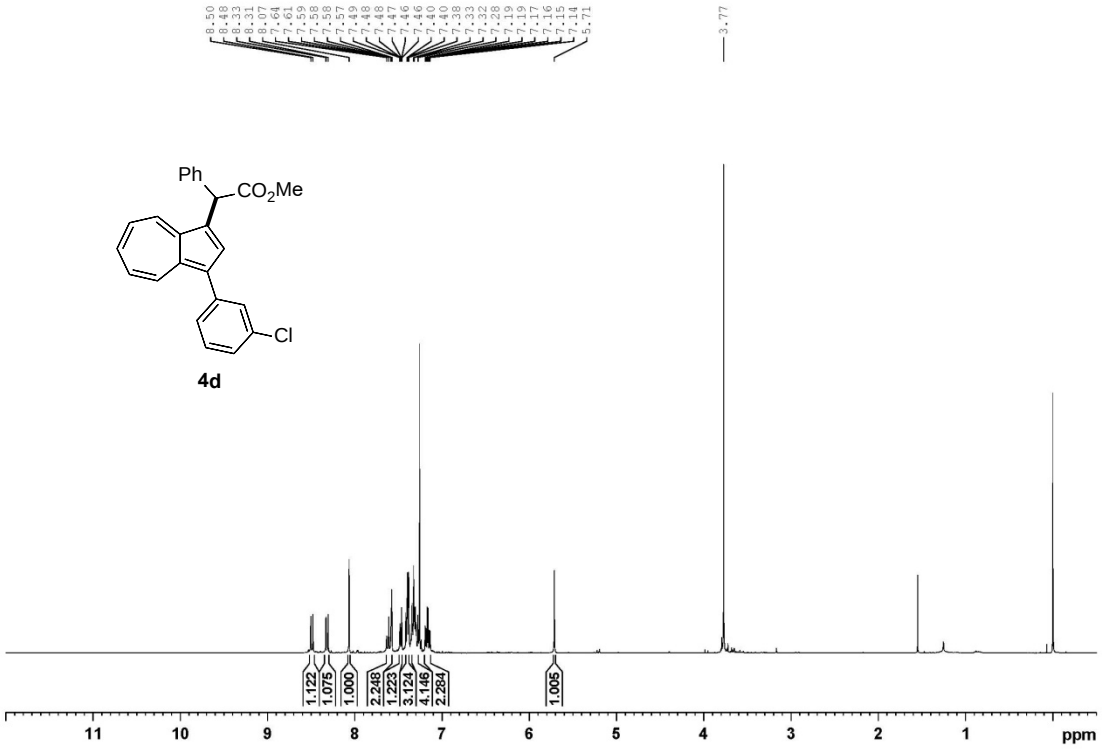

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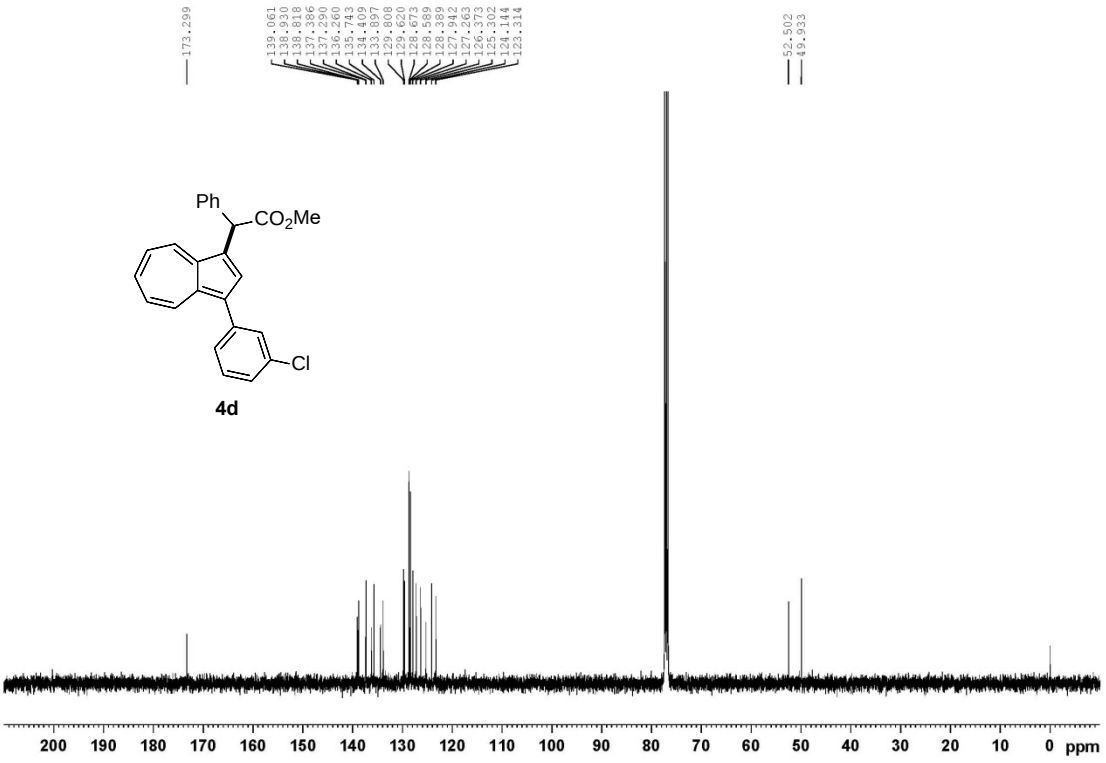

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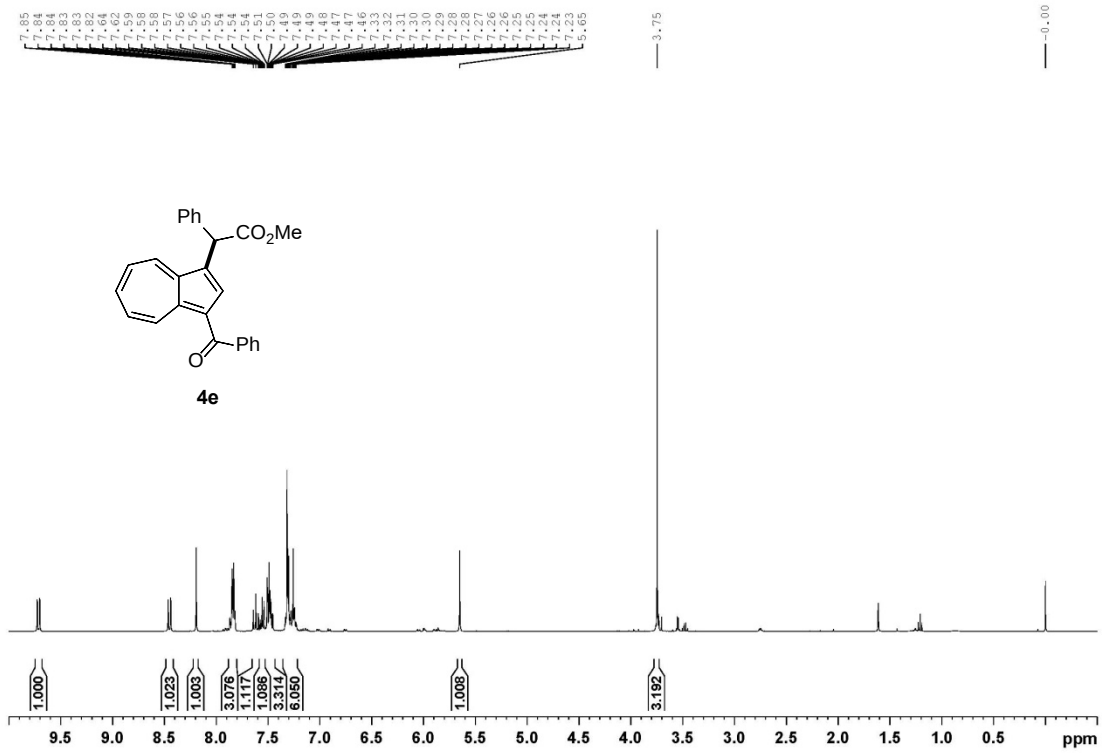
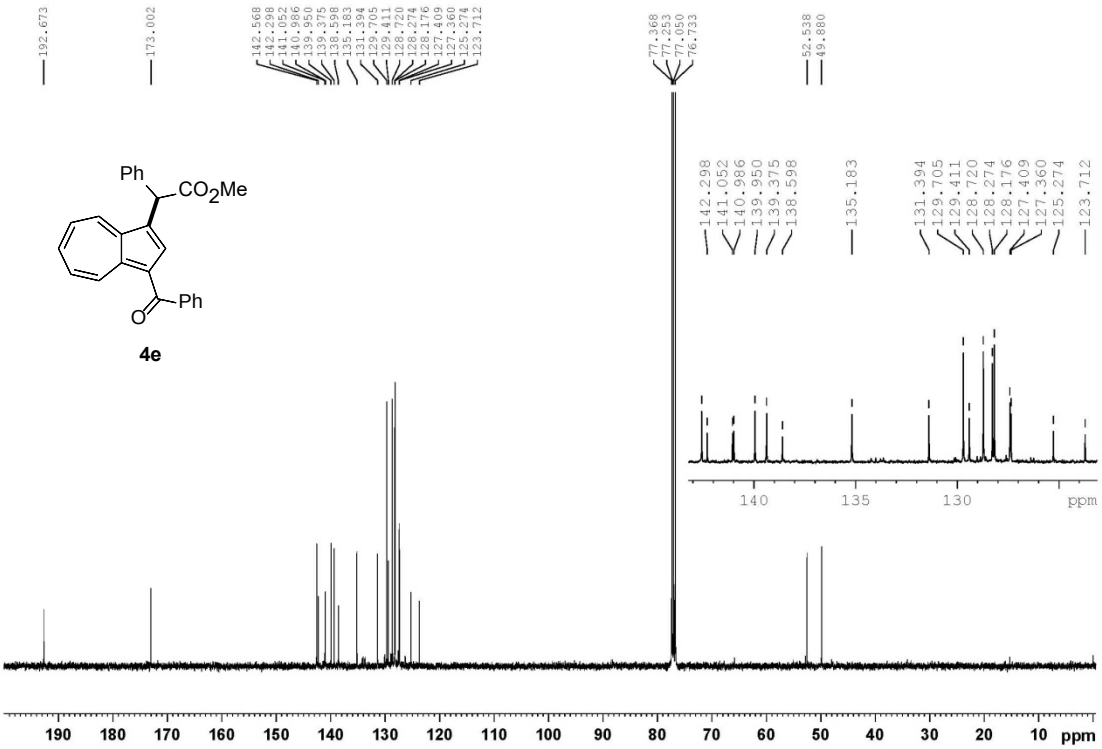


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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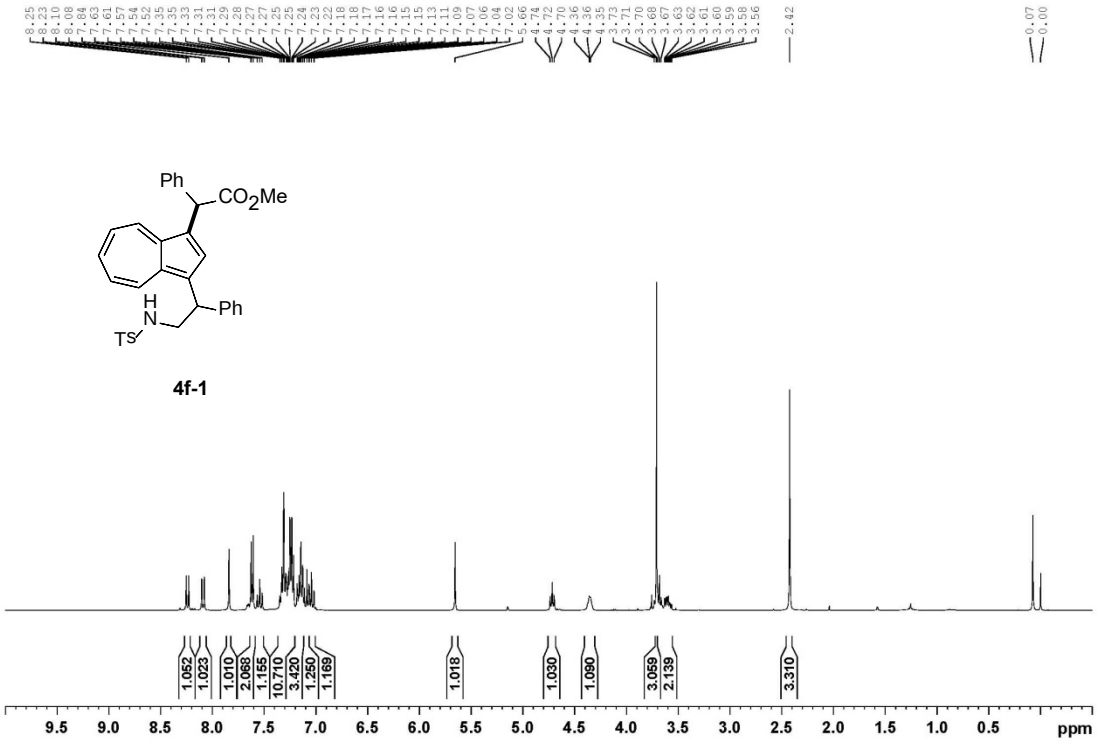

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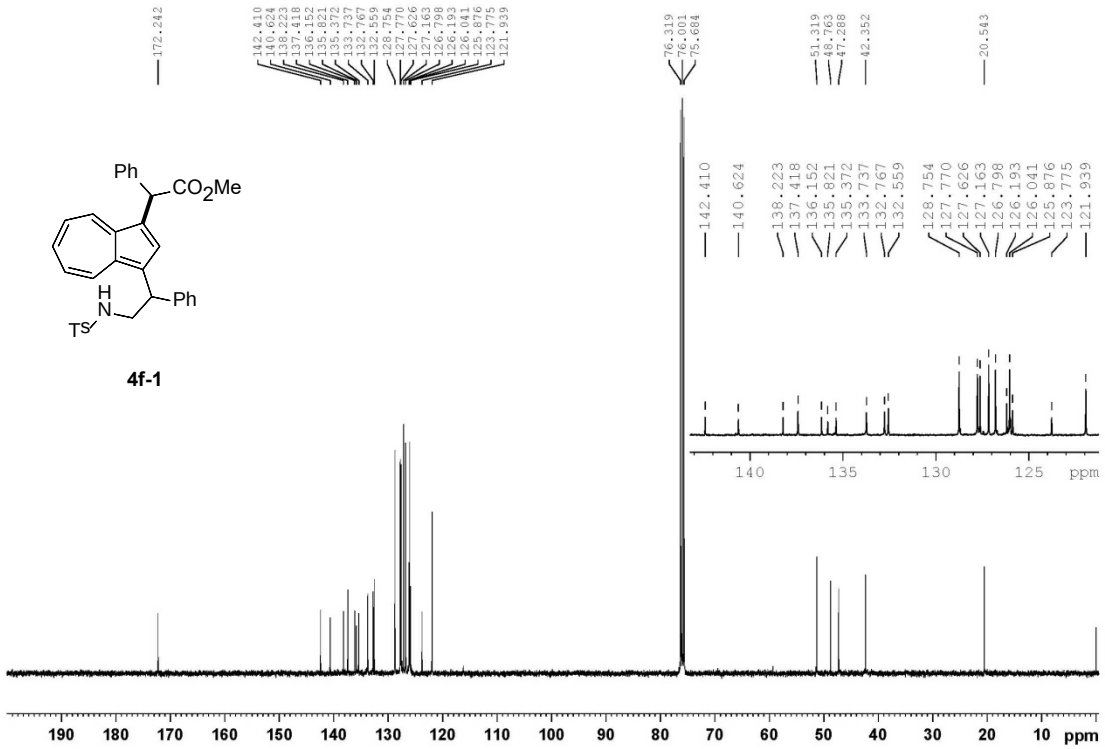

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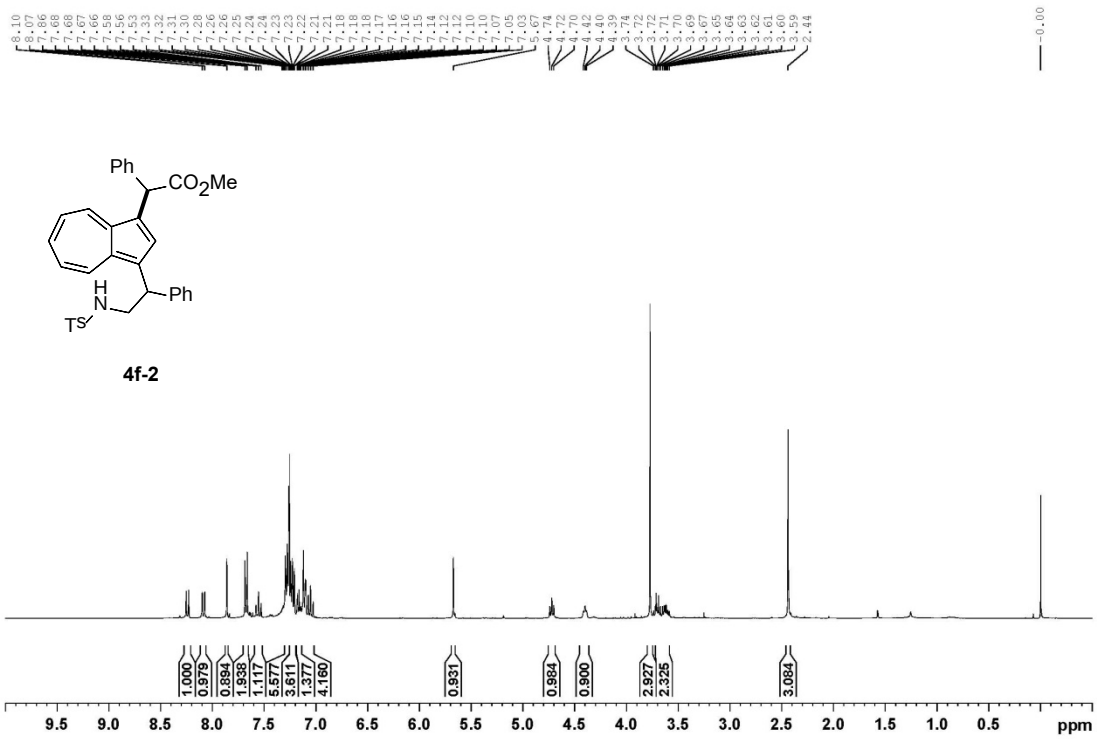

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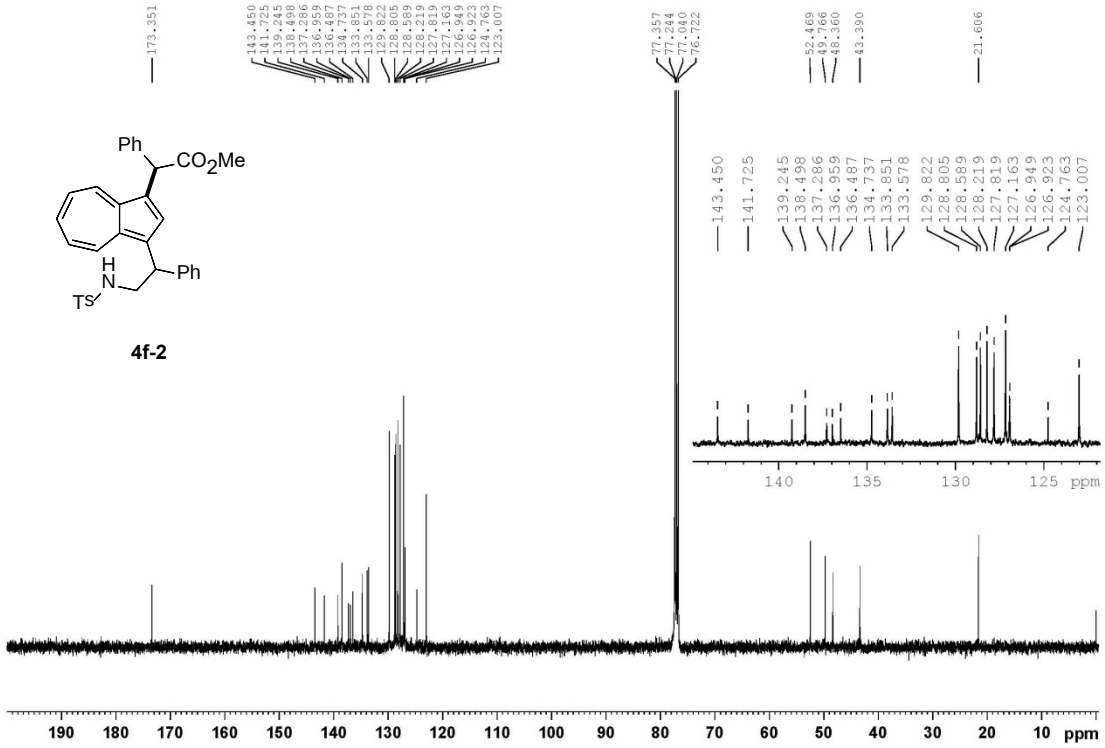

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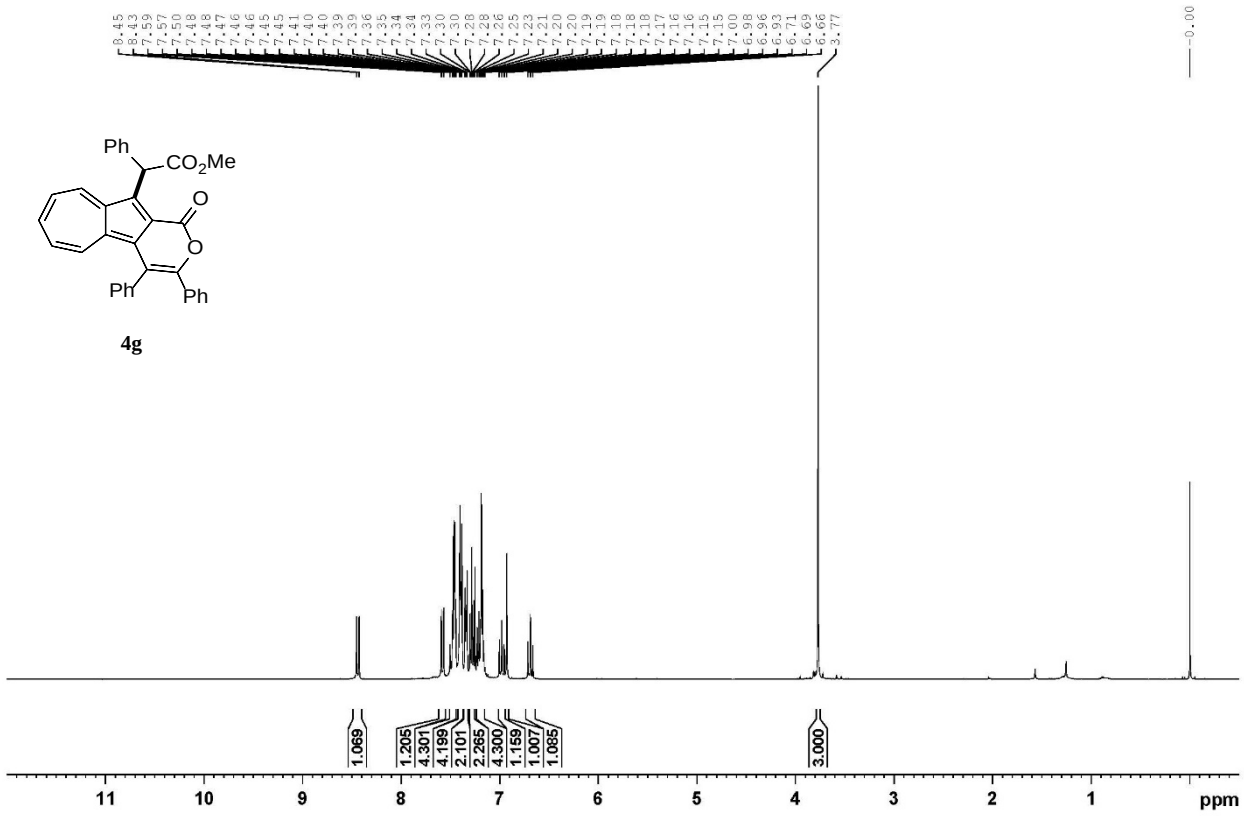

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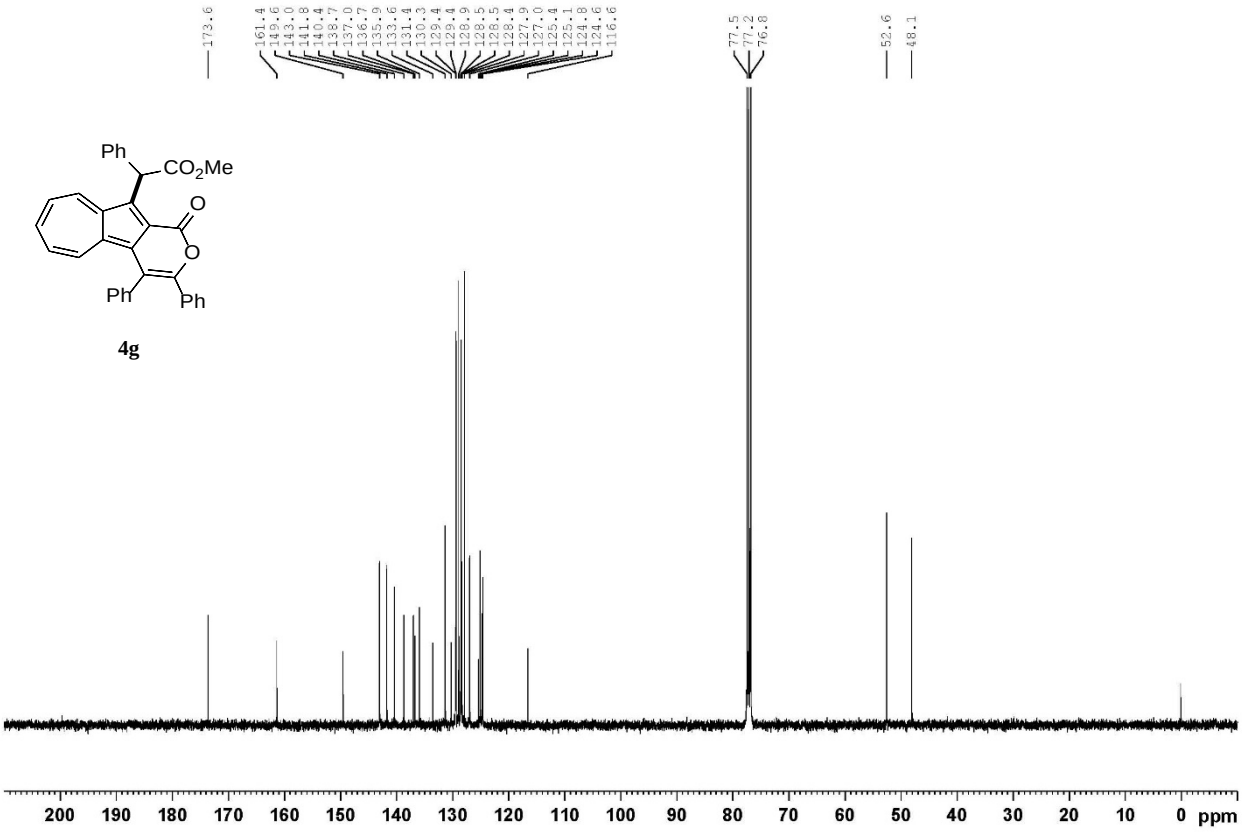

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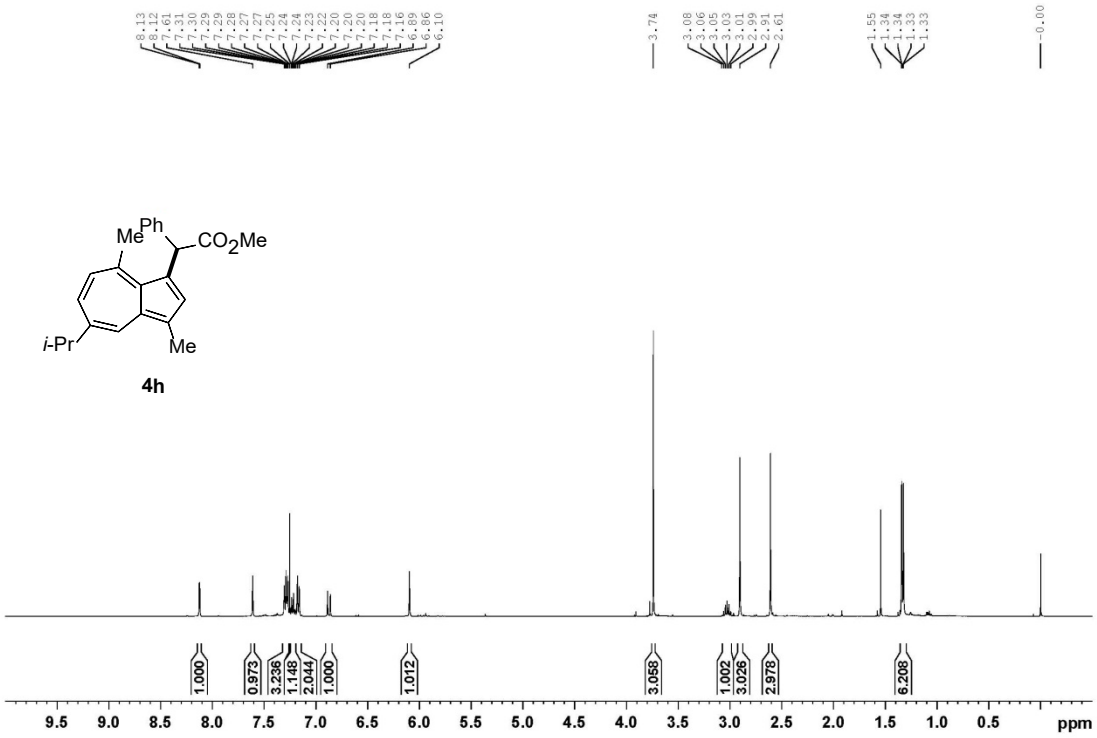
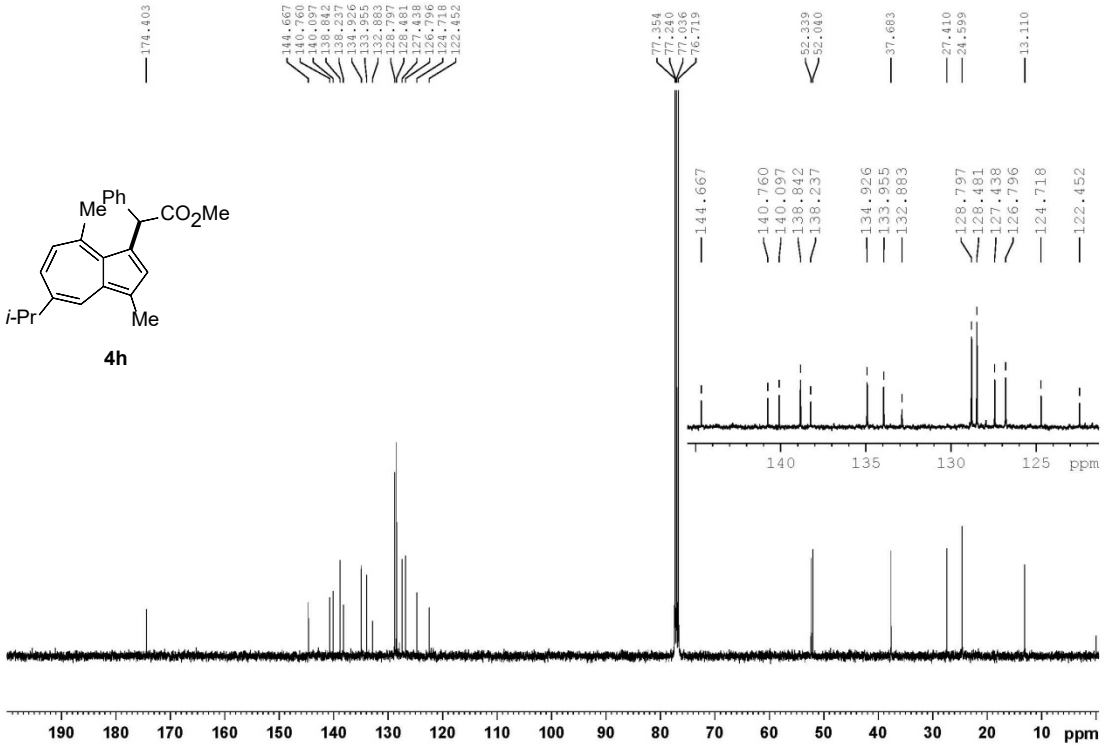


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



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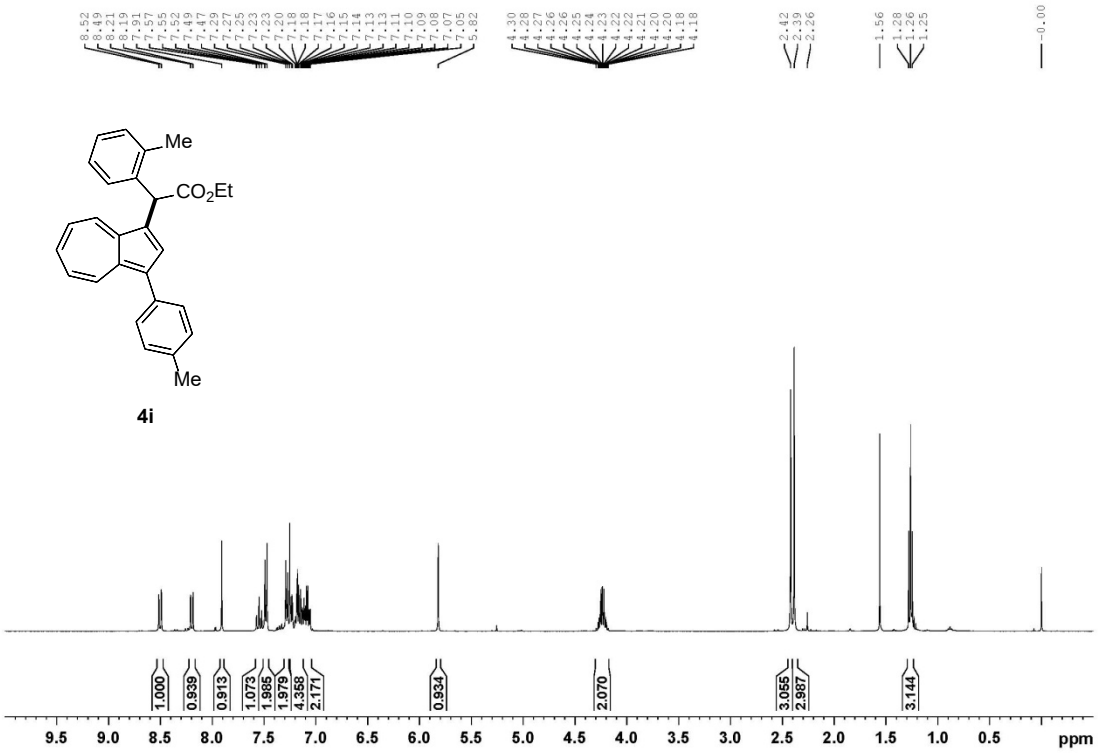
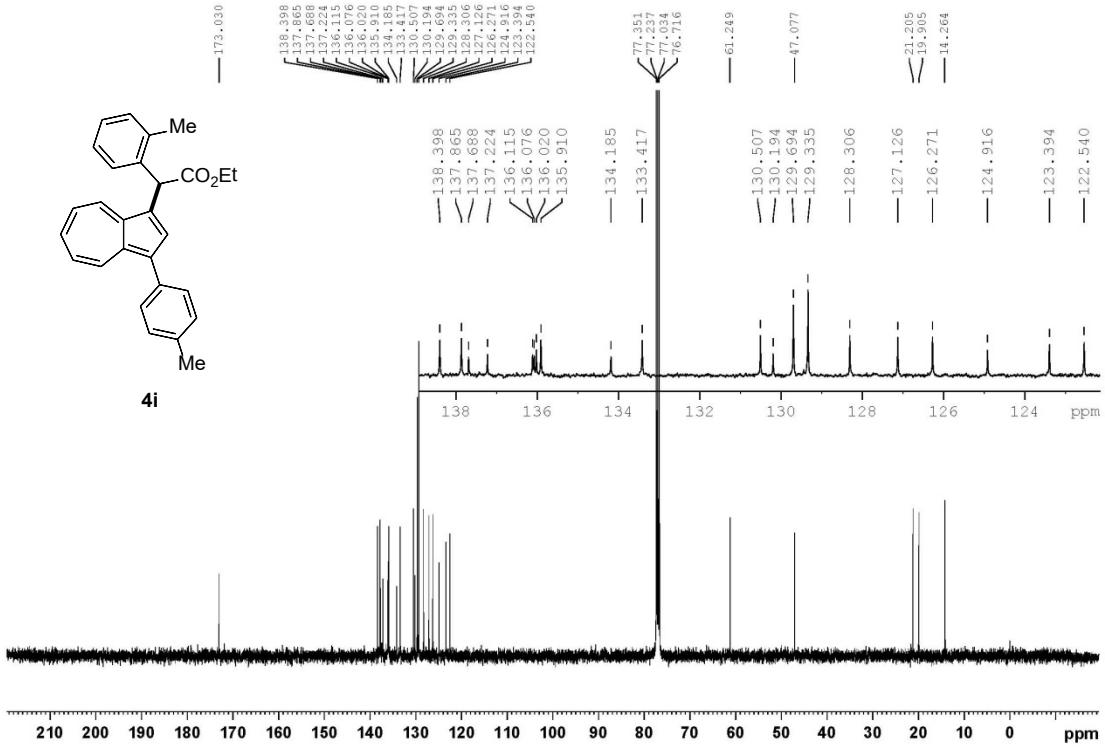
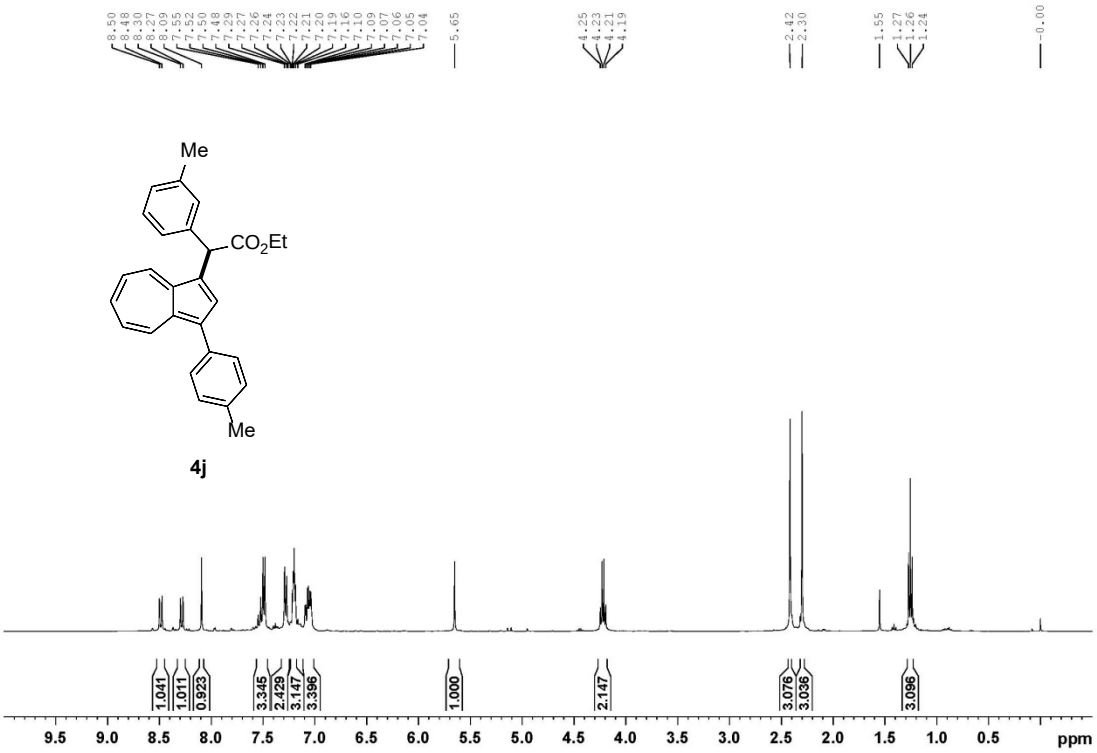


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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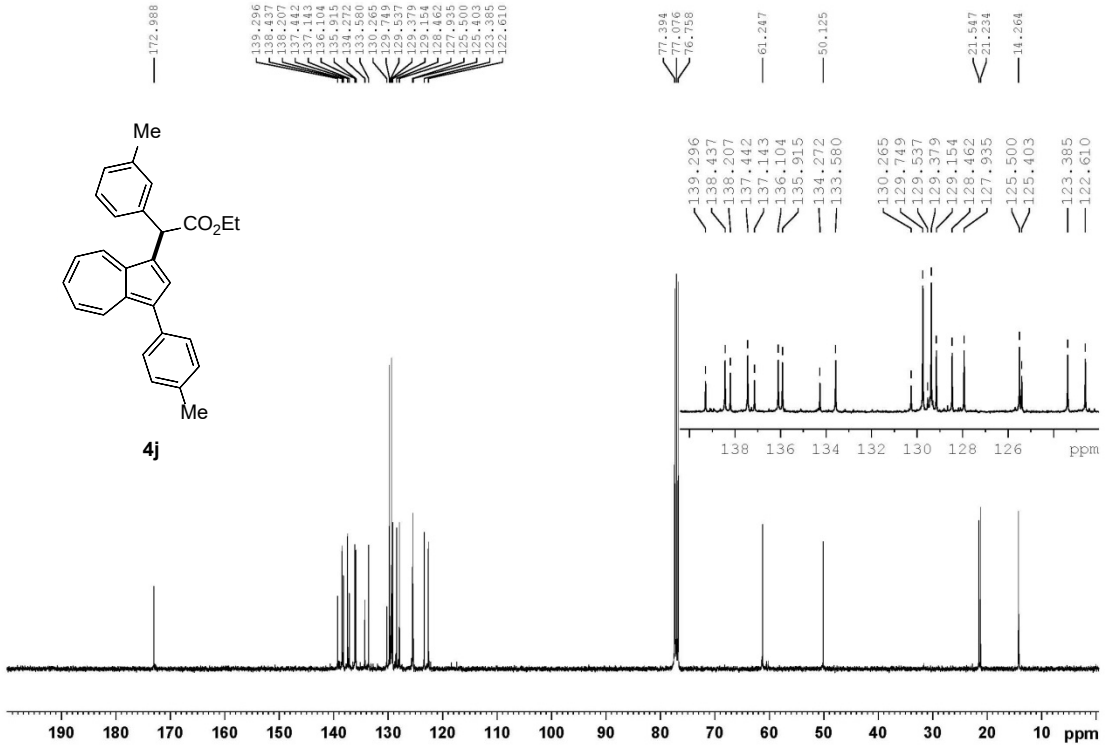
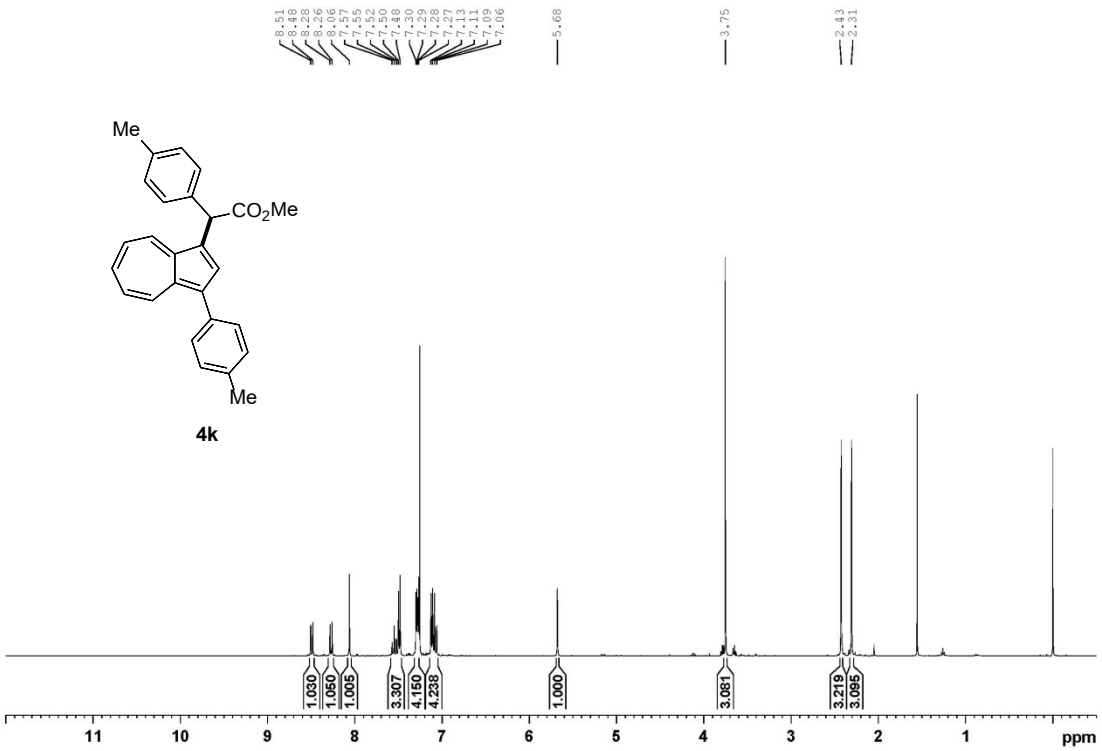


^{1}H NMR (400 MHz, $CDCl_3$)



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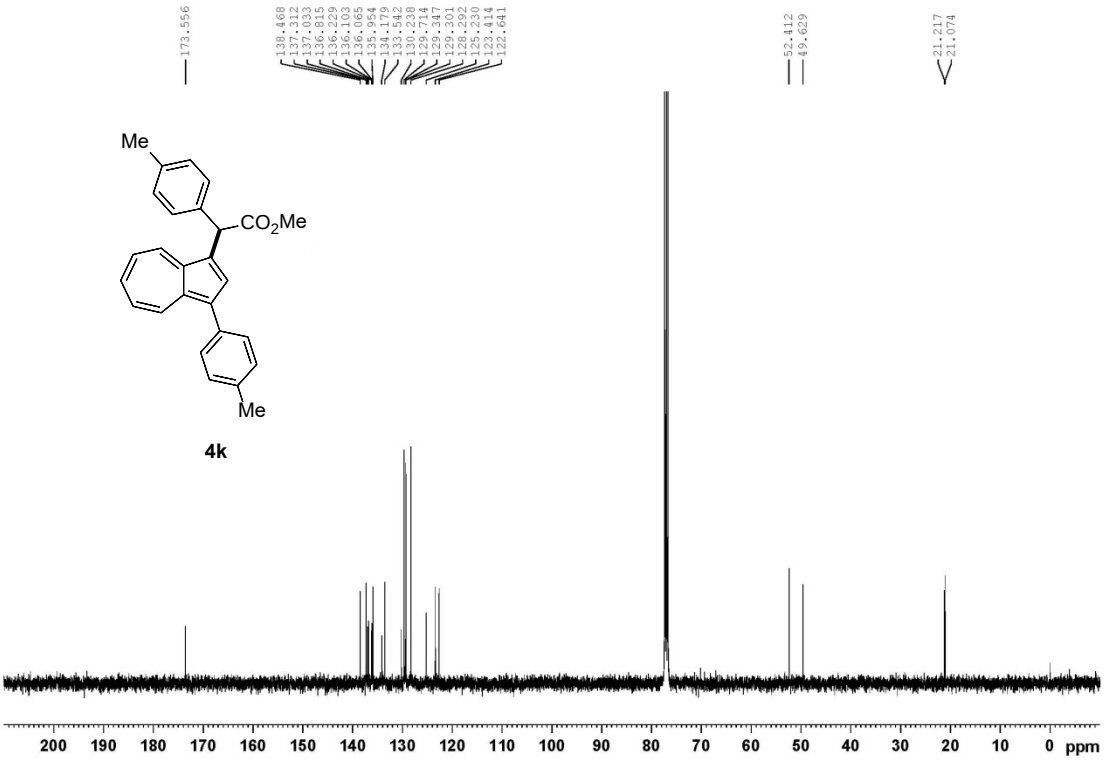
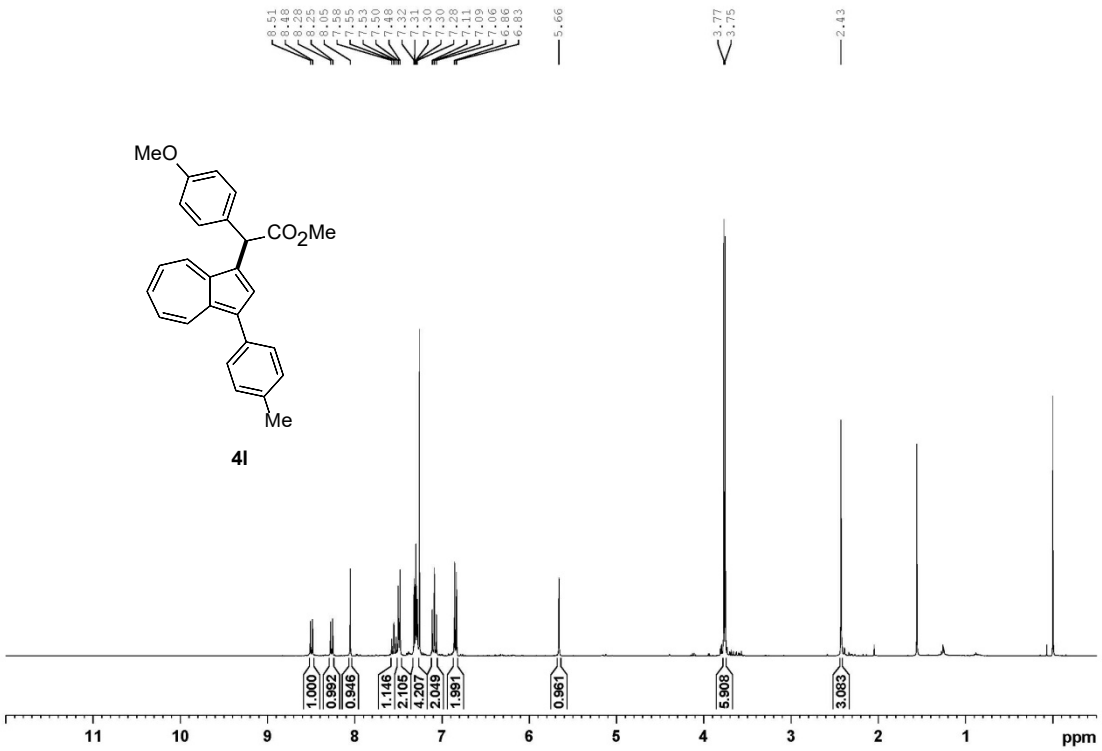
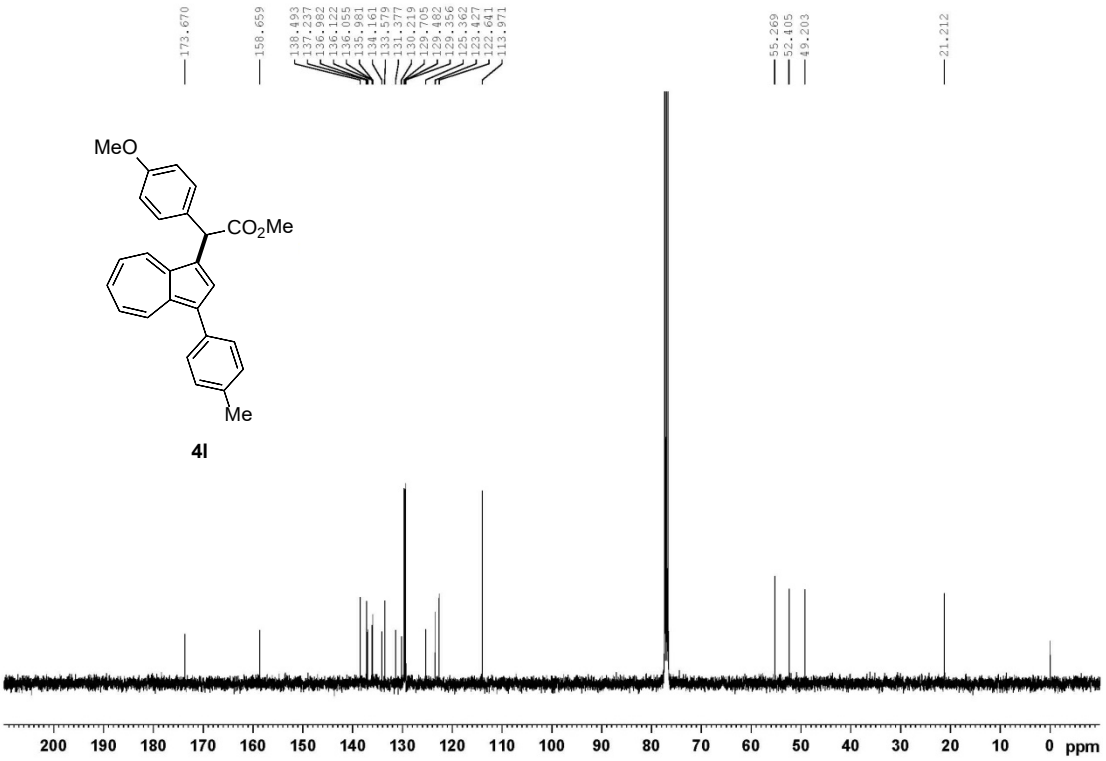


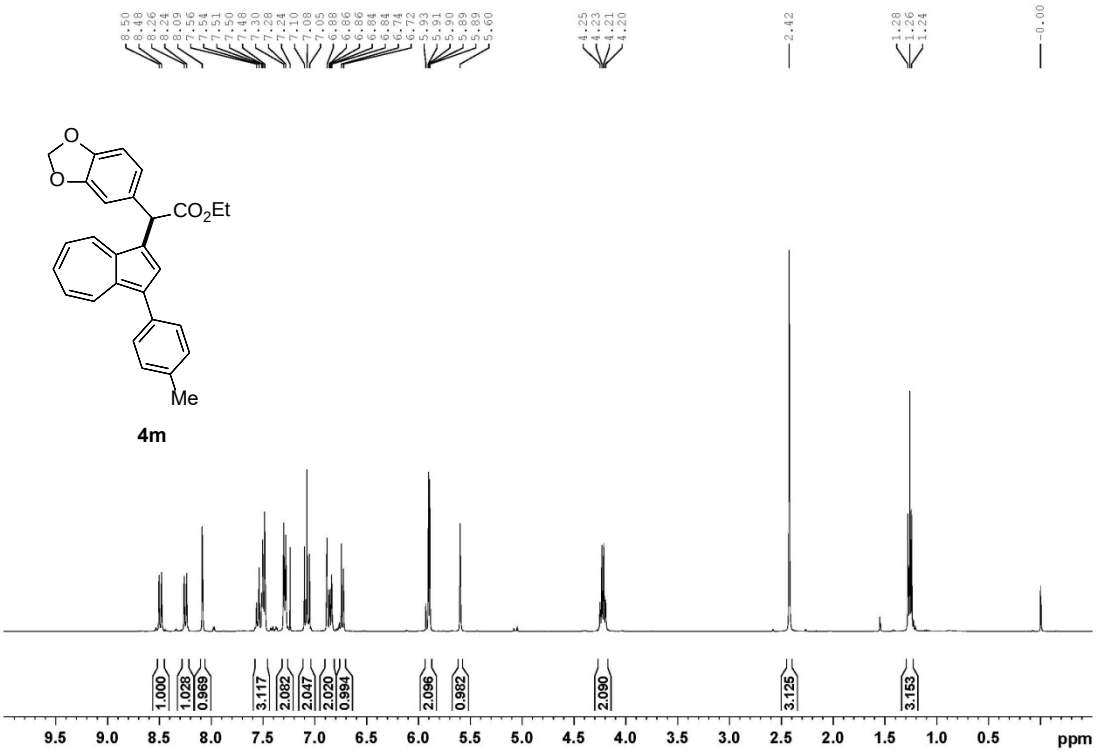
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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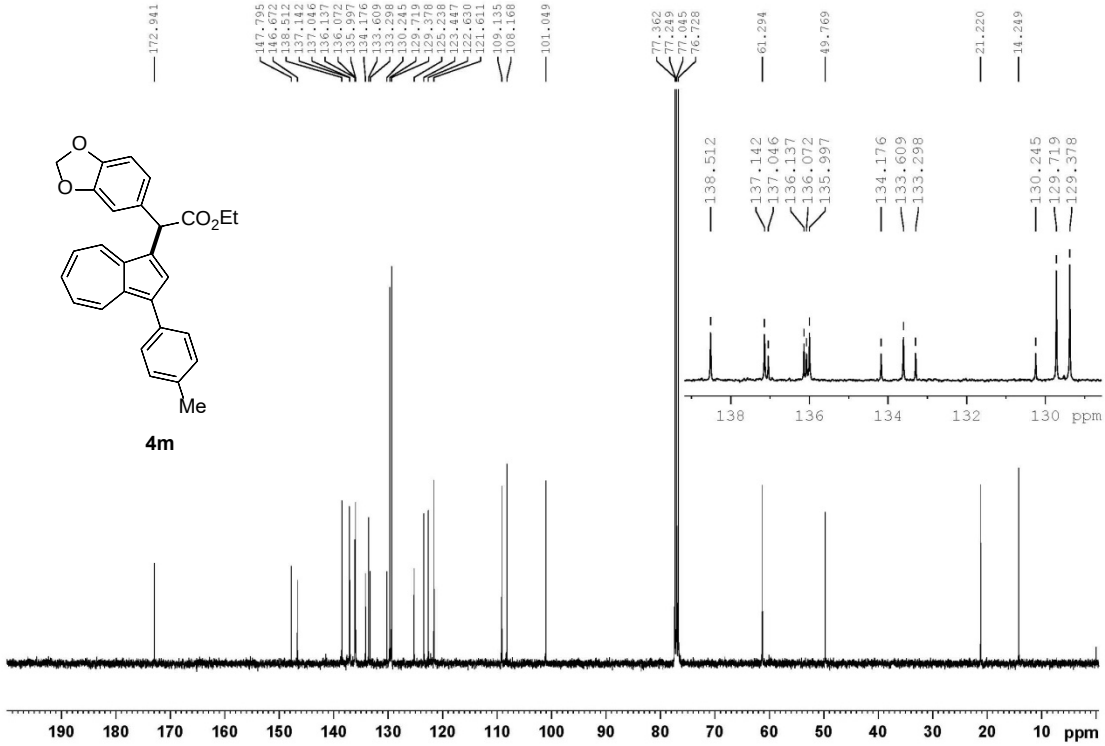
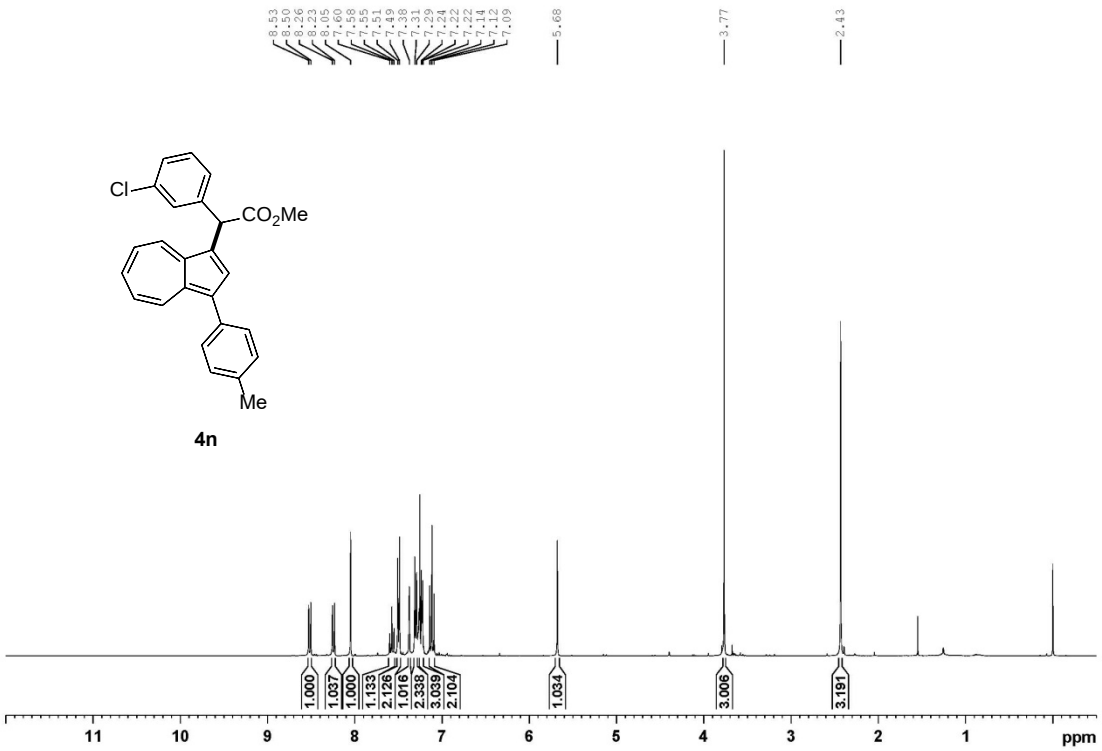
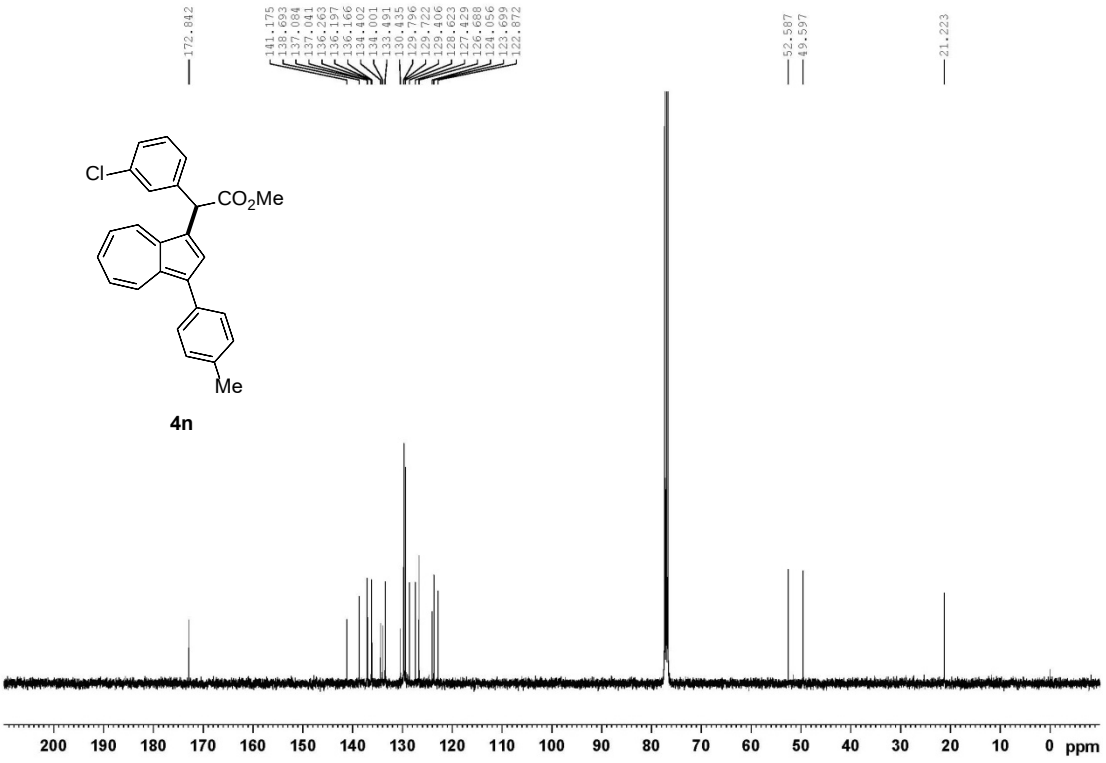


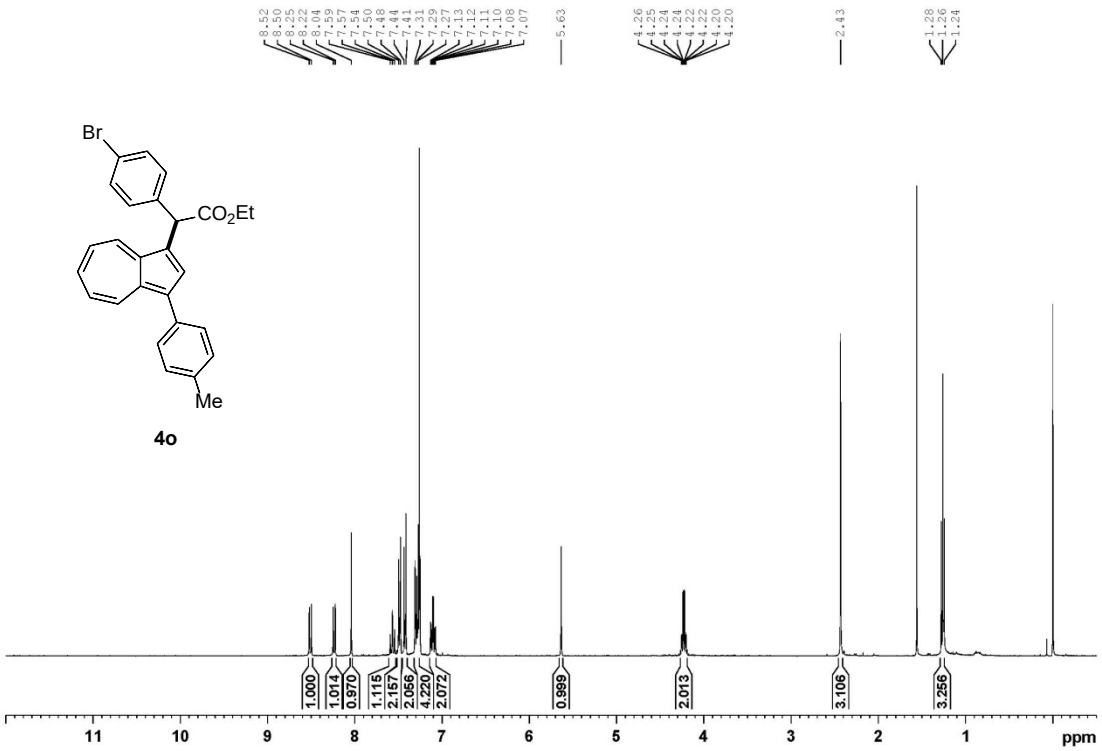
^{1}H NMR (400 MHz, $CDCl_3$)



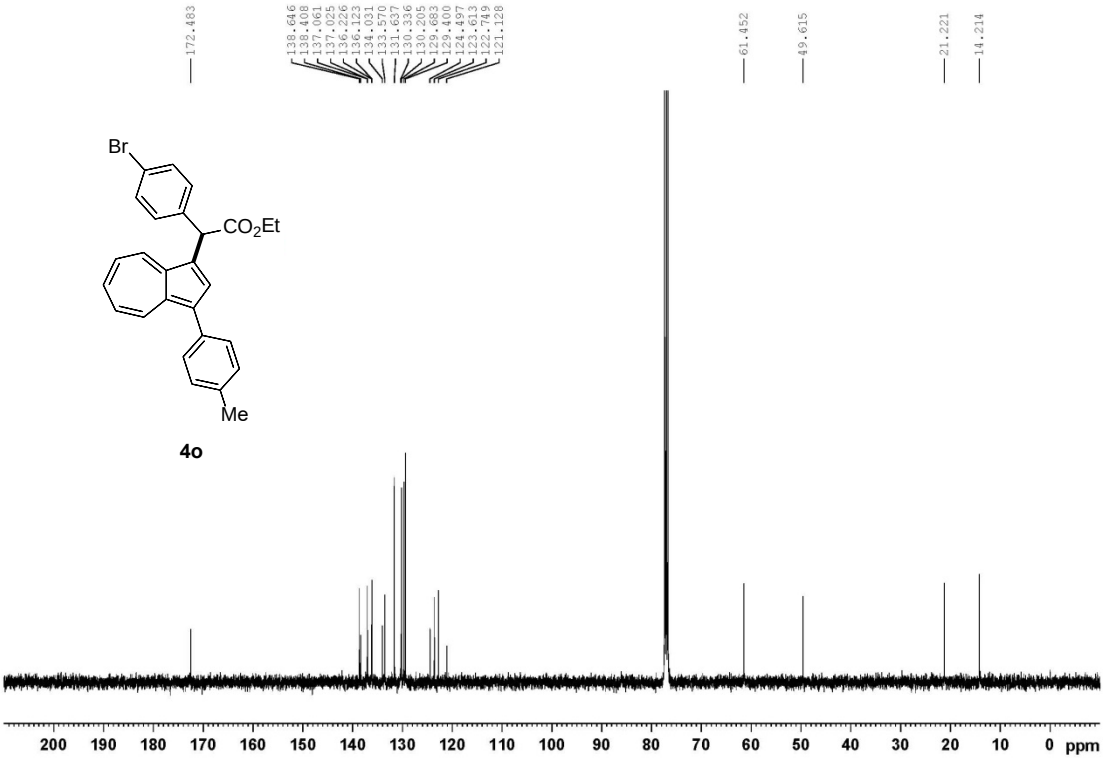
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



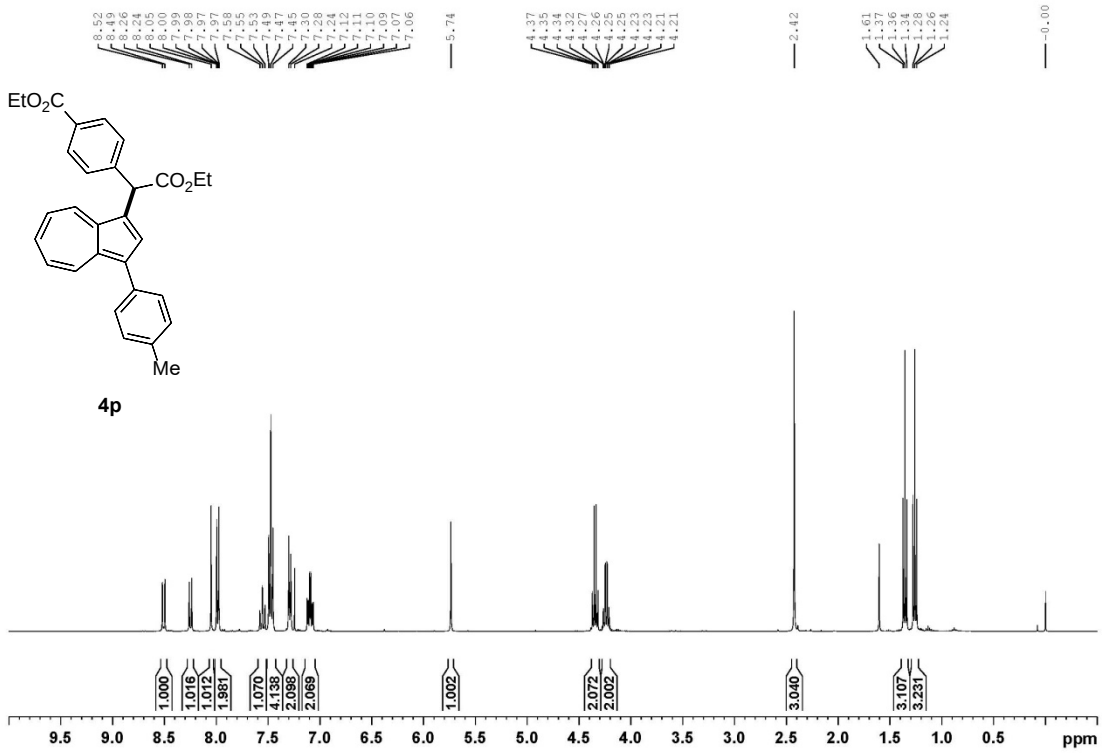
^{1}H NMR (400 MHz, $CDCl_3$)



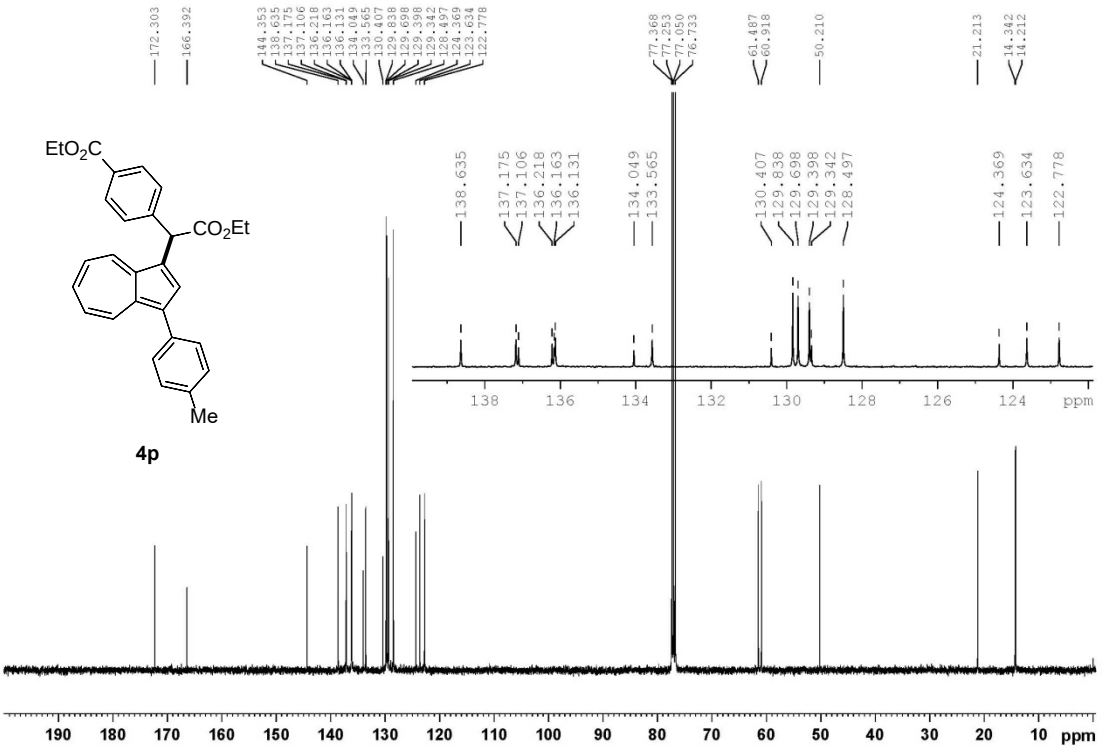
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



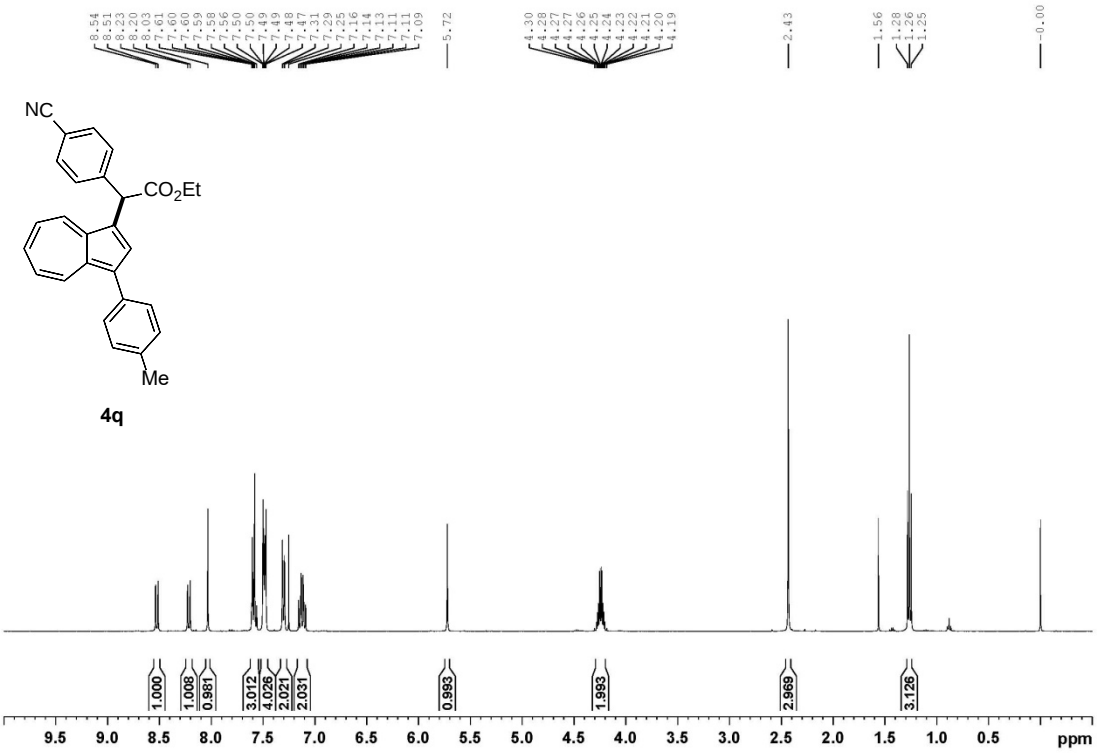
^{1}H NMR (400 MHz, $CDCl_3$)



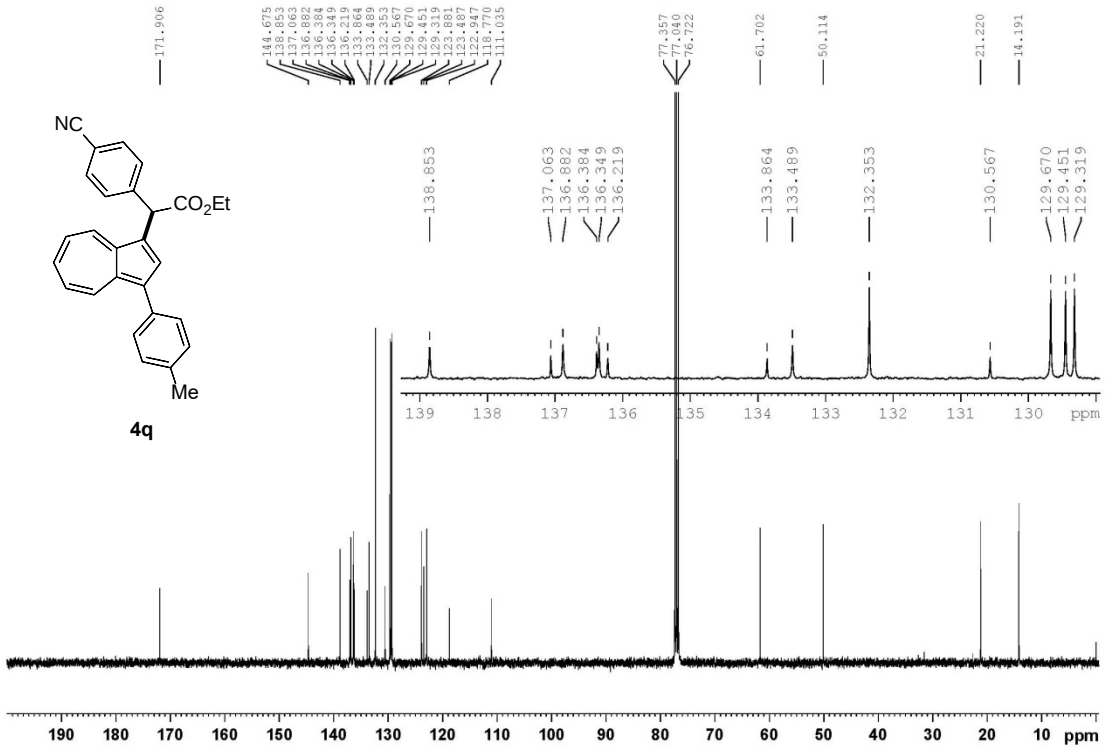
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



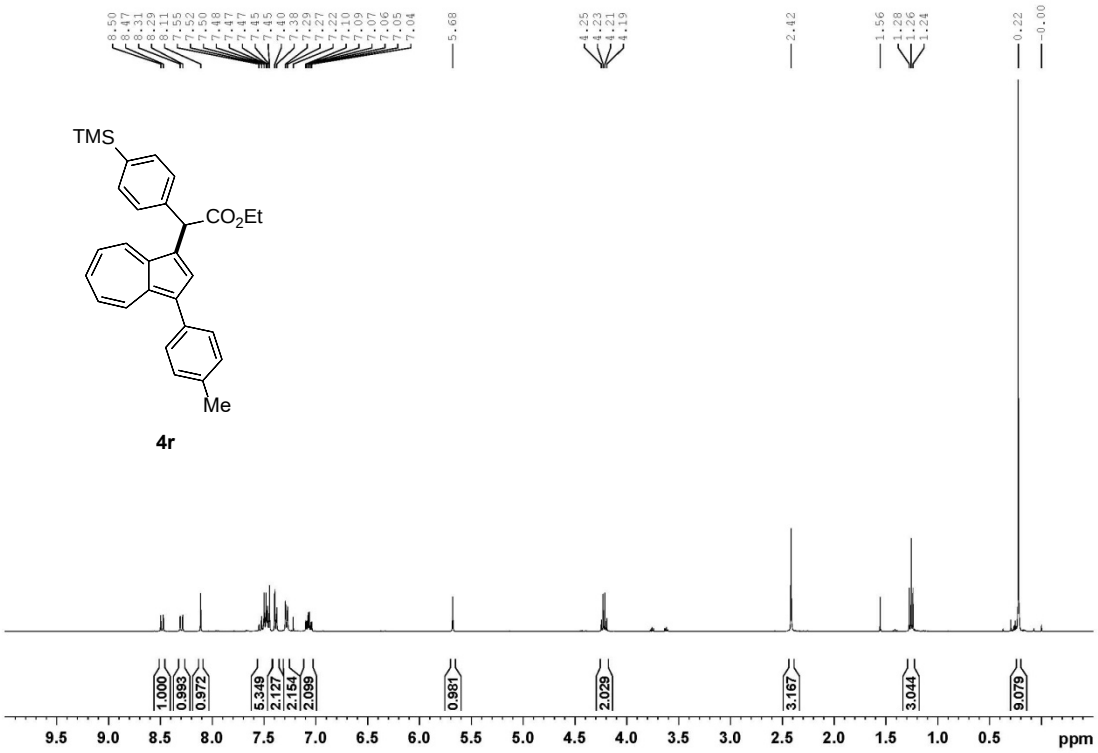
^{1}H NMR (400 MHz, $CDCl_3$)



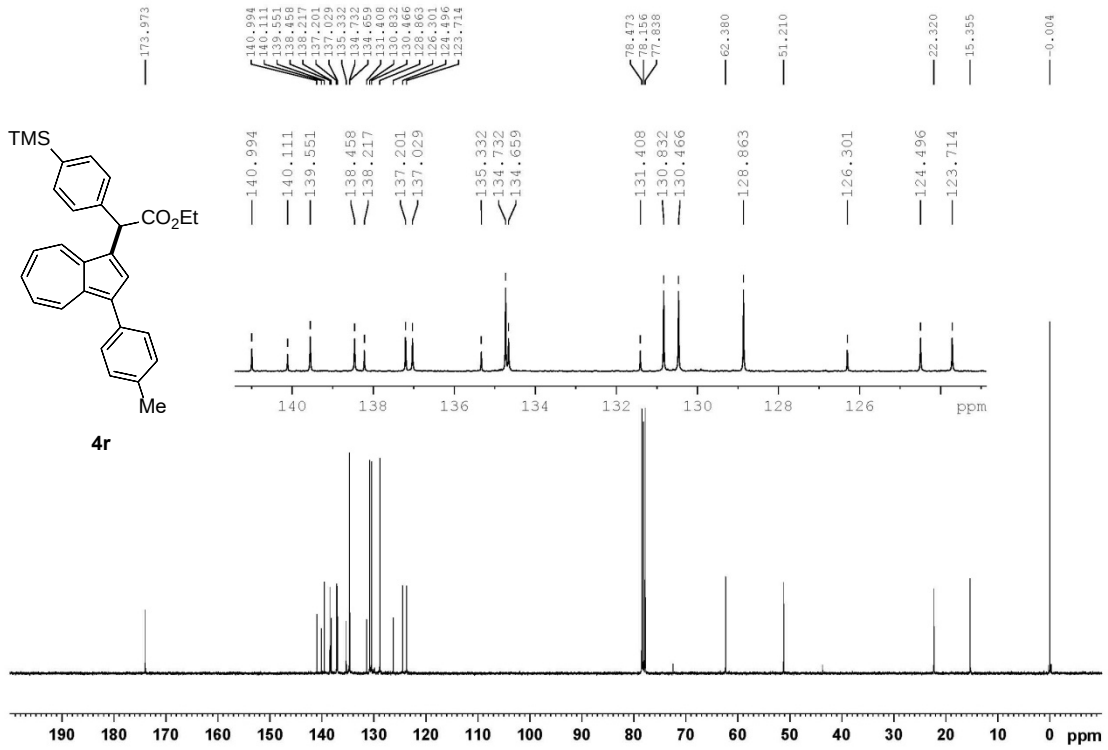
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



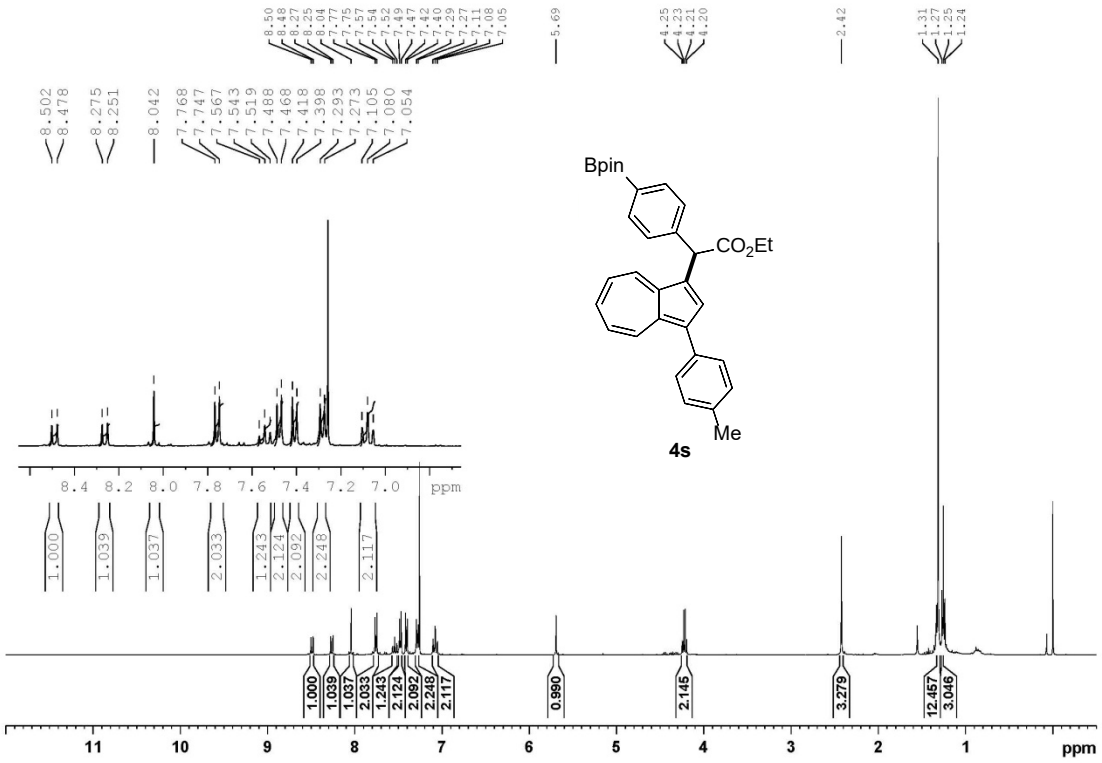
^{1}H NMR (400 MHz, $CDCl_3$)



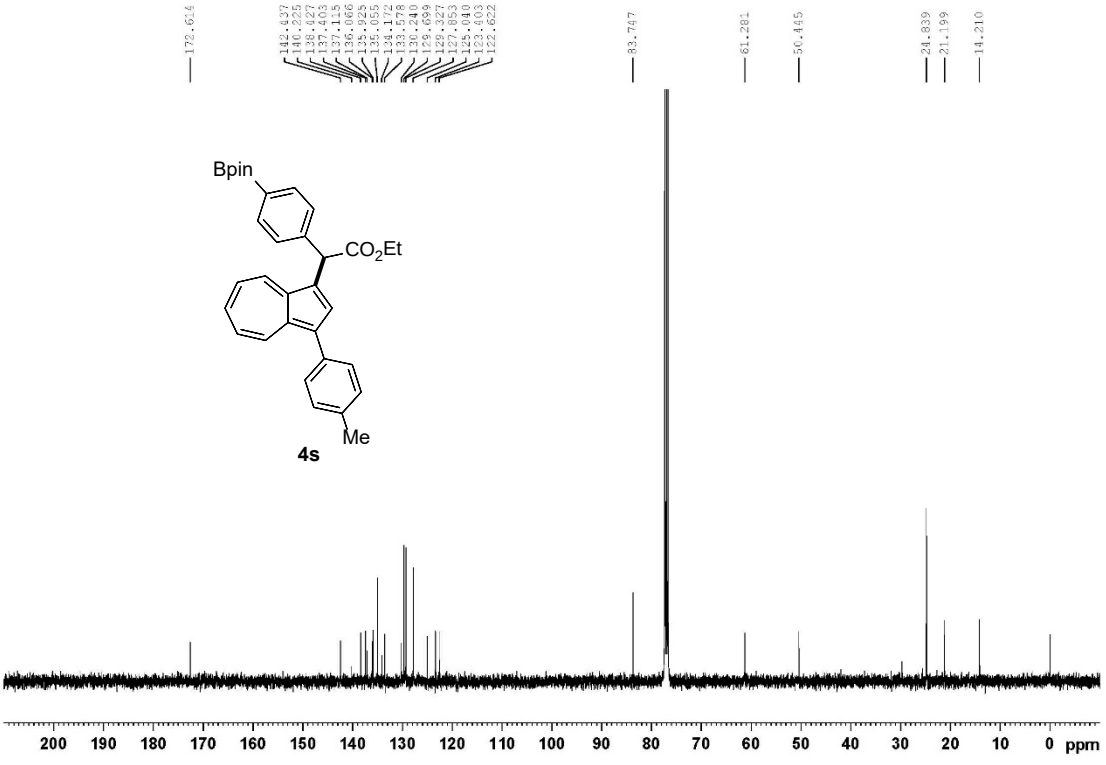
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



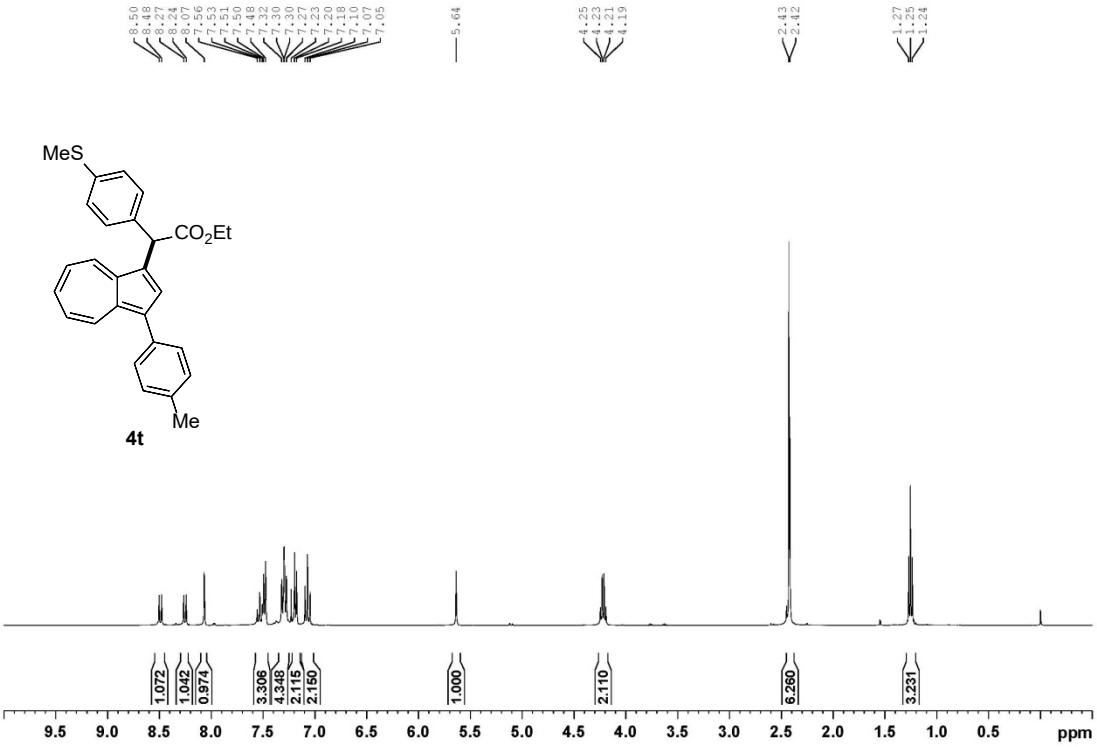
^{1}H NMR (400 MHz, $CDCl_3$)



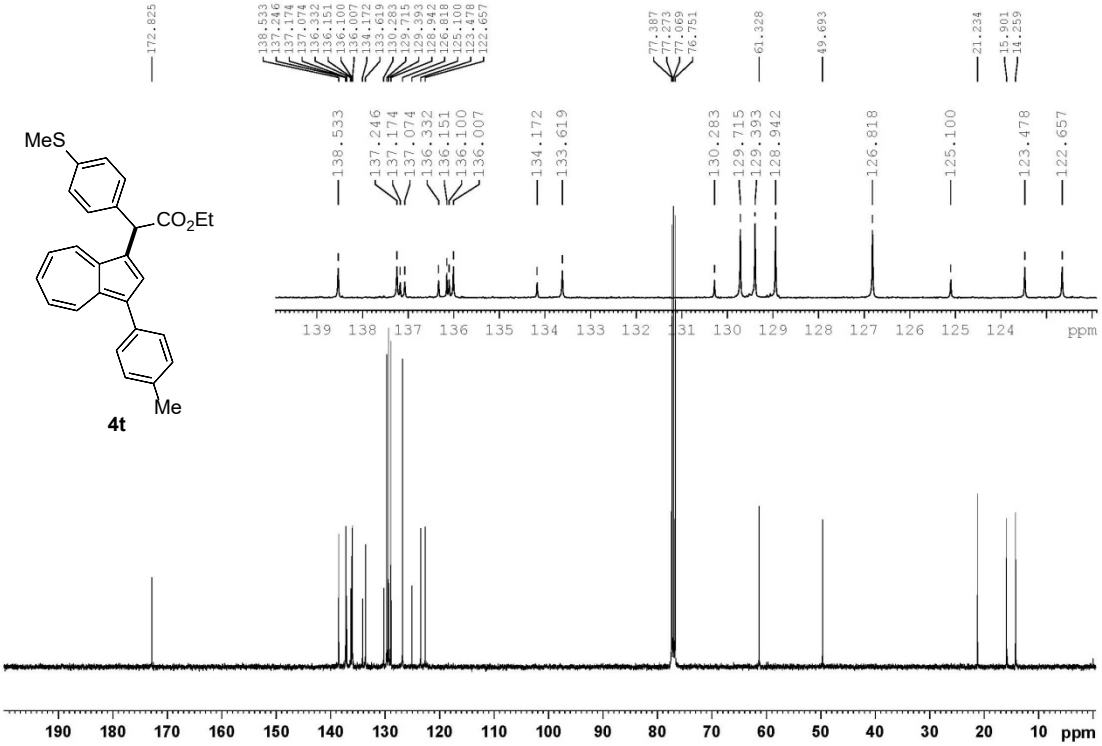
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



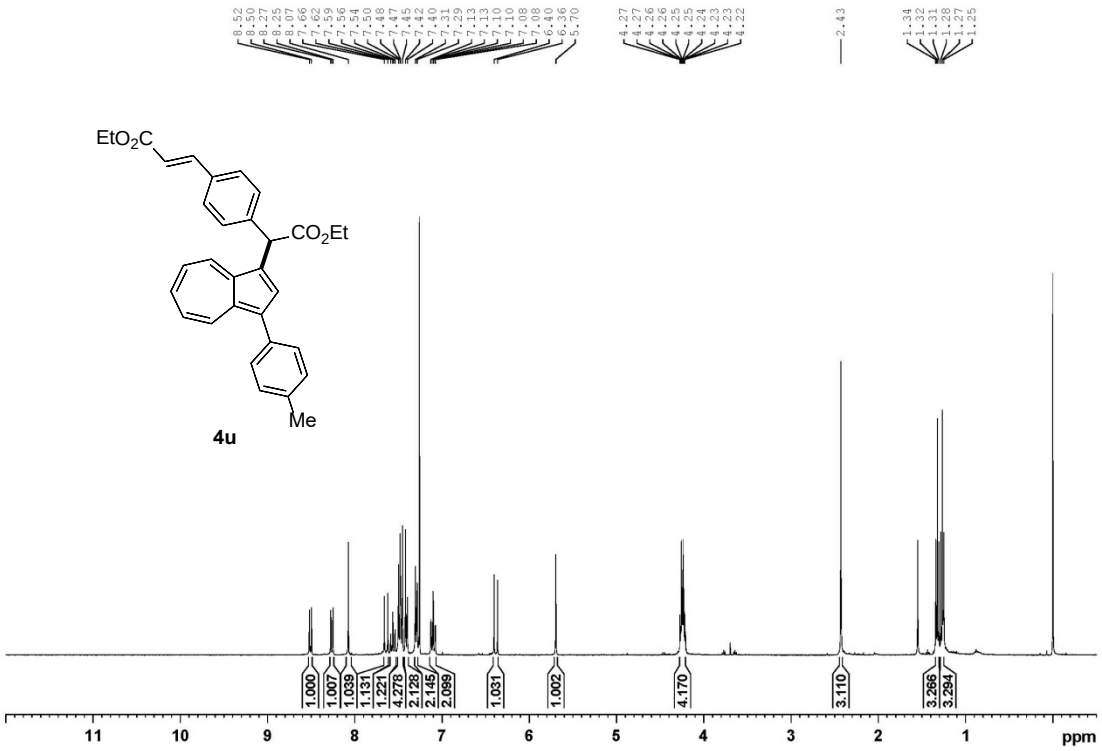
^{1}H NMR (400 MHz, $CDCl_3$)



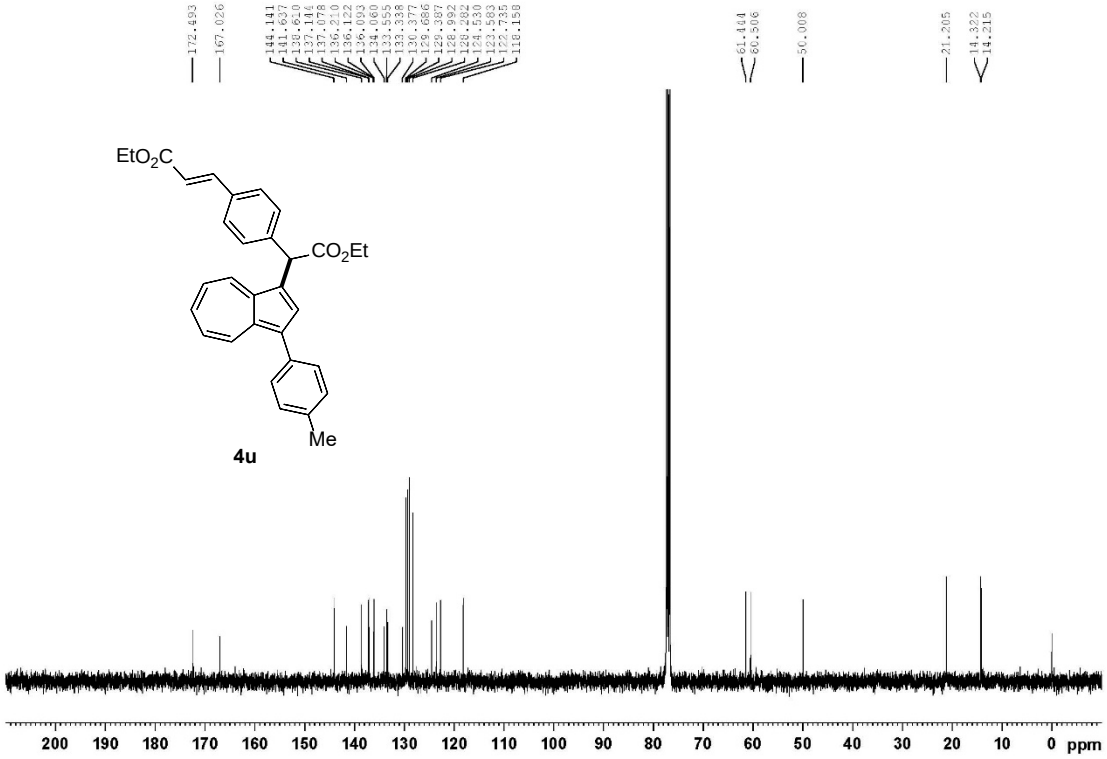
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



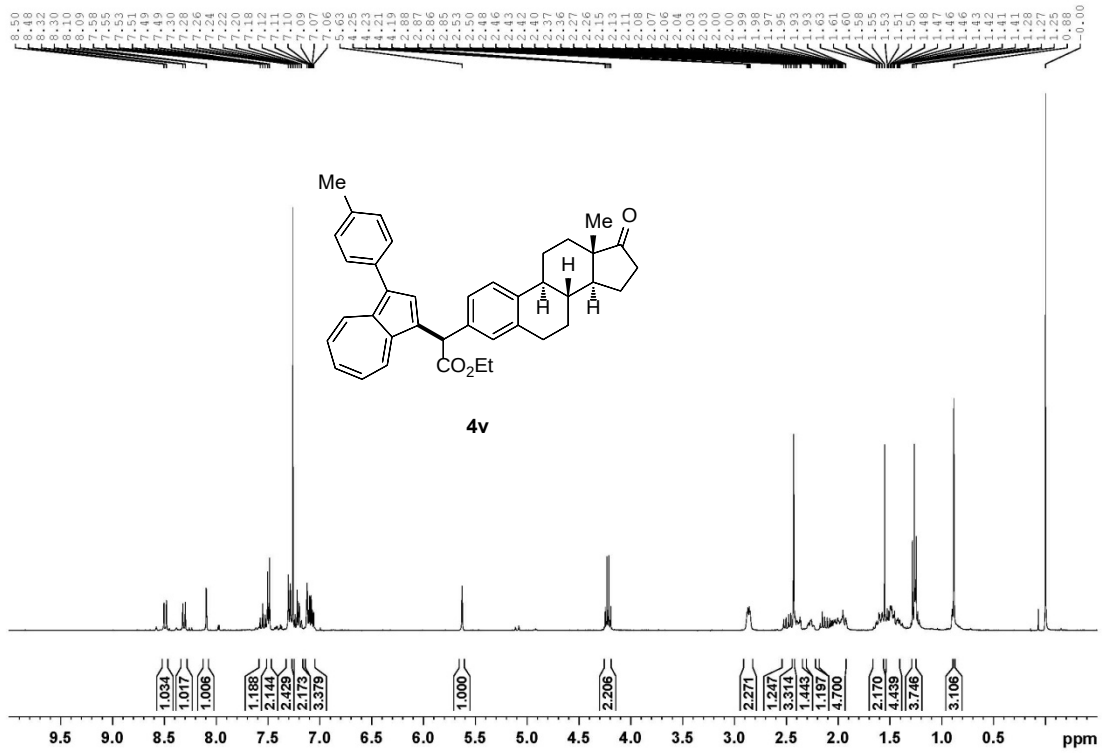
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)