Supporting Information

Catalytically Reversible C–C Bond Formation Using Palladium Catalysis

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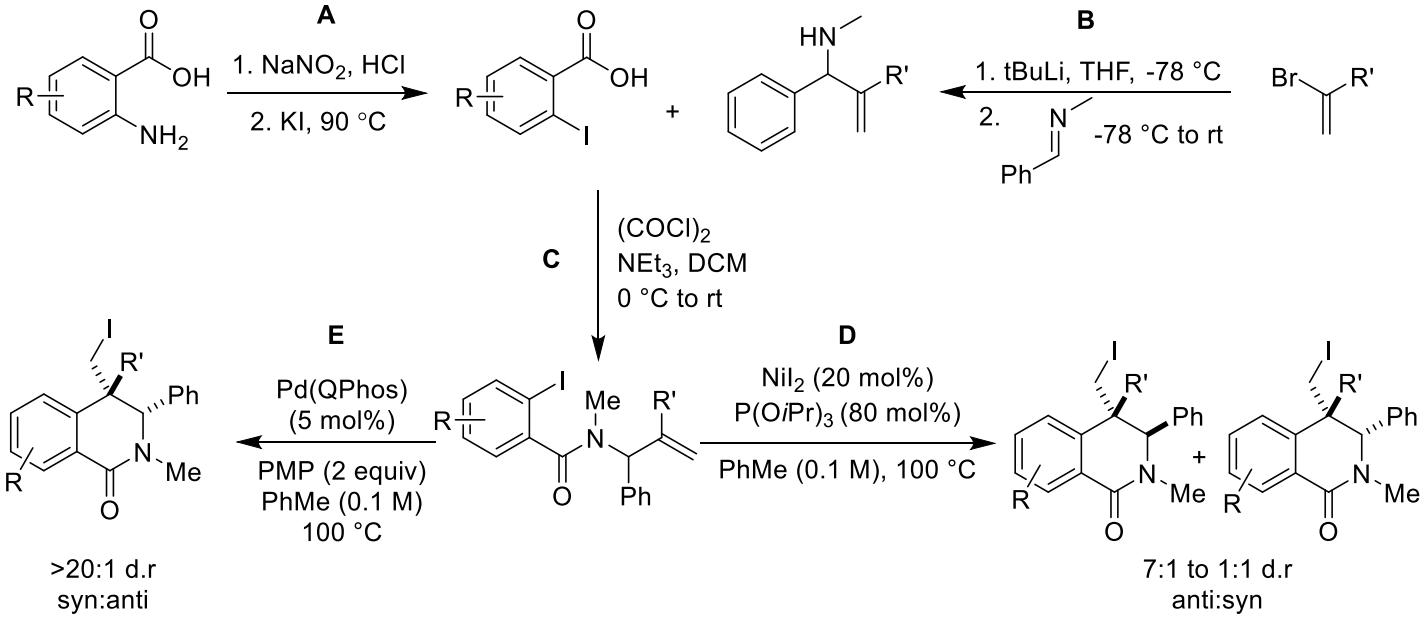
General Considerations

All reactions were performed in a dry environment under an inert atmosphere of argon unless otherwise stated. Reactions were monitored by thin layer chromatography (TLC) and visualized under UV light or by iodine staining. Flash column chromatography was performed with Silicycle 46-60 µm silica gel. Catalytic reactions were performed in 2-dram vials equipped with a Teflon cap. THF was distilled over sodium/benzophenone. Toluene and DCM were distilled over CaH_2. 1,3,5-Trimethoxybenzene was dried over night under vacuum and stored in a desiccator.

All reagents and organic building blocks were purchased from commercial suppliers (Sigma-Aldrich, Alfa Aesar, TCI, Combi-Blocks, Oakwood Chemical, AK Scientific) and used as received. NMR characterization data was collected at 296 K on a Varian Mercury 400 or an Agilent DD2 500 equipped with a 5mm Xses Cold Probe. Spectra were internally referenced to the residual solvent signal (^{1}H NMR: $CDCl_3$ = 7.26 ppm, ^{13}C NMR: $CDCl_3$ = 77.0 ppm). Data for ^{1}HNMR is reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constant (Hz), integration. Coupling constants were rounded to the nearest 0.5 Hz. Infrared (IR) spectra were recorded on a PerkinElmer Spectrum 100 instrument equipped with a single-bounce diamond / ZnSe ATR accessory. Melting point ranges were determined on a Fisher-Johns Melting Point Apparatus and are reported uncorrected. High resolution mass spectra (HRMS) were obtained on a Micromass 70S-250 spectrometer (EI) or an ABI/Sciex QStar Mass Spectrometer (ESI) or a JEOL AccuTOF model JMS-T1000LC mass spectrometer equipped with and IONICS® Direct Analysis in Real Time (DART) ion source at Advanced Instrumentation for Molecular Structure (AIMS) in the Department of Chemistry at the University of Toronto. Chiral HPLC was performed on Agilent 1100 or 1200 Series operated by ChemStation LC 3D software.

General Procedure 1: Synthesis of Starting Materials



Synthesis of 2-iodo benzoic acids (A): Synthesized according to Lautens.(*1–3*) The 2-amino benzoic acid (typically 5 mmol) was stirred in aq. HCl (1:1 HCl:H_2O, 0.36 M with respect to substrate) at 0 °C. $NaNO_2$ (1.2 equiv) was added, and the reaction was stirred at 0 °C for 30 min. KI (2 equiv) in H_2O (4.0 M) was added in one aliquot, and the reaction was refluxed for 90 minutes. The reaction was cooled, quenched with $Na_2S_2O_3$. The reaction was acidified with HCl and extracted with EtOAc (3 times). The organic phase collected and dried over $MgSO_4$, filtered and was concentrated *in-vacuo*.

Synthesis of phenylprop-2-en-1-amines (B): All reactions were run using a flame dried flask and an oven-dried Teflon stir bar under argon. To this flask was added vinyl bromide (1 equiv) and dried THF (0.4 M). The reaction vessel was cooled to -78 °C, upon which 1.8 equiv of tBuLi was added dropwise. After the addition of the tBuLi, the reaction mixture was a slight yellow colour; the addition of excess tBuLi led to a vibrant yellow solution, which led to a substantial amount of side product derived from the direct addition of tBuLi to the imine. The reaction was allowed to stir for 30 min, upon which the corresponding N-methyl-1-phenylmethanimine (1 equiv) was added dropwise, upon which an orange reaction mixture formed. The reaction was kept at -78 °C for at least 30 min and was allowed to warm to room temperature overnight, with the reaction mixture continually darkening from orange to dark red. The reaction was quenched with H_2O,

extracted 3x with EtOAc and concentrated in vacuo. The crude product was used in the following amidation step.

Synthesis of 2-Iodo-allylamine substrates (C): Synthesized according to Lautens.(*1*, *2*) In a separate flame dried flask, 2-iodo benzoic acid was mixed under an atmosphere of argon with $(COCl)_2$ (1.2 equiv) and catalytic amounts of DMF in DCM (0.5M) at 0 °C. The reaction was allowed to warm to room temperature and stir for 3h and the solvent was removed in vacuo. The resulting acyl chloride was again put under argon, dissolved in DCM (0.5M), cooled to 0 °C and 1 equiv of NEt_3 was added dropwise, with sufficient argon flow to purge the flask of the gas generated in this step. The corresponding amine was purged with argon and dissolved in a dried round bottom flask with DCM (0.5 M) and Et_3N (1 equiv) and the solution was added dropwise to the acyl chloride. The reaction was monitored by TLC and was stirred from 1h to 10h until the starting material had been consumed. The reaction was quenched with distilled water and was extracted with 3x25mL with DCM. The crude mixture was pushed through a pad of silica gel and dried in vacuo. Note** Full purification was not necessary/possible at this step. Additionally, the nickel-carboiodination reaction proved to be quite robust. However, it was found crucial to remove unreacted iodo-benzoic acid, and we made our best effort to remove the majority of the polar by-products and side products for the reaction. To achieve full purification of these intermediates, multiple rounds silica gel flash chromatography is required.

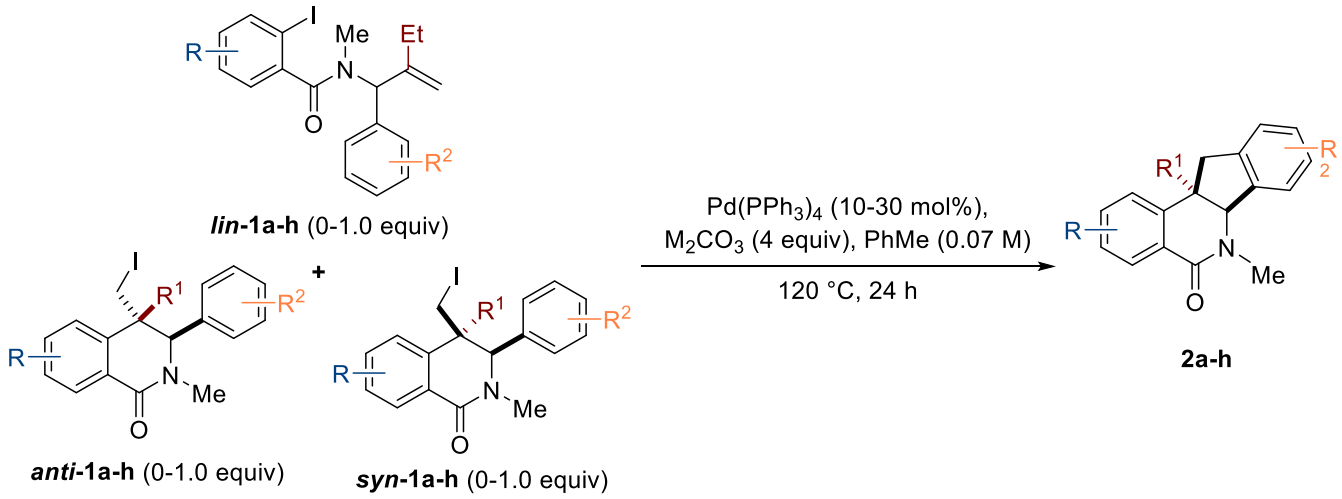
General synthetic remarks for the metal-catalyzed carboiodination reactions: For all substrates where R' = ethyl, sufficient amounts of both the syn and anti diastereomers were obtained using the nickel carboiodination reaction (D). For the starting material where R' = Me, the syn compound was obtained from Lautens[1] using the palladium carboiodination reaction (E), while the anti was obtained using a separate method from Lautens[2] using the nickel carboiodination reaction (D).

Nickel Carboidoination Reaction (D): Synthesized according to Lautens.(*2*) In an oven dried scintillation vial under argon, was charged with 20 mol% NiI_2 and 80 mol% $P(O\textit{i}Pr)_3$. The crude substrate was transferred to the reaction vial in 2 aliquots with dry toluene (0.1 M). The vial was fitted with a Teflon cap and Teflon tape. The reactions were heated at 100 °C for 18 hours. The reaction mixture was pushed through a pad of silica, eluting with 100% EtOAc, concentrated in vacuo and a crude 1H NMR was obtained to determine the d.r of the reaction. The products were then purified via flash silica gel chromatography. The diastereomers were identified by 1H NMR splitting patterns as well as NOESY experiments.

Palladium Carboidoination Reaction (E): Synthesized according to Lautens.(*1*) One oven-dried 2 dram vial was cooled under argon, charged with the liquid racemic or chiral N-ally carboxamides (0.2 mmol, 1 equiv, 1), and purged with argon for 10 minutes. A second ovendried vial was cooled under argon, charged with $Pd(QPhos)_2$ (0.01 mmol, 5 mol% [Pd]), and purged with argon for 10 minutes. The amide was dissolved in dry and degassed toluene (2 mL, 0.1 M) and 1,2,2,6,6-pentamethylpiperidine (72.4 µL, 0.4 mmol, 2 equiv) was added via a dry microsyringe. This well-mixed solution of amide and base was added into the vial containing the catalyst. The vial was

fitted with a Teflon lined screw cap under a stream of argon passed through a large inverted glass funnel, sealed using Teflon tape, and placed in a pre-heated oil bath at 100 °C for 22 hours. At this time either TLC analysis or ^{1}H NMR analysis of a small aliquot indicated full conversion of starting material, and the reaction vial was cooled, and its contents were filtered through a 2 cm plug of silica gel in a pipette eluting with 100% EtOAc.

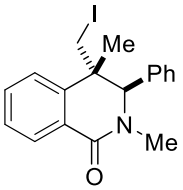
General Procedure 2: Catalytic Procedure



General remarks: Reactions were run in an oven-dried 2 dram vial fitted with an oven-dried Teflon coated stir bar, and a Teflon cap under argon. The $Pd(PPh_3)_4$ that was used was stored under argon in a freezer. Prior to every reaction set up, the carbonate base used was flame-dried under vacuum prior to every use, and the toluene was freshly distilled. **Procedure**: To an oven-dried 2 dram vial was cooled under argon for 10 minutes, was added $Pd(PPh_3)_4$ (10-30 mol%), a carbonate base (either K_2CO_3 or Cs_2CO_3, 4 equiv with respect to substrate), and substrate (0.065-0.1 mmol). The reaction was allowed to purge under argon for another 3 minutes, at which time a layer of Teflon tape was placed around the edge of the vial. Toluene (0.07 M) was added, and the vial was fitted with a Teflon screw-cap, sealed using Teflon tape, and placed in a pre-heated oil bath at 120 °C for 24 hours. The reaction vial was cooled to room temperature, and its contents were filtered through a 2 cm plug of silica gel in a pipette eluting with 100% EtOAc and dried in-vacuo. A ^{1}H NMR analysis of the crude was obtained to check for conversion. The products were then purified via silica gel flash chromatography and dried in-vacuo. Note** when using any ***lin*-1** substrates either alone or in the 3-component convergence experiment, the *lin*-substrate was first weighed into a separate oven-dried vial under argon. The substrate was then transferred to the reaction vial via 2 aliquots of toluene with a syringe under argon.

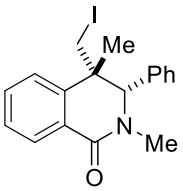
Starting Materials

<u>*anti* and *syn* 1a:</u>



anti-4-(iodomethyl)-2,4-dimethyl-3-phenyl-3,4-dihydroisoquinolin-1(2H)-one

***anti*-1a** was synthesized by **General Procedure 1(b-d)**. For full characterization and the complete synthesis of this compound, refer to our previous report of nickel-carboiodination.[2]



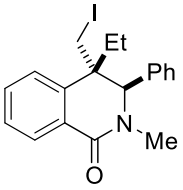
syn-4-(iodomethyl)-2,4-dimethyl-3-phenyl-3,4-dihydroisoquinolin-1(2H)-one

***syn*-1a** was synthesized by **General Procedure 1(b-c,e)**. For full characterization and the complete synthesis of this compound, refer to our previous report of palladium-carboiodination.(*1*, *2*)

<u>anti and syn 1b:</u>

***anti* and *syn*-1a** were synthesized by **General Procedure 1(b-d)** on various scales giving roughly a 1.1:1 d.r (anti:syn) of the alkyl iodides. Each diastereomer was Isolated by flash column chromatography using 2:1 Pentane:EtOAc, each followed by 3 rounds of trituration using pentanes in a sonicator to yield white solids. On a 4 mmol scale, **syn-1b** (top spot) was obtained in a 3.0% yield (0.12 mmol, 48.4 mg) while **anti-1b** (bottom spot) was obtained in a 5.1% yield (0.20 mmol, 82.2 mg) over 2 steps (**C**, **D**). note** the general crude yields of the carboiodination reactions were higher than what is reported, as pure compound could only be obtained via multiple rounds of trituration in pentane using a sonicator. Additionally, d.r was obtained from the crude ^{1}H NMR; even though in some cases the anti-isomer was the major diastereomer of the reaction, the isolated yields do not always accurately reflect this due to purification

difficulties. In some cases, the isomers were more soluble in pentanes, and thus each trituration was followed by cooling the reaction vial to 0 °C overnight.



anti-4-ethyl-4-(iodomethyl)-2-methyl-3-phenyl-3,4-dihydroisoquinolin-1(2H)-one

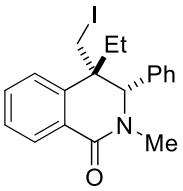
^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.91 (t, *J* = 7.4 Hz, 3H), 1.41 – 1.62 (m, 1H), 1.93 (dq, *J* = 14.7, 7.3 Hz, 1H), 3.04 (s, 3H), 3.56 (dd, *J* = 10.3, 0.8 Hz, 1H), 3.73 (d, *J* = 10.3 Hz, 1H), 4.48 (s, 1H), 6.85 – 6.91 (m, 2H), 7.11 – 7.17 (m, 2H), 7.19 – 7.24 (m, 1H), 7.27 – 7.31 (m, 1H), 7.41 – 7.62 (m, 2H), 8.13 – 8.38 (m, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 8.4, 19.6, 26.4, 34.1, 43.2, 70.2, 126.2, 128.0, 128.1, 128.5, 128.7, 129.1, 131.9, 136.9, 139.5, 163.3.

IR (thin film, cm^{-1}): 3061, 3023, 2978, 2957, 2875, 1632, 1598, 1574, 1490, 1309, 1254, 1093, 821, 706.

HRMS (DART, M+H): Calc. for $C_{19}H_{21}INO$ 406.0662, found 406.0661.

m.p: 144-149 °C



syn-4-ethyl-4-(iodomethyl)-2-methyl-3-phenyl-3,4-dihydroisoquinolin-1(2H)-one

^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.64 (t, *J* = 7.4 Hz, 3H), 2.03 (dq, *J* = 14.4, 7.3 Hz, 1H), 2.12 (dtd, *J* = 15.0, 7.5, 1.9 Hz, 1H), 2.79 (dd, *J* = 10.2, 1.9 Hz, 1H), 3.06 (s, 3H), 3.93 (d, *J* = 10.3 Hz, 1H), 4.31 (s, 1H), 7.06 (d, *J* = 7.8 Hz, 2H), 7.13 (t, *J* = 7.9 Hz, 3H), 7.20 – 7.25 (m, 1H), 7.46 (pd, *J* = 7.4, 1.6 Hz, 2H), 8.22 (dd, *J* = 7.0, 2.2 Hz, 1H).

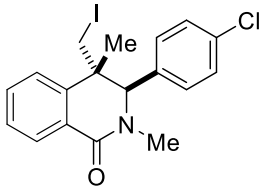
^{13}C NMR (126 MHz, Chloroform-*d*) δ 7.5, 12.8, 33.4, 34.3, 43.4, 72.4, 125.4, 127.7, 128.4, 128.6, 128.7, 128.9, 129.1, 131.5, 136.4, 137.4, 163.6.

IR (thin film, cm^{-1}): 3025, 2961, 2915, 2875, 1636, 1596, 1474, 1453, 1317, 1254, 1087, 759.

HRMS (ESI, M+H): Calc. for $C_{19}H_{21}INO$ 406.0668, found 406.0666.

m.p: 122-124 ^{o}C

***anti*-1c**

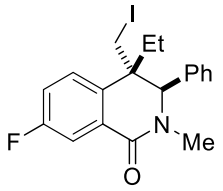


3-(4-chlorophenyl)-4-(iodomethyl)-2,4-dimethyl-3,4-dihydroisoquinolin-1(2H)-one

***anti*-1c** was synthesized by **General Procedure 1(a-d)**. For full characterization and the complete synthesis of this compound, refer to our previous report of nickel-carboiodination.(*2*)

***anti* and *syn* 1d:**

***anti* and *syn*-1d** were synthesized by **General Procedure 1(b-d)**on a 3.6 scale giving roughly a 1:1.5 d.r (anti:syn) of the alkyl iodides. Each diastereomer was Isolated by flash column chromatography using 2:1 Pentane:EtOAc, each followed by 3 rounds of trituration using pentanes in a sonicator to yield white solids. **syn-1d** (top spot) was obtained in an 8.9% yield (0.32 mmol,136.5 mg) while **anti-1d** (bottom spot) was obtained in a 7.2% yield (0.26 mmol, 112.0 mg).



anti-4-ethyl-7-fluoro-4-(iodomethyl)-2-methyl-3-phenyl-3,4-dihydroisoquinolin-1(2H)-one

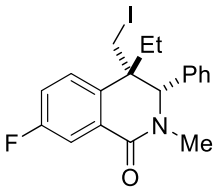
^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.90 (t, *J* = 7.4 Hz, 3H), 1.44 (dq, *J* = 14.8, 7.5, 1H), 1.93 (dq, *J* = 14.7, 7.4 Hz, 1H), 3.04 (s, 3H), 3.54 (dd, *J* = 10.3, 0.9 Hz, 1H), 3.70 (d, *J* = 10.3 Hz, 1H), 4.48 (s, 1H), 6.80 – 6.91 (m, 2H), 7.10 – 7.21 (m, 3H), 7.21 – 7.39 (m, 2H), 7.92 (dd, *J* = 9.0, 2.9 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 8.2, 19.3 (d, *J* = 1.8 Hz), 26.5, 34.2, 43.0, 70.0, 115.6 (d, *J* = 23.4 Hz), 118.7 (d, *J* = 21.5 Hz), 128.0, 128.3 (d, *J* = 7.6 Hz), 128.6, 128.6, 131.2 (d, *J* = 7.3 Hz), 135.3, 136.5, 162.2 (d, *J* = 2.3 Hz), 162.3 (d, *J* = 247.9 Hz).

IR (thin film, cm^{-1}): 3066, 3029, 2967, 2936, 1647, 1610, 1588, 1484, 1451, 1355, 1257, 1147, 1097,899, 700.

HRMS (DART, M+H): Calc. for $C_{19}H_{20}FINO$ 424.0568, found 424.0570.

m.p: 156-158 °C



syn-4-ethyl-7-fluoro-4-(iodomethyl)-2-methyl-3-phenyl-3,4-dihydroisoquinolin-1(2H)-one

^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.63 (t, *J* = 7.4 Hz, 3H), 1.93 – 2.21 (m, 2H), 2.76 (dd, *J* = 10.3, 1.8 Hz, 1H), 3.05 (s, 3H), 3.88 (d, *J* = 10.3 Hz, 1H), 4.31 (s, 1H), 7.06 (d, *J* = 7.3 Hz, 2H), 7.10 (dd, *J* = 8.6, 5.0 Hz, 1H), 7.13 – 7.19 (m, 3H), 7.23 – 7.36 (m, 1H), 7.93 (dd, *J* = 9.0, 2.9 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 7.5, 12.2, 33.3, 34.3, 43.2, 72.4, 115.9 (d, *J* = 23.4 Hz), 118.2 (d, *J* = 21.6 Hz), 127.3 (d, *J* = 7.4 Hz), 128.5, 128.6, 128.7, 131.3 (d, *J* = 7.2 Hz), 133.1 (d, *J* = 3.5 Hz), 136.0, 162.2 (d, *J* = 247.7 Hz), 162.5 (d, *J* = 2.2 Hz).

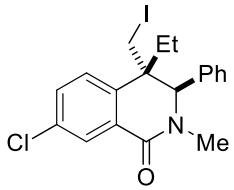
IR (thin film, cm^{-1}): 3065, 3031, 2967, 2936, 2877, 1645, 1588, 1482, 1316, 1255, 1092, 904, 699.

HRMS (DART, M+H): Calc. for $C_{19}H_{20}FINO$ 424.0568, found 424.0559.

m.p: 138-141 °C

***anti* and *syn*-1e:**

***anti* and *syn*-1e** were synthesized by **General Procedure 1(b-d)** on a 4 mmol scale giving roughly an 1:1.6 d.r (anti:syn) of the of the alkyl iodides. Each diastereomer was Isolated by flash column chromatography using 2:1 Pentane:EtOAc, each followed by 3 rounds of trituration in a sonicator using pentanes to yield white solids. **syn-1e** (top spot) was obtained in a 5.7% yield (0.23 mmol, 99.7 mg) while **anti-1e** (bottom spot) was obtained in a 6.2% yield (0.25 mmol, 109.0 mg).



anti-7-chloro-4-ethyl-4-(iodomethyl)-2-methyl-3-phenyl-3,4-dihydroisoquinolin-1(2H)-one

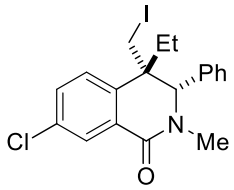
^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.90 (t, *J* = 7.4 Hz, 3H), 1.44 (dqd, *J* = 14.7, 7.4, 0.9 Hz, 1H), 1.93 (dq, *J* = 14.7, 7.4 Hz, 1H), 3.04 (s, 3H), 3.54 (dd, *J* = 10.3, 0.9 Hz, 1H), 3.70 (d, *J* = 10.3 Hz, 1H), 4.47 (s, 1H), 6.60 – 7.03 (m, 2H), 7.16 – 7.21 (m, 2H), 7.22 – 7.28 (m, 2H), 7.45 (dd, *J* = 8.3, 2.4 Hz, 1H), 8.21 (d, *J* = 2.4 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 8.2, 18.9, 26.3, 34.2, 43.1, 70.0, 127.8, 128.0, 128.6, 128.7, 128.7, 130.6, 131.8, 134.3, 136.5, 138.0, 162.1.

IR (thin film, cm^{-1}): 3066, 3029, 2970, 2941, 1646, 1594, 1474, 1451, 1352, 1249, 908, 732

HRMS (DART, M+H): Calc. for $C_{19}H_{20}ClINO$ 440.0273, found 440.0275.

m.p: 119-122 °C



syn-7-chloro-4-ethyl-4-(iodomethyl)-2-methyl-3-phenyl-3,4-dihydroisoquinolin-1(2H)-one

^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.63 (t, *J* = 7.4 Hz, 3H), 1.96 – 2.27 (m, 2H), 2.75 (dd, *J* = 10.3, 1.7 Hz, 1H), 3.04 (s, 3H), 3.86 (d, *J* = 10.3 Hz, 1H), 4.31 (s, 1H), 7.06 (m, 3H), 7.15 (td, *J* = 7.5, 0.8 Hz, 2H), 7.21 – 7.30 (m, 1H), 7.44 (dd, *J* = 8.2, 2.4 Hz, 1H), 8.21 (d, *J* = 2.4 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 7.5, 12.0, 33.4, 34.4, 43.3, 72.2, 127.0, 128.5, 128.6, 128.8, 128.9, 130.7, 131.3, 134.1, 135.8, 136.0, 162.3.

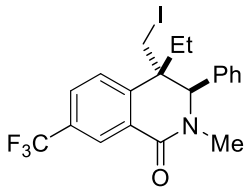
IR (thin film, cm^{-1}): 3066, 3031, 2966, 2936, 2876, 1645, 1593, 1487, 1315, 1278, 1185, 908, 698.

HRMS (DART, M+H): Calc. for $C_{19}H_{20}ClINO$ 440.0273, found 440.0264.

m.p: 184-187 °C

***anti* and *syn*-1f:**

***anti* and *syn*-1f** were synthesized by **General Procedure 1(a-d)** on a 4 mmol scale giving roughly a 1.2:1 d.r (anti:syn) of the alkyl iodides. Each diastereomer was Isolated by flash column chromatography using 2:1 Pentane:EtOAc, each followed by 3 rounds of trituration using pentanes in a sonicator to yield white solids. **syn-1f** (top spot) was obtained in a 5.4% yield (0.22 mmol 101.3 mg) while **anti-1f** (bottom spot) was obtained in a 4.2% yield (0.17 mmol, 81.0 mg).



anti-4-ethyl-4-(iodomethyl)-2-methyl-3-phenyl-7-(trifluoromethyl)-3,4-dihydroisoquinolin-1(2H)-one

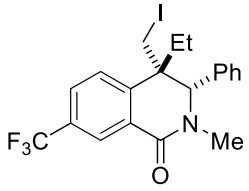
^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.92 (t, *J* = 7.4 Hz, 3H), 1.49 (dd, *J* = 14.7, 7.4 Hz, 1H), 2.00 (dq, *J* = 14.7, 7.4 Hz, 1H), 3.06 (s, 3H), 3.55 (dd, *J* = 10.4, 0.9 Hz, 1H), 3.72 (d, *J* = 10.4 Hz, 1H), 4.51 (s, 1H), 6.86 (d, *J* = 7.3 Hz, 2H), 7.19 (dd, *J* = 8.1, 6.8 Hz, 2H), 7.26 (s, 1H), 7.43 (d, *J* = 8.1 Hz, 1H), 7.74 (dd, *J* = 7.8, 2.1 Hz, 1H), 8.52 (d, *J* = 2.1 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 8.1, 18.4, 26.3, 34.2, 43.5, 69.9, 124.5 (q, *J* = 272.6 Hz), 125.8 (q, *J* = 3.8 Hz), 127.0, 127.9, 128.3 (q, *J* = 3.7 Hz), 128.7, 128.8, 129.7, 130.5 (q, *J* = 33.3 Hz), 136.3, 143.5 (d, *J* = 1.2 Hz), 162.0.

IR (thin film, cm^{-1}): 3083, 3023, 2967, 2918, 1649, 1593, 1569, 1474, 1451, 1393, 1243, 1113, 1082, 847, 556.

HRMS (DART, M+H): Calc. for $C_{20}H_{20}IF_3ON$ 473.0536, found 474.0545.

m.p: 106-111 °C



syn-4-ethyl-4-(iodomethyl)-2-methyl-3-phenyl-7-(trifluoromethyl)-3,4-dihydroisoquinolin-1(2H)-one

^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.64 (t, *J* = 7.4 Hz, 3H), 1.94 – 2.19 (m, 2H), 2.80 (dd, *J* = 10.3, 1.7 Hz, 1H), 3.07 (s, 3H), 3.92 (d, *J* = 10.3 Hz, 1H), 4.37 (s, 1H), 7.00 – 7.11 (m, 2H), 7.16 (t, *J* = 7.9 Hz, 2H), 7.23 – 7.42 (m, 2H), 7.73 (dd, *J* = 8.1, 1.3 Hz, 1H), 8.51 (d, *J* = 1.4 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 7.5, 11.4, 33.5, 34.4, 43.7, 72.1, 123.7 (q, *J* = 272.4 Hz), 125.9 (q, *J* = 3.7 Hz), 126.1, 128.0 (q, *J* = 3.7 Hz), 128.5, 128.6, 128.9, 129.9, 130.3 (q, *J* = 33.3 Hz), 135.8, 141.4 (d, *J* = 1.1 Hz), 162.2

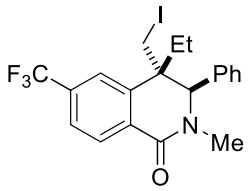
IR (thin film, cm^{-1}): 3033, 2969, 2939, 1649, 1616, 1581, 1487, 1454, 1333, 1248, 1126, 1095, 909, 728.

HRMS (DART, M+H): Calc. for $C_{20}H_{20}IF_3ON$ 474.0536, found 474.0539.

m.p: 173-177 °C

***anti* and *syn*-1g:**

***anti* and *syn*-1g** were synthesized by **General Procedure 1(a-d)** on a 3.91 mmol scale giving roughly a 1.7:1 d.r (anti:syn) of the alkyl iodides. Each diastereomer was Isolated by flash column chromatography using 2:1 Pentane:EtOAc, each followed by 3 rounds of trituration using pentanes in a sonicator to yield white solids. **syn-1f** (top spot) was obtained in a 4.9% yield (0.19 mmol, 90.0 mg) while **anti-1f** (bottom spot) was obtained in a 5.1% yield (0.20 92.1 mg).



anti-4-ethyl-4-(iodomethyl)-2-methyl-3-phenyl-6-(trifluoromethyl)-3,4-dihydroisoquinolin-1(2H)-one

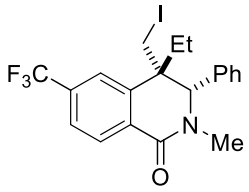
^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.93 (t, *J* = 7.4 Hz, 3H), 1.49 (tdd, *J* = 14.8, 7.4, 0.9 Hz, 1H), 2.00 (dq, *J* = 14.7, 7.3 Hz, 1H), 3.06 (s, 3H), 3.56 (dd, *J* = 10.3, 0.9 Hz, 1H), 3.71 (d, *J* = 10.4 Hz, 1H), 4.52 (s, 1H), 6.76 – 6.96 (m, 2H), 7.18 (dd, *J* = 8.2, 6.9 Hz, 2H), 7.25 (tt, *J* = 6.7, 1.3 Hz, 1H), 7.52 (d, *J* = 1.7 Hz, 1H), 7.65 – 7.95 (m, 1H), 8.29 – 8.47 (m, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 8.1, 18.4, 26.2, 34.3, 43.4, 69.9, 123.3 (q, *J* = 3.8 Hz), 123.6 (q, *J* = 272.9 Hz), 124.9 (q, *J* = 3.7 Hz), 127.9, 128.7, 128.8, 129.3, 132.0 (d, *J* = 1.4 Hz), 133.4 (q, *J* = 32.5 Hz), 136.3, 140.7, 162.0.

IR (thin film, cm^{-1}): 3031, 2972, 2943, 1652, 1601, 1495, 1452, 1329, 1255, 1127, 898, 730, 699.

HRMS (DART, M+H): Calc. for $C_{20}H_{20}IF_3ON$ 474.0536, found 474.0537.

m.p: 177-180 °C



syn-4-ethyl-4-(iodomethyl)-2-methyl-3-phenyl-6-(trifluoromethyl)-3,4-dihydroisoquinolin-1(2H)-one

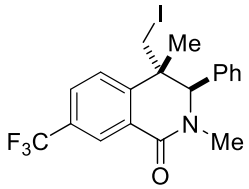
^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.64 (t, *J* = 7.4 Hz, 3H), 1.96 – 2.35 (m, 2H), 2.81 (dd, *J* = 10.3, 1.6 Hz, 1H), 3.07 (s, 3H), 3.91 (d, *J* = 10.3 Hz, 1H), 4.37 (s, 1H), 7.04 (d, *J* = 7.3 Hz, 1H), 7.12 – 7.21 (m, 2H), 7.23 – 7.30 (m, 1H), 7.36 (d, *J* = 1.6 Hz, 1H), 7.64 – 7.98 (m, 1H), 8.36 (d, *J* = 8.0 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 7.5, 11.4, 33.5, 34.4, 43.6, 72.1, 122.54 (q, *J* = 272.9 Hz), 122.3 (q, *J* = 3.6 Hz), 124.7 (q, *J* = 3.6 Hz), 128.5, 128.6, 128.9, 129.4, 132.1 (d, *J* = 1.3 Hz), 133.1 (q, *J* = 32.5 Hz), 135.7, 138.5, 162.3.
IR (thin film, cm^{-1}): 3034,2967,2937, 1650, 1578, 1325, 1158, 1128, 1079, 700

HRMS (DART, M+H): Calc. for $C_{20}H_{20}IF_3ON$ 474.0536, found 474.0541.

m.p: 107-110 °C

***anti*-1h:**



anti-4-(iodomethyl)-2,4-dimethyl-3-phenyl-7-(trifluoromethyl)-3,4-dihydroisoquinolin-1(2H)-one

***anti* 1h** were synthesized by **General Procedure 1(a-d)** on a 2 mmol scale giving roughly a 5:1 d.r (anti:syn) of the alkyl iodides. Isolated by flash column chromatography using 12:8:1 Pentane:DCM:EtOAc yielding a white solid (Yield: 17%, 0.34 mmol, 158.2 mg).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 1.26 (s, 3H), 3.09 (s, 3H), 3.34 (d, *J* = 10.3 Hz, 1H), 3.75 (d, *J* = 9.4 Hz, 1H), 4.64 (s, 1H), 6.89 (d, *J* = 6.8 Hz, 2H), 7.06 – 7.27 (m, 3H), 7.34 (d, *J* = 7.7 Hz, 1H), 7.72 (ddd, *J* = 8.1, 2.0, 0.8 Hz, 1H), 8.40 – 8.56 (m, 1H).

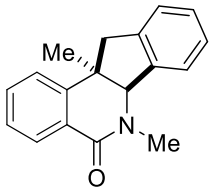
^{13}C NMR (126 MHz, Chloroform-*d*) δ 21.2, 22.9, 34.4, 41.2, 70.6, 123.6 (q, *J* = 272.5 Hz), 125.7 (q, *J* = 3.8 Hz), 126.0, 127.8, 128.6, 128.6, 129.0 (q, *J* = 3.6 Hz), 129.6, 130.7 (q, *J* = 33.2 Hz), 135.9, 142.7 (d, *J* = 1.4 Hz), 162.0.

IR (thin film, cm^{-1}): 3071, 3027, 2964, 2919, 2878, 1650, 1595, 1460, 1315, 1293, 1177, 1092, 908.

HRMS (DART, M+H): Calc. for $C_{19}H_{18}IF_3O$ 460.0380, found 460.0378.

m.p: 115-118 °C

Products



2a: 6,11a-dimethyl-6,6a,11,11a-tetrahydro-5H-indeno[1,2-c]isoquinolin-5-one

2a was synthesized according to **General Procedure 2** using 30 mol% catalyst. Isolated by flash column chromatography using 2:1 Pentane:EtOAc yielding a white solid. From 1:1 ***syn*-1a:*anti*-1a** mix (0.1 mmol scale, base = Cs_2CO_3), Yield: 58%, 0.058 mmol, 15.1 mg, >20:1 d.r. From just ***anti*-1a** (0.1 mmol scale, base = K_2CO_3) Yield: 45% yield, 0.045mmol, 11.8 mg, >20:1 d.r. From just ***syn*-1a** (0.1 mmol scale, base = K_2CO_3) Yield: 79% yield, 0.079mmol, 20.8 mg, >20:1 d.r

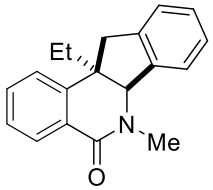
^{1}H NMR (500 MHz, Chloroform-*d*) δ 1.57 (s, 3H), 3.10 (dd, *J* = 15.4, 1.0 Hz, 1H), 3.52 (s, 3H), 3.56 (d, *J* = 15.5 Hz, 1H), 4.64 (s, 1H), 7.08 – 7.14 (m, 3H), 7.23 (m, 2H), 7.35 – 7.42 (m, 2H), 8.05 (dd, *J* = 7.8, 1.0 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 27.2, 36.8, 44.2, 48.7, 72.5, 123.0, 124.4, 124.9, 126.8, 126.9, 127.9, 128.2, 128.3, 132.0, 140.0, 142.6, 143.8, 163.3.

IR (thin film, cm^{-1}): 3036, 2954, 2922, 2852, 1645, 1601, 1575, 1468, 1457, 1376, 1267, 1155, 1099, 889, 700.

HRMS (ESI, M+H): Calc. for $C_{18}H_{18}NO$ 264.1388, found 648.1388.

m.p: 130-136 °C



2b: 11a-ethyl-6-methyl-6,6a,11,11a-tetrahydro-5H-indeno[1,2-c]isoquinolin-5-one

2b was synthesized according to **General Procedure 2** using 10 mol% catalyst and Cs_2CO_3 as the base. Isolated by flash column chromatography using 2:1 Pentane:EtOAc yielding a white solid. From 1:1 ***syn*-1b:*anti*-1b** mix (0.08 mmol scale), Yield: 72%, 0.058 mmol, 15.9 mg, >20:1 d.r. From just ***anti*-1b** (0.1 mmol) Yield:73%, 0.073 mmol, 20.2 mg, >20:1 d.r.

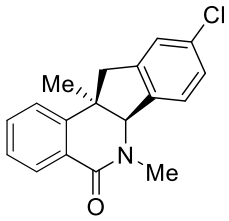
^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.89 (t, *J* = 7.5 Hz, 3H), 1.86 – 2.06 (m, 2H), 3.11 (d, *J* = 15.5 Hz, 1H), 3.52 (d, *J* = 15.3 Hz, 1zH), 3.52 (s, 3H), 4.72 (s, 1H), 7.05 – 7.14 (m, 3H), 7.19 – 7.26 (m, 2H), 7.33 – 7.43 (m, 2H), 8.06 (dd, *J* = 7.7, 1.4 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 9.7, 34.1, 36.7, 42.4, 52.8, 71.1, 122.6, 124.3, 125.7, 126.8, 126.9, 127.8, 128.2, 129.3, 131.6, 139.6, 141.9, 142.8, 163.3.

IR (thin film, cm^{-1}): 3066, 3025, 2962, 2923, 2852, 1636, 1598, 1490, 1459, 1332, 1261, 804, 733.

HRMS (ESI, M+H): Calc. for $C_{19}H_{20}NO$ 278.1545, found 278.1539.

m.p: 137-142 °C



2c: (6aS,11aR)-9-chloro-6,11a-dimethyl-6,6a,11,11a-tetrahydro-5H-indeno[1,2-c]isoquinolin-5-one

2c was synthesized according to **General Procedure 2** using 30 mol% catalyst and Cs_2CO_3 as the base using the enantioenriched starting material. Isolated by flash column chromatography using 2:1 Pentane:EtOAc yielding a white solid. From **lin-1c** mix (0.1 mmol scale), Yield: 75%, 0.075 mmol, 22.3 mg, >20:1 d.r, 99.5:0.5 e.r. From just ***anti*-1e** (0.1 mmol) Yield: 47%, 0.047 mmol, 14.1 mg, >20:1 d.r, 99.5:0.5 e.r.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 1.57 (s, 3H), 3.08 (dd, *J* = 15.6, 1.1 Hz, 1H), 3.50 (s, 3H), 3.52 (d, *J* = 15.6 Hz, 1H), 4.59 (s, 1H), 7.08 (d, *J* = 7.2 Hz, 2H), 7.15 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.21 – 7.27 (m, 1H), 7.38 – 7.47 (m, 1H), 8.05 (dd, *J* = 7.7, 1.3 Hz, 1H).

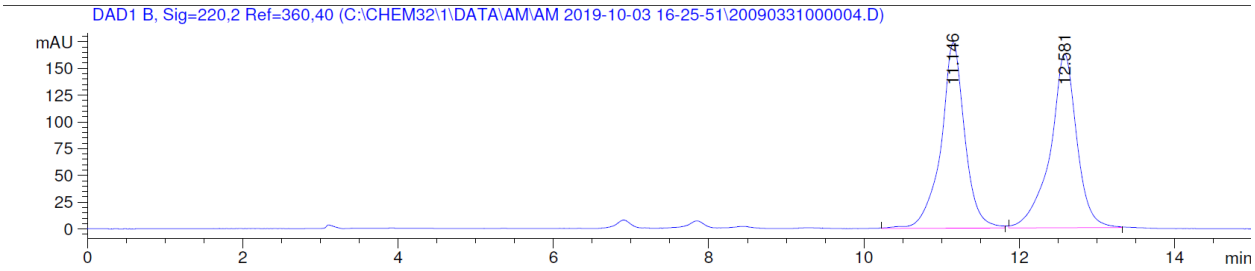
^{13}C NMR (126 MHz, Chloroform-*d*) δ 27.0, 36.7, 43.9, 49.1, 71.9, 124.1, 124.7, 124.9, 127.0, 127.1, 128.1, 128.4, 132.2, 133.6, 141.2, 141.9, 143.3, 163.2.

IR (thin film, cm^{-1}): 3050, 2954, 2921, 2863, 1645, 1600, 1467, 1327, 1264, 1066, 883, 770.

HRMS (DART, M+H): Calc. for $C_{18}H_{17}ClNO$ 298.0993, found 298.0998.

m.p: 187-194 °C

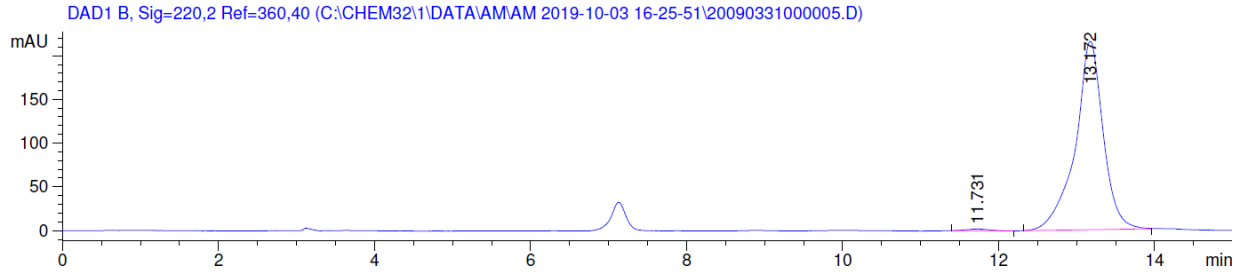
Enantiomeric purity was determined by HPLC analysis. T_{R1} = 11.46 T_{R2} =12.58 (99.5:0.5 e.r; Chiralcel IA column, 10% iPrOH in hexanes 1 mL/min, 220nm). In both cases, the same enantiomer of compound **2c** was observed, as indicated in the below HPLC traces.



Signal 2: DAD1 B, Sig=220,2 Ref=360,40

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.146	BB	0.3053	3691.79663	173.44479	49.0055
2	12.581	BB	0.3421	3841.63672	162.30217	50.9945
Totals :				7533.43335	335.74696	

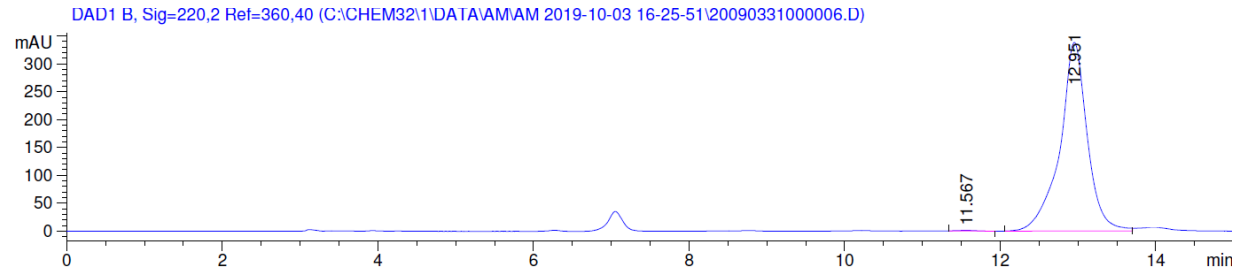
From *lin*-1c



Signal 2: DAD1 B, Sig=220,2 Ref=360,40

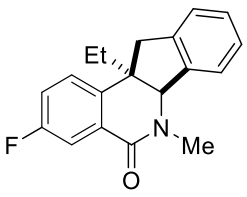
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.731	BB	0.2396	40.12095	2.06530	0.7455
2	13.172	BB	0.3573	5341.78271	215.43042	99.2545
Totals :				5381.90366	217.49572	

From *anti*-1c



Signal 2: DAD1 B, Sig=220,2 Ref=360,40

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.567	BB	0.1876	15.56489	1.00530	0.1876
2	12.951	BB	0.3517	8280.71094	338.19363	99.8124
Totals :				8296.27583	339.19893	



2d: 11a-ethyl-3-fluoro-6-methyl-6,6a,11,11a-tetrahydro-5H-indeno[1,2-c]isoquinolin-5-one

2d was synthesized according to **General Procedure 2** using 10 mol% catalyst and Cs_2CO_3 as the base. Isolated by flash column chromatography using 2:1 Pentane:EtOAc yielding a white solid. From 1:1 ***syn*-1d:*anti*-1d** mix (0.1 mmol scale), Yield: 74%, 0.074 mmol, 21.7 mg, >20:1 d.r. From just ***anti*-1d** (0.1 mmol) Yield: 65%, 0.065 mmol, 19.2 mg, >20:1 d.r.

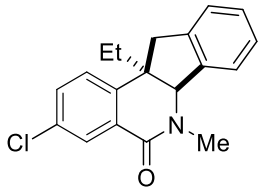
^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.89 (t, *J* = 7.5 Hz, 3H), 1.83 – 2.05 (m, 2H), 3.11 (d, *J* = 15.4 Hz, 1H), 3.47 (d, *J* = 15.5 Hz, 1H), 3.52 (s, 3H), 4.71 (s, 1H), 7.01 – 7.15 (m, 4H), 7.19 – 7.24 (m, 1H), 7.34 (dd, *J* = 8.7, 5.1 Hz, 1H), 7.73 (dd, *J* = 9.4, 2.9 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 9.7, 34.0, 36.7, 42.5, 52.6, 71.2, 114.7 (d, *J* = 23.0 Hz), 118.8 (d, *J* = 21.9 Hz), 122.6, 124.4, 127.0, 127.7 (d, *J* = 7.5 Hz), 128.0, 131.3 (d, *J* = 7.4 Hz), 137.6 (d, *J* = 3.2 Hz), 139.3, 142.5, 161.6 (d, *J* = 245.6 Hz), 162.2 (d, *J* = 2.5 Hz).

IR (thin film, cm^{-1}): 3072, 2964, 2920, 2878, 1648, 1612, 1482, 1460, 1302, 1268, 1100, 887, 774.

HRMS (DART, M+H): Calc. for $C_{19}H_{19}FNO$ 296.1445, found 296.1448

m.p: 133-135 °C



2e: 3-chloro-11a-ethyl-6-methyl-6,6a,11,11a-tetrahydro-5H-indeno[1,2-c]isoquinolin-5-one

2e was synthesized according to **General Procedure 2** using 10 mol% catalyst and Cs_2CO_3 as the base. Isolated by flash column chromatography using 2:1 Pentane:EtOAc yielding a white solid. From 1:1 ***syn*-1e:*anti*-1e** mix (0.1 mmol scale), Yield: 73%, 0.073 mmol, 22.7 mg, >20:1 d.r. From just ***anti*-1e** (0.065 mmol) Yield: 77%, 0.050 mmol, 15.6 mg, >20:1 d.r.

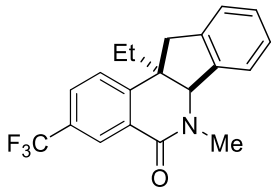
^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.88 (t, *J* = 7.5 Hz, 3H), 1.82 – 2.10 (m, 2H), 3.10 (dd, *J* = 15.5, 1.2 Hz, 1H), 3.45 (d, *J* = 15.5 Hz, 1H), 3.51 (s, 3H), 4.71 (t, *J* = 0.8 Hz, 1H), 7.06 – 7.15 (m, 3H), 7.17 – 7.25 (m, 1H), 7.28 – 7.36 (m, 2H), 8.03 (d, *J* = 2.3 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 9.7, 33.8, 36.8, 42.3, 52.7, 71.1, 122.6, 124.4, 127.1, 127.5, 128.0, 128.1, 130.9, 131.6, 133.0, 139.3, 140.4, 142.5, 162.1.

IR (thin film, cm^{-1}): 3070, 3027, 2964, 2918, 2872, 1649, 1595, 1460, 1315, 1261, 1092, 908, 759.

HRMS (DART, M+H): Calc. for $C_{19}H_{19}ClNO$ 312.1150, found 312.1150.

m.p: 129-134 °C



2f: 11a-ethyl-6-methyl-3-(trifluoromethyl)-6,6a,11,11a-tetrahydro-5H-indeno[1,2-c]isoquinolin-5-one

2f was synthesized according to **General Procedure 2** using 10 mol% catalyst and Cs_2CO_3 as the base. Isolated by flash column chromatography using 2:1 Pentane:EtOAc yielding a white solid. From 1:1 ***syn*-1f:*anti*-1f** mix (0.1 mmol scale), Yield: 95%, 0.095 mmol, 32.6 mg, >20:1 d.r. From just ***anti*-1f** (0.1 mmol) Yield: 94%, 0.094 mmol, 32.4 mg, >20:1 d.r.

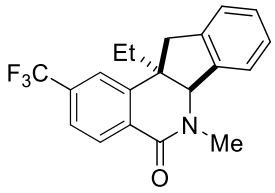
^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.90 (t, *J* = 7.5 Hz, 3H), 1.98 (qd, *J* = 7.5, 5.0 Hz, 2H), 3.16 (d, *J* = 15.5 Hz, 1H), 3.52 (d, *J* = 15.6 Hz, 1H), 3.54 (s, 3H), 4.76 (s, 1H), 7.05 – 7.16 (m, 3H), 7.20 – 7.25 (m, 1H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.63 (ddd, *J* = 8.2, 2.2, 0.7 Hz, 1H), 8.29 – 8.38 (m, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 9.7, 33.8, 36.8, 42.3, 53.1, 70.9, 122.6, 123.7 (q, *J* = 272.3 Hz), 124.4, 125.5 (q, *J* = 3.9 Hz), 126.5, 127.2, 128.0 (q, *J* = 3.6 Hz), 128.1, 129.4 (q, *J* = 33.1 Hz), 129.9, 139.1, 142.3, 145.9 (d, *J* = 1.3 Hz), 162.0.

IR (thin film, cm^{-1}): 3073, 2965, 2922, 2879, 2854, 1651, 1579, 1459, 1333, 1258, 1094, 961, 807, 722.

HRMS (DART, M+H): Calc. for $C_{20}H_{19}F_3ON$ 346.1413, found 346.1420.

m.p: 185-188 °C



2g: 11a-ethyl-6-methyl-2-(trifluoromethyl)-6,6a,11,11a-tetrahydro-5H-indeno[1,2-c]isoquinolin-5-one

2g was synthesized according to **General Procedure 2** using 10 mol% catalyst and Cs_2CO_3 as the base. Isolated by flash column chromatography using 2:1 Pentane:EtOAc yielding a white solid. From just ***anti*-1g** (0.076 mmol) Yield: 86%, 0.065 mmol, 22.8 mg.

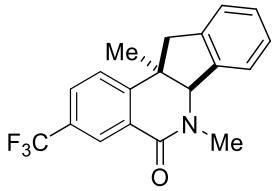
^{1}H NMR (500 MHz, Chloroform-*d*) δ 0.90 (t, *J* = 7.5 Hz, 3H), 1.99 (qd, *J* = 7.5, 4.8 Hz, 2H), 3.17 (d, *J* = 15.6 Hz, 1H), 3.51 (d, *J* = 15.6 Hz, 1H), 3.54 (s, 3H), 4.77 (s, 1H), 7.09 – 7.19 (m, 3H), 7.23 (ddt, *J* = 5.7, 4.5, 2.3 Hz, 1H), 7.49 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.61 (d, *J* = 1.7 Hz, 1H), 8.18 (d, *J* = 8.2 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 9.7, 33.9, 36.8, 42.4, 52.9, 70.9, 122.6, 122.7 (q, *J* = 3.9 Hz), 123.8 (q, *J* = 3.7 Hz), 124.5, 120.3 – 127.1 (m), 127.2, 128.1, 129.0, 132.2 (d, *J* = 1.3 Hz), 133.2 (q, *J* = 32.3 Hz), 139.0, 142.2, 143.0, 162.0.

IR (thin film, cm^{-1}): 3047, 2967, 2923, 2854, 1657, 1579, 1461, 1332, 1259, 1168, 1080, 900, 745.

HRMS (DART, M+H): Calc. for $C_{20}H_{19}F_3ON$ 346.1413, found 346.1414.

m.p: 147-151 °C



2h: 6,11a-dimethyl-3-(trifluoromethyl)-6,6a,11,11a-tetrahydro-5H-indeno[1,2-c]isoquinolin-5-one

2h was synthesized according to **General Procedure 2** using 10 mol% catalyst and Cs_2CO_3 as the base. Isolated by flash column chromatography using 2:1 Pentane:EtOAc yielding a white solid. From just ***anti*-1h** (0.1 mmol) Yield: 47%, 0.047 mmol, 15.5 mg, >20:1 d.r.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 1.59 (s, 3H), 3.16 (d, *J* = 15.5 Hz, 1H), 3.54 (s, 3H), 3.57 (d, *J* = 15.6 Hz, 1H), 4.69 (s, 1H), 6.97 – 7.19 (m, 3H), 7.20 – 7.33 (m, 1H), 7.54 (d, *J* = 8.2 Hz, 1H), 7.64 (dd, *J* = 8.2, 2.1 Hz, 1H), 8.18 – 8.41 (m, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 26.9, 36.9, 44.1, 49.0, 72.3, 123.0, 123.7 (q, *J* = 272.2 Hz), 124.4, 125.6 (q, *J* = 3.8 Hz), 125.8, 127.2, 128.2, 128.5 (q, *J* = 3.6 Hz), 128.9, 129.4 (q, *J* = 33.1 Hz), 139.4, 142.1, 147.7 (d, *J* = 1.3 Hz), 162.0.

IR (thin film, cm^{-1}): 3045, 2960, 2925, 1654, 1619, 1491, 1459, 1333, 1252, 1164, 1113, 982, 759.

HRMS (DART, M+H): Calc. for $C_{20}H_{19}F_3ON$ 346.1413, found 346.1420.

m.p: 184-188 °C

X-Ray Data

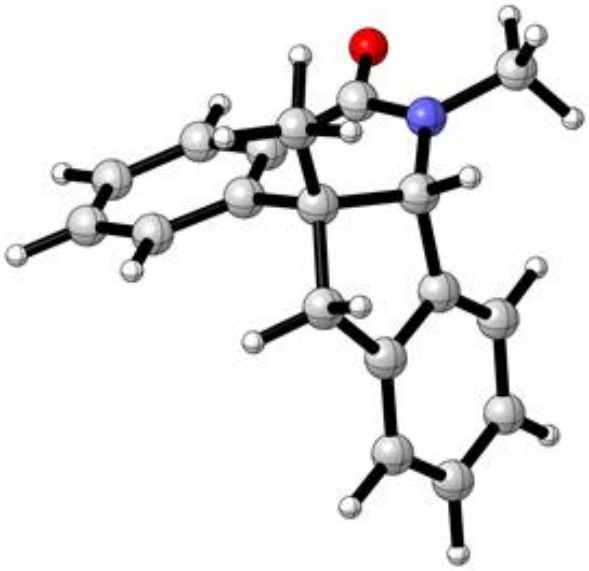


Table 1. Crystal data and structure refinement for d19121a_a.

Identification code	d19121a_a
Empirical formula	C18 H18 N O1.50
Formula weight	272.33
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 17.6395(11) Å a= 90°.
	b = 11.2890(7) Å b= 120.080(2)°.
	c = 16.5674(15) Å g = 90°.
Volume	2854.8(4) Å3
Z	8
Density (calculated)	1.267 Mg/m3
Absorption coefficient	0.080 mm-1
F(000)	1160

Crystal size	0.180 x 0.170 x 0.120 mm3
Theta range for data collection	2.244 to 27.523°.
Index ranges	-22<=h<=22, -14<=k<=14, -17<=l<=21
Reflections collected	17327
Independent reflections	3289 [R(int) = 0.0444]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.7012
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	3289 / 0 / 190
Goodness-of-fit on F2	1.005
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.1151
R indices (all data)	R1 = 0.1047, wR2 = 0.1507
Extinction coefficient	0.0021(5)
Largest diff. peak and hole	0.293 and -0.262 e.Å-3

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for d19121a_a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	6173(1)	8084(1)	2944(1)	44(1)
N(1)	5832(1)	7014(1)	1654(1)	34(1)
C(1)	6879(1)	5443(2)	1699(1)	38(1)
C(2)	7280(1)	5483(2)	2756(1)	34(1)
C(3)	7973(1)	4754(2)	3349(1)	47(1)
C(4)	8339(2)	4825(2)	4307(1)	52(1)
C(5)	8022(1)	5631(2)	4695(1)	45(1)
C(6)	7356(1)	6381(2)	4123(1)	37(1)
C(7)	6983(1)	6319(2)	3154(1)	31(1)
C(8)	6292(1)	7197(2)	2580(1)	32(1)
C(9)	5930(1)	5927(2)	1240(1)	33(1)
C(10)	5112(1)	7810(2)	1065(1)	42(1)
C(11)	7458(1)	6124(2)	1416(1)	51(1)
C(12)	5411(1)	4874(2)	1269(1)	36(1)
C(13)	4620(1)	4842(2)	1256(1)	41(1)
C(14)	4275(2)	3754(2)	1294(1)	54(1)
C(15)	4720(2)	2718(2)	1351(1)	62(1)
C(16)	5517(2)	2750(2)	1367(1)	56(1)
C(17)	5862(1)	3836(2)	1327(1)	43(1)
C(18)	6699(1)	4142(2)	1342(1)	50(1)
O(1W)	5000	10055(2)	2500	79(1)

Table 3. Bond lengths [Å] and angles [°] for d19121a_a.

O(1)-C(8)	1.240(2)
N(1)-C(8)	1.344(2)
N(1)-C(9)	1.458(2)
N(1)-C(10)	1.460(2)
C(1)-C(2)	1.525(2)
C(1)-C(11)	1.528(3)
C(1)-C(9)	1.550(3)
C(1)-C(18)	1.556(3)
C(2)-C(3)	1.390(3)
C(2)-C(7)	1.396(2)
C(3)-C(4)	1.384(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.383(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.371(3)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.398(2)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.486(3)
C(9)-C(12)	1.517(3)
C(9)-H(9A)	1.0000
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(10)-H(10D)	0.9800
C(10)-H(10E)	0.9800
C(10)-H(10F)	0.9800

C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(13)	1.384(3)
C(12)-C(17)	1.393(3)
C(13)-C(14)	1.386(3)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.385(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.393(4)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.385(3)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.504(3)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
O(1W)-H(1W)	0.8400
O(1W)-H(1W)#1	0.8400

C(8)-N(1)-C(9)	121.35(14)
C(8)-N(1)-C(10)	119.62(15)
C(9)-N(1)-C(10)	118.17(14)
C(2)-C(1)-C(11)	109.91(16)
C(2)-C(1)-C(9)	108.60(14)
C(11)-C(1)-C(9)	113.31(16)
C(2)-C(1)-C(18)	110.68(16)
C(11)-C(1)-C(18)	113.50(16)
C(9)-C(1)-C(18)	100.47(15)
C(3)-C(2)-C(7)	118.13(16)

C(3)-C(2)-C(1) 122.15(17)

C(7)-C(2)-C(1) 119.61(16)

C(4)-C(3)-C(2) 121.06(19)

C(4)-C(3)-H(3A) 119.5

C(2)-C(3)-H(3A) 119.5

C(5)-C(4)-C(3) 120.42(19)

C(5)-C(4)-H(4A) 119.8

C(3)-C(4)-H(4A) 119.8

C(6)-C(5)-C(4) 119.41(17)

C(6)-C(5)-H(5A) 120.3

C(4)-C(5)-H(5A) 120.3

C(5)-C(6)-C(7) 120.64(18)

C(5)-C(6)-H(6A) 119.7

C(7)-C(6)-H(6A) 119.7

C(2)-C(7)-C(6) 120.28(17)

C(2)-C(7)-C(8) 122.01(15)

C(6)-C(7)-C(8) 117.68(16)

O(1)-C(8)-N(1) 121.77(17)

O(1)-C(8)-C(7) 120.76(16)

N(1)-C(8)-C(7) 117.42(15)

N(1)-C(9)-C(12) 115.34(14)

N(1)-C(9)-C(1) 114.81(14)

C(12)-C(9)-C(1) 103.24(15)

N(1)-C(9)-H(9A) 107.7

C(12)-C(9)-H(9A) 107.7

C(1)-C(9)-H(9A) 107.7

N(1)-C(10)-H(10A) 109.5

N(1)-C(10)-H(10B) 109.5

H(10A)-C(10)-H(10B) 109.5

N(1)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(1)-C(10)-H(10D)	109.5
H(10A)-C(10)-H(10D)	141.1
H(10B)-C(10)-H(10D)	56.3
H(10C)-C(10)-H(10D)	56.3
N(1)-C(10)-H(10E)	109.5
H(10A)-C(10)-H(10E)	56.3
H(10B)-C(10)-H(10E)	141.1
H(10C)-C(10)-H(10E)	56.3
H(10D)-C(10)-H(10E)	109.5
N(1)-C(10)-H(10F)	109.5
H(10A)-C(10)-H(10F)	56.3
H(10B)-C(10)-H(10F)	56.3
H(10C)-C(10)-H(10F)	141.1
H(10D)-C(10)-H(10F)	109.5
H(10E)-C(10)-H(10F)	109.5
C(1)-C(11)-H(11A)	109.5
C(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(13)-C(12)-C(17)	121.06(19)
C(13)-C(12)-C(9)	129.78(18)
C(17)-C(12)-C(9)	109.15(17)
C(12)-C(13)-C(14)	119.0(2)
C(12)-C(13)-H(13A)	120.5

C(14)-C(13)-H(13A)	120.5
C(15)-C(14)-C(13)	120.3(2)
C(15)-C(14)-H(14A)	119.9
C(13)-C(14)-H(14A)	119.9
C(14)-C(15)-C(16)	120.8(2)
C(14)-C(15)-H(15A)	119.6
C(16)-C(15)-H(15A)	119.6
C(17)-C(16)-C(15)	119.1(2)
C(17)-C(16)-H(16A)	120.5
C(15)-C(16)-H(16A)	120.5
C(16)-C(17)-C(12)	119.8(2)
C(16)-C(17)-C(18)	130.9(2)
C(12)-C(17)-C(18)	109.27(18)
C(17)-C(18)-C(1)	103.59(15)
C(17)-C(18)-H(18A)	111.0
C(1)-C(18)-H(18A)	111.0
C(17)-C(18)-H(18B)	111.0
C(1)-C(18)-H(18B)	111.0
H(18A)-C(18)-H(18B)	109.0
H(1W)-O(1W)-H(1W)#1	99.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2

Table 4. Anisotropic displacement parameters (Å2x 103) for d19121a_a. The anisotropic displacement factor exponent takes the form: -2p2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	40(1)	45(1)	42(1)	-14(1)	18(1)	2(1)
N(1)	31(1)	37(1)	30(1)	-3(1)	12(1)	5(1)
C(1)	32(1)	48(1)	29(1)	-7(1)	11(1)	8(1)
C(2)	31(1)	38(1)	28(1)	-5(1)	10(1)	0(1)
C(3)	42(1)	50(1)	36(1)	-4(1)	10(1)	11(1)
C(4)	46(1)	52(1)	36(1)	3(1)	5(1)	8(1)
C(5)	46(1)	54(1)	26(1)	-1(1)	10(1)	-9(1)
C(6)	37(1)	43(1)	28(1)	-7(1)	14(1)	-9(1)
C(7)	27(1)	36(1)	27(1)	-4(1)	10(1)	-6(1)
C(8)	30(1)	36(1)	32(1)	-7(1)	17(1)	-4(1)
C(9)	32(1)	40(1)	23(1)	-4(1)	10(1)	6(1)
C(10)	37(1)	46(1)	38(1)	1(1)	14(1)	10(1)
C(11)	35(1)	82(2)	36(1)	-5(1)	18(1)	5(1)
C(12)	36(1)	41(1)	21(1)	-4(1)	7(1)	1(1)
C(13)	40(1)	48(1)	27(1)	-2(1)	12(1)	-2(1)
C(14)	56(1)	67(2)	31(1)	-2(1)	16(1)	-16(1)
C(15)	85(2)	53(2)	31(1)	-2(1)	16(1)	-21(1)
C(16)	75(2)	40(1)	29(1)	-3(1)	7(1)	5(1)
C(17)	46(1)	42(1)	24(1)	-7(1)	4(1)	5(1)
C(18)	44(1)	55(1)	33(1)	-13(1)	8(1)	16(1)
O(1W)	98(2)	38(1)	112(2)	0	61(2)	0

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3) for d19121a_a.

	x	y	z	U(eq)
H(3A)	8199	4198	3093	56
H(4A)	8810	4317	4700	62
H(5A)	8263	5663	5352	54
H(6A)	7147	6950	4387	44
H(9A)	5732	6096	570	40
H(10A)	5334	8623	1141	64
H(10B)	4663	7771	1246	64
H(10C)	4857	7571	411	64
H(10D)	4569	7354	724	64
H(10E)	5240	8205	619	64
H(10F)	5045	8406	1455	64
H(11A)	7504	6952	1613	76
H(11B)	7199	6089	737	76
H(11C)	8043	5767	1717	76
H(13A)	4319	5555	1221	49
H(14A)	3731	3719	1281	65
H(15A)	4478	1978	1379	74
H(16A)	5819	2037	1406	67
H(18A)	6625	4083	710	59
H(18B)	7182	3613	1769	59
H(1W)	5409	9572	2636	118

Table 6. Torsion angles [°] for d19121a_a.

C(11)-C(1)-C(2)-C(3)	-79.0(2)
C(9)-C(1)-C(2)-C(3)	156.56(19)
C(18)-C(1)-C(2)-C(3)	47.2(3)
C(11)-C(1)-C(2)-C(7)	97.3(2)
C(9)-C(1)-C(2)-C(7)	-27.2(2)
C(18)-C(1)-C(2)-C(7)	-136.57(18)
C(7)-C(2)-C(3)-C(4)	2.2(3)
C(1)-C(2)-C(3)-C(4)	178.53(19)
C(2)-C(3)-C(4)-C(5)	-0.2(3)
C(3)-C(4)-C(5)-C(6)	-1.7(3)
C(4)-C(5)-C(6)-C(7)	1.6(3)
C(3)-C(2)-C(7)-C(6)	-2.4(3)
C(1)-C(2)-C(7)-C(6)	-178.76(17)
C(3)-C(2)-C(7)-C(8)	175.32(18)
C(1)-C(2)-C(7)-C(8)	-1.1(3)
C(5)-C(6)-C(7)-C(2)	0.5(3)
C(5)-C(6)-C(7)-C(8)	-177.28(17)
C(9)-N(1)-C(8)-O(1)	-175.35(16)
C(10)-N(1)-C(8)-O(1)	-6.1(3)
C(9)-N(1)-C(8)-C(7)	7.2(2)
C(10)-N(1)-C(8)-C(7)	176.45(16)
C(2)-C(7)-C(8)-O(1)	-164.06(17)
C(6)-C(7)-C(8)-O(1)	13.7(3)
C(2)-C(7)-C(8)-N(1)	13.4(3)
C(6)-C(7)-C(8)-N(1)	-168.88(16)
C(8)-N(1)-C(9)-C(12)	81.8(2)
C(10)-N(1)-C(9)-C(12)	-87.51(19)

C(8)-N(1)-C(9)-C(1)	-38.0(2)
C(10)-N(1)-C(9)-C(1)	152.61(16)
C(2)-C(1)-C(9)-N(1)	45.5(2)
C(11)-C(1)-C(9)-N(1)	-76.9(2)
C(18)-C(1)-C(9)-N(1)	161.71(15)
C(2)-C(1)-C(9)-C(12)	-80.85(17)
C(11)-C(1)-C(9)-C(12)	156.73(15)
C(18)-C(1)-C(9)-C(12)	35.32(17)
N(1)-C(9)-C(12)-C(13)	30.0(3)
C(1)-C(9)-C(12)-C(13)	156.07(18)
N(1)-C(9)-C(12)-C(17)	-149.31(15)
C(1)-C(9)-C(12)-C(17)	-23.26(18)
C(17)-C(12)-C(13)-C(14)	-0.4(3)
C(9)-C(12)-C(13)-C(14)	-179.70(17)
C(12)-C(13)-C(14)-C(15)	0.4(3)
C(13)-C(14)-C(15)-C(16)	-0.2(3)
C(14)-C(15)-C(16)-C(17)	0.0(3)
C(15)-C(16)-C(17)-C(12)	-0.1(3)
C(15)-C(16)-C(17)-C(18)	179.29(18)
C(13)-C(12)-C(17)-C(16)	0.3(3)
C(9)-C(12)-C(17)-C(16)	179.68(16)
C(13)-C(12)-C(17)-C(18)	-179.21(16)
C(9)-C(12)-C(17)-C(18)	0.19(19)
C(16)-C(17)-C(18)-C(1)	-156.5(2)
C(12)-C(17)-C(18)-C(1)	22.9(2)
C(2)-C(1)-C(18)-C(17)	79.21(18)
C(11)-C(1)-C(18)-C(17)	-156.67(16)
C(9)-C(1)-C(18)-C(17)	-35.40(18)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2

Table 7. Hydrogen bonds for d19121a_a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1W)...O(1)	0.84	2.05	2.872(2)	165.1

Symmetry transformations used to generate equivalent atoms:

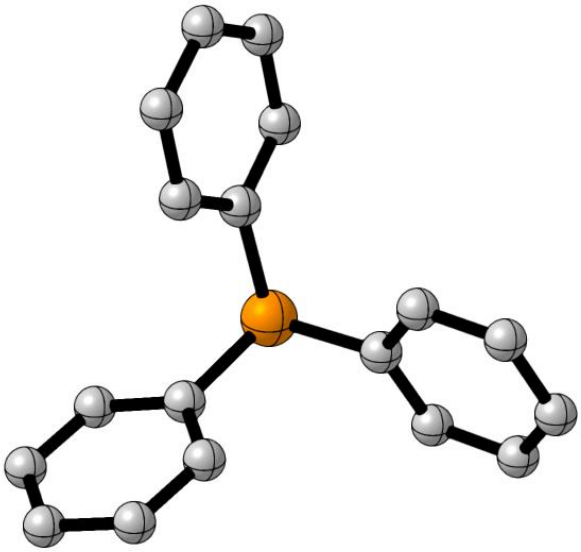
#1 -x+1,y,-z+1/2

Computational Details

The computational analyses in this manuscript were performed on the oxidative addition complex of ***anti*-1a** as a model substrate. All geometry optimizations were performed at the BP86(*4–6*) level of theory without any constraints at 298 K and 1 atm, using an ultrafine integration grid and Grimme's D3 dispersion(*7*) with Becke-Johnson damping.(*8*) The Berny algorithm was used for geometry optimizations.(*9*) The use of the standard double- ζ basis set (LANL2DZ) and its effective core potentials (ECPs)(*10–13*) were used for Pd and I. The 6-31g(d) Pople basis set was used for all other atoms (C, H, O, P, K).(*14–16*) All frequency calculations were performed at the same level of theory for all intermediates and transition states to confirm minima (no imaginary frequencies) or first order saddle points (exactly one imaginary frequency). Single-point energies were calculated at the M06L(*17*) level of theory with the addition of Grimme's D3 dispersion with the original D3 damping function. The Karlsruhe triple- ζ basis set def2-TZVPP(*18*, *19*) was used for all atoms. Solvent effects were assessed using the SMD model developed by Truhlar(*20*) using default parameters for toluene. This method has previously been shown to provide accurate results for similar systems.(*21*) Solution phase-corrected zero-point energies, enthalpies, and Gibbs free energies were obtained by adding the respective gas phase thermodynamic contributions to the single-point energies. Gibbs free energies are reported relative to **1** (the oxidative addition complex of ***anti*-1a**) and are reported in kcal mol^{-1}. The Gibbs free energies are converted to standard state by addition of 2.71 kcal mol^{-1} to all species (based on RT ln (c/c_0)(*22*) at 393.15 K). Grimme's quasi-harmonic approximation was used with a frequency cutoff value of 100 cm^{-1} to correct for the effect of small frequency vibrational modes.[23] All calculations were performed using the Gaussian16 package.[24] The images of the computed structures were created with CYLview[25] (unimportant hydrogens omitted for clarity).

Energies and Cartesian Coordinates

PPh_3



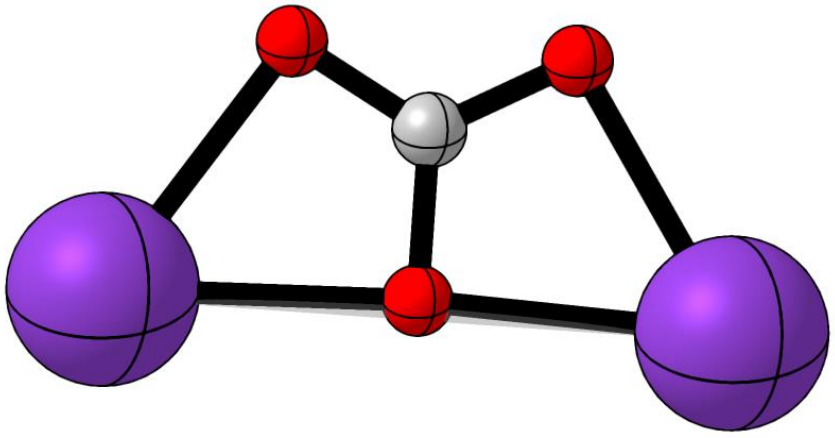
Zero-point correction = 0.266319 (Hartree/particle)
Thermal correction to energy = 0.282710
Thermal correction to enthalpy = 0.283654
Thermal correction to Gibbs free energy = 0.219336
Sum of electronic and zero-point energies = -1036.202358
Sum of electronic and thermal energies = -1036.185967
Sum of electronic and thermal enthalpies = -1036.185023
Sum of electronic and thermal free energies = -1036.249341

E_{SCF} (M06L/def2-TZVPP) = -1036.468677

15	0.000241000	-0.000303000	-1.269969000
6	1.601839000	-0.446212000	-0.442983000
6	2.345240000	-1.504496000	-1.012216000
6	2.106720000	0.201714000	0.704426000
6	3.556954000	-1.916528000	-0.437912000
1	1.969104000	-2.009895000	-1.910454000
6	3.326717000	-0.203415000	1.270027000
1	1.542867000	1.024126000	1.158054000
6	4.052555000	-1.263890000	0.703523000
1	4.119826000	-2.742361000	-0.887808000
1	3.708585000	0.310157000	2.160095000
1	5.003893000	-1.578577000	1.147399000
6	-0.414415000	1.609848000	-0.443316000
6	-1.233124000	1.724500000	0.700232000
6	0.136112000	2.781903000	-1.008994000

6	-1.492061000	2.983896000	1.265293000
1	-1.667703000	0.825806000	1.151299000
6	-0.112772000	4.037606000	-0.435311000
1	0.766258000	2.707879000	-1.903975000
6	-0.931091000	4.141774000	0.702324000
1	-2.131802000	3.058808000	2.152366000
1	0.325442000	4.937112000	-0.882821000
1	-1.134129000	5.123206000	1.145792000
6	-1.187341000	-1.164189000	-0.443630000
6	-2.477275000	-1.273750000	-1.009900000
6	-0.877401000	-1.930466000	0.700089000
6	-3.440432000	-2.116801000	-0.435991000
1	-2.727817000	-0.691759000	-1.905610000
6	-1.838806000	-2.783948000	1.265374000
1	0.118030000	-1.857671000	1.151272000
6	-3.121960000	-2.876916000	0.702164000
1	-4.438435000	-2.187673000	-0.883615000
1	-1.583939000	-3.375141000	2.152683000
1	-3.870541000	-3.543247000	1.145669000

K_2CO_3



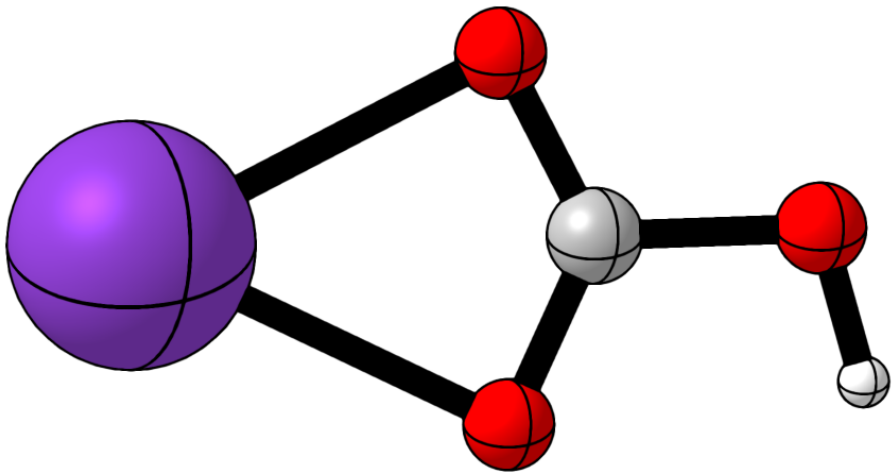
Zero-point correction = 0.016015 (Hartree/particle)
Thermal correction to energy = 0.022770
Thermal correction to enthalpy = 0.023714
Thermal correction to Gibbs free energy = -0.017105
Sum of electronic and zero-point energies = -1463.832696
Sum of electronic and thermal enthalpies = -1463.825941
Sum of electronic and thermal free energies = -1463.824997

Sum of electronic and thermal Free Energies = -1463.865816

E_{SCF} (M06L/def2-TZVPP) = -1463.848711

8	1.134062000	1.444263000	-0.049314000
8	0.000071000	-0.538104000	-0.013922000
6	-0.000365000	0.816466000	-0.003760000
8	-1.136010000	1.442847000	0.051883000
19	-2.505517000	-0.623679000	-0.006665000
19	2.506422000	-0.623207000	0.012633000

$KHCO_3$

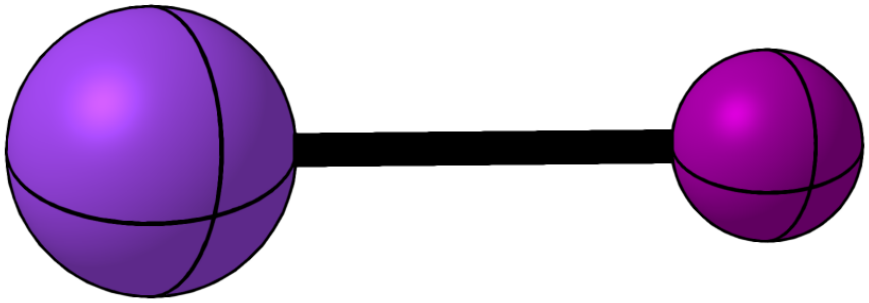


Zero-point correction = 0.027091 (Hartree/particle)
Thermal correction to energy = 0.032384
Thermal correction to enthalpy = 0.033328
Thermal correction to Gibbs free energy = -0.002630
Sum of electronic and zero-point energies = -864.460273
Sum of electronic and thermal enthalpies = -864.454980
Sum of electronic and thermal free energies = -864.454036
Sum of electronic and thermal Free Energies = -864.489994

E_{SCF} (M06L/def2-TZVPP) = -864.487364

8	2.402806000	0.086367000	0.000642000
8	0.477428000	-1.124586000	-0.000678000
6	1.007371000	0.038949000	-0.000298000
8	0.427296000	1.164674000	-0.000559000
19	-1.851128000	-0.020265000	0.000274000
1	2.666965000	-0.860293000	0.001348000

KI

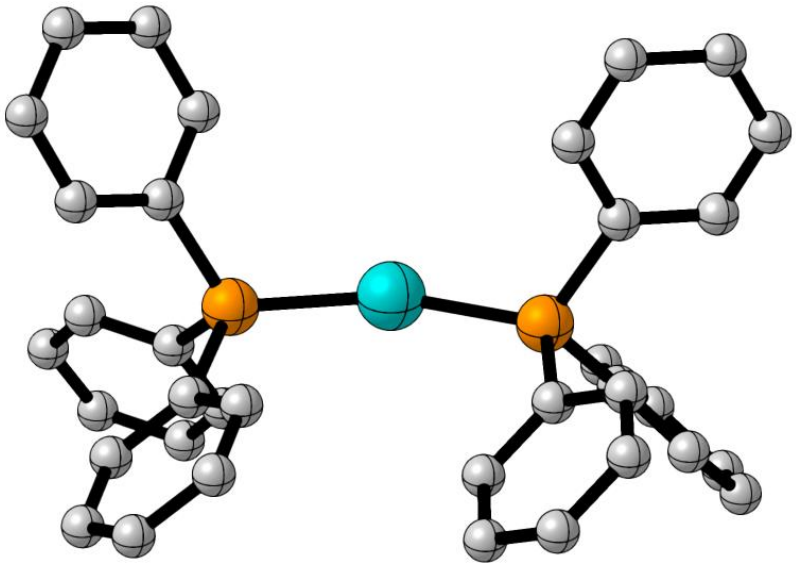


Zero-point correction = 0.000388 (Hartree/particle)
Thermal correction to energy = 0.003357
Thermal correction to enthalpy = 0.004301
Thermal correction to Gibbs free energy = -0.025121
Sum of electronic and zero-point energies = -897.887844
Sum of electronic and thermal enthalpies = -897.884875
Sum of electronic and thermal free energies = -897.883931
Sum of electronic and thermal Free Energies = -897.913353

E_{SCF} (M06L/def2-TZVPP) = -897.888232

19	0.000000000	0.000000000	-2.400154000
53	0.000000000	0.000000000	0.860432000

PdL_2 (L = PPh_3)



Zero-point correction = 0.535165 (Hartree/particle)
Thermal correction to energy = 0.571820
Thermal correction to enthalpy = 0.572765
Thermal correction to Gibbs free energy = 0.456629
Sum of electronic and zero-point energies = -2200.492686
Sum of electronic and thermal enthalpies = -2200.456031
Sum of electronic and thermal free energies = -2200.455086
Sum of electronic and thermal Free Energies = -2200.571222

E_{SCF} (M06L/def2-TZVPP) = -2201.027850

46	0.000021000	-0.000177000	-0.645273000
15	2.245612000	-0.011771000	-0.222691000
15	-2.245655000	0.011623000	-0.222851000
6	-3.259301000	-1.370366000	-0.923520000
6	-4.605777000	-1.230307000	-1.319687000
6	-2.630219000	-2.629070000	-1.047131000
6	-5.311895000	-2.334889000	-1.825124000
1	-5.102769000	-0.257510000	-1.235875000
6	-3.341205000	-3.732236000	-1.541782000
1	-1.576420000	-2.730975000	-0.756963000
6	-4.683565000	-3.586511000	-1.933867000
1	-6.356448000	-2.215267000	-2.135244000
1	-2.843598000	-4.704606000	-1.631497000
1	-5.236489000	-4.445826000	-2.330094000
6	-3.197074000	1.523418000	-0.705178000
6	-4.274000000	2.035207000	0.049177000
6	-2.815791000	2.177041000	-1.897074000
6	-4.963556000	3.177556000	-0.389627000

1	-4.570237000	1.542473000	0.982024000
6	-3.511965000	3.312751000	-2.337408000
1	-1.962955000	1.791296000	-2.470086000
6	-4.586539000	3.815600000	-1.583322000
1	-5.796369000	3.570850000	0.204701000
1	-3.208393000	3.812341000	-3.264446000
1	-5.124417000	4.708575000	-1.921557000
6	-2.567230000	-0.123147000	1.598722000
6	-3.650526000	-0.846023000	2.140858000
6	-1.669828000	0.531814000	2.471443000
6	-3.831749000	-0.909777000	3.533063000
1	-4.349751000	-1.365432000	1.476245000
6	-1.857150000	0.471686000	3.860002000
1	-0.810522000	1.069338000	2.051738000
6	-2.937975000	-0.251936000	4.394333000
1	-4.673188000	-1.479282000	3.944448000
1	-1.147509000	0.978851000	4.523325000
1	-3.079528000	-0.308528000	5.479716000
6	3.259002000	1.370579000	-0.923061000
6	2.629656000	2.629151000	-1.046627000
6	4.605573000	1.230873000	-1.319041000
6	3.340454000	3.732526000	-1.541086000
1	1.575801000	2.730789000	-0.756568000
6	5.311507000	2.335662000	-1.824277000
1	5.102782000	0.258185000	-1.235226000
6	4.682897000	3.587147000	-1.933007000
1	2.842634000	4.704791000	-1.630770000
1	6.356134000	2.216315000	-2.134253000
1	5.235676000	4.446623000	-2.329088000
6	2.567165000	0.122642000	1.598902000
6	1.669586000	-0.532255000	2.471493000
6	3.650580000	0.845225000	2.141186000
6	1.856845000	-0.472336000	3.860070000
1	0.810191000	-1.069544000	2.051667000
6	3.831745000	0.908766000	3.533408000
1	4.349947000	1.364570000	1.476671000
6	2.937789000	0.251002000	4.394546000
1	1.147068000	-0.979440000	4.523295000
1	4.673277000	1.478051000	3.944907000
1	3.079291000	0.307430000	5.479945000
6	3.197387000	-1.523208000	-0.705465000
6	4.273995000	-2.035402000	0.049055000
6	2.816698000	-2.176107000	-1.897956000
6	4.963829000	-3.177432000	-0.390161000
1	4.569804000	-1.543227000	0.982330000
6	3.513158000	-3.311474000	-2.338699000
1	1.964091000	-1.790073000	-2.471116000
6	4.587419000	-3.814739000	-1.584434000

1	5.796390000	-3.571047000	0.204307000
1	3.210052000	-3.810490000	-3.266200000
1	5.125511000	-4.707462000	-1.922991000

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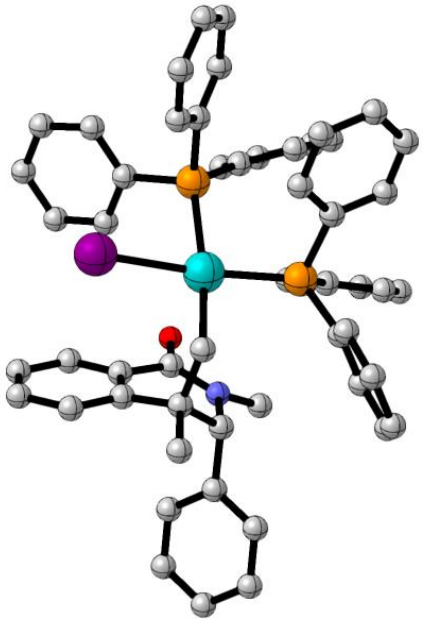


Zero-point correction = 0.849919 (Hartree/particle)
Thermal correction to energy = 0.905883
Thermal correction to enthalpy = 0.906827
Thermal correction to Gibbs free energy = 0.757369
Sum of electronic and zero-point energies = -3325.071968
Sum of electronic and thermal enthalpies = -3325.016004
Sum of electronic and thermal free energies = -3325.015060
Sum of electronic and thermal Free Energies = -3325.164518

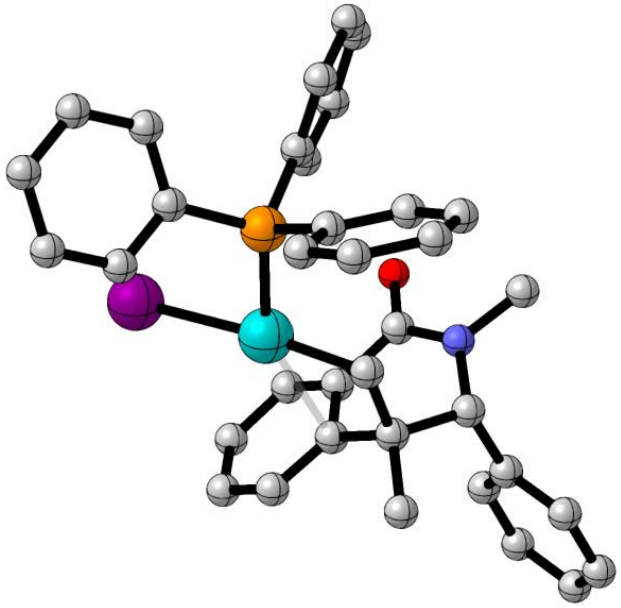
E_{SCF} (M06L/def2-TZVPP) = -3325.921887

46	0.154261000	-0.269861000	-0.686179000
53	0.440289000	-2.775469000	-1.769695000
15	0.104262000	2.009542000	-0.352107000
15	2.327462000	-0.672523000	0.389887000
6	2.419706000	-2.359414000	1.110097000
6	3.549819000	-3.179806000	0.945863000
6	1.321811000	-2.811338000	1.871316000
6	3.579423000	-4.453554000	1.533908000
1	4.396447000	-2.830995000	0.346704000
6	1.369405000	-4.076528000	2.471448000
1	0.432215000	-2.182328000	1.999137000
6	2.492048000	-4.903086000	2.298852000
1	4.455024000	-5.096469000	1.390195000

1	0.516708000	-4.422675000	3.065771000
1	2.517422000	-5.898439000	2.756435000
6	3.792337000	-0.576532000	-0.737130000
6	3.655073000	-0.969551000	-2.084840000
6	5.052368000	-0.138784000	-0.278610000
6	4.751601000	-0.913653000	-2.955940000
1	2.686794000	-1.336836000	-2.440515000
6	6.144033000	-0.068923000	-1.157739000
1	5.181828000	0.154583000	0.766808000
6	5.997435000	-0.452776000	-2.499506000
1	4.626974000	-1.230290000	-3.997632000
1	7.113882000	0.281223000	-0.787040000
1	6.851772000	-0.400210000	-3.183769000
6	2.880852000	0.367391000	1.816568000
6	3.279700000	1.701703000	1.585379000
6	2.841320000	-0.110807000	3.141373000
6	3.600828000	2.547279000	2.653499000
1	3.350300000	2.076991000	0.562918000
6	3.171076000	0.737337000	4.209877000
1	2.545684000	-1.144935000	3.339098000
6	3.540072000	2.070140000	3.972652000
1	3.895332000	3.582745000	2.450847000
1	3.134968000	0.350704000	5.234561000
1	3.784053000	2.732426000	4.810400000
6	1.633310000	2.701796000	-1.128347000
6	2.223333000	3.920786000	-0.735506000
6	2.231737000	1.945551000	-2.155570000
6	3.404990000	4.359800000	-1.347881000
1	1.789687000	4.504099000	0.080592000
6	3.411715000	2.390067000	-2.771197000
1	1.780688000	0.985909000	-2.436678000
6	4.003836000	3.593405000	-2.363298000
1	3.867086000	5.298449000	-1.022464000
1	3.884013000	1.771341000	-3.539865000
1	4.936652000	3.931382000	-2.827460000
6	0.069767000	2.615253000	1.374982000
6	-0.028498000	3.985575000	1.707434000
6	0.133709000	1.656702000	2.403156000
6	-0.020272000	4.384998000	3.051140000
1	-0.144741000	4.736726000	0.919230000
6	0.138281000	2.060097000	3.744895000
1	0.129793000	0.591938000	2.155605000
6	0.073045000	3.422329000	4.070863000
1	-0.097577000	5.448648000	3.302074000
1	0.180866000	1.298866000	4.528940000
1	0.077388000	3.737301000	5.120204000
6	-1.183504000	3.024206000	-1.202281000
6	-1.108886000	3.165082000	-2.604968000

6	-2.297712000	3.555040000	-0.523368000
6	-2.128671000	3.818838000	-3.309904000
1	-0.248333000	2.756100000	-3.145333000
6	-3.316146000	4.214399000	-1.230114000
1	-2.368848000	3.462740000	0.563445000
6	-3.238315000	4.342442000	-2.625411000
1	-2.056878000	3.916996000	-4.398411000
1	-4.170756000	4.628586000	-0.683743000
1	-4.035895000	4.851042000	-3.177398000
8	-1.402516000	-1.156624000	2.668029000
7	-2.703607000	0.116314000	1.264409000
6	-2.997416000	-0.668393000	-1.123929000
6	-2.857167000	-2.077580000	-0.573280000
6	-3.180262000	-3.230852000	-1.301991000
1	-3.597799000	-3.139562000	-2.308385000
6	-2.945815000	-4.507491000	-0.767895000
1	-3.194655000	-5.394719000	-1.360370000
6	-2.381093000	-4.649267000	0.508329000
1	-2.187037000	-5.644795000	0.921112000
6	-2.069034000	-3.506945000	1.252823000
1	-1.657004000	-3.573973000	2.263261000
6	-2.308409000	-2.228553000	0.720132000
6	-2.066351000	-1.058129000	1.610915000
6	-3.482763000	0.275564000	0.024415000
1	-3.290034000	1.303885000	-0.331856000
6	-2.949288000	1.111583000	2.304674000
1	-2.519626000	2.090474000	2.038605000
1	-2.471080000	0.758368000	3.227270000
1	-4.038420000	1.225129000	2.456320000
6	-4.038879000	-0.588932000	-2.269900000
1	-3.664966000	-1.116026000	-3.163271000
1	-4.207423000	0.465097000	-2.552773000
1	-5.007658000	-1.027478000	-1.977303000
6	-1.668640000	-0.168743000	-1.757236000
6	-4.978164000	0.172342000	0.313322000
6	-5.522097000	-0.927611000	1.005814000
1	-4.860704000	-1.722610000	1.363655000
6	-6.903246000	-1.007170000	1.234306000
1	-7.314653000	-1.870354000	1.769366000
6	-7.757853000	0.012807000	0.782619000
6	-7.221639000	1.118186000	0.104102000
1	-7.878901000	1.923501000	-0.243047000
6	-5.839205000	1.195298000	-0.124225000
1	-5.413950000	2.056755000	-0.654294000
1	-8.836200000	-0.051607000	0.965310000
1	-1.826064000	0.864484000	-2.103010000
1	-1.447977000	-0.794667000	-2.635088000

2



Zero-point correction = 0.579281 (Hartree/particle)
Thermal correction to energy = 0.618503
Thermal correction to enthalpy = 0.619447
Thermal correction to Gibbs free energy = 0.501729
Sum of electronic and zero-point energies = -2288.832792
Sum of electronic and thermal enthalpies = -2288.79357
Sum of electronic and thermal free energies = -2288.792626
Sum of electronic and thermal Free Energies = -2288.910344

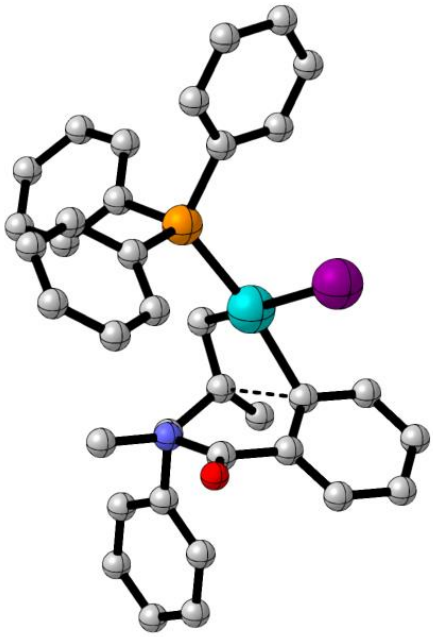
E_{SCF} (M06L/def2-TZVPP) = -2289.412073

46	0.230860000	-0.567795000	-0.561882000
53	1.494339000	-2.905596000	0.100286000
15	1.995618000	0.712105000	-0.048407000
6	1.944030000	2.427404000	-0.708207000
6	2.550441000	2.737044000	-1.942053000
6	1.199026000	3.420615000	-0.035620000
6	2.421228000	4.022120000	-2.488962000
1	3.134849000	1.974012000	-2.466606000
6	1.075389000	4.704700000	-0.584941000
1	0.734279000	3.189850000	0.928817000
6	1.684511000	5.008422000	-1.813174000
1	2.904938000	4.254782000	-3.443948000
1	0.502950000	5.470395000	-0.049806000
1	1.588056000	6.012148000	-2.241068000
6	2.082417000	0.960429000	1.762376000
6	1.291066000	0.149335000	2.598929000
6	2.876263000	1.986199000	2.324203000

6	1.295262000	0.358836000	3.985624000
1	0.665659000	-0.635164000	2.162105000
6	2.890082000	2.177495000	3.712658000
1	3.458133000	2.649100000	1.674784000
6	2.098570000	1.365014000	4.543560000
1	0.653658000	-0.261479000	4.618504000
1	3.509389000	2.970909000	4.145340000
1	2.101105000	1.527753000	5.627103000
6	3.608777000	0.083260000	-0.645961000
6	4.809185000	0.320182000	0.048135000
6	3.628555000	-0.616470000	-1.869520000
6	6.024495000	-0.132146000	-0.487621000
1	4.794469000	0.832407000	1.014774000
6	4.847303000	-1.048829000	-2.408728000
1	2.681222000	-0.847385000	-2.369422000
6	6.046363000	-0.808137000	-1.717681000
1	6.955967000	0.039202000	0.062815000
1	4.857048000	-1.598448000	-3.355896000
1	6.997225000	-1.161752000	-2.131045000
8	-1.912890000	-0.450531000	2.851093000
7	-2.664267000	1.013751000	1.237020000
6	-2.319562000	0.511118000	-1.176173000
6	-2.198218000	-0.974440000	-0.772922000
6	-2.129967000	-2.037038000	-1.704121000
1	-2.133281000	-1.817231000	-2.775367000
6	-2.088657000	-3.370185000	-1.267455000
1	-2.031056000	-4.177153000	-2.004450000
6	-2.090179000	-3.667474000	0.103290000
1	-2.037559000	-4.707137000	0.439504000
6	-2.120531000	-2.630171000	1.043940000
1	-2.081319000	-2.824751000	2.119087000
6	-2.168099000	-1.293066000	0.619769000
6	-2.226528000	-0.221415000	1.670039000
6	-3.198194000	1.243815000	-0.114556000
1	-3.053731000	2.322535000	-0.317713000
6	-2.855628000	2.078313000	2.212464000
1	-3.929030000	2.328871000	2.309659000
1	-2.305751000	2.985145000	1.898327000
1	-2.468370000	1.720525000	3.176629000
6	-2.918162000	0.687949000	-2.579544000
1	-2.224540000	0.296910000	-3.343669000
1	-3.067942000	1.761281000	-2.792216000
1	-3.888645000	0.174149000	-2.683940000
6	-0.888146000	1.085028000	-1.115357000
6	-4.694150000	0.961263000	-0.214101000
6	-5.277337000	-0.205094000	0.319502000
1	-4.661584000	-0.926915000	0.863221000
6	-6.649727000	-0.448859000	0.164177000

1	-7.086358000	-1.361763000	0.583814000
6	-7.462113000	0.470611000	-0.518801000
6	-6.893556000	1.642302000	-1.041845000
1	-7.519539000	2.373860000	-1.564645000
6	-5.520649000	1.882948000	-0.885523000
1	-5.078068000	2.801226000	-1.291092000
1	-8.534350000	0.278773000	-0.634726000
1	-0.505567000	1.424048000	-2.093390000
1	-0.774458000	1.886424000	-0.370636000

TS 2-3



Zero-point correction = 0.576440 (Hartree/particle)
Thermal correction to energy = 0.615618
Thermal correction to enthalpy = 0.616562
Thermal correction to Gibbs free energy = 0.500139
Sum of electronic and zero-point energies = -2288.777191
Sum of electronic and thermal enthalpies = -2288.738013
Sum of electronic and thermal free energies = -2288.737069
Sum of electronic and thermal Free Energies = -2288.853492

E_{SCF} (M06L/def2-TZVPP) = -2289.353631

Imaginary Frequency = -219.92 cm^{-1}

46	0.062504000	-0.496287000	-0.697855000
53	1.152976000	-2.825330000	0.237713000
15	1.980291000	0.640272000	-0.065635000
6	2.144651000	2.355003000	-0.722022000
6	2.987574000	2.642718000	-1.812786000

6	1.319185000	3.377516000	-0.202522000
6	3.009104000	3.931438000	-2.369206000
1	3.634867000	1.858676000	-2.219035000
6	1.345739000	4.664171000	-0.758191000
1	0.670787000	3.164812000	0.655429000
6	2.190596000	4.944287000	-1.845428000
1	3.675508000	4.144912000	-3.212185000
1	0.708345000	5.450509000	-0.338764000
1	2.212353000	5.949532000	-2.279815000
6	1.950650000	0.923654000	1.749396000
6	1.118700000	0.128284000	2.562484000
6	2.720160000	1.953001000	2.337755000
6	1.061452000	0.354396000	3.945627000
1	0.519056000	-0.669070000	2.115274000
6	2.665421000	2.168645000	3.722068000
1	3.343638000	2.598066000	1.709422000
6	1.835026000	1.370272000	4.527668000
1	0.398770000	-0.266672000	4.556812000
1	3.267075000	2.966649000	4.171059000
1	1.788257000	1.546974000	5.608004000
6	3.590804000	-0.116851000	-0.496073000
6	4.746605000	0.067614000	0.284264000
6	3.658629000	-0.864324000	-1.689241000
6	5.966117000	-0.485515000	-0.134143000
1	4.689770000	0.622771000	1.225781000
6	4.882613000	-1.400846000	-2.111066000
1	2.740879000	-1.045069000	-2.259717000
6	6.036990000	-1.212947000	-1.333069000
1	6.862067000	-0.352211000	0.481956000
1	4.929612000	-1.986701000	-3.035218000
1	6.990585000	-1.645602000	-1.654964000
8	-2.189474000	-1.055557000	2.728171000
7	-2.121283000	0.650601000	1.183078000
6	-2.017442000	0.585044000	-1.388225000
6	-1.795126000	-1.518349000	-0.800663000
6	-1.958484000	-2.485464000	-1.808011000
1	-1.434064000	-2.379718000	-2.763864000
6	-2.744476000	-3.620023000	-1.563592000
1	-2.845725000	-4.387161000	-2.339579000
6	-3.376734000	-3.789777000	-0.317294000
1	-3.981629000	-4.682411000	-0.126141000
6	-3.219916000	-2.824072000	0.683142000
1	-3.670982000	-2.946590000	1.673316000
6	-2.452464000	-1.669052000	0.433499000
6	-2.258003000	-0.686230000	1.545463000
6	-2.594700000	1.228845000	-0.087041000
1	-2.152303000	2.242572000	-0.086855000
6	-1.958450000	1.629063000	2.256413000

1	-2.883769000	2.220886000	2.393623000
1	-1.121596000	2.310016000	2.017241000
1	-1.735413000	1.081310000	3.180506000
6	-3.006366000	0.232374000	-2.487220000
1	-2.490913000	-0.263679000	-3.323940000
1	-3.443329000	1.176687000	-2.866628000
1	-3.828031000	-0.408003000	-2.135692000
6	-0.744368000	1.114777000	-1.785658000
6	-4.107267000	1.441835000	-0.125488000
6	-5.028532000	0.469012000	0.305968000
1	-4.672308000	-0.484830000	0.702413000
6	-6.407420000	0.710394000	0.219650000
1	-7.111072000	-0.057658000	0.558614000
6	-6.886172000	1.926244000	-0.294534000
6	-5.975165000	2.905407000	-0.719927000
1	-6.336242000	3.862352000	-1.112424000
6	-4.596706000	2.661843000	-0.631040000
1	-3.884484000	3.430069000	-0.958582000
1	-7.963860000	2.111937000	-0.356824000
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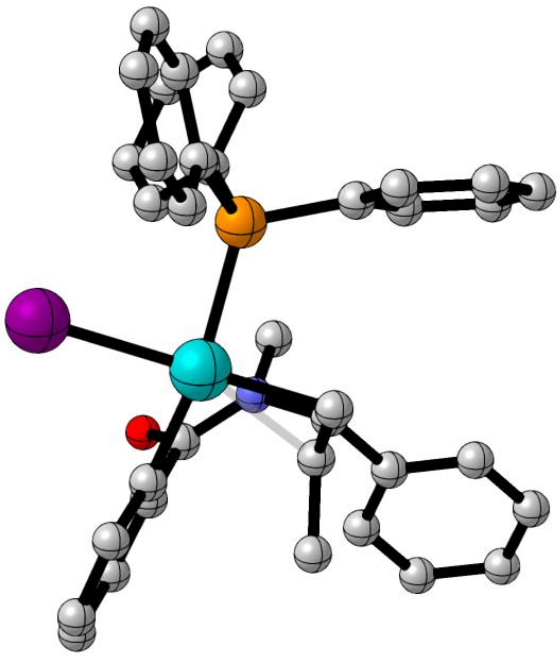
1	-0.384894000	2.036230000	-1.314652000

3



Zero-point correction = 0.577108 (Hartree/particle)
Thermal correction to energy = 0.617097
Thermal correction to enthalpy = 0.618041
Thermal correction to Gibbs free energy = 0.499025
Sum of electronic and zero-point energies = -2288.790101

Sum of electronic and thermal enthalpies = -2288.750112
Sum of electronic and thermal free energies = -2288.749168
Sum of electronic and thermal Free Energies = -2288.868184

E_{SCF} (M06L/def2-TZVPP) = -2289.367209

46	0.061518000	-0.796252000	-0.655998000
53	1.713671000	-2.717015000	0.258413000
15	1.730225000	0.818815000	-0.030715000
6	1.454919000	2.544580000	-0.623830000
6	2.040544000	2.996905000	-1.823904000
6	0.499551000	3.362438000	0.020883000
6	1.676295000	4.238979000	-2.366711000
1	2.785122000	2.374288000	-2.331074000
6	0.135143000	4.601580000	-0.525491000
1	0.057138000	3.033943000	0.967063000
6	0.720525000	5.042300000	-1.724079000
1	2.145379000	4.580946000	-3.295793000
1	-0.602029000	5.225746000	-0.008476000
1	0.436719000	6.009631000	-2.152048000
6	1.776481000	1.050619000	1.790878000
6	1.171282000	0.096432000	2.632826000
6	2.383548000	2.192934000	2.361347000
6	1.186817000	0.274005000	4.024477000
1	0.691368000	-0.783876000	2.197047000
6	2.398860000	2.363882000	3.752664000
1	2.824423000	2.958434000	1.713885000
6	1.801515000	1.403255000	4.586471000
1	0.710471000	-0.475212000	4.665454000
1	2.873586000	3.251267000	4.185496000
1	1.810540000	1.540474000	5.673329000
6	3.438167000	0.463901000	-0.593267000
6	4.584637000	0.857055000	0.120640000
6	3.574650000	-0.202878000	-1.828478000
6	5.858626000	0.596084000	-0.405720000
1	4.483343000	1.345571000	1.094622000
6	4.849115000	-0.446739000	-2.358180000
1	2.675597000	-0.553463000	-2.348445000
6	5.992443000	-0.047862000	-1.646386000
1	6.749663000	0.892305000	0.158544000
1	4.949588000	-0.969431000	-3.315394000
1	6.989204000	-0.251664000	-2.052546000
8	-2.625881000	-1.525313000	2.612425000
7	-2.053122000	0.161944000	1.178178000
6	-1.962996000	0.233889000	-1.390877000
6	-1.345376000	-2.271952000	-0.652440000
6	-1.360874000	-3.317916000	-1.586646000
1	-0.579835000	-3.378354000	-2.351603000

6	-2.359833000	-4.303429000	-1.524435000
1	-2.367833000	-5.114213000	-2.262515000
6	-3.329236000	-4.266775000	-0.506396000
1	-4.099061000	-5.043749000	-0.448031000
6	-3.295067000	-3.241793000	0.444304000
1	-4.014336000	-3.208884000	1.269362000
6	-2.323383000	-2.217662000	0.361177000
6	-2.362135000	-1.182418000	1.448496000
6	-2.304939000	0.930970000	-0.067401000
1	-1.605853000	1.784413000	-0.001180000
6	-2.055318000	1.034008000	2.359860000
1	-3.072056000	1.396803000	2.602476000
1	-1.402556000	1.899897000	2.159516000
1	-1.669109000	0.470037000	3.216618000
6	-3.041300000	-0.536678000	-2.120047000
1	-2.609639000	-1.162395000	-2.915490000
1	-3.719197000	0.205677000	-2.583275000
1	-3.646095000	-1.175658000	-1.461443000
6	-0.834307000	0.668090000	-2.087692000
6	-3.717817000	1.510398000	-0.121172000
6	-4.826396000	0.817147000	0.395740000
1	-4.679452000	-0.140987000	0.905580000
6	-6.115315000	1.357907000	0.274148000
1	-6.972426000	0.812629000	0.684025000
6	-6.307157000	2.593011000	-0.365904000
6	-5.201639000	3.291499000	-0.879106000
1	-5.343042000	4.259748000	-1.372029000
6	-3.913312000	2.752371000	-0.753017000
1	-3.044756000	3.293669000	-1.149516000
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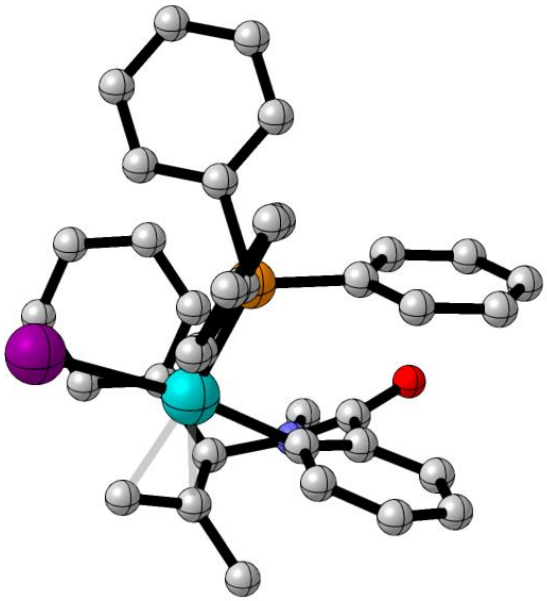
1	-0.328237000	1.598342000	-1.821737000



Zero-point correction = 0.577693 (Hartree/particle)
Thermal correction to energy = 0.617116
Thermal correction to enthalpy = 0.618061
Thermal correction to Gibbs free energy = 0.504668
Sum of electronic and zero-point energies = -2288.791826
Sum of electronic and thermal enthalpies = -2288.752403
Sum of electronic and thermal free energies = -2288.751458
Sum of electronic and thermal Free Energies = -2288.864851

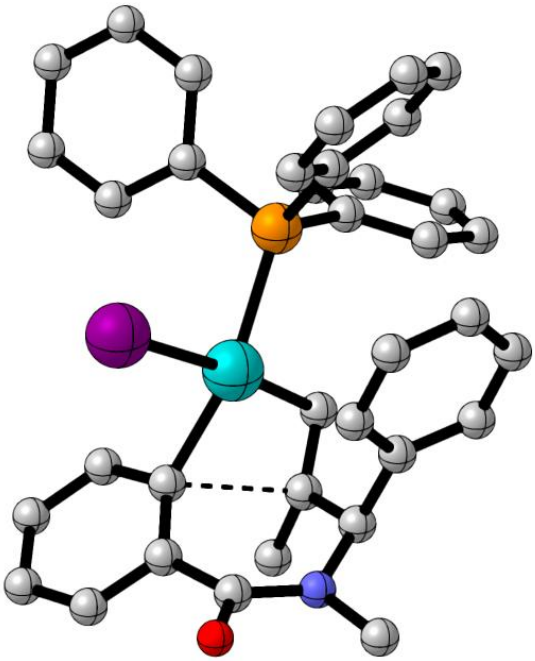
E_{SCF} (M06L/def2-TZVPP) = -2289.369519

46	-0.422745000	-0.457436000	-0.928919000
53	1.024923000	-2.778222000	-1.479659000
15	1.275039000	0.495178000	0.357242000
6	0.836141000	2.140155000	1.048139000
6	1.231392000	3.333226000	0.414277000
6	-0.010950000	2.200835000	2.173632000
6	0.786260000	4.568155000	0.907065000
1	1.873405000	3.295292000	-0.469614000
6	-0.453532000	3.435550000	2.661765000
1	-0.330918000	1.278002000	2.668471000
6	-0.053228000	4.622783000	2.029996000
1	1.091346000	5.490985000	0.401942000
1	-1.132933000	3.464304000	3.518037000
1	-0.407378000	5.589200000	2.404648000
6	1.925745000	-0.375902000	1.852045000
6	1.974601000	-1.781609000	1.905902000

6	2.451462000	0.373256000	2.930275000
6	2.544769000	-2.427078000	3.013106000
1	1.566985000	-2.368654000	1.078467000
6	3.014984000	-0.278167000	4.036715000
1	2.406352000	1.465854000	2.914221000
6	3.064007000	-1.680843000	4.081730000
1	2.574252000	-3.521898000	3.036183000
1	3.414682000	0.315610000	4.866097000
1	3.503923000	-2.187803000	4.947742000
6	2.770519000	0.833331000	-0.655855000
6	3.905144000	1.435912000	-0.073798000
6	2.777616000	0.511239000	-2.025558000
6	5.027978000	1.724006000	-0.860798000
1	3.910465000	1.676470000	0.994223000
6	3.903741000	0.801569000	-2.810581000
1	1.911581000	-0.000473000	-2.457754000
6	5.027322000	1.410046000	-2.230972000
1	5.907214000	2.190260000	-0.403026000
1	3.904129000	0.539203000	-3.873891000
1	5.907918000	1.633303000	-2.843339000
8	-3.176611000	2.305193000	1.730553000
7	-3.720260000	0.439096000	0.561021000
6	-2.816390000	-0.586455000	-1.587208000
6	-1.108447000	1.445361000	-1.133953000
6	-0.459711000	2.116205000	-2.190087000
1	0.273021000	1.581923000	-2.804058000
6	-0.709481000	3.472141000	-2.451218000
1	-0.188800000	3.970779000	-3.277046000
6	-1.603080000	4.182891000	-1.635860000
1	-1.788064000	5.248608000	-1.807975000
6	-2.259865000	3.520062000	-0.596085000
1	-2.960554000	4.050485000	0.054949000
6	-2.059826000	2.136698000	-0.357760000
6	-2.955782000	1.597535000	0.730056000
6	-3.428278000	-0.793288000	-0.200563000
1	-4.430063000	-1.226863000	-0.418332000
6	-4.683648000	0.209734000	1.649990000
1	-5.196896000	1.152908000	1.881922000
1	-4.188749000	-0.149856000	2.570883000
1	-5.409499000	-0.549771000	1.317121000
6	-3.484406000	0.438056000	-2.478435000
1	-4.417006000	-0.019355000	-2.866059000
1	-2.845155000	0.694315000	-3.337012000
1	-3.755022000	1.362656000	-1.951500000
6	-2.004467000	-1.561342000	-2.150366000
6	-2.678103000	-1.801337000	0.670179000
6	-1.785201000	-1.361708000	1.665911000
1	-1.674479000	-0.290129000	1.856343000

6	-1.076904000	-2.288419000	2.443372000
1	-0.396601000	-1.933357000	3.222098000
6	-1.227594000	-3.663507000	2.209582000
6	-2.122419000	-4.109400000	1.225105000
1	-2.253974000	-5.181417000	1.044720000
6	-2.861773000	-3.180991000	0.476517000
1	-3.575250000	-3.531427000	-0.279604000
1	-0.655664000	-4.386247000	2.800976000
1	-1.738449000	-1.491761000	-3.210771000
1	-1.836908000	-2.528431000	-1.674627000

TS 4-5



Zero-point correction = 0.576615 (Hartree/particle)
Thermal correction to energy = 0.615527
Thermal correction to enthalpy = 0.616471
Thermal correction to Gibbs free energy = 0.503633
Sum of electronic and zero-point energies = -2288.778607
Sum of electronic and thermal enthalpies = -2288.739695
Sum of electronic and thermal free energies = -2288.738751
Sum of electronic and thermal Free Energies = -2288.851589

E_{SCF} (M06L/def2-TZVPP) = -2289.355222

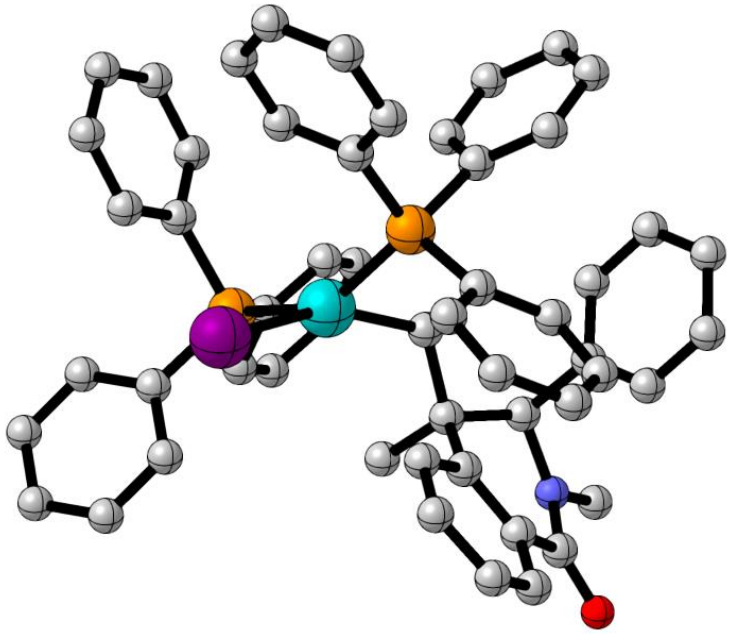
Imaginary Frequency = -137.79 cm^{-1}

46	0.573755000	0.279754000	0.384064000
53	0.804277000	1.857952000	-1.847651000
15	-1.786132000	0.159863000	0.216036000
6	-2.541138000	-0.672429000	1.675778000

6	-3.083398000	0.071016000	2.742030000
6	-2.462610000	-2.078914000	1.787685000
6	-3.546629000	-0.581818000	3.895689000
1	-3.147650000	1.160943000	2.667173000
6	-2.935228000	-2.727102000	2.937204000
1	-2.032261000	-2.664517000	0.967352000
6	-3.477343000	-1.980012000	3.996310000
1	-3.969725000	0.007673000	4.716559000
1	-2.876089000	-3.819073000	3.006212000
1	-3.842932000	-2.486123000	4.896316000
6	-2.516375000	1.842635000	0.292738000
6	-1.724142000	2.917184000	0.739665000
6	-3.869333000	2.058529000	-0.037675000
6	-2.283652000	4.196928000	0.866871000
1	-0.663807000	2.745463000	0.954268000
6	-4.423377000	3.340414000	0.085333000
1	-4.481860000	1.224743000	-0.397184000
6	-3.632189000	4.409445000	0.539301000
1	-1.659504000	5.031231000	1.204282000
1	-5.473350000	3.506805000	-0.179258000
1	-4.066260000	5.411398000	0.628399000
6	-2.653272000	-0.613981000	-1.216368000
6	-2.221640000	-0.277253000	-2.516014000
6	-3.744303000	-1.492529000	-1.057508000
6	-2.859365000	-0.828630000	-3.635232000
1	-1.378296000	0.411024000	-2.642505000
6	-4.371716000	-2.050698000	-2.182585000
1	-4.106325000	-1.746779000	-0.057710000
6	-3.928262000	-1.725749000	-3.473918000
1	-2.511795000	-0.558798000	-4.638573000
1	-5.214447000	-2.737382000	-2.045186000
1	-4.419708000	-2.162171000	-4.350558000
8	4.974055000	-0.753697000	-1.342829000
7	3.681264000	-1.931208000	0.122562000
6	1.991499000	-1.117804000	1.845609000
6	2.523802000	0.902867000	0.801891000
6	2.398928000	2.085552000	1.557042000
1	1.457274000	2.307806000	2.074155000
6	3.449113000	3.012374000	1.602244000
1	3.326246000	3.947330000	2.160894000
6	4.647878000	2.740575000	0.919700000
1	5.471855000	3.461660000	0.940905000
6	4.796033000	1.531650000	0.235411000
1	5.725953000	1.278902000	-0.282470000
6	3.750476000	0.577602000	0.201604000
6	4.124114000	-0.727546000	-0.438313000
6	2.427112000	-2.200696000	0.846819000
1	2.655836000	-3.072203000	1.501590000

6	4.248164000	-3.138212000	-0.492046000
1	4.185357000	-3.965411000	0.235396000
1	5.293886000	-2.937281000	-0.758828000
1	3.702706000	-3.428837000	-1.409574000
6	3.009776000	-0.776225000	2.916722000
1	3.049413000	-1.638937000	3.613659000
1	2.706667000	0.112319000	3.489642000
1	4.017027000	-0.613074000	2.507465000
6	0.609759000	-0.988744000	2.133771000
6	1.329794000	-2.646487000	-0.117739000
6	0.454026000	-3.686119000	0.236504000
1	0.587007000	-4.200308000	1.197059000
6	-0.595642000	-4.059073000	-0.621719000
1	-1.275811000	-4.868197000	-0.331960000
6	-0.763418000	-3.401913000	-1.850407000
6	0.134730000	-2.390254000	-2.225334000
1	0.018786000	-1.877078000	-3.183526000
6	1.174510000	-2.010004000	-1.365720000
1	1.873061000	-1.227948000	-1.678622000
1	-1.592564000	-3.669901000	-2.512910000
1	-0.083505000	-1.771060000	1.820820000
1	0.316020000	-0.439776000	3.037357000

5



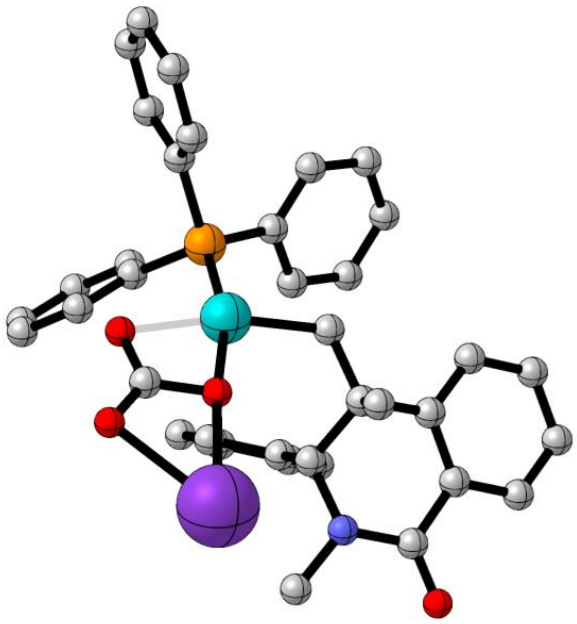
Zero-point correction = 0.848464 (Hartree/particle)
Thermal correction to energy = 0.905177
Thermal correction to enthalpy = 0.906121
Thermal correction to Gibbs free energy = 0.751847

Sum of electronic and zero-point energies = -3325.076234
Sum of electronic and thermal enthalpies = -3325.019521
Sum of electronic and thermal free energies = -3325.018577
Sum of electronic and thermal Free Energies = -3325.172851

E_{SCF} (M06L/def2-TZVPP) = -3325.924698

1	-4.890837000	1.989577000	-1.569728000
1	-1.974465000	3.689243000	-4.289010000
1	-4.323775000	2.973526000	-3.805516000
6	-0.935621000	2.389585000	1.782215000
6	-1.908897000	3.364529000	2.072503000
6	-0.346954000	1.660983000	2.834728000
6	-2.286683000	3.604832000	3.401634000
1	-2.369777000	3.934375000	1.259402000
6	-0.723455000	1.904177000	4.162202000
1	0.420130000	0.915788000	2.590008000
6	-1.693431000	2.879757000	4.447828000
1	-3.045356000	4.364036000	3.620861000
1	-0.256310000	1.337114000	4.975155000
1	-1.986675000	3.075127000	5.485312000
8	-5.279367000	-3.525701000	-1.691344000
7	-3.954746000	-3.078882000	0.137788000
6	-1.815699000	-1.785840000	-0.096620000
6	-2.333054000	-1.335610000	-1.459985000
6	-1.603876000	-0.489447000	-2.309275000
1	-0.643474000	-0.070640000	-1.975971000
6	-2.060028000	-0.165408000	-3.592864000
1	-1.459315000	0.504645000	-4.215318000
6	-3.275231000	-0.691645000	-4.059561000
1	-3.643184000	-0.436108000	-5.059366000
6	-4.002441000	-1.564349000	-3.243291000
1	-4.935734000	-2.028009000	-3.577350000
6	-3.534199000	-1.897417000	-1.957759000
6	-4.339445000	-2.892647000	-1.179893000
6	-3.052201000	-2.145867000	0.819623000
1	-2.623781000	-2.697803000	1.678601000
6	-4.761808000	-3.942444000	0.990568000
1	-5.434893000	-4.517819000	0.339527000
1	-5.362127000	-3.342732000	1.702310000
1	-4.107772000	-4.624658000	1.563680000
6	-1.008597000	-3.089522000	-0.307112000
1	-0.666803000	-3.495130000	0.659854000
1	-0.122971000	-2.889932000	-0.931365000
1	-1.621424000	-3.853427000	-0.812784000
6	-1.013072000	-0.738349000	0.699716000
6	-3.813272000	-0.946429000	1.389115000
6	-4.848868000	-0.311443000	0.677002000

1	-5.146910000	-0.685678000	-0.305666000
6	-5.502287000	0.808881000	1.215115000
1	-6.306510000	1.289489000	0.646660000
6	-5.130023000	1.313117000	2.470786000
6	-4.113715000	0.673858000	3.197815000
1	-3.814226000	1.053894000	4.178603000
6	-3.469705000	-0.448550000	2.661743000
1	-2.670903000	-0.940067000	3.229619000
1	-5.634550000	2.192685000	2.885021000
1	-0.704441000	-1.183646000	1.657391000
1	-1.662967000	0.113879000	0.931074000
15	2.195159000	-1.561212000	0.454049000
6	1.669815000	-2.758611000	1.745839000
6	0.982749000	-2.280437000	2.885556000
6	1.812743000	-4.149921000	1.572959000
6	0.458897000	-3.172358000	3.831920000
1	0.847622000	-1.203274000	3.026619000
6	1.279822000	-5.040917000	2.516987000
1	2.327210000	-4.536244000	0.688368000
6	0.600475000	-4.557290000	3.646260000
1	-0.069045000	-2.783945000	4.709760000
1	1.393319000	-6.119730000	2.364706000
1	0.180643000	-5.255920000	4.377826000
6	3.069297000	-2.576703000	-0.791552000
6	4.296936000	-3.205760000	-0.495987000
6	2.493378000	-2.722072000	-2.068054000
6	4.930692000	-3.991860000	-1.468224000
1	4.753036000	-3.072171000	0.491233000
6	3.129453000	-3.513210000	-3.036273000
1	1.569601000	-2.184410000	-2.305693000
6	4.344576000	-4.148647000	-2.736630000
1	5.885132000	-4.478326000	-1.239060000
1	2.682104000	-3.616825000	-4.030256000
1	4.844417000	-4.759479000	-3.496434000
6	3.547885000	-0.583774000	1.247358000
6	4.408810000	0.149422000	0.400597000
6	3.698085000	-0.472123000	2.644102000
6	5.385399000	0.992761000	0.946380000
1	4.289542000	0.083864000	-0.685354000
6	4.673082000	0.381020000	3.184805000
1	3.068669000	-1.061900000	3.315948000
6	5.514145000	1.121123000	2.339872000
1	6.041366000	1.557190000	0.274867000
1	4.777293000	0.459783000	4.272623000
1	6.272166000	1.788080000	2.765027000



Zero-point correction = 0.596620 (Hartree/particle)
Thermal correction to energy = 0.639352
Thermal correction to enthalpy = 0.640296
Thermal correction to Gibbs free energy = 0.517825
Sum of electronic and zero-point energies = -2854.805664
Sum of electronic and thermal enthalpies = -2854.762932
Sum of electronic and thermal free energies = -2854.761988
Sum of electronic and thermal Free Energies = -2854.884459

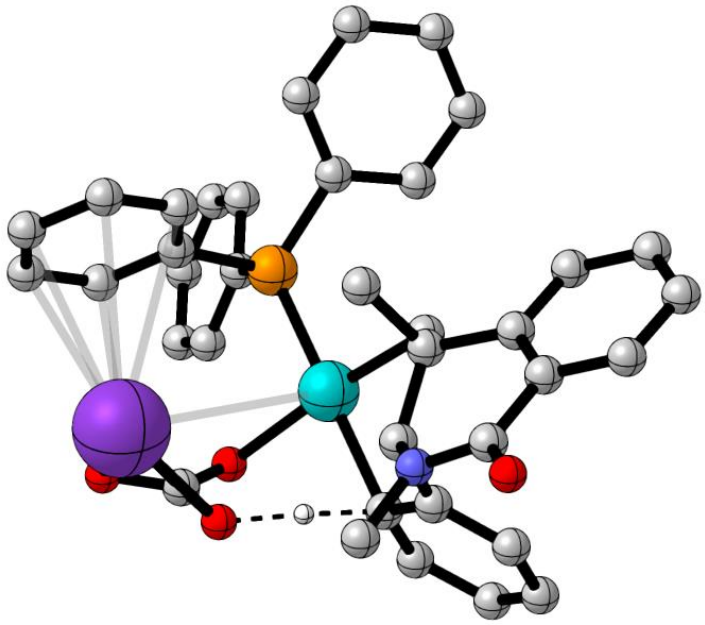
E_{SCF} (M06L/def2-TZVPP) = -2855.402284

8	6.061299000	0.065882000	0.472438000
7	3.875701000	0.783432000	0.579100000
6	2.199813000	-0.086460000	-1.065856000
6	3.088640000	-1.328371000	-1.176441000
6	2.689143000	-2.502408000	-1.836415000
1	1.673489000	-2.575954000	-2.235993000
6	3.574343000	-3.583850000	-1.973647000
1	3.239568000	-4.494124000	-2.484056000
6	4.879574000	-3.503837000	-1.460623000
1	5.571016000	-4.346033000	-1.572950000
6	5.288292000	-2.342335000	-0.793791000
1	6.290205000	-2.242341000	-0.364858000
6	4.397790000	-1.264095000	-0.641664000
6	4.866487000	-0.092432000	0.164871000
6	2.435966000	0.554307000	0.338766000
1	1.959638000	1.550566000	0.284979000
6	4.214247000	1.791898000	1.567522000
1	3.596494000	1.664188000	2.475496000

1	4.038058000	2.819221000	1.178677000
1	5.281594000	1.685569000	1.809952000
6	2.651101000	0.899448000	-2.177584000
1	2.608934000	0.390727000	-3.156428000
1	3.691572000	1.237933000	-2.020179000
1	1.966926000	1.763421000	-2.201508000
6	1.791348000	-0.185046000	1.512005000
6	2.265107000	-1.432428000	1.967514000
1	3.117158000	-1.906865000	1.473490000
6	1.653457000	-2.073206000	3.056212000
1	2.035566000	-3.042636000	3.395977000
6	0.559995000	-1.477723000	3.708841000
1	0.078559000	-1.982433000	4.553651000
6	0.086172000	-0.231545000	3.270742000
1	-0.768851000	0.241079000	3.763743000
6	0.702495000	0.407995000	2.182719000
6	0.711124000	-0.429315000	-1.240327000
1	0.474967000	-1.324123000	-0.648916000
1	0.482588000	-0.642467000	-2.302357000
6	-3.227300000	-1.143783000	2.352414000
6	-3.675246000	0.436283000	4.147234000
6	-3.262148000	1.493760000	3.317770000
1	-3.271810000	2.523238000	3.692414000
6	-2.820589000	1.241035000	2.010744000
1	-2.466644000	2.062140000	1.372523000
6	-2.303101000	-2.940583000	-1.346317000
1	-3.006132000	-2.520561000	-2.072936000
6	-1.865744000	-4.269011000	-1.474786000
1	-2.235949000	-4.882783000	-2.303490000
6	-0.957827000	-4.808275000	-0.549598000
1	-0.613353000	-5.842627000	-0.657960000
6	-3.658344000	-0.881236000	3.662043000
1	-4.008300000	0.638657000	5.171362000
15	-2.200257000	-0.352949000	-0.190278000
6	-2.801691000	-0.085323000	1.525900000
6	-1.836546000	-2.145942000	-0.282017000
6	-0.487313000	-4.015991000	0.511462000
1	0.231754000	-4.419217000	1.232291000
6	-0.919616000	-2.690913000	0.644385000
1	-0.534964000	-2.073014000	1.460976000
6	-3.694587000	-0.136740000	-1.233436000
6	-4.930886000	-0.711529000	-0.873822000
1	-5.016811000	-1.281026000	0.058177000
6	-6.047203000	-0.542860000	-1.704128000
1	-7.008067000	-0.987852000	-1.422968000
6	-5.935824000	0.202395000	-2.891294000
1	-6.811934000	0.336577000	-3.535399000
6	-4.708104000	0.782831000	-3.246673000

1	-4.623328000	1.373929000	-4.164960000
6	-3.587334000	0.615913000	-2.418654000
1	-2.622361000	1.075460000	-2.665965000
1	-3.978066000	-1.709232000	4.304594000
1	-3.200426000	-2.173251000	1.981267000
46	-0.579969000	1.107947000	-0.700651000
8	-1.443912000	3.108446000	-0.157163000
8	0.658803000	2.849441000	-0.888075000
6	-0.291879000	3.681608000	-0.373496000
8	0.004963000	4.884471000	-0.135175000
1	0.322689000	1.376621000	1.836743000
19	2.502455000	4.530132000	-0.664453000

TS 6-7



Zero-point correction = 0.591098 (Hartree/particle)
Thermal correction to energy = 0.633216
Thermal correction to enthalpy = 0.634160
Thermal correction to Gibbs free energy = 0.514578
Sum of electronic and zero-point energies = -2854.755108
Sum of electronic and thermal enthalpies = -2854.712990
Sum of electronic and thermal free energies = -2854.712046
Sum of electronic and thermal Free Energies = -2854.831628

E_{SCF} (M06L/def2-TZVPP) = -2855.346206

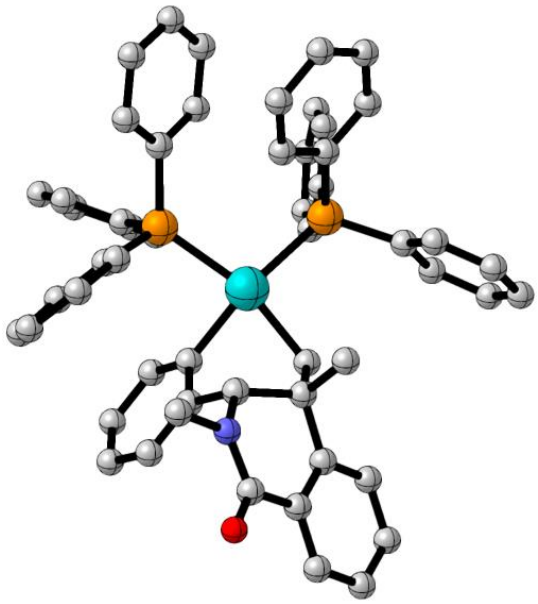
Imaginary Frequency = -762.73 cm^{-1}

6	2.178530000	0.623420000	0.471931000
6	3.376794000	1.567493000	0.341982000

6	3.219407000	2.925097000	0.005358000
1	2.220048000	3.312368000	-0.216755000
6	4.325310000	3.785602000	-0.054575000
1	4.178526000	4.837312000	-0.325782000
6	5.614607000	3.303911000	0.229196000
1	6.479234000	3.974716000	0.180871000
6	5.784643000	1.960353000	0.577784000
1	6.767341000	1.543069000	0.818069000
6	4.676536000	1.094033000	0.634571000
6	4.941448000	-0.325340000	1.031139000
6	2.635465000	-0.839153000	0.195705000
1	1.839146000	-1.479237000	0.627593000
6	4.082220000	-2.614009000	1.135843000
1	3.930814000	-3.194352000	0.207017000
1	3.364889000	-2.982247000	1.897060000
1	5.110130000	-2.745622000	1.502449000
6	1.664312000	0.692427000	1.928883000
1	1.365016000	1.723281000	2.188578000
1	2.438326000	0.364265000	2.644865000
1	0.776177000	0.040684000	2.028134000
6	2.642278000	-1.152370000	-1.290410000
6	3.758439000	-0.986629000	-2.117733000
1	4.727762000	-0.695990000	-1.697592000
6	3.618202000	-1.183654000	-3.504608000
1	4.486615000	-1.045936000	-4.159183000
6	2.377959000	-1.553384000	-4.056472000
1	2.286700000	-1.704816000	-5.138357000
6	1.268026000	-1.736526000	-3.217190000
1	0.301529000	-2.055688000	-3.623837000
6	1.387448000	-1.542473000	-1.821327000
6	1.051344000	1.032077000	-0.506355000
1	1.473198000	1.290947000	-1.494700000
1	0.547506000	1.922869000	-0.103613000
6	-2.470696000	3.094744000	1.422167000
6	-1.749225000	5.257009000	0.567634000
6	-1.252266000	4.633429000	-0.589314000
1	-0.782566000	5.229886000	-1.378709000
6	-1.350932000	3.243129000	-0.734366000
1	-0.964002000	2.751090000	-1.634230000
6	-3.409212000	-1.207729000	1.608063000
1	-3.917933000	-1.538930000	0.699937000
6	-3.636333000	-1.882590000	2.820831000
1	-4.339737000	-2.721696000	2.840941000
6	-2.960260000	-1.494389000	3.991983000
1	-3.154780000	-2.010939000	4.939137000
6	-2.361925000	4.487092000	1.568507000
1	-1.663829000	6.342582000	0.685819000
15	-2.107784000	0.662470000	-0.063605000

6	-1.953312000	2.460596000	0.275406000
6	-2.505369000	-0.123474000	1.557901000
6	-2.039969000	-0.426779000	3.943414000
1	-1.513281000	-0.108970000	4.850793000
6	-1.810567000	0.250222000	2.734031000
1	-1.096370000	1.078227000	2.704818000
6	-3.690175000	0.583109000	-1.006402000
6	-4.601809000	1.660423000	-0.980657000
1	-4.366945000	2.571518000	-0.422523000
6	-5.814080000	1.566831000	-1.679140000
1	-6.516087000	2.407902000	-1.658436000
6	-6.125374000	0.403768000	-2.402109000
1	-7.073625000	0.335283000	-2.947092000
6	-5.217307000	-0.666399000	-2.427512000
1	-5.452959000	-1.575416000	-2.991937000
6	-3.996353000	-0.584151000	-1.739878000
1	-3.274606000	-1.414509000	-1.747053000
1	-2.765001000	4.970625000	2.465055000
1	-2.971054000	2.504166000	2.195793000
46	-0.321725000	-0.456660000	-0.935745000
8	-1.556741000	-2.217136000	-1.365015000
8	0.115012000	-3.288129000	-0.246069000
6	-1.204015000	-3.085790000	-0.435794000
8	-2.035514000	-3.679798000	0.314120000
1	0.728906000	-2.363617000	-1.062925000
19	-0.376388000	-3.180964000	2.245413000

7



Zero-point correction = 0.836193 (Hartree/particle)
Thermal correction to energy = 0.889940
Thermal correction to enthalpy = 0.890884
Thermal correction to Gibbs free energy = 0.745132
Sum of electronic and zero-point energies = -3026.542501
Sum of electronic and thermal enthalpies = -3026.488754
Sum of electronic and thermal free energies = -3026.487810
Sum of electronic and thermal Free Energies = -3026.633562

E_{SCF} (M06L/def2-TZVPP) = -3027.378694

8	6.239809000	-1.086854000	1.850266000
7	3.956912000	-0.918536000	1.588209000
6	2.913178000	0.897570000	0.199809000
6	4.320857000	1.140210000	-0.346858000
6	4.570183000	2.124856000	-1.321407000
1	3.731570000	2.705287000	-1.719754000
6	5.869979000	2.366213000	-1.788648000
1	6.037542000	3.133954000	-2.553026000
6	6.952828000	1.625917000	-1.283219000
1	7.968565000	1.809364000	-1.650674000
6	6.723166000	0.657211000	-0.301434000
1	7.536453000	0.069566000	0.135500000
6	5.418597000	0.415183000	0.168925000
6	5.260220000	-0.596162000	1.259223000
6	2.818853000	-0.573864000	0.731952000
1	1.920988000	-0.594085000	1.384322000
6	3.724442000	-1.930344000	2.608540000
1	4.684871000	-2.131838000	3.104097000
1	3.330580000	-2.859822000	2.157852000
1	2.983210000	-1.561250000	3.341483000
6	2.682628000	1.847422000	1.400477000
1	3.393806000	1.635258000	2.217553000
1	1.652480000	1.713237000	1.780899000
1	2.801840000	2.899648000	1.093380000
6	2.566807000	-1.574351000	-0.390001000
6	3.478928000	-2.586696000	-0.724926000
1	4.400195000	-2.706305000	-0.143121000
6	3.217059000	-3.441477000	-1.809533000
1	3.930652000	-4.232873000	-2.065767000
6	2.055549000	-3.258907000	-2.572122000
1	1.855865000	-3.903626000	-3.437168000
6	1.138298000	-2.245458000	-2.229425000
1	0.232029000	-2.128302000	-2.832595000
6	1.367024000	-1.417003000	-1.117531000
6	1.843294000	1.159389000	-0.883189000
1	2.197244000	0.838944000	-1.875485000
1	1.602812000	2.233604000	-0.927444000

6	0.152443000	4.202493000	1.150280000
6	1.205814000	6.002437000	-0.102746000
6	0.720334000	5.447488000	-1.297265000
1	0.936509000	5.930419000	-2.256568000
6	-0.045306000	4.272319000	-1.271113000
1	-0.422594000	3.851997000	-2.208536000
6	-2.978541000	3.174068000	1.893698000
1	-3.107978000	3.996592000	1.182027000
6	-3.669925000	3.185099000	3.113462000
1	-4.362571000	4.003188000	3.339792000
6	-3.465596000	2.155828000	4.048558000
1	-4.010728000	2.165054000	4.998681000
6	0.916582000	5.377667000	1.120800000
1	1.807361000	6.917423000	-0.125123000
15	-1.176842000	1.996200000	0.009763000
15	-1.435596000	-1.670292000	0.057168000
6	-0.338165000	3.639355000	-0.046226000
6	-2.096395000	2.114801000	1.591235000
6	-2.551973000	1.126719000	3.774131000
1	-2.381366000	0.329473000	4.504095000
6	-1.869059000	1.109609000	2.550380000
1	-1.153009000	0.315200000	2.314783000
6	-2.407983000	2.104673000	-1.359972000
6	-3.781843000	2.367240000	-1.197107000
1	-4.186368000	2.561520000	-0.199350000
6	-4.643378000	2.345156000	-2.305630000
1	-5.712726000	2.536146000	-2.162866000
6	-4.142202000	2.078476000	-3.589369000
1	-4.818205000	2.062928000	-4.450970000
6	-2.772424000	1.821244000	-3.762334000
1	-2.372852000	1.602723000	-4.758774000
6	-1.913217000	1.819084000	-2.654266000
1	-0.853013000	1.561991000	-2.775071000
6	-2.943864000	-1.460812000	1.107384000
6	-3.187995000	-2.144447000	2.312687000
1	-2.485540000	-2.906103000	2.663464000
6	-4.332926000	-1.847646000	3.071135000
1	-4.510244000	-2.381302000	4.011787000
6	-5.245515000	-0.877676000	2.630274000
1	-6.130008000	-0.640507000	3.231257000
6	-5.024019000	-0.219193000	1.408841000
1	-5.735668000	0.531529000	1.048361000
6	-3.883453000	-0.510788000	0.653996000
1	-3.711707000	0.007926000	-0.294277000
1	-0.343668000	-1.866478000	2.750780000
1	1.290406000	5.803078000	2.058504000
1	-0.062207000	3.718044000	2.107974000
6	-2.220988000	-2.441589000	-1.413717000

6	-2.887968000	-3.681597000	-1.345817000
1	-2.888337000	-4.249593000	-0.409103000
6	-3.553159000	-4.180756000	-2.474132000
1	-4.063777000	-5.148631000	-2.421214000
6	-3.576141000	-3.436833000	-3.667320000
1	-4.103337000	-3.827900000	-4.544490000
6	-2.930658000	-2.192214000	-3.731545000
1	-2.954339000	-1.603022000	-4.654652000
6	-2.249996000	-1.699018000	-2.608543000
1	-1.739701000	-0.730761000	-2.640432000
6	-0.475127000	-2.991107000	0.890205000
6	0.850124000	-5.034674000	0.819919000
1	1.219175000	-5.899047000	0.258293000
6	-0.017924000	-4.127647000	0.195789000
1	-0.310109000	-4.283754000	-0.845202000
6	-0.035132000	-2.770889000	2.213901000
6	0.801917000	-3.699435000	2.846919000
1	1.123577000	-3.524942000	3.879301000
6	1.249936000	-4.833327000	2.149619000
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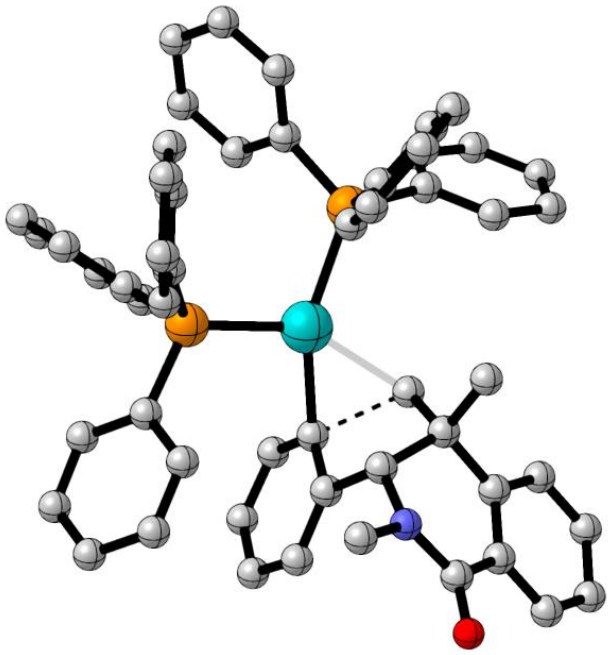
46	0.086105000	0.069703000	-0.458131000

TS 7-8



Zero-point correction = 0.834308 (Hartree/particle)
Thermal correction to energy = 0.888000
Thermal correction to enthalpy = 0.888944
Thermal correction to Gibbs free energy = 0.743005

Sum of electronic and zero-point energies = -3026.517298
Sum of electronic and thermal enthalpies = -3026.463606
Sum of electronic and thermal free energies = -3026.462662
Sum of electronic and thermal Free Energies = -3026.608601

E_{SCF} (M06L/def2-TZVPP) = -3027.351606

Imaginary Frequency = -399.59 cm^{-1}

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6	4.436257000	1.289579000	-0.400035000
6	4.729456000	2.244719000	-1.391626000
1	3.909516000	2.809971000	-1.849526000
6	6.049704000	2.477989000	-1.800944000
1	6.253188000	3.220451000	-2.580921000
6	7.107117000	1.760194000	-1.215229000
1	8.139326000	1.935568000	-1.537241000
6	6.832657000	0.828167000	-0.209925000
1	7.626448000	0.265621000	0.290858000
6	5.507260000	0.594114000	0.204215000
6	5.306265000	-0.358990000	1.341205000
6	2.896633000	-0.348602000	0.739207000
1	1.965873000	-0.326423000	1.348090000
6	3.714307000	-1.556165000	2.756162000
1	4.623762000	-1.629167000	3.369390000
1	3.452042000	-2.565501000	2.384322000
1	2.871581000	-1.172624000	3.359508000
6	2.622544000	2.139065000	1.099817000
1	3.242846000	2.030223000	2.006838000
1	1.560025000	2.032114000	1.388370000
1	2.785469000	3.151777000	0.694248000
6	2.701609000	-1.333554000	-0.393896000
6	3.462104000	-2.477411000	-0.644746000
1	4.238175000	-2.783522000	0.066799000
6	3.233227000	-3.219854000	-1.816417000
1	3.808904000	-4.130205000	-2.012133000
6	2.289689000	-2.761571000	-2.753741000
1	2.131544000	-3.318935000	-3.684900000
6	1.560864000	-1.583193000	-2.525155000
1	0.869075000	-1.212435000	-3.290982000
6	1.711563000	-0.889504000	-1.301051000
6	2.026217000	1.054223000	-1.145361000
1	1.397102000	1.963982000	-1.166136000
1	2.537264000	1.013951000	-2.115140000
6	0.162290000	4.182127000	-0.598779000
6	-0.021511000	5.625471000	-2.549050000

6	-1.158201000	4.909927000	-2.962017000
1	-1.682708000	5.196016000	-3.880678000
6	-1.635450000	3.833886000	-2.200087000
1	-2.526437000	3.286863000	-2.526014000
6	-1.760996000	3.748378000	2.082733000
1	-2.001808000	4.514905000	1.337985000
6	-1.771339000	4.063201000	3.449680000
1	-2.029878000	5.077810000	3.772751000
6	-1.450603000	3.080663000	4.402623000
1	-1.461867000	3.329999000	5.469484000
6	0.633966000	5.259903000	-1.362500000
1	0.348602000	6.465047000	-3.147279000
15	-1.437754000	1.924974000	-0.101746000
15	-1.285609000	-1.809546000	0.038746000
6	-0.981254000	3.458273000	-1.007774000
6	-1.426230000	2.444372000	1.659671000
6	-1.108561000	1.784226000	3.986456000
1	-0.859086000	1.012611000	4.722021000
6	-1.088394000	1.469009000	2.620548000
1	-0.816625000	0.462483000	2.286380000
6	-3.220417000	1.717023000	-0.505406000
6	-4.267306000	2.206457000	0.300179000
1	-4.037466000	2.805948000	1.186675000
6	-5.598077000	1.885636000	-0.008347000
1	-6.407660000	2.256423000	0.630529000
6	-5.894575000	1.083192000	-1.123931000
1	-6.934119000	0.820816000	-1.349070000
6	-4.856325000	0.611343000	-1.943771000
1	-5.072198000	-0.030688000	-2.803626000
6	-3.525989000	0.924578000	-1.631726000
1	-2.708460000	0.515894000	-2.234254000
6	-2.252034000	-1.648528000	1.598691000
6	-1.777461000	-2.143859000	2.831013000
1	-0.899846000	-2.797155000	2.855252000
6	-2.429336000	-1.809798000	4.028505000
1	-2.048700000	-2.205024000	4.977235000
6	-3.564541000	-0.983337000	4.014371000
1	-4.064232000	-0.716207000	4.951694000
6	-4.055812000	-0.506107000	2.788519000
1	-4.942269000	0.136284000	2.756385000
6	-3.406754000	-0.833378000	1.592069000
1	-3.795757000	-0.449828000	0.646706000
1	1.055756000	-2.435021000	1.624487000
1	1.516099000	5.816095000	-1.025801000
1	0.667276000	3.913994000	0.333707000
6	-2.549411000	-2.267077000	-1.218286000
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1	-4.055955000	-3.020190000	0.150796000

6	-4.715728000	-3.143042000	-1.911920000
1	-5.688797000	-3.573486000	-1.650588000
6	-4.388473000	-2.907854000	-3.257346000
1	-5.106202000	-3.152751000	-4.048122000
6	-3.135328000	-2.362375000	-3.586786000
1	-2.871245000	-2.181513000	-4.634634000
6	-2.223655000	-2.039943000	-2.572186000
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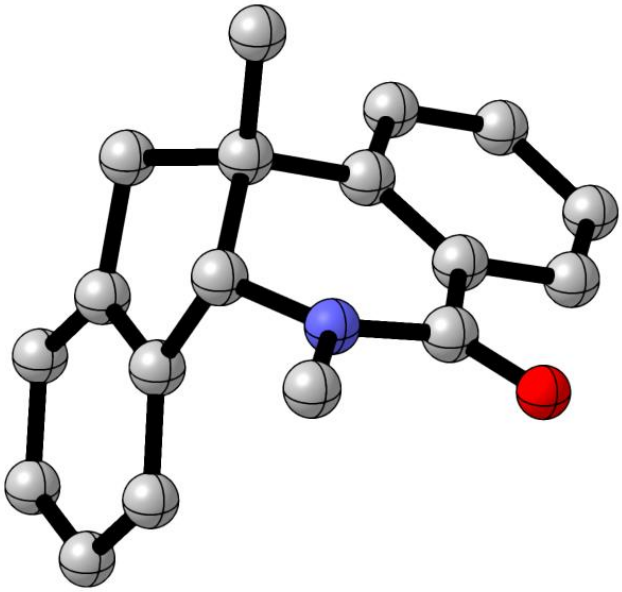
6	-0.336981000	-3.368637000	0.243768000
6	0.144994000	-5.693477000	-0.310330000
1	-0.099546000	-6.600599000	-0.874196000
6	-0.643456000	-4.545296000	-0.469444000
1	-1.500410000	-4.561205000	-1.149450000
6	0.782044000	-3.358703000	1.103931000
6	1.549528000	-4.517151000	1.282473000
1	2.410070000	-4.501332000	1.960250000
6	1.238627000	-5.685020000	0.570182000
1	1.851876000	-6.583965000	0.695477000
46	-0.032304000	0.075827000	-0.559799000

8

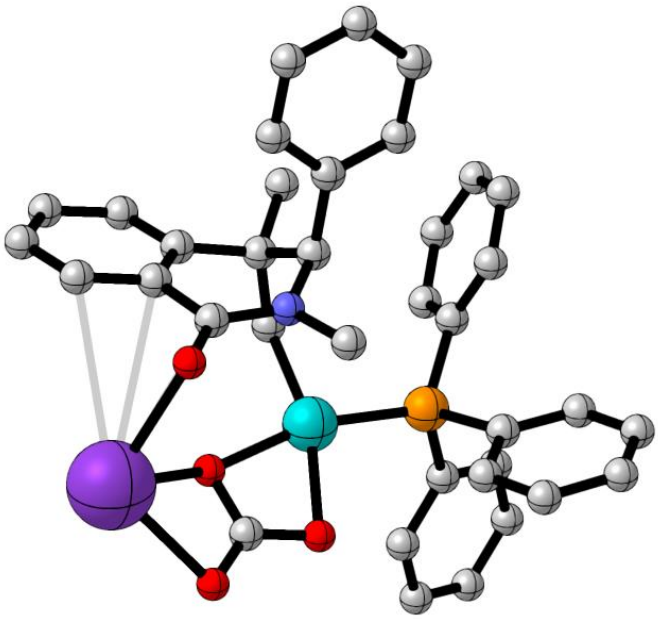


Zero-point correction = 0.299340 (Hartree/particle)
Thermal correction to energy = 0.315781
Thermal correction to enthalpy = 0.316725
Thermal correction to Gibbs free energy = 0.256198
Sum of electronic and zero-point energies = -826.06491
Sum of electronic and thermal enthalpies = -826.048460
Sum of electronic and thermal free energies = -826.04752

Sum of electronic and thermal Free Energies = -826.108050

E_{SCF} (M06L/def2-TZVPP) = -826.364245

8	-1.866642000	2.511850000	-1.129290000
7	-0.239417000	1.943561000	0.397222000
6	-0.177955000	-0.363532000	1.470775000
6	-1.184606000	-0.768982000	0.388176000
6	-1.708150000	-2.074301000	0.326359000
1	-1.376084000	-2.826732000	1.050436000
6	-2.648657000	-2.433388000	-0.649755000
1	-3.031381000	-3.459834000	-0.683264000
6	-3.095719000	-1.480720000	-1.581282000
1	-3.826257000	-1.757414000	-2.349375000
6	-2.610481000	-0.171204000	-1.511657000
1	-2.957758000	0.603868000	-2.202025000
6	-1.663880000	0.193041000	-0.533086000
6	-1.266288000	1.641022000	-0.473398000
6	0.600632000	0.900335000	0.980793000
1	1.088259000	1.356043000	1.867111000
6	0.178658000	3.330501000	0.575806000
1	1.181680000	3.510103000	0.144951000
1	0.211189000	3.578509000	1.652934000
1	-0.550669000	3.977400000	0.067867000
6	-0.920633000	-0.118212000	2.796176000
1	-1.665286000	0.689123000	2.678318000
1	-0.214537000	0.172815000	3.596088000
1	-1.456105000	-1.027617000	3.121424000
6	1.678571000	0.310458000	0.076139000
6	2.380919000	0.896166000	-0.981375000
1	2.169895000	1.924800000	-1.294330000
6	3.343967000	0.124087000	-1.658400000
1	3.898124000	0.560261000	-2.497220000
6	3.591103000	-1.206237000	-1.274161000
1	4.338606000	-1.797602000	-1.815218000
6	2.873271000	-1.791968000	-0.213804000
1	3.051208000	-2.836751000	0.067668000
6	1.912640000	-1.025242000	0.456018000
6	0.985228000	-1.403445000	1.593247000
1	1.488587000	-1.264427000	2.572396000
1	0.647867000	-2.452549000	1.556574000



Zero-point correction = 0.596470 (Hartree/particle)
Thermal correction to energy = 0.639049
Thermal correction to enthalpy = 0.639993
Thermal correction to Gibbs free energy = 0.518402
Sum of electronic and zero-point energies = -2854.814440
Sum of electronic and thermal enthalpies = -2854.771860
Sum of electronic and thermal free energies = -2854.770920
Sum of electronic and thermal Free Energies = -2854.892510

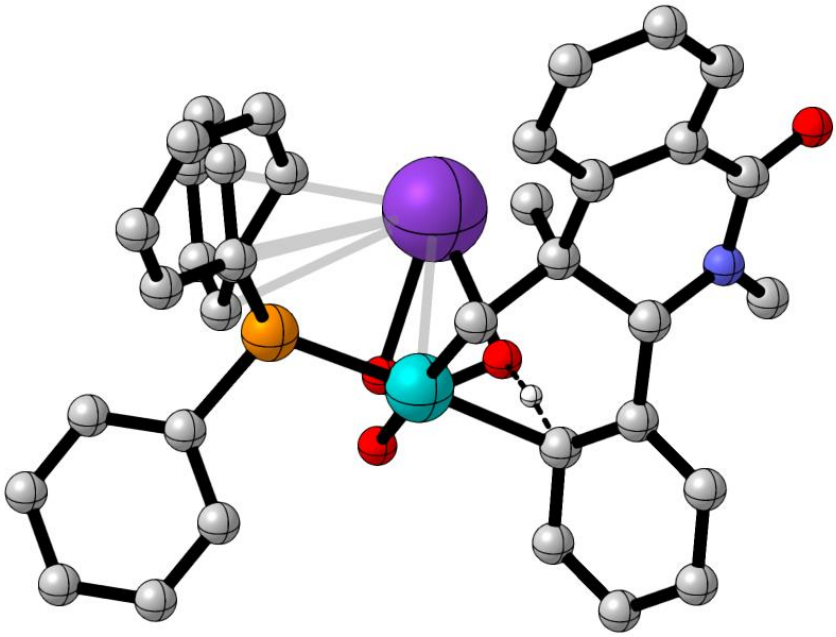
E_{SCF} (M06L/def2-TZVPP) = -2855.410910

46	0.510107000	-1.203207000	-0.381507000
15	2.205368000	0.239096000	-0.164558000
6	3.716792000	-0.423114000	-0.983509000
6	4.770890000	0.404381000	-1.419817000
6	3.829916000	-1.825421000	-1.091311000
6	5.922866000	-0.166287000	-1.980590000
1	4.687513000	1.492886000	-1.331234000
6	4.990465000	-2.387837000	-1.643570000
1	3.014672000	-2.460743000	-0.721409000
6	6.033174000	-1.562155000	-2.094475000
1	6.736770000	0.480521000	-2.327073000
1	5.076151000	-3.476964000	-1.724083000
1	6.934400000	-2.005293000	-2.532752000
6	2.770911000	0.466928000	1.574444000
6	3.631271000	1.518618000	1.954626000
6	2.396066000	-0.509546000	2.521532000
6	4.076398000	1.617758000	3.280236000
1	3.951275000	2.261101000	1.215922000

6	2.853994000	-0.406868000	3.844909000
1	1.785814000	-1.365212000	2.202179000
6	3.682070000	0.659051000	4.229272000
1	4.737081000	2.441924000	3.571734000
1	2.563065000	-1.169903000	4.575169000
1	4.031872000	0.738714000	5.264607000
6	2.030321000	1.938221000	-0.834440000
6	2.141762000	2.140685000	-2.228116000
6	1.627843000	3.016230000	-0.019225000
6	1.876620000	3.398386000	-2.788021000
1	2.447515000	1.309026000	-2.872034000
6	1.369146000	4.275979000	-0.582112000
1	1.529294000	2.871483000	1.061779000
6	1.491278000	4.470764000	-1.966925000
1	1.968993000	3.539730000	-3.870265000
1	1.070431000	5.107947000	0.065201000
1	1.284385000	5.453098000	-2.404548000
8	-3.200742000	-1.914463000	1.639043000
7	-1.921792000	-0.063324000	1.163526000
6	-1.769673000	0.822815000	-1.192831000
6	-3.058625000	0.055357000	-1.454585000
6	-3.744251000	0.130371000	-2.681669000
1	-3.367532000	0.789596000	-3.469139000
6	-4.905446000	-0.621090000	-2.914179000
1	-5.421514000	-0.536653000	-3.877055000
6	-5.415094000	-1.465255000	-1.912995000
1	-6.334547000	-2.036140000	-2.082688000
6	-4.741444000	-1.556262000	-0.689707000
1	-5.126722000	-2.174419000	0.129198000
6	-3.564218000	-0.815039000	-0.461925000
6	-2.884092000	-0.976524000	0.859979000
6	-1.662732000	1.130605000	0.338931000
1	-0.603448000	1.387264000	0.510955000
6	-1.260748000	-0.108452000	2.462776000
1	-0.171006000	-0.026083000	2.317098000
1	-1.502740000	-1.067762000	2.938489000
1	-1.610802000	0.725652000	3.100203000
6	-1.745922000	2.171273000	-1.950923000
1	-1.645928000	1.999952000	-3.036031000
1	-0.866857000	2.758378000	-1.635730000
1	-2.651977000	2.773325000	-1.766617000
6	-0.561081000	-0.035200000	-1.708927000
6	-2.513664000	2.304455000	0.822748000
6	-3.905115000	2.192895000	1.017148000
1	-4.407261000	1.237951000	0.837998000
6	-4.656631000	3.299213000	1.438534000
1	-5.737938000	3.194861000	1.581920000
6	-4.030747000	4.533235000	1.680828000

6	-2.644241000	4.651134000	1.501557000
1	-2.142097000	5.605488000	1.696898000
6	-1.896182000	3.542387000	1.078607000
1	-0.815740000	3.634120000	0.929996000
1	-4.620262000	5.394573000	2.013728000
1	0.124909000	0.631023000	-2.258033000
1	-0.927965000	-0.802604000	-2.415528000
8	1.223529000	-2.863022000	0.799247000
8	-0.150428000	-4.674002000	1.011568000
6	0.134308000	-3.555157000	0.515948000
8	-0.703450000	-2.939213000	-0.347158000
19	-2.671111000	-4.280847000	0.643644000

TS 9-10



Zero-point correction = 0.591085 (Hartree/particle)
Thermal correction to energy = 0.633074
Thermal correction to enthalpy = 0.634018
Thermal correction to Gibbs free energy = 0.515339
Sum of electronic and zero-point energies = -2854.744364
Sum of electronic and thermal enthalpies = -2854.702375
Sum of electronic and thermal free energies = -2854.701431
Sum of electronic and thermal Free Energies = -2854.820110

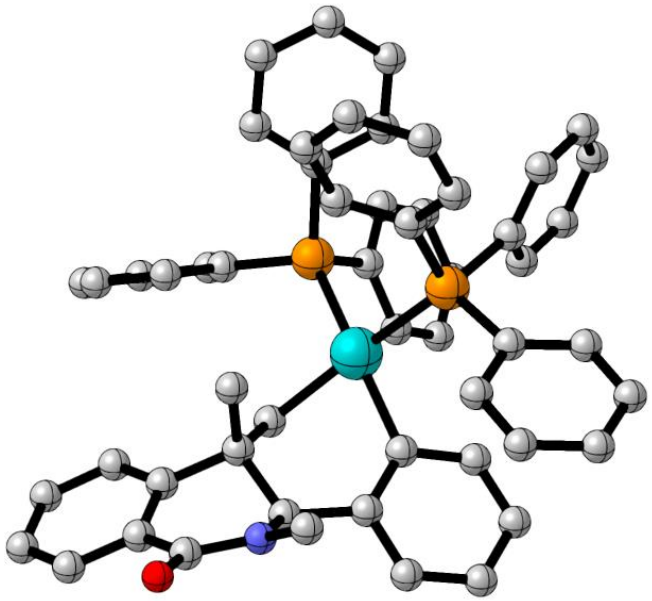
E_{SCF} (M06L/def2-TZVPP) = -2855.335449

Imaginary Frequency = -789.17 cm^{-1}

6	-5.009593000	0.176789000	0.723871000
6	-2.291811000	0.527959000	-0.245682000

6	-3.227056000	-0.599214000	-0.775658000
1	-3.744666000	-0.133216000	-1.640764000
6	-1.089218000	0.656768000	-1.194515000
1	-1.388068000	0.479601000	-2.244793000
6	-1.841089000	0.303569000	1.230313000
1	-1.321152000	-0.663153000	1.339020000
1	-2.700561000	0.334362000	1.922391000
1	-1.144892000	1.112098000	1.519646000
6	-3.329522000	-2.525322000	-2.349580000
6	-2.588373000	-1.851823000	-1.358813000
6	-2.797678000	-3.632894000	-3.025575000
1	-3.392805000	-4.136390000	-3.796107000
6	-1.284287000	-2.303684000	-1.034818000
6	-1.497581000	-4.077769000	-2.728998000
1	-1.071729000	-4.933926000	-3.264790000
6	-0.755710000	-3.414960000	-1.744929000
1	0.252226000	-3.749863000	-1.475145000
1	-4.332203000	-2.161489000	-2.609028000
7	-4.273913000	-0.882784000	0.232477000
6	-5.442441000	2.611842000	0.394599000
6	-4.548312000	1.535938000	0.262725000
6	-5.048249000	3.906973000	0.034740000
1	-5.750765000	4.742375000	0.127839000
6	-3.226422000	1.752462000	-0.210966000
6	-3.747029000	4.125186000	-0.446194000
1	-3.431720000	5.133119000	-0.740330000
6	-2.841917000	3.056311000	-0.560627000
1	-1.833628000	3.243466000	-0.941316000
1	-6.440984000	2.401445000	0.791027000
8	-5.959578000	0.039487000	1.515946000
6	-4.500328000	-2.227105000	0.748570000
1	-5.224523000	-2.132211000	1.570987000
1	-4.912264000	-2.900120000	-0.024490000
1	-3.552895000	-2.662851000	1.113848000
1	-0.620723000	1.648411000	-1.139553000
46	0.288927000	-0.792012000	-0.668975000
15	2.005853000	0.644320000	-0.287685000
6	2.613662000	0.530332000	1.456668000
6	2.369292000	1.524590000	2.430737000
1	1.874657000	2.459533000	2.152349000
6	2.790493000	1.335095000	3.758367000
1	2.608276000	2.120889000	4.500640000
6	3.473271000	0.157970000	4.124106000
1	3.816564000	0.019730000	5.156104000
6	3.721987000	-0.831188000	3.155479000
1	4.225271000	-1.764256000	3.427247000
6	3.290487000	-0.655234000	1.829826000
1	3.415031000	-1.461068000	1.101399000

6	3.479943000	0.154553000	-1.255809000
6	4.772957000	0.609854000	-0.922474000
1	4.913639000	1.267152000	-0.057390000
6	5.873532000	0.211600000	-1.693501000
1	6.877588000	0.564201000	-1.433461000
6	5.689200000	-0.646085000	-2.792221000
1	6.552482000	-0.961509000	-3.388452000
6	4.404528000	-1.107983000	-3.119066000
1	4.262351000	-1.788309000	-3.965413000
6	3.299258000	-0.710416000	-2.352011000
1	2.290641000	-1.079750000	-2.573812000
6	1.814694000	2.448508000	-0.583376000
6	2.421057000	4.510149000	-1.739173000
1	3.060925000	5.035754000	-2.456304000
6	2.627241000	3.142114000	-1.502592000
1	3.422544000	2.610459000	-2.033282000
1	0.106086000	2.618823000	0.757303000
6	0.776796000	3.149037000	0.073558000
6	0.580961000	4.518561000	-0.155438000
1	-0.228474000	5.041973000	0.364716000
6	1.404057000	5.202977000	-1.064050000
1	1.246804000	6.270494000	-1.251746000
8	1.542425000	-2.423430000	0.087589000
6	1.029823000	-2.781002000	1.249475000
8	-0.306497000	-2.683670000	1.424037000
8	1.745254000	-3.138989000	2.233835000
19	0.272738000	-1.491347000	3.614525000
1	-0.848680000	-2.346853000	0.183423000



Zero-point correction = 0.835915 (Hartree/particle)
Thermal correction to energy = 0.889620
Thermal correction to enthalpy = 0.890565
Thermal correction to Gibbs free energy = 0.746760
Sum of electronic and zero-point energies = -3026.527114
Sum of electronic and thermal enthalpies = -3026.473409
Sum of electronic and thermal free energies = -3026.472464
Sum of electronic and thermal Free Energies = -3026.616269

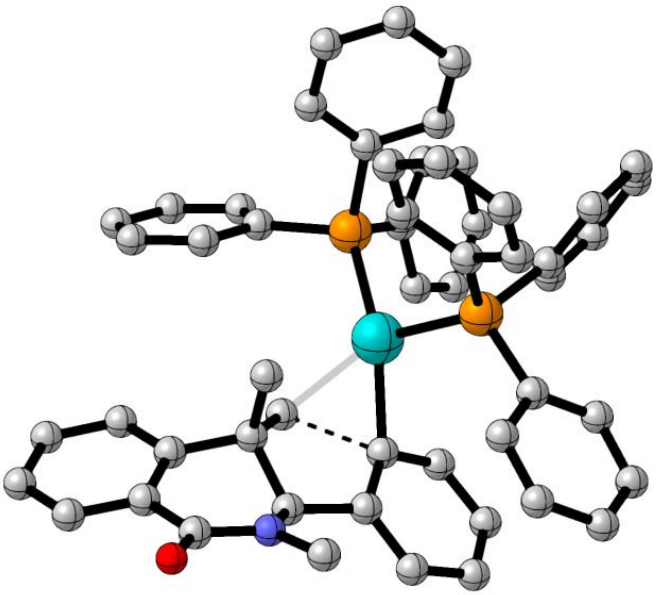
E_{SCF} (M06L/def2-TZVPP) = -3027.363029

6	0.283344000	2.411999000	-2.332610000
1	-0.775565000	2.154419000	-2.451479000
1	4.017339000	3.362408000	-1.989214000
7	4.390567000	1.810782000	0.246690000
6	6.747232000	-1.023172000	0.528084000
6	5.526501000	-0.343489000	0.375010000
6	6.821259000	-2.402714000	0.299980000
1	7.776224000	-2.928789000	0.407997000
6	4.347854000	-1.049052000	0.012094000
6	5.659914000	-3.106889000	-0.058874000
1	5.705571000	-4.187422000	-0.238691000
6	4.433418000	-2.435738000	-0.193380000
1	3.539268000	-3.000333000	-0.472437000
1	7.620978000	-0.443363000	0.842523000
8	6.312582000	1.618451000	1.519976000
6	3.987430000	3.046146000	0.906837000
1	3.884697000	3.882447000	0.196492000
1	3.016428000	2.911631000	1.421793000

1	4.770026000	3.277531000	1.644331000
1	1.851882000	-1.951499000	-0.776208000
46	0.153339000	0.065364000	-0.541992000
15	-1.479524000	1.531288000	0.391921000
15	-1.002235000	-2.004067000	-0.226059000
6	-1.145162000	3.322787000	0.160922000
6	0.121398000	3.796565000	0.564203000
6	-0.387023000	5.977175000	-0.374187000
6	-1.654111000	5.516782000	-0.759916000
1	-2.348877000	6.187315000	-1.278022000
6	-2.035281000	4.190558000	-0.495129000
1	-3.016725000	3.826124000	-0.815561000
6	-1.604373000	1.411050000	2.221035000
6	-2.188474000	2.437845000	2.993806000
1	-2.534404000	3.354736000	2.503658000
6	-2.301581000	2.293651000	4.383835000
1	-2.756698000	3.093169000	4.978879000
6	-1.822115000	1.131847000	5.013416000
1	-1.911844000	1.021941000	6.099786000
6	-1.212610000	0.122404000	4.252465000
1	-0.825065000	-0.779211000	4.737733000
6	-1.096740000	0.266039000	2.862816000
1	-0.605938000	-0.503955000	2.262122000
6	-3.203623000	1.342463000	-0.225947000
6	-4.354484000	1.556349000	0.557691000
1	-4.254150000	1.898254000	1.592382000
6	-5.624861000	1.279779000	0.029618000
1	-6.515567000	1.435582000	0.648764000
6	-5.756827000	0.789232000	-1.281178000
1	-6.749735000	0.555554000	-1.680796000
6	-4.614232000	0.593407000	-2.074486000
1	-4.701405000	0.196059000	-3.090786000
6	-3.345301000	0.871416000	-1.547795000
1	-2.449255000	0.674810000	-2.144078000
6	-2.237332000	-2.283271000	1.119599000
6	-1.903570000	-3.005654000	2.284185000
1	-0.959103000	-3.555673000	2.336139000
6	-2.775774000	-3.025045000	3.382491000
1	-2.500133000	-3.589891000	4.280053000
6	-3.993797000	-2.329142000	3.333650000
1	-4.667341000	-2.335323000	4.197297000
6	-4.346128000	-1.634588000	2.166374000
1	-5.297885000	-1.096596000	2.104455000
6	-3.478196000	-1.613045000	1.066860000
1	-3.768375000	-1.072961000	0.163903000
6	-1.972428000	-2.219667000	-1.774658000
6	-3.173266000	-2.953178000	-1.839009000
1	-3.564292000	-3.436681000	-0.938164000

6	-3.877549000	-3.045451000	-3.049410000
1	-4.816777000	-3.608063000	-3.089213000
6	-3.382246000	-2.418029000	-4.204516000
1	-3.936165000	-2.489525000	-5.147174000
6	-2.173268000	-1.703033000	-4.150740000
1	-1.779817000	-1.215444000	-5.049290000
6	-1.470519000	-1.603140000	-2.941579000
1	-0.539892000	-1.023513000	-2.873878000
6	0.017387000	-3.537264000	-0.140742000
6	0.685358000	-5.738554000	-0.945932000
1	0.553912000	-6.565325000	-1.652653000
6	-0.143060000	-4.609068000	-1.039401000
1	-0.912877000	-4.557644000	-1.815548000
1	1.189248000	-2.763092000	1.516255000
6	1.029181000	-3.610836000	0.841465000
6	1.847699000	-4.744614000	0.942053000
1	2.633942000	-4.779747000	1.703378000
6	1.677702000	-5.811513000	0.044495000
1	2.324714000	-6.692825000	0.110624000
1	0.823145000	3.112043000	1.051242000
6	0.499084000	5.115109000	0.296532000
1	1.493144000	5.465886000	0.592441000
1	-0.085148000	7.006037000	-0.598578000

TS 10-11



Zero-point correction = 0.833287 (Hartree/particle)
Thermal correction to energy = 0.887117
Thermal correction to enthalpy = 0.888061

Thermal correction to Gibbs free energy = 0.743385
Sum of electronic and zero-point energies = -3026.500330
Sum of electronic and thermal enthalpies = -3026.446500
Sum of electronic and thermal free energies = -3026.445560
Sum of electronic and thermal Free Energies = -3026.590230

E_{SCF} (M06L/def2-TZVPP) = -3027.333617

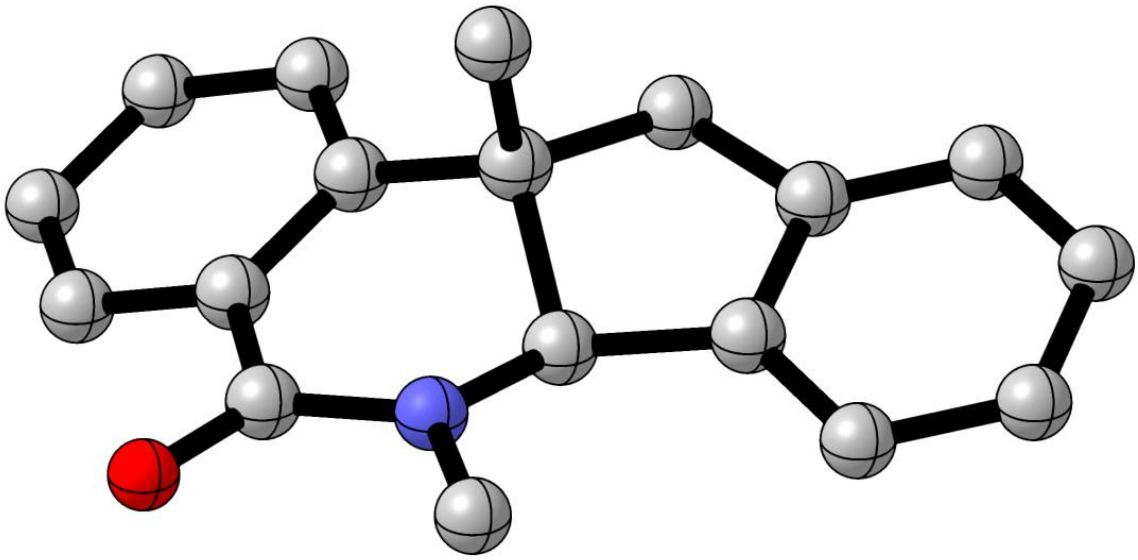
Imaginary Frequency = -335.78 cm^{-1}

6	-5.596641000	-0.465601000	0.718969000
6	-3.063294000	0.591533000	-0.218232000
6	-3.713996000	-0.674646000	-0.820872000
1	-4.353376000	-0.307462000	-1.657678000
6	-1.990708000	1.038650000	-1.218034000
1	-2.396013000	1.224139000	-2.225694000
6	-2.452227000	0.304843000	1.177783000
1	-1.670224000	-0.475131000	1.117000000
1	-3.224682000	-0.025362000	1.891217000
1	-1.990922000	1.220862000	1.581899000
6	-2.966518000	-2.691097000	-2.217989000
6	-2.657838000	-1.510357000	-1.515415000
6	-2.079586000	-3.221946000	-3.162478000
1	-2.311176000	-4.164074000	-3.668890000
6	-1.432427000	-0.839908000	-1.766455000
6	-0.923939000	-2.495524000	-3.498603000
1	-0.244997000	-2.867811000	-4.274626000
6	-0.633293000	-1.286943000	-2.851201000
1	0.260330000	-0.724356000	-3.145477000
1	-3.928899000	-3.185292000	-2.045263000
7	-4.625232000	-1.280113000	0.165417000
6	-6.544152000	1.845476000	0.705098000
6	-5.447857000	1.008472000	0.434738000
6	-6.441063000	3.229113000	0.510361000
1	-7.300481000	3.877547000	0.713011000
6	-4.222838000	1.564290000	-0.017528000
6	-5.230607000	3.780836000	0.057495000
1	-5.145036000	4.862041000	-0.101656000
6	-4.124753000	2.952432000	-0.196088000
1	-3.181227000	3.387868000	-0.541373000
1	-7.463730000	1.381287000	1.075577000
8	-6.509961000	-0.910239000	1.435773000
6	-4.629313000	-2.695593000	0.502534000
1	-5.273221000	-3.291613000	-0.174855000
1	-3.601584000	-3.082988000	0.445375000
1	-5.029533000	-2.799274000	1.522594000
1	-1.482214000	1.966940000	-0.901643000
46	0.007477000	0.112490000	-0.532632000

15	1.053127000	-1.790689000	0.363559000
15	1.486905000	1.898844000	-0.153860000
6	0.389696000	-3.421175000	-0.148435000
6	-0.862549000	-3.823281000	0.366525000
6	-0.824803000	-5.804767000	-1.041375000
6	0.415312000	-5.406301000	-1.563614000
1	0.917089000	-6.022132000	-2.318550000
6	1.021186000	-4.221341000	-1.121269000
1	1.992137000	-3.917141000	-1.525668000
6	1.064092000	-1.909147000	2.196526000
6	1.248314000	-3.126797000	2.886432000
1	1.344893000	-4.060276000	2.321424000
6	1.293040000	-3.140728000	4.288260000
1	1.434785000	-4.088994000	4.818867000
6	1.155076000	-1.942807000	5.011062000
1	1.192057000	-1.957761000	6.106056000
6	0.959690000	-0.730976000	4.329761000
1	0.849642000	0.206539000	4.884342000
6	0.905950000	-0.715701000	2.929086000
1	0.744752000	0.221712000	2.388866000
6	2.833194000	-1.885434000	-0.101465000
6	3.841719000	-2.361114000	0.759388000
1	3.572568000	-2.774355000	1.736648000
6	5.190720000	-2.257989000	0.385686000
1	5.971345000	-2.615044000	1.067111000
6	5.543487000	-1.686380000	-0.849189000
1	6.598954000	-1.589166000	-1.126399000
6	4.541151000	-1.232545000	-1.722953000
1	4.803268000	-0.767860000	-2.679050000
6	3.194350000	-1.331632000	-1.347881000
1	2.409208000	-0.933890000	-1.998676000
6	2.502755000	1.895042000	1.380850000
6	2.144858000	2.658246000	2.511255000
1	1.344795000	3.401907000	2.437000000
6	2.808618000	2.468012000	3.733481000
1	2.519894000	3.068894000	4.603350000
6	3.838919000	1.520343000	3.842237000
1	4.347787000	1.367037000	4.799926000
6	4.212836000	0.771833000	2.714435000
1	5.014979000	0.029133000	2.781002000
6	3.550986000	0.953995000	1.494196000
1	3.845795000	0.358713000	0.626927000
6	2.724748000	2.029797000	-1.509624000
6	4.051372000	2.463186000	-1.322054000
1	4.389721000	2.759765000	-0.324268000
6	4.943343000	2.494201000	-2.405563000
1	5.976958000	2.821630000	-2.247767000
6	4.515104000	2.108803000	-3.686326000

1	5.214675000	2.131656000	-4.529185000
6	3.185722000	1.696062000	-3.884921000
1	2.843700000	1.398642000	-4.882342000
6	2.298474000	1.652998000	-2.801083000
1	1.263785000	1.313127000	-2.936238000
6	0.694988000	3.560351000	-0.148467000
6	0.452046000	5.856955000	-0.933104000
1	0.815756000	6.689183000	-1.546162000
6	1.150648000	4.640388000	-0.931873000
1	2.053239000	4.525424000	-1.540603000
1	-0.854741000	2.879305000	1.213562000
6	-0.480473000	3.721170000	0.620453000
6	-1.167496000	4.944559000	0.632253000
1	-2.074262000	5.050270000	1.237592000
6	-0.704235000	6.014529000	-0.150030000
1	-1.245895000	6.966588000	-0.155077000
1	-1.361488000	-3.202348000	1.119493000
6	-1.457718000	-5.013173000	-0.068219000
1	-2.424952000	-5.319892000	0.345450000
1	-1.295986000	-6.731445000	-1.386813000

11



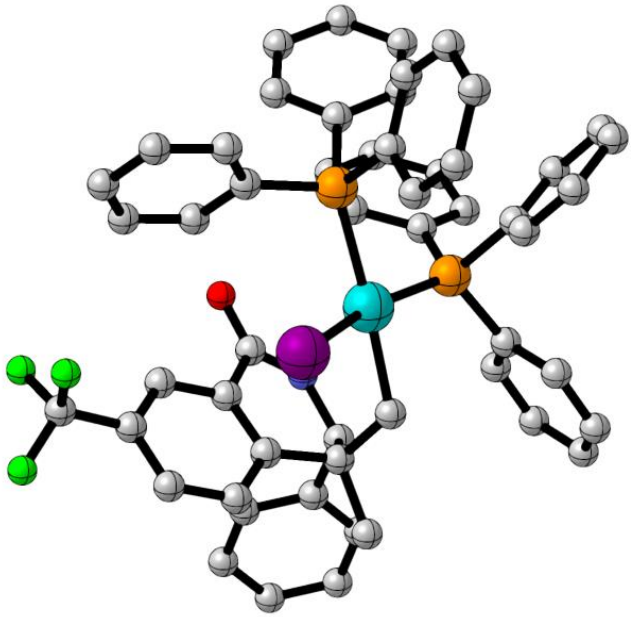
Zero-point correction = 0.299580 (Hartree/particle)
Thermal correction to energy = 0.315833
Thermal correction to enthalpy = 0.316778
Thermal correction to Gibbs free energy = 0.256995
Sum of electronic and zero-point energies = -826.054748
Sum of electronic and thermal enthalpies = -826.038495

Sum of electronic and thermal free energies = -826.037550
Sum of electronic and thermal Free Energies = -826.097333

E_{SCF} (M06L/def2-TZVPP) = -826.354328

6	1.564168000	1.709198000	0.023553000
6	0.107084000	-0.759024000	0.440577000
6	-0.475567000	0.435667000	-0.376806000
1	-0.204031000	0.256759000	-1.443900000
6	-0.849127000	-1.909018000	0.026941000
1	-0.548298000	-2.328087000	-0.955104000
6	-0.015458000	-0.520490000	1.967788000
1	-1.071705000	-0.401946000	2.268154000
1	0.537193000	0.379645000	2.283323000
1	0.405388000	-1.386303000	2.508502000
6	-3.077856000	1.052637000	-0.494994000
6	-1.978444000	0.207528000	-0.292177000
6	-4.376766000	0.510134000	-0.451705000
1	-5.240064000	1.170050000	-0.593179000
6	-2.178957000	-1.182663000	-0.096003000
6	-4.574274000	-0.862961000	-0.233218000
1	-5.591089000	-1.270010000	-0.197670000
6	-3.470324000	-1.719343000	-0.063993000
1	-3.619294000	-2.793633000	0.097108000
1	-2.946437000	2.120486000	-0.689660000
7	0.176948000	1.685669000	0.037063000
6	3.623387000	0.368639000	-0.451535000
6	2.250927000	0.372510000	-0.141333000
6	4.319333000	-0.842159000	-0.566639000
1	5.385843000	-0.838918000	-0.817382000
6	1.571519000	-0.856009000	0.068501000
6	3.647895000	-2.058684000	-0.354220000
1	4.189326000	-3.007587000	-0.441920000
6	2.281073000	-2.062805000	-0.029204000
1	1.759599000	-3.011410000	0.143853000
1	4.126031000	1.330749000	-0.594263000
8	2.217677000	2.757934000	0.168818000
6	-0.553118000	2.931319000	0.228308000
1	-0.973832000	3.313053000	-0.722599000
1	-1.370293000	2.784619000	0.953803000
1	0.157349000	3.675235000	0.617273000
1	-0.868719000	-2.742700000	0.750628000

p-CF_3-1



Zero-point correction = 0.854445
Thermal correction to energy = 0.914201
Thermal correction to enthalpy = 0.915145
Thermal correction to Gibbs free energy = 0.756560
Sum of electronic and zero-point energies = -3662.211648
Sum of electronic and thermal enthalpies = -3662.151892
Sum of electronic and thermal free energies = -3662.150948
Sum of electronic and thermal Free Energies = -3662.309533

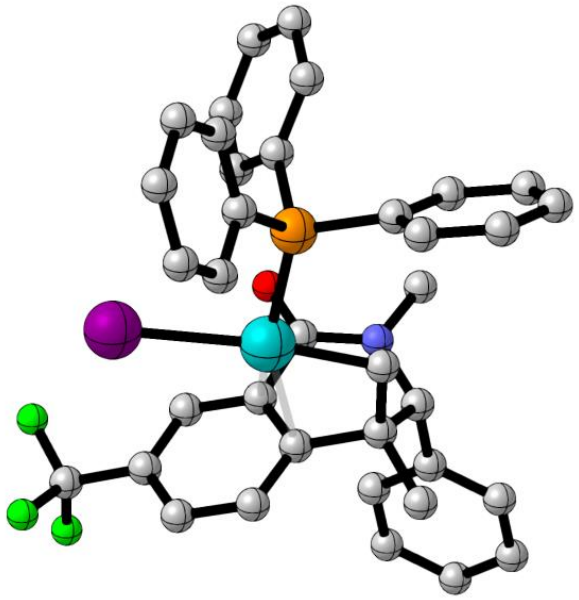
E_{SCF} (M06L/def2-TZVPP) = -3663.066093

46	-0.312919000	-0.037953000	-0.734388000
53	0.414556000	2.248190000	-2.069535000
15	-1.225035000	-2.088453000	-0.212062000
15	-2.046743000	1.322518000	0.353855000
6	-1.375095000	2.953340000	0.863570000
6	-2.043711000	4.156121000	0.575449000
6	-0.138929000	2.976667000	1.543195000
6	-1.469407000	5.380424000	0.950258000
1	-2.997027000	4.137656000	0.038787000
6	0.420048000	4.202903000	1.925803000
1	0.388330000	2.040735000	1.765091000
6	-0.237472000	5.406017000	1.620731000
1	-1.983772000	6.316735000	0.706728000
1	1.387569000	4.226715000	2.436417000
1	0.217598000	6.362912000	1.898343000
6	-3.496581000	1.744280000	-0.714989000
6	-3.289180000	1.974735000	-2.091443000
6	-4.799895000	1.867465000	-0.190970000

6	-4.364792000	2.308876000	-2.925162000
1	-2.275740000	1.906523000	-2.500663000
6	-5.877604000	2.182310000	-1.033058000
1	-4.977558000	1.713145000	0.876721000
6	-5.665277000	2.401619000	-2.402535000
1	-4.182213000	2.492864000	-3.989921000
1	-6.885473000	2.264554000	-0.611149000
1	-6.507548000	2.651955000	-3.057311000
6	-2.861900000	0.735966000	1.906264000
6	-3.796614000	-0.320513000	1.844492000
6	-2.516040000	1.265789000	3.165252000
6	-4.356998000	-0.848495000	3.013404000
1	-4.095823000	-0.724088000	0.875340000
6	-3.080914000	0.735177000	4.335388000
1	-1.801562000	2.091098000	3.231616000
6	-3.995103000	-0.327158000	4.265796000
1	-5.073216000	-1.674285000	2.942477000
1	-2.801603000	1.157890000	5.306954000
1	-4.426510000	-0.744379000	5.182180000
6	-2.945863000	-2.096756000	-0.886866000
6	-3.986732000	-2.885992000	-0.355720000
6	-3.210017000	-1.255814000	-1.986497000
6	-5.273049000	-2.818157000	-0.908167000
1	-3.806658000	-3.517872000	0.517902000
6	-4.496359000	-1.197633000	-2.543680000
1	-2.403850000	-0.620461000	-2.373726000
6	-5.530881000	-1.972283000	-2.001022000
1	-6.080159000	-3.420147000	-0.476186000
1	-4.692889000	-0.513902000	-3.374519000
1	-6.540784000	-1.910677000	-2.420542000
6	-1.347297000	-2.555107000	1.552811000
6	-1.823164000	-3.814952000	1.982160000
6	-0.935128000	-1.607902000	2.507951000
6	-1.919402000	-4.098977000	3.351705000
1	-2.087985000	-4.583117000	1.247976000
6	-1.028051000	-1.897753000	3.875536000
1	-0.497167000	-0.661467000	2.181800000
6	-1.530013000	-3.136633000	4.299398000
1	-2.288472000	-5.077244000	3.678876000
1	-0.694410000	-1.150716000	4.601125000
1	-1.604140000	-3.362951000	5.368798000
6	-0.542509000	-3.602207000	-1.021109000
6	-0.761527000	-3.786387000	-2.403311000
6	0.292115000	-4.508328000	-0.337886000
6	-0.154529000	-4.850409000	-3.084411000
1	-1.407370000	-3.088996000	-2.947376000
6	0.896276000	-5.576276000	-1.020373000
1	0.465049000	-4.387668000	0.734565000

6	0.680315000	-5.746862000	-2.396459000
1	-0.333072000	-4.977764000	-4.157504000
1	1.535211000	-6.275822000	-0.470045000
1	1.156094000	-6.576386000	-2.930303000
8	1.615598000	0.271288000	2.528752000
7	2.218073000	-1.502826000	1.193280000
6	2.689703000	-1.040549000	-1.254004000
6	3.150895000	0.333903000	-0.803538000
6	3.869388000	1.222409000	-1.617767000
1	4.181108000	0.914770000	-2.619039000
6	4.164907000	2.520168000	-1.181218000
1	4.710356000	3.207813000	-1.834034000
6	3.747873000	2.946275000	0.090547000
6	3.064491000	2.059727000	0.928965000
1	2.770374000	2.342506000	1.941227000
6	2.766652000	0.764248000	0.485249000
6	2.124099000	-0.155975000	1.468444000
6	2.804106000	-2.034075000	-0.050341000
1	2.192075000	-2.910826000	-0.330176000
6	2.079685000	-2.453792000	2.293626000
1	1.258010000	-3.165126000	2.113680000
1	1.855089000	-1.884289000	3.204651000
1	3.024298000	-3.014535000	2.414319000
6	3.555266000	-1.598127000	-2.412362000
1	3.386809000	-1.011866000	-3.330804000
1	3.266502000	-2.641729000	-2.628074000
1	4.631194000	-1.581172000	-2.170057000
6	1.240308000	-0.987858000	-1.817342000
6	4.224234000	-2.534314000	0.199705000
6	5.198536000	-1.715618000	0.804213000
1	4.933200000	-0.703309000	1.124413000
6	6.503218000	-2.191876000	0.996349000
1	7.253153000	-1.543688000	1.463109000
6	6.849626000	-3.493502000	0.595755000
6	5.880650000	-4.319942000	0.005975000
1	6.138849000	-5.340079000	-0.299760000
6	4.575821000	-3.840647000	-0.186208000
1	3.813816000	-4.481959000	-0.646673000
1	7.869242000	-3.863355000	0.749865000
1	0.937897000	-2.017781000	-2.060622000
1	1.253072000	-0.404644000	-2.750337000
6	3.977338000	4.369551000	0.522989000
9	3.981682000	4.497548000	1.886299000
9	5.170340000	4.854916000	0.067545000
9	3.007443000	5.204435000	0.053480000

***p*-CF_3-2**



Zero-point correction = 0.583468
Thermal correction to energy = 0.626531
Thermal correction to enthalpy = 0.627475
Thermal correction to Gibbs free energy = 0.500448
Sum of electronic and zero-point energies = -2625.969703
Sum of electronic and thermal enthalpies = -2625.926640
Sum of electronic and thermal free energies = -2625.925696
Sum of electronic and thermal Free Energies = -2625.052723

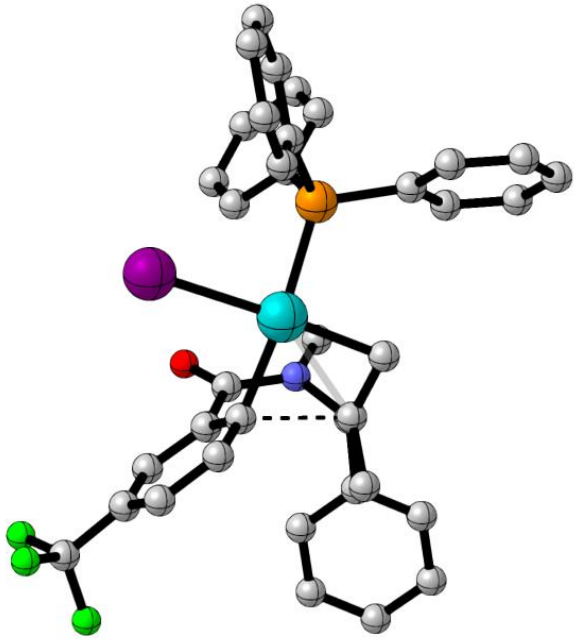
E_{SCF} (M06L/def2-TZVPP) = -2626.553171

46	-0.362745000	0.183414000	-0.618336000
53	-1.020434000	2.793371000	-0.153593000
15	-2.367374000	-0.603615000	-0.003602000
6	-2.718228000	-2.335819000	-0.506515000
6	-3.393535000	-2.606549000	-1.713351000
6	-2.212809000	-3.408716000	0.259845000
6	-3.569135000	-3.930806000	-2.141049000
1	-3.792700000	-1.779698000	-2.309996000
6	-2.394269000	-4.730782000	-0.170279000
1	-1.695062000	-3.204498000	1.203182000
6	-3.071235000	-4.995092000	-1.371965000
1	-4.104086000	-4.131037000	-3.075794000
1	-2.007235000	-5.556499000	0.436909000
1	-3.213151000	-6.028340000	-1.706699000
6	-2.493491000	-0.657502000	1.820316000
6	-1.536451000	0.028550000	2.593220000
6	-3.499125000	-1.418676000	2.458936000
6	-1.587763000	-0.040234000	3.993036000

1	-0.749106000	0.604964000	2.098245000
6	-3.554405000	-1.468267000	3.858482000
1	-4.217907000	-1.990787000	1.862477000
6	-2.598420000	-0.779770000	4.625882000
1	-0.823131000	0.477759000	4.579613000
1	-4.337478000	-2.055574000	4.350427000
1	-2.637226000	-0.832035000	5.719573000
6	-3.791660000	0.328632000	-0.678219000
6	-5.013017000	0.430596000	0.012635000
6	-3.651945000	0.912464000	-1.953526000
6	-6.092080000	1.105831000	-0.577309000
1	-5.114868000	0.008465000	1.016826000
6	-4.738729000	1.570062000	-2.544700000
1	-2.678178000	0.876932000	-2.454714000
6	-5.959406000	1.668228000	-1.856660000
1	-7.036869000	1.198297000	-0.030786000
1	-4.623286000	2.029313000	-3.532100000
1	-6.803542000	2.197466000	-2.311948000
8	1.730135000	-0.231276000	2.774488000
7	2.117376000	-1.930482000	1.263639000
6	1.848916000	-1.513665000	-1.174823000
6	2.093800000	-0.020988000	-0.873084000
6	2.263966000	0.967691000	-1.869688000
1	2.202604000	0.689987000	-2.925207000
6	2.534402000	2.297651000	-1.521576000
1	2.652854000	3.054662000	-2.300832000
6	2.613294000	2.669601000	-0.170584000
6	2.416287000	1.716161000	0.836461000
1	2.430164000	1.988697000	1.894285000
6	2.151342000	0.382794000	0.495454000
6	1.972185000	-0.604730000	1.614361000
6	2.558465000	-2.361665000	-0.072440000
1	2.166735000	-3.388665000	-0.204205000
6	2.077372000	-2.947015000	2.306509000
1	3.065128000	-3.434171000	2.410744000
1	1.324406000	-3.717883000	2.057358000
1	1.806292000	-2.449401000	3.248007000
6	2.349368000	-1.916608000	-2.569632000
1	1.748799000	-1.418743000	-3.350303000
1	2.231151000	-3.005351000	-2.711092000
1	3.411573000	-1.660120000	-2.719868000
6	0.323535000	-1.723550000	-1.056910000
6	4.077113000	-2.433621000	-0.198192000
6	4.920974000	-1.410488000	0.277129000
1	4.498300000	-0.547166000	0.798429000
6	6.309327000	-1.491641000	0.095481000
1	6.950260000	-0.686007000	0.469711000
6	6.876719000	-2.598699000	-0.555682000

6	6.046156000	-3.630804000	-1.019235000
1	6.478648000	-4.506438000	-1.515659000
6	4.658143000	-3.546337000	-0.836858000
1	4.010447000	-4.355835000	-1.195584000
1	7.961711000	-2.660815000	-0.692443000
1	-0.153518000	-2.029303000	-2.003822000
1	0.044866000	-2.422441000	-0.254828000
6	2.961162000	4.091726000	0.200059000
9	2.434600000	4.450135000	1.398671000
9	4.319819000	4.244928000	0.297546000
9	2.529982000	4.980337000	-0.734716000

p-CF_3-TS 2-3



Zero-point correction = 0.580847 (Hartree/particle)
Thermal correction to energy = 0.623835
Thermal correction to enthalpy = 0.624779
Thermal correction to Gibbs free energy = 0.498625
Sum of electronic and zero-point energies = -2625.915309
Sum of electronic and thermal enthalpies = -2625.872321
Sum of electronic and thermal free energies = -2625.871377
Sum of electronic and thermal Free Energies = -2625.997531

E_{SCF} (M06L/def2-TZVPP) = -2626.496156

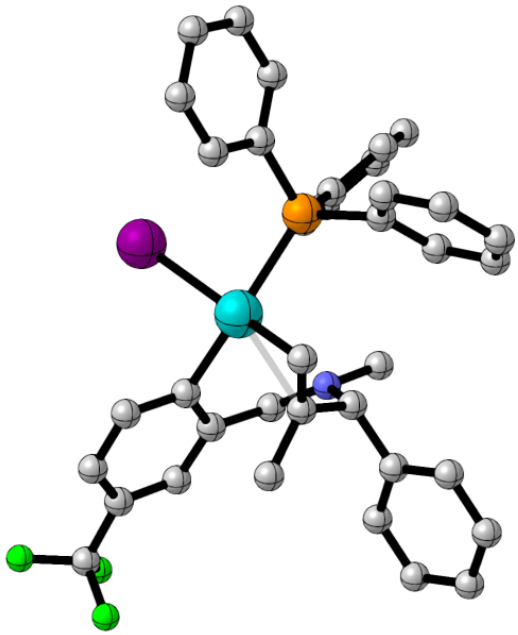
Imaginary Frequency = -217.23 cm^{-1}

46	0.372886000	-0.176839000	-0.683132000
53	0.504847000	-2.765872000	0.183081000
15	2.581502000	0.134481000	-0.058718000

6	3.377078000	1.669871000	-0.696858000
6	4.226722000	1.635221000	-1.819519000
6	3.037682000	2.918359000	-0.129082000
6	4.732369000	2.827708000	-2.360545000
1	4.501123000	0.672210000	-2.262376000
6	3.547206000	4.107072000	-0.670049000
1	2.390294000	2.952582000	0.754881000
6	4.395285000	4.064838000	-1.789388000
1	5.399544000	2.787011000	-3.228532000
1	3.284873000	5.067902000	-0.213516000
1	4.794480000	4.993211000	-2.211741000
6	2.673458000	0.371609000	1.759182000
6	1.598093000	-0.048174000	2.567250000
6	3.786318000	1.006802000	2.355904000
6	1.635675000	0.159986000	3.953886000
1	0.734338000	-0.542380000	2.114722000
6	3.823090000	1.202456000	3.743715000
1	4.611046000	1.367616000	1.732036000
6	2.747103000	0.780914000	4.544185000
1	0.783470000	-0.162035000	4.560763000
1	4.690493000	1.692378000	4.199635000
1	2.775515000	0.943635000	5.627303000
6	3.774803000	-1.171223000	-0.529251000
6	4.915718000	-1.463925000	0.239673000
6	3.545638000	-1.856823000	-1.739426000
6	5.827916000	-2.431542000	-0.207305000
1	5.079700000	-0.954262000	1.194148000
6	4.468728000	-2.810247000	-2.189617000
1	2.626104000	-1.658306000	-2.301084000
6	5.609806000	-3.099248000	-1.423035000
1	6.708481000	-2.668157000	0.399792000
1	4.283759000	-3.345613000	-3.126932000
1	6.323105000	-3.856092000	-1.767157000
8	-1.837741000	0.087311000	2.745605000
7	-1.266700000	1.700677000	1.201570000
6	-1.166621000	1.605799000	-1.356471000
6	-1.734069000	-0.426917000	-0.790994000
6	-2.254177000	-1.258348000	-1.800168000
1	-1.747750000	-1.335899000	-2.767777000
6	-3.384187000	-2.042042000	-1.547744000
1	-3.772256000	-2.715089000	-2.318120000
6	-4.001812000	-1.999319000	-0.281477000
6	-3.490756000	-1.171256000	0.724953000
1	-3.932997000	-1.156584000	1.725098000
6	-2.376816000	-0.357021000	0.458171000
6	-1.821171000	0.480907000	1.569364000
6	-1.561895000	2.392862000	-0.063077000
1	-0.855027000	3.243259000	-0.063795000

6	-0.728036000	2.552636000	2.259084000
1	-1.393594000	3.416450000	2.448199000
1	0.272564000	2.919692000	1.967263000
1	-0.647393000	1.947755000	3.171133000
6	-2.146487000	1.637436000	-2.517516000
1	-1.794076000	0.988992000	-3.334703000
1	-2.189619000	2.674043000	-2.903367000
1	-3.163845000	1.338732000	-2.226254000
6	0.233317000	1.669961000	-1.672147000
6	-2.951858000	3.026900000	-0.118359000
6	-4.099061000	2.439323000	0.444605000
1	-4.026705000	1.491393000	0.980822000
6	-5.349856000	3.064337000	0.325297000
1	-6.232194000	2.589441000	0.767439000
6	-5.472178000	4.287886000	-0.350798000
6	-4.330277000	4.892274000	-0.900341000
1	-4.408953000	5.855859000	-1.415455000
6	-3.082372000	4.266184000	-0.777727000
1	-2.189498000	4.745297000	-1.199858000
1	-6.449959000	4.773197000	-0.439967000
1	0.544749000	1.491865000	-2.711505000
1	0.861917000	2.384720000	-1.129415000
6	-5.254660000	-2.799118000	-0.034400000
9	-6.370164000	-2.105779000	-0.424602000
9	-5.257589000	-3.969633000	-0.733067000
9	-5.419286000	-3.101734000	1.282577000

***p*-CF_3-3**



Zero-point correction = 0.581661 (Hartree/particle)

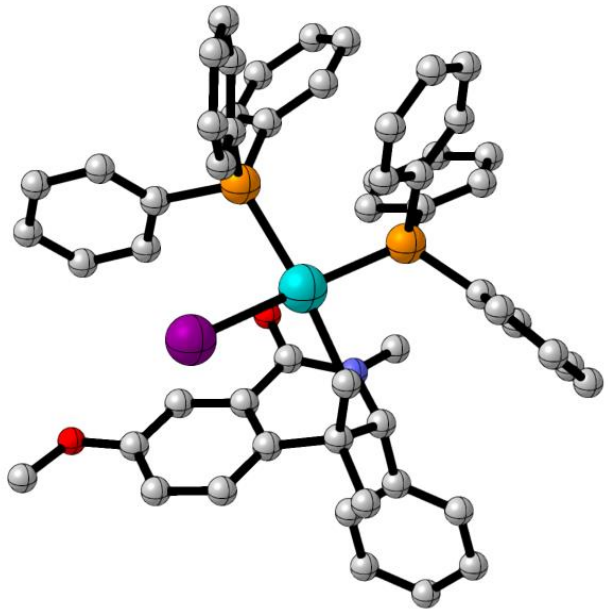
Thermal correction to energy = 0.625379
Thermal correction to enthalpy = 0.626323
Thermal correction to Gibbs free energy = 0.498263
Sum of electronic and zero-point energies = -2625.928634
Sum of electronic and thermal enthalpies = -2625.884916
Sum of electronic and thermal free energies = -2625.883972
Sum of electronic and thermal Free Energies = -2626.012032

E_{SCF} (M06L/def2-TZVPP) = -2626.510295

46	0.372886000	-0.176839000	-0.683132000
53	0.504847000	-2.765872000	0.183081000
15	2.581502000	0.134481000	-0.058718000
6	3.377078000	1.669871000	-0.696858000
6	4.226722000	1.635221000	-1.819519000
6	3.037682000	2.918359000	-0.129082000
6	4.732369000	2.827708000	-2.360545000
1	4.501123000	0.672210000	-2.262376000
6	3.547206000	4.107072000	-0.670049000
1	2.390294000	2.952582000	0.754881000
6	4.395285000	4.064838000	-1.789388000
1	5.399544000	2.787011000	-3.228532000
1	3.284873000	5.067902000	-0.213516000
1	4.794480000	4.993211000	-2.211741000
6	2.673458000	0.371609000	1.759182000
6	1.598093000	-0.048174000	2.567250000
6	3.786318000	1.006802000	2.355904000
6	1.635675000	0.159986000	3.953886000
1	0.734338000	-0.542380000	2.114722000
6	3.823090000	1.202456000	3.743715000
1	4.611046000	1.367616000	1.732036000
6	2.747103000	0.780914000	4.544185000
1	0.783470000	-0.162035000	4.560763000
1	4.690493000	1.692378000	4.199635000
1	2.775515000	0.943635000	5.627303000
6	3.774803000	-1.171223000	-0.529251000
6	4.915718000	-1.463925000	0.239673000
6	3.545638000	-1.856823000	-1.739426000
6	5.827916000	-2.431542000	-0.207305000
1	5.079700000	-0.954262000	1.194148000
6	4.468728000	-2.810247000	-2.189617000
1	2.626104000	-1.658306000	-2.301084000
6	5.609806000	-3.099248000	-1.423035000
1	6.708481000	-2.668157000	0.399792000
1	4.283759000	-3.345613000	-3.126932000
1	6.323105000	-3.856092000	-1.767157000
8	-1.837741000	0.087311000	2.745605000
7	-1.266700000	1.700677000	1.201570000

6	-1.166621000	1.605799000	-1.356471000
6	-1.734069000	-0.426917000	-0.790994000
6	-2.254177000	-1.258348000	-1.800168000
1	-1.747750000	-1.335899000	-2.767777000
6	-3.384187000	-2.042042000	-1.547744000
1	-3.772256000	-2.715089000	-2.318120000
6	-4.001812000	-1.999319000	-0.281477000
6	-3.490756000	-1.171256000	0.724953000
1	-3.932997000	-1.156584000	1.725098000
6	-2.376816000	-0.357021000	0.458171000
6	-1.821171000	0.480907000	1.569364000
6	-1.561895000	2.392862000	-0.063077000
1	-0.855027000	3.243259000	-0.063795000
6	-0.728036000	2.552636000	2.259084000
1	-1.393594000	3.416450000	2.448199000
1	0.272564000	2.919692000	1.967263000
1	-0.647393000	1.947755000	3.171133000
6	-2.146487000	1.637436000	-2.517516000
1	-1.794076000	0.988992000	-3.334703000
1	-2.189619000	2.674043000	-2.903367000
1	-3.163845000	1.338732000	-2.226254000
6	0.233317000	1.669961000	-1.672147000
6	-2.951858000	3.026900000	-0.118359000
6	-4.099061000	2.439323000	0.444605000
1	-4.026705000	1.491393000	0.980822000
6	-5.349856000	3.064337000	0.325297000
1	-6.232194000	2.589441000	0.767439000
6	-5.472178000	4.287886000	-0.350798000
6	-4.330277000	4.892274000	-0.900341000
1	-4.408953000	5.855859000	-1.415455000
6	-3.082372000	4.266184000	-0.777727000
1	-2.189498000	4.745297000	-1.199858000
1	-6.449959000	4.773197000	-0.439967000
1	0.544749000	1.491865000	-2.711505000
1	0.861917000	2.384720000	-1.129415000
6	-5.254660000	-2.799118000	-0.034400000
9	-6.370164000	-2.105779000	-0.424602000
9	-5.257589000	-3.969633000	-0.733067000
9	-5.419286000	-3.101734000	1.282577000

p-OMe-1



Zero-point correction = 0.881665 (Hartree/particle)
Thermal correction to energy = 0.940369
Thermal correction to enthalpy = 0.941314
Thermal correction to Gibbs free energy = 0.785526
Sum of electronic and zero-point energies = -3439.594649
Sum of electronic and thermal enthalpies = -3439.535945
Sum of electronic and thermal free energies = -3439.535000
Sum of electronic and thermal Free Energies = -3439.690791

E_{SCF} (M06L/def2-TZVPP) = -3440.476314

46	-0.202856000	0.085013000	-0.702273000
53	-0.101511000	2.540540000	-1.940871000
15	-0.553449000	-2.154190000	-0.306418000
15	-2.248807000	0.878966000	0.410995000
6	-2.045946000	2.608484000	0.993466000
6	-3.033541000	3.587147000	0.783150000
6	-0.844487000	2.945697000	1.650390000
6	-2.813280000	4.903927000	1.215062000
1	-3.960963000	3.326466000	0.264138000
6	-0.635313000	4.261085000	2.085332000
1	-0.073545000	2.184178000	1.815185000
6	-1.614509000	5.243024000	1.861119000
1	-3.578290000	5.667836000	1.036084000
1	0.309711000	4.529780000	2.567715000
1	-1.439440000	6.274994000	2.185506000
6	-3.756332000	0.943638000	-0.660483000
6	-3.612949000	1.317912000	-2.013471000

6	-5.044710000	0.656833000	-0.164890000
6	-4.732941000	1.391677000	-2.852183000
1	-2.618318000	1.565827000	-2.399320000
6	-6.161186000	0.710825000	-1.013862000
1	-5.179925000	0.386110000	0.885668000
6	-6.010154000	1.075973000	-2.360042000
1	-4.601962000	1.692741000	-3.897764000
1	-7.153878000	0.474594000	-0.614558000
1	-6.883998000	1.122237000	-3.019726000
6	-2.877805000	0.032838000	1.929549000
6	-3.496380000	-1.231738000	1.819347000
6	-2.682170000	0.584893000	3.211171000
6	-3.899423000	-1.932796000	2.961850000
1	-3.672668000	-1.665283000	0.833010000
6	-3.085933000	-0.121257000	4.354860000
1	-2.209421000	1.565525000	3.315494000
6	-3.689540000	-1.382589000	4.236279000
1	-4.370307000	-2.915835000	2.853082000
1	-2.925944000	0.321197000	5.344463000
1	-3.996206000	-1.933578000	5.132032000
6	-2.208419000	-2.563599000	-1.022583000
6	-3.027384000	-3.608515000	-0.547504000
6	-2.657000000	-1.770784000	-2.098171000
6	-4.280188000	-3.841928000	-1.131312000
1	-2.709069000	-4.210698000	0.307662000
6	-3.905898000	-2.015222000	-2.688773000
1	-2.030349000	-0.937103000	-2.439229000
6	-4.722470000	-3.045018000	-2.201447000
1	-4.918093000	-4.643082000	-0.741767000
1	-4.253167000	-1.369987000	-3.500799000
1	-5.707876000	-3.221219000	-2.646036000
6	-0.569603000	-2.738376000	1.427339000
6	-0.713308000	-4.100784000	1.775508000
6	-0.419735000	-1.775726000	2.442247000
6	-0.746609000	-4.480291000	3.124786000
1	-0.767456000	-4.865959000	0.993889000
6	-0.446960000	-2.160167000	3.789260000
1	-0.232976000	-0.731325000	2.180958000
6	-0.622151000	-3.508344000	4.132729000
1	-0.857978000	-5.537704000	3.389058000
1	-0.318224000	-1.396921000	4.561723000
1	-0.645270000	-3.808904000	5.186098000
6	0.502588000	-3.395051000	-1.176525000
6	0.347311000	-3.559004000	-2.569756000
6	1.540480000	-4.086676000	-0.521561000
6	1.213997000	-4.393228000	-3.288974000
1	-0.454082000	-3.026114000	-3.092363000
6	2.405819000	-4.924772000	-1.242561000

1	1.670030000	-3.979922000	0.558441000
6	2.249320000	-5.076004000	-2.628866000
1	1.080959000	-4.507892000	-4.370115000
1	3.202309000	-5.460512000	-0.714283000
1	2.927898000	-5.725133000	-3.192524000
8	1.537162000	0.686982000	2.653583000
7	2.596261000	-0.777428000	1.229513000
6	2.957003000	-0.055382000	-1.172987000
6	3.029338000	1.361625000	-0.631509000
6	3.470347000	2.464196000	-1.371375000
1	3.848335000	2.323004000	-2.387711000
6	3.401358000	3.770968000	-0.859185000
1	3.731667000	4.605679000	-1.482549000
6	2.881568000	3.988925000	0.429629000
6	2.481382000	2.889489000	1.205017000
1	2.123935000	3.032792000	2.227174000
6	2.541837000	1.596786000	0.674965000
6	2.154555000	0.480652000	1.584830000
6	3.319968000	-1.054692000	-0.024785000
1	2.971014000	-2.045889000	-0.368342000
6	2.706871000	-1.797398000	2.269099000
1	2.105376000	-2.688893000	2.029533000
1	2.331645000	-1.365026000	3.205674000
1	3.765537000	-2.094901000	2.380893000
6	3.959517000	-0.285752000	-2.333229000
1	3.654753000	0.294195000	-3.220105000
1	3.967853000	-1.352029000	-2.620568000
1	4.985819000	0.005361000	-2.053115000
6	1.561754000	-0.369348000	-1.781054000
6	4.818893000	-1.170458000	0.238368000
6	5.531051000	-0.155571000	0.907976000
1	5.000567000	0.731880000	1.266322000
6	6.912636000	-0.278415000	1.113623000
1	7.455928000	0.519967000	1.631415000
6	7.599644000	-1.418020000	0.661908000
6	6.894649000	-2.439308000	0.006339000
1	7.419734000	-3.336662000	-0.340164000
6	5.512177000	-2.313734000	-0.199294000
1	4.955386000	-3.108923000	-0.710930000
1	8.678663000	-1.511745000	0.827228000
1	1.546174000	-1.429184000	-2.077610000
1	1.430480000	0.242975000	-2.685797000
8	2.737819000	5.219381000	1.023367000
6	2.974892000	6.359677000	0.199675000
1	4.035845000	6.425398000	-0.113993000
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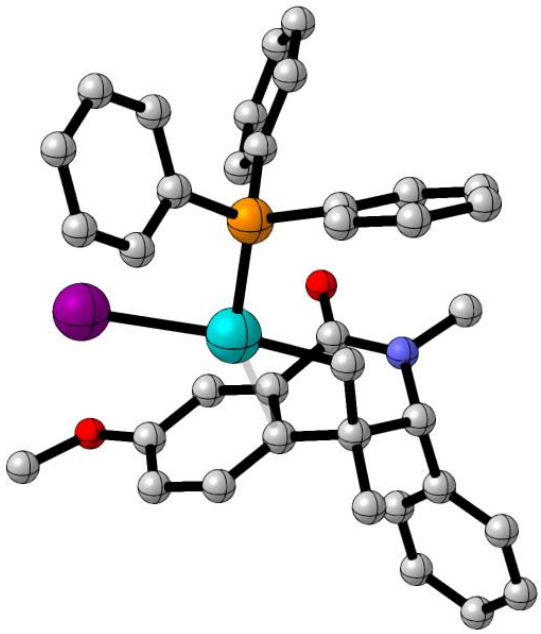
p-OMe-2



Zero-point correction = 0.611238
Thermal correction to energy = 0.653006
Thermal correction to enthalpy = 0.653950
Thermal correction to Gibbs free energy = 0.531546
Sum of electronic and zero-point energies = -2403.358405
Sum of electronic and thermal enthalpies = -2403.316637
Sum of electronic and thermal free energies = -2403.315693
Sum of electronic and thermal Free Energies = -2403.438097

E_{SCF} (M06L/def2-TZVPP) = -2403.969643

46	-0.282326000	0.342110000	-0.621738000
53	-1.402120000	2.821873000	-0.178808000
15	-2.134828000	-0.774098000	-0.025470000
6	-2.192509000	-2.538584000	-0.537393000
6	-2.821536000	-2.914437000	-1.741209000
6	-1.505586000	-3.514141000	0.217893000
6	-2.771505000	-4.246511000	-2.177382000
1	-3.361383000	-2.164655000	-2.328937000
6	-1.461278000	-4.845104000	-0.220946000
1	-1.024385000	-3.231207000	1.160084000
6	-2.092262000	-5.214535000	-1.419782000
1	-3.272219000	-4.529741000	-3.109715000
1	-0.933864000	-5.595838000	0.377900000
1	-2.057767000	-6.254830000	-1.761113000
6	-2.232936000	-0.863107000	1.800166000
6	-1.380113000	-0.045113000	2.567181000
6	-3.093641000	-1.780039000	2.445257000

6	-1.390264000	-0.138926000	3.966271000
1	-0.704293000	0.653539000	2.063925000
6	-3.112617000	-1.854725000	3.844725000
1	-3.723887000	-2.452184000	1.853029000
6	-2.259967000	-1.035434000	4.605376000
1	-0.700316000	0.480483000	4.546815000
1	-3.783571000	-2.564039000	4.341699000
1	-2.266189000	-1.108596000	5.698568000
6	-3.706313000	-0.096501000	-0.678985000
6	-4.920642000	-0.202818000	0.023383000
6	-3.680780000	0.502812000	-1.954598000
6	-6.104651000	0.278926000	-0.554962000
1	-4.939324000	-0.636464000	1.027616000
6	-4.869468000	0.964729000	-2.535059000
1	-2.720006000	0.633196000	-2.464971000
6	-6.082375000	0.854261000	-1.835308000
1	-7.046120000	0.209392000	0.000762000
1	-4.843556000	1.435754000	-3.523417000
1	-7.008895000	1.231041000	-2.282203000
8	1.943118000	-0.124870000	2.921799000
7	2.625943000	-1.529702000	1.226446000
6	2.186383000	-0.918365000	-1.144600000
6	2.157826000	0.553655000	-0.682480000
6	2.139270000	1.664879000	-1.555613000
1	2.120901000	1.502888000	-2.637070000
6	2.154069000	2.980253000	-1.067400000
1	2.099170000	3.810429000	-1.773982000
6	2.168466000	3.211941000	0.321453000
6	2.202956000	2.118937000	1.213826000
1	2.193278000	2.289097000	2.293281000
6	2.181735000	0.814393000	0.725533000
6	2.225484000	-0.305774000	1.725368000
6	3.083999000	-1.728620000	-0.158407000
1	2.885165000	-2.792533000	-0.392847000
6	2.829815000	-2.637484000	2.150316000
1	3.895308000	-2.934773000	2.167055000
1	2.222459000	-3.509358000	1.842392000
1	2.520553000	-2.300114000	3.149475000
6	2.695041000	-1.067697000	-2.584900000
1	1.978489000	-0.612451000	-3.290553000
1	2.779005000	-2.137429000	-2.846525000
1	3.682195000	-0.596849000	-2.726674000
6	0.732135000	-1.418900000	-1.024076000
6	4.581836000	-1.496264000	-0.323375000
6	5.229464000	-0.366893000	0.215700000
1	4.665788000	0.355442000	0.812792000
6	6.599817000	-0.162412000	-0.001705000
1	7.087374000	0.721853000	0.423206000

6	7.345643000	-1.084915000	-0.753181000
6	6.712575000	-2.220033000	-1.282924000
1	7.286833000	-2.953725000	-1.859398000
6	5.341745000	-2.421455000	-1.064835000
1	4.848422000	-3.310882000	-1.476092000
1	8.416701000	-0.924090000	-0.917383000
1	0.321561000	-1.838529000	-1.958133000
1	0.584984000	-2.124654000	-0.193368000
8	2.139030000	4.442463000	0.900186000
6	1.780037000	5.544892000	0.058158000
1	2.567190000	5.757199000	-0.691180000
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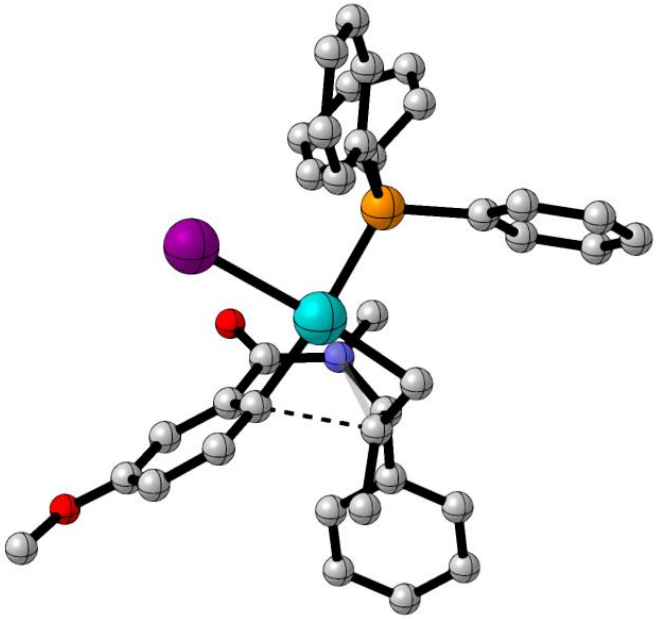
1	1.677002000	6.408276000	0.731318000

p-OMe-TS 2-3



Zero-point correction = 0.608182
Thermal correction to energy = 0.650068
Thermal correction to enthalpy = 0.651012
Thermal correction to Gibbs free energy = 0.528585
Sum of electronic and zero-point energies = -2403.300297
Sum of electronic and thermal enthalpies = -2403.258411
Sum of electronic and thermal free energies = -2403.257467
Sum of electronic and thermal Free Energies = -2403.379894

E_{SCF} (M06L/def2-TZVPP) = -2403.908479

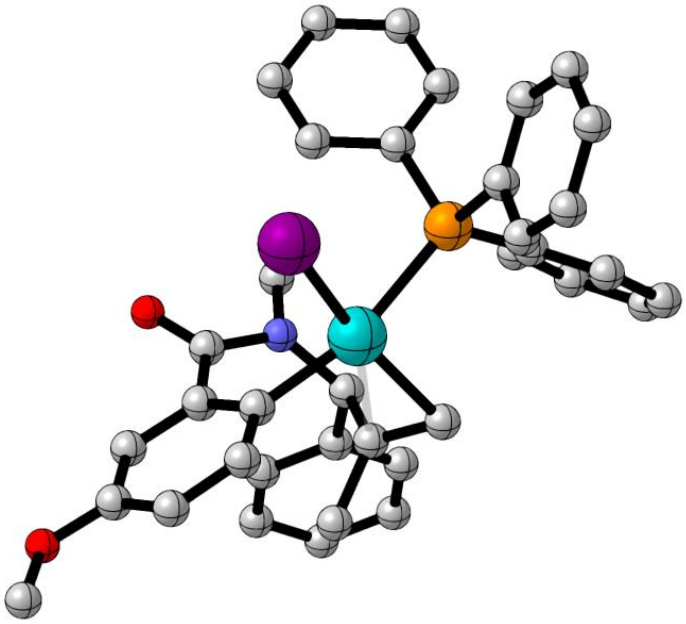
Imaginary Frequency = -201.92 cm^{-1}

46	0.147321000	-0.377968000	-0.663374000

53	0.733477000	-2.840312000	0.370734000
15	2.286433000	0.355553000	-0.100077000
6	2.804269000	1.964754000	-0.835612000
6	3.680616000	2.018362000	-1.936857000
6	2.212871000	3.160695000	-0.369597000
6	3.965189000	3.245176000	-2.554864000
1	4.147825000	1.098182000	-2.302544000
6	2.501833000	4.385499000	-0.987651000
1	1.540580000	3.129317000	0.495980000
6	3.378584000	4.430190000	-2.083925000
1	4.654963000	3.274529000	-3.405740000
1	2.044454000	5.306436000	-0.609198000
1	3.605027000	5.386809000	-2.567464000
6	2.348903000	0.719008000	1.700332000
6	1.388429000	0.144044000	2.557556000
6	3.321200000	1.595350000	2.234664000
6	1.405008000	0.435073000	3.929594000
1	0.630882000	-0.531239000	2.152519000
6	3.336564000	1.876714000	3.608170000
1	4.050125000	2.073137000	1.571366000
6	2.378272000	1.297487000	4.456933000
1	0.642855000	-0.012431000	4.575618000
1	4.095078000	2.555229000	4.014035000
1	2.388779000	1.525782000	5.528533000
6	3.696538000	-0.744348000	-0.498407000
6	4.881023000	-0.762558000	0.260421000
6	3.583244000	-1.552325000	-1.647216000
6	5.949927000	-1.579002000	-0.135629000
1	4.959482000	-0.156688000	1.168580000
6	4.660706000	-2.355218000	-2.047591000
1	2.637950000	-1.567841000	-2.199199000
6	5.844337000	-2.369531000	-1.291375000
1	6.866460000	-1.602364000	0.464035000
1	4.566857000	-2.987253000	-2.937131000
1	6.681043000	-3.007792000	-1.595951000
8	-2.140063000	-0.277707000	2.792240000
7	-1.667710000	1.296540000	1.180227000
6	-1.632296000	1.153664000	-1.400251000
6	-1.846740000	-1.017478000	-0.691582000
6	-2.261247000	-1.949597000	-1.651146000
1	-1.716142000	-2.046785000	-2.596938000
6	-3.332501000	-2.816438000	-1.389444000
1	-3.615974000	-3.559059000	-2.140615000
6	-3.999395000	-2.747279000	-0.146898000
6	-3.604049000	-1.794298000	0.808378000
1	-4.102688000	-1.758320000	1.781710000
6	-2.551449000	-0.912354000	0.523878000
6	-2.122929000	0.044911000	1.594812000

6	-1.992650000	1.943816000	-0.105754000
1	-1.301090000	2.807882000	-0.133371000
6	-1.274711000	2.244701000	2.221164000
1	-2.028553000	3.049392000	2.325698000
1	-0.295257000	2.691701000	1.968709000
1	-1.195519000	1.694526000	3.166566000
6	-2.731572000	0.928342000	-2.419563000
1	-2.373348000	0.291185000	-3.242532000
1	-3.001549000	1.916400000	-2.844067000
1	-3.639545000	0.485608000	-1.985801000
6	-0.299004000	1.330624000	-1.861387000
6	-3.401164000	2.538326000	-0.133385000
6	-4.532955000	1.834332000	0.319277000
1	-4.423702000	0.822543000	0.720569000
6	-5.805294000	2.417373000	0.246981000
1	-6.677055000	1.856841000	0.602212000
6	-5.966209000	3.710820000	-0.276794000
6	-4.842688000	4.421360000	-0.725663000
1	-4.955207000	5.434884000	-1.126647000
6	-3.570711000	3.836315000	-0.649936000
1	-2.691425000	4.394749000	-0.996479000
1	-6.962382000	4.164514000	-0.328918000
1	-0.058802000	1.056727000	-2.898246000
1	0.309070000	2.140756000	-1.445980000
8	-5.040089000	-3.560986000	0.219945000
6	-5.411125000	-4.592946000	-0.692174000
1	-5.777572000	-4.178532000	-1.652448000
1	-4.566061000	-5.279532000	-0.893538000
1	-6.224841000	-5.147152000	-0.201693000

***p*-OMe-3**



Zero-point correction = 0.608921 (Hartree/particle)
Thermal correction to energy = 0.651502
Thermal correction to enthalpy = 0.652446
Thermal correction to Gibbs free energy = 0.528791
Sum of electronic and zero-point energies = -2403.310645
Sum of electronic and thermal enthalpies = -2403.268064
Sum of electronic and thermal free energies = -2403.267120
Sum of electronic and thermal Free Energies = -2403.390775

E_{SCF} (M06L/def2-TZVPP) = -2403.919566

46	0.002822000	-0.639583000	-0.588233000
53	0.895779000	-2.980606000	0.398419000
15	2.158048000	0.296403000	-0.081887000
6	2.490373000	1.983459000	-0.752576000
6	3.143425000	2.153182000	-1.990513000
6	1.918477000	3.111155000	-0.121374000
6	3.219793000	3.422959000	-2.583744000
1	3.594108000	1.287680000	-2.487693000
6	1.993688000	4.378176000	-0.717888000
1	1.432066000	2.995644000	0.852820000
6	2.642014000	4.537186000	-1.953990000
1	3.736840000	3.541239000	-3.542324000
1	1.550834000	5.242642000	-0.211020000
1	2.701128000	5.525924000	-2.421271000
6	2.359242000	0.568214000	1.723515000
6	1.479005000	-0.058953000	2.627520000
6	3.365907000	1.428068000	2.219454000
6	1.614088000	0.157221000	4.007282000

1	0.691811000	-0.716448000	2.249229000
6	3.498807000	1.637801000	3.599147000
1	4.030493000	1.950041000	1.522690000
6	2.623658000	1.000739000	4.495337000
1	0.921379000	-0.335972000	4.697232000
1	4.283573000	2.303939000	3.974078000
1	2.726135000	1.168896000	5.573024000
6	3.602998000	-0.667114000	-0.668709000
6	4.840756000	-0.693030000	-0.001121000
6	3.442569000	-1.377004000	-1.876839000
6	5.914111000	-1.412637000	-0.547376000
1	4.960048000	-0.171287000	0.953353000
6	4.522457000	-2.080441000	-2.427536000
1	2.457827000	-1.396557000	-2.358001000
6	5.759502000	-2.099177000	-1.762471000
1	6.873042000	-1.440981000	-0.018451000
1	4.390910000	-2.633643000	-3.363631000
1	6.599801000	-2.661265000	-2.184381000
8	-2.664137000	-0.191122000	2.752224000
7	-1.566494000	1.099496000	1.219191000
6	-1.544689000	1.016938000	-1.350501000
6	-1.838713000	-1.508255000	-0.482346000
6	-2.268166000	-2.521910000	-1.345073000
1	-1.592933000	-2.906831000	-2.116300000
6	-3.553718000	-3.080643000	-1.223662000
1	-3.861301000	-3.869071000	-1.916362000
6	-4.412083000	-2.638182000	-0.197176000
6	-3.974471000	-1.642904000	0.692286000
1	-4.623590000	-1.328107000	1.514551000
6	-2.703636000	-1.056600000	0.537710000
6	-2.332782000	-0.026023000	1.567470000
6	-1.563774000	1.850700000	-0.063361000
1	-0.599908000	2.391050000	-0.055151000
6	-1.227883000	1.967116000	2.355349000
1	-2.066864000	2.633294000	2.631340000
1	-0.356701000	2.582832000	2.077482000
1	-0.977717000	1.341304000	3.219991000
6	-2.853441000	0.651758000	-2.014667000
1	-2.702612000	-0.120845000	-2.783348000
1	-3.239940000	1.566674000	-2.503603000
1	-3.620761000	0.299978000	-1.310764000
6	-0.361938000	0.979755000	-2.089907000
6	-2.670153000	2.902354000	-0.123875000
6	-3.942482000	2.674618000	0.429943000
1	-4.142311000	1.742972000	0.970099000
6	-4.949412000	3.643364000	0.304593000
1	-5.936190000	3.458652000	0.742871000
6	-4.694319000	4.845435000	-0.375322000

6	-3.423112000	5.079236000	-0.925408000
1	-3.214647000	6.018497000	-1.449665000
6	-2.415994000	4.111931000	-0.796149000
1	-1.419630000	4.288762000	-1.221115000
1	-5.481866000	5.600771000	-0.470580000
1	-0.371474000	0.522963000	-3.087251000
1	0.455710000	1.674253000	-1.886880000
8	-5.683766000	-3.116595000	0.021950000
6	-6.135035000	-4.161497000	-0.834935000
1	-6.176053000	-3.835135000	-1.893614000
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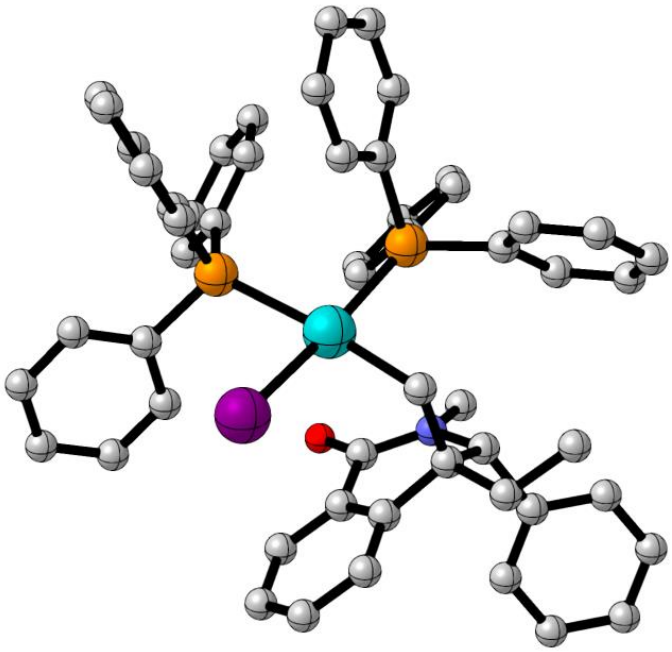
1	-7.150310000	-4.412749000	-0.492680000

Et-1



Zero-point correction = 0.878018 (Hartree/particle)
Thermal correction to energy = 0.935401
Thermal correction to enthalpy = 0.936345
Thermal correction to Gibbs free energy = 0.784398
Sum of electronic and zero-point energies = -3364.364132
Sum of electronic and thermal enthalpies = -3364.306749
Sum of electronic and thermal free energies = -3364.305805
Sum of electronic and thermal Free Energies = -3364.457752

E_{SCF} (M06L/def2-TZVPP) = -3365.242150

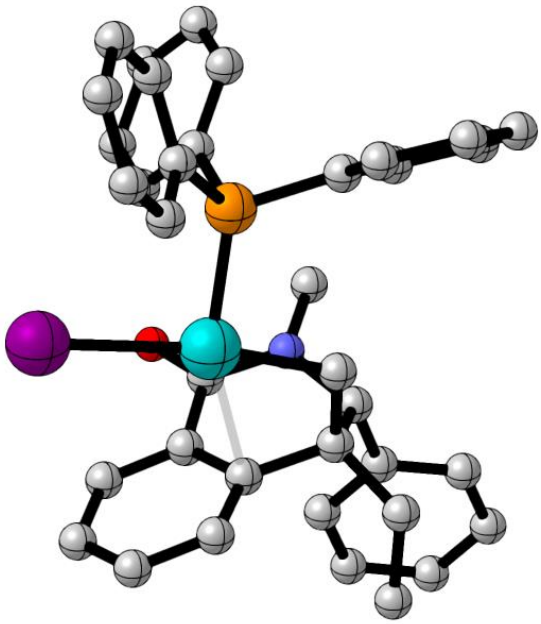
46	0.207531000	-0.276238000	-0.646861000
53	0.498951000	-2.753044000	-1.791585000
15	0.145991000	2.001956000	-0.297429000
15	2.406177000	-0.666525000	0.376129000

6	2.530739000	-2.362636000	1.069205000
6	3.663460000	-3.170969000	0.867068000
6	1.452738000	-2.836428000	1.845262000
6	3.715695000	-4.453879000	1.433130000
1	4.494478000	-2.805680000	0.256028000
6	1.523124000	-4.110951000	2.423063000
1	0.561850000	-2.215544000	2.001521000
6	2.648477000	-4.925025000	2.213302000
1	4.593141000	-5.087025000	1.260254000
1	0.686106000	-4.474581000	3.029151000
1	2.691534000	-5.927517000	2.653652000
6	3.852329000	-0.539599000	-0.771670000
6	3.699050000	-0.920954000	-2.120982000
6	5.114629000	-0.093857000	-0.327410000
6	4.781900000	-0.845328000	-3.007552000
1	2.729404000	-1.294926000	-2.465926000
6	6.192215000	-0.003734000	-1.221917000
1	5.257015000	0.189564000	0.719060000
6	6.029573000	-0.375850000	-2.565136000
1	4.645050000	-1.153223000	-4.050336000
1	7.163897000	0.352618000	-0.862079000
1	6.873046000	-0.307745000	-3.261404000
6	2.967413000	0.362054000	1.807935000
6	3.357352000	1.700745000	1.586731000
6	2.941032000	-0.129090000	3.128379000
6	3.684285000	2.537178000	2.660353000
1	3.417059000	2.086692000	0.567591000
6	3.275982000	0.710111000	4.202295000
1	2.652427000	-1.166645000	3.318490000
6	3.637408000	2.046831000	3.975115000
1	3.972241000	3.575957000	2.465325000
1	3.250462000	0.313206000	5.223369000
1	3.885978000	2.701809000	4.817243000
6	1.659527000	2.711739000	-1.087860000
6	2.249509000	3.928146000	-0.687275000
6	2.243598000	1.974256000	-2.136781000
6	3.417007000	4.383709000	-1.314605000
1	1.827360000	4.495789000	0.145860000
6	3.409084000	2.435648000	-2.767447000
1	1.793428000	1.015964000	-2.423957000
6	4.001349000	3.636539000	-2.352530000
1	3.879627000	5.320083000	-0.983406000
1	3.870918000	1.831618000	-3.553943000
1	4.923275000	3.987286000	-2.828813000
6	0.125252000	2.609809000	1.428809000
6	0.008025000	3.979106000	1.759502000
6	0.223312000	1.654815000	2.457366000
6	0.030502000	4.381804000	3.102083000

1	-0.132837000	4.725812000	0.971032000
6	0.242332000	2.061692000	3.798039000
1	0.234149000	0.589646000	2.212299000
6	0.157374000	3.423299000	4.122210000
1	-0.061786000	5.444497000	3.352072000
1	0.311551000	1.303415000	4.583083000
1	0.172580000	3.740823000	5.170699000
6	-1.158683000	3.008219000	-1.134157000
6	-1.084549000	3.179901000	-2.533341000
6	-2.280122000	3.511221000	-0.445912000
6	-2.109124000	3.840781000	-3.224931000
1	-0.219371000	2.792040000	-3.081595000
6	-3.303548000	4.176530000	-1.139570000
1	-2.350728000	3.396024000	0.638796000
6	-3.223801000	4.339654000	-2.530822000
1	-2.036391000	3.964614000	-4.310742000
1	-4.162859000	4.570996000	-0.585829000
1	-4.025570000	4.852476000	-3.072453000
8	-1.250803000	-1.175529000	2.708230000
7	-2.616232000	0.076620000	1.347542000
6	-2.956339000	-0.698179000	-1.037442000
6	-2.768618000	-2.112747000	-0.500388000
6	-3.085635000	-3.275882000	-1.217677000
1	-3.530254000	-3.202971000	-2.212958000
6	-2.816564000	-4.547466000	-0.686879000
1	-3.063882000	-5.438900000	-1.273662000
6	-2.221473000	-4.678676000	0.575734000
1	-2.001142000	-5.669745000	0.985942000
6	-1.913305000	-3.528672000	1.309675000
1	-1.480347000	-3.585051000	2.311872000
6	-2.186457000	-2.255908000	0.780485000
6	-1.946213000	-1.085128000	1.670547000
6	-3.446902000	0.213913000	0.134386000
1	-3.306761000	1.255219000	-0.205822000
6	-2.853125000	1.060006000	2.400834000
1	-2.459385000	2.051648000	2.125679000
1	-2.333765000	0.715569000	3.304154000
1	-3.938627000	1.144012000	2.592014000
6	-4.028178000	-0.670089000	-2.176545000
1	-3.669265000	-1.335043000	-2.982271000
1	-4.963871000	-1.114711000	-1.789714000
6	-1.641808000	-0.168782000	-1.673203000
6	-4.924705000	0.054991000	0.495175000
6	-5.442603000	-1.148551000	1.017748000
1	-4.780795000	-2.007021000	1.161528000
6	-6.800530000	-1.251420000	1.350497000
1	-7.188871000	-2.196103000	1.747235000
6	-7.660834000	-0.153002000	1.182378000

6	-7.150605000	1.055798000	0.686521000
1	-7.807690000	1.924454000	0.565913000
6	-5.791270000	1.154645000	0.350728000
1	-5.387910000	2.103050000	-0.025475000
1	-8.720918000	-0.237839000	1.445716000
1	-1.795921000	0.875570000	-1.972961000
1	-1.434298000	-0.760582000	-2.578308000
6	-4.328662000	0.701325000	-2.799408000
1	-3.443739000	1.135263000	-3.293165000
1	-5.120958000	0.596449000	-3.561842000
1	-4.685604000	1.433445000	-2.057098000

Et-2



Zero-point correction = 0.878018 (Hartree/particle)
Thermal correction to energy = 0.935401
Thermal correction to enthalpy = 0.936345
Thermal correction to Gibbs free energy = 0.784398
Sum of electronic and zero-point energies = -2328.121633
Sum of electronic and thermal enthalpies = -2328.081073
Sum of electronic and thermal free energies = -2328.080129
Sum of electronic and thermal Free Energies = -2328.198714

E_{SCF} (M06L/def2-TZVPP) = -2328.728810

46	0.359923000	-0.679507000	-0.647108000
53	1.720109000	-2.866764000	0.272819000
15	1.947642000	0.788797000	-0.063650000
6	1.815954000	2.470182000	-0.796024000
6	2.545796000	2.810390000	-1.951548000

6	0.896351000	3.399436000	-0.261195000
6	2.366427000	4.064306000	-2.555492000
1	3.262972000	2.096958000	-2.370307000
6	0.723783000	4.652633000	-0.864680000
1	0.331754000	3.141543000	0.641456000
6	1.457616000	4.987689000	-2.014865000
1	2.945770000	4.321984000	-3.448805000
1	0.014983000	5.369162000	-0.435087000
1	1.322396000	5.966869000	-2.486753000
6	1.885748000	1.118810000	1.737748000
6	1.201552000	0.217546000	2.575514000
6	2.472066000	2.281111000	2.289049000
6	1.099627000	0.475840000	3.950455000
1	0.743608000	-0.679958000	2.150268000
6	2.379847000	2.525525000	3.666210000
1	2.975702000	3.004210000	1.638813000
6	1.690616000	1.625076000	4.497415000
1	0.538996000	-0.221443000	4.579944000
1	2.837250000	3.426837000	4.088989000
1	1.608273000	1.827416000	5.571112000
6	3.654190000	0.287369000	-0.503250000
6	4.770226000	0.734471000	0.228209000
6	3.835632000	-0.518258000	-1.644821000
6	6.062463000	0.380639000	-0.187445000
1	4.630825000	1.337034000	1.131099000
6	5.129774000	-0.854282000	-2.064900000
1	2.955738000	-0.901480000	-2.173336000
6	6.243741000	-0.406631000	-1.335924000
1	6.929295000	0.716441000	0.392079000
1	5.266266000	-1.487317000	-2.948031000
1	7.254453000	-0.683125000	-1.655511000
8	-1.776105000	-0.823039000	2.802451000
7	-2.189310000	0.770777000	1.189533000
6	-2.257553000	0.243668000	-1.263281000
6	-2.051974000	-1.225580000	-0.842219000
6	-1.864022000	-2.258347000	-1.794350000
1	-1.835359000	-2.007004000	-2.859167000
6	-1.763093000	-3.599095000	-1.390911000
1	-1.620834000	-4.379768000	-2.144631000
6	-1.821659000	-3.933129000	-0.030290000
1	-1.731656000	-4.977209000	0.283736000
6	-1.934499000	-2.921517000	0.931639000
1	-1.900113000	-3.138563000	2.002557000
6	-2.028786000	-1.576668000	0.540974000
6	-2.008124000	-0.530436000	1.617264000
6	-2.868691000	1.069247000	-0.082667000
1	-2.616923000	2.120353000	-0.318953000
6	-2.185988000	1.832831000	2.187923000

1	-3.215577000	2.103018000	2.493828000
1	-1.694868000	2.727115000	1.764779000
1	-1.627403000	1.476729000	3.063711000
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1	-2.441561000	0.108276000	-3.404355000
1	-3.312041000	1.465581000	-2.705528000
6	-0.829606000	0.770390000	-1.515144000
6	-4.384554000	1.016168000	0.078193000
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1	-4.463018000	-0.916698000	1.071755000
6	-6.440323000	-0.103800000	0.762935000
1	-6.936687000	-0.964339000	1.224492000
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1	-4.769812000	-0.361714000	-3.739413000
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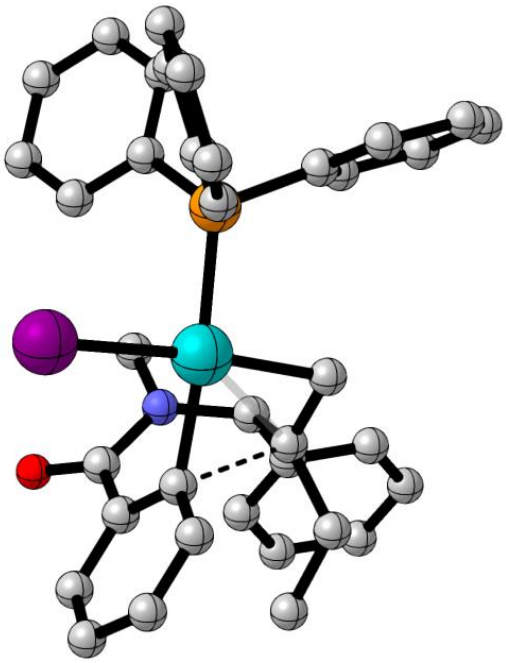
Et-TS 2-3



Zero-point correction = 0.604622 (Hartree/particle)
Thermal correction to energy = 0.645025
Thermal correction to enthalpy = 0.645969

Thermal correction to Gibbs free energy = 0.526569
Sum of electronic and zero-point energies = -2328.068737
Sum of electronic and thermal enthalpies = -2328.028334
Sum of electronic and thermal free energies = -2328.027390
Sum of electronic and thermal Free Energies = -2328.146790

E_{SCF} (M06L/def2-TZVPP) = -2328.673359

Imaginary Frequency = -185.66 cm^{-1}

46	0.121784000	-0.594615000	-0.583984000
53	1.325769000	-2.749590000	0.593813000
15	1.977084000	0.714143000	-0.078184000
6	1.961611000	2.389208000	-0.846968000
6	2.694736000	2.666678000	-2.016333000
6	1.086557000	3.372868000	-0.332604000
6	2.561328000	3.909738000	-2.655520000
1	3.375988000	1.910912000	-2.420770000
6	0.957021000	4.613459000	-0.972457000
1	0.520736000	3.167983000	0.583956000
6	1.694253000	4.884592000	-2.137713000
1	3.143462000	4.117657000	-3.560043000
1	0.282139000	5.370616000	-0.558192000
1	1.594240000	5.853787000	-2.637995000
6	2.095114000	1.130623000	1.708255000
6	1.408238000	0.347618000	2.657055000
6	2.851085000	2.243862000	2.141114000
6	1.490544000	0.664868000	4.021481000
1	0.821876000	-0.513386000	2.321962000
6	2.932670000	2.552920000	3.506034000
1	3.357751000	2.879836000	1.407468000
6	2.253355000	1.762463000	4.448623000
1	0.952595000	0.048117000	4.749194000
1	3.523165000	3.415815000	3.833031000
1	2.315038000	2.007702000	5.514620000
6	3.595041000	0.031618000	-0.599350000
6	4.805766000	0.377623000	0.028720000
6	3.602516000	-0.833054000	-1.712519000
6	6.017026000	-0.132161000	-0.461752000
1	4.800890000	1.025841000	0.910521000
6	4.816587000	-1.328122000	-2.207863000
1	2.648491000	-1.134004000	-2.159878000
6	6.024531000	-0.978878000	-1.582141000
1	6.957000000	0.128284000	0.036920000
1	4.816765000	-2.005308000	-3.068615000
1	6.972351000	-1.377516000	-1.960109000
8	-2.761903000	-1.636340000	2.611831000
7	-2.141544000	0.156728000	1.317520000

6	-2.009519000	0.335367000	-1.260767000
6	-1.589769000	-1.795818000	-0.808556000
6	-1.536066000	-2.682296000	-1.899023000
1	-0.910480000	-2.449392000	-2.768020000
6	-2.235833000	-3.896500000	-1.843048000
1	-2.161892000	-4.605074000	-2.675890000
6	-3.019504000	-4.211076000	-0.715349000
1	-3.562430000	-5.161131000	-0.672859000
6	-3.109391000	-3.305549000	0.346882000
1	-3.703711000	-3.523432000	1.239521000
6	-2.411934000	-2.081394000	0.296348000
6	-2.483410000	-1.186847000	1.488774000
6	-2.365541000	0.976037000	0.114355000
1	-1.626480000	1.794188000	0.221147000
6	-1.984544000	0.955624000	2.533683000
1	-2.891792000	1.545774000	2.763992000
1	-1.129979000	1.642181000	2.399964000
1	-1.789122000	0.270393000	3.368187000
6	-3.113086000	-0.015396000	-2.270720000
1	-2.616678000	-0.448241000	-3.157220000
1	-3.480356000	0.981550000	-2.592973000
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6	-3.740899000	1.650510000	0.116020000
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6	-5.170702000	3.450349000	-0.706332000
1	-5.301436000	4.346953000	-1.322229000
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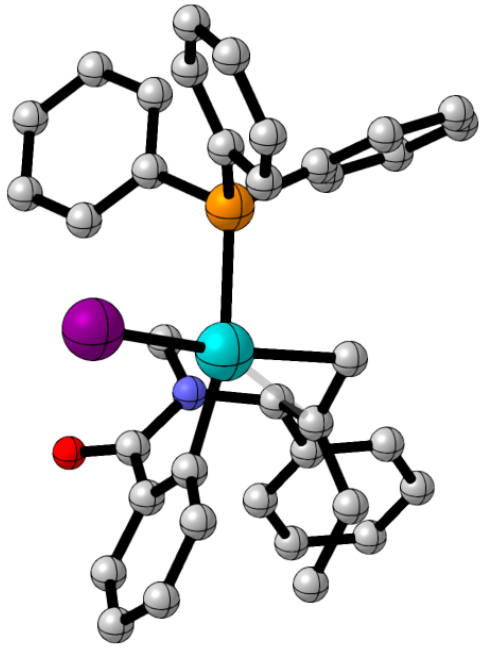
Et-3



Zero-point correction = 0.605416 (Hartree/particle)
Thermal correction to energy = 0.646487
Thermal correction to enthalpy = 0.647431
Thermal correction to Gibbs free energy = 0.528152
Sum of electronic and zero-point energies = -2328.073878
Sum of electronic and thermal enthalpies = -2328.032807
Sum of electronic and thermal free energies = -2328.031863
Sum of electronic and thermal Free Energies = -2328.151142

E_{SCF} (M06L/def2-TZVPP) = -2328.679294

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15	1.888674000	0.757188000	-0.052191000
6	1.767189000	2.496876000	-0.656422000
6	2.421811000	2.906835000	-1.834772000
6	0.869809000	3.388312000	-0.025630000
6	2.186605000	4.184141000	-2.367699000
1	3.121001000	2.225926000	-2.331051000
6	0.635877000	4.662635000	-0.561035000
1	0.367656000	3.085666000	0.899616000
6	1.293212000	5.063799000	-1.736199000
1	2.709160000	4.493489000	-3.279557000
1	-0.057714000	5.344077000	-0.056317000
1	1.111485000	6.059122000	-2.155518000
6	2.003104000	1.007359000	1.764336000
6	1.342936000	0.122175000	2.639617000
6	2.722425000	2.101784000	2.296744000
6	1.413408000	0.320245000	4.026720000

1	0.777972000	-0.721172000	2.233510000
6	2.793280000	2.292253000	3.683794000
1	3.209244000	2.814993000	1.623134000
6	2.139472000	1.400459000	4.551008000
1	0.892788000	-0.374481000	4.694119000
1	3.355478000	3.141594000	4.087161000
1	2.191880000	1.553404000	5.634553000
6	3.540630000	0.238575000	-0.652667000
6	4.733484000	0.513171000	0.039742000
6	3.586833000	-0.426563000	-1.895368000
6	5.965393000	0.133974000	-0.514598000
1	4.699523000	1.001780000	1.018374000
6	4.820527000	-0.788066000	-2.452965000
1	2.647856000	-0.683225000	-2.399310000
6	6.011340000	-0.508930000	-1.761928000
1	6.891966000	0.337132000	0.033359000
1	4.850649000	-1.309113000	-3.415865000
1	6.975224000	-0.805070000	-2.189998000
8	-2.560536000	-1.302696000	2.738865000
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6	-1.473856000	-3.150454000	-1.506394000
1	-0.763109000	-3.184800000	-2.338484000
6	-2.389159000	-4.199845000	-1.324916000
1	-2.410850000	-5.029610000	-2.041164000
6	-3.252892000	-4.203748000	-0.213288000
1	-3.952889000	-5.032179000	-0.061070000
6	-3.211526000	-3.144591000	0.697159000
1	-3.861542000	-3.124505000	1.577552000
6	-2.324681000	-2.060934000	0.498352000
6	-2.321966000	-1.002945000	1.557004000
6	-2.297915000	1.057703000	-0.013490000
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6	-1.815812000	1.224018000	2.376086000
1	-2.753710000	1.759430000	2.617599000
1	-1.031446000	1.962054000	2.136904000
1	-1.514377000	0.633431000	3.248712000
6	-2.963130000	-0.221188000	-2.300260000
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6	-6.013893000	1.702292000	0.802461000
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6	-6.320291000	2.714775000	-0.119941000

6	-5.321429000	3.192066000	-0.984544000
1	-5.548375000	3.988563000	-1.701809000
6	-4.028532000	2.653377000	-0.925845000
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6	-4.171193000	-1.039109000	-1.824937000
1	-4.915255000	-1.057861000	-2.641592000
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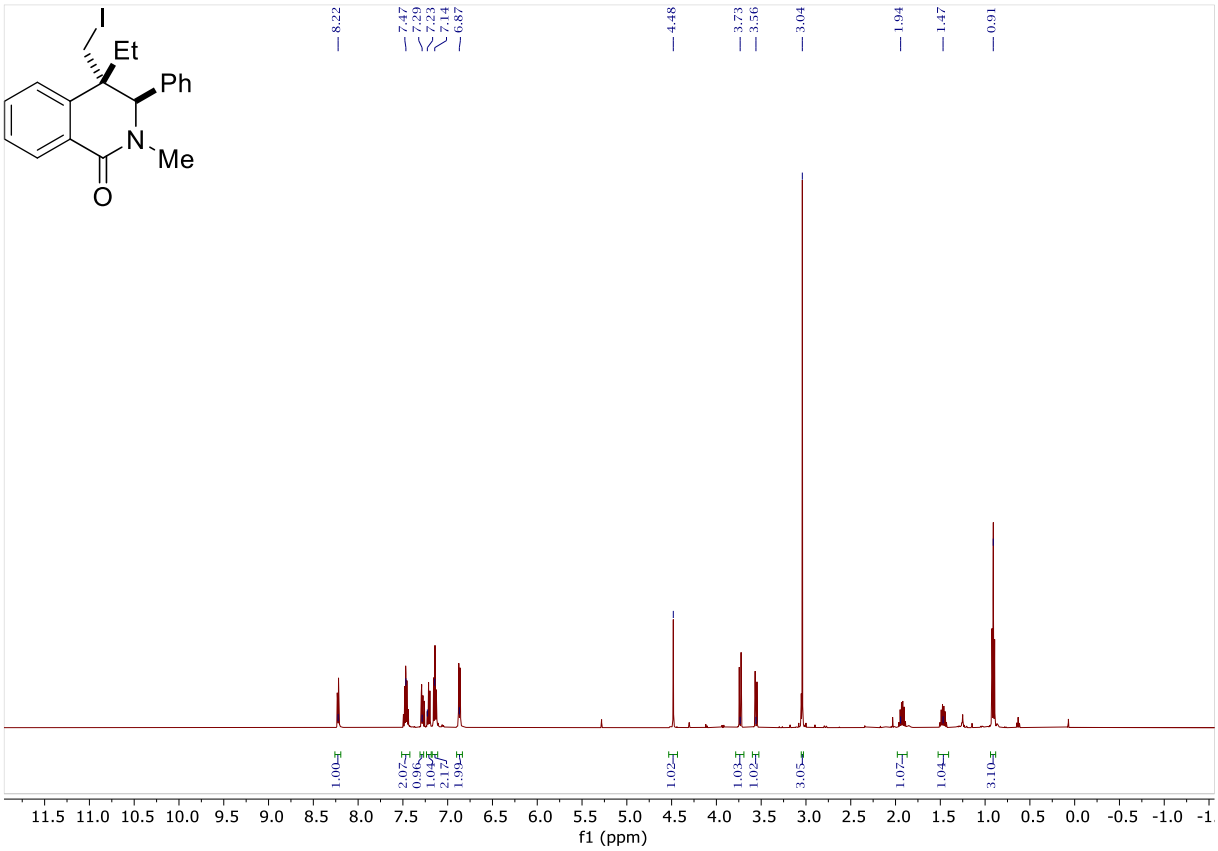
Spectra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Et
Ph
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Me
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3.04
1.94
1.47
0.91
1.00
2.07
0.96
1.04
2.17
1.99
1.02
1.03
1.02
3.05
1.07
1.04
3.10
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1
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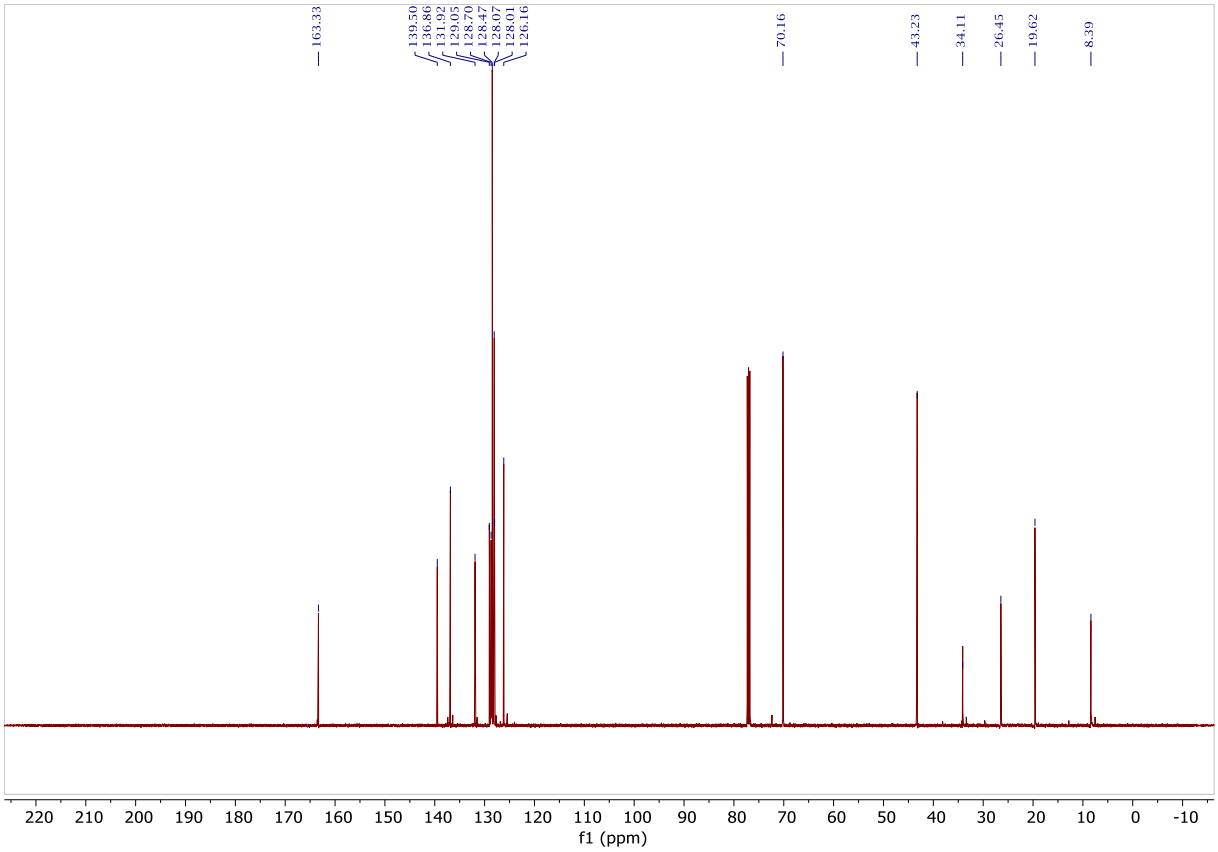
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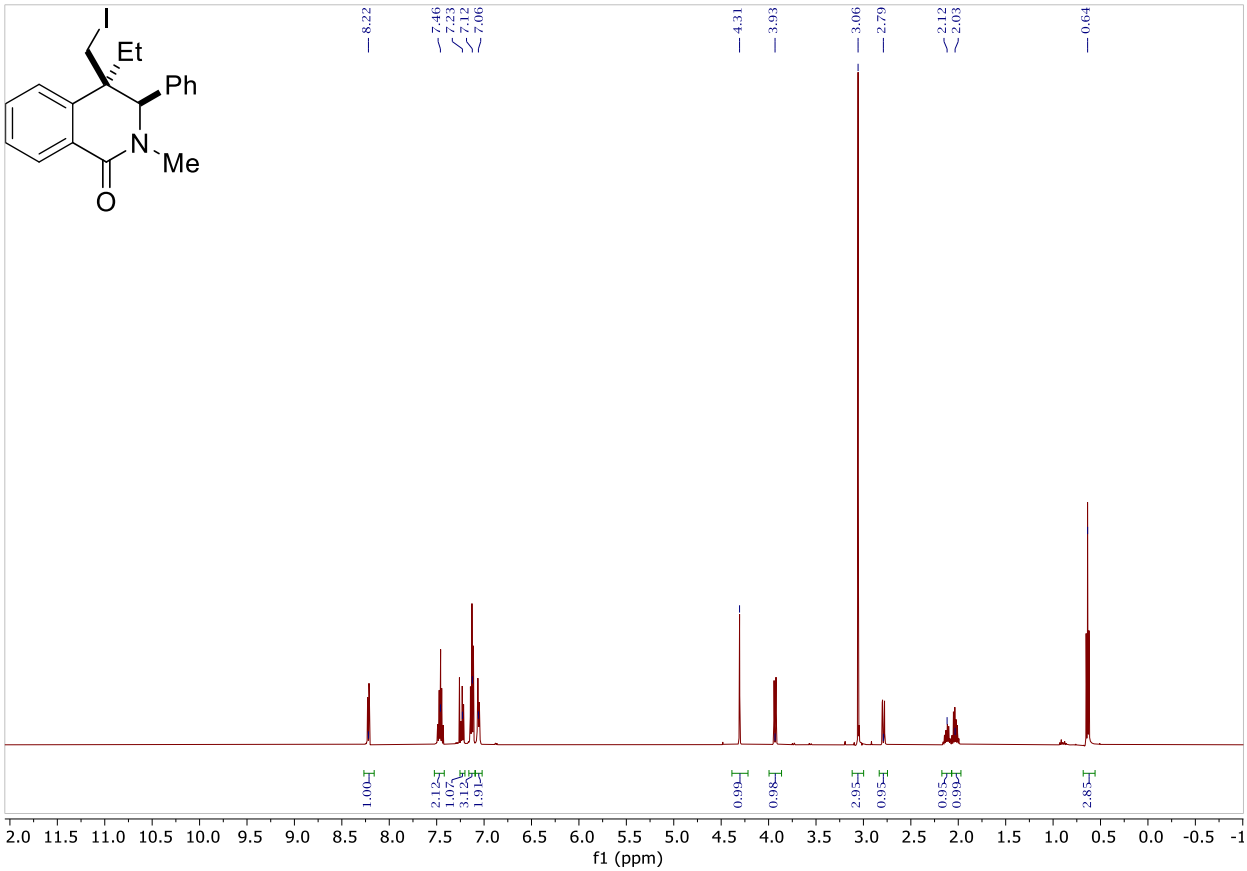
f1 (ppm)


I
Et
Ph
N
Me
O
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2.12
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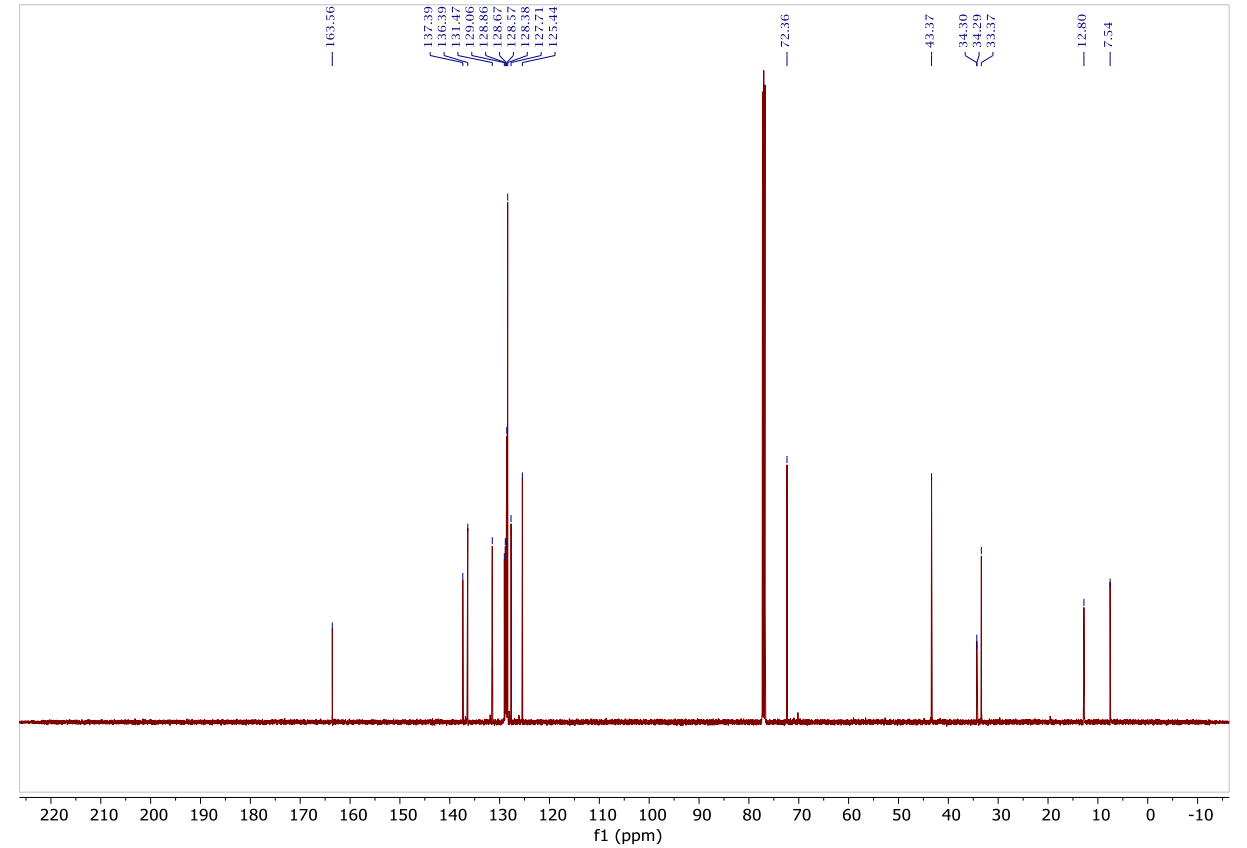
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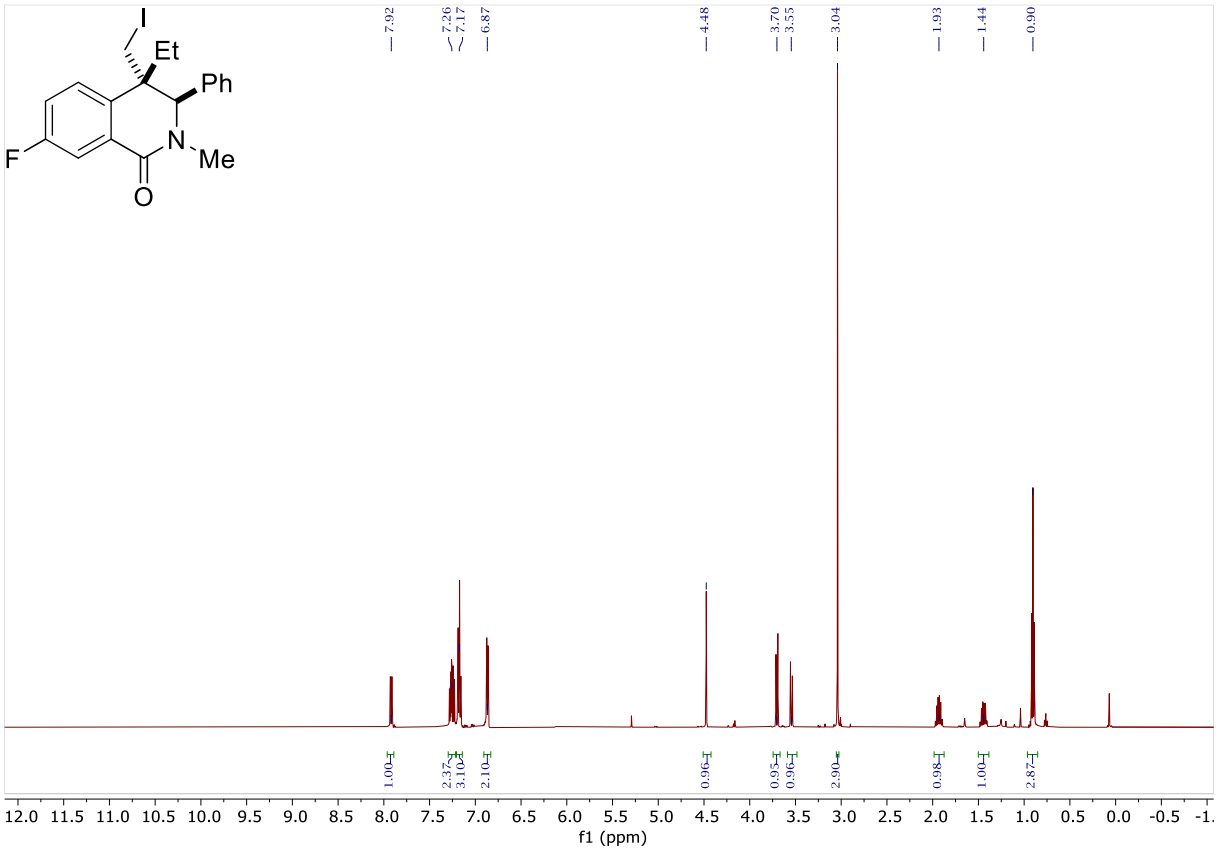
f1 (ppm)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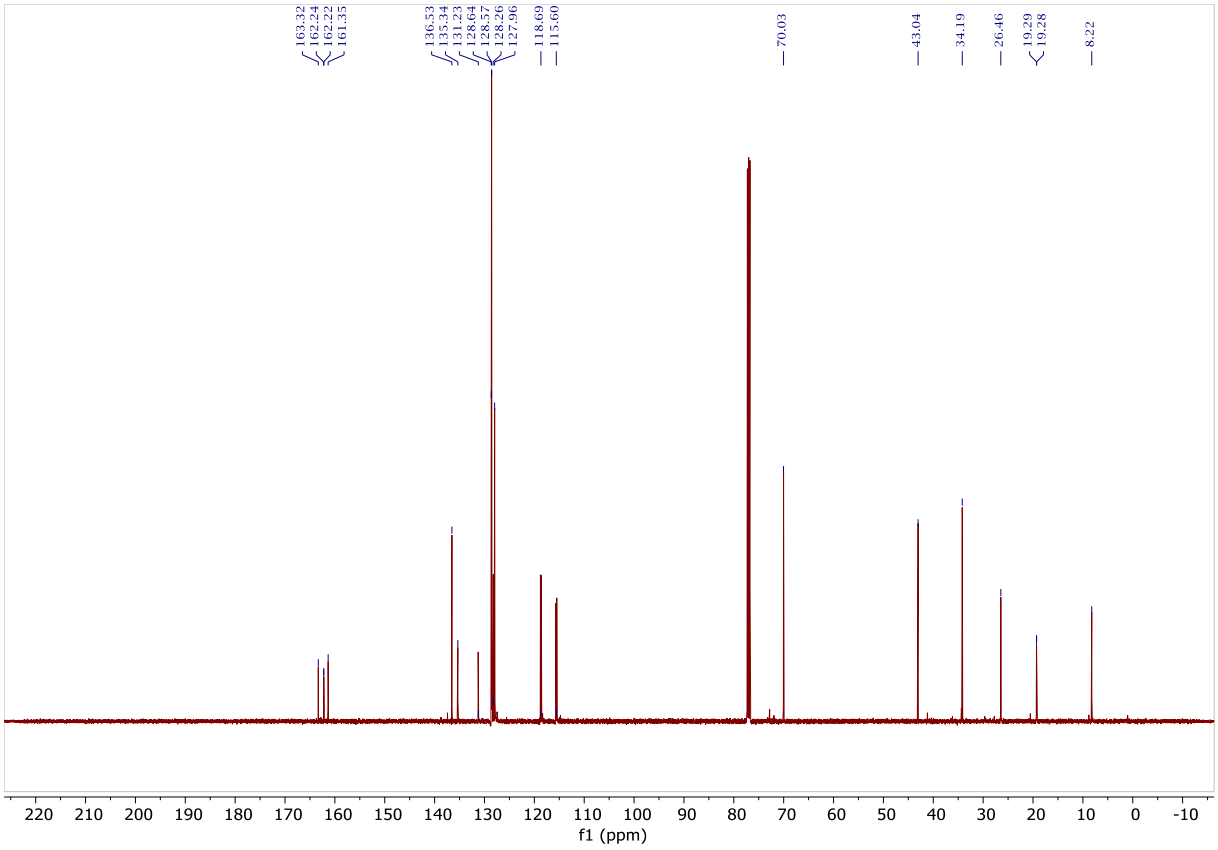
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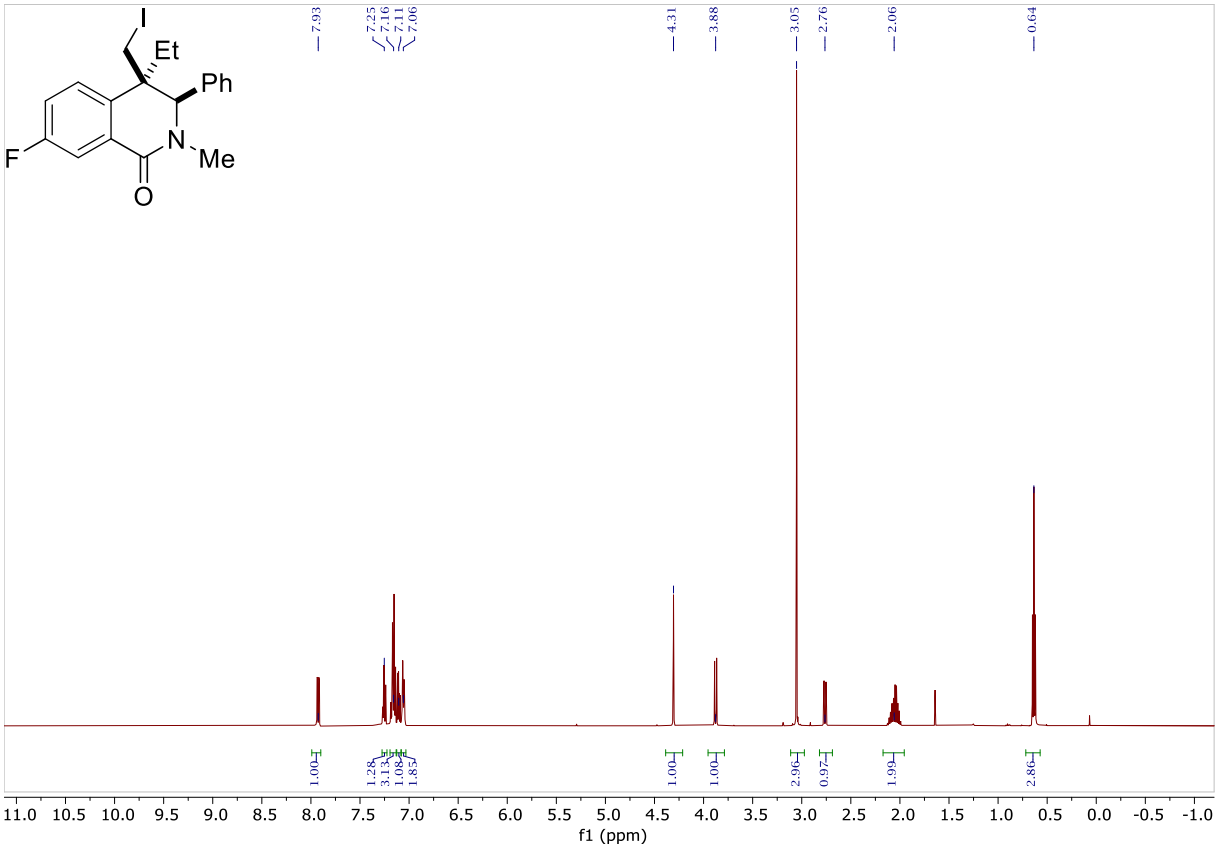
19.29
19.28
8.22
f1 (ppm)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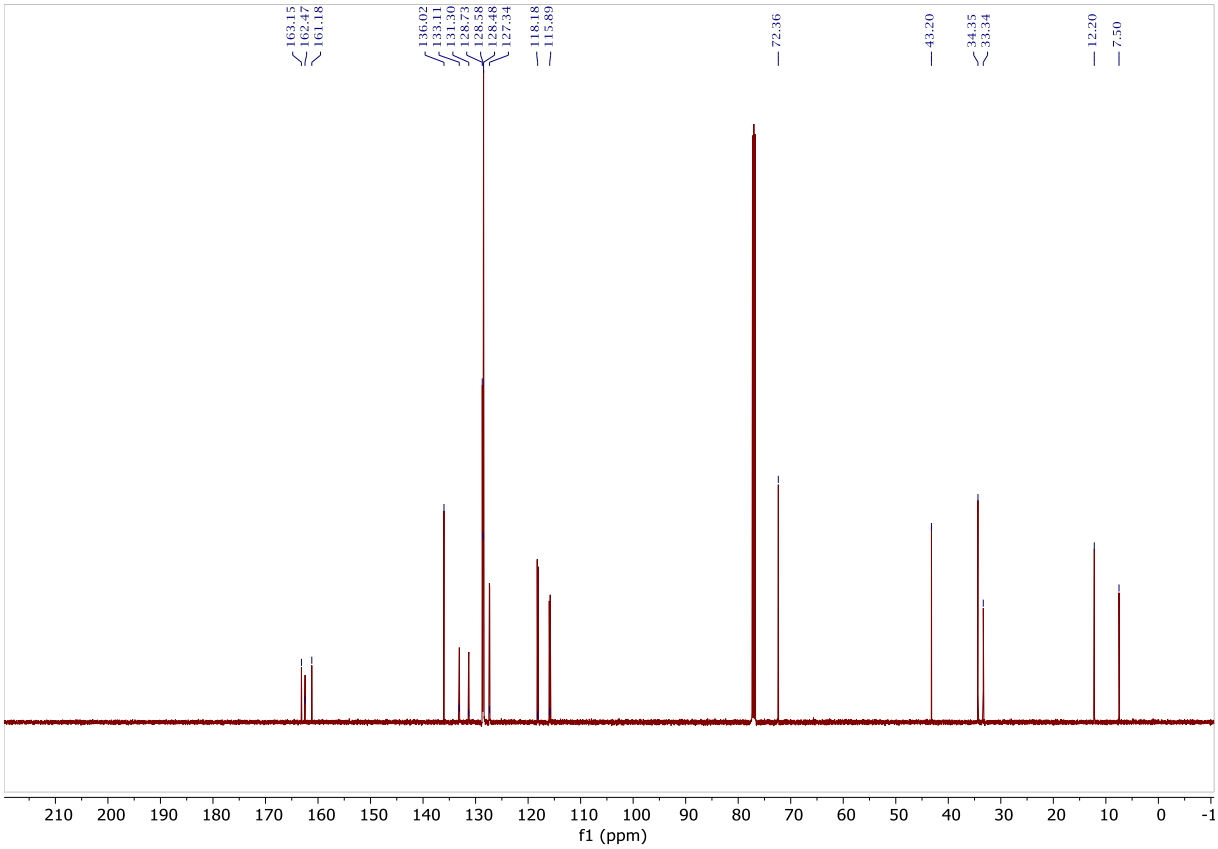
Et
Ph
N
Me
F
O
7.93
7.25
7.16
7.11
7.06
4.31
3.88
3.05
2.76
2.06
0.64
1.00
1.28
3.13
1.08
1.85
1.00
1.00
2.96
0.97
1.99
2.86
f1 (ppm)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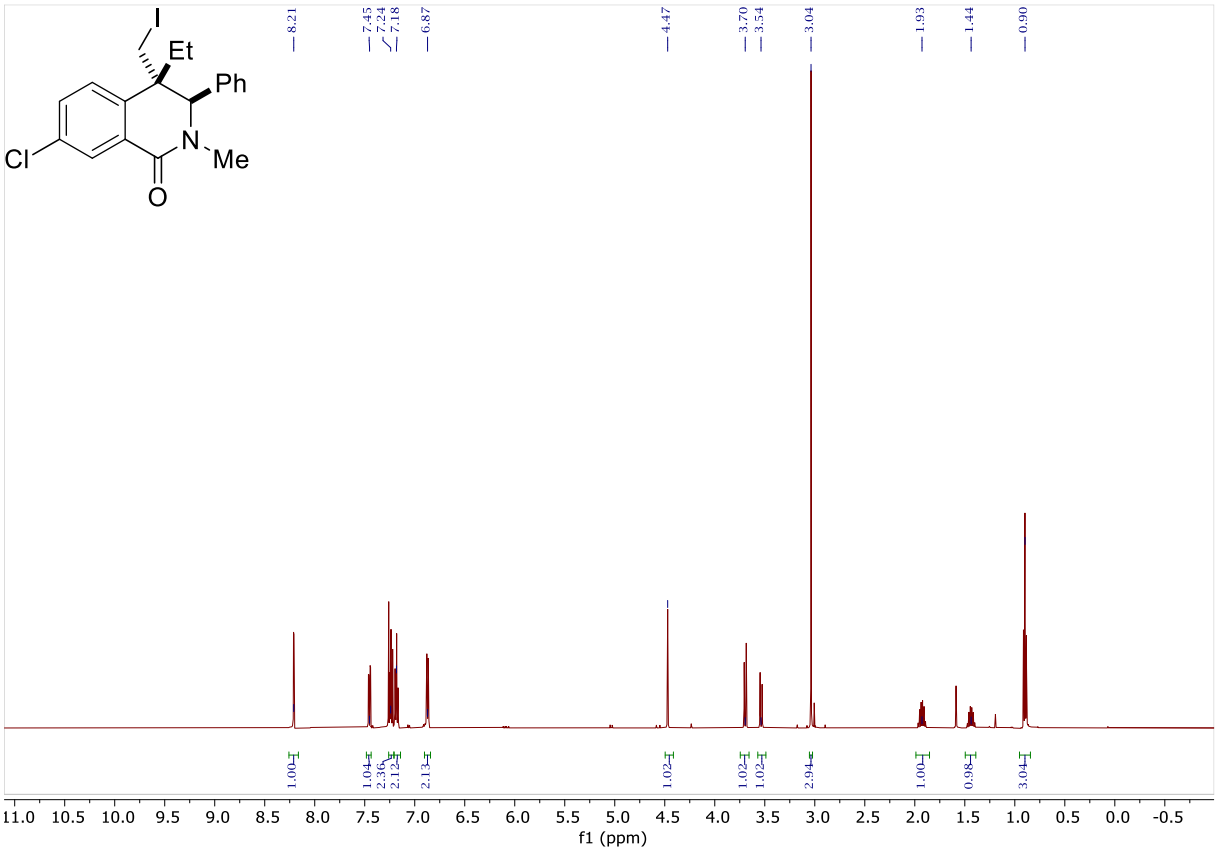
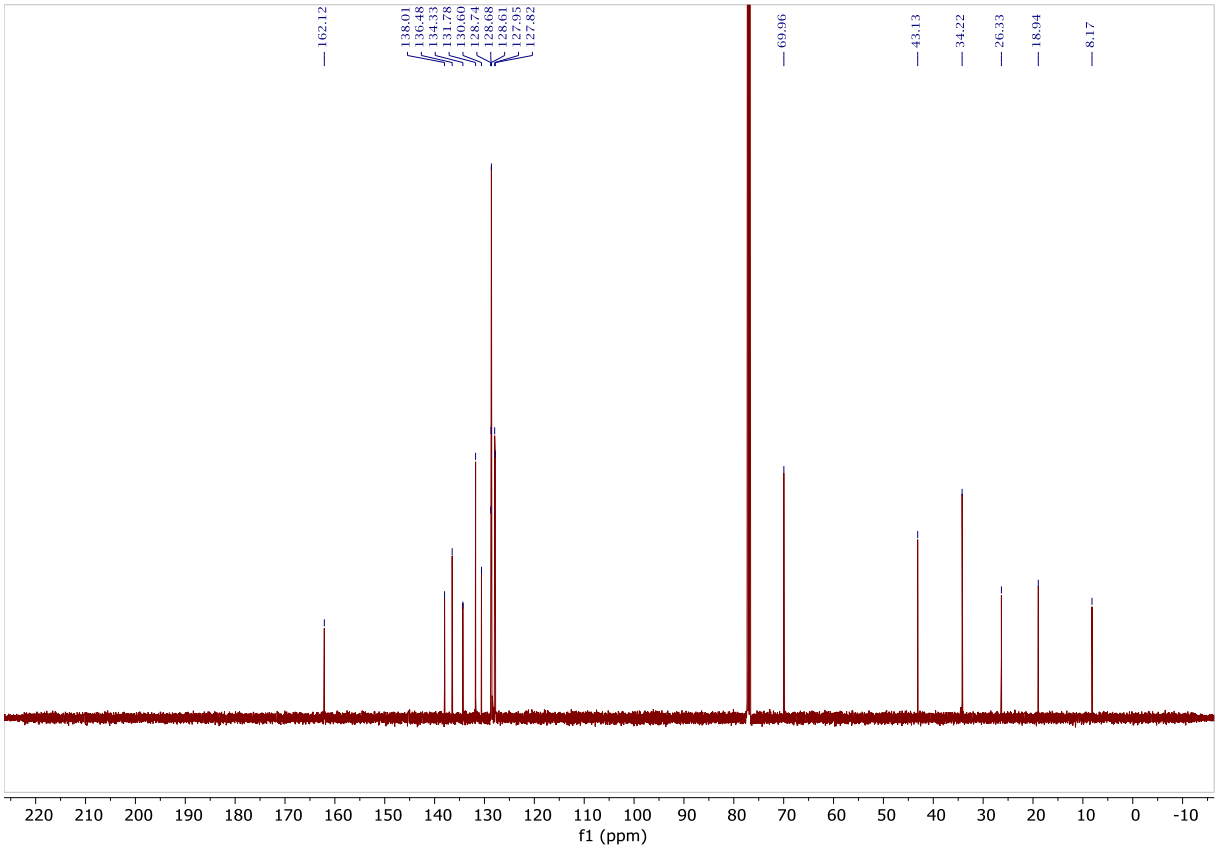
162.47
161.18
136.02
133.11
131.20
128.73
128.58
128.48
127.34
118.18
115.89
72.36
43.20
34.35
33.34
12.20
7.50
f1 (ppm)


I
Et
Ph
N
Me
Cl
O
8.21
7.45
7.24
7.18
6.87
4.47
3.70
3.54
3.04
1.93
1.44
0.90
1.00
1.04
2.36
2.12
2.13
1.02
1.02
1.02
2.94
1.00
0.98
3.04
f1 (ppm)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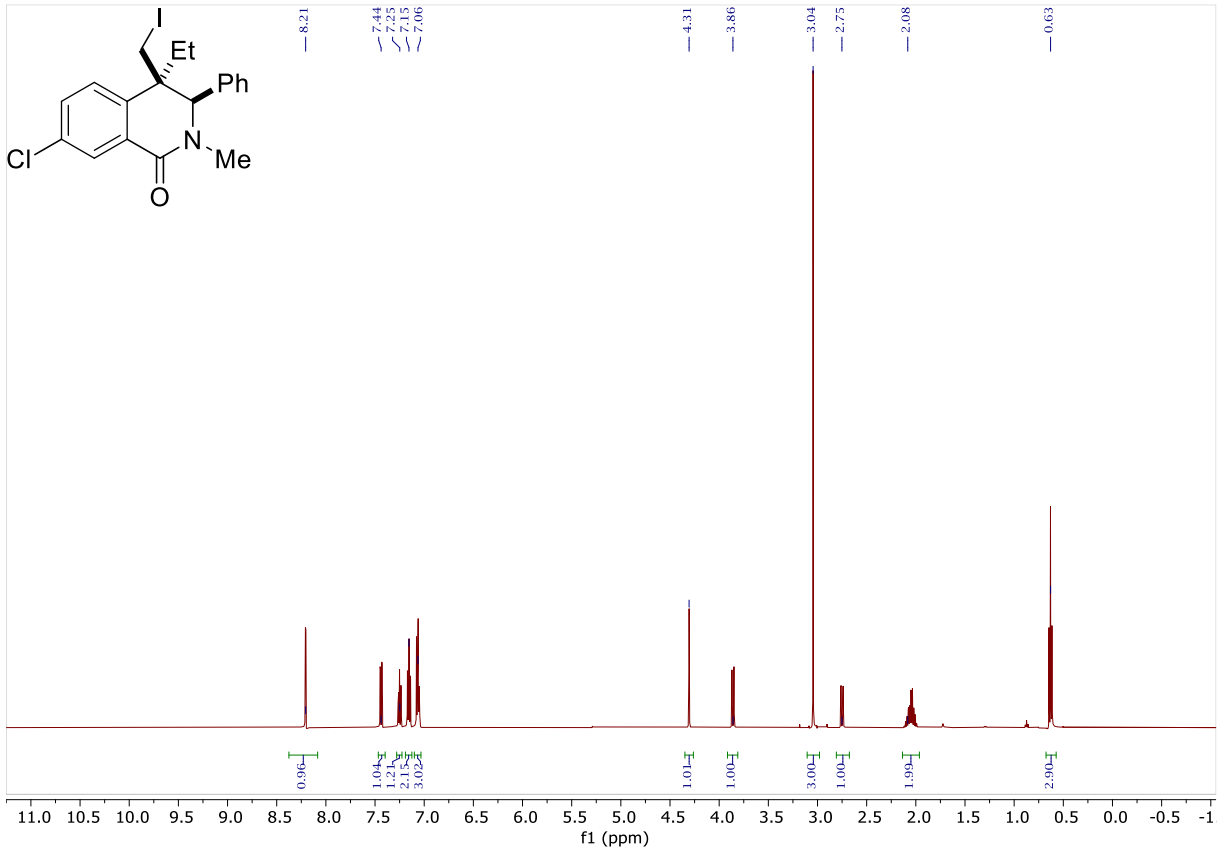
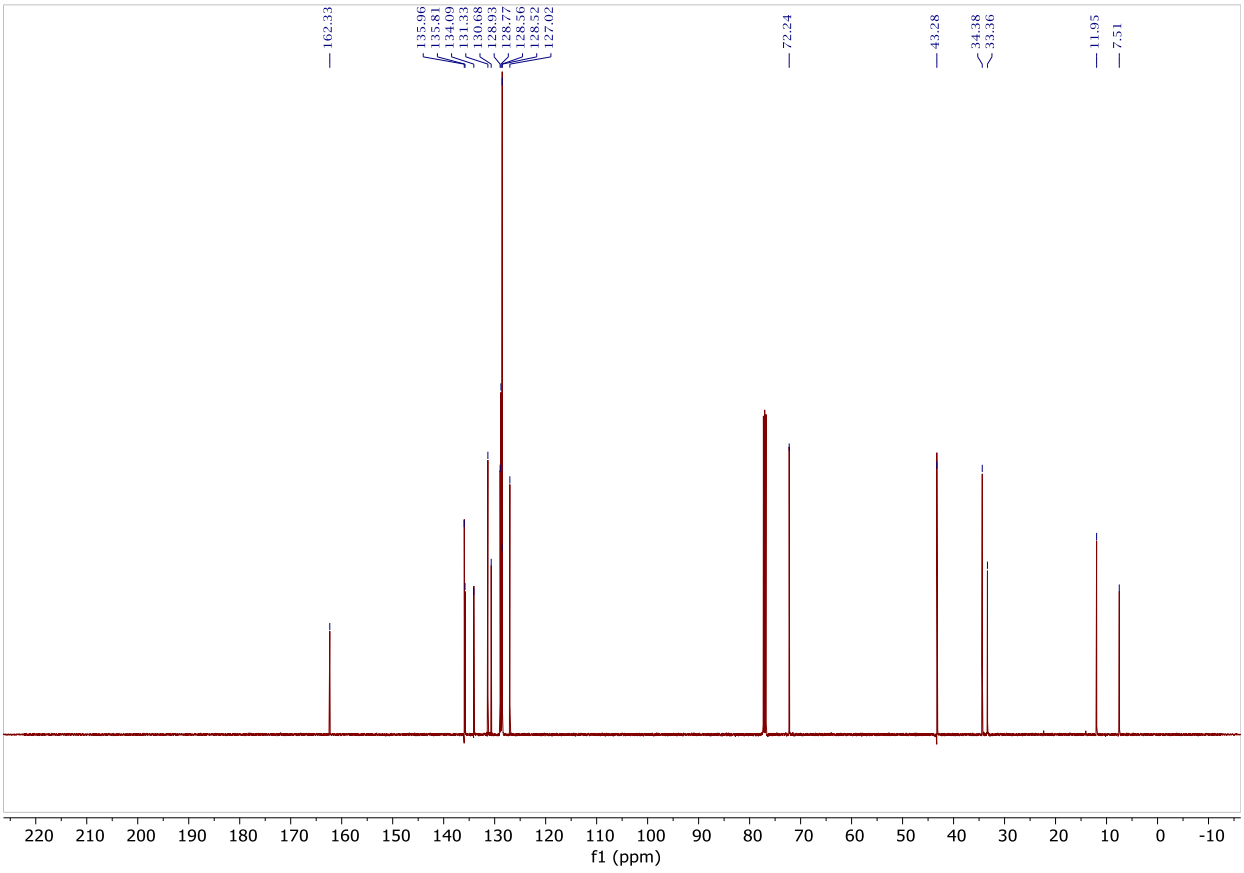
138.01
136.48
134.33
131.78
130.60
128.74
128.68
128.61
127.95
127.82
69.96
43.13
34.22
26.33
18.94
8.17
f1 (ppm)


I
Et
Ph
N
Me
Cl
O
8.21
7.44
7.25
7.15
7.06
4.31
3.86
3.04
2.75
2.08
0.63
0.96
1.04
1.21
2.15
3.02
1.01
1.00
3.00
1.00
1.99
2.90
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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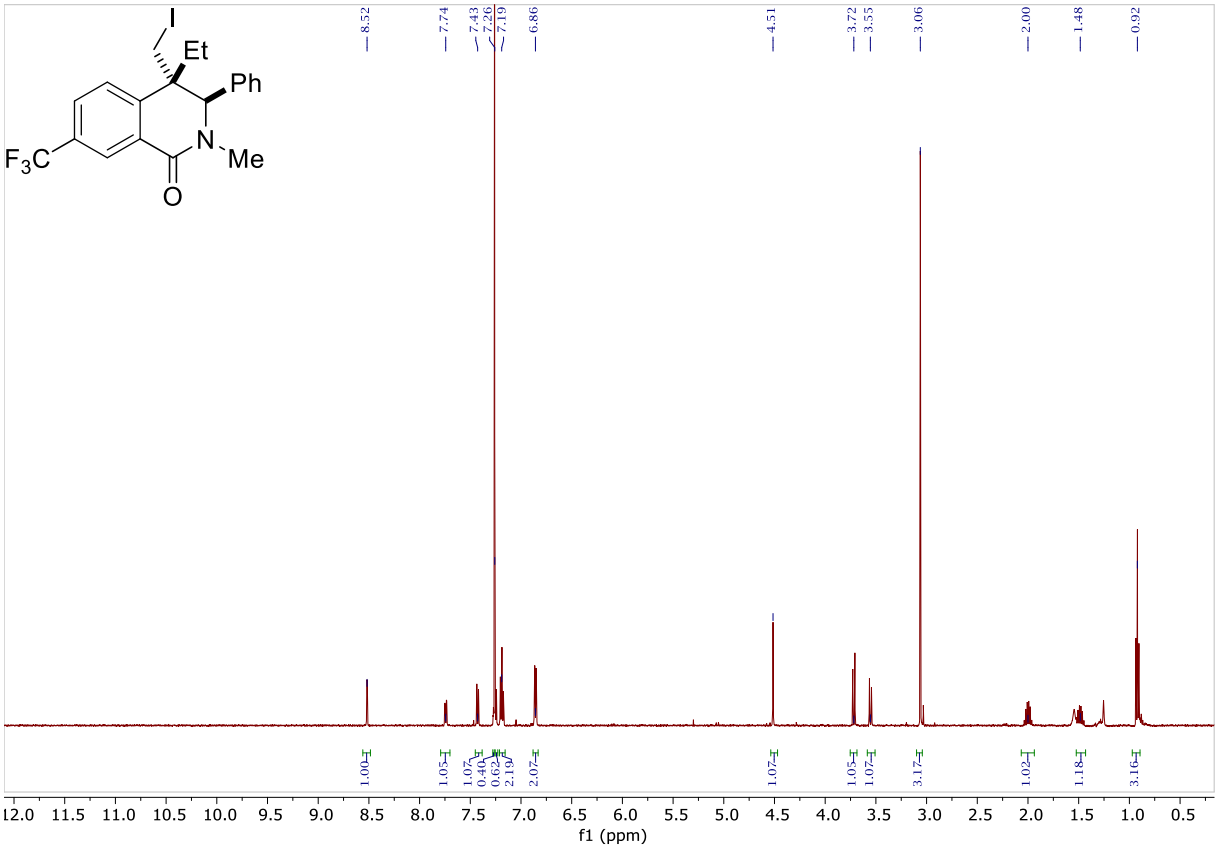
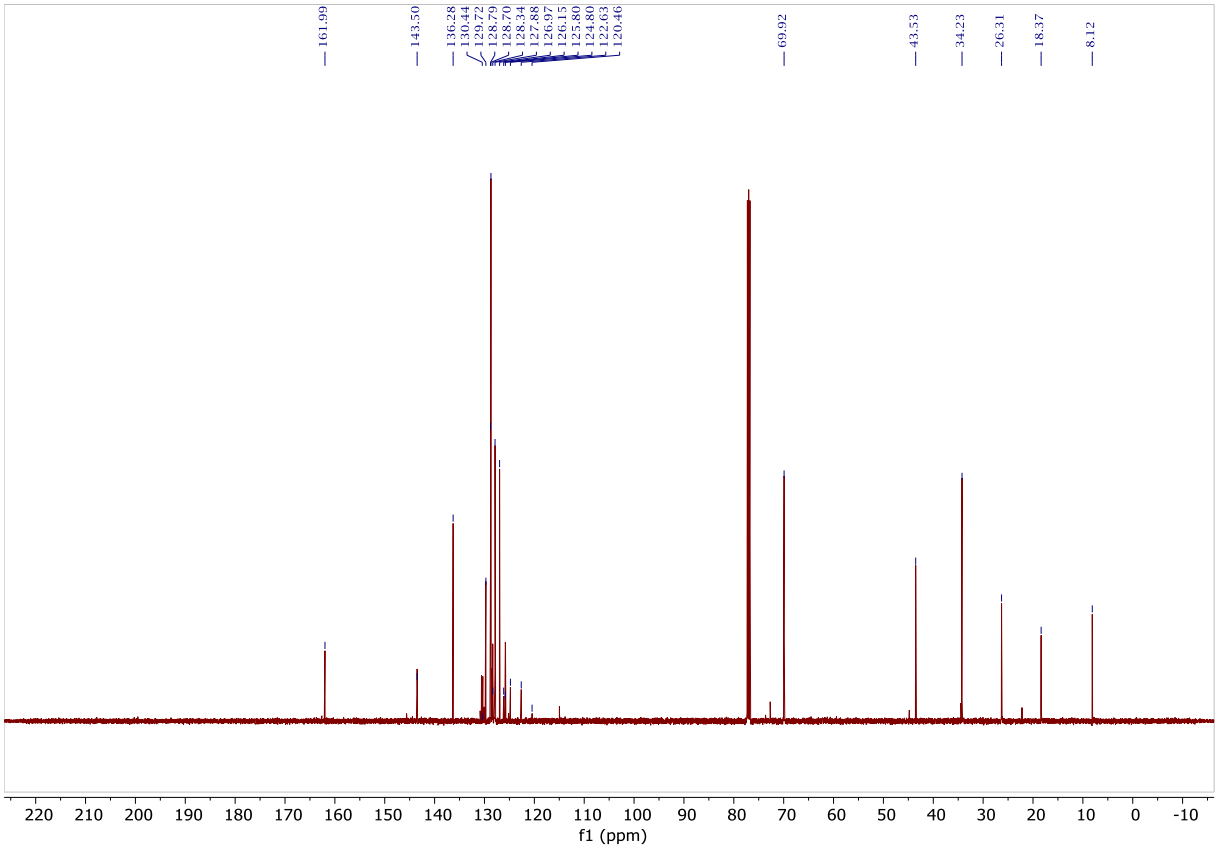
135.81
134.09
131.33
130.68
128.93
128.77
128.56
128.52
127.02
72.24
43.28
34.38
33.36
11.95
7.51
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


I
Et
Ph
N
Me
F3C
O
8.52
7.74
7.43
7.26
7.19
6.86
4.51
3.72
3.55
3.06
2.00
1.48
0.92
1.00
1.05
1.07
0.40
0.62
2.19
2.07
1.07
1.05
1.07
3.17
1.02
1.18
3.16
f1 (ppm)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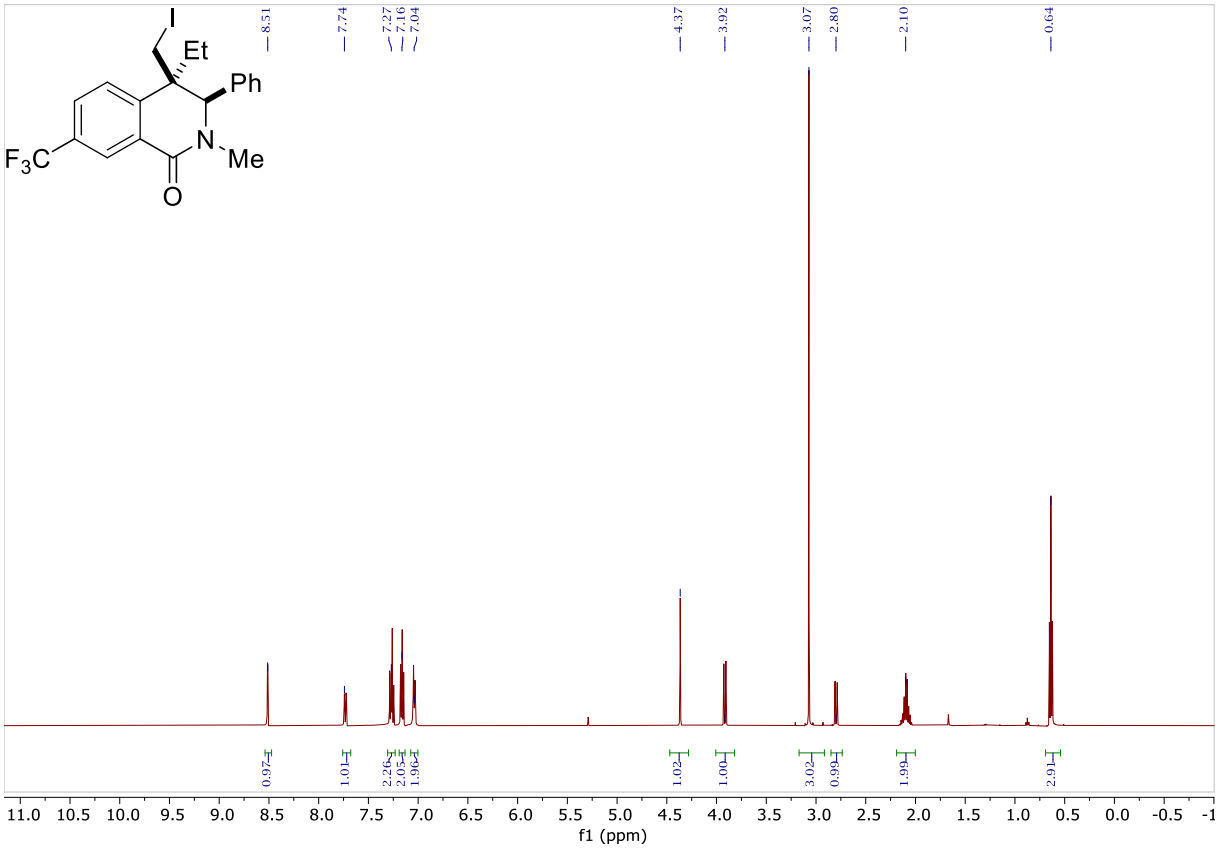
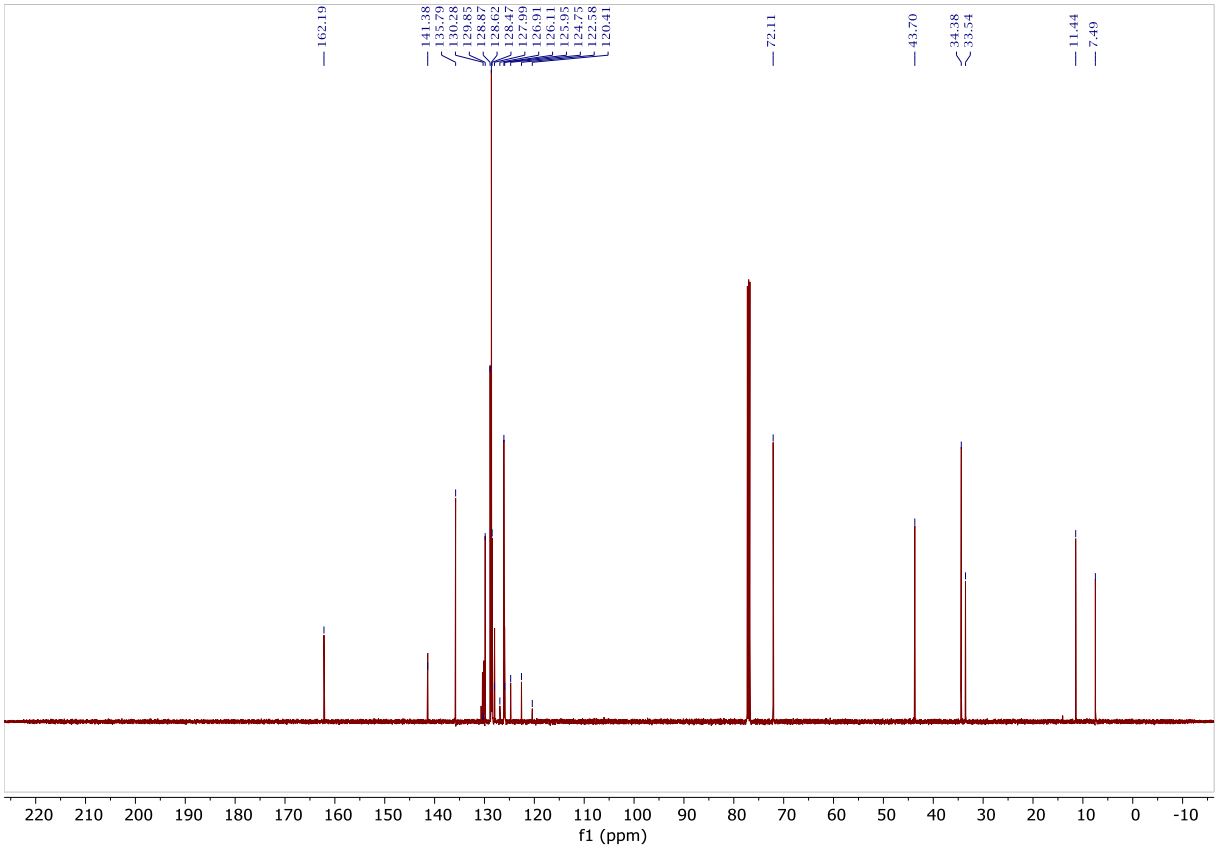
143.50
136.28
130.44
129.72
128.79
128.70
128.34
127.88
126.97
126.15
125.80
124.80
122.63
120.46
69.92
43.53
34.23
26.31
18.37
8.12
f1 (ppm)


I
Et
Ph
N
Me
O
F3C
8.51
7.74
7.27
7.16
7.04
4.37
3.92
3.07
2.80
2.10
0.64
0.97
1.01
2.26
2.05
1.96
1.02
1.00
3.02
0.99
1.99
2.91
f1 (ppm)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135.79
130.28
129.85
128.87
128.62
128.47
127.99
126.91
126.11
125.95
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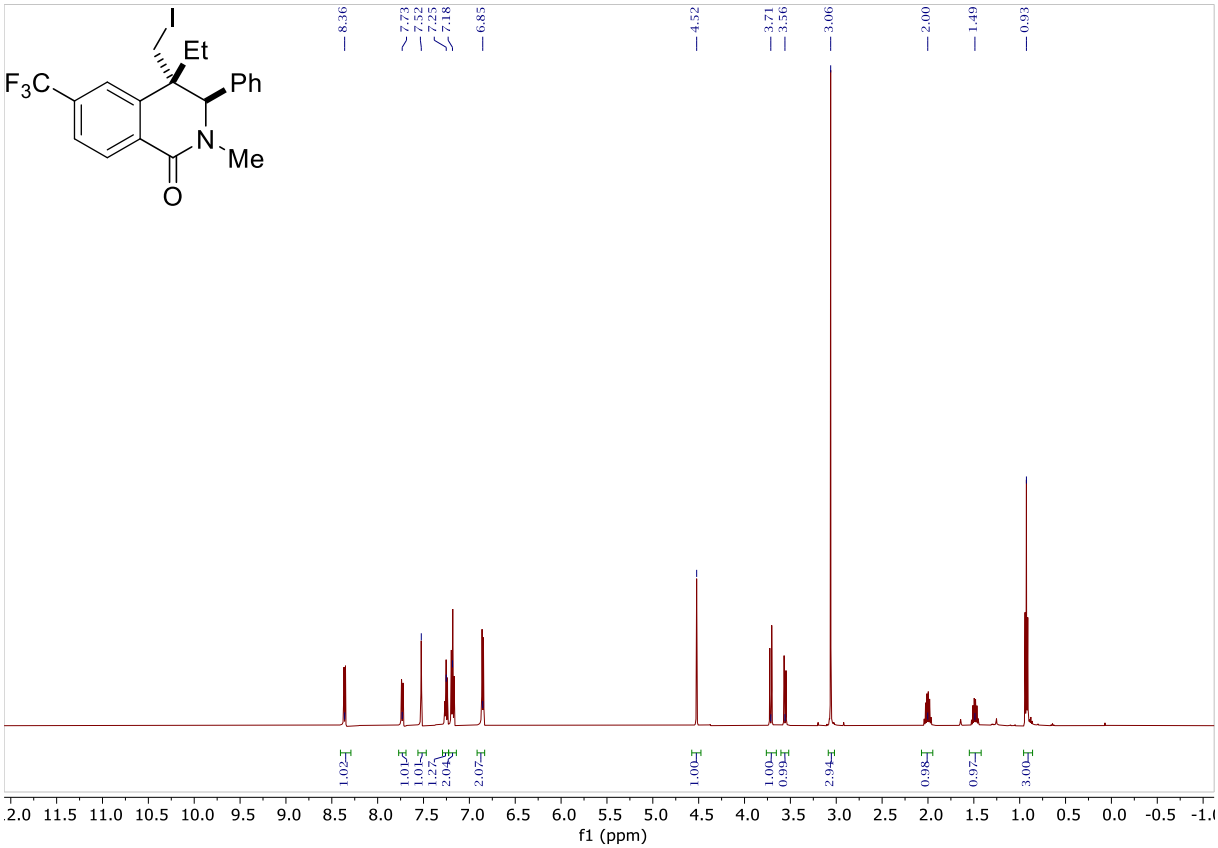
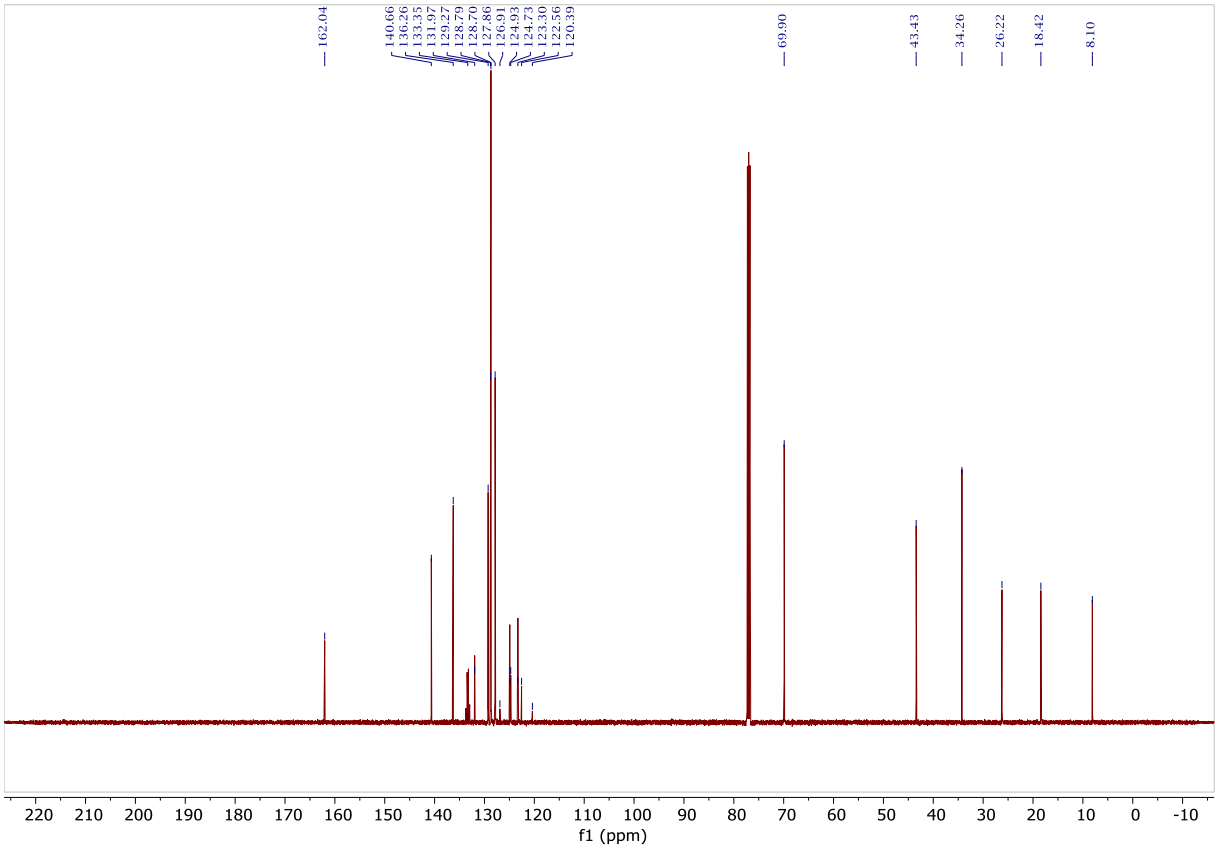
122.58
120.41
72.11
43.70
34.38
33.54
11.44
7.49
f1 (ppm)


I
Et
F3C
Ph
N
Me
O
8.36
7.73
7.52
7.25
7.18
6.85
4.52
3.71
3.56
3.06
2.00
1.49
0.93
1.02
1.01
1.01
1.25
2.04
2.07
1.00
1.00
0.99
2.94
0.98
0.97
3.00
f1 (ppm)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131.97
129.27
128.79
128.70
127.86
126.91
124.93
124.73
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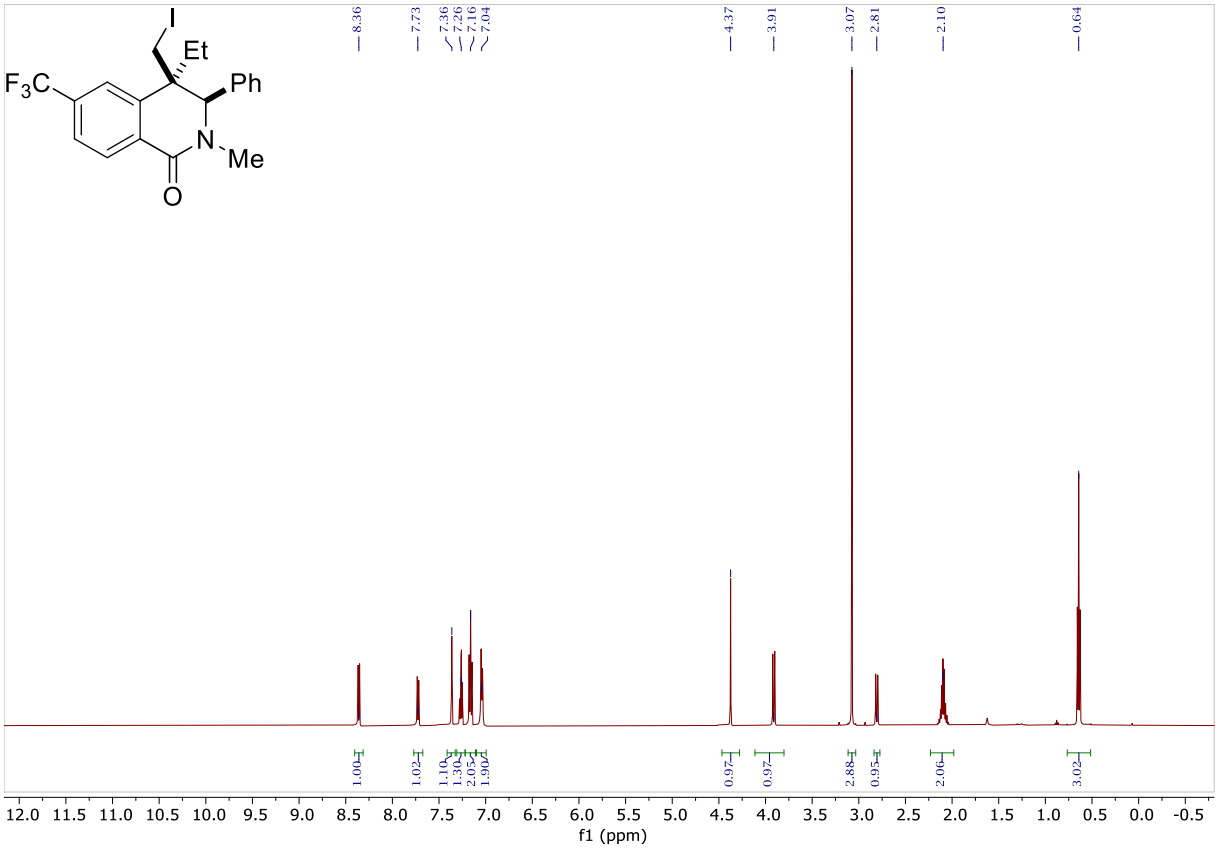
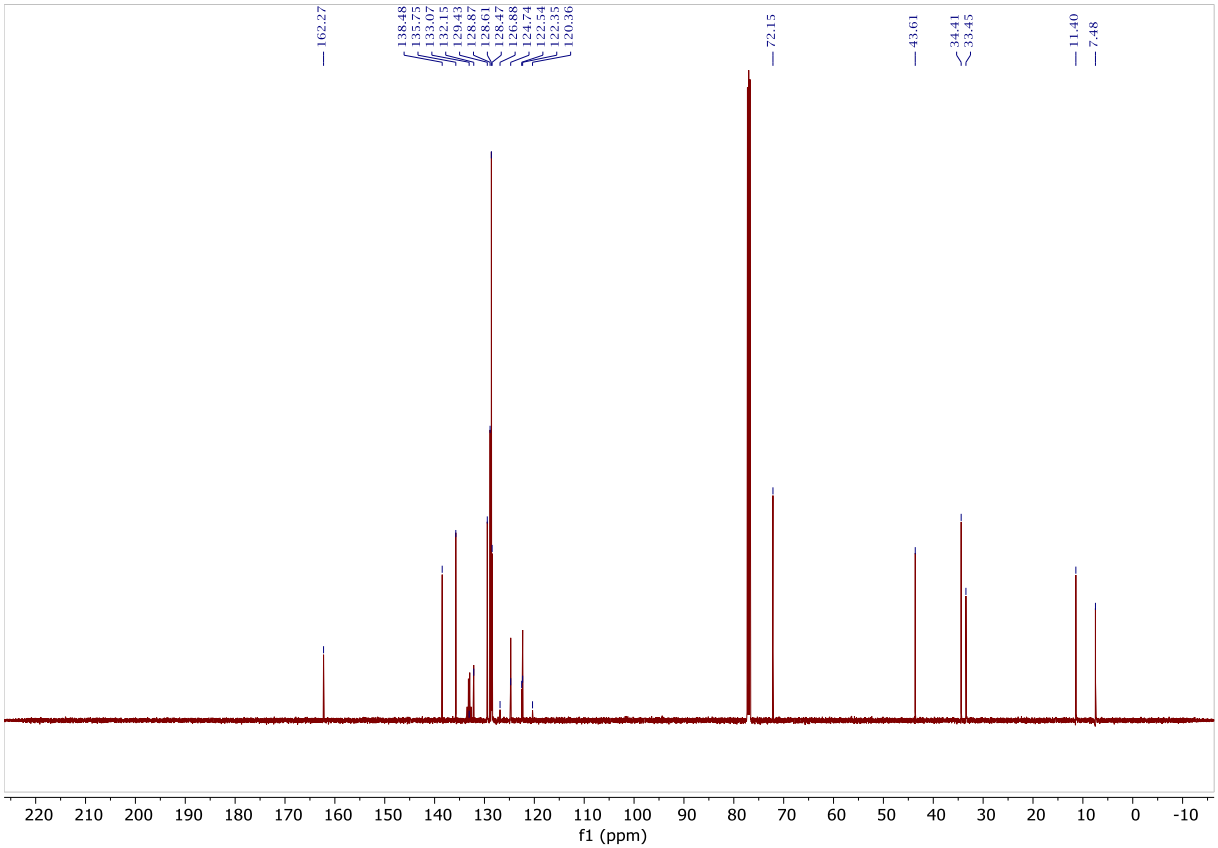
34.26
26.22
18.42
8.10
f1 (ppm)


I
Et
Ph
F3C
N
Me
O
8.36
7.73
7.36
7.26
7.16
7.04
4.37
3.91
3.07
2.81
2.10
0.64
1.00
1.02
1.10
1.30
2.05
1.90
0.97
0.97
2.88
0.95
2.06
3.02
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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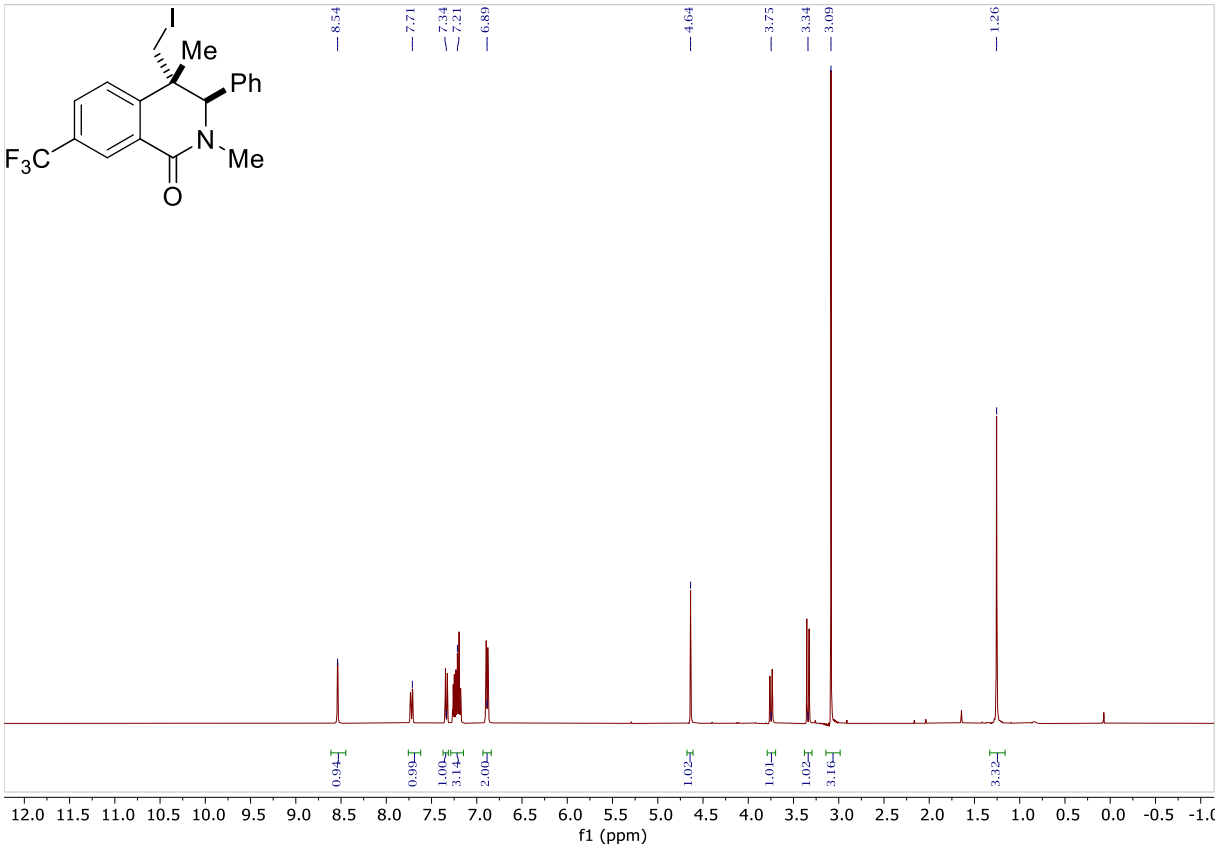
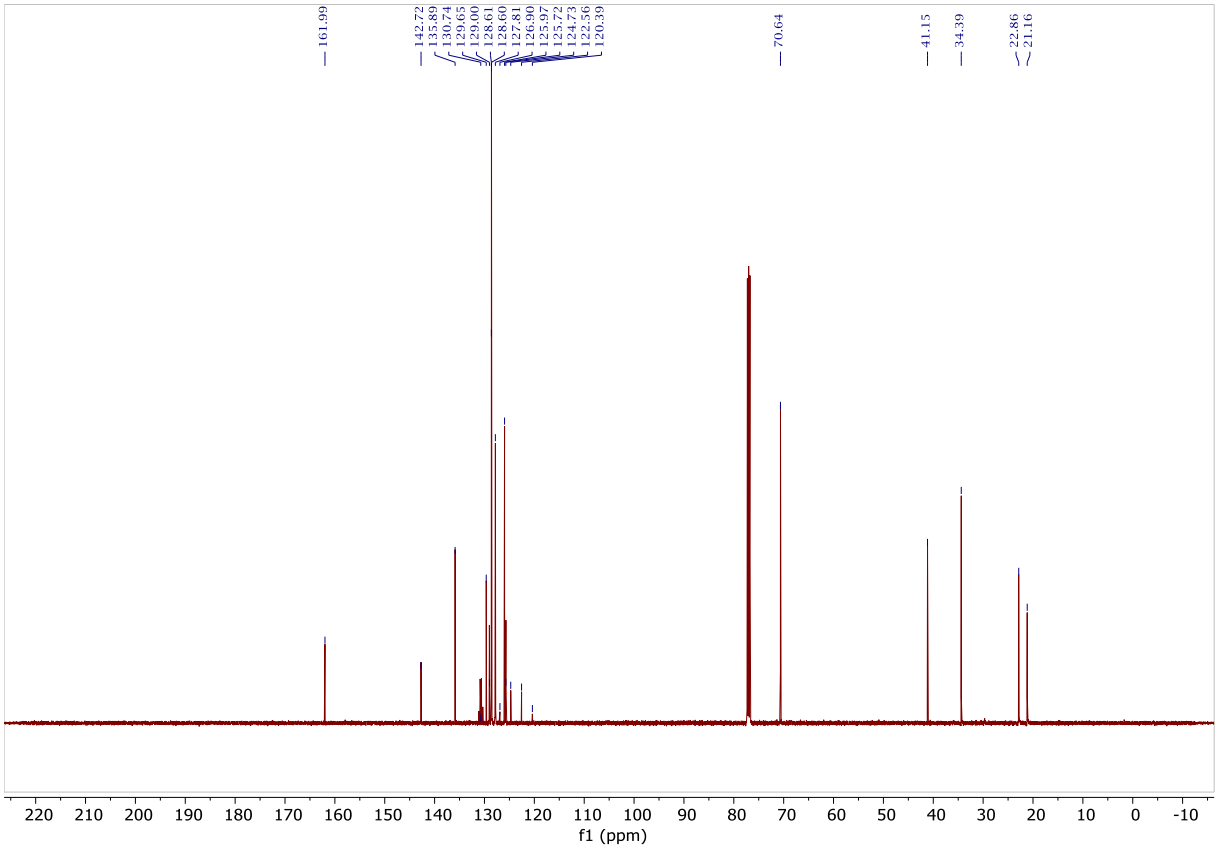
138.48
135.75
133.07
132.15
129.43
128.87
128.61
128.47
126.88
124.74
122.54
122.35
120.36
72.15
43.61
34.41
33.45
11.40
7.48
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


I
Me
Ph
N
Me
F3C
O
8.54
7.71
7.34
7.21
6.89
4.64
3.75
3.34
3.09
1.26
0.94
0.99
1.00
3.14
2.00
1.02
1.01
1.02
3.16
3.32
f1 (ppm)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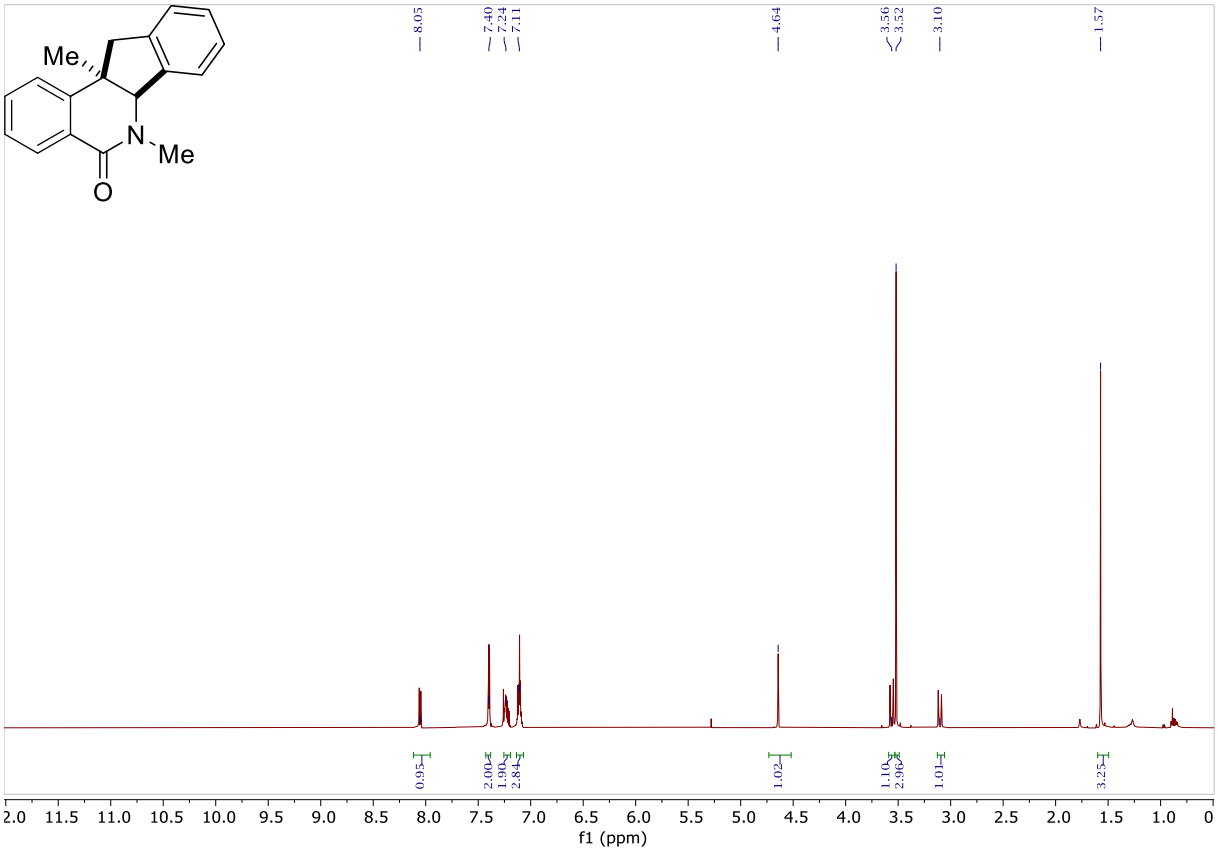
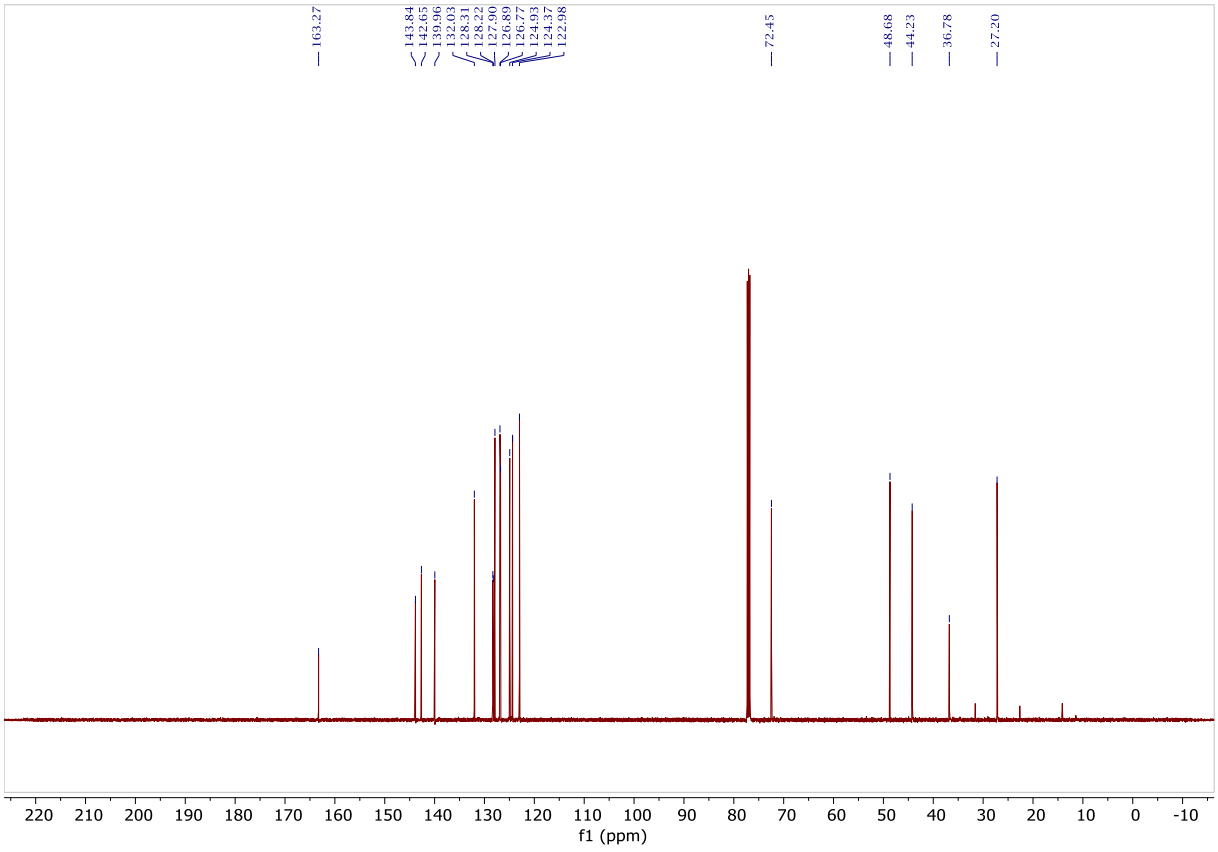
142.72
135.89
130.74
129.65
129.00
128.61
128.60
127.81
126.90
125.97
125.72
124.73
122.56
120.39
70.64
41.15
34.39
22.86
21.16
f1 (ppm)


Me
N
Me
O
8.05
7.40
7.24
7.11
4.64
3.56
3.52
3.10
1.57
0.95
2.00
1.90
2.84
1.02
1.10
2.96
1.01
3.25
f1 (ppm)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128.31
127.22
127.00
126.89
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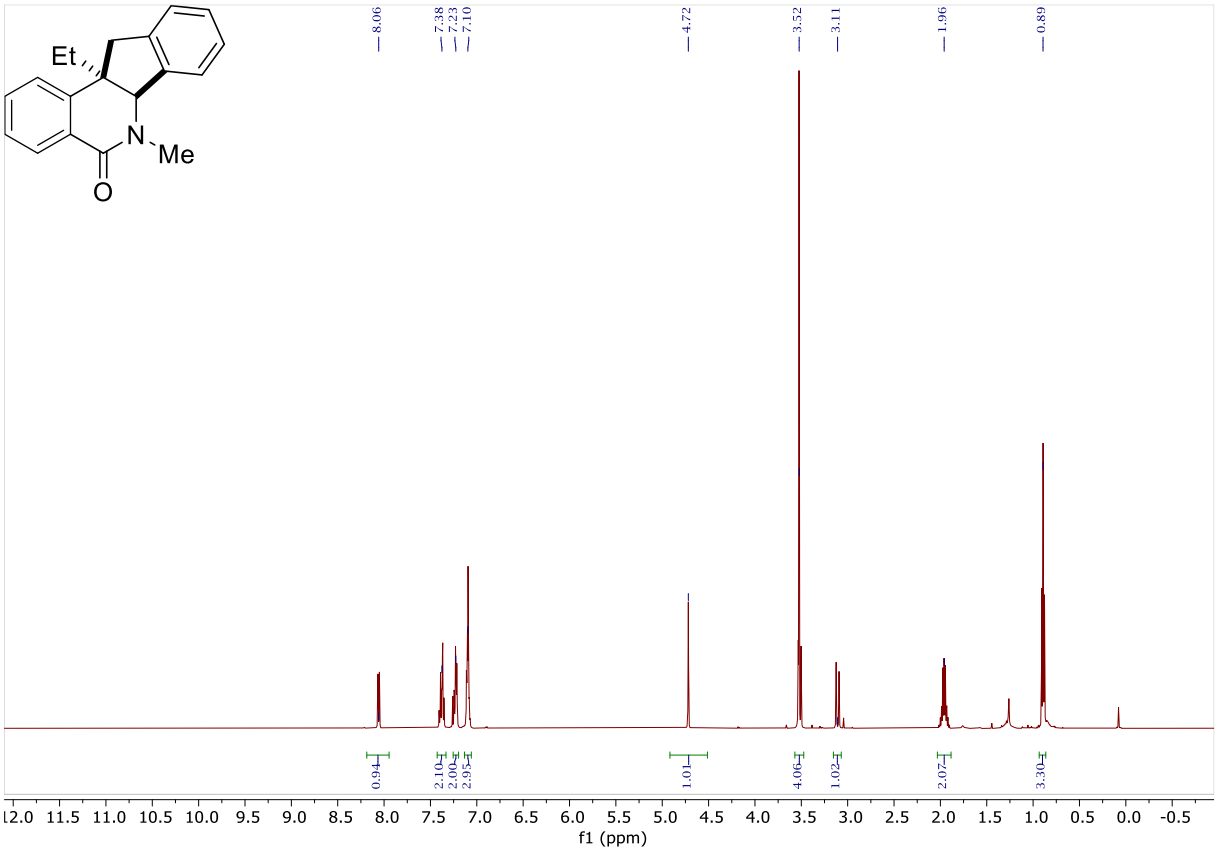
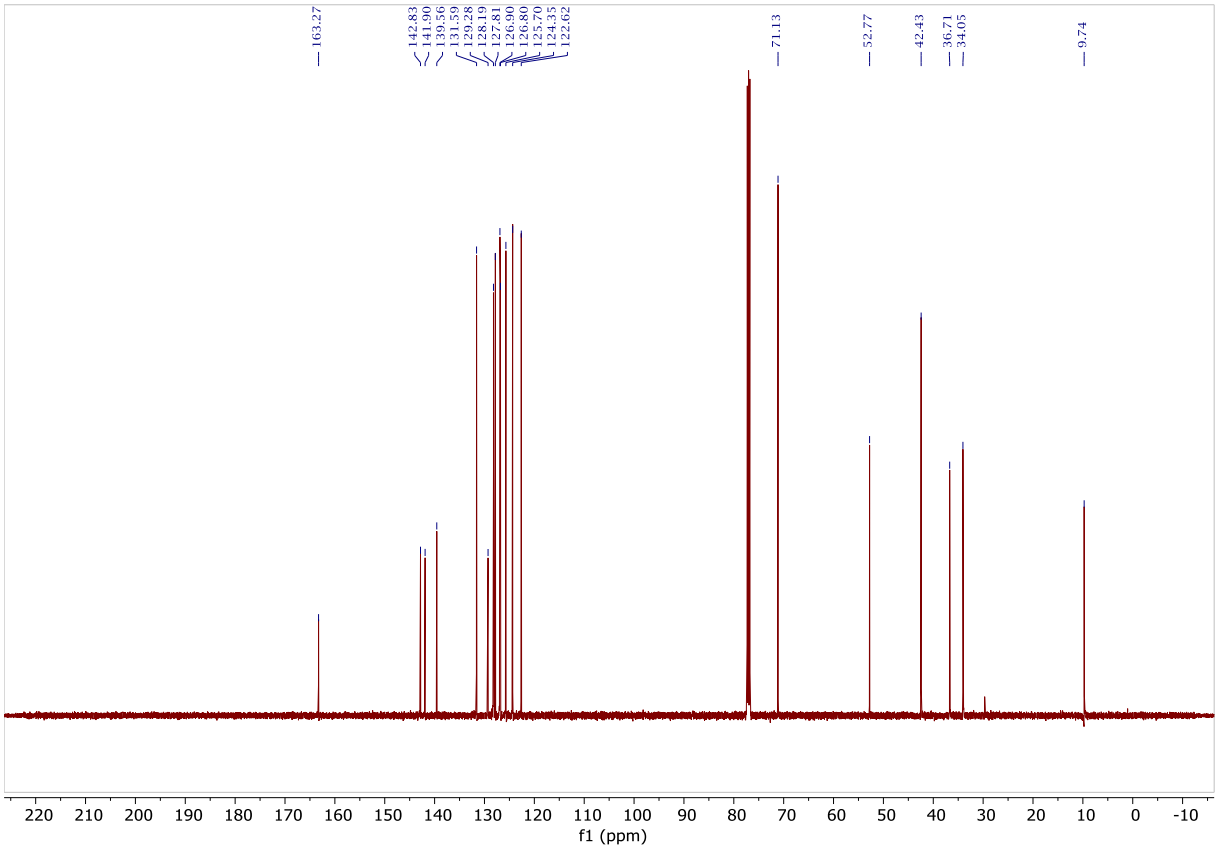
124.93
124.37
122.98
72.45
48.68
44.23
36.78
27.20
f1 (ppm)


Et
N
Me
O
8.06
7.38
7.23
7.10
4.72
3.52
3.11
1.96
0.89
0.94
2.10
2.00
2.95
1.01
4.06
1.02
2.07
3.30
f1 (ppm)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127.81
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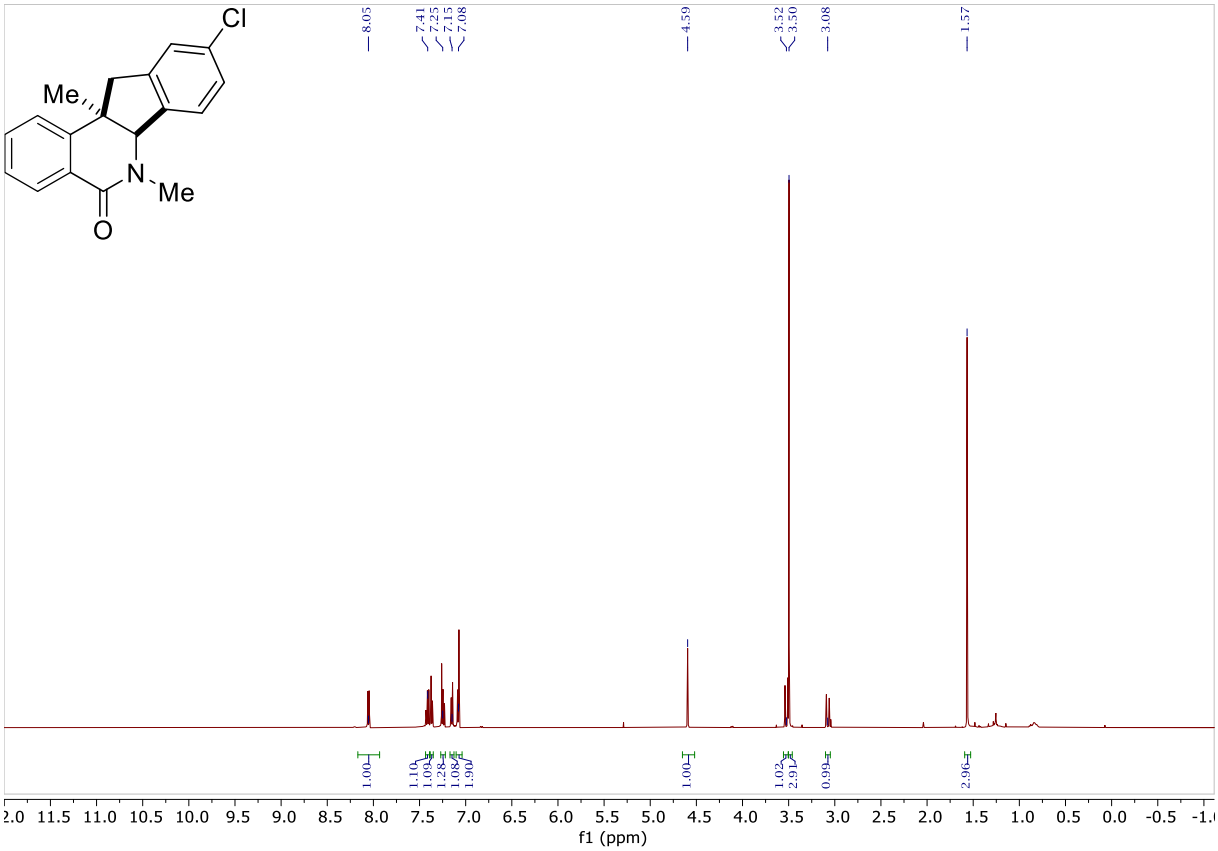
124.35
122.62
71.13
52.77
42.43
36.71
34.05
9.74
f1 (ppm)


Cl
Me
N
Me
O
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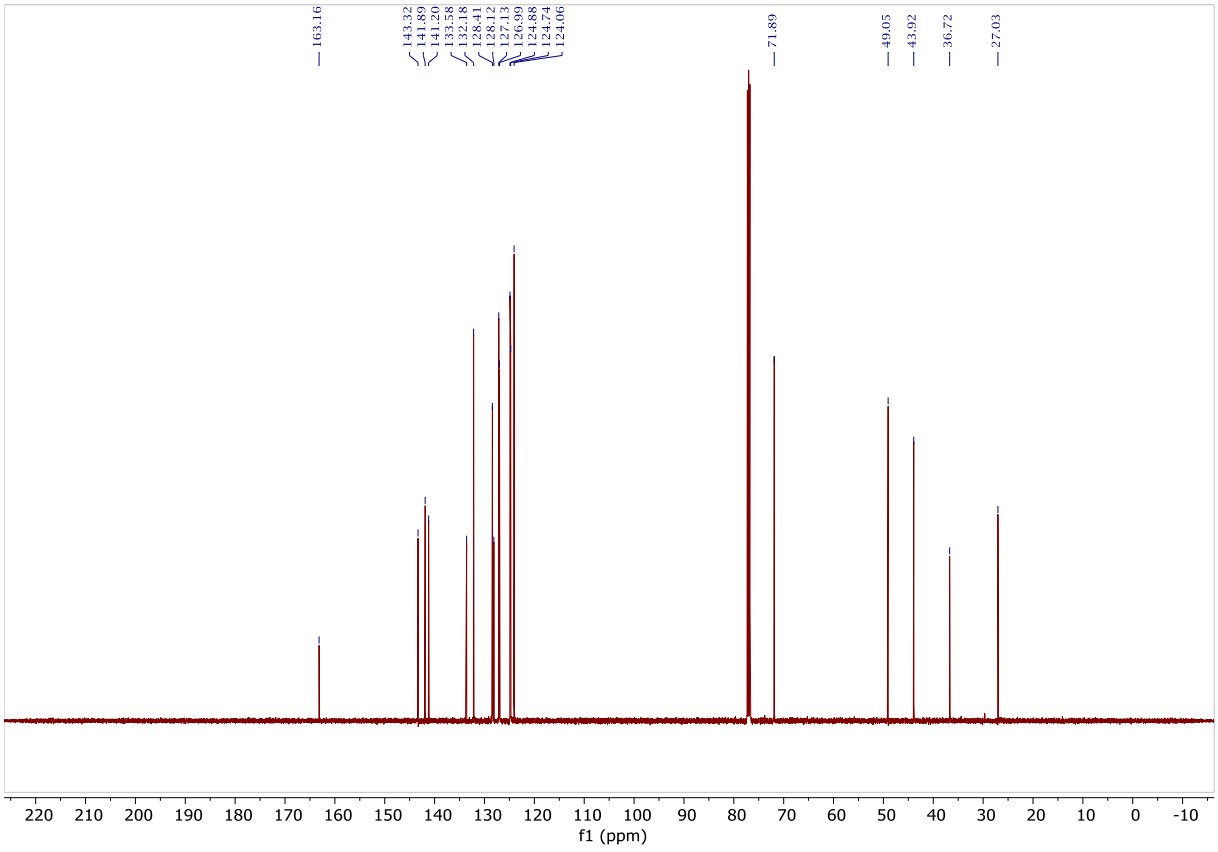
7.41
7.25
7.15
7.08
4.59
3.52
3.50
3.08
1.57
1.00
1.10
1.09
1.28
1.08
1.90
1.00
1.02
2.91
0.99
2.96
f1 (ppm)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141.20
133.58
132.18
128.41
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127.13
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124.88
124.74
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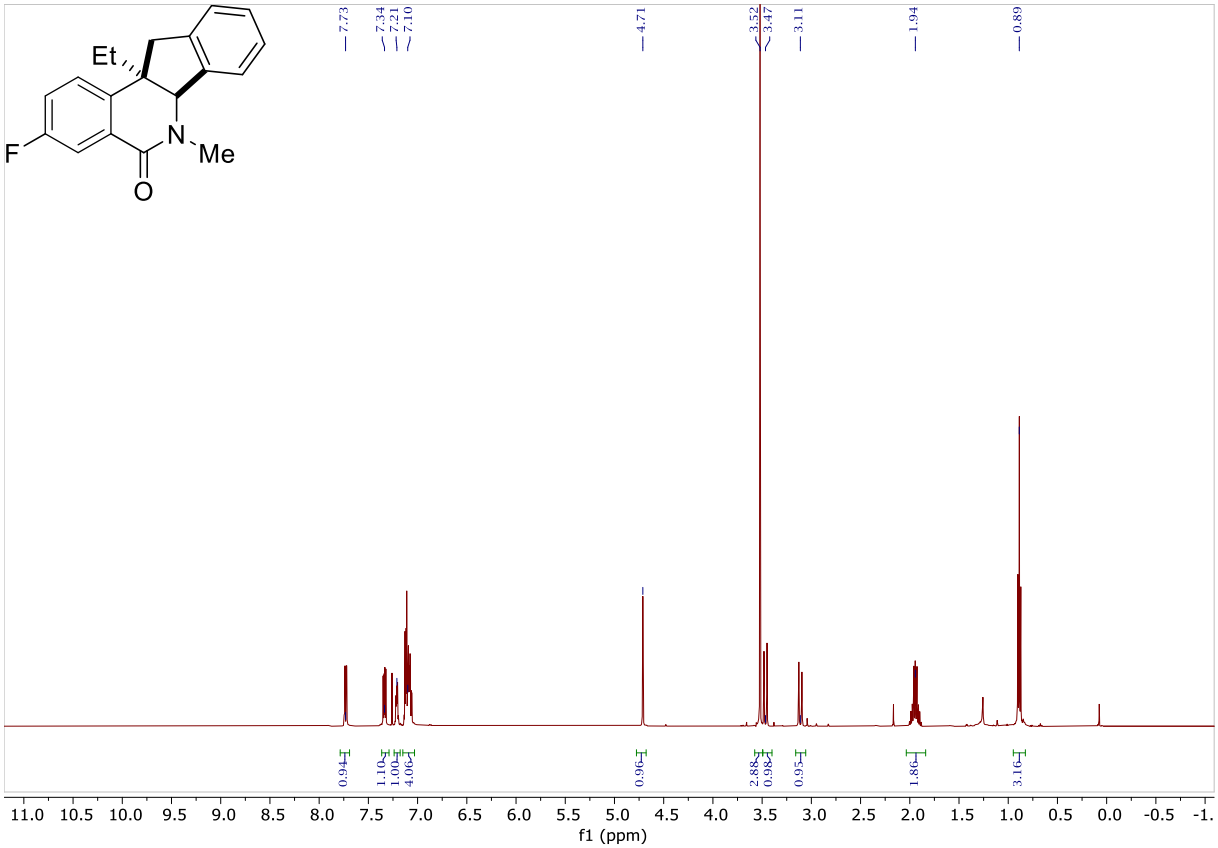
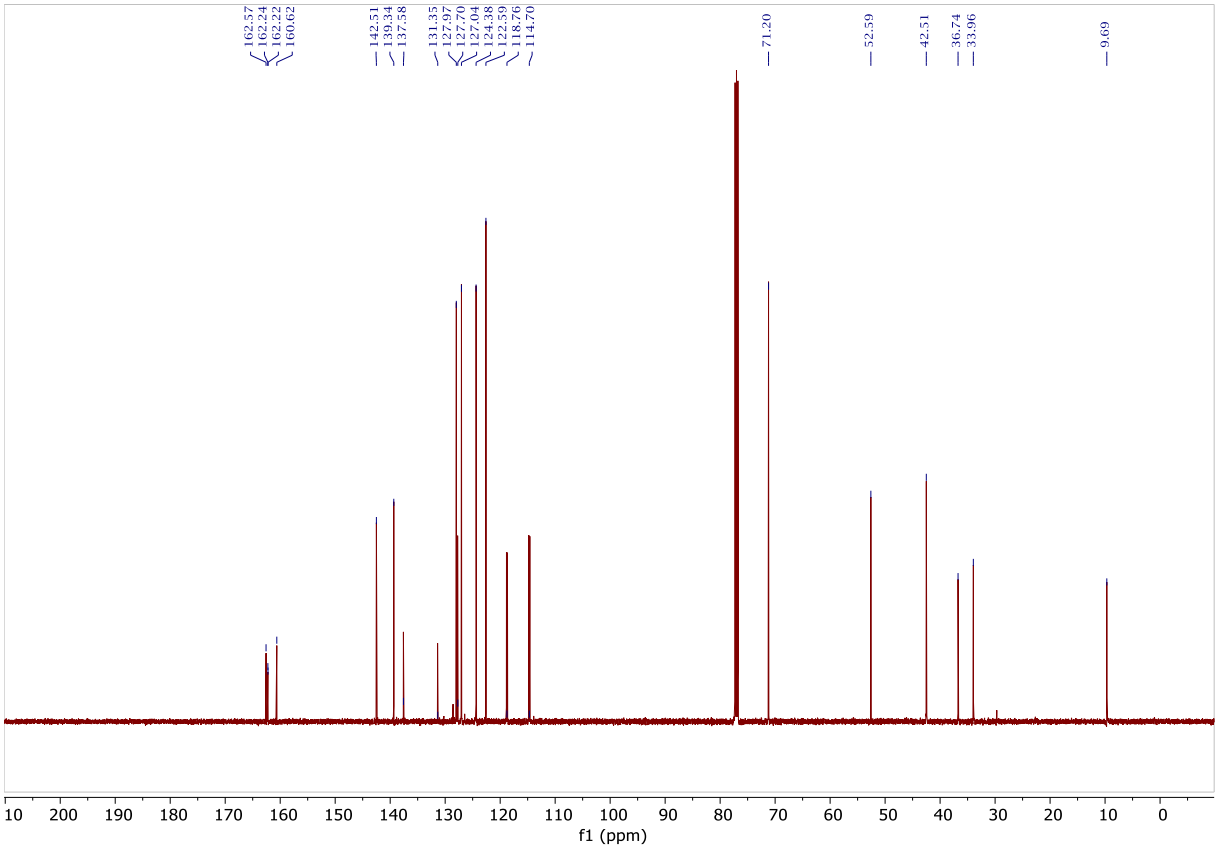
49.05
43.92
36.72
27.03
f1 (ppm)


Et
F
N
Me
O
7.73
7.34
7.31
7.10
4.71
3.52
3.47
3.11
1.94
0.89
0.94
1.10
1.00
4.06
0.96
2.88
0.98
0.95
1.86
3.16
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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162.24
162.22
160.62
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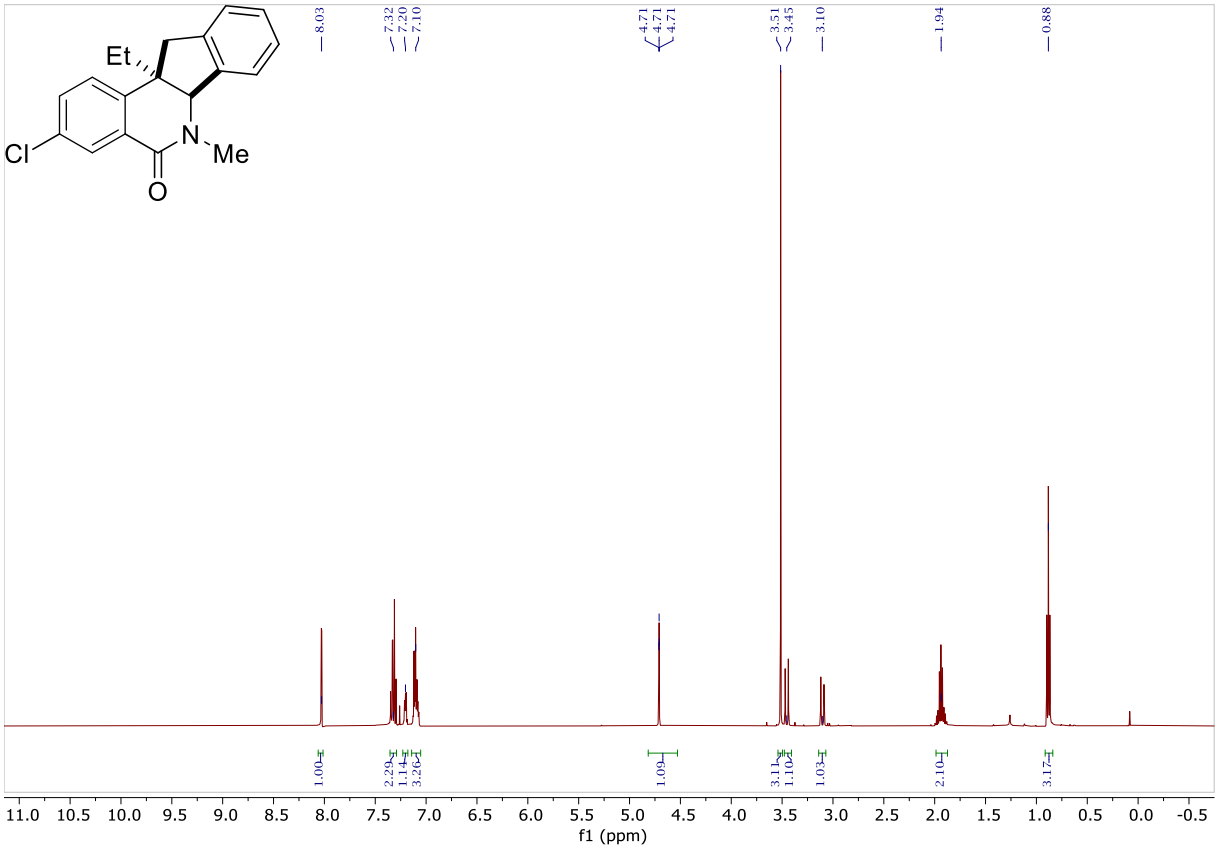
137.58
131.35
127.97
127.70
127.04
124.38
122.59
118.76
114.70
71.20
52.59
42.51
36.74
33.96
9.69
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Et
Cl
N
Me
O
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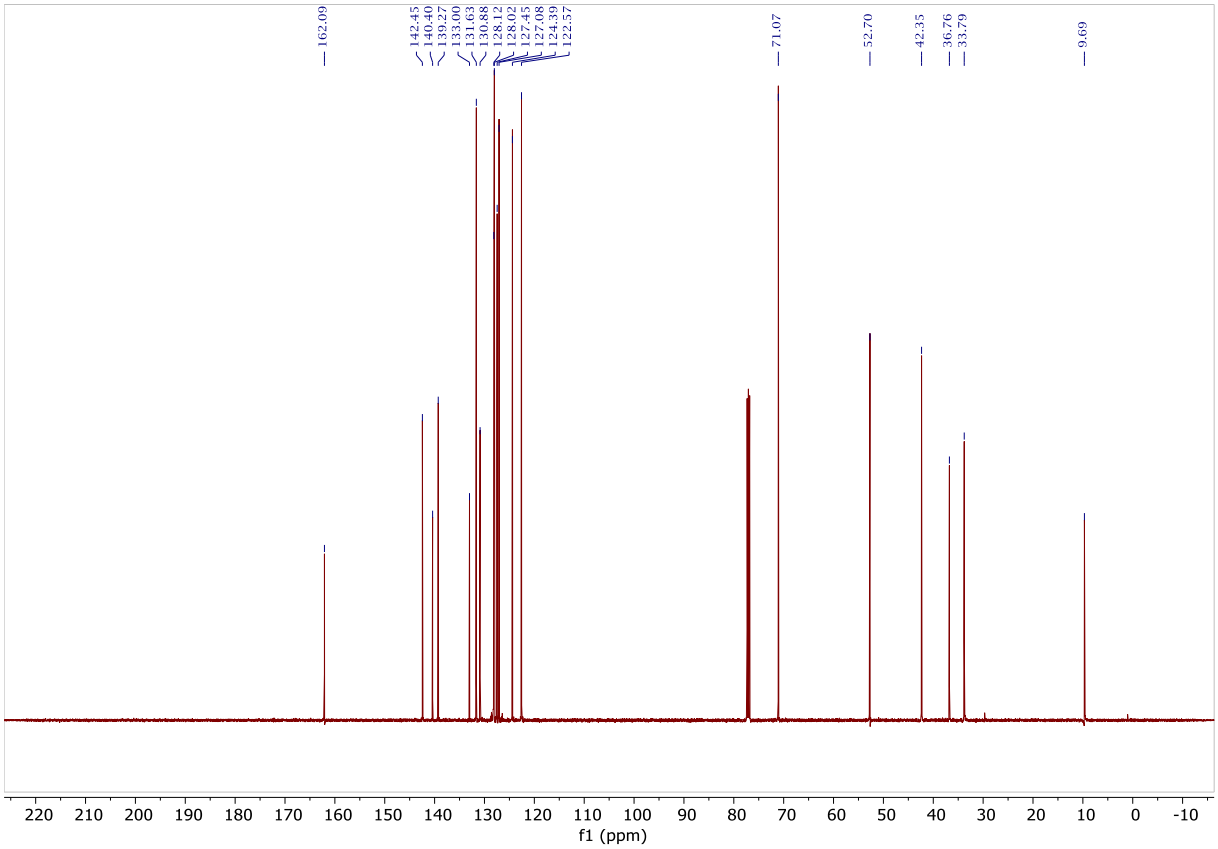
7.32
7.20
7.10
4.71
4.71
4.71
3.51
3.45
3.10
1.94
0.88
1.00
2.29
1.14
3.26
1.09
3.11
1.10
1.03
2.10
3.17
f1 (ppm)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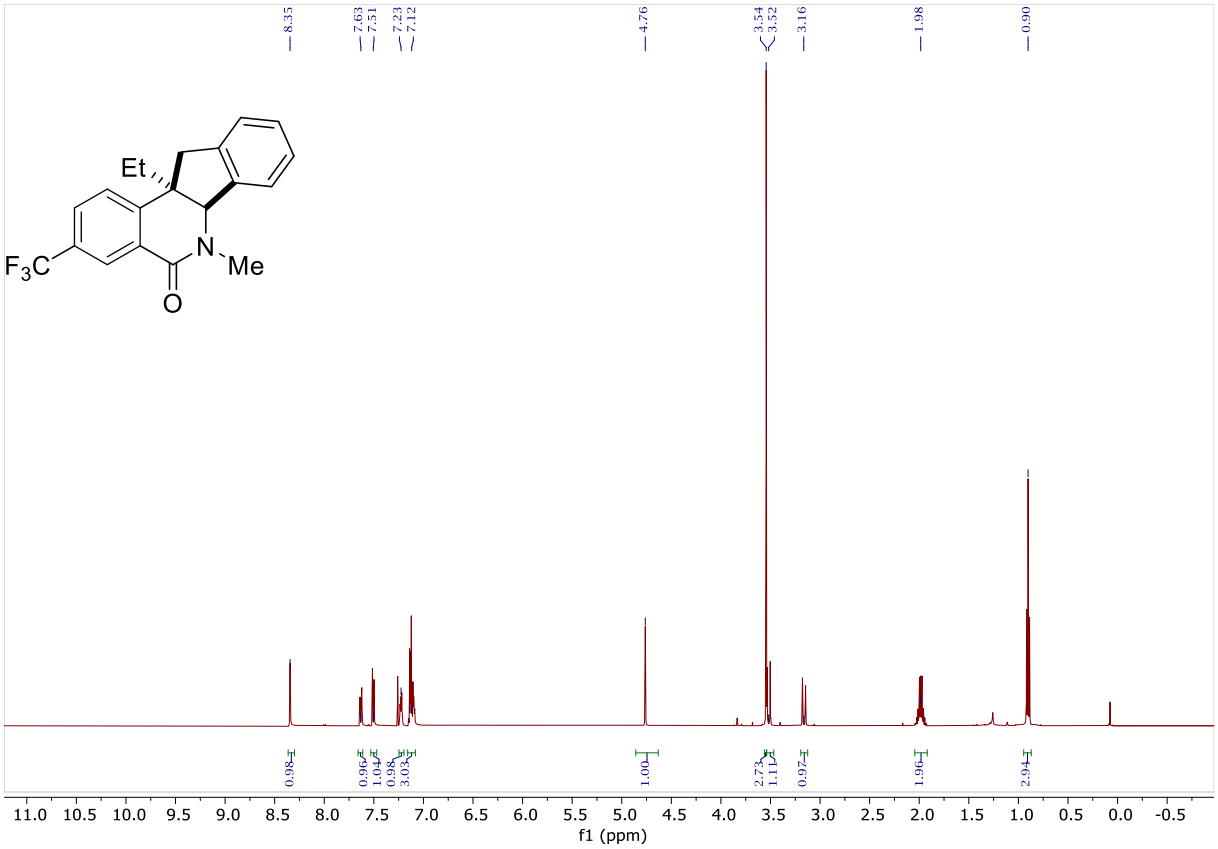
139.27
133.00
131.63
130.88
128.12
128.02
127.45
127.08
124.39
122.57
71.07
52.70
42.35
36.76
33.79
9.69
f1 (ppm)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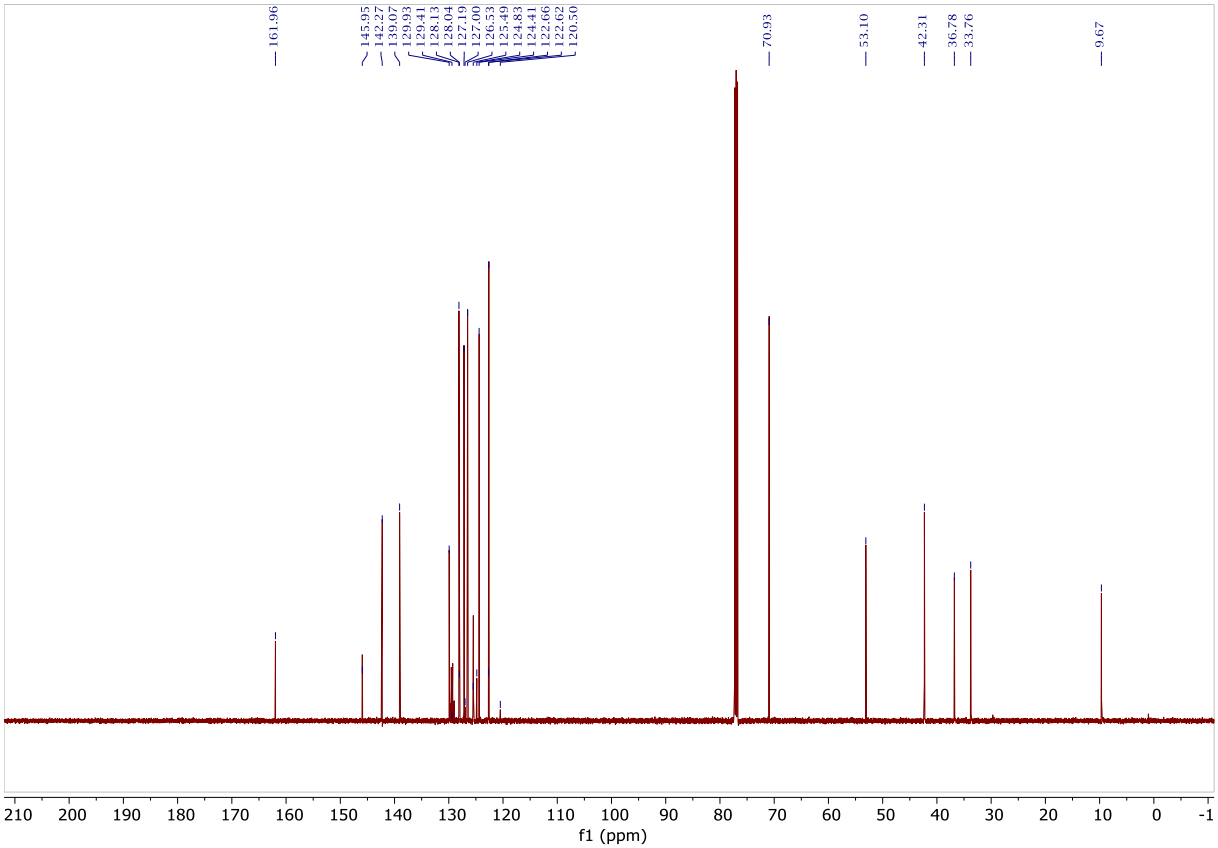
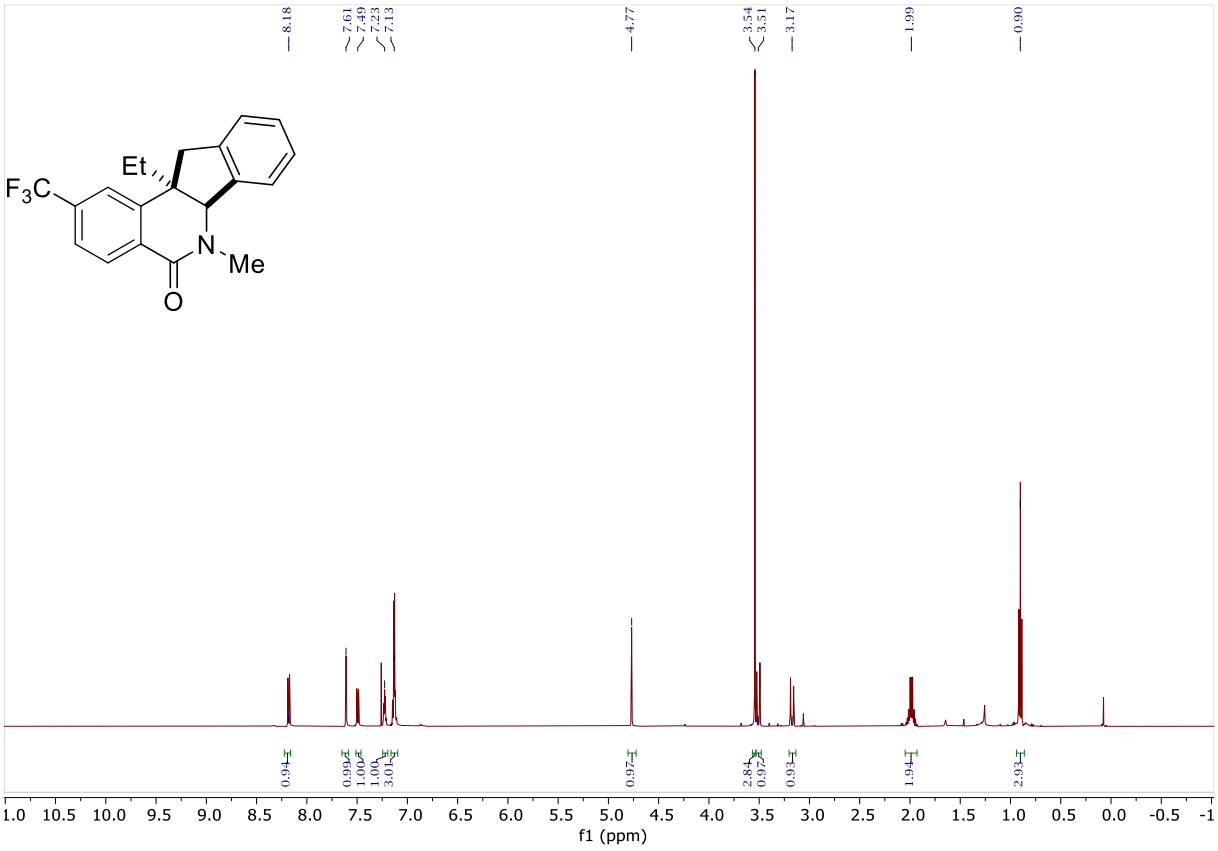
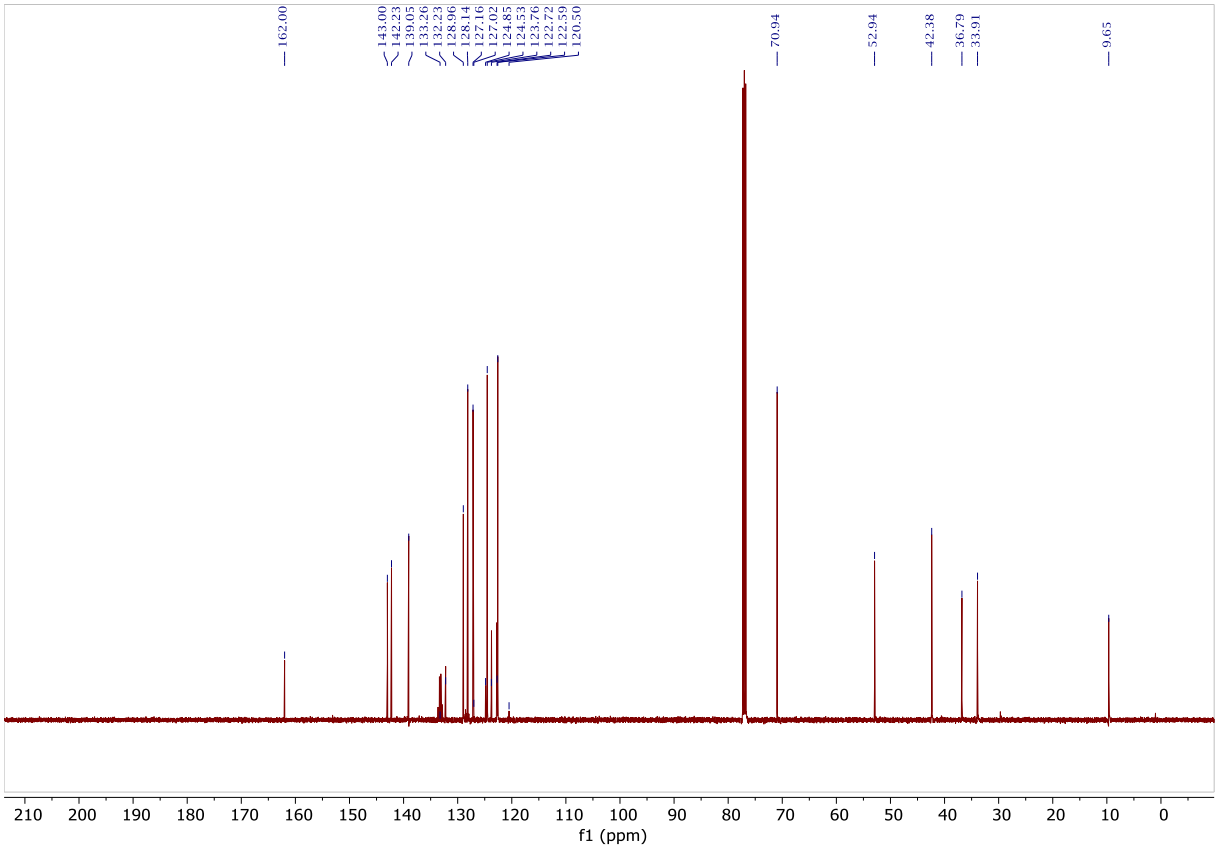
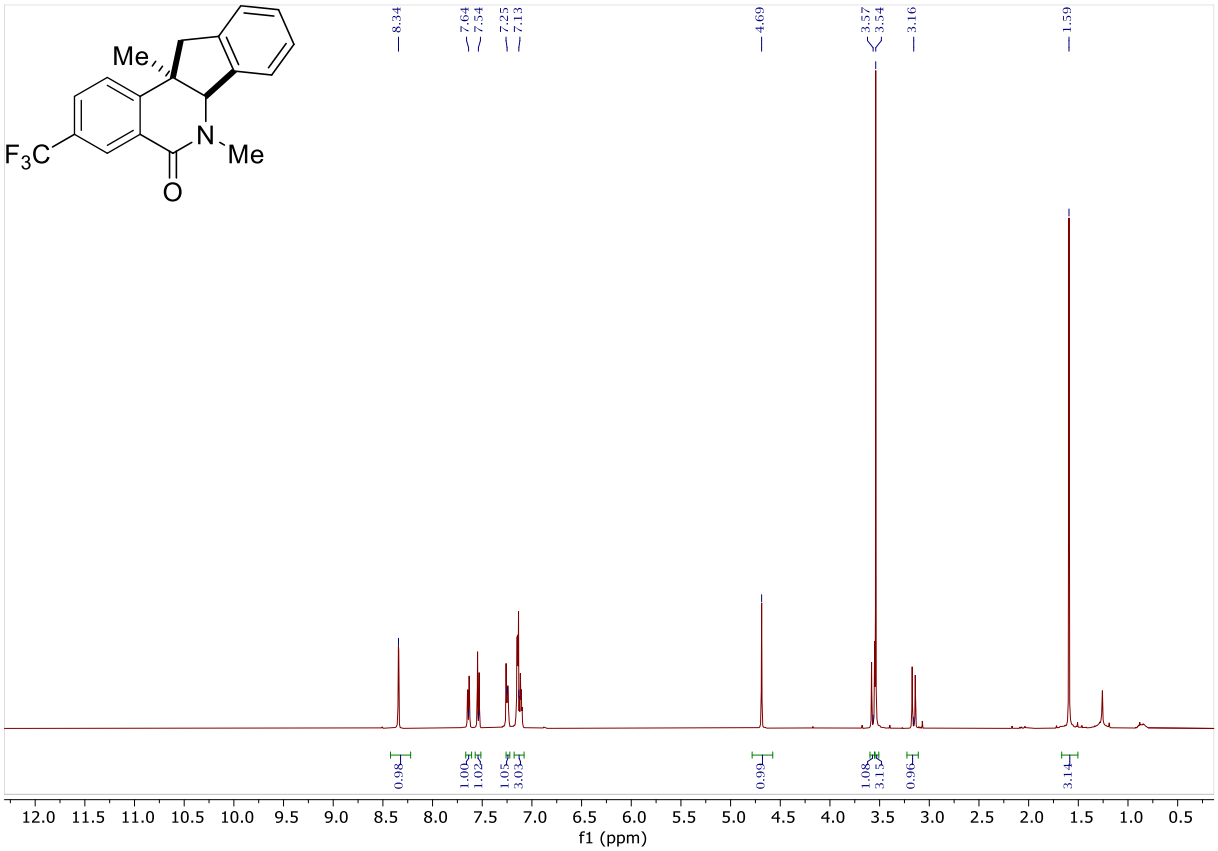
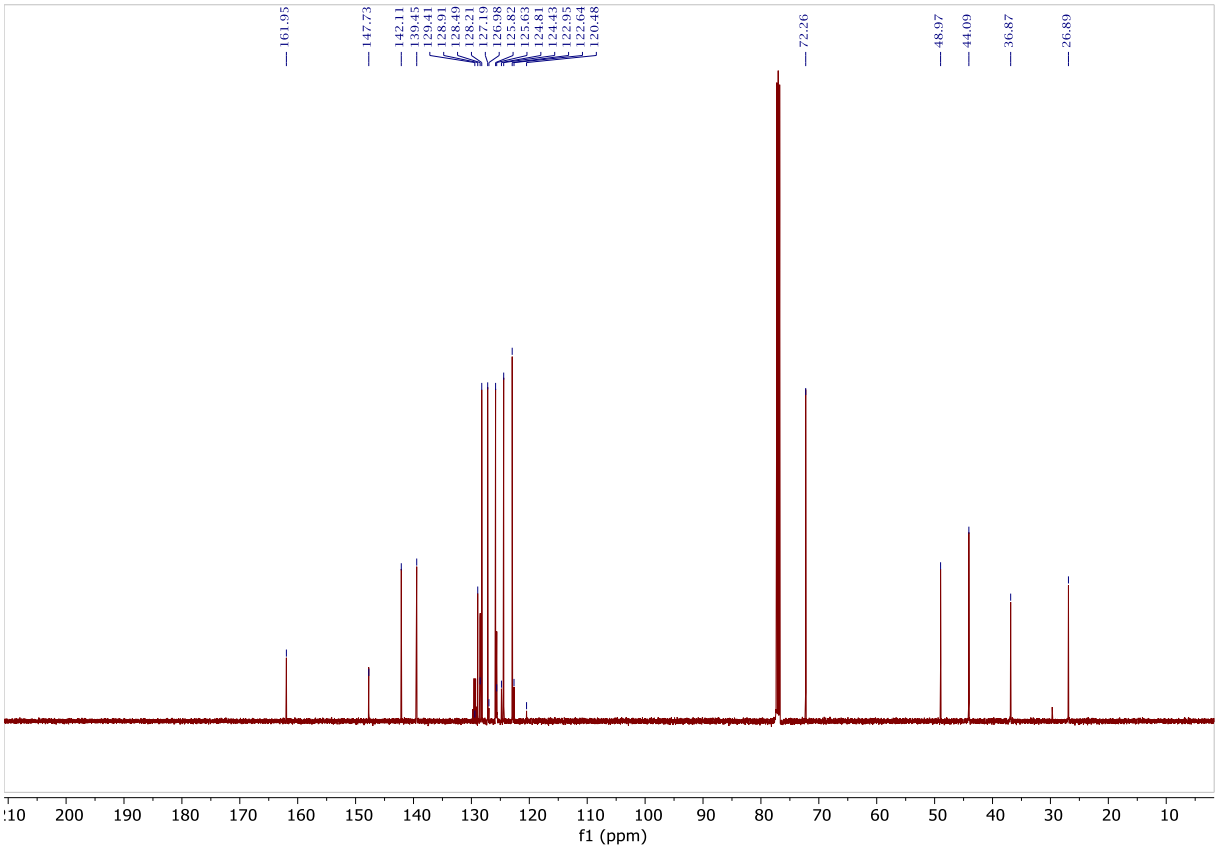
7.63
7.51
7.23
7.12
4.76
3.54
3.52
3.16
1.98
0.90
Et
N
Me
F3C
O
0.98
0.96
1.04
0.98
3.03
1.00
2.73
1.11
0.97
1.96
2.94
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


161.96
145.95
142.27
139.07
129.93
129.41
128.13
128.04
127.19
127.00
126.53
125.49
124.83
124.41
122.66
122.62
120.50
70.93
53.10
42.31
36.78
33.76
9.67
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


8.18
7.61
7.49
7.23
7.13
4.77
3.54
3.51
3.17
1.99
0.90
Et
F3C
N
Me
O
0.94
0.99
1.00
1.00
3.01
0.97
2.84
0.92
0.93
1.94
2.93
f1 (ppm)


162.00
143.00
142.23
139.05
133.26
132.23
128.96
128.14
127.16
127.02
124.65
124.53
123.76
122.72
122.59
120.50
70.94
52.94
42.38
36.79
33.91
9.65
f1 (ppm)


Me
F3C
N
Me
O
8.34
7.64
7.54
7.25
7.13
4.69
3.57
3.54
3.16
1.59
0.98
1.00
1.02
1.05
3.03
0.99
1.08
3.15
0.96
3.14
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

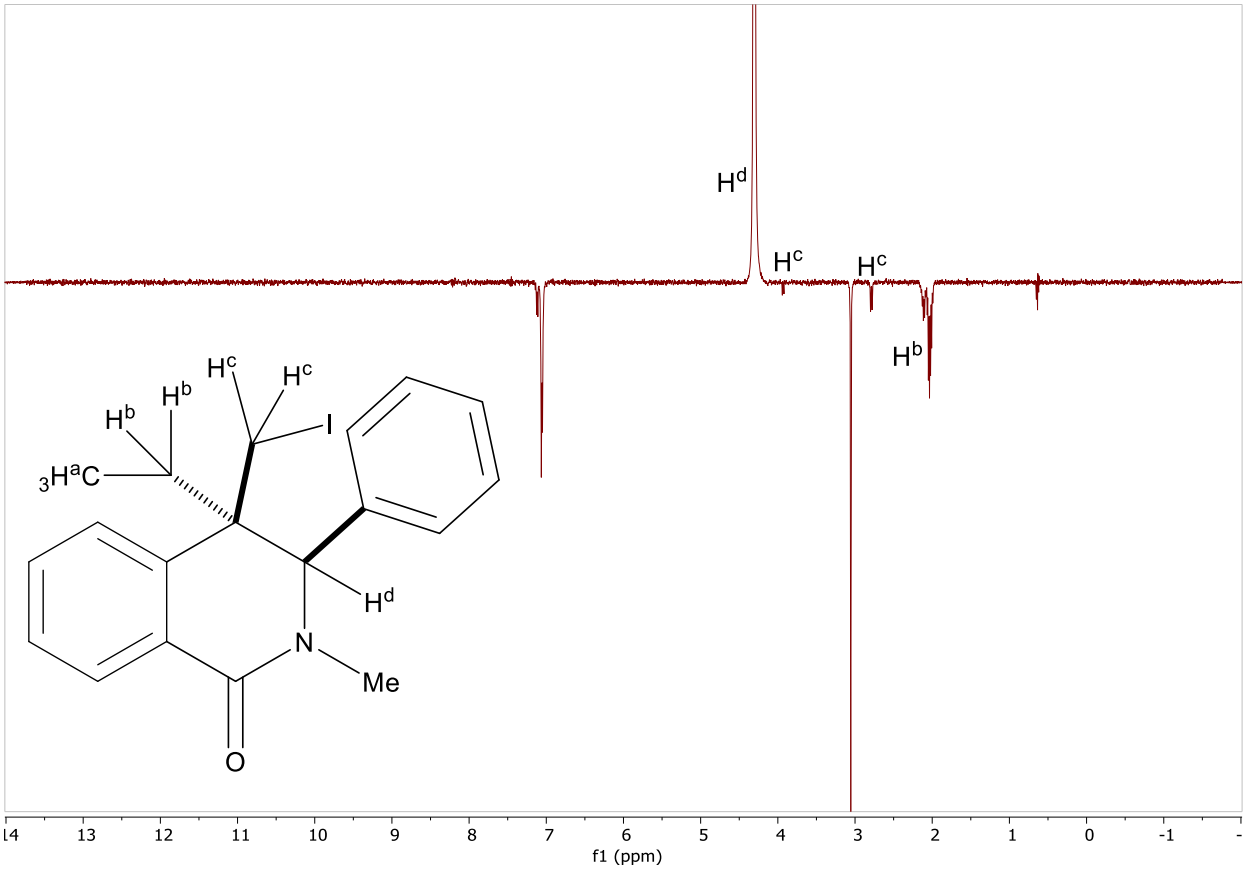

161.95
147.73
142.11
139.45
129.41
128.91
128.49
128.21
127.19
126.98
125.82
125.63
124.81
124.43
122.95
122.64
120.48
72.26
48.97
44.09
36.87
26.89
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

NOESY Experiments

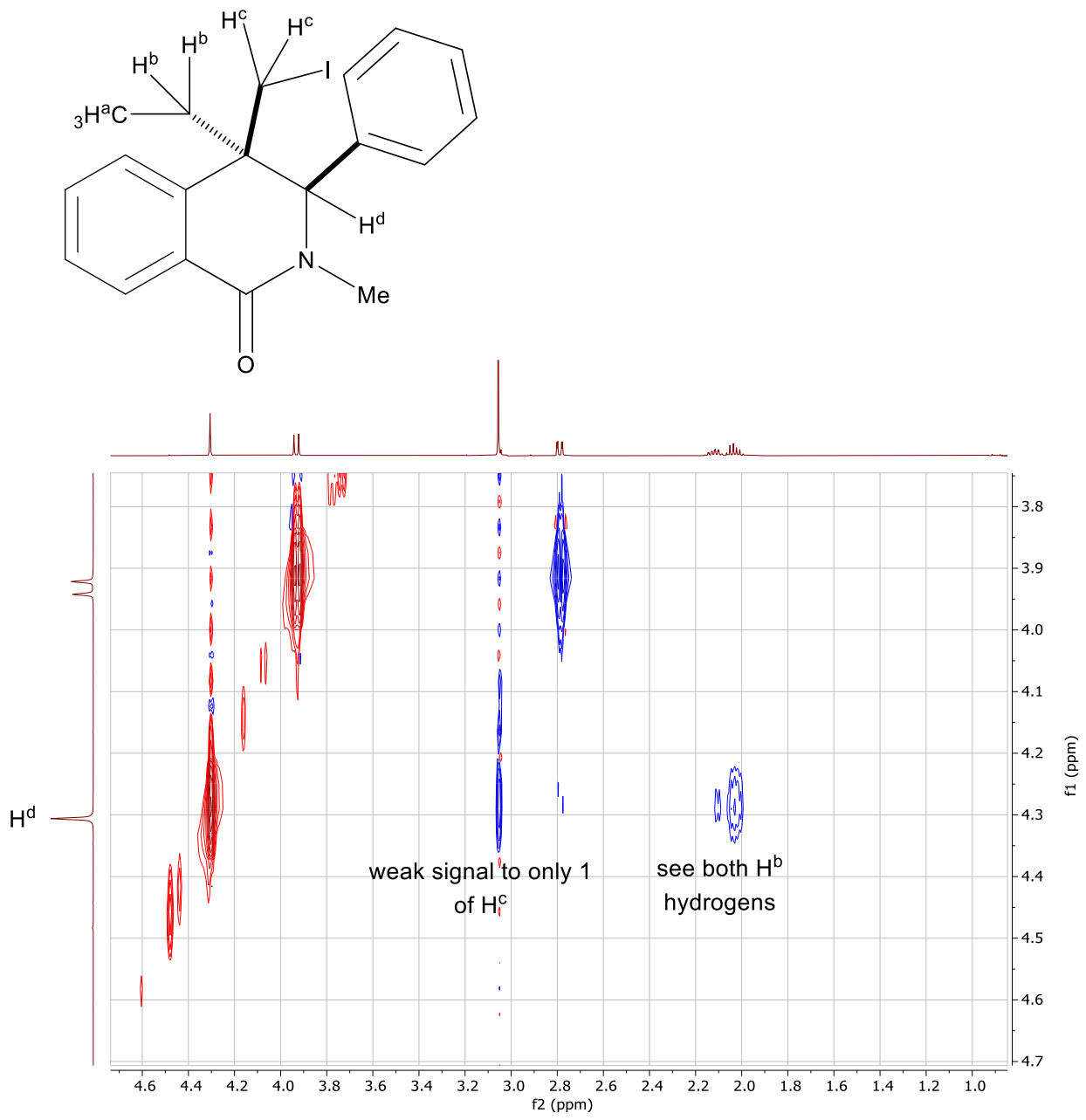
For all neopentyl-iodides: In the literature, the syn-isomer consistently has the larger chemical shift between the 2-CH_2I diastereotopic protons when compared to the anti-products (Δppm = ~0.3 ppm vs Δppm = ~0.9). These were corroborated with x-ray crystallographic evidence. However, to confirm the identity of each diastereomers, we used 1D and 2D NOESY experiments.

1D-NOESY

***syn*-1b**: H^d correlates H^b the strongest, very weak correlation to H^a and H^c

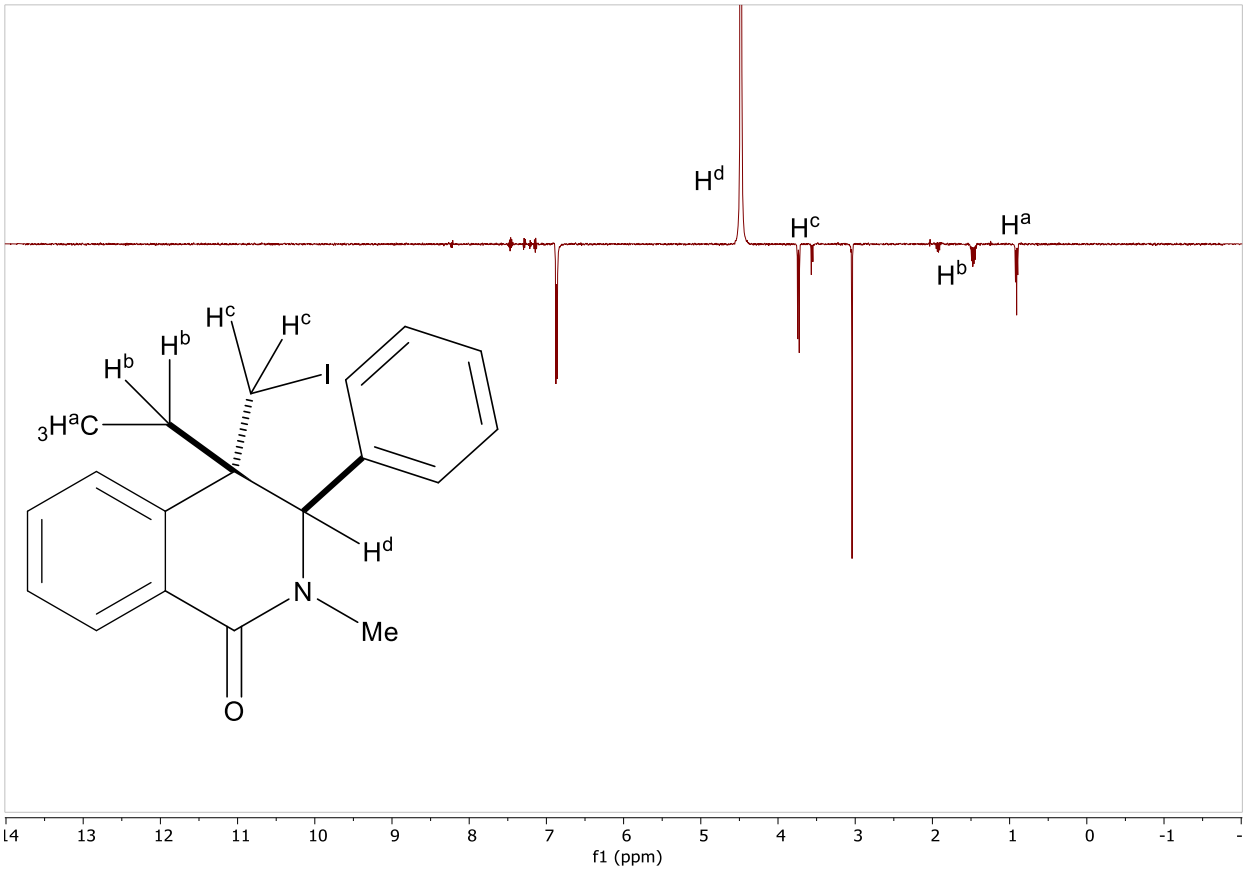


2D-NOESY

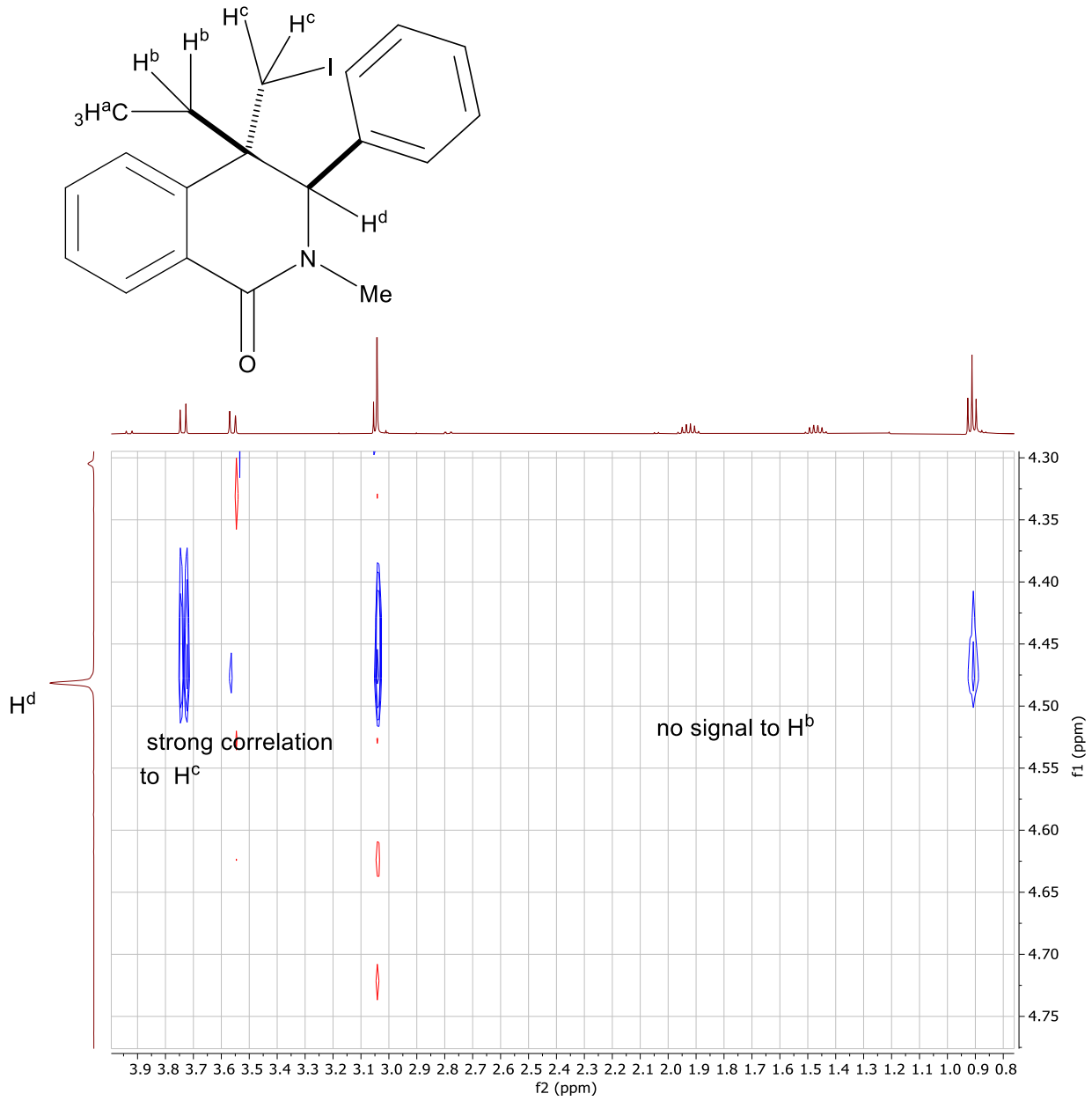

Hc
Hc
Hb
Hb
I
3HaC
Hd
N
Me
O
Hd
weak signal to only 1
of Hc
see both Hb
hydrogens
f2 (ppm)
f1 (ppm)

1D-NOESY

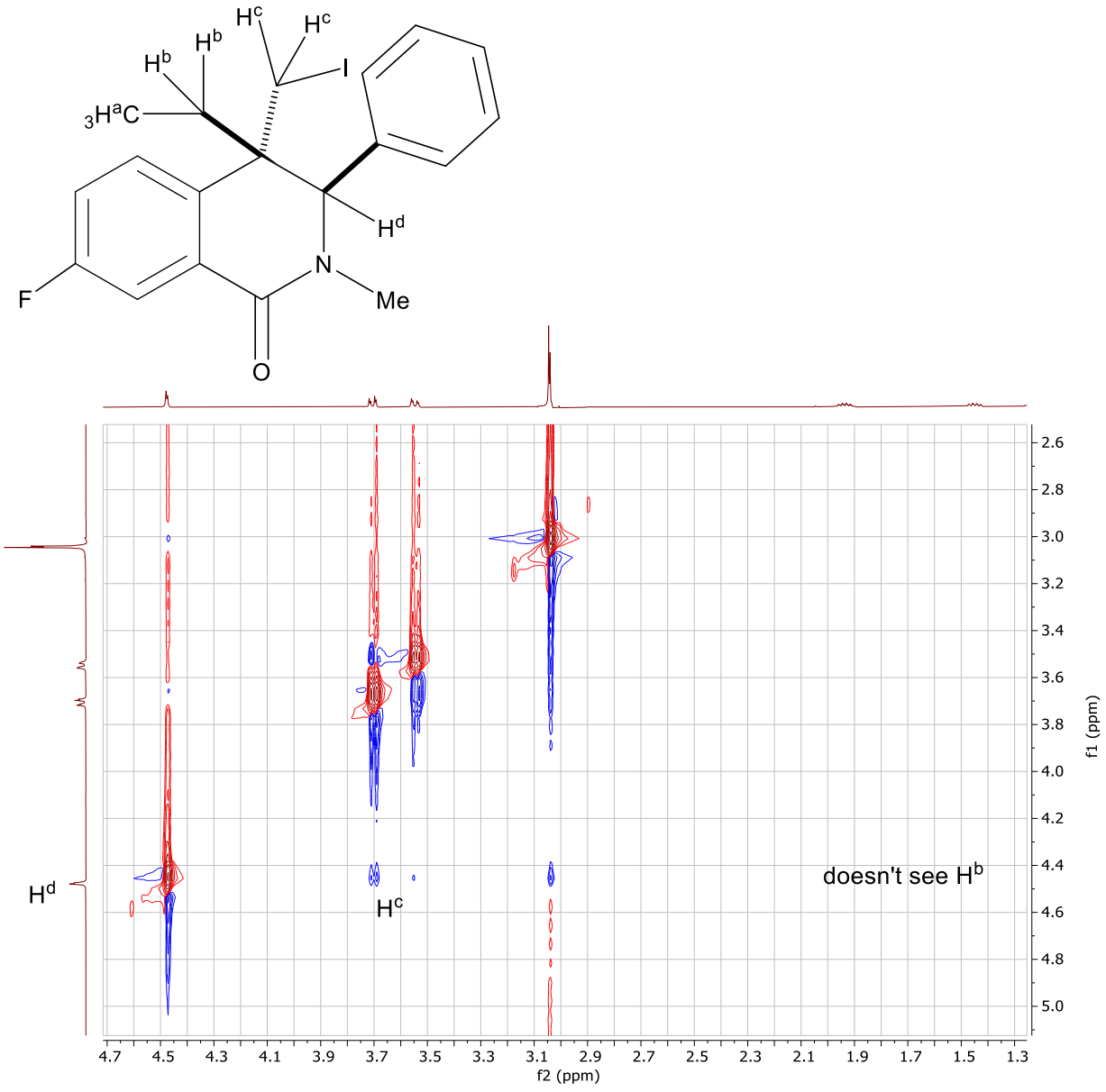
***anti*-1b**: H^d has the strongest correlation to H^c, weak correlation to H^b, moderate to H^a



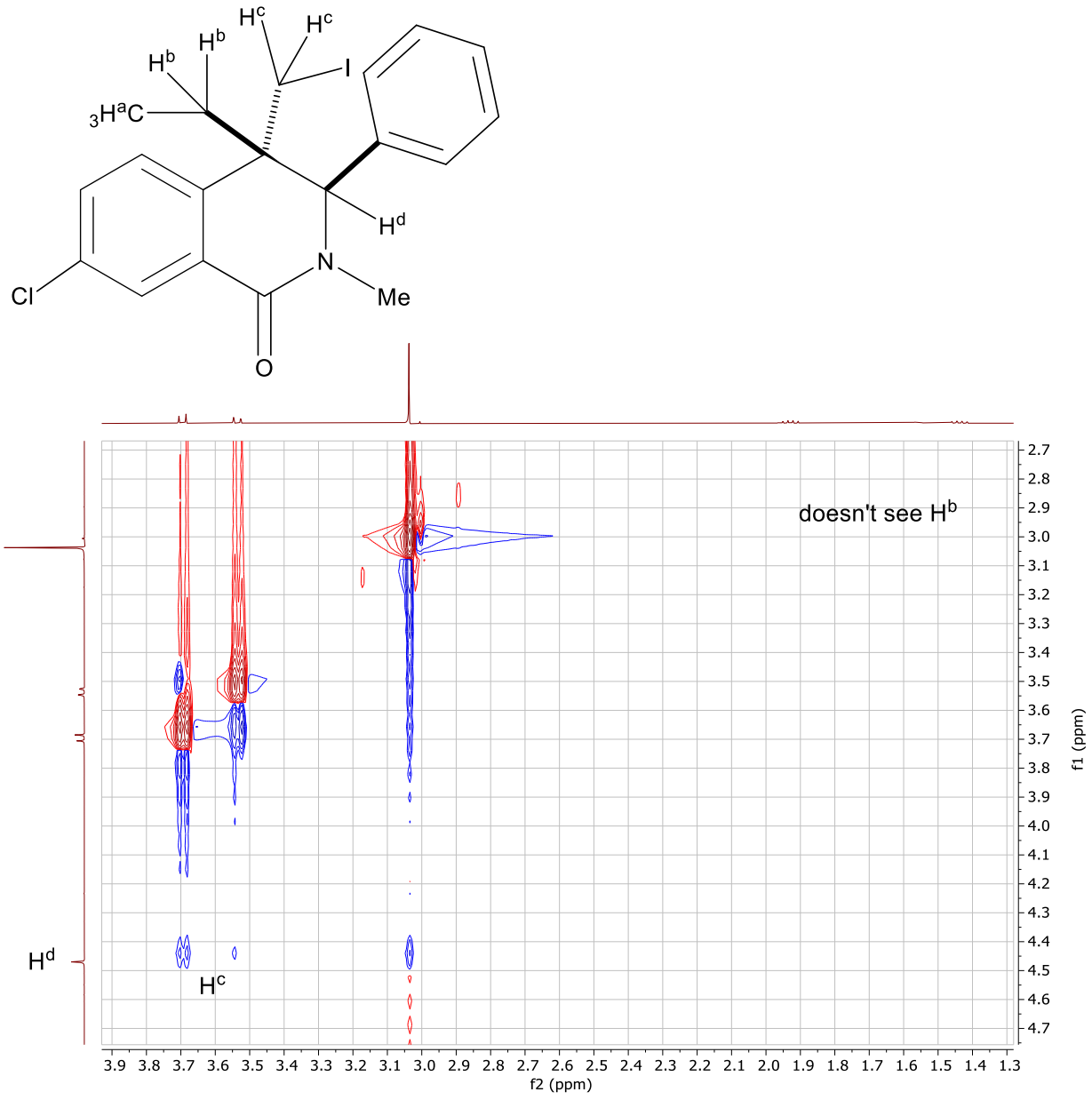
2D-NOESY


Hc
Hc
Hb
Hb
I
3HaC
Hd
N
Me
O
Hd
strong correlation
to Hc
no signal to Hb
4.30
4.35
4.40
4.45
4.50
4.55
4.60
4.65
4.70
4.75
f1 (ppm)
3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8
f2 (ppm)

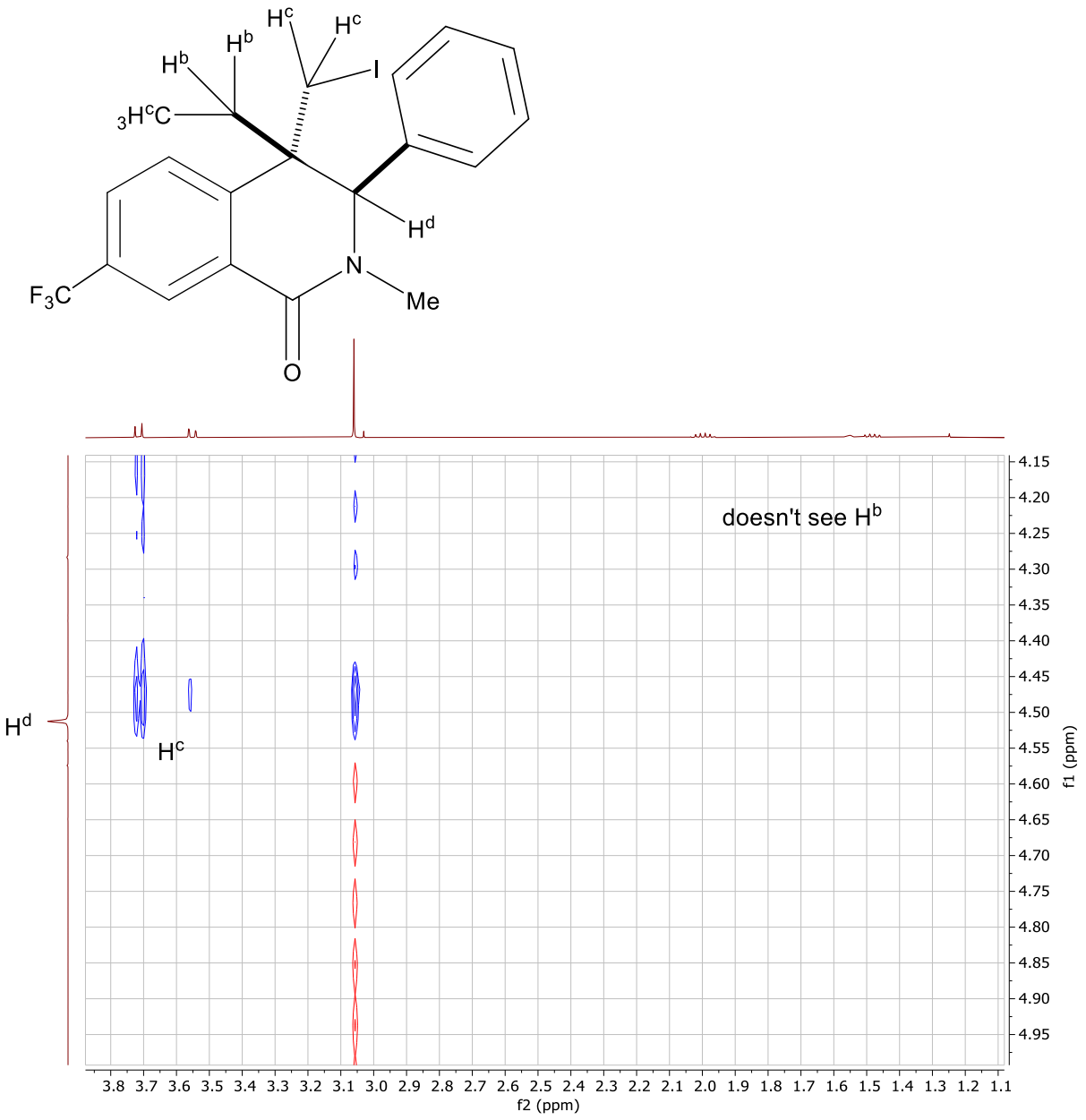
***anti*-1d:**


Hc
Hc
Hb
Hb
I
3HaC
Hd
N
Me
F
O
2.6
2.8
3.0
3.2
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
5.0
f1 (ppm)
Hd
Hc
doesn't see Hb
4.7
4.5
4.3
4.1
3.9
3.7
3.5
3.3
3.1
2.9
2.7
2.5
2.3
2.1
1.9
1.7
1.5
1.3
f2 (ppm)

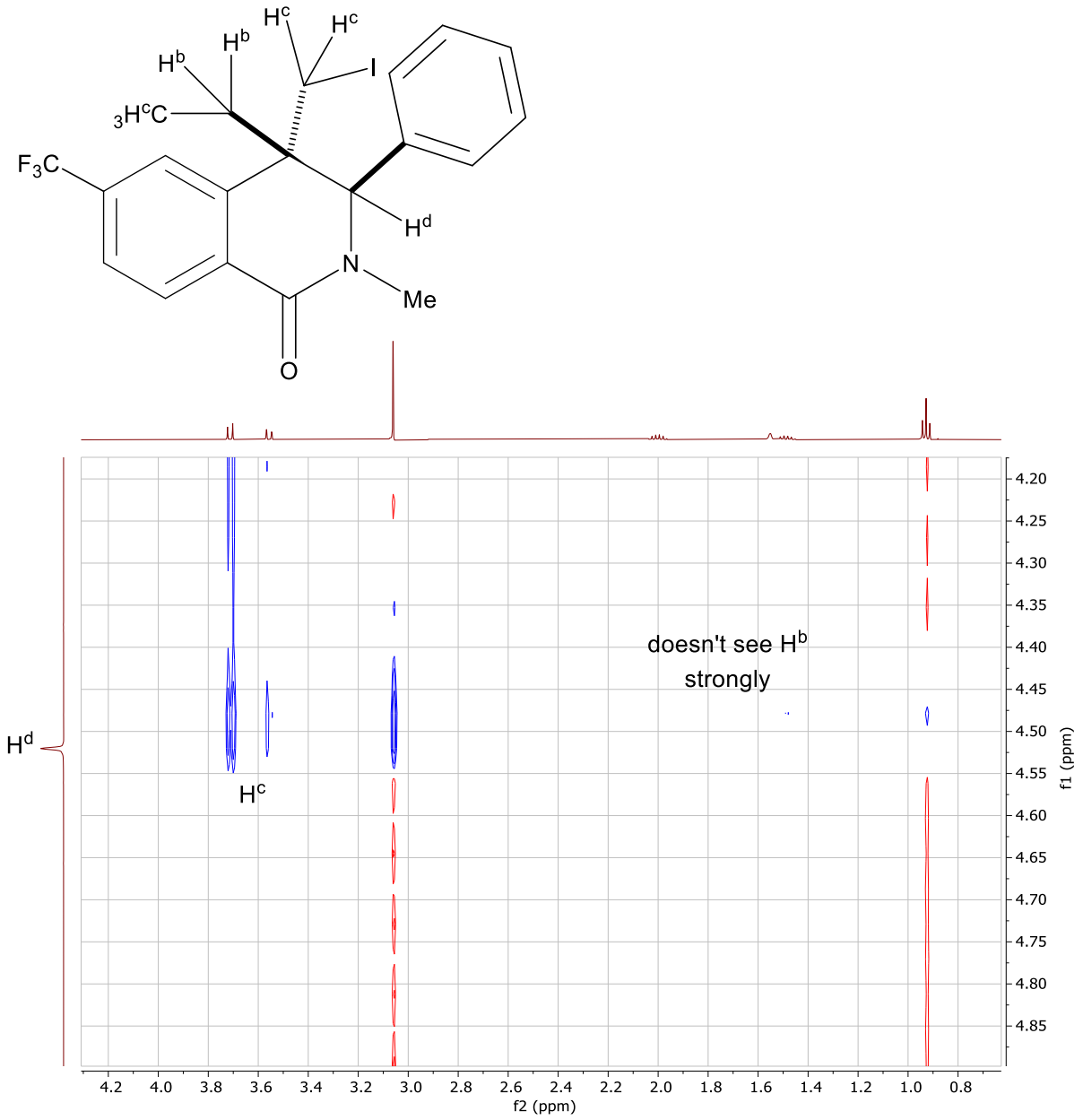
***anti*-1e:**



***anti*-1f:**



***anti*-1g:**



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