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Supporting Information

Development of a web-based platform for studying lithiation reactions *in silico*

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Content

General

All reactions involving air-sensitive reagents were performed in oven-dried glassware under an atmosphere of nitrogen using syringe-septum cap technique. Tetrahydrofuran (THF) was freshly distilled under a nitrogen atmosphere over sodium / benzophenone. ^{1}H-NMR spectra were recorded on either Bruker Avance DPX-400 or Bruker Avance DPX-600 spectrometer, as specified, with the residual solvent peak as the internal reference ($CDCl_3$ = 7.26 ppm). ^{1}H resonances are reported to the nearest 0.01 ppm. ^{13}C-NMR spectra were recorded on the same spectrometer, as specified, with the central resonance of the solvent peak as the internal reference ($CDCl_3$ = 77.00 ppm). All ^{13}C resonances are reported to the nearest 0.01 ppm. DEPT 135, COSY, HMQC, and HMBC experiments were used to aid structural determination and spectral assignment. The multiplicity of ^{1}H signals are indicated as: s = singlet, d = doublet, dd = doublet of doublet, ddd = doublet of doublet of doublet, t = triplet, q = quadruplet, sext = sextet, m = multiplet, br = broad, or combinations of thereof. Coupling constants (*J*) are quoted in Hz and reported to the nearest 0.1 Hz. Where appropriate, averages of the signals from peaks displaying multiplicity were used to calculate the value of the coupling constant. ^{19}F-NMR spectra were recorded on the same spectrometer, as specified, with the central resonance of α,α,α-Trifluorotoluene as the internal reference ($C_6H_5CF_3$ = -63.72 ppm). Infrared spectra were recorded neat on a PerkinElmer Spectrum One FT-IR spectrometer using Universal ATR sampling accessories. The removal of solvent under reduced pressure was carried out on a standard rotary evaporator. High resolution mass spectrometry (HR-MS) was performed using a Waters Micromass LCT Premier™ spectrometer using time of flight with positive ESI, or a Bruker BioApex 47e FTICR spectrometer using (positive or negative) ESI or EI at 70 eV to within a tolerance of 5 ppm of the theoretically calculated value. Melting points were uncorrected. TLC was performed on Merck silica gel plates with F-254 indicator; detection was accomplished by UV light (254 nm), by exposing to I2 vapours and spraying a solution of (5% W/V) ammonium molibdate and 0.2% W/V cerium(III)sulphate in 100 ml 17.6% aq. sulphuric acid and heating to 200 °C for some time until blue spots appear. *N*,*N*,*N*',*N*'-tetramethylethylenediamine (TMEDA) and Diisopropylamine (DIPA) were distilled over finely powdered CaH_2. Commercial solution of *n*-BuLi (1.6 M hexane solution) was tritated by using *N*-pivaloyl-*o*-toluidine prior use.[i] Unless stated otherwise, reagents were obtained from commercial sources and used without purification.

Representative procedure for the lithiation - trapping sequence of 1a, 1b and 1d.

n-BuLi (1.6 M in hexane, 2.0 mmol) was added dropwise to a stirred solution of TMEDA (300 µl, 2.0 mmol) and **1a** (160 mg, 1.0 mmol) in THF (10 mL) at -78 °C. After 2h stirring at this temperature, MeOH-d_4 (100 µL, 2.5 mmol) was added. The mixture was allowed to warm slowly to room temperature. After the addition of saturated aqueous NH_4Cl (10 mL), the mixture was extracted with Et_2O (3 x 10 mL). The combined organic layers were dried ($MgSO_4$), filtered and evaporated under reduced pressure. Purification by SiO2 flash chromatography (Hexane:AcOEt, 80:10) gave the compound **3a**.

Representative procedure for the lithiation - trapping sequence of 1c and 4.

n-BuLi (1.6 M in hexane, 2.0 mmol) was added dropwise to a stirred solution of DIPA (328 µl, 2.34 mmol) in THF (5 mL) at -78 °C. The solution was allowed to warm at 0 °C and kept stirring for 15 minutes. After this time, the mixture was cooled down to -78 °C and the solution of **1c** (156 mg, 1.0 mmol) in THF (5ml) was added. After 2h stirring at this temperature, MeOH-d_4 (100 µL, 2.5 mmol) was added. The mixture was allowed to warm slowly to room temperature. Saturated aqueous NH_4Cl (10 mL) was added and the mixture was extracted with Et_2O (3 x 10 mL). The

combined organic layers were dried ($MgSO_4$), filtered and evaporated under reduced pressure. Purification by SiO_2 flash chromatography (Hexane : AcOEt, 80:10) gave the compound **3c**.

1-Chloro-4-deuterium-3-fluoro-2-methoxybenzene (3a). Colourless oil; yield 95%; %D 99%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.16 (dd, *J* = 8.2, 1.5 Hz, 1H), 6.98 – 6.95 (m , 1H), 3.98 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.2 (d, *J* = 249.3 Hz), 144.4 (d, *J* = 13.2 Hz), 128.5 (d, *J* = 3.7 Hz), 125.5 (d, *J* = 1.1 Hz), 123.7 (d, *J* = 8.5 Hz), 115.2 (dt, *J* = 25.2, 19.3 Hz), 61.5 (d, 4.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -129.31. GC-MS (70 eV) m/z (%): 163 (26), 161 (83), 148 (30), 146 (102), 118 (100). FT-IR (Neat, υ_{max} cm^{-1}) 1470, 1430, 1242, 904, 843, 786, 750.

1-Chloro-2-deuterium-3-fluoro-4-methoxybenzene (3b). Colourless oil; yield 95%; %D 99%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.04 (dd, *J* = 8.8, 1.5 Hz, 1H), 6.87 (t, *J* = 8.8 Hz, 1H), 3.87 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 152.1 (d, *J* = 249.6 Hz), 144.6 (d, *J* = 10.3 Hz), 125.2 (d, *J* = 8.8 Hz), 124.2 (d, *J* = 3.9 Hz), 116.4 – 116.9 (m), 114.1 (d, *J* = 2.4 Hz), 56.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -129.32. GC-MS (70 eV) m/z (%): 163 (27), 161 (84), 148 (28), 146 (88), 120 (32), 118 (100). FT-IR (Neat, υ_{max} cm^{-1}) 1471, 1430, 1445, 1427, 1242, 1000, 904.

2-Chloro-5-deuterium-6-fluorobenzonitrile (3c). White solid; yield 65%; %D 80%; mp 59 – 60 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.53 (m, 1H), 7.34 (dd, *J* = 8.3, 0.9 Hz, 1H), 7.17 (dt, *J* = 8.4, 0.8 Hz, 0.2 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.7 (d, *J* = 262.2 Hz), 163.71 (d, *J* = 262.3 Hz), 137.8 (d, *J* = 2.1 Hz), 134.8 (d, *J* = 9.5 Hz), 134.7 (d, *J* = 9.4 Hz), 125.7 (d, *J* = 3.4 Hz), 114.6 (d, *J* = 19.7 Hz), 114.4 (dt, *J* = 29.9, 19.4 Hz), 111.1, 103.3 (d, *J* = 17.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.69, -103.97. GC-MS (70 eV) m/z (%): 158 (32), 156 (100), 121 (37), 101 (16). FT-IR (Neat, υ_{max} cm^{-1}) 2235, 1594, 1444, 1429, 904, 845, 789, 751.

1-Chloro-2-deuterium-3-fluoro-6-methoxybenzene (3d). Colourless oil; yield 95%; %D 99%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.93 (dd, *J* = 9.0, 8.0 Hz, 1H), 6.85 (dd, *J* = 9.1, 4.8 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.3 (d, *J* = 241.8 Hz), 151.6 (d, *J* = 2.4 Hz), 122.8 (d, *J* = 10.4 Hz), 117.3 (q, *J* = 25.6 Hz)), 113.9 (d, *J* = 22.4 Hz), 112.5 (d, *J* = 8.7 Hz), 56.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.43 (d, *J* = 3.4 Hz). GC-MS (70 eV) m/z (%): 163 (25), 161 (75), 148 (31), 146 (88), 118 (100). FT-IR (Neat, υ_{max} cm^{-1}) 1479, 1437, 1248, 1103, 920, 807, 724.

2-Chloro-1-deuterium-10-methylacridin-9(10*H*)-one (4-D). Yellow solid; yield 95%; %D 80%; mp 169.7 – 170.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, *J* = 8.0, 1.7 Hz, 1H), 8.27 (d, *J* = 2.6, 0.2H), 7.60 (ddd, *J* = 8.6, 7.0, 1.7 Hz, 1H), 7.43 (dt, *J* = 9.2, 1.2 Hz, 1H), 7.33 (d, *J* = 8.7 Hz, 1H), 7.24 (d, *J* = 9.2 Hz, 1H), 7.17 (ddd, *J* = 7.8, 7.0, 0.8 Hz, 1H), 3.69 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 176.7, 142.2, 140.7, 134.0, 133.7, 127.5, 127.1, 127.0, 126.6, 126.3 (t, *J* = 25.5 Hz), 123.0, 122.9, 122.1, 121.5, 116.5, 114.8, 33.7. FT-IR (Neat, υ_{max} cm^{-1}) 2844, 2721, 1630, 1592, 1489, 1451, 1274, 1177, 805, 743. HRMS *m/z* calculated for C14H10DClNO $[M+H]^+$ 245.0586, found 245.0585.

Computational data.

Cartesian coordinates (in Å) and uncorrected electronic energies (in hartrees) for the computed structures (substrates and lithiated intermediates) are given. Lithiated intermediates are sorted by energy starting from the lowest for every substrate. Only selected intermediates (within 10 kcal mol^{-1} threshold after initial optimisation; see the main text for the explanation of the algorithm) are shown for which full geometry optimisation and frequency analysis were performed confirming that they are genuine minima on the potential energy surface (PES). Screenshots of HTML5 representations of 3D structures for all the intermediates are also provided.

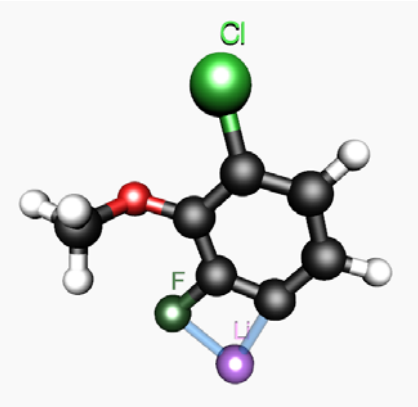
Substrate 1a

C -2.49479895 -1.21932971 0.32112036
O -1.68468418 -0.18746445 -0.25523351
C -0.33832927 -0.2212225 -0.10780649
C 0.35452061 1.0028837 -0.03876082
Cl -0.56166182 2.49343291 -0.09249754
C 1.742419 1.05670121 0.07382042
C 2.47999213 -0.12458794 0.13235782
C 1.82776243 -1.35433936 0.0651
C 0.44735315 -1.38438939 -0.06611563
F -0.16255109 -2.5911491 -0.16463904
H -3.50468638 -0.80782495 0.35090194
H -2.16800476 -1.45644851 1.33898948
H -2.4819324 -2.1277194 -0.28431264
H 2.23030146 2.02308121 0.12361516
H 3.55952855 -0.08560656 0.22786176
H 2.36557619 -2.29535642 0.09598852

E(B3LYP) = -905.607940717

Intermediate 1

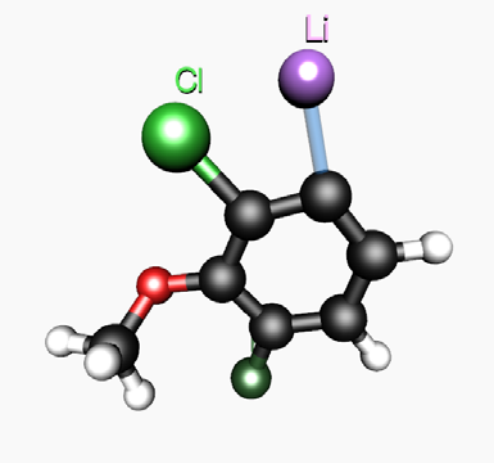
C -2.6320 -0.023830 0.50807
O -1.6689 0.30445 -0.49773
C -0.37865 -0.034011 -0.19961
C 0.60717 0.93454 0.039055
Cl 0.15195 2.6307 0.046831
C 1.9374 0.56656 0.27106
C 2.3009 -0.78218 0.27630
C 1.3677 -1.8133 0.049329
C 0.10077 -1.3442 -0.17097
F -0.89233 -2.3813 -0.42907
H -3.5950 0.32524 0.13144
H -2.4043 0.48704 1.4511
H -2.6780 -1.1047 0.67913
H 2.6721 1.3460 0.44716
H 3.3456 -1.0236 0.46388
Li 0.55165 -3.5987 -0.25891



E(B3LYP) = -912.539147731

Intermediate 2

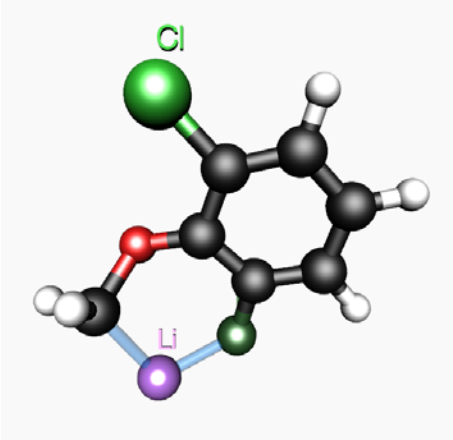
C -2.2788 -1.5569 0.45450
O -1.6260 -0.65289 -0.44533
C -0.29806 -0.42943 -0.22228
C 0.21892 0.85574 -0.017285
Cl -1.0515 2.2187 0.0052100
C 1.5354 1.2325 0.15691
C 2.4392 0.15034 0.13142
C 2.0251 -1.1690 -0.065399
C 0.67359 -1.4379 -0.24752
F 0.27106 -2.7160 -0.46263
H -3.3362 -1.5343 0.18546
H -2.1616 -1.2251 1.4932
H -1.8934 -2.5741 0.34992
Li 1.1151 3.1578 0.30984
H 3.5035 0.33317 0.26755
H 2.7257 -1.9984 -0.092707



E(B3LYP) = -912.532357117

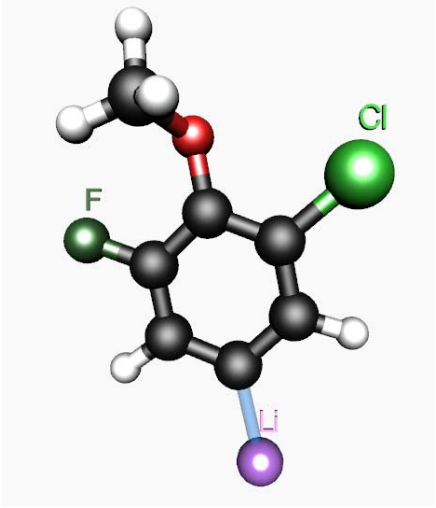
Intermediate 3

C -2.2568 -1.5414 0.51931
O -1.5651 -0.50146 -0.37440
C -0.27318 -0.25966 -0.17804
C 0.18661 1.0672 0.010182
Cl -0.99929 2.3518 0.063334
C 1.5372 1.3847 0.14598
C 2.5019 0.37950 0.11111
C 2.1091 -0.94624 -0.072339
C 0.76141 -1.2139 -0.21546
F 0.42899 -2.5565 -0.45945
H -3.2700 -1.5084 0.10199
H -2.3316 -1.0398 1.4954
Li -1.1671 -3.1735 0.17248
H 1.8234 2.4205 0.28747
H 3.5520 0.62511 0.22479
H 2.8239 -1.7599 -0.12449



E(B3LYP) = -912.527842233

Intermediate 4



C -1.4519 2.3752 0.47046
O -0.62105 1.7204 -0.49250
C -0.36664 0.39808 -0.25555
C 0.93556 -0.063950 -0.023935
Cl 2.2495 1.1124 0.045891
C 1.2096 -1.4232 0.14559
C 0.20027 -2.4107 0.11431
C -1.1084 -1.9289 -0.11419
C -1.3687 -0.57907 -0.29993
F -2.6424 -0.16519 -0.53800
H -1.5083 3.4197 0.15868
H -1.0085 2.3210 1.4723
H -2.4570 1.9438 0.49066
H 2.2518 -1.6920 0.30923
Li 0.63305 -4.3230 0.35201
H -1.9684 -2.5956 -0.16386

E(B3LYP) = -912.525605024

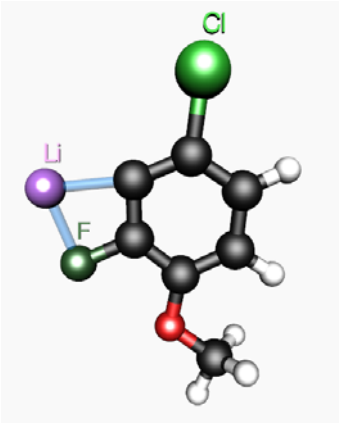
Substrate 1b

C 1.24119316 -3.35862863 0.0
O 0.04048938 -2.59963573 0.0
C 0.14789291 -1.24452619 0.0
C 1.33778363 -0.51209548 0.0
C 1.31768658 0.88688405 0.0
C 0.10112623 1.55773999 0.0
Cl 0.0695364 3.31522565 0.0
C -1.10535624 0.85294517 0.0
C -1.06379292 -0.53009497 0.0
F -2.21480817 -1.22562348 0.0
H 0.93279666 -4.40425903 0.0
H 1.84420451 -3.15817224 0.89451414
H 1.84420451 -3.15817224 -0.89451414
H 2.29204177 -1.02400258 0.0
H 2.24684934 1.4447915 0.0
H -2.06432738 1.35627305 0.0

E(B3LYP) = -905.613086914

Intermediate 1

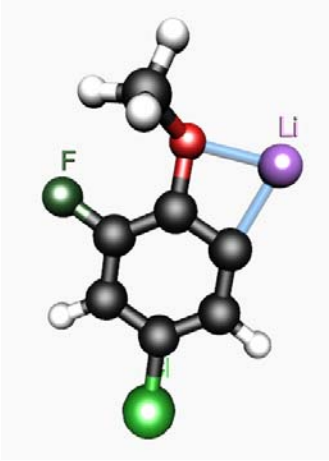
C 1.0085 -3.4642 0.0000
O -0.11147 -2.5915 0.0000
C 0.13798 -1.2512 0.0000
C 1.3967 -0.63804 0.0000
C 1.4997 0.76039 0.0000
C 0.34474 1.5399 0.0000
Cl 0.55804 3.3142 0.0000
C -0.94045 1.0010 0.0000
C -0.94193 -0.36599 0.0000
F -2.2645 -0.96317 0.0000
H 0.60110 -4.4761 0.0000
H 1.6300 -3.3243 0.89375
H 1.6300 -3.3243 -0.89375
H 2.3003 -1.2358 0.0000
H 2.4804 1.2245 0.0000
Li -2.9183 0.81220 0.0000



E(B3LYP) = -912.552466746

Intermediate 2

C -0.11791 3.3655 0.47600
O 0.66437 2.4794 -0.34217
C 0.41986 1.0735 -0.18996
C 1.5658 0.29147 -0.056274
C 1.3569 -1.0912 0.069146
C 0.066956 -1.6248 0.057494
Cl -0.16815 -3.3691 0.23822
C -1.0640 -0.82206 -0.10225
C -0.86835 0.54476 -0.24375
F -1.9543 1.3427 -0.43438
H 0.35337 4.3490 0.41217
H -0.12292 3.0213 1.5170
H -1.1433 3.4246 0.11040
Li 2.5416 2.0063 -0.23167
H 2.1940 -1.7760 0.17639
H -2.0654 -1.2331 -0.13087



E(B3LYP) = -912.543527795

Intermediate 3

C 1.3724 -3.3745 0.0000
O 0.14669 -2.6611 0.0000
C 0.20499 -1.2976 0.0000
C 1.3661 -0.51795 0.0000
C 1.3401 0.89628 0.0000
C 0.067516 1.4196 0.0000
Cl -0.070778 3.2893 0.0000
C -1.1459 0.73271 0.0000
C -1.0445 -0.64676 0.0000
F -2.1657 -1.3952 0.0000
H 1.1030 -4.4318 0.0000
H 1.9718 -3.1530 0.89258
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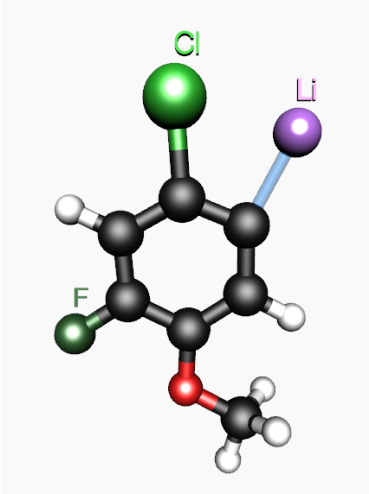
H 2.3261 -1.0267 0.0000

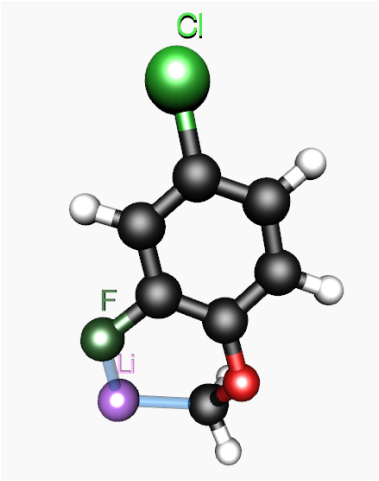


Li 2.2254 2.6598 0.0000
H -2.1195 1.2087 0.0000

E(B3LYP) = -912.536834347

Intermediate 4

C 0.25025 -3.4304 -0.54556
O 0.92155 -2.3904 0.34820
C 0.58694 -1.1080 0.19492
C 1.6121 -0.14757 0.074040
C 1.3581 1.2178 -0.014794
C 0.041265 1.6767 -0.00077821
Cl -0.30105 3.3950 -0.13281
C -1.0154 0.77611 0.11818
C -0.71307 -0.56934 0.21976
F -1.8181 -1.4171 0.40111
H 0.69279 -4.3511 -0.14633
H 0.72952 -3.2859 -1.5269
Li -1.6935 -3.1259 -0.21972
H 2.6299 -0.52234 0.058313
H 2.1771 1.9224 -0.10473
H -2.0472 1.1048 0.15326



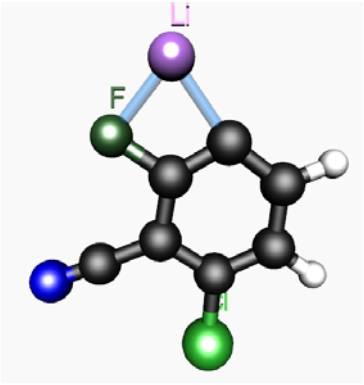
E(B3LYP) = -912.529112716

Substrate 1c
F -1.03293858 2.47562387 0.0
C -0.0795104 1.53680748 0.0
C 1.25276712 1.919657 0.0
C 2.23011964 0.9253818 0.0
C 1.8809769 -0.42618592 0.0
C 0.53650577 -0.78800591 0.0
Cl 0.10520323 -2.47873818 0.0
C -0.47841925 0.19014524 0.0
C -1.8693934 -0.13281417 0.0
N -3.00570924 -0.37623381 0.0
H 1.50078755 2.97446258 0.0
H 3.27843179 1.20473106 0.0
H 2.6405245 -1.19834005 0.0

E(B3LYP) = -883.328887388

Intermediate 1

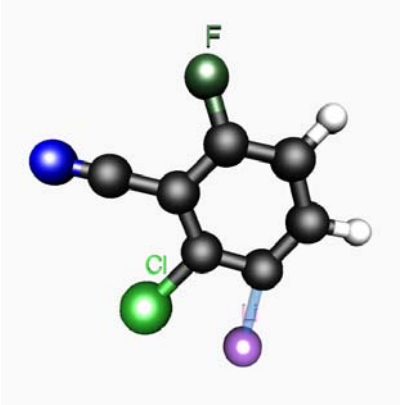
F -1.4147 2.2406 0.0000
C -0.23893 1.4127 0.0000
C 0.94195 2.1052 0.0000
C 2.0652 1.2547 0.0000
C 1.9606 -0.14092 0.0000
C 0.70509 -0.74871 0.0000
Cl 0.58304 -2.4938 0.0000
C -0.46903 0.031757 0.0000
C -1.7866 -0.51592 0.0000
N -2.8743 -0.92792 0.0000
Li -0.20531 3.7367 0.0000
H 3.0671 1.6808 0.0000
H 2.8462 -0.76733 0.0000



E(B3LYP) = -890.263658285

Intermediate 2

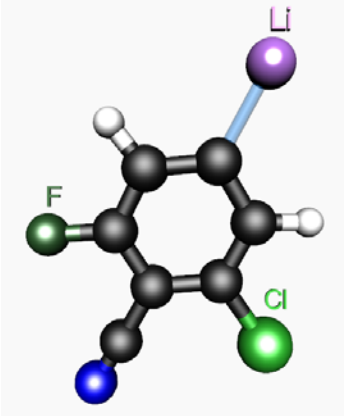
F 0.28495 2.7500 0.0000
C 0.67789 1.4653 0.0000
C 2.0322 1.1579 0.0000
C 2.4208 -0.18333 0.0000
C 1.5036 -1.2576 0.0000
C 0.18469 -0.85207 0.0000
Cl -1.0763 -2.1915 0.0000
C -0.30837 0.46847 0.0000
C -1.6903 0.81867 0.0000
N -2.8197 1.0986 0.0000
H 2.7533 1.9687 0.0000
H 3.4889 -0.39389 0.0000
Li 1.1215 -3.2056 0.0000



E(B3LYP) = -890.256961836

Intermediate 3

F -2.5810 0.77719 0.0000
C -1.2362 0.86053 0.0000
C -0.62246 2.1043 0.0000
C 0.78263 2.2373 0.0000
C 1.5148 1.0268 0.0000
C 0.89470 -0.21953 0.0000
Cl 1.8801 -1.6778 0.0000
C -0.50834 -0.33945 0.0000
C -1.1930 -1.5906 0.0000
N -1.7733 -2.5975 0.0000
H -1.2850 2.9679 0.0000
Li 1.6913 4.0075 0.0000
H 2.6024 1.0310 0.0000

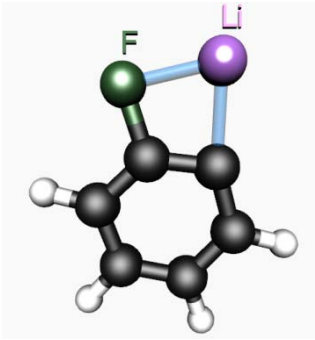


E(B3LYP) = -890.252825181

Substrate 1d
F 0.0 0.0 2.27937068
C 0.0 0.0 0.92861465
C 0.0 1.21752811 0.25793058
C 0.0 1.20832088 -1.13775291
C 0.0 0.0 -1.8382857
C 0.0 -1.20832088 -1.13775291
C 0.0 -1.21752811 0.25793058
H 0.0 2.14221725 0.82461427
H 0.0 2.15063799 -1.67732585
H 0.0 0.0 -2.92358051
H 0.0 -2.15063799 -1.67732585
H 0.0 -2.14221725 0.82461427

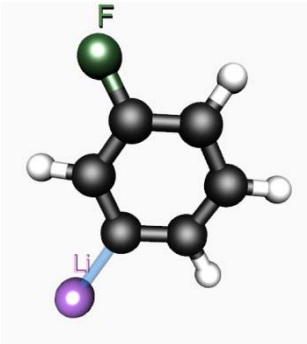
E(B3LYP) = -331.497380663

Intermediate 1
F 0.63921 2.0946 0.0000
C 0.20986 0.69258 0.0000
C 1.2184 -0.25383 0.0000
C 0.77926 -1.5821 0.0000
C -0.59229 -1.8626 0.0000
C -1.5326 -0.82550 0.0000
C -1.1553 0.53229 0.0000
H 2.2702 0.011489 0.0000
H 1.5071 -2.3885 0.0000
H -0.92378 -2.8981 0.0000
H -2.5892 -1.0918 0.0000
Li -1.1899 2.5127 0.0000



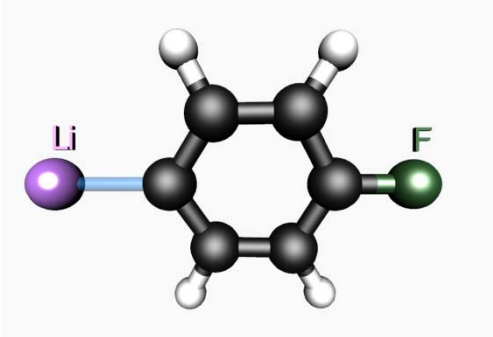
E(B3LYP) = -338.426740594

Intermediate 2
F -0.89579 2.1971 0.0000
C -0.31482 0.96672 0.0000
C 1.0717 0.88922 0.0000
C 1.6476 -0.38276 0.0000
C 0.83827 -1.5231 0.0000
C -0.57676 -1.4671 0.0000
C -1.1249 -0.16426 0.0000
H 1.6658 1.7972 0.0000
H 2.7316 -0.47784 0.0000
H 1.3431 -2.4906 0.0000
Li -1.7033 -3.0891 0.0000
H -2.2013 0.0084100 0.0000



E(B3LYP) = -338.410390108

Intermediate 3



F 0.0000 0.0000 2.4515
C 0.0000 0.0000 1.0938
C 0.0000 1.2120 0.41712
C 0.0000 1.1900 -0.98234
C 0.0000 0.0000 -1.7481
C 0.0000 -1.1900 -0.98234
C 0.0000 -1.2120 0.41712
H 0.0000 2.1401 0.98170
H 0.0000 2.1597 -1.4836
Li 0.0000 0.0000 -3.7195
H 0.0000 -2.1597 -1.4836
H 0.0000 -2.1401 0.98170

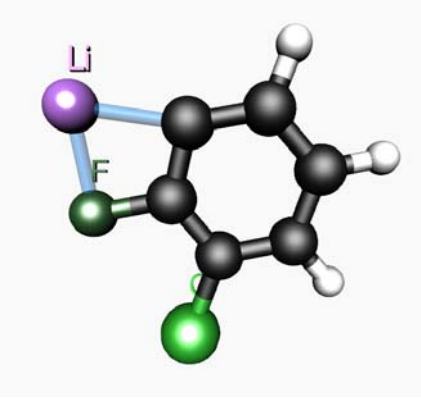
E(B3LYP) = -338.408867593

Substrate 1e

F -2.02507334 -0.60816812 0.0
C -0.92550963 0.16308362 0.0
C -1.06642476 1.54532098 0.0
C 0.07439301 2.34741274 0.0
C 1.34259434 1.76297865 0.0
C 1.47555472 0.37476425 0.0
C 0.33795931 -0.43252039 0.0
Cl 0.47362366 -2.17396785 0.0
H -2.06558061 1.96710577 0.0
H -0.03046604 3.42750065 0.0
H 2.23202338 2.38437353 0.0
H 2.45462483 -0.09194497 0.0

E(B3LYP) = -791.089140336

Intermediate 1

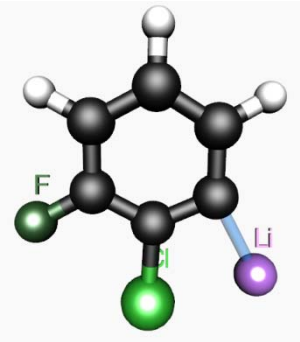


F -2.0871 0.30990 0.0000
C -0.66564 0.57843 0.0000
C -0.33911 1.9124 0.0000
C 1.0473 2.1528 0.0000
C 1.9784 1.1087 0.0000
C 1.5588 -0.22607 0.0000
C 0.19262 -0.51066 0.0000
Cl -0.38811 -2.1688 0.0000
Li -2.3099 2.1905 0.0000
H 1.4199 3.1756 0.0000
H 3.0445 1.3225 0.0000
H 2.2730 -1.0420 0.0000

E(B3LYP) = -798.021190449

Intermediate 2

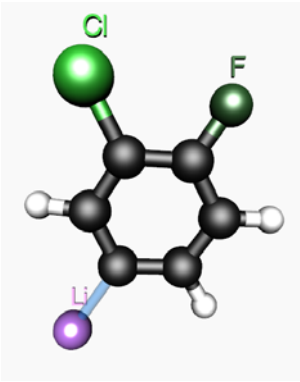
F -2.0764 -0.30674 0.0000
C -0.89771 0.34730 0.0000
C -0.87008 1.7357 0.0000
C 0.37117 2.3818 0.0000
C 1.5582 1.6456 0.0000
C 1.5715 0.23419 0.0000
C 0.31468 -0.33506 0.0000
Cl 0.20738 -2.1892 0.0000
H -1.8087 2.2798 0.0000
H 0.40043 3.4687 0.0000
H 2.5006 2.1905 0.0000
Li 2.5044 -1.5137 0.0000



E(B3LYP) = -798.014057072

Intermediate 3

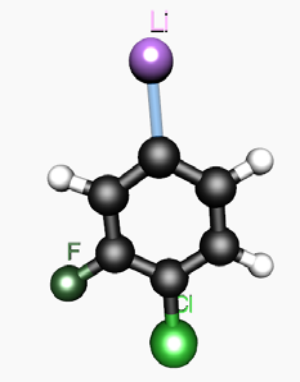
F 1.7306 1.4183 0.0000
C 0.97979 0.29913 0.0000
C 1.6006 -0.94294 0.0000
C 0.81094 -2.0959 0.0000
C -0.60355 -2.0714 0.0000
C -1.1780 -0.78051 0.0000
C -0.41039 0.38701 0.0000
Cl -1.1741 1.9745 0.0000
H 2.6864 -0.98193 0.0000
H 1.3393 -3.0498 0.0000
Li -1.7145 -3.7046 0.0000
H -2.2588 -0.64679 0.0000



E(B3LYP) = -798.005262601

Intermediate 4

F -2.0322 -0.71442 0.0000
C -0.91547 0.045032 0.0000
C -1.0276 1.4327 0.0000
C 0.098299 2.2844 0.0000
C 1.3466 1.6172 0.0000
C 1.4777 0.22569 0.0000
C 0.33415 -0.57091 0.0000
Cl 0.45120 -2.3229 0.0000
H -2.0455 1.8223 0.0000
Li -0.061810 4.2553 0.0000
H 2.2731 2.1925 0.0000
H 2.4539 -0.25030 0.0000



E(B3LYP) = -798.005156243

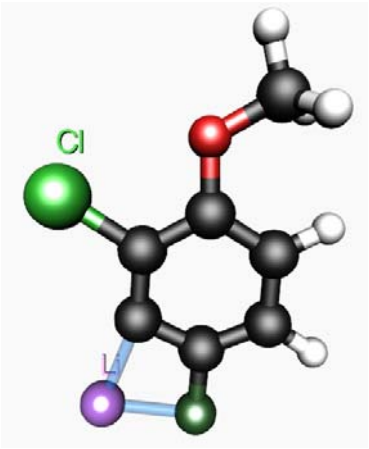
Substrate 1f

C 2.10960914 2.46673067 -0.06119334
O 0.77983071 1.9699843 -0.06548693
C 0.59410018 0.62465919 -0.0298011
C 1.62375537 -0.32299922 0.01936813
C 1.34211432 -1.69055372 0.05995092
C 0.01990521 -2.1042035 0.05061321
F -0.266756 -3.42309717 0.09256268
C -1.03079998 -1.19397647 0.00076096
C -0.73810365 0.16440596 -0.04039597
Cl -2.04880466 1.32115933 -0.10547319
H 2.02034885 3.55298234 -0.0942058
H 2.67234438 2.12333399 -0.93833713
H 2.64634118 2.17566625 0.85049054
H 2.65741995 -3.749e-05 0.02408807
H 2.13790871 -2.42548842 0.09851453
H -2.05648809 -1.54164139 -0.00667494

E(B3LYP) = -905.613971739

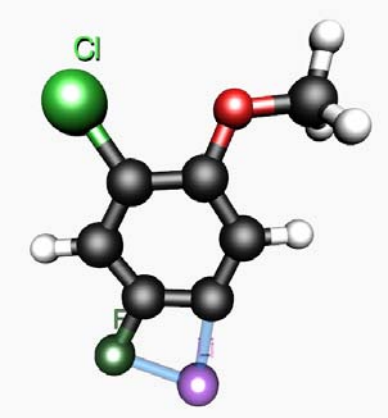
Intermediate 1

C 1.6967 2.8609 0.019319
O 0.46414 2.1629 0.023115
C 0.48835 0.80003 0.028486
C 1.6703 0.041405 0.024067
C 1.6147 -1.3575 0.019228
C 0.34690 -1.8945 0.012449
F 0.23846 -3.3491 0.0041698
C -0.86955 -1.2544 0.025467
C -0.75467 0.12564 0.037355
Cl -2.2218 1.1294 0.065640
H 1.4411 3.9214 0.011992
H 2.2939 2.6290 -0.87258
H 2.2929 2.6411 0.91503
H 2.6352 0.53200 0.029216
H 2.5137 -1.9643 0.026990
Li -1.6244 -3.0870 0.069446



E(B3LYP) = -912.552885532

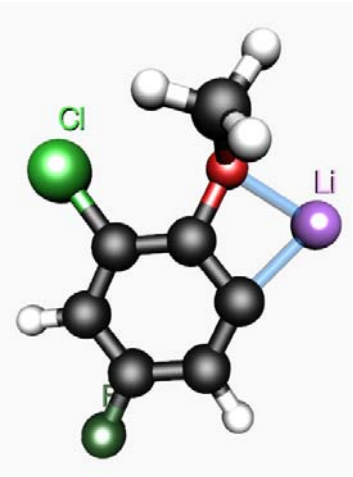
Intermediate 2



C 2.6901 1.9085 -0.059377
O 1.2797 1.7651 -0.060897
C 0.75825 0.50568 -0.024224
C 1.5148 -0.67706 0.015565
C 0.92580 -1.9549 0.049749
C -0.44479 -1.9121 0.039627
F -1.0876 -3.2224 0.073003
C -1.2903 -0.81721 0.0037029
C -0.65131 0.41923 -0.028520
Cl -1.6176 1.8826 -0.074875
H 2.8796 2.9825 -0.094393
H 3.1484 1.4320 -0.93526
H 3.1402 1.4912 0.85035
H 2.5976 -0.59178 0.020486
Li 0.66183 -3.9200 0.10552
H -2.3709 -0.89649 0.00026590

E(B3LYP) = -912.545411164

Intermediate 3



C 1.0820 2.5539 0.66717
O 1.3094 1.6072 -0.39413
C 0.67844 0.32888 -0.20405
C 1.5510 -0.72888 0.061981
C 0.95933 -1.9915 0.21686
C -0.41860 -2.1419 0.10723
F -0.97630 -3.3651 0.27573
C -1.2701 -1.0803 -0.19330
C -0.70096 0.17896 -0.36838
Cl -1.7532 1.5240 -0.83645
H 1.6837 3.4365 0.43762
H 1.3873 2.1299 1.6320
H 0.029077 2.8387 0.71089
Li 2.9582 0.58703 -0.39685
H 1.5518 -2.8799 0.42286
H -2.3358 -1.2397 -0.29826

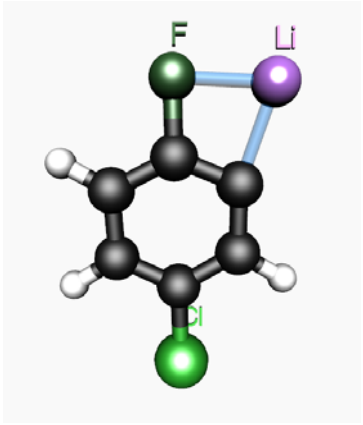
E(B3LYP) = -912.54167599

Substrate 1g

F 0.0 0.0 3.15195363
C 0.0 0.0 1.80418218
C 0.0 1.21617332 1.13145825
C 0.0 1.21472775 -0.26277722
C 0.0 0.0 -0.94887569
Cl 0.0 0.0 -2.70725707
C 0.0 -1.21472775 -0.26277722
C 0.0 -1.21617332 1.13145825
H 0.0 2.14321767 1.69345739
H 0.0 2.14947828 -0.81236782
H 0.0 -2.14947828 -0.81236782
H 0.0 -2.14321767 1.69345739

E(B3LYP) = -791.091712702

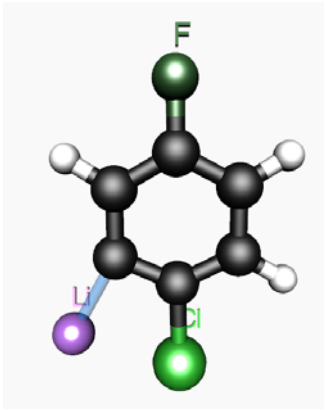
Intermediate 1



F 0.11604 3.0480 0.0000
C 0.081618 1.5894 0.0000
C 1.3050 0.94455 0.0000
C 1.2431 -0.45136 0.0000
C -0.010742 -1.0696 0.0000
Cl -0.073933 -2.8384 0.0000
C -1.2037 -0.34096 0.0000
C -1.1892 1.0654 0.0000
H 2.2504 1.4768 0.0000
H 2.1487 -1.0465 0.0000
H -2.1414 -0.89103 0.0000
Li -1.7712 2.9646 0.0000

E(B3LYP) = -798.025033517

Intermediate 2



F 0.045946 3.2461 0.0000
C 0.027573 1.8918 0.0000
C 1.2327 1.1964 0.0000
C 1.2573 -0.21210 0.0000
C -0.0046089 -0.77750 0.0000
Cl -0.059151 -2.6542 0.0000
C -1.2401 -0.14011 0.0000
C -1.2120 1.2542 0.0000
H 2.1511 1.7800 0.0000
Li 2.2139 -1.9427 0.0000
H -2.1783 -0.68493 0.0000
H -2.1246 1.8399 0.0000

E(B3LYP) = -798.017093861

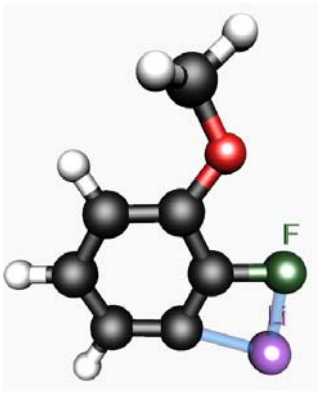
Substrate 1h

C -0.75205223 2.74083991 0.15969754
O 0.29180142 1.78080797 0.09586548
C -0.05789302 0.46562001 0.07119664
C 1.00680815 -0.45172971 0.01108071
F 2.26477477 0.03147411 -0.0189634
C 0.79394478 -1.817944 -0.01696816
C -0.51613507 -2.31033917 0.01220772
C -1.58355886 -1.41997994 0.06718702
C -1.3614597 -0.03854826 0.0964996
H -0.26218342 3.71457318 0.17871931
H -1.3555778 2.62322788 1.06920009
H -1.40903207 2.68299323 -0.7177303
H 1.65470842 -2.47657372 -0.06170181
H -0.69094386 -3.38054982 -0.00808736
H -2.60328776 -1.79101773 0.08785309
H -2.20596384 0.63877881 0.13424519

E(B3LYP) = -446.019023891

Intermediate 1

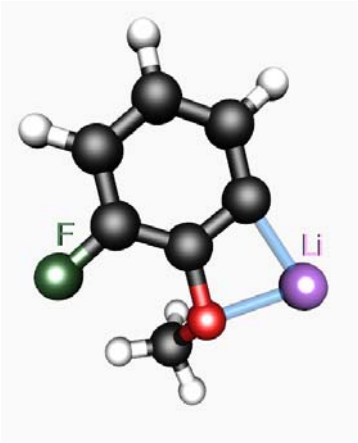
C 0.13399 2.8717 0.19542
O 0.78853 1.6156 0.12131
C 0.0012118 0.50008 0.081094
C 0.61499 -0.75250 0.014569
F 2.0746 -0.74544 -0.0084318
C 0.045831 -1.9947 -0.031655
C -1.3651 -1.9672 -0.0091912
C -2.0664 -0.76310 0.055369
C -1.3977 0.47045 0.10175
H 0.92515 3.6228 0.22037
H -0.47558 2.9583 1.1043
H -0.50482 3.0489 -0.67958
Li 1.9344 -2.6074 -0.089383
H -1.9305 -2.8970 -0.039746
H -3.1541 -0.76406 0.072602
H -1.9655 1.3924 0.15158



E(B3LYP) = -452.949377761

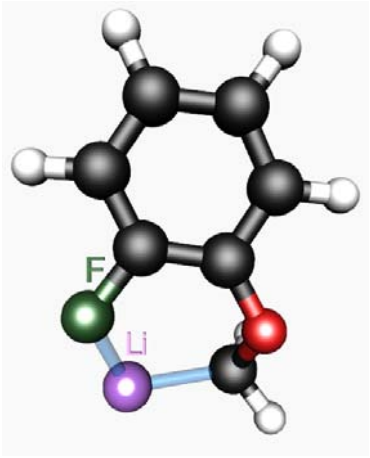
Intermediate 2

C 0.025533 -2.6135 -0.29043
O 0.71628 -1.6379 0.50714
C 0.37420 -0.26189 0.25535
C -0.94386 0.17858 0.36370
F -1.9490 -0.68488 0.68740
C -1.2441 1.5151 0.14432
C -0.19794 2.3952 -0.15342
C 1.1190 1.9300 -0.22090
C 1.4518 0.57813 -0.018465
H 0.47479 -3.5832 -0.063031
H 0.14226 -2.3899 -1.3583
H -1.0349 -2.6331 -0.037144
H -2.2751 1.8442 0.22130
H -0.42242 3.4460 -0.32184
H 1.9052 2.6510 -0.44094
Li 2.5439 -1.0344 0.31125



E(B3LYP) = -452.945577756

Intermediate 3



C 0.70398 -2.5312 -0.34995
O 1.1168 -1.3243 0.48772
C 0.49050 -0.16146 0.27761
C -0.89872 0.057910 0.32164
F -1.7639 -1.0184 0.59916
C -1.5078 1.2878 0.15753
C -0.70634 2.4105 -0.054326
C 0.68100 2.2553 -0.093145
C 1.2606 0.99829 0.059528
H 1.3703 -3.2990 0.061593
H 1.1050 -2.3116 -1.3527
Li -1.2497 -2.6630 0.031027
H -2.5892 1.3545 0.21701
H -1.1629 3.3860 -0.18184
H 1.3183 3.1194 -0.25568
H 2.3368 0.86563 0.021370

E(B3LYP) = -452.935282063

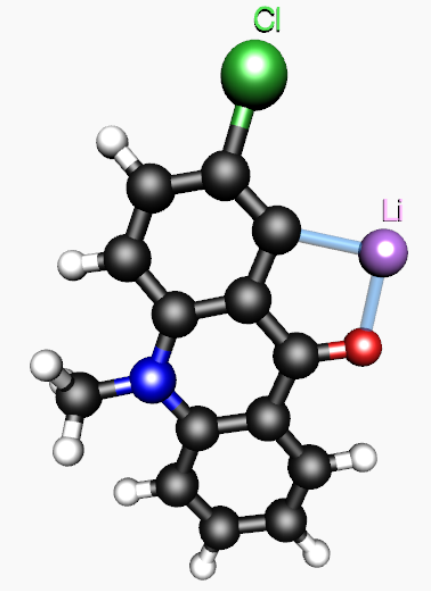
Substrate 4

C -2.85104449 -1.13684862 -0.24159641
N -1.41875436 -0.90124126 -0.07606146
C -0.94017307 0.40702248 -0.01453896
C -1.81612815 1.50836778 0.1172916
C -1.32831148 2.80556278 0.15062426
C 0.04878754 3.042646 0.05933071
Cl 0.64425004 4.69633816 0.09754441
C 0.92992033 1.98420346 -0.04571023
C 0.4498863 0.66627037 -0.07682309
C 1.42990506 -0.43346696 -0.16252149
O 2.63970038 -0.22917093 -0.27439834
C 0.8569064 -1.78606876 -0.06406314
C -0.54369215 -1.98785517 -0.00034911
C -1.02305444 -3.30868623 0.14627487
C -0.13904163 -4.37733228 0.1919601
C 1.24551536 -4.17873694 0.10060979
C 1.72752341 -2.88710924 -0.01920506
H -3.00599737 -2.05635069 -0.80475268
H -3.28904113 -0.32704925 -0.8244219
H -3.37857834 -1.21259778 0.71718209
H -2.88283401 1.36121018 0.22481642
H -2.01454574 3.63825666 0.25874452
H 2.00254008 2.12846666 -0.10472787
H -2.08182133 -3.50505629 0.25495503
H -0.53684198 -5.38108309 0.31099135
H 1.92568199 -5.02340892 0.13573001
H 2.78935721 -2.67299085 -0.07929727

E(B3LYP) = -1129.74596148

Intermediate 1

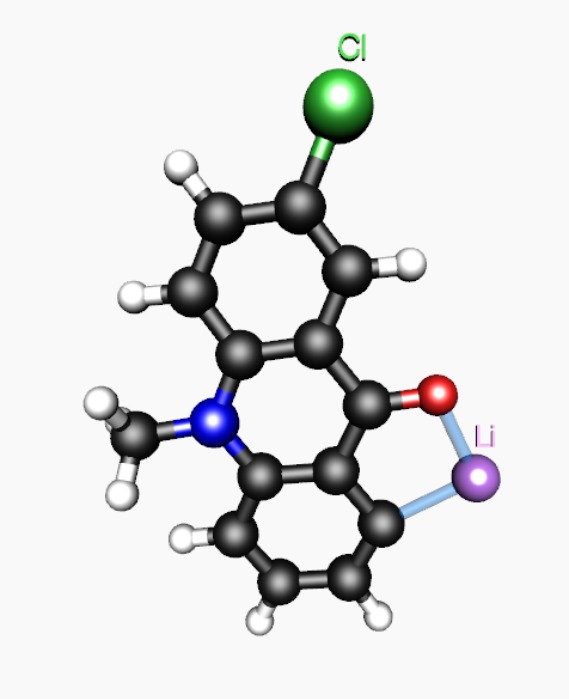
C -2.8851 -1.2077 0.23377
N -1.4543 -0.95158 0.071378
C -0.99458 0.36862 0.0058068
C -1.8933 1.4473 -0.11876
C -1.4130 2.7489 -0.14702
C -0.035285 2.9859 -0.047042
Cl 0.46728 4.7103 -0.062675
C 0.91875 1.9970 0.045898
C 0.39820 0.66609 0.059092
C 1.3561 -0.43016 0.11684
O 2.6053 -0.23059 0.20007
C 0.83150 -1.7858 0.041404
C -0.56988 -2.0167 0.0015337
C -1.0231 -3.3532 -0.11786
C -0.12029 -4.4018 -0.16219
C 1.2646 -4.1753 -0.094713
C 1.7232 -2.8764 -0.00050867
H -3.0320 -2.1268 0.79942
H -3.4055 -1.2911 -0.72780
H -3.3322 -0.39925 0.81038
H -2.9579 1.2865 -0.22824
H -2.1109 3.5737 -0.25460
Li 2.8872 1.5904 0.18482
H -2.0788 -3.5721 -0.20891
H -0.49883 -5.4151 -0.26149
H 1.9594 -5.0080 -0.12888
H 2.7823 -2.6479 0.040098



E(B3LYP) = -1136.69977344

Intermediate 2

C -2.9485 -1.0327 0.22478
N -1.5085 -0.83369 0.064481
C -0.99887 0.45107 0.0087216
C -1.8407 1.5854 -0.10099
C -1.3129 2.8636 -0.13284
C 0.075117 3.0565 -0.060645
Cl 0.72044 4.6929 -0.097031
C 0.92302 1.9732 0.023745
C 0.40333 0.66504 0.052585
C 1.3252 -0.46391 0.12193
O 2.5725 -0.25215 0.20938
C 0.75896 -1.8014 0.052408
C -0.66019 -1.9482 -0.011800
C -1.1861 -3.2455 -0.15562
C -0.32229 -4.3335 -0.18886
C 1.0666 -4.1705 -0.077948
C 1.6640 -2.9135 0.034130
H -3.1237 -1.9490 0.78621
H -3.4707 -1.0983 -0.73721
H -3.3709 -0.21299 0.80479
H -2.9126 1.4731 -0.19455
H -1.9726 3.7192 -0.22590
H 1.9989 2.0901 0.067230
H -2.2490 -3.4125 -0.27361
H -0.74832 -5.3279 -0.31083
H 1.6841 -5.0681 -0.095326
Li 3.3963 -1.8937 0.18310



E(B3LYP) = -1136.68941164

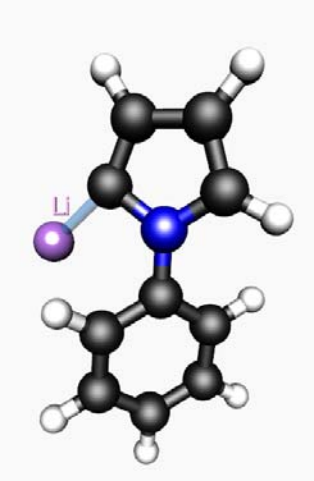
Substrate 5

C 0.26386025 -0.66232658 3.12213404
C 0.41150828 -1.04574419 1.81046824
N 0.0 0.0 1.00124456
C -0.41150828 1.04574419 1.81046824
C -0.26386025 0.66232658 3.12213404
C 0.0 0.0 -0.41580811
C 0.30671817 1.17148297 -1.11975841
C 0.29454051 1.16871914 -2.51341406
C 0.0 0.0 -3.21735502
C -0.29454051 -1.16871914 -2.51341406
C -0.30671817 -1.17148297 -1.11975841
H 0.51641862 -1.26112854 3.98578643
H 0.81638019 -1.94731392 1.37768246
H -0.81638019 1.94731392 1.37768246
H -0.51641862 1.26112854 3.98578643
H 0.57409207 2.07014736 -0.5743324
H 0.53371284 2.08231757 -3.04955565
H 0.0 0.0 -4.30282704
H -0.53371284 -2.08231757 -3.04955565
H -0.57409207 -2.07014736 -0.5743324

E(B3LYP) = -441.248390533

Intermediate 1

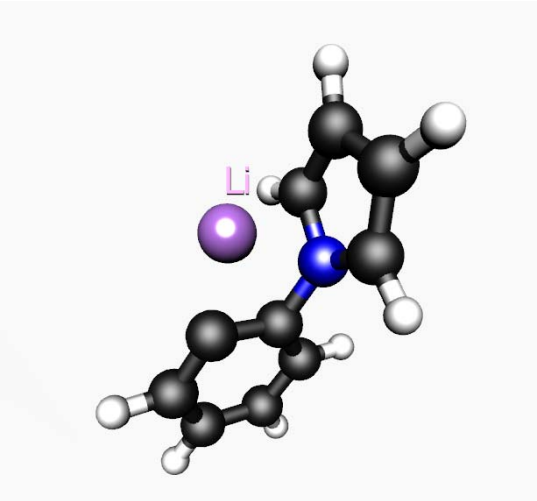
C -0.90705 3.0875 -0.26944
C -1.2539 1.7705 -0.44167
N -0.14052 1.0082 -0.11084
C 0.94906 1.8237 0.31460
C 0.44238 3.1118 0.20393
C -0.079908 -0.38823 -0.079624
C 1.1221 -1.0498 -0.42238
C 1.2299 -2.4401 -0.30747
C 0.14322 -3.1992 0.12392
C -1.0616 -2.5523 0.42014
C -1.1766 -1.1679 0.32839
H -1.5499 3.9355 -0.47020
H -2.1574 1.3164 -0.82332
Li 2.2800 0.56356 1.0147
H 0.99151 4.0099 0.46244
H 1.9110 -0.47657 -0.90746
H 2.1570 -2.9295 -0.59436
H 0.22460 -4.2779 0.21018
H -1.9192 -3.1335 0.74738
H -2.1021 -0.67193 0.60058



E(B3LYP) = -448.169564509

Intermediate 2

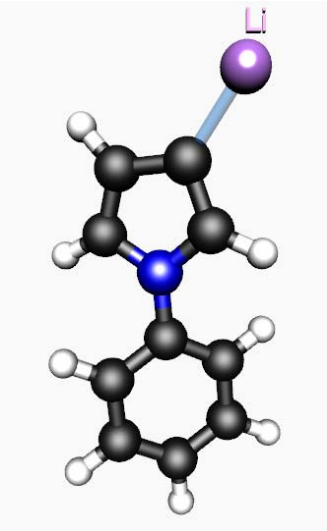
C -0.69514 2.9733 0.45527
C -0.52998 1.7181 1.0182
N 0.33212 0.98494 0.22538
C 0.71352 1.7707 -0.84589
C 0.098794 3.0073 -0.73308
C 0.26509 -0.48536 0.13949
C 1.2478 -1.2592 0.75415
C 1.1426 -2.6458 0.63232
C 0.074795 -3.1920 -0.086377
C -0.88505 -2.3635 -0.68015
C -0.83786 -0.95809 -0.59591
H -1.2763 3.7853 0.86962
H -0.96857 1.2700 1.8972
H 1.3711 1.3697 -1.6025
H 0.23745 3.8498 -1.3962
H 2.0628 -0.80030 1.3083
H 1.8846 -3.2910 1.0940
H -0.0057248 -4.2731 -0.18154
H -1.6974 -2.8411 -1.2283
Li -1.4924 0.94069 -0.99691



E(B3LYP) = -448.167752751

Intermediate 3

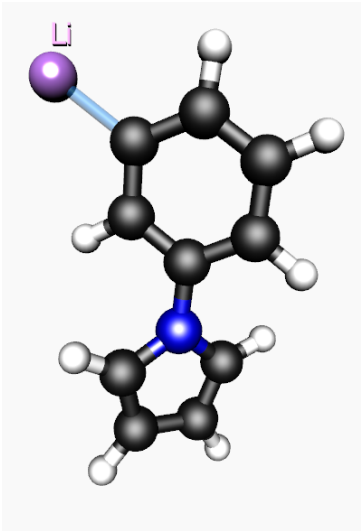
C -0.96935 2.9106 -0.26834
C -1.2668 1.5761 -0.38475
N -0.13285 0.85692 -0.033467
C 0.85763 1.7789 0.30666
C 0.39716 3.0812 0.18967
C -0.015600 -0.54673 -0.014405
C 1.2133 -1.1601 -0.30399
C 1.3300 -2.5481 -0.27097
C 0.22633 -3.3482 0.030009
C -0.99905 -2.7400 0.30861
C -1.1220 -1.3523 0.29779
H -1.6709 3.7047 -0.50122
H -2.1511 1.0664 -0.73862
H 1.8065 1.3982 0.66266
Li 1.3916 4.7031 0.60645
H 2.0636 -0.54525 -0.57789
H 2.2884 -3.0064 -0.49878
H 0.31953 -4.4298 0.046561
H -1.8658 -3.3483 0.55185
H -2.0668 -0.88484 0.55316



E(B3LYP) = -448.162816572

Intermediate 4

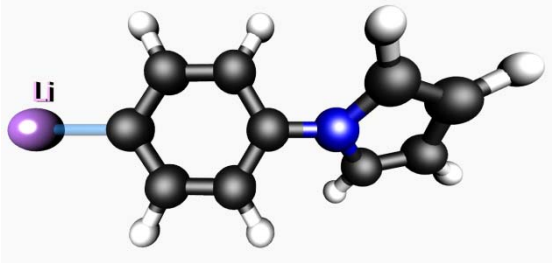
C 0.36555 -3.2811 -0.32827
C 0.88393 -2.0151 -0.48524
N -0.030791 -1.1033 0.0059223
C -1.1298 -1.7956 0.47655
C -0.91195 -3.1419 0.28645
C 0.12997 0.31274 0.020120
C -0.95408 1.1516 -0.27551
C -0.86027 2.5604 -0.26854
C 0.42208 3.0728 0.040374
C 1.5175 2.2529 0.32545
C 1.3767 0.86620 0.32742
H 0.84614 -4.2014 -0.62978
H 1.8017 -1.6756 -0.94007
H -1.9465 -1.2680 0.94449
H -1.5887 -3.9367 0.56806
H -1.8921 0.66204 -0.53812
Li -2.3949 3.7291 -0.70072
H 0.58715 4.1515 0.061022
H 2.4850 2.6903 0.56321
H 2.2093 0.21890 0.58475



E(B3LYP) = -448.160706386

Intermediate 5

C 0.27492 -0.65718 3.2810
C 0.42999 -1.0360 1.9668
N 0.0000 0.0000 1.1591
C -0.42999 1.0360 1.9668
C -0.27492 0.65718 3.2810
C 0.0000 0.0000 -0.26341
C 0.32025 1.1624 -0.97197
C 0.30435 1.1475 -2.3686
C 0.0000 0.0000 -3.1383
C -0.30435 -1.1475 -2.3686
C -0.32025 -1.1624 -0.97197
H 0.53689 -1.2533 4.1441
H 0.84607 -1.9311 1.5310
H -0.84607 1.9311 1.5310
H -0.53689 1.2533 4.1441
H 0.59872 2.0611 -0.42840
H 0.56000 2.0842 -2.8677
Li 0.0000 0.0000 -5.1116
H -0.56000 -2.0842 -2.8677
H -0.59872 -2.0611 -0.42840



E(B3LYP) = -448.16005468

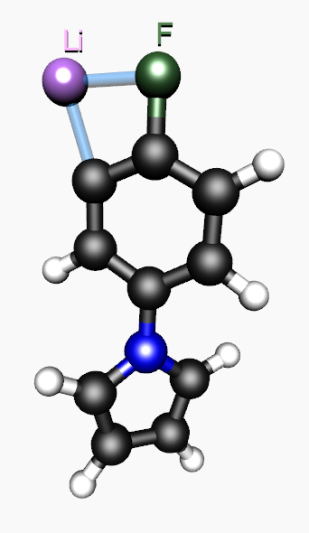
Substrate 6

F 0.0 0.0 4.10385187
C 0.0 0.0 2.75436463
C -0.31205669 1.17333452 2.07791054
C -0.32258523 1.16678146 0.68483777
C 0.0 0.0 -0.02040788
C 0.32258523 -1.16678146 0.68483777
C 0.31205669 -1.17333452 2.07791054
N 0.0 0.0 -1.43722509
C -0.43184312 -1.03772013 -2.24594343
C -0.27592954 -0.65717859 -3.55775296
C 0.27592954 0.65717859 -3.55775296
C 0.43184312 1.03772013 -2.24594343
H -0.55962865 2.06699783 2.63981891
H -0.60149003 2.06244077 0.14070057
H 0.60149003 -2.06244077 0.14070057
H 0.55962865 -2.06699783 2.63981891
H -0.85542445 -1.93057765 -1.81256845
H -0.53964451 -1.25114963 -4.42135796
H 0.53964451 1.25114963 -4.42135796
H 0.85542445 1.93057765 -1.81256845

E(B3LYP) = -540.478291685

Intermediate 1

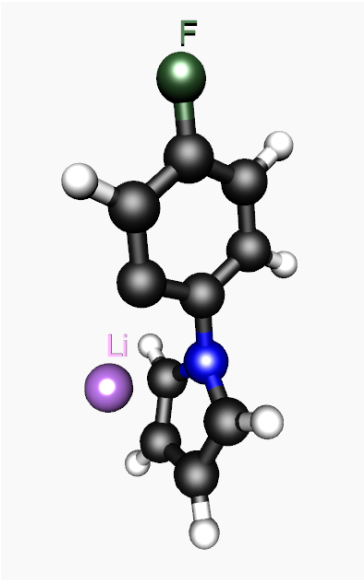
F 0.21692 4.0186 0.0069627
C 0.16392 2.5593 0.0068972
C 1.3328 1.8984 0.33684
C 1.2508 0.50515 0.33932
C 0.041508 -0.12124 -0.0012595
C -1.0892 0.64300 -0.33367
C -1.0666 2.0475 -0.32889
N -0.028144 -1.5418 -0.0058281
C -1.0983 -2.2977 0.43597
C -0.78876 -3.6282 0.27040
C 0.51571 -3.6930 -0.29913
C 0.95950 -2.3998 -0.45464
H 2.2487 2.4201 0.59373
H 2.1093 -0.093186 0.62424
H -1.9938 0.10895 -0.61749
Li -1.6006 3.9528 -0.49043
H -1.9634 -1.8186 0.86746
H -1.4238 -4.4611 0.53844
H 1.0626 -4.5843 -0.57337
H 1.8680 -2.0092 -0.88677



E(B3LYP) = -547.40996257

Intermediate 2

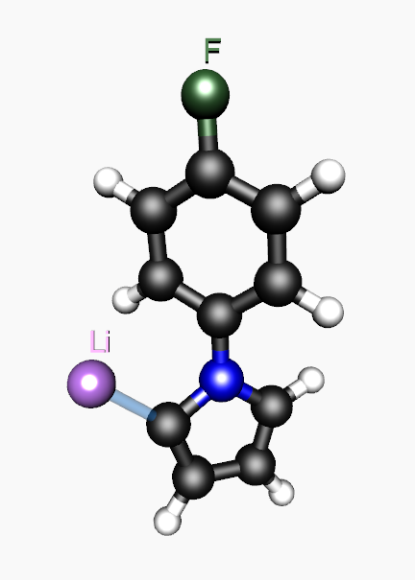
F -0.11696 4.0845 0.19150
C 0.0066900 2.7377 0.078981
C 1.0900 2.2414 -0.64162
C 1.2184 0.85698 -0.75708
C 0.25280 0.061915 -0.14280
C -0.85848 0.51737 0.59503
C -0.94399 1.9179 0.68270
N 0.34604 -1.4042 -0.22800
C -0.50668 -2.1526 -1.0178
C -0.64929 -3.4095 -0.45335
C 0.14742 -3.4287 0.73370
C 0.74166 -2.1823 0.84425
H 1.8004 2.9256 -1.0920
H 2.0451 0.41881 -1.3100
Li -1.4807 -1.3959 0.99501
H -1.7529 2.4063 1.2230
H -0.95402 -1.7135 -1.8965
H -1.2204 -4.2306 -0.86378
H 0.29850 -4.2670 1.3993
H 1.3936 -1.7697 1.5994



E(B3LYP) = -547.401322064

Intermediate 3

F -0.19265 4.0924 0.21295
C -0.10488 2.7476 0.11114
C 1.0958 2.1182 0.42937
C 1.1866 0.73180 0.34376
C 0.086969 -0.037023 -0.078233
C -1.1032 0.63456 -0.43284
C -1.2067 2.0257 -0.32578
N 0.13791 -1.4356 -0.11015
C -0.94913 -2.2468 0.32176
C -0.44838 -3.5381 0.20484
C 0.89660 -3.5177 -0.27744
C 1.2450 -2.2004 -0.45101
H 1.9375 2.7169 0.76131
H 2.1040 0.22783 0.62734
H -1.9012 0.066597 -0.90698
H -2.1111 2.5497 -0.61691
Li -2.3144 -1.0441 1.0514
H -1.0022 -4.4333 0.46382
H 1.5369 -4.3658 -0.48524
H 2.1459 -1.7503 -0.84378



E(B3LYP) = -547.399288228

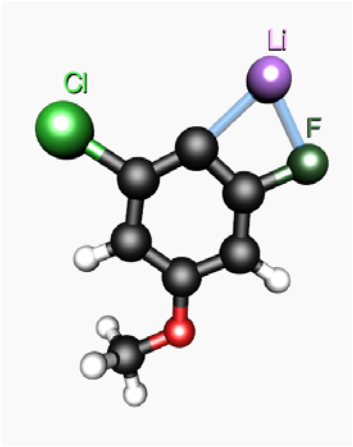
Substrate 7

C -1.12182456 -3.370547 0.20989816
O -1.56080636 -2.02360249 0.09001904
C -0.62321252 -1.03975737 0.0558544
C -1.12743901 0.26630457 -0.05733628
C -0.23612433 1.32913877 -0.09804513
Cl -0.86608702 2.9637376 -0.23561546
C 1.14786763 1.14762431 -0.03195973
C 1.60049173 -0.15867669 0.07420351
F 2.9297301 -0.3756404 0.13618447
C 0.75671267 -1.26463371 0.11965494
H -2.02671849 -3.97845457 0.22909364
H -0.55934915 -3.52935648 1.13809015
H -0.50305436 -3.66991947 -0.64492768
H -2.19755401 0.42061414 -0.11045969
H 1.84208866 1.97695454 -0.06362282
H 1.18982103 -2.25252479 0.19671594

E(B3LYP) = -905.618192951

Intermediate 1

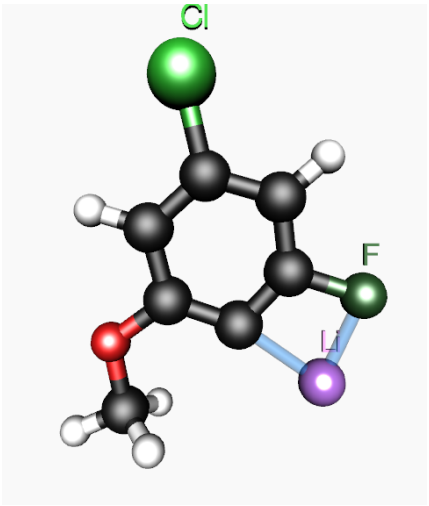
C -1.1604 -3.2978 0.0000
O 0.11762 -2.6806 0.0000
C 0.17558 -1.3161 0.0000
C -0.94700 -0.47517 0.0000
C -0.74790 0.91152 0.0000
Cl -2.2325 1.9088 0.0000
C 0.48956 1.5392 0.0000
C 1.5078 0.61342 0.0000
F 2.8307 1.2157 0.0000
C 1.4675 -0.76485 0.0000
H -0.97426 -4.3728 0.0000
H -1.7391 -3.0313 -0.89349
H -1.7391 -3.0313 0.89349
H -1.9511 -0.87767 0.0000
Li 1.9281 2.8929 0.0000
H 2.3460 -1.3984 0.0000



E(B3LYP) = -912.555561718

Intermediate 2

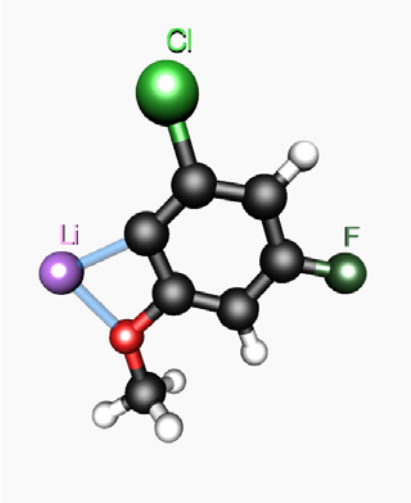
C -1.6865 -3.1290 0.22090
O -1.9067 -1.7338 0.12234
C -0.81109 -0.91288 0.071718
C -1.1334 0.45400 -0.030641
C -0.10417 1.3869 -0.086198
Cl -0.49889 3.0999 -0.21340
C 1.2414 1.0084 -0.045026
C 1.4198 -0.35924 0.054882
F 2.8097 -0.80731 0.10033
C 0.50966 -1.3841 0.11908
H -2.6784 -3.5843 0.25922
H -1.1259 -3.3881 1.1274
H -1.1377 -3.5152 -0.64716
H -2.1712 0.76359 -0.064638
H 2.0536 1.7221 -0.088040
Li 2.1144 -2.5375 0.21410



E(B3LYP) = -912.55509406

Intermediate 3

C -1.2026 -3.2979 0.0054889
O -1.5626 -1.9226 -0.0027477
C -0.52987 -0.93275 -0.0013013
C -1.0564 0.36176 0.00046886
C -0.084675 1.3468 0.00082108
Cl -0.58285 3.0653 0.0034178
C 1.2977 1.1146 -0.00032209
C 1.7117 -0.20849 -0.0021136
F 3.0372 -0.48133 -0.0036461
C 0.81943 -1.2806 -0.0026954
H -2.1331 -3.8684 0.0086242
H -0.62161 -3.5467 0.90075
H -0.62133 -3.5576 -0.88649
Li -2.8495 -0.47196 -0.0022579
H 2.0265 1.9157 0.00033087
H 1.2032 -2.2934 -0.0045010



E(B3LYP) = -912.553150886

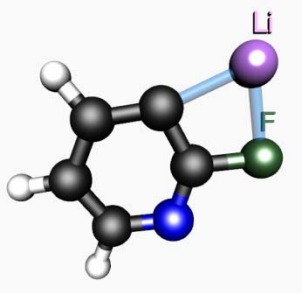
Substrate 8

F 2.23424002 0.00445929 2.83e-05
N 0.32473324 -1.19511088 -1.795e-05
C -1.17021173 1.16699572 -1.699e-05
C 0.22133364 1.21449225 -2.048e-05
C -1.80933128 -0.07623324 4.231e-05
C 0.89127885 -0.00749361 -1.462e-05
C -1.0167855 -1.22232991 -1.512e-05
H -1.74577229 2.08758105 -2.169e-05
H 0.77219913 2.14779336 -3.255e-05
H -2.8909432 -0.15490921 3.787e-05
H -1.46917489 -2.21210482 -2.108e-05

E(B3LYP) = -347.540166136

Intermediate 1

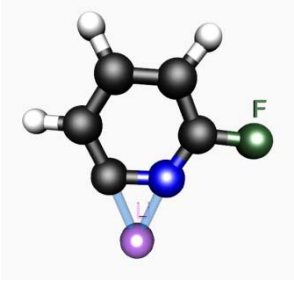
F 2.1643 0.15825 0.000012900
N 0.34497 -1.2596 0.0000034500
C -1.3438 0.97452 -0.0000022000
C 0.042812 1.1988 9.3000e-7
C -1.8722 -0.32767 0.000031900
C 0.71924 -0.0095861 -0.0000061100
C -0.99945 -1.4106 0.0000075900
H -2.0344 1.8164 -2.2000e-7
Li 1.8233 2.0478 -0.000010660
H -2.9448 -0.50035 0.000030100
H -1.3645 -2.4346 0.000013480



E(B3LYP) = -354.472952788

Intermediate 2

F 2.2368 -0.12812 0.000010300
N 0.17293 -1.0781 0.0000079300
C -1.0180 1.4135 0.0000047800
C 0.37259 1.3105 0.000010530
C -1.7987 0.25740 0.000013330
C 0.89744 0.027920 0.000015950
C -1.2189 -1.0213 0.000010280
H -1.4830 2.3958 -3.0000e-7
H 1.0307 2.1725 0.0000087300
H -2.8812 0.34896 0.0000057900
Li -0.56194 -2.8147 0.0000032200



E(B3LYP) = -354.465652701

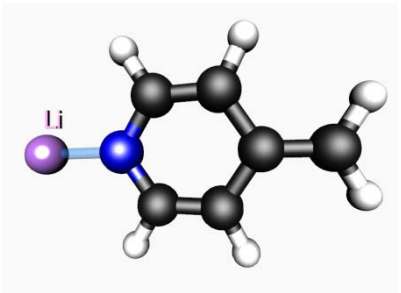
Substrate 9

N -1.92699825 -2.878e-05 0.01127809
C 0.90552635 -0.00031762 -0.01307588
C 0.17162055 1.19106554 -0.00900665
C 0.17134309 -1.19161607 -0.00894453
C 2.41337138 -0.00057111 0.00521786
C -1.22170654 1.13825682 0.00430569
C -1.22189457 -1.13853555 0.00435326
H 0.67785989 2.15250242 -0.01844339
H 0.67746589 -2.153117 -0.01856125
H 2.81940208 -0.88667925 -0.49078242
H 2.81990702 0.88709256 -0.48751313
H 2.7886557 -0.00296915 1.03578477
H -1.80107987 2.06016214 0.00576884
H -1.80155367 -2.06026047 0.00582552

E(B3LYP) = -287.62415428

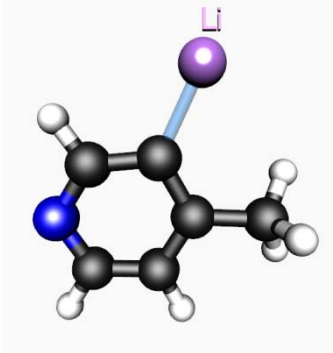
Intermediate 1

N -1.6691 -0.10804 -0.22440
C 1.2222 0.072511 0.19909
C 0.37232 1.2173 -0.11288
C 0.46632 -1.1742 0.26946
C 2.5621 0.15776 0.40292
C -0.96542 1.0836 -0.29989
C -0.87547 -1.2067 0.066308
H 0.82365 2.2023 -0.19705
H 0.99242 -2.0995 0.48959
Li -3.4530 -0.24778 -0.50133
H 3.0843 1.1070 0.34013
H 3.1549 -0.72085 0.63715
H -1.5667 1.9654 -0.52949
H -1.4045 -2.1596 0.13193



E(B3LYP) = -294.552805024

Intermediate 2



N -1.9720 -0.14435 0.015577
C 0.84252 -0.11651 -0.015505
C 0.14971 1.1184 -0.0083709
C 0.12567 -1.3198 -0.010644
C 2.3566 -0.16747 0.0027046
C -1.2547 0.99392 0.010218
C -1.2675 -1.2809 0.0052478
Li 0.96696 2.9228 -0.016610
H 0.63788 -2.2803 -0.021349
H 2.7473 -1.0643 -0.48993
H 2.7891 0.70594 -0.50126
H 2.7402 -0.17344 1.0319
H -1.8772 1.8942 0.016400
H -1.8426 -2.2071 0.0056969

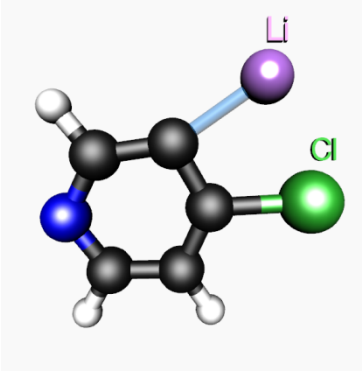
E(B3LYP) = -294.538317318

Substrate 10

Cl 2.25657485 0.00018947 -1.548e-05
N -2.28871879 -0.0001437 -3.6e-05
C 0.50435362 5.685e-05 9.955e-05
C -0.19420823 1.20441489 0.00011251
C -0.19402938 -1.2044014 3.647e-05
C -1.58873318 1.14009965 -6.3e-07
C -1.58856575 -1.14028383 3.463e-05
H 0.32451234 2.15592788 0.00013979
H 0.32481977 -2.15584389 7.596e-05
H -2.16770047 2.06146946 -5.003e-05
H -2.16739271 -2.06174227 2.566e-05

E(B3LYP) = -707.89615721

Intermediate 1



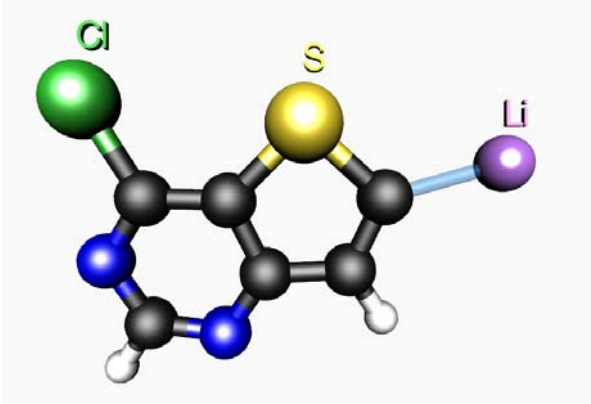
Cl 2.2205 -0.076100 0.000017730
N -2.3626 0.23063 -0.000086790
C 0.34197 0.035920 -0.000044250
C -0.20324 1.3105 -0.000044290
C -0.33522 -1.1626 -0.000044960
C -1.6009 1.3316 -0.000052910
C -1.7333 -0.95474 -0.000087310
H 0.38395 2.2215 -0.0000046500
Li 1.2828 -2.2991 0.0000076600
H -2.1236 2.2869 -0.000048980
H -2.4005 -1.8171 -0.000097050

E(B3LYP) = -714.82299928

Substrate 11
Cl -2.00874016 1.72966828 -6.93e-06
S 1.41136991 1.37957388 -1.767e-05
N 0.03350076 -2.29136889 4.703e-05
N -1.93063214 -0.910378 -4.585e-05
C 0.78293206 -1.17201978 1.007e-05
C 0.20205088 0.12235329 1.21e-05
C 2.21913373 -1.11171957 -4.23e-06
C -1.19188869 0.17758593 -2.375e-05
C 2.67582853 0.16805843 -2.06e-05
C -1.27743834 -2.09373557 4.26e-06
H 2.8492468 -1.99182991 -1.288e-05
H 3.70704323 0.49534766 -3.677e-05
H -1.90956586 -2.97721133 1.383e-05

E(B3LYP) = -1198.34546845

Intermediate 1
Cl -2.1603 1.6857 -0.000016180
S 1.3041 1.3348 -0.0000090500
N -0.078310 -2.3173 0.000017680
N -2.0566 -0.95453 0.0000081200
C 0.66732 -1.1894 0.000015240
C 0.072677 0.10212 0.0000074400
C 2.1011 -1.1127 0.0000084600
C -1.3195 0.13722 0.0000013700
C 2.6317 0.15863 -0.0000070900
C -1.3906 -2.1306 0.000015570
H 2.7004 -2.0186 0.000011270
Li 4.5212 0.70960 -0.000020410
H -2.0157 -3.0203 0.000020130



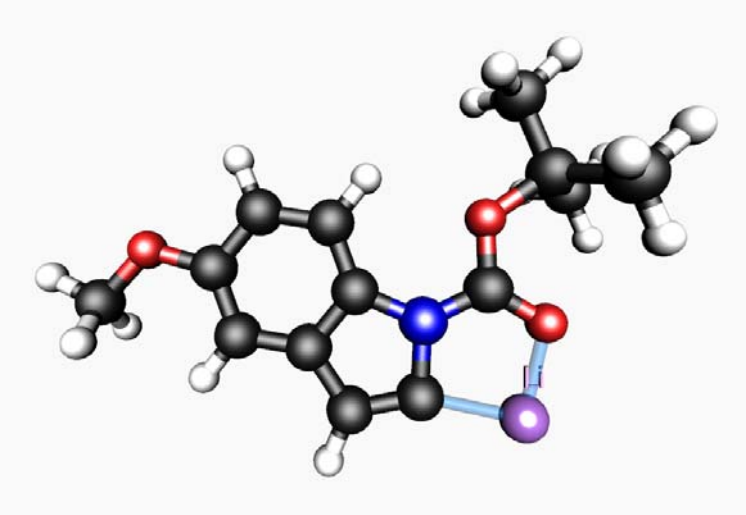
E(B3LYP) = -1205.28521776

Substrate 12

O 2.52621838 -0.27509927 -0.6488336
O -5.01698239 0.53571239 0.87759784
O 1.36010399 1.6711135 -0.34353512
N 0.32551176 -0.37766082 -0.22214112
C 3.83687745 0.37027442 -0.88245389
C -0.98956838 0.04808806 0.05401575
C 4.25873736 1.15306804 0.36416987
C 4.75561903 -0.83123794 -1.11085848
C 3.76588838 1.25094901 -2.13292319
C -1.79014473 -1.11049551 0.1634433
C 1.42680427 0.45880699 -0.40459127
C 0.32691294 -1.77941379 -0.28100633
C -0.92841137 -2.24776127 -0.05328426
C -1.52768034 1.32845119 0.21607837
C -3.1627247 -0.99743775 0.44195587
C -3.69977621 0.27802472 0.60367274
C -2.88424435 1.42541758 0.48982254
C -5.89745912 -0.56632559 1.0047654
H 4.24631922 0.50306266 1.24437932
H 5.27938688 1.52544194 0.23124718
H 3.59727281 2.00149106 0.53973752
H 4.42066165 -1.41621287 -1.9720984
H 4.76670943 -1.48260945 -0.23239848
H 5.77690332 -0.48917413 -1.30111457
H 3.09767534 2.09866921 -1.98149341
H 4.76590495 1.62886463 -2.36791151
H 3.41396645 0.66818733 -2.98969541
H 1.24788043 -2.30026643 -0.48236277
H -1.21909872 -3.28895521 -0.0432894
H -0.90491826 2.2079575 0.12903518
H -3.7735645 -1.88816673 0.52498912
H -3.35307476 2.39421974 0.6245093
H -5.95077577 -1.15324355 0.07814568
H -6.88122997 -0.14585988 1.21920692
H -5.60208305 -1.22989341 1.82839283

E(B3LYP) = -824.213882321

Intermediate 1

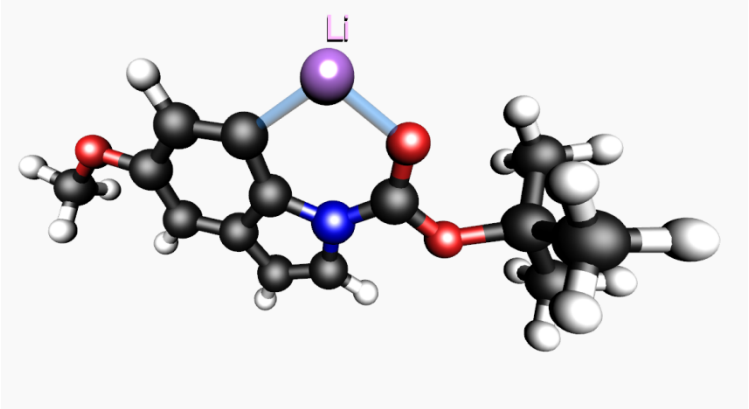


O 1.8027 0.90708 -0.14620
O -4.7031 0.23795 -0.38722
O 2.9487 -0.99029 0.37490
N 0.66180 -1.0075 0.23507
C 3.0069 1.7572 -0.28297
C -0.63983 -0.47837 0.027308
C 3.8900 1.2344 -1.4192
C 2.4049 3.1161 -0.64654
C 3.7468 1.8327 1.0554
C -1.5307 -1.5511 0.25068
C 1.8712 -0.38713 0.16387
C 0.60496 -2.4221 0.58825
C -0.73248 -2.7107 0.58915
C -1.1051 0.78925 -0.32461
C -2.9136 -1.3549 0.12063
C -3.3789 -0.085901 -0.22982
C -2.4790 0.97364 -0.45011
C -5.6645 -0.77883 -0.17596
H 3.3041 1.1265 -2.3370
H 4.6940 1.9517 -1.6118
H 4.3339 0.27154 -1.1668
H 1.7384 3.4690 0.14538
H 1.8339 3.0505 -1.5769
H 3.2028 3.8519 -0.78116
H 4.1880 0.87185 1.3199
H 4.5452 2.5783 0.98630
H 3.0621 2.1417 1.8510
Li 2.5563 -2.7598 0.79848
H -1.1451 -3.6869 0.81709
H -0.42726 1.6141 -0.49402
H -3.5930 -2.1812 0.29351
H -2.8863 1.9422 -0.71954
H -5.5400 -1.6112 -0.88157
H -6.6391 -0.31485 -0.33920
H -5.6222 -1.1748 0.84746

E(B3LYP) = -831.162748724

Intermediate 2

O 2.5212 -0.65077 0.46516
O -4.9509 0.94195 -0.83450
O 1.4968 1.3187 0.94426
N 0.33998 -0.44531 -0.0028191
C 3.8584 -0.23167 0.94086
C -0.99117 0.11112 -0.13531
C 3.8071 0.084092 2.4380
C 4.6965 -1.4857 0.68044
C 4.3685 0.94376 0.10304
C -1.7731 -0.91396 -0.71160
C 1.4551 0.15723 0.49960
C 0.31713 -1.7699 -0.49899
C -0.93169 -2.0697 -0.92589
C -1.4500 1.3919 0.21702
C -3.1309 -0.68420 -0.97224
C -3.6409 0.57149 -0.63916
C -2.8145 1.5627 -0.066988
C -5.8296 -0.0041124 -1.4099
H 3.3691 -0.75385 2.9885
H 4.8246 0.23898 2.8104
H 3.2225 0.98218 2.6374
H 4.6875 -1.7425 -0.38242
H 4.3059 -2.3362 1.2461
H 5.7318 -1.3118 0.98648
H 3.7852 1.8465 0.28414
H 5.4131 1.1451 0.36022
H 4.3232 0.69949 -0.96253
H 1.2177 -2.3596 -0.48860
H -1.2335 -3.0176 -1.3520
Li 0.050856 2.4278 0.98675
H -3.7429 -1.4608 -1.4156
H -3.3093 2.5080 0.15282
H -5.5110 -0.29886 -2.4195
H -6.8053 0.48213 -1.4727
H -5.9201 -0.90875 -0.79267



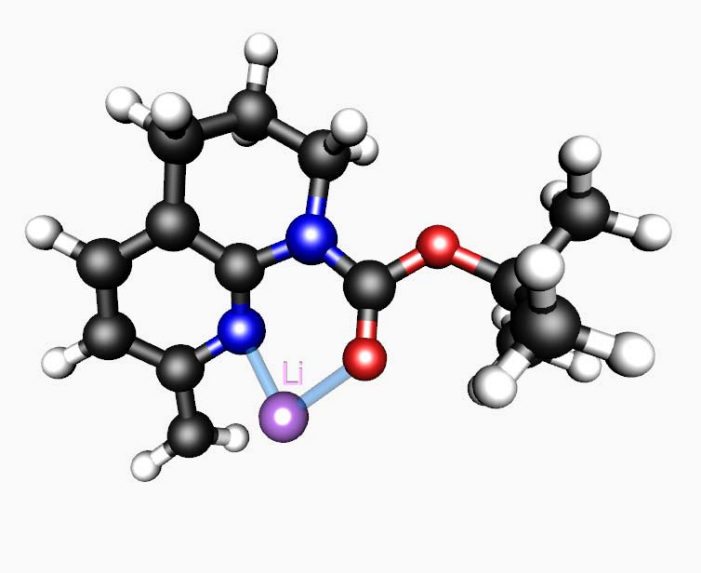
E(B3LYP) = -831.155351871

Substrate 13

O 1.13665897 -0.49380201 -0.89296295
O 2.61370291 0.93814517 0.08997885
N 0.38434242 1.03467536 0.60498477
N -0.9996541 -0.87003004 0.73853132
C -0.4798016 3.32027687 0.51022006
C 0.53686745 2.3839226 1.16468491
C -1.90311162 2.83272637 0.80874262
C -2.0267109 1.32072682 0.78248589
C -0.90898597 0.46085193 0.68651935
C 2.15567803 -1.3358378 -1.5406566
C 1.48526405 0.49335128 -0.05832107
C -3.27175088 0.70332544 0.89552202
C 3.03833573 -2.00139538 -0.48036479
C 1.30150251 -2.37793571 -2.26657798
C 2.96724552 -0.50280055 -2.53790875
C -2.20669944 -1.44202958 0.83341216
C -3.37936323 -0.68370614 0.91123578
C -2.23020993 -2.95014365 0.8595807
H -0.29552683 3.33238341 -0.57011724
H -0.34304696 4.34412124 0.87442135
H 1.56434827 2.69378615 0.98369746
H 0.3803717 2.34581403 2.25091512
H -2.61812299 3.27713348 0.10613688
H -2.20350753 3.18494804 1.80554778
H -4.16467601 1.3205447 0.96765208
H 3.64212902 -1.26402284 0.04933188
H 2.41703268 -2.53839221 0.24260136
H 3.70685377 -2.7224816 -0.96160715
H 0.684377 -2.9284818 -1.55170288
H 0.64037655 -1.89579867 -2.9923705
H 1.94355205 -3.08651648 -2.79831606
H 2.29935691 -0.00943086 -3.25104268
H 3.64080528 -1.15742674 -3.10082093
H 3.55701709 0.25539343 -2.02293146
H -4.34662964 -1.16848618 0.99367267
H -3.22706994 -3.33576706 1.08846595
H -1.91997826 -3.35443201 -0.11055446
H -1.52463788 -3.32845668 1.60511088

E(B3LYP) = -805.580166463

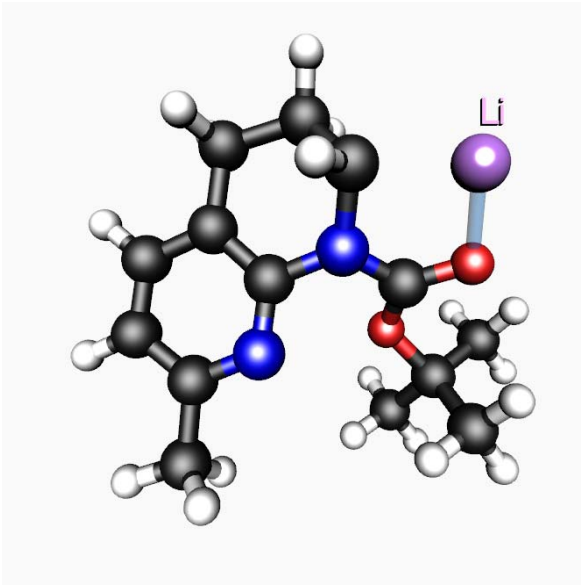
Intermediate 1



O 2.1038 0.56637 0.10703
O 0.84860 -1.2237 0.72990
N -0.071009 0.61087 -0.38139
N -1.4569 -1.2432 -0.68332
C -1.1509 2.7511 -1.0975
C 0.14621 2.0470 -0.69446
C -2.3019 2.3775 -0.15135
C -2.4944 0.88572 -0.22337
C -1.3957 0.062310 -0.44941
C 3.3666 0.052742 0.67846
C 0.94599 -0.11096 0.18471
C -3.7371 0.20880 -0.14059
C 3.7688 -1.2468 -0.024287
C 4.3511 1.1758 0.34216
C 3.2312 -0.11263 2.1945
C -2.6352 -1.9369 -0.46936
C -3.8214 -1.1613 -0.21532
C -2.5200 -3.3346 -0.41873
H -1.4280 2.4708 -2.1199
H -0.95496 3.8293 -1.0958
H 0.89423 2.1282 -1.4885
H 0.56741 2.5282 0.19433
H -3.2220 2.8961 -0.44500
H -2.0642 2.7237 0.86737
H -4.6412 0.79625 0.010596
H 3.0718 -2.0530 0.20307
H 3.8003 -1.0995 -1.1080
H 4.7688 -1.5438 0.30707
H 4.4093 1.3282 -0.73911
H 4.0410 2.1153 0.80818
H 5.3486 0.91973 0.71022
H 2.8910 0.82226 2.6504
H 4.2084 -0.36051 2.6208
H 2.5281 -0.90593 2.4472
H -4.7751 -1.6674 -0.10618
H -1.7607 -3.8007 -1.0473
Li -0.57526 -2.4830 0.43267
H -3.3995 -3.9399 -0.22959

E(B3LYP) = -812.534129239

Intermediate 2



O 1.2352 -0.67529 -0.55517
O 2.5616 0.89822 0.40250
N 0.27909 1.1453 0.39963
N -1.1982 -0.68337 0.68933
C -0.38782 3.3230 -0.41383
C 0.37578 2.6182 0.71313
C -1.8639 2.8771 -0.50117
C -2.0718 1.4168 -0.14709
C -1.0228 0.57941 0.28903
C 2.2614 -1.7294 -0.62392
C 1.4171 0.46350 0.11330
C -3.3396 0.83765 -0.18822
C 2.7046 -2.1164 0.78981
C 1.4962 -2.8790 -1.2843
C 3.4286 -1.2745 -1.5050
C -2.4251 -1.2203 0.63626
C -3.5300 -0.48843 0.19157
C -2.5489 -2.6554 1.0864
H 0.10985 3.1239 -1.3738
H -0.35006 4.4096 -0.26873
Li 2.3927 2.6313 0.94414
H -0.19767 2.7474 1.6457
H -2.2875 3.0772 -1.4954
H -2.4618 3.4736 0.20290
H -4.1853 1.4367 -0.51952
H 3.2535 -1.3047 1.2694
H 1.8311 -2.3639 1.3997
H 3.3549 -2.9957 0.74242
H 0.63494 -3.1608 -0.67351
H 1.1347 -2.5816 -2.2728
H 2.1497 -3.7489 -1.4001
H 3.0608 -0.95487 -2.4850
H 4.1201 -2.1098 -1.6578
H 3.9681 -0.44723 -1.0444
H -4.5151 -0.94297 0.15854
H -2.0556 -3.3273 0.37427
H -2.0572 -2.7952 2.0536
H -3.5944 -2.9626 1.1748

E(B3LYP) = -812.511752017

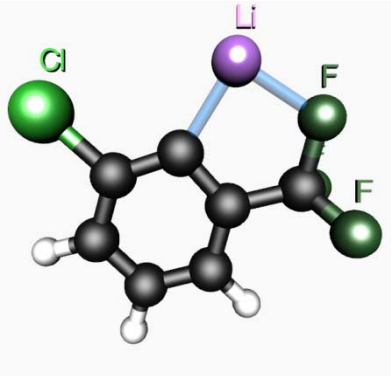
Substrate 14

Cl -2.97690685 1.51473687 0.00109884
F 2.24302877 1.37218325 -0.00282518
F 2.68454503 -0.46433221 1.08366761
F 2.68230228 -0.46605581 -1.08679853
C 0.58786031 -0.33235547 0.00075166
C -0.39353438 0.65810387 0.00058443
C 0.23713336 -1.68608761 0.00144172
C 2.05022559 0.03724099 -0.00134153
C -1.7344025 0.27557651 0.00102426
C -1.1078461 -2.04589671 0.00193391
C -2.10437146 -1.06819819 0.00171048
H -0.11966707 1.70522456 -8.77e-05
H 1.01059007 -2.44641918 0.00140403
H -1.38873611 -3.09426346 0.00247448
H -3.15337094 -1.34164076 0.00201155

E(B3LYP) = -1028.89519858

Intermediate 1

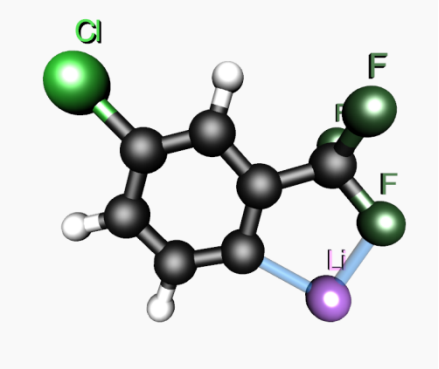
Cl -3.0202 1.4307 -0.087401
F 2.2311 1.3415 0.15303
F 2.7462 -0.62804 0.95988
F 2.6083 -0.34580 -1.1783
C 0.55081 -0.39661 0.040919
C -0.38906 0.65063 -0.028884
C 0.22134 -1.7592 0.11649
C 2.0126 -0.057570 -0.0074037
C -1.7095 0.20752 -0.017377
C -1.1225 -2.1168 0.11880
C -2.1077 -1.1259 0.050446
Li 0.63791 2.3441 0.0078641
H 0.99311 -2.5218 0.17521
H -1.4116 -3.1617 0.17704
H -3.1594 -1.3931 0.054282



E(B3LYP) = -1035.83478345

Intermediate 2

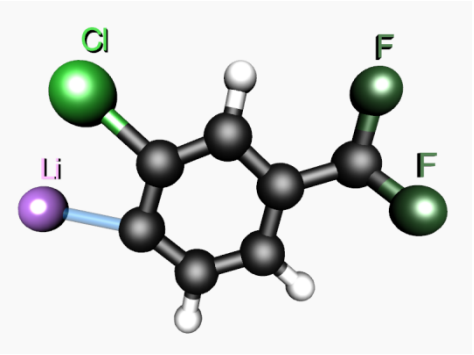
Cl -2.9761 1.6664 -0.23796
F 2.2770 1.2013 0.63005
F 2.8190 -0.91617 0.46287
F 2.4189 0.27459 -1.3183
C 0.52051 -0.30649 0.017679
C -0.41506 0.73538 -0.098788
C 0.19620 -1.6751 0.14160
C 1.9632 0.099508 -0.064059
C -1.7600 0.39598 -0.098977
C -1.1908 -1.9322 0.13388
C -2.1617 -0.93654 0.014587
H -0.11112 1.7736 -0.18333
Li 1.9437 -2.5632 0.46697
H -1.5455 -2.9580 0.22793
H -3.2199 -1.1796 0.013709



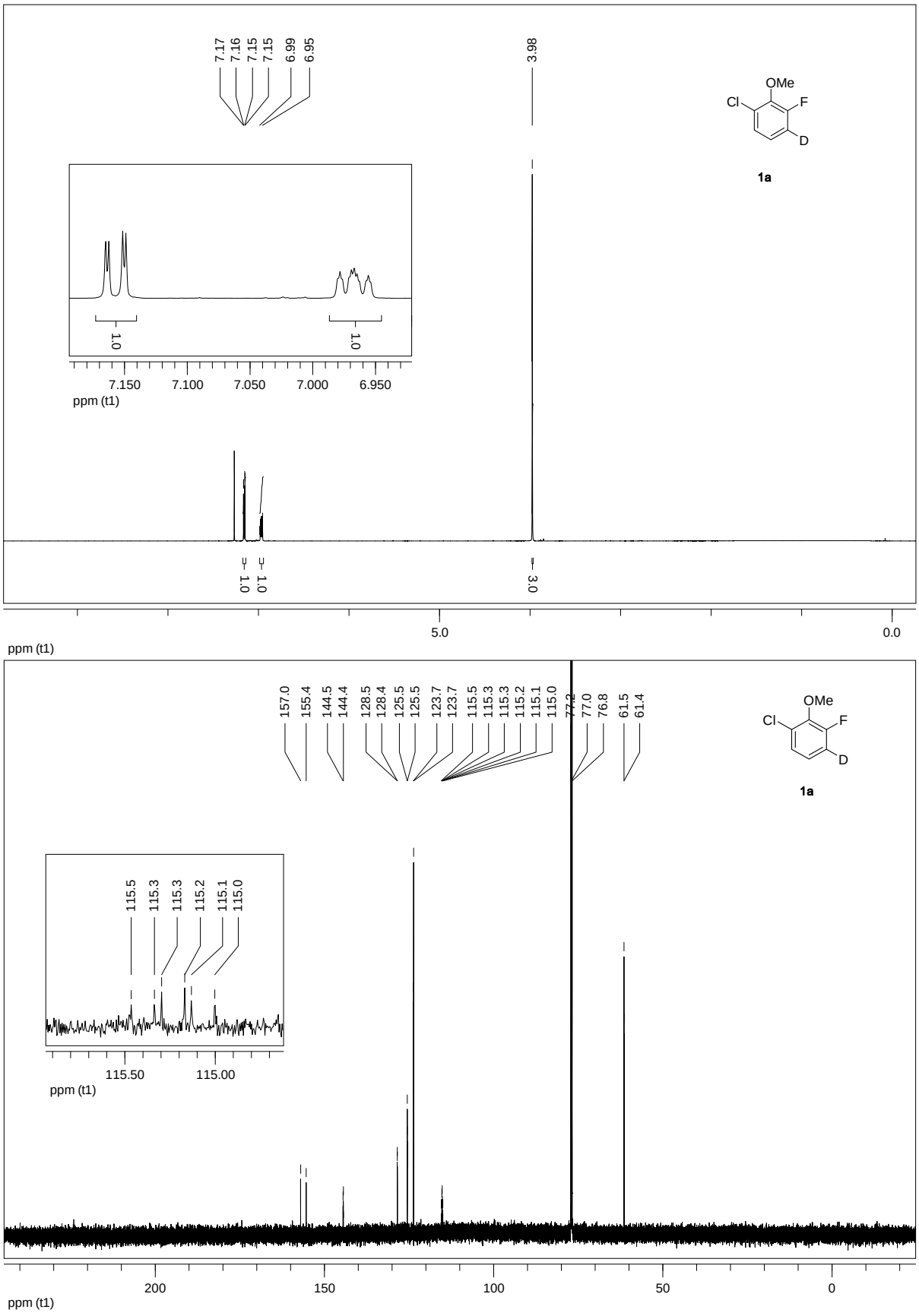
E(B3LYP) = -1035.8268941

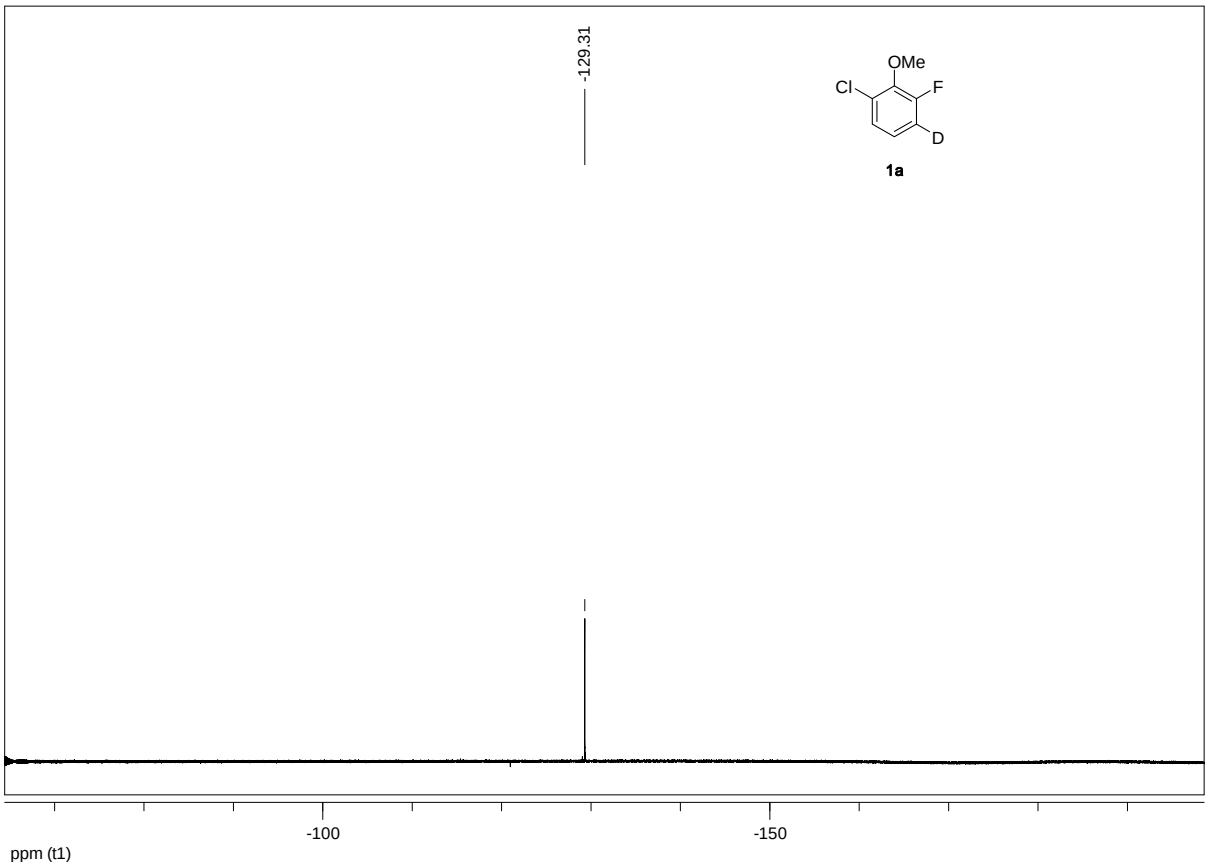
Intermediate 3

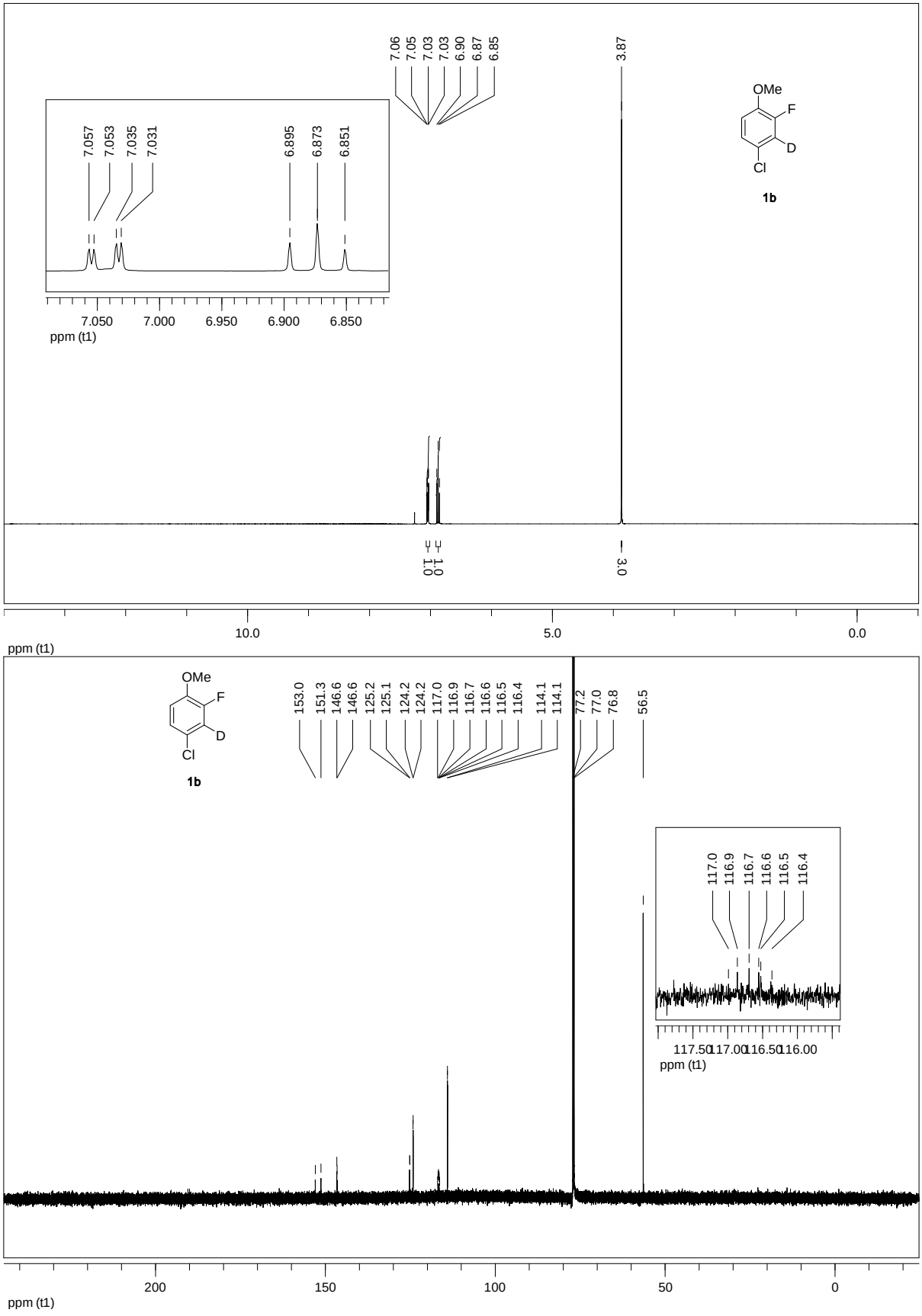
Cl -2.9641 1.4250 -0.090216
F 2.3020 1.4718 0.16214
F 2.8905 -0.46835 0.96274
F 2.7441 -0.18100 -1.1821
C 0.71966 -0.29291 0.040448
C -0.30315 0.65526 -0.023034
C 0.41000 -1.6579 0.11048
C 2.1585 0.13742 -0.0020072
C -1.5950 0.14579 -0.010548
C -0.92055 -2.0742 0.11677
C -2.0052 -1.1706 0.055396
H -0.085537 1.7148 -0.074351
H 1.2157 -2.3842 0.16560
H -1.1191 -3.1431 0.17435
Li -3.9444 -0.75864 0.016009

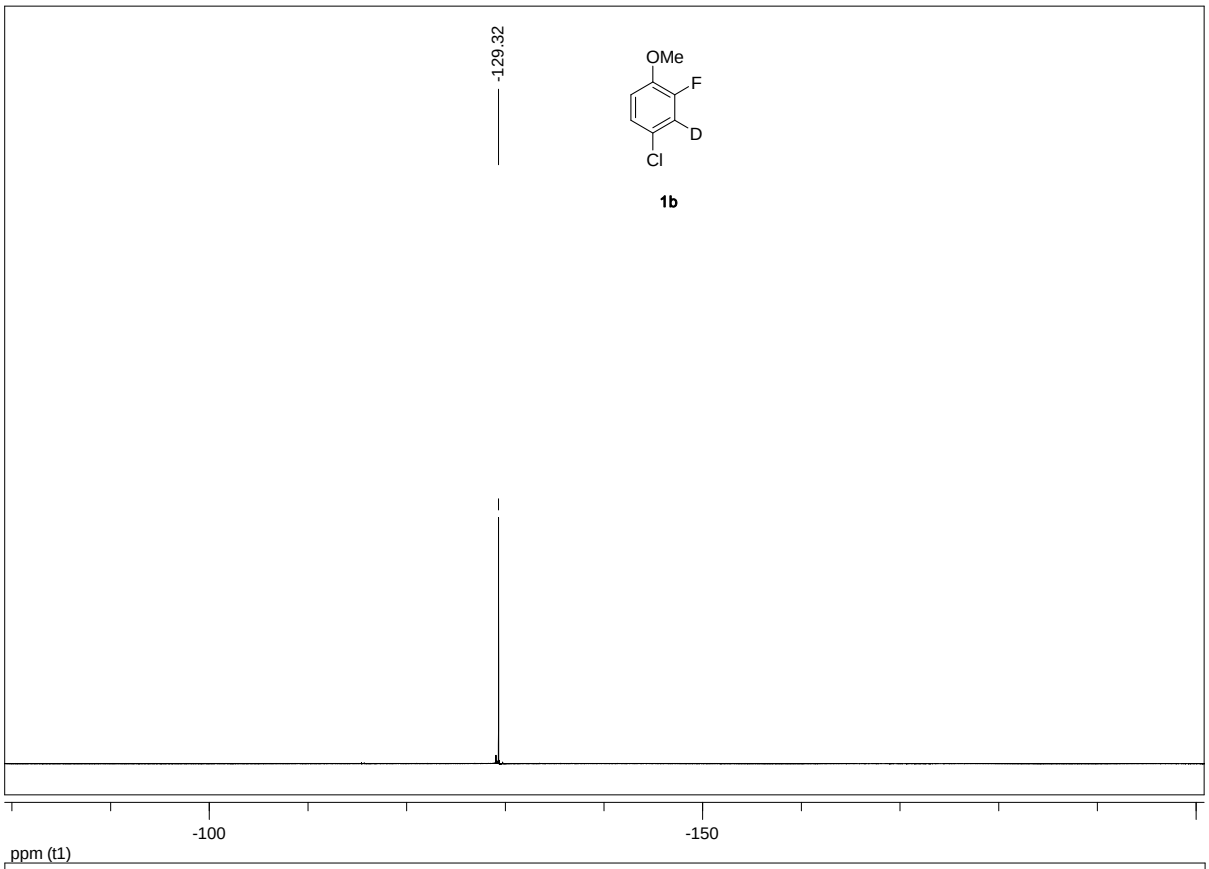


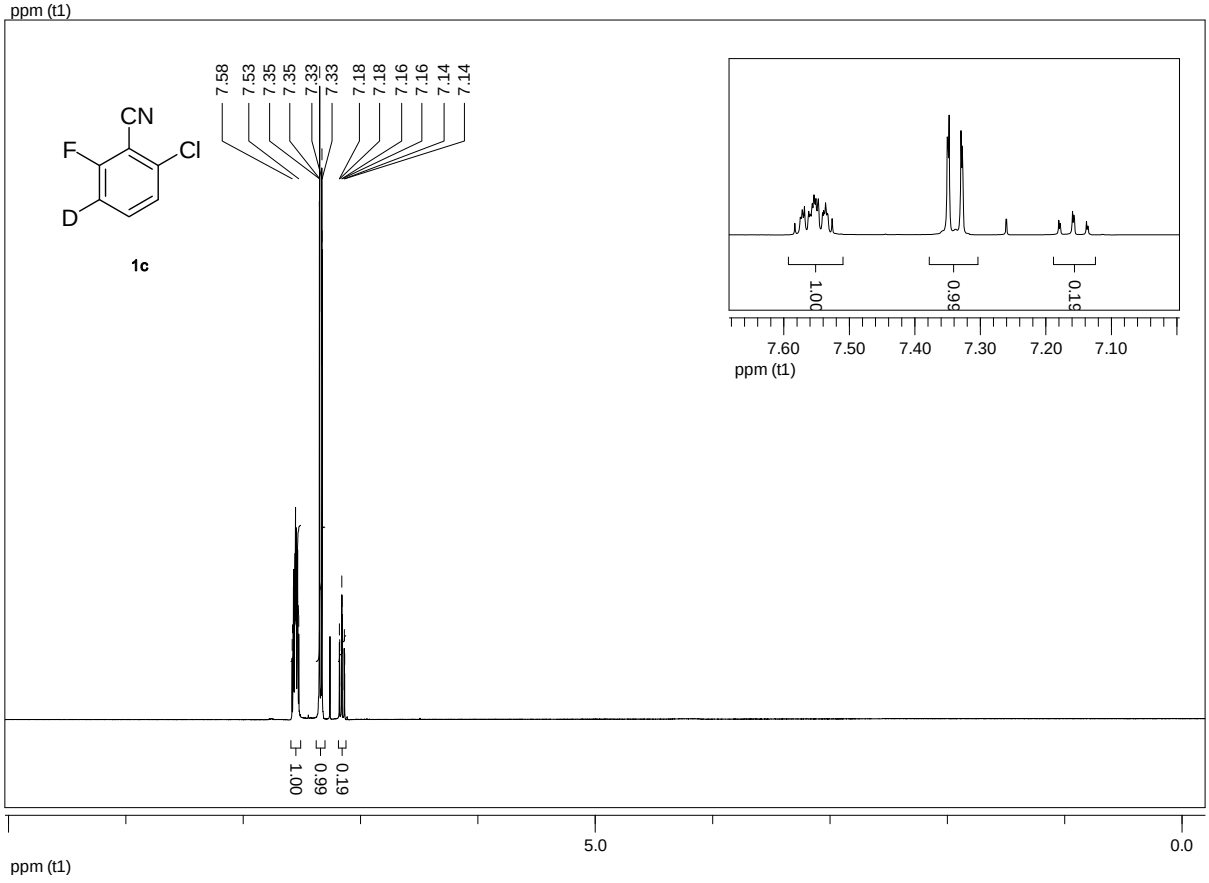
E(B3LYP) = -1035.8209973

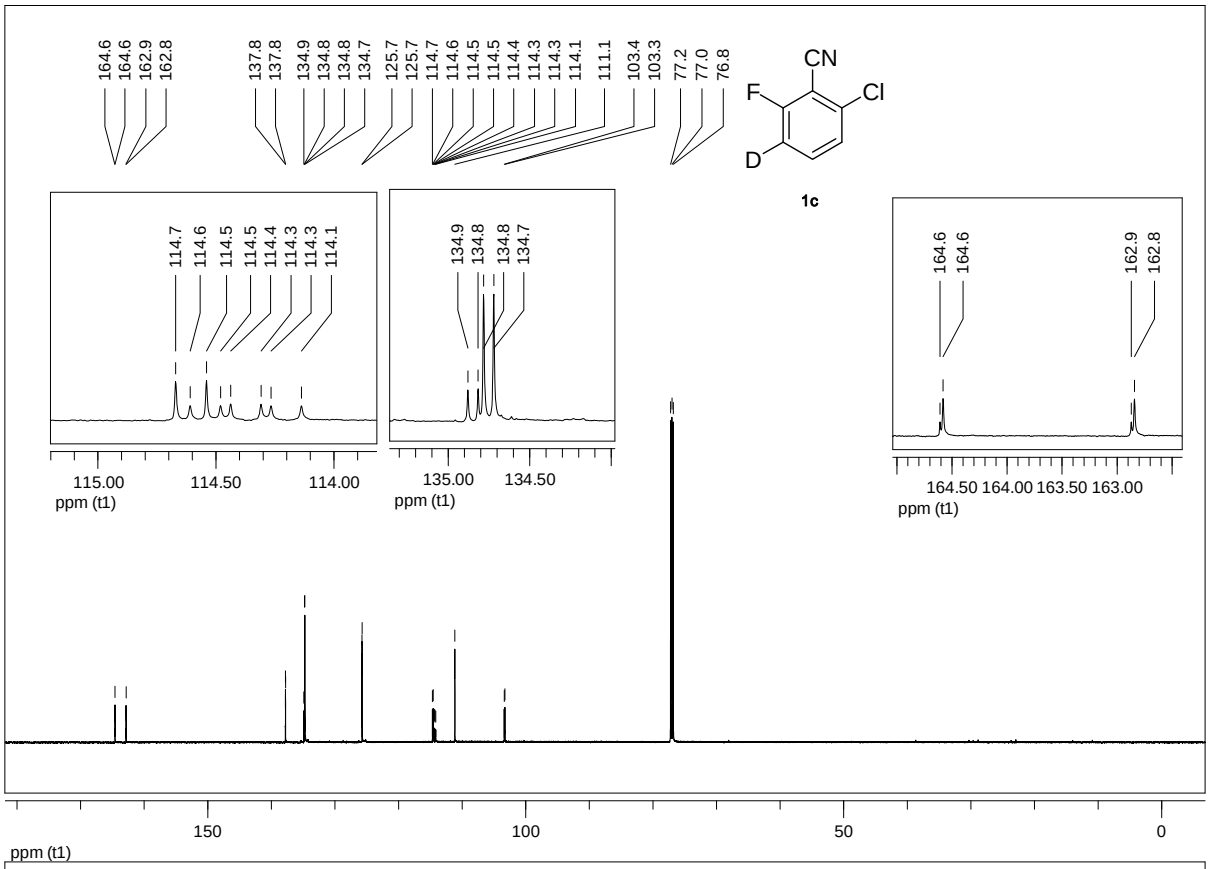

7.17
7.16
7.15
7.15
6.99
6.95
3.98
OMe
Cl
F
D
1a
1.0
1.0
7.150
7.100
7.050
7.000
6.950
ppm (t1)
1.0
1.0
3.0
5.0
0.0
ppm (t1)
157.0
155.4
144.5
144.4
128.5
128.4
125.5
125.5
123.7
123.7
115.5
115.3
115.3
115.2
115.1
115.0
77.2
77.0
76.8
61.5
61.4
OMe
Cl
F
D
1a
115.5
115.3
115.3
115.2
115.1
115.0
115.50
115.00
ppm (t1)
200
150
100
50
0
ppm (t1)

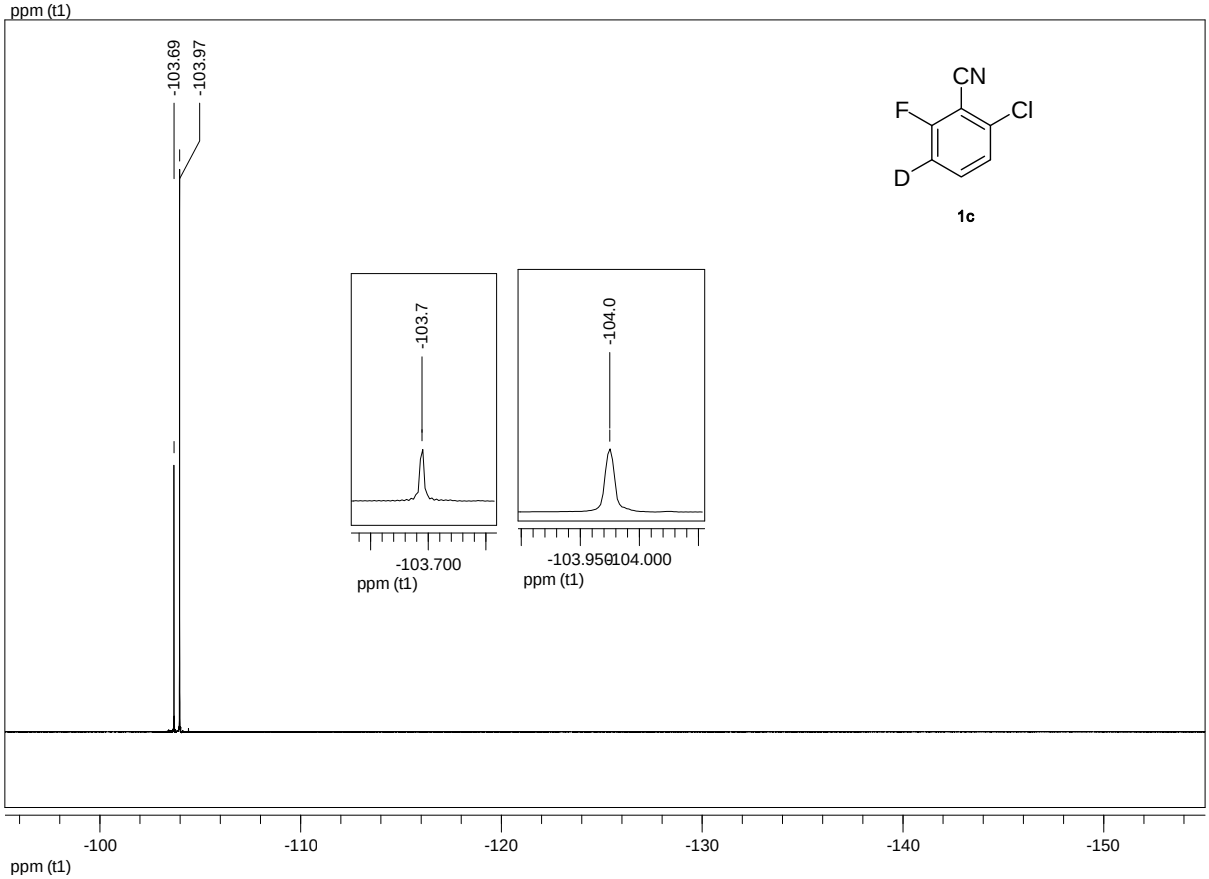

-129.31
OMe
Cl
F
D
1a
-100
-150
ppm (t1)

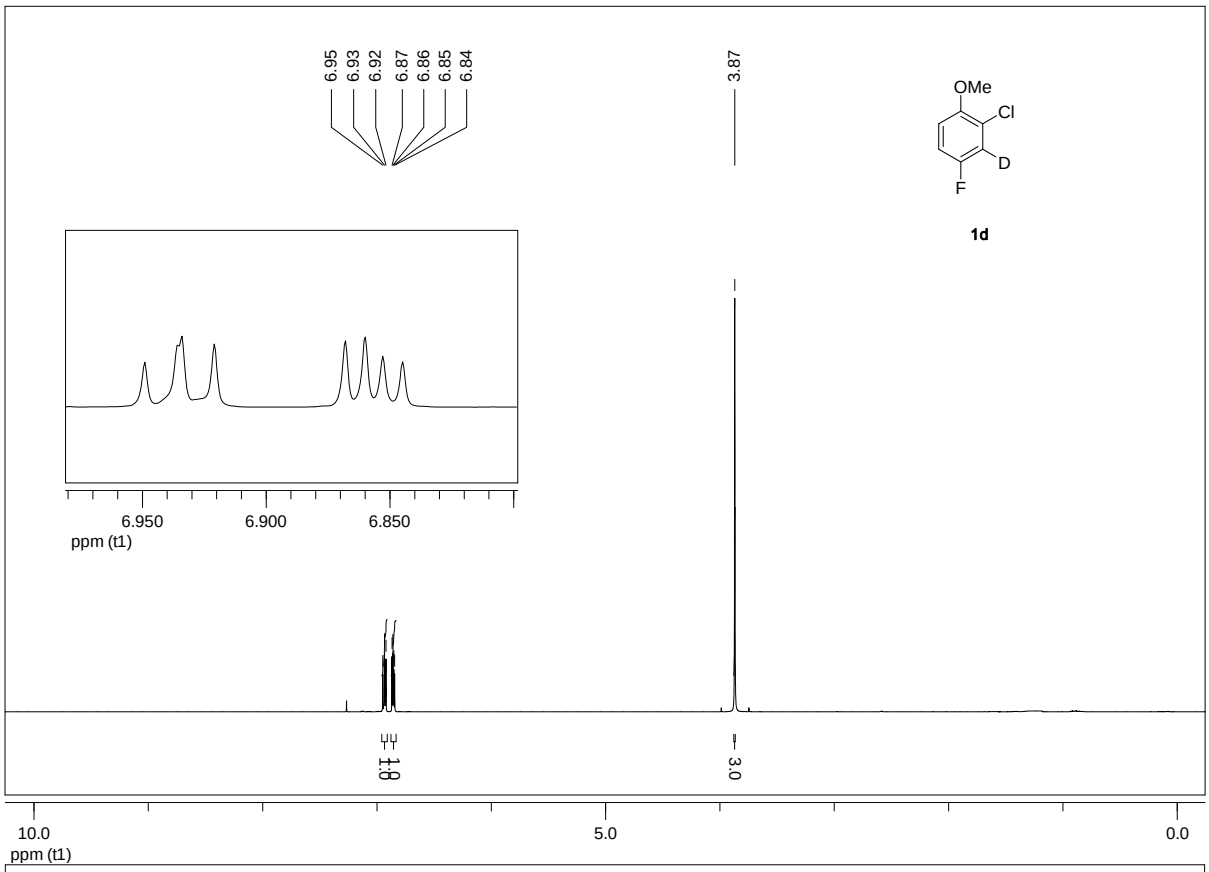

7.06
7.05
7.03
7.03
6.90
6.87
6.85
3.87
7.057
7.053
7.035
7.031
6.895
6.873
6.851
7.050
7.000
6.950
6.900
6.850
ppm (t1)
OMe
F
D
Cl
1b
1.0
1.0
3.0
10.0
5.0
0.0
ppm (t1)
153.0
151.3
146.6
146.6
125.2
125.1
124.2
124.2
117.0
116.9
116.7
116.6
116.5
116.4
114.1
114.1
77.2
77.0
76.8
56.5
117.0
116.9
116.7
116.6
116.5
116.4
117.50
117.00
116.50
116.00
ppm (t1)
200
150
100
50
0
ppm (t1)

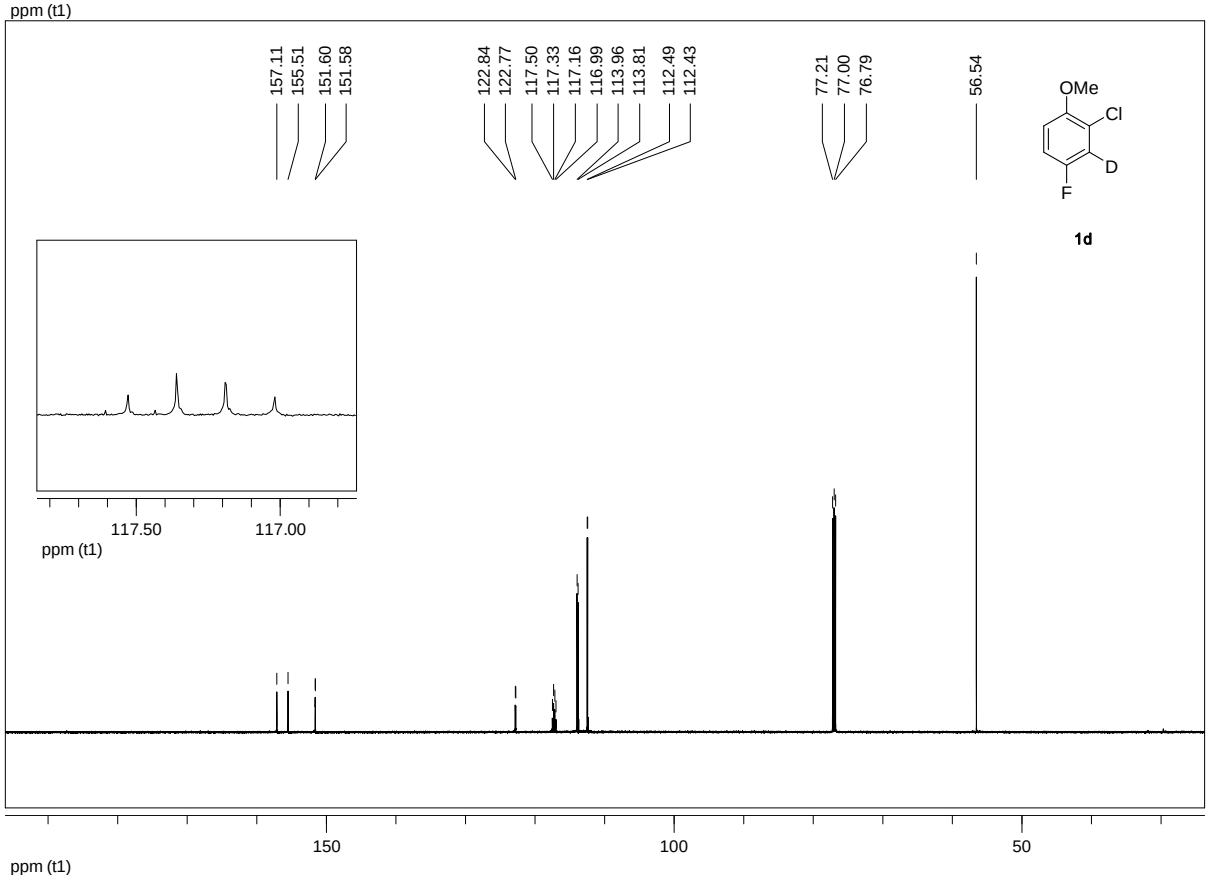

-129.32
OMe
F
D
Cl
1b
-100
-150
ppm (t1)

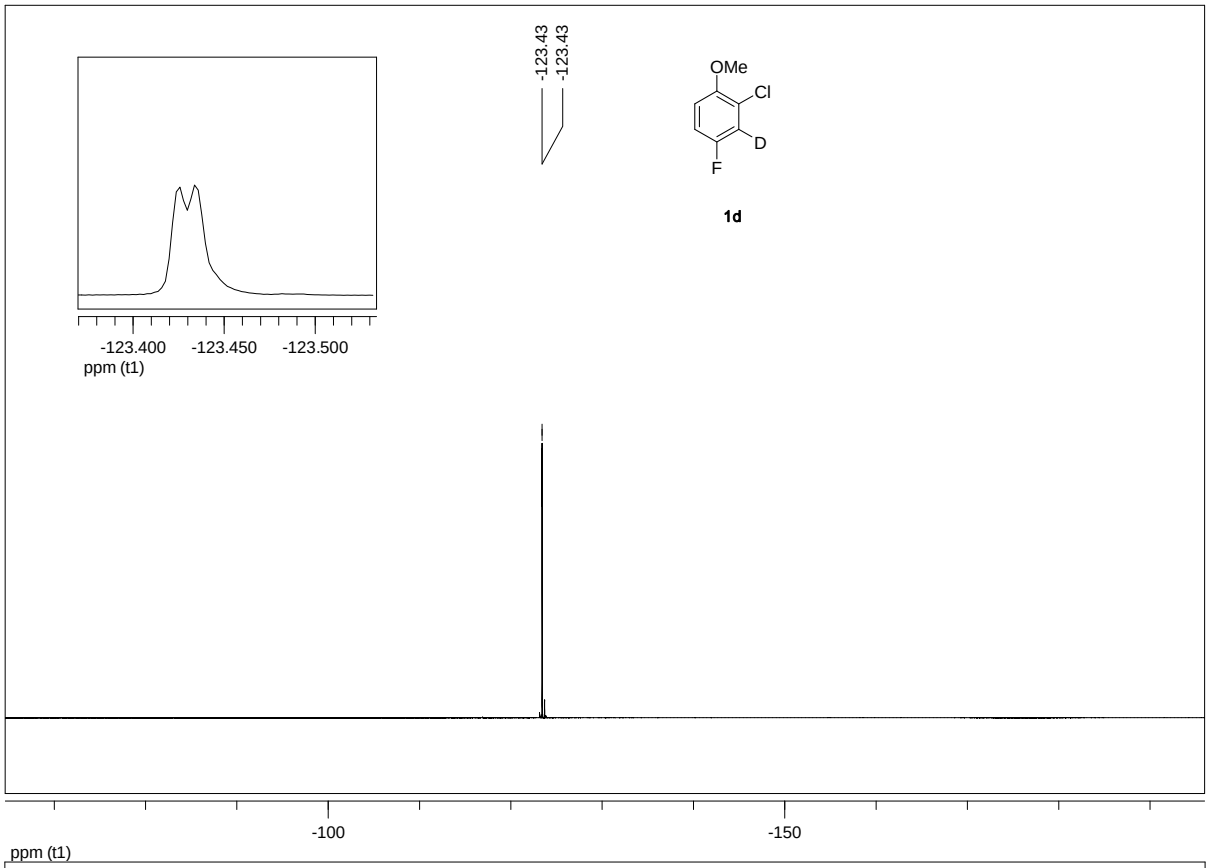

7.58
7.53
7.35
7.35
7.33
7.33
7.18
7.18
7.16
7.16
7.14
7.14
CN
F
Cl
D
1c
1.00
0.99
0.19
7.60
7.50
7.40
7.30
7.20
7.10
ppm (t1)
1.00
0.99
0.19
5.0
0.0
ppm (t1)

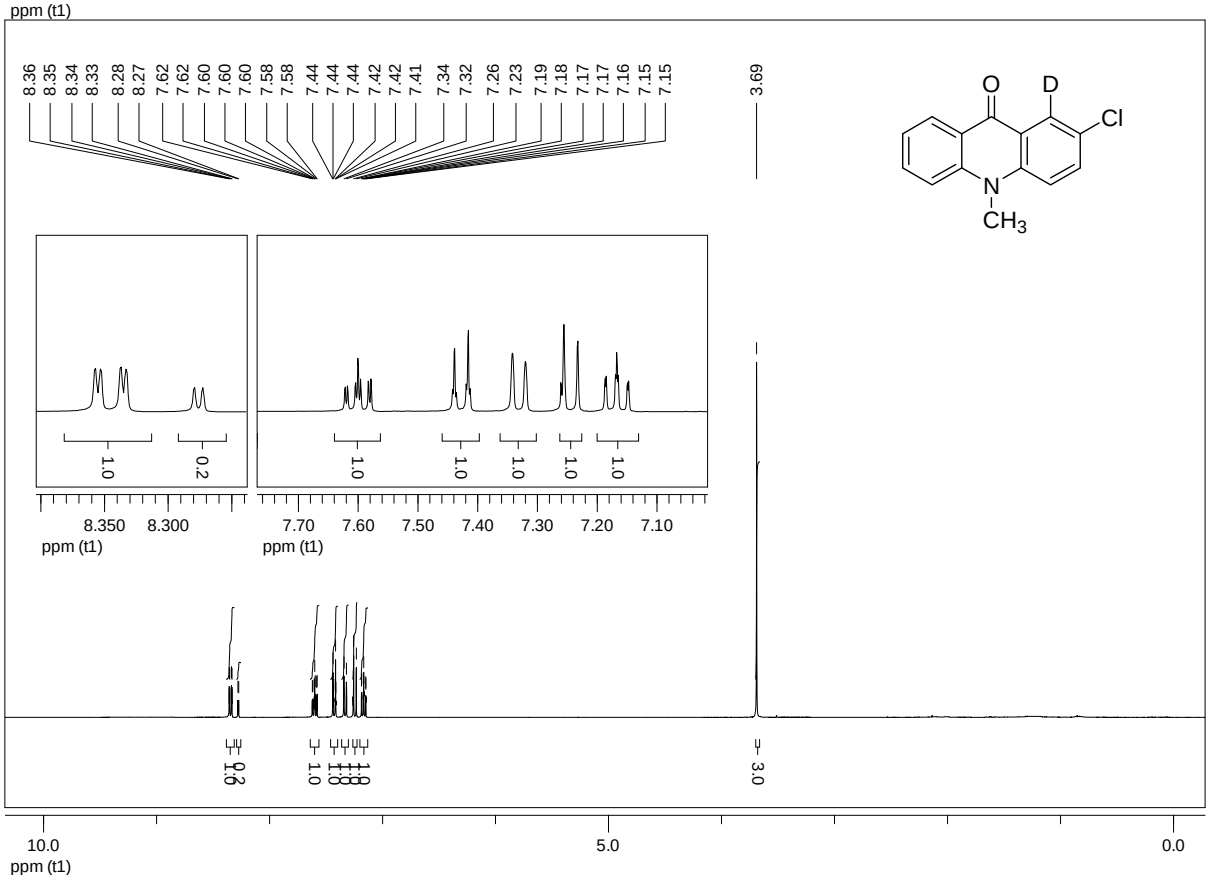

164.6
164.6
162.9
162.8
137.8
137.8
134.9
134.8
134.8
134.7
125.7
125.7
114.7
114.6
114.5
114.5
114.4
114.3
114.3
114.1
111.1
103.4
103.3
77.2
77.0
76.8
CN
F
Cl
D
1c
114.7
114.6
114.5
114.5
114.4
114.3
114.3
114.1
115.00
114.50
114.00
ppm (t1)
134.9
134.8
134.8
134.7
135.00
134.50
ppm (t1)
164.6
164.6
162.9
162.8
164.50 164.00 163.50 163.00
ppm (t1)
150
100
50
0
ppm (t1)

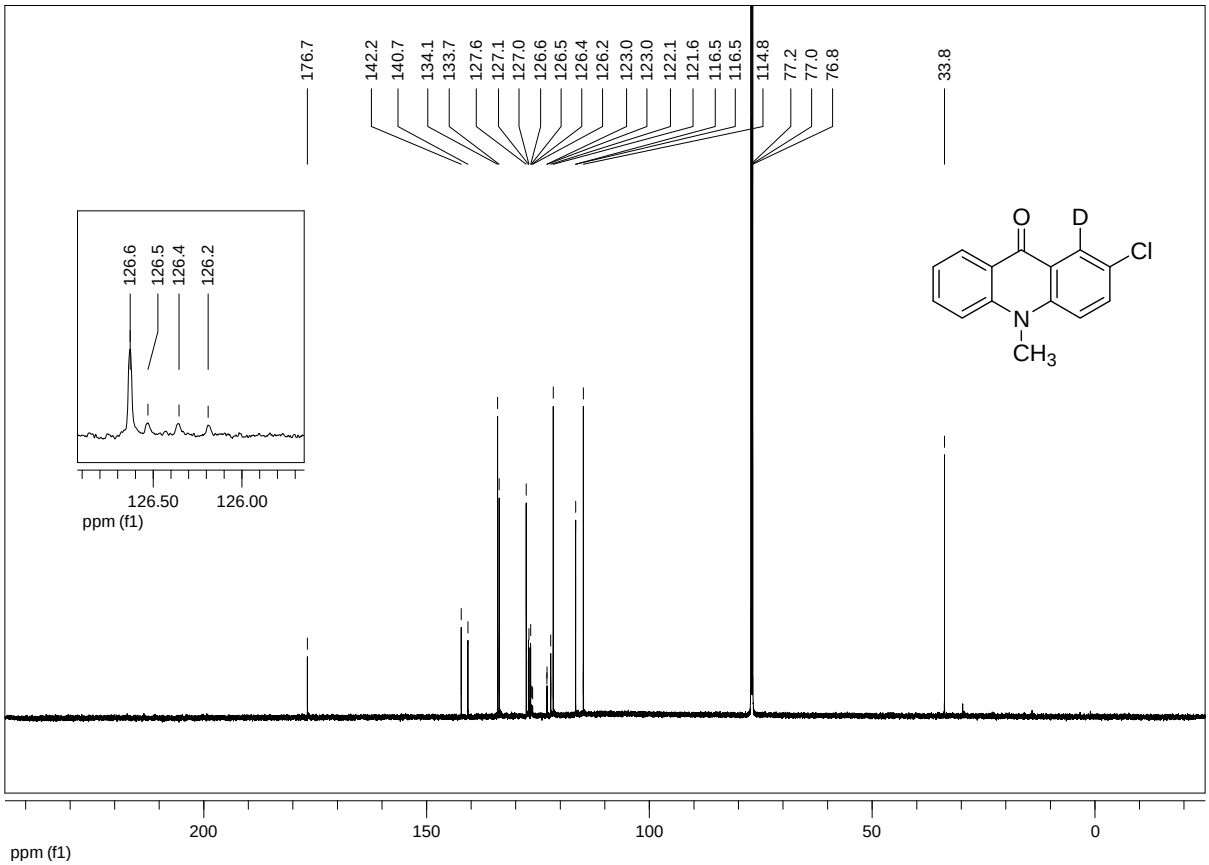

-103.69
-103.97
CN
F
Cl
D
1c
-103.7
-103.700
ppm (t1)
-104.0
-103.950
-104.000
ppm (t1)
-100
-110
-120
-130
-140
-150
ppm (t1)


6.95
6.93
6.92
6.87
6.86
6.85
6.84
3.87
OMe
Cl
D
F
1d
6.950
6.900
6.850
ppm (t1)
3.18
3.00
10.0
5.0
0.0
ppm (t1)


157.11
155.51
151.60
151.58
122.84
122.77
117.50
117.33
117.16
116.99
113.96
113.81
112.49
112.43
77.21
77.00
76.79
56.54
OMe
Cl
D
F
1d
117.50
117.00
ppm (t1)
150
100
50
ppm (t1)


-123.43
-123.43
OMe
Cl
D
F
1d
-123.400
-123.450
-123.500
ppm (t1)
-100
-150
ppm (t1)


8.36
8.35
8.34
8.33
8.28
8.27
7.62
7.62
7.60
7.60
7.60
7.58
7.58
7.44
7.44
7.44
7.42
7.42
7.41
7.34
7.32
7.26
7.23
7.19
7.18
7.17
7.17
7.16
7.15
7.15
3.69
O
D
Cl
N
CH3
1.0
0.2
1.0
1.0
1.0
1.0
1.0
8.350
8.300
ppm (t1)
7.70
7.60
7.50
7.40
7.30
7.20
7.10
ppm (t1)
0.9
1.0
3.0
10.0
ppm (t1)
5.0
0.0



[i] Suffert, J. *J. Org. Chem*. **1989**, *54*, 509-510.