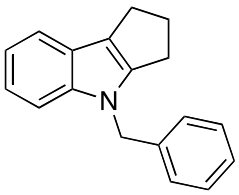
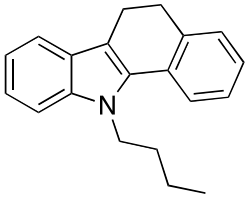
General Procedures. All chemicals were purchased from commercial suppliers and used without further purification. Analytical thin layer chromatography was carried out on pre-coated plates (silica gel 60 F254, 250 μm thickness) and visualized with UV light or I_2 chamber. Flash chromatography was performed using 60 Å, 32-63 μm silica gel (Scientific Adsorbents). ^{1}H NMR spectra were recorded at 600 MHz at ambient temperature with $CDCl_3$ as the solvent. ^{13}C NMR spectra were recorded at 150 MHz at ambient temperature with $CDCl_3$ as the solvent. Chemical shifts are reported in parts per million (ppm) relative to the residual solvent peak. Infrared spectra were recorded on an ATR-FTIR spectrometer and frequency is reported in cm^{-1}. The specifications of the LC/MS are as follows: electrospray (+) ionization, mass range 150 - 1500 Da, 20 V cone voltage, and Xterra® MS C18 column (2.1 mm x 50 mm x 3.5 μm). Preparative HPLC specifications are as follows: 15 mL/min flow rate, Xterra Prep MS C18 OBD column (19 mm x 100 mm) and dual wavelength absorbance detector.

Gerneral Procedure for Synthesis of Indoles. A 10 mL vial was charged with Cs_2CO_3 (0.720 g, 2.2 mmol), DPPF (0.028 g, 0.05 mmol), Pd_2dba_3 (0.018 g, 0.02 mmol), $MgSO_4$ (0.600 g, 5 mmol) dry toluene (2 mL) and a small stir bar. Vial was sealed with a teflon cap and solution was degassed by bubbling Ar through for 5 min. The appropriate *o*-bromoiodoarene (1 mmol) and primary amine (1 mmol) were added to the reaction vessel via a syringe and the reaction was stirred at 130 ^{o}C for 6 hours. The appropriate aldehyde or ketone (3 mmol) was then added via a syringe and the reaction was again stirred and heated at 130 ^{o}C for 48 hours. The reaction was allowed to cool to room temperature diluted with EtOAc (50 mL) and filtered through a bed of celite. The crude mixture was isolated under reduced pressure and purified via column chromatography. All reactions were run by strictly avoiding oxygen.

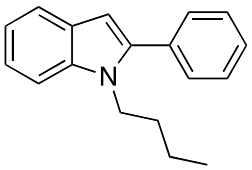
Reactions were also examined with all components present by the following method: A 10mL vial was charged with the aproprate *o*-dihaloarene (1 mmol), amine (1 mmol), aldehyde/ketone (1 mmol), Cs_2CO_3 (2.2 mmol), $MgSO_4$ (5 mmol), 1.5 mL dry toluene and a small stir bar. Solution was brought to 130 ^{o}C followed by addition of $Pd_2(dba)_3$ (0.02 mmol) and DPPF (0.05 mmol) dissolved in 0.5 mL toluene. Reaction was allowed to stir at 130^{o}C for 48 hours. The reaction was allowed to cool to room temperature diluted with EtOAc (50 mL) and filtered through a bed of celite. The crude mixture was isolated under reduced pressure and purified via column chromatography.



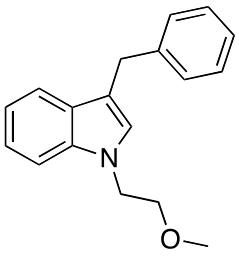
4-benzyl-1,2,3,4-tetrahydrocyclopenta[*b*]indole (11). Yellow oil (68%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.48 (dd, J = 5.8, 3.2, 1H), 7.30 (t, J = 7.3, 2H), 7.27 – 7.25 (m, 1H), 7.22 (dd, J = 6.0, 3.2, 1H), 7.12 – 7.08 (m, 4H), 5.25 (s, 2H), 2.90 (t, J = 6.9, 2H), 2.79 (t, J = 6.9, 2H), 2.54 (quint, J = 6.9, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.25, 141.11, 138.01, 128.68, 127.34, 126.60, 124.56, 120.12, 119.14, 118.56, 118.26, 109.84, 48.30, 28.41, 25.11, 24.69. IR (neat): 3086, 3051, 3030, 3005, 2950, 2921, 2899, 2850, 2818, 1666, 1612, 1580, 1494, 1454, 1376. ESI-MS *m/z* $[M+H]^+$: 248.14.



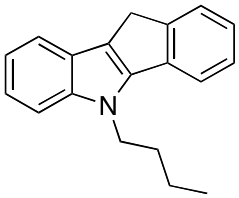
11-butyl-6,11-dihydro-5*H*-benzo[*a*]carbazole (12). Yellow oil (62%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, J = 7.8, 1H), 7.60 (d, J = 7.7, 1H), 7.42 (d, J = 8.2, 1H), 7.39 – 7.34 (m, J = 7.6, 2H), 7.28 (t, J = 7.0, 1H), 7.24 (t, J = 7.4, 1H), 7.18 (t, J = 7.0, 1H), 4.44 (t, J = 8.0, 2H), 3.02 (dd, J = 7.2, 2.1, 2H), 2.97 (dd, J = 7.6, 2.1, 2H), 1.98 (quint, J = 7.7, 2H), 1.51 (sextet, J = 7.3, 2H), 1.05 (t, J = 7.3, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.74, 138.26, 134.28, 129.80, 128.76, 126.74, 126.23, 126.17, 122.01, 121.98, 119.46, 118.81, 114.24, 109.75, 45.01, 32.63, 30.86, 20.33, 20.15, 13.91. IR (neat): 3056, 3032, 2956, 2928, 2891, 2871, 1600, 1577, 1536, 1491, 1462, 1442, 1426, 1306. ESI-MS *m/z* $[M+H]^+$: 276.16.



1-butyl-2-phenyl-1*H*-indole (13). Yellow oil (69%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 (ddd, J = 7.8, 1.1, 0.6, 1H), 7.52 – 7.46 (m, 4H), 7.43 – 7.39 (m, 2H), 7.24 (td, J = 7.0, 1.2, 1H), 7.14 (td, J = 7.1, 1.2, 1H), 4.16 (t, J = 7.4, 2H), 1.68 (quint, J = 7.4, 2H), 1.20 (sextet, J = 7.4, 2H), 0.80 (t, J = 7.4, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.36, 137.33, 133.30, 129.44, 128.44, 128.17, 127.86, 121.41, 120.52, 119.68, 110.04, 102.00, 43.73, 32.07, 19.99, 13.61. IR (neat): 3075, 308, 3030, 2957, 2930, 2872, 1601, 1509, 1460, 1393. ESI-MS *m/z* $[M+H]^+$: 250.18.

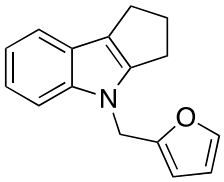


3-benzyl-1-(2-methoxyethyl)-1*H*-indole (14). Yellow oil (65%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.50 (d, J = 7.8, 1H), 7.33 (d, J = 7.8, 1H), 7.30 – 7.26 (m, 4H), 7.20 (t, J = 7.0, 2H), 7.06 (t, J = 7.43, 1H), 6.88 (s, 1H), 4.23 (t, J = 5.7, 2H), 4.11 (s, 2H), 3.69 (t, J = 5.7, 2H), 3.30 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.34, 136.58, 128.66, 128.26, 128.00, 126.64, 125.78, 121.52, 119.32, 118.85, 114.45, 109.18, 71.60, 59.03, 46.00, 31.52. IR (neat): 3057, 3025, 2893, 2829, 2135, 1930, 1681, 1602, 1466, 1453, 1359, 1332. ESI-MS *m/z* $[M+H]^+$: 266.13.

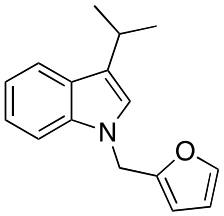


5-butyl-5,10-dihydroindeno[1,2-*b*]indole (15). Yellow oil (59%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 (d, J = 7.8, 1H), 7.59 (d, J = 7.6, 1H), 7.56 (d, J = 7.4, 1H), 7.42 – 7.40 (d, J = 7.5, 1H), 7.36 (t, J = 7.5, 1H), 7.25 – 7.20 (m, 2H), 7.15 (td, J = 7.7, 1.3, 1H), 4.44 (t, J = 7.2, 2H), 3.74 (s, 2H), 1.91 (quint, J = 7.5, 2H), 1.45 (sextet, J =

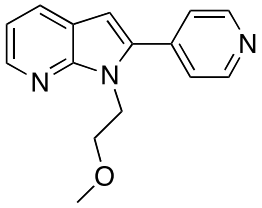
7.3, 2H), 0.96 (t, J = 7.3, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.27, 144.21, 141.27, 135.44, 126.54, 125.62, 124.53, 124.06, 121.07, 120.37, 119.43, 119.08, 117.76, 110.00, 44.62, 32.97, 30.15, 20.35, 13.93. IR (neat): 3351, 3247, 3072, 2957, 2925, 2872, 1737, 1461, 1439. ESI-MS *m/z* $[M+H]^+$: 262.04.



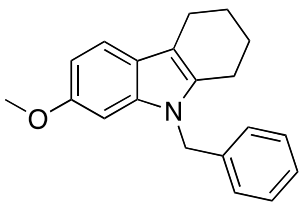
4-(furan-2-ylmethyl)-1,2,3,4-tetrahydrocyclopenta[*b*]indole (16). Yellow oil (63%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.44 (d, J = 7.8, 1H), 7.35 (d, J = 8.2, 1H), 7.34 – 7.33 (m, 1H), 7.13 (t, J = 7.6, 1H), 7.09 (t, J = 7.6, 1H), 6.29 (dd, J = 3.0, 1.8, 1H), 6.19 (d, J = 3.3, 1H), 5.17 (s, 3H), 2.87 (t, J = 7.1, 4H), 2.55 (quint, J = 7.2, 2H); 13C NMR (151 MHz, $CDCl_3$) δ 150.86, 145.92, 142.31, 140.86, 124.59, 120.14, 119.23, 118.57, 118.36, 110.36, 109.63, 107.66, 41.55, 28.35, 24.94, 24.63. IR (neat): ESI-MS *m/z* $[M+H]^+$: 238.11.



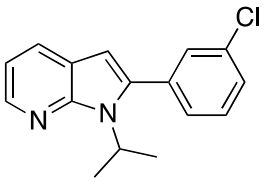
1-(furan-2-ylmethyl)-3-isopropyl-1*H*-indole (17). Yellow oil (58%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, J = 7.8, 1H), 7.37 (d, J = 8.3, 1H), 7.34 (dd, J = 1.8, 0.8, 1H), 7.20 (t, J = 7.3, 1H), 7.10 (t, J = 7.8, 1H), 6.88 (s, 1H), 6.30 – 6.29 (m, 1H), 6.21 – 6.19 (m, 1H), 5.20 (s, 2H), 3.19 (septet, J = 6.9, 1H), 1.35 (d, J = 6.6, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.75, 142.41, 136.63, 127.43, 123.24, 123.06, 121.56, 119.55, 118.72, 110.36, 109.38, 107.87, 42.90, 25.44, 23.34 (^{13}C spectrum includes grease peak at 29.70.) IR (neat): 3116, 3054, 2765, 2711, 2665, 2511, 2364, 2173, 2016, 1954, 1529. ESI-MS *m/z* $[M+H]^+$: 240.22.



1-(2-methoxyethyl)-2-(pyridin-4-yl)-1*H*-pyrrolo[2,3-*b*]pyridine (18). Deep orange oil (60%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.72 (d, J = 4.4, 2H), 8.38 (d, J = 4.8, 1H), 7.93 (d, J = 7.8, 1H), 7.60 (d, J = 4.5, 1H), 7.12 (dd, J = 7.7, 4.7, 1H), 6.62 (s, 1H), 4.53 (t, J = 5.6, 2H), 3.80 (t, J = 5.6, 2H), 3.20 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.05, 149.44, 143.60, 140.22, 139.09, 128.80, 123.69, 120.40, 116.67, 101.69, 70.89, 58.81, 42.91. IR (neat): 3382, 3128, 3050, 2923, 2889, 2860, 2815, 2182, 1597, 1572, 1476. ESI-MS m/z [M+H]+: 254.13.



9-benzyl-7-methoxy-2,3,4,9-tetrahydro-1*H*-carbazole (19). Yellow oil (52%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37 (d, J = 8.4, 1H), 7.27 (t, J = 7.2, 2H), 7.22 (t, J = 7.0, 1H), 7.01 (d, J = 7.6, 2H), 6.75 (dd, J = 8.5, 2.2, 1H), 6.70 (s, 1H), 5.19 (s, 2H), 3.78 (s, 3H), 2.73 (t, J = 5.6, 2H), 2.60 (t, J = 5.6, 2H), 1.93 – 1.87 (m, 2H), 1.87 – 1.81 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 155.72, 138.20, 137.22, 134.39, 128.66, 127.11, 126.14, 122.03, 118.22, 109.66, 107.81, 93.62, 55.81, 46.21, 23.21, 23.18, 22.10, 21.10. IR (neat): 3364, 3139, 3077, 3033, 2920, 2871, 2727, 2670, 1947, 1492. ESI-MS *m/z* $[M+H]^+$: 292.25.



2-(3-chlorophenyl)-1-isopropyl-1*H*-pyrrolo[2,3-*b*]pyridine (20). Deep orange oil (54%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.33 (d, J = 5.0, 1H), 7.87 (d, J = 7.7, 1H), 7.48 (s, 1H),

7.42 – 7.40 (m, 2H), 7.36 – 7.34 (m, 1H), 7.06 (ddd, J = 7.8, 4.7, 0.9, 1H), 6.40 (s, 1H), 4.67 (sept., J = 6.9, 1H), 1.71 (d, J = 7.0, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.79, 142.38, 139.90, 135.10, 134.38, 129.67, 129.55, 128.34, 128.13, 127.67, 120.86, 115.91, 100.55, 48.44, 21.40. IR (neat): 3157, 3068, 2888, 2777, 2737, 1580, 1467. ESI-MS *m/z* $[M+H]^+$: 271.14.

Computational Methods

All calculations were carried out using GAUSSIAN09:

Gaussian 09, Revision B.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

All structures were optimized (in the gas phase) using B3LYP (Becke, A. D. *J. Chem. Phys.,* 1993, **98**, 5648-5652; Becke, A. D. *J. Chem. Phys.* 1993, **98**, 1372-1377; Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B.,* 1988, **37**, 785-789; Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.,* 1994, **98**, 11623-11627) with the 6-31G(d) basis set for C, H, N and O and the LANL2DZ basis set (Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* 1985, **82**, 270–283) for Pd, P and Br. This level of theory has been used previously for studying Heck reactions (e.g., Wu, W.-Q.; Peng, Q.; Dong, D.-X.; Hou, X.-L.; Wu, Y.-D. *J. Am. Chem. Soc.* **2008**, *130*, 9717-9725). Frequency analysis was used to confirm that optimized structures were minima or transition state structures. Energies reported in the text are free energies (298K) and include zero point energy corrections (unscaled). For the system in Figure 1, intrinsic reaction coordinate (IRC) calculations (Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.,* 1990, **94**, 5523-5527; Fukui, K. *Acc. Chem. Res.,* 1981, **14**, 363-368; Fukui, K., *Acc. Chem. Res.,* 1981, **14**, 363-368) were used to verify the nature of transition state structures (IRC plots are shown below).

Coordinates, energies, and IRC plots follow.

Structures from Figure 1 in text

A

```
Zero-point correction=                0.222212 (Hartree/Particle)
 Thermal correction to Energy=          0.239928
 Thermal correction to Enthalpy=        0.240873
 Thermal correction to Gibbs Free Energy=     0.174718
 Sum of electronic and zero-point Energies=      -546.572610
 Sum of electronic and thermal Energies=       -546.554893
 Sum of electronic and thermal Enthalpies=      -546.553949
 Sum of electronic and thermal Free Energies=     -546.620104
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.166582	0.588630	-2.426110
2	6	0	0.824515	0.257254	-1.119107
3	6	0	1.787796	-0.223267	-0.245948
4	6	0	3.119863	-0.400473	-0.603455
5	6	0	3.465601	-0.068192	-1.918700
6	6	0	2.504147	0.416656	-2.812658
7	1	0	0.448304	0.972868	-3.144128
8	1	0	3.860399	-0.781221	0.093539
9	1	0	4.492921	-0.187715	-2.248543
10	1	0	2.798634	0.668648	-3.827563
11	7	0	1.162444	-0.457638	1.071769
12	6	0	1.678760	0.459579	2.126401
13	1	0	1.635315	1.485342	1.759617
14	1	0	1.059462	0.365893	3.022340
15	1	0	2.714095	0.204618	2.380007
16	6	0	1.107742	-1.827183	1.525564
17	6	0	1.378105	-2.912262	0.801063
18	1	0	0.793060	-1.901542	2.563354
19	1	0	1.277589	-3.892089	1.254558
20	1	0	1.694495	-2.869526	-0.235194
21	46	0	-0.741265	0.202171	0.136095
22	15	0	-2.328997	0.981451	-1.471658
23	1	0	-3.406292	0.107821	-1.803587
24	1	0	-3.043051	2.174460	-1.154976
25	1	0	-1.837969	1.301547	-2.768590
26	15	0	-2.418390	-0.052032	2.052750
27	1	0	-3.371418	0.977772	2.327703
28	1	0	-3.302181	-1.175341	2.031686
29	1	0	-1.890088	-0.212759	3.371482

TS A-to-B

```
Zero-point correction=                0.221404 (Hartree/Particle)
 Thermal correction to Energy=          0.238532
 Thermal correction to Enthalpy=        0.239476
 Thermal correction to Gibbs Free Energy=     0.175353
 Sum of electronic and zero-point Energies=      -546.559127
 Sum of electronic and thermal Energies=       -546.541999
 Sum of electronic and thermal Enthalpies=      -546.541054
 Sum of electronic and thermal Free Energies=     -546.605177
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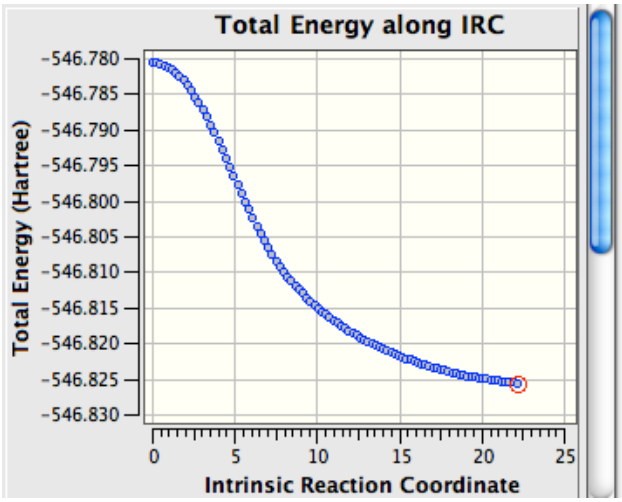
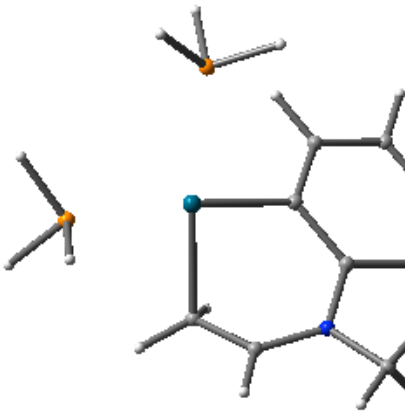
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.271396	0.420541	-0.155966
2	6	0	0.060247	0.246491	1.204562
3	6	0	1.132309	0.038283	2.076147
4	6	0	2.441983	0.007430	1.603225
5	6	0	2.663156	0.194252	0.233785
6	6	0	1.591029	0.388363	-0.636726
7	1	0	-0.540799	0.567080	-0.862078
8	1	0	3.275042	-0.150196	2.282012
9	1	0	3.677652	0.180218	-0.152168
10	1	0	1.770932	0.512805	-1.700595
11	7	0	0.735175	-0.127176	3.458034
12	6	0	1.540207	0.545731	4.486483
13	1	0	1.738626	1.571246	4.169844
14	1	0	0.978467	0.569491	5.424644
15	1	0	2.493699	0.031798	4.666861
16	6	0	0.147932	-1.368594	3.824113
17	6	0	-0.143168	-2.409381	3.019184
18	1	0	-0.089885	-1.409895	4.885324
19	1	0	-0.656428	-3.268482	3.435280
20	1	0	0.140078	-2.449214	1.974041
21	46	0	-1.527578	0.197597	2.447461
22	15	0	-2.863029	1.262912	0.815937
23	1	0	-3.107919	0.529898	-0.380479
24	1	0	-4.186919	1.635139	1.188465
25	1	0	-2.363154	2.490406	0.296357
26	15	0	-3.275503	0.051561	4.312131
27	1	0	-4.433392	0.890362	4.295292
28	1	0	-3.914807	-1.208000	4.526538
29	1	0	-2.835158	0.314340	5.646500

forward…





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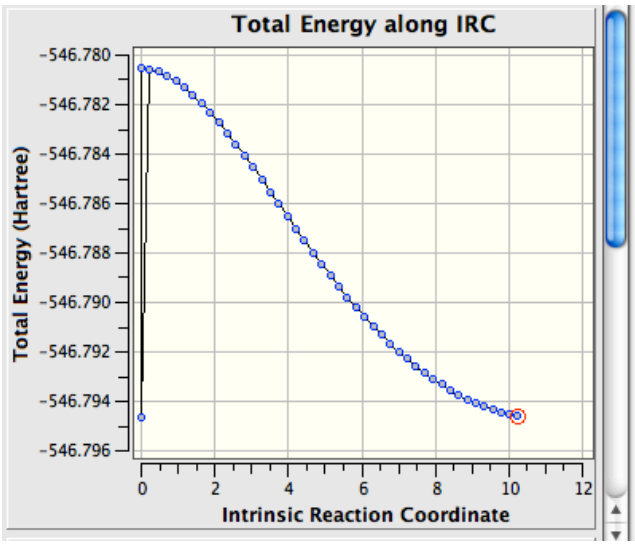
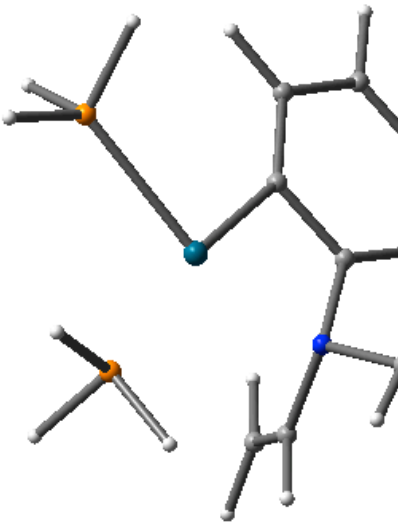




B

```
Zero-point correction=                0.223038 (Hartree/Particle)
 Thermal correction to Energy=          0.240353
 Thermal correction to Enthalpy=         0.241297
 Thermal correction to Gibbs Free Energy=     0.175888
 Sum of electronic and zero-point Energies=      -546.602983
 Sum of electronic and thermal Energies=       -546.585669
 Sum of electronic and thermal Enthalpies=      -546.584724
 Sum of electronic and thermal Free Energies=     -546.650134
```

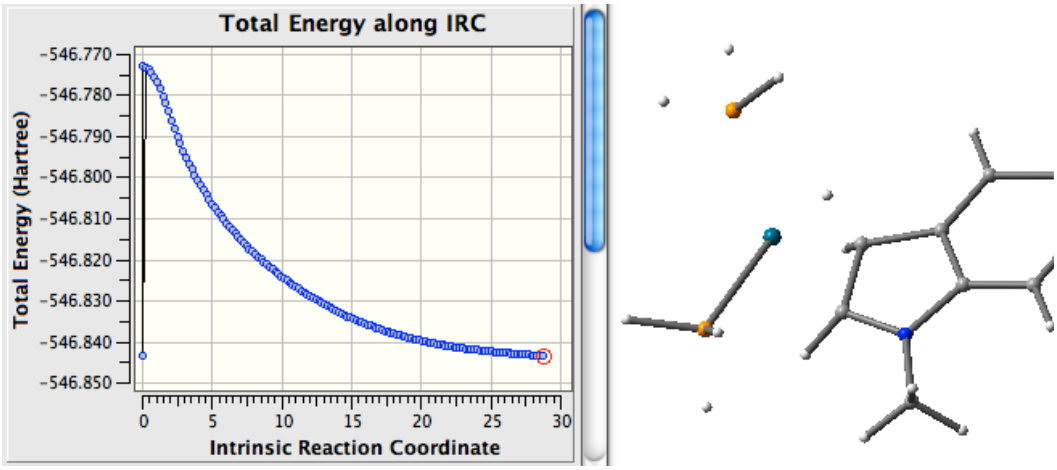
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.916850	-0.126857	-2.228876
2	6	0	0.888113	-0.059034	-0.833515
3	6	0	2.130858	-0.055232	-0.159309
4	6	0	3.341555	-0.043655	-0.862567
5	6	0	3.336629	-0.056045	-2.256371
6	6	0	2.124130	-0.107264	-2.940060
7	1	0	-0.012087	-0.179494	-2.789544
8	1	0	4.286810	-0.062598	-0.329238
9	1	0	4.276820	-0.046379	-2.798327
10	1	0	2.108759	-0.122872	-4.026017
11	7	0	2.151663	-0.069726	1.273879
12	6	0	3.161638	0.723787	1.988357
13	1	0	3.205345	1.727858	1.559793
14	1	0	2.891192	0.782908	3.043874
15	1	0	4.145987	0.254275	1.907000
16	6	0	1.208128	-0.728355	1.925090
17	6	0	0.241057	-1.586213	1.319101
18	1	0	1.186585	-0.560553	2.999970
19	1	0	-0.368722	-2.125477	2.040030
20	1	0	0.615491	-2.222586	0.514920
21	46	0	-0.882791	-0.154648	0.207126
22	15	0	-1.812204	1.710218	-1.159780
23	1	0	-1.911289	1.528429	-2.573428
24	1	0	-3.105491	2.267898	-0.908701
25	1	0	-1.036778	2.908336	-1.134684
26	15	0	-3.014372	-0.529271	1.508650
27	1	0	-3.840395	0.566540	1.914189
28	1	0	-4.015059	-1.337919	0.883821
29	1	0	-2.930909	-1.214845	2.760960

TS B-to-C

```
Zero-point correction=                0.219965 (Hartree/Particle)
 Thermal correction to Energy=          0.237631
 Thermal correction to Enthalpy=         0.238575
 Thermal correction to Gibbs Free Energy=     0.172162
 Sum of electronic and zero-point Energies=      -546.552903
 Sum of electronic and thermal Energies=       -546.535237
 Sum of electronic and thermal Enthalpies=      -546.534293
 Sum of electronic and thermal Free Energies=     -546.600706
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.004728	0.217748	0.076949
2	6	0	0.016494	0.147832	1.465108
3	6	0	1.259407	0.055187	2.137118
4	6	0	2.460728	0.157909	1.449848
5	6	0	2.424651	0.329551	0.057777
6	6	0	1.208830	0.344851	-0.621567
7	1	0	-0.943748	0.213296	-0.466572
8	1	0	3.410871	0.071422	1.967657
9	1	0	3.356089	0.419578	-0.491731
10	1	0	1.191043	0.464998	-1.700560
11	7	0	1.129428	-0.225809	3.530320
12	6	0	2.117354	0.213429	4.509446
13	1	0	2.288749	1.292929	4.424558
14	1	0	1.757283	-0.024915	5.511882
15	1	0	3.063063	-0.312421	4.351807
16	6	0	-0.143774	-0.544702	3.832804
17	6	0	-0.955522	-1.002119	2.738049
18	1	0	-0.449187	-0.575733	4.872267
19	1	0	-2.018667	-1.143593	2.947522
20	1	0	-0.581235	-1.824162	2.128474
21	46	0	-1.473961	1.194465	2.652277
22	15	0	-2.712071	2.594768	0.851088
23	1	0	-2.015259	3.715249	0.289920
24	1	0	-3.069500	1.958763	-0.384075
25	1	0	-3.965265	3.250937	1.091608
26	15	0	-2.245633	2.494482	4.636960
27	1	0	-1.741181	3.827213	4.773123
28	1	0	-3.642754	2.794460	4.720796
29	1	0	-2.054581	2.069725	5.992579

forward…



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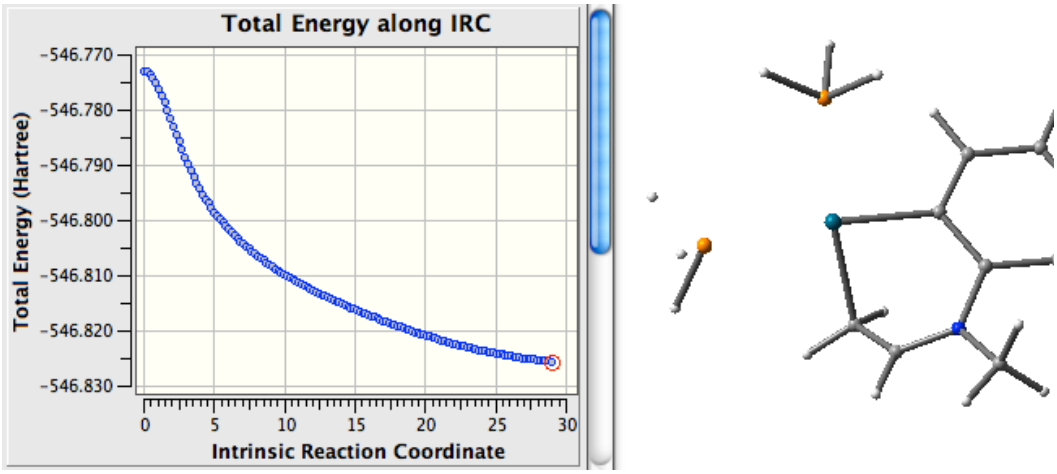
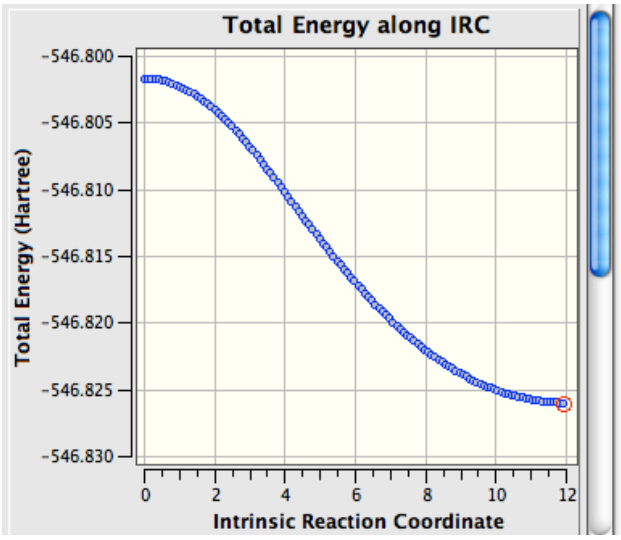


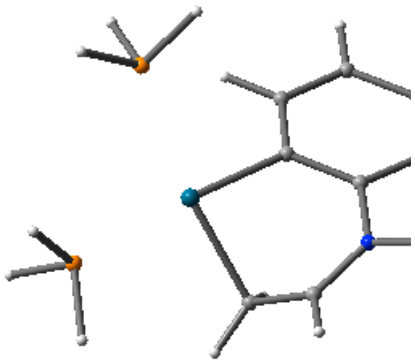
TS B-to-B′

```
Zero-point correction=                0.222711 (Hartree/Particle)
 Thermal correction to Energy=           0.239064
 Thermal correction to Enthalpy=         0.240009
 Thermal correction to Gibbs Free Energy=     0.177939
 Sum of electronic and zero-point Energies=      -546.578927
 Sum of electronic and thermal Energies=       -546.562573
 Sum of electronic and thermal Enthalpies=      -546.561629
 Sum of electronic and thermal Free Energies=     -546.623699
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.078818	0.773423	-1.970104
2	6	0	0.988493	0.178155	-0.696624
3	6	0	2.203722	0.119390	0.023953
4	6	0	3.379780	0.730059	-0.457621
5	6	0	3.400841	1.348938	-1.699100
6	6	0	2.247201	1.338982	-2.477974
7	1	0	0.211623	0.780999	-2.618475
8	1	0	4.293029	0.732736	0.120795
9	1	0	4.314426	1.813998	-2.054744
10	1	0	2.248309	1.774309	-3.473073
11	7	0	2.334222	-0.643823	1.248180
12	6	0	3.682234	-0.749327	1.863846
13	1	0	4.018857	0.240492	2.176232
14	1	0	3.622595	-1.396210	2.737222
15	1	0	4.382933	-1.172787	1.143304
16	6	0	1.374366	-1.315021	1.817175
17	6	0	-0.045372	-1.331494	1.499336
18	1	0	1.697122	-1.919315	2.664148
19	1	0	-0.389203	-2.369416	1.602390
20	46	0	-0.880776	-0.417779	-0.115769
21	15	0	-2.209433	1.061361	-1.757807
22	1	0	-2.301558	0.774614	-3.158183
23	1	0	-3.602291	1.273711	-1.501467
24	1	0	-1.800915	2.428540	-1.840780
25	15	0	-3.121193	-1.423446	0.594560
26	1	0	-3.123305	-2.288945	1.734627
27	1	0	-4.245699	-0.607849	0.941838
28	1	0	-3.767453	-2.294816	-0.338168
29	1	0	-0.531503	-0.776281	2.324492

forward…





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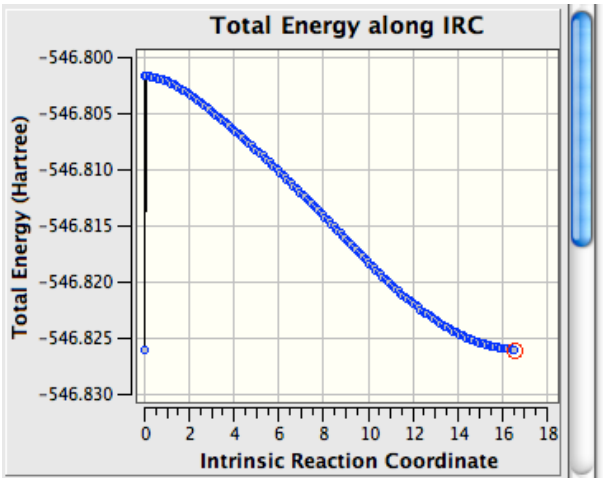


c

```
Zero-point correction=                0.221699 (Hartree/Particle)
 Thermal correction to Energy=          0.239348
 Thermal correction to Enthalpy=         0.240292
 Thermal correction to Gibbs Free Energy=     0.171933
 Sum of electronic and zero-point Energies=      -546.622016
 Sum of electronic and thermal Energies=       -546.604367
 Sum of electronic and thermal Enthalpies=      -546.603423
 Sum of electronic and thermal Free Energies=     -546.671782
```

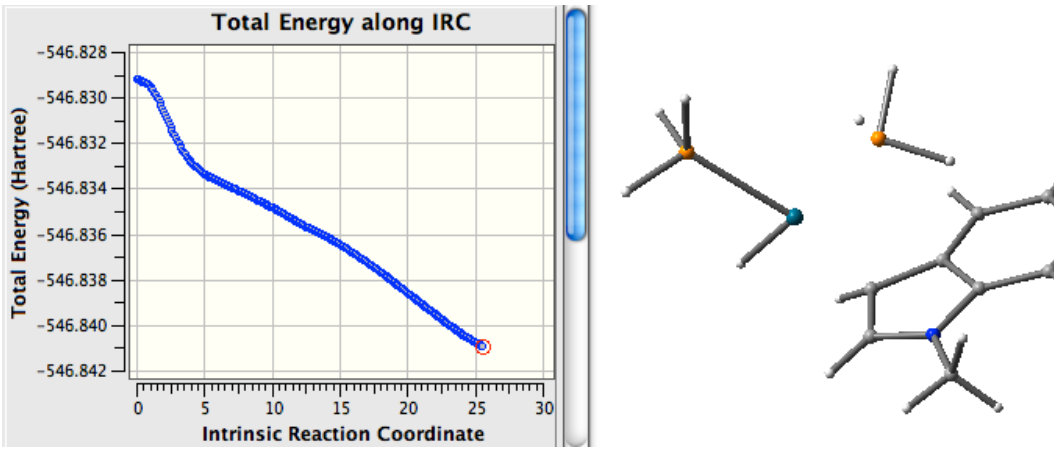
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.109357	0.025020	-0.049290
2	6	0	0.059559	0.037785	1.340843
3	6	0	1.246656	-0.030019	2.089007
4	6	0	2.502241	-0.104316	1.485899
5	6	0	2.535125	-0.130154	0.090442
6	6	0	1.358307	-0.070446	-0.669727
7	1	0	-0.799331	0.076827	-0.642396
8	1	0	3.418641	-0.140841	2.065536
9	1	0	3.493923	-0.197082	-0.414312
10	1	0	1.418823	-0.098685	-1.752933
11	7	0	0.927096	-0.034743	3.458195
12	6	0	1.901481	-0.211031	4.522094
13	1	0	2.457980	0.716531	4.701838
14	1	0	1.385399	-0.504856	5.438548
15	1	0	2.606154	-1.000684	4.248187
16	6	0	-0.416875	0.138819	3.652524
17	6	0	-1.084780	0.166596	2.300419
18	1	0	-0.859820	-0.335737	4.524631
19	1	0	-1.604470	1.184803	2.147365
20	1	0	-1.911568	-0.544179	2.201910
21	46	0	-1.159660	2.188236	3.817615
22	15	0	-2.275152	4.332227	3.058012
23	1	0	-1.621076	5.126626	2.063119
24	1	0	-3.576689	4.285404	2.464080
25	1	0	-2.527517	5.369288	4.011597
26	15	0	-0.454499	2.628113	6.128222
27	1	0	0.644256	3.519861	6.341754
28	1	0	-1.426543	3.288375	6.942981
29	1	0	-0.074490	1.600754	7.053371

TS C-to-D

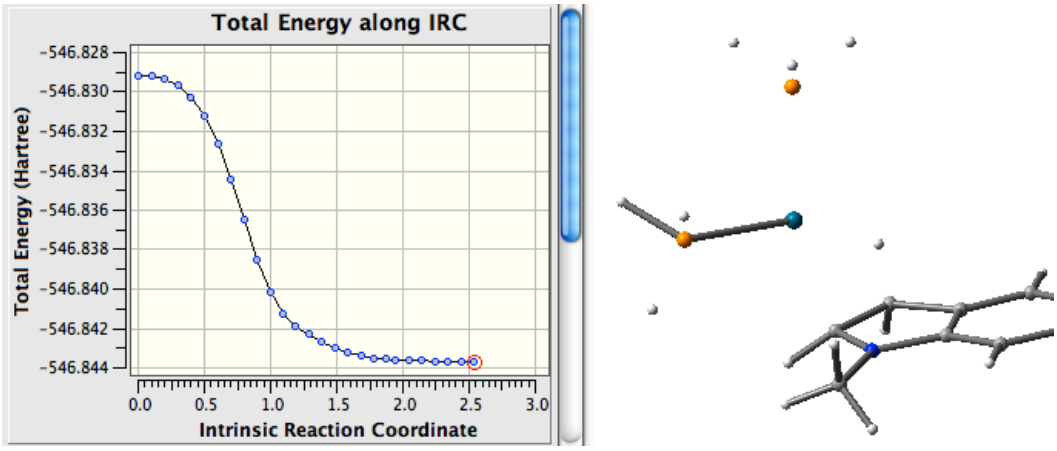
```
Zero-point correction=                0.218606 (Hartree/Particle)
 Thermal correction to Energy=          0.235799
 Thermal correction to Enthalpy=         0.236743
 Thermal correction to Gibbs Free Energy=     0.170978
 Sum of electronic and zero-point Energies=      -546.610559
 Sum of electronic and thermal Energies=       -546.593366
 Sum of electronic and thermal Enthalpies=      -546.592422
 Sum of electronic and thermal Free Energies=     -546.658187
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.021684	-0.106063	0.028390
2	6	0	0.041120	-0.093915	1.431048
3	6	0	1.296690	-0.009256	2.082096
4	6	0	2.494930	0.097171	1.365131
5	6	0	2.405663	0.079203	-0.022066
6	6	0	1.164917	-0.028093	-0.686268
7	1	0	-0.976993	-0.178010	-0.483441
8	1	0	3.456032	0.180504	1.861811
9	1	0	3.315857	0.146468	-0.610325
10	1	0	1.143542	-0.046172	-1.771176
11	7	0	1.093400	-0.062811	3.455561
12	6	0	2.145538	-0.018929	4.457720
13	1	0	2.564614	0.989741	4.553966
14	1	0	1.737740	-0.332956	5.421033
15	1	0	2.947006	-0.710179	4.182839
16	6	0	-0.262004	-0.128478	3.714211
17	6	0	-0.962191	-0.157797	2.467942
18	1	0	-0.607563	-0.552865	4.649230
19	1	0	-1.681263	1.580095	2.358887
20	1	0	-1.971278	-0.533888	2.357650
21	46	0	-1.296925	1.949364	3.835481
22	15	0	-2.470745	4.029149	3.371487
23	1	0	-1.969231	4.823742	2.298686
24	1	0	-3.835207	3.910669	2.973986
25	1	0	-2.598746	5.033290	4.380009
26	15	0	-0.670792	2.351362	6.266001
27	1	0	-0.393633	1.263207	7.154374
28	1	0	0.475342	3.157276	6.556710
29	1	0	-1.624043	3.041213	7.078970

forward…



reverse…



D (complexed to $HPd(PH_3)_2$+)

```
Zero-point correction=                0.220723 (Hartree/Particle)
 Thermal correction to Energy=          0.237958
 Thermal correction to Enthalpy=        0.238903
 Thermal correction to Gibbs Free Energy=     0.173356
 Sum of electronic and zero-point Energies=      -546.620951
 Sum of electronic and thermal Energies=       -546.603716
 Sum of electronic and thermal Enthalpies=      -546.602771
 Sum of electronic and thermal Free Energies=     -546.668318
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.540197	-0.114414	-2.501382
2	6	0	0.192086	-0.691974	-1.272963
3	6	0	1.216019	-1.063563	-0.370662
4	6	0	2.570450	-0.848296	-0.634299
5	6	0	2.890018	-0.265843	-1.859478
6	6	0	1.889147	0.090351	-2.782882
7	1	0	-0.224898	0.160567	-3.221896
8	1	0	3.346315	-1.134844	0.068541
9	1	0	3.932195	-0.093893	-2.109866
10	1	0	2.177068	0.526673	-3.734400
11	7	0	0.613671	-1.665693	0.745587
12	6	0	1.337108	-2.174502	1.905903
13	1	0	1.835145	-1.357057	2.436809
14	1	0	0.632432	-2.663088	2.580404
15	1	0	2.086191	-2.903189	1.583764
16	6	0	-0.722857	-1.687064	0.571212
17	6	0	-1.080371	-1.047317	-0.645163
18	1	0	-1.361756	-2.206841	1.272237
19	1	0	-3.191848	-0.346965	0.643437
20	1	0	-1.971505	-1.320001	-1.202003
21	46	0	-2.004091	0.651847	0.503758
22	15	0	-3.604757	2.098424	1.600911
23	1	0	-4.820430	2.324731	0.892901
24	1	0	-4.116083	1.640446	2.849568
25	1	0	-3.254823	3.439730	1.945331
26	15	0	-0.110024	2.331472	0.253780
27	1	0	-0.097345	3.535957	1.025663
28	1	0	1.225410	1.888527	0.499671
29	1	0	0.077338	2.895820	-1.044483

E

```
Zero-point correction=                0.209235 (Hartree/Particle)
 Thermal correction to Energy=          0.226441
 Thermal correction to Enthalpy=         0.227385
 Thermal correction to Gibbs Free Energy=     0.162939
 Sum of electronic and zero-point Energies=      -546.179244
 Sum of electronic and thermal Energies=       -546.162038
 Sum of electronic and thermal Enthalpies=      -546.161094
 Sum of electronic and thermal Free Energies=     -546.225540
```

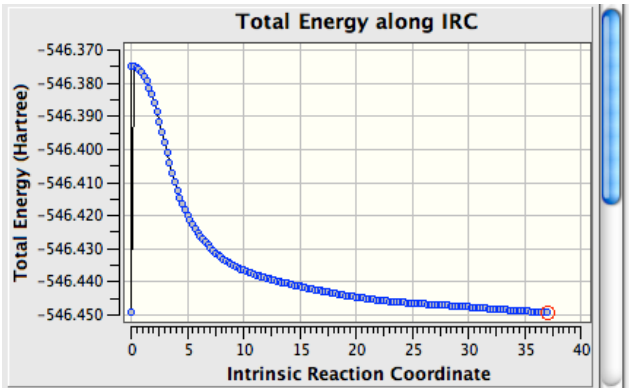
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.671669	1.316688	-1.299730
2	6	0	-0.570442	1.129813	-0.444832
3	6	0	-0.311364	2.147843	0.508215
4	6	0	-1.225555	3.219073	0.647223
5	6	0	-2.330815	3.339707	-0.187303
6	6	0	-2.548376	2.397711	-1.190917
7	1	0	-1.853119	0.598357	-2.095810
8	1	0	-1.059336	3.986463	1.394343
9	1	0	-3.005652	4.182866	-0.061294
10	1	0	-3.387319	2.494677	-1.875637
11	7	0	0.851094	2.143331	1.289731
12	6	0	1.033236	3.148914	2.322468
13	1	0	0.199592	3.132846	3.034058
14	1	0	1.948187	2.927141	2.874929
15	1	0	1.114497	4.166612	1.911710
16	6	0	1.952097	1.371112	0.930138
17	6	0	1.974777	0.328954	0.085660
18	1	0	2.872461	1.708668	1.406538
19	1	0	2.954329	-0.100540	-0.122506
20	15	0	-1.763305	-1.981959	-1.080185
21	1	0	-2.442524	-2.024713	-2.349271
22	1	0	-1.851746	-3.391068	-0.800518
23	1	0	-2.885297	-1.569555	-0.291523
24	15	0	1.816410	-2.741982	-0.862806
25	1	0	3.227427	-2.525768	-0.720514
26	1	0	1.708635	-3.838478	0.062148
27	1	0	1.871632	-3.538520	-2.060408
28	46	0	0.397679	-0.657777	-0.615270

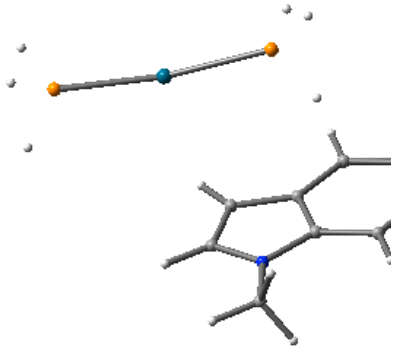
TS E-to-D

```
Zero-point correction=                0.206974 (Hartree/Particle)
 Thermal correction to Energy=          0.224201
 Thermal correction to Enthalpy=        0.225145
 Thermal correction to Gibbs Free Energy=     0.159767
 Sum of electronic and zero-point Energies=      -546.167837
 Sum of electronic and thermal Energies=       -546.150610
 Sum of electronic and thermal Enthalpies=      -546.149665
 Sum of electronic and thermal Free Energies=     -546.215044
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.271779	1.509569	-1.187380
2	6	0	0.977424	0.274297	-0.574789
3	6	0	2.011071	-0.345533	0.178858
4	6	0	3.198303	0.347992	0.476192
5	6	0	3.421699	1.605236	-0.077963
6	6	0	2.476933	2.170107	-0.943958
7	1	0	0.534048	1.975370	-1.835911
8	1	0	3.963457	-0.111569	1.094950
9	1	0	4.350708	2.127572	0.135735
10	1	0	2.670746	3.132623	-1.411652
11	7	0	1.837839	-1.699221	0.452310
12	6	0	2.856528	-2.480319	1.124574
13	1	0	3.043256	-2.091880	2.132188
14	1	0	2.506464	-3.510448	1.221121
15	1	0	3.809012	-2.481782	0.573742
16	6	0	0.882440	-2.301824	-0.357974
17	6	0	-0.031122	-1.542722	-1.007353
18	1	0	1.017550	-3.368957	-0.524587
19	1	0	-0.582998	-1.978899	-1.839797
20	46	0	-1.032499	0.009090	-0.146318
21	15	0	-1.496507	2.229948	0.999796
22	1	0	-1.433565	3.413183	0.183504
23	1	0	-2.638111	2.641899	1.782652
24	1	0	-0.496080	2.634642	1.947599
25	15	0	-3.344742	-1.031647	-0.042771
26	1	0	-3.580685	-2.089149	-0.990063
27	1	0	-3.662682	-1.800896	1.131950
28	1	0	-4.642640	-0.410640	-0.173578

forward…





System with two PMe_3 ligands:

A

Zero-point correction= 0.402030 (Hartree/Particle)
Thermal correction to Energy= 0.428743
Thermal correction to Enthalpy= 0.429687
Thermal correction to Gibbs Free Energy= 0.345915
Sum of electronic and zero-point Energies= -782.347902
Sum of electronic and thermal Energies= -782.321189
Sum of electronic and thermal Enthalpies= -782.320245
Sum of electronic and thermal Free Energies= -782.404017

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.306303	0.526869	-2.445582
2	6	0	0.869268	0.257480	-1.148376
3	6	0	1.773274	-0.279237	-0.240006
4	6	0	3.099832	-0.569577	-0.545546
5	6	0	3.526537	-0.295370	-1.848106
6	6	0	2.638059	0.246449	-2.782199
7	1	0	0.655258	0.947923	-3.200942
8	1	0	3.776296	-0.996100	0.189434
9	1	0	4.552990	-0.503400	-2.134392
10	1	0	2.985540	0.456684	-3.790162
11	7	0	1.130539	-0.441754	1.078413
12	6	0	1.697152	0.490579	2.091288
13	1	0	1.685753	1.502560	1.685693
14	1	0	1.090507	0.458127	2.999053
15	1	0	2.727692	0.210383	2.339447
16	6	0	1.024712	-1.787742	1.577490
17	6	0	1.189439	-2.911570	0.878769
18	1	0	0.766905	-1.817041	2.633075
19	1	0	1.058011	-3.869183	1.370379
20	1	0	1.455183	-2.918428	-0.172471
21	46	0	-0.749154	0.298199	0.073650
22	15	0	-2.351172	1.164312	-1.480143
23	15	0	-2.428549	-0.064857	1.976548
24	6	0	-1.715603	0.070874	3.718364
25	1	0	-0.887412	-0.630435	3.841113
26	1	0	-1.353183	1.087397	3.892579
27	1	0	-2.488929	-0.166051	4.455696
28	6	0	-3.057715	-1.841518	1.945047
29	1	0	-3.651041	-2.006168	1.041878
30	1	0	-2.202509	-2.521882	1.923977
31	1	0	-3.673046	-2.050959	2.825528
32	6	0	-4.019312	0.926065	2.197734
33	1	0	-3.775230	1.974774	2.387870
34	1	0	-4.646236	0.861172	1.305592
35	1	0	-4.581711	0.533443	3.050564
36	6	0	-3.852884	0.055049	-1.704626
37	1	0	-4.348961	-0.119673	-0.748172
38	1	0	-4.560344	0.524800	-2.395114
39	1	0	-3.529896	-0.904909	-2.115612
40	6	0	-3.053714	2.820675	-0.939334
41	1	0	-3.816733	3.151425	-1.650937
42	1	0	-3.495279	2.739478	0.054907
43	1	0	-2.245141	3.555543	-0.907800
44	6	0	-1.878687	1.511658	-3.261207
45	1	0	-1.097953	2.274051	-3.299158
46	1	0	-1.522726	0.597698	-3.741079
47	1	0	-2.763347	1.877352	-3.792102

TS A-to-B

```
Zero-point correction=                0.401250 (Hartree/Particle)
 Thermal correction to Energy=          0.427535
 Thermal correction to Enthalpy=        0.428480
 Thermal correction to Gibbs Free Energy=     0.345007
 Sum of electronic and zero-point Energies=      -782.338031
 Sum of electronic and thermal Energies=       -782.311746
 Sum of electronic and thermal Enthalpies=      -782.310802
 Sum of electronic and thermal Free Energies=     -782.394274
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.313281	0.249836	-0.139735
2	6	0	0.053883	0.284551	1.228665
3	6	0	1.128353	0.280354	2.126012
4	6	0	2.450169	0.269750	1.681854
5	6	0	2.701841	0.264100	0.306939
6	6	0	1.639972	0.239183	-0.596403
7	1	0	-0.483637	0.221105	-0.875835
8	1	0	3.271694	0.264651	2.392569
9	1	0	3.725552	0.264326	-0.054621
10	1	0	1.836129	0.207811	-1.664542
11	7	0	0.749084	0.247221	3.522153
12	6	0	1.463304	1.142310	4.440618
13	1	0	1.504258	2.142345	4.004573
14	1	0	0.919957	1.195455	5.388734
15	1	0	2.486072	0.800201	4.649827
16	6	0	0.350751	-1.005236	4.044683
17	6	0	0.154002	-2.155897	3.372382
18	1	0	0.169277	-0.961937	5.115862
19	1	0	-0.212672	-3.023152	3.909668
20	1	0	0.378674	-2.275706	2.319211
21	46	0	-1.578556	0.238228	2.442068
22	15	0	-2.915755	1.164559	0.722895
23	15	0	-3.343446	-0.051411	4.275737
24	6	0	-4.240513	1.451563	4.977077
25	1	0	-3.504943	2.171417	5.346168
26	1	0	-4.842802	1.931140	4.202927
27	1	0	-4.894770	1.150708	5.801297
28	6	0	-4.751876	-1.231076	3.854225
29	1	0	-5.337169	-0.842716	3.017265
30	1	0	-4.333508	-2.199451	3.567190
31	1	0	-5.410897	-1.363327	4.717852
32	6	0	-2.673702	-0.838652	5.853398
33	1	0	-2.207239	-1.796621	5.614061
34	1	0	-1.929740	-0.180018	6.308884
35	1	0	-3.490930	-0.998804	6.563307
36	6	0	-4.586308	1.831085	1.260498
37	1	0	-5.102040	2.241479	0.386463
38	1	0	-5.196844	1.033843	1.688759
39	1	0	-4.447876	2.624193	1.998266
40	6	0	-3.381187	-0.053857	-0.627305
41	1	0	-3.940487	0.462336	-1.413887
42	1	0	-2.488060	-0.513341	-1.053164
43	1	0	-4.003924	-0.839663	-0.192180
44	6	0	-2.175428	2.654845	-0.144185
45	1	0	-2.845678	2.982390	-0.945027
46	1	0	-2.059383	3.459196	0.586822
47	1	0	-1.195809	2.407241	-0.552485

B

```
Zero-point correction=                0.402446 (Hartree/Particle)
 Thermal correction to Energy=          0.428982
 Thermal correction to Enthalpy=         0.429926
 Thermal correction to Gibbs Free Energy=     0.345956
 Sum of electronic and zero-point Energies=      -782.375349
 Sum of electronic and thermal Energies=       -782.348813
 Sum of electronic and thermal Enthalpies=      -782.347868
 Sum of electronic and thermal Free Energies=     -782.431838
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.087359	-0.209079	-2.118597
2	6	0	0.953868	0.006665	-0.743296
3	6	0	2.151347	0.128461	-0.001526
4	6	0	3.407347	0.112670	-0.618841
5	6	0	3.500031	-0.047766	-2.000776
6	6	0	2.338512	-0.221923	-2.750157
7	1	0	0.200295	-0.355912	-2.729289
8	1	0	4.312751	0.189110	-0.024135
9	1	0	4.474308	-0.058780	-2.479053
10	1	0	2.398581	-0.361029	-3.826027
11	7	0	2.071583	0.250643	1.425148
12	6	0	2.946135	1.201050	2.120021
13	1	0	2.924554	2.164616	1.604108
14	1	0	2.599270	1.325624	3.147588
15	1	0	3.976079	0.832898	2.144647
16	6	0	1.131711	-0.428716	2.070142
17	6	0	0.291704	-1.418301	1.495573
18	1	0	1.011203	-0.160244	3.118097
19	1	0	-0.307068	-1.961134	2.219800
20	1	0	0.742208	-2.055501	0.734016
21	46	0	-0.873194	-0.109613	0.221093
22	15	0	-1.811225	1.619593	-1.293191
23	15	0	-3.036658	-0.600100	1.429252
24	6	0	-4.545609	-0.916758	0.343974
25	1	0	-4.785414	-0.027256	-0.243579
26	1	0	-4.329917	-1.741592	-0.340713
27	1	0	-5.410965	-1.178453	0.960738
28	6	0	-3.668754	0.676436	2.664356
29	1	0	-2.906873	0.845139	3.430178
30	1	0	-3.866907	1.623320	2.157511
31	1	0	-4.587939	0.324096	3.142790
32	6	0	-3.027251	-2.163381	2.482662
33	1	0	-2.715244	-3.016833	1.875112
34	1	0	-2.332440	-2.049604	3.318851
35	1	0	-4.029024	-2.350864	2.881197
36	6	0	-3.139624	2.748550	-0.576959
37	1	0	-4.028983	2.171820	-0.312933
38	1	0	-2.754470	3.240902	0.319913
39	1	0	-3.418536	3.510401	-1.311651
40	6	0	-2.624778	0.997176	-2.874165
41	1	0	-1.906743	0.410651	-3.452464
42	1	0	-3.475741	0.358445	-2.624006
43	1	0	-2.969448	1.840911	-3.480022
44	6	0	-0.568896	2.881609	-1.926202
45	1	0	-0.135000	3.414358	-1.076077
46	1	0	0.231247	2.371816	-2.464766
47	1	0	-1.067880	3.596058	-2.588221

TS B-to-C

Zero-point correction= 0.399722 (Hartree/Particle)
Thermal correction to Energy= 0.426230
Thermal correction to Enthalpy= 0.427174
Thermal correction to Gibbs Free Energy= 0.342683
Sum of electronic and zero-point Energies= -782.321320
Sum of electronic and thermal Energies= -782.294812
Sum of electronic and thermal Enthalpies= -782.293868
Sum of electronic and thermal Free Energies= -782.378359

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.073073	0.272563	0.006358
2	6	0	0.027453	0.233726	1.393769
3	6	0	1.226809	0.173650	2.142753
4	6	0	2.457339	0.297723	1.507911
5	6	0	2.491222	0.431559	0.111775
6	6	0	1.316598	0.399843	-0.636503
7	1	0	-0.837202	0.235925	-0.582447
8	1	0	3.382781	0.247455	2.072998
9	1	0	3.450176	0.525192	-0.388426
10	1	0	1.355673	0.479783	-1.718719
11	7	0	1.039266	-0.118522	3.524873
12	6	0	1.857716	0.531147	4.540303
13	1	0	1.718927	1.623058	4.541492
14	1	0	1.596458	0.128184	5.521651
15	1	0	2.913085	0.312509	4.364033
16	6	0	-0.308394	-0.368643	3.751057
17	6	0	-0.983718	-1.004328	2.657645
18	1	0	-0.650820	-0.423365	4.776785
19	1	0	-2.054108	-1.184061	2.763696
20	1	0	-0.496668	-1.790038	2.086340
21	46	0	-1.475196	1.226872	2.643094
22	15	0	-2.626591	2.646116	0.829714
23	15	0	-2.316127	2.391815	4.662157
24	6	0	-1.825831	1.707498	6.349800
25	1	0	-2.202476	0.686552	6.460811
26	1	0	-0.736950	1.700330	6.445809
27	1	0	-2.249503	2.327324	7.146188
28	6	0	-1.787314	4.193945	4.819924
29	1	0	-0.697650	4.248989	4.887056
30	1	0	-2.110589	4.754444	3.939618
31	1	0	-2.228448	4.643384	5.715252
32	6	0	-4.188941	2.487208	4.839220
33	1	0	-4.617381	3.002858	3.977683
34	1	0	-4.602113	1.476075	4.884567
35	1	0	-4.455426	3.028235	5.752663
36	6	0	-3.908437	3.974529	1.232140
37	1	0	-4.782257	3.517297	1.703824
38	1	0	-3.482648	4.717533	1.911504
39	1	0	-4.227514	4.478949	0.314394
40	6	0	-1.413100	3.626609	-0.230221
41	1	0	-0.946180	4.404578	0.380264
42	1	0	-0.630761	2.959425	-0.598010
43	1	0	-1.930060	4.092118	-1.075154
44	6	0	-3.583259	1.649850	-0.460335
45	1	0	-2.939220	0.891266	-0.911224
46	1	0	-4.425398	1.147294	0.023252
47	1	0	-3.961450	2.309503	-1.247933

E

```
Zero-point correction=                0.388611 (Hartree/Particle)
 Thermal correction to Energy=          0.415001
 Thermal correction to Enthalpy=         0.415946
 Thermal correction to Gibbs Free Energy=     0.331956
 Sum of electronic and zero-point Energies=      -781.937582
 Sum of electronic and thermal Energies=       -781.911192
 Sum of electronic and thermal Enthalpies=      -781.910248
 Sum of electronic and thermal Free Energies=     -781.994238
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.497100	1.382870	-1.473497
2	6	0	-0.537883	1.106427	-0.484397
3	6	0	-0.376217	2.071504	0.541800
4	6	0	-1.265220	3.168221	0.618204
5	6	0	-2.241199	3.373932	-0.352301
6	6	0	-2.343580	2.495012	-1.429266
7	1	0	-1.595450	0.701083	-2.315450
8	1	0	-1.175602	3.892103	1.420616
9	1	0	-2.899590	4.235945	-0.274252
10	1	0	-3.072598	2.663264	-2.218695
11	7	0	0.685632	1.982319	1.453810
12	6	0	0.775657	2.926580	2.552292
13	1	0	-0.143433	2.914872	3.148925
14	1	0	1.599994	2.631883	3.205264
15	1	0	0.952103	3.961198	2.216400
16	6	0	1.845627	1.284455	1.102038
17	6	0	1.955759	0.309480	0.186456
18	1	0	2.722471	1.633783	1.649293
19	1	0	2.967161	-0.041593	-0.007353
20	15	0	-1.783450	-1.966490	-1.017448
21	15	0	1.881756	-2.742525	-0.913884
22	46	0	0.416803	-0.704423	-0.595822
23	6	0	1.619742	-3.790520	-2.468188
24	1	0	0.607950	-4.204740	-2.475921
25	1	0	1.738714	-3.154136	-3.349705
26	1	0	2.342587	-4.612109	-2.515197
27	6	0	1.909768	-4.075637	0.427535
28	1	0	2.174740	-3.608969	1.380281
29	1	0	0.917700	-4.523157	0.526690
30	1	0	2.637682	-4.859184	0.190170
31	6	0	3.730931	-2.396348	-1.073354
32	1	0	3.897326	-1.678934	-1.881223
33	1	0	4.103560	-1.962992	-0.142139
34	1	0	4.277038	-3.321428	-1.285165
35	6	0	-2.532500	-2.156249	-2.746689
36	1	0	-2.675620	-1.167085	-3.188846
37	1	0	-1.844778	-2.722889	-3.381192
38	1	0	-3.496983	-2.674012	-2.704033
39	6	0	-1.892488	-3.757055	-0.411725
40	1	0	-1.220647	-4.395838	-0.991790
41	1	0	-1.592925	-3.796708	0.639347
42	1	0	-2.914278	-4.139486	-0.507741
43	6	0	-3.233126	-1.225968	-0.064279
44	1	0	-2.991774	-1.235941	1.002112
45	1	0	-3.371360	-0.188476	-0.374237
46	1	0	-4.148911	-1.800740	-0.240324

TS E-to-D

```
Zero-point correction=                0.386560 (Hartree/Particle)
 Thermal correction to Energy=          0.412834
 Thermal correction to Enthalpy=        0.413778
 Thermal correction to Gibbs Free Energy=     0.329249
 Sum of electronic and zero-point Energies=      -781.925387
 Sum of electronic and thermal Energies=       -781.899113
 Sum of electronic and thermal Enthalpies=      -781.898169
 Sum of electronic and thermal Free Energies=     -781.982699
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.232801	1.460659	-1.299975
2	6	0	0.932826	0.268987	-0.607407
3	6	0	1.969233	-0.296501	0.188263
4	6	0	3.143383	0.426052	0.463864
5	6	0	3.362899	1.652112	-0.161192
6	6	0	2.428425	2.147855	-1.081079
7	1	0	0.500835	1.875012	-1.989074
8	1	0	3.905175	0.011578	1.118128
9	1	0	4.283420	2.196567	0.033572
10	1	0	2.624175	3.078064	-1.610056
11	7	0	1.804305	-1.637791	0.520437
12	6	0	2.831936	-2.380965	1.220438
13	1	0	3.016401	-1.951341	2.211692
14	1	0	2.492961	-3.410220	1.358845
15	1	0	3.784487	-2.394593	0.669007
16	6	0	0.876616	-2.283802	-0.294848
17	6	0	-0.031536	-1.554067	-0.987872
18	1	0	1.042912	-3.351040	-0.432071
19	1	0	-0.546009	-2.024929	-1.825428
20	46	0	-1.074757	-0.001813	-0.154436
21	15	0	-1.454839	2.194341	1.065312
22	15	0	-3.386292	-1.039546	-0.099049
23	6	0	-3.602974	-2.478405	-1.304534
24	1	0	-3.542799	-2.101226	-2.329669
25	1	0	-2.787580	-3.190523	-1.151989
26	1	0	-4.564092	-2.983405	-1.159906
27	6	0	-3.855412	-1.883397	1.528486
28	1	0	-3.069199	-2.594189	1.797645
29	1	0	-3.924843	-1.131398	2.319721
30	1	0	-4.812033	-2.411493	1.446408
31	6	0	-4.972580	-0.064947	-0.450910
32	1	0	-5.072686	0.741791	0.281012
33	1	0	-4.907285	0.379679	-1.448233
34	1	0	-5.858908	-0.707109	-0.399783
35	6	0	-2.905235	2.540720	2.235018
36	1	0	-3.846140	2.482837	1.679384
37	1	0	-2.920601	1.783096	3.024266
38	1	0	-2.822459	3.532587	2.693245
39	6	0	-1.511429	3.745841	-0.015555
40	1	0	-0.622841	3.754884	-0.651693
41	1	0	-2.399615	3.717442	-0.653463
42	1	0	-1.530750	4.655480	0.594843
43	6	0	0.003479	2.613162	2.190598
44	1	0	0.061880	1.871536	2.992229
45	1	0	0.923673	2.560871	1.602885
46	1	0	-0.104641	3.612959	2.625885

System with *cis* methyl groups on the enamine carbons:

A, the **A→B** transition state structure, **B**, and the **B→C** transition state structure were recomputed using a reactant with *cis* methyl groups on the two alkene carbons of the enamine. Energies (kcal/mol) relative to that of **A:** +9.9 (**A→B**), -15.5 (**B**), +9.8 (**B→C**). Also, the predicted **E→D** barrier for this system is 1.7 kcal/mol. Although not by much, the **A→B** barrier is predicted to be larger for this system than that for the system shown in Figure 1, an effect that is likely to be larger with larger groups on the enamine or phosphines, since the [Pd(PR3)] group moves from the nitrogen over the enamine C=C bond during the **A→B** reaction.

A

```
Zero-point correction=              0.279009 (Hartree/Particle)
 Thermal correction to Energy=          0.299594
 Thermal correction to Enthalpy=         0.300538
 Thermal correction to Gibbs Free Energy=     0.228559
 Sum of electronic and zero-point Energies=      -625.148041
 Sum of electronic and thermal Energies=       -625.127456
 Sum of electronic and thermal Enthalpies=      -625.126512
 Sum of electronic and thermal Free Energies=     -625.198491
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.138358	0.501827	-2.383808
2	6	0	0.802646	0.194085	-1.068529
3	6	0	1.765739	-0.280910	-0.194012
4	6	0	3.096872	-0.461740	-0.557554
5	6	0	3.436768	-0.153474	-1.879569
6	6	0	2.471475	0.316971	-2.777360
7	1	0	0.417999	0.881450	-3.102272
8	1	0	3.841127	-0.832864	0.140600
9	1	0	4.462400	-0.280247	-2.212186
10	1	0	2.760478	0.550450	-3.798277
11	7	0	1.151104	-0.474462	1.137489
12	6	0	1.724750	0.496085	2.116091
13	1	0	1.756364	1.479397	1.646558
14	1	0	1.105272	0.548351	3.011326
15	1	0	2.741502	0.197815	2.398434
16	6	0	1.087795	-1.858652	1.634595
17	6	0	1.355663	-2.892864	0.820840
18	1	0	1.641099	-2.676338	-0.204467
19	46	0	-0.750607	0.224218	0.200418
20	15	0	-2.332978	0.971706	-1.433134
21	1	0	-3.446983	0.121647	-1.701500
22	1	0	-3.002821	2.205394	-1.179016
23	1	0	-1.854118	1.200067	-2.754066
24	15	0	-2.454499	0.182813	2.115832
25	1	0	-3.717540	0.836817	1.961192
26	1	0	-2.925196	-1.084949	2.579820
27	1	0	-2.077166	0.755252	3.370688
28	6	0	0.662789	-1.983755	3.074820
29	1	0	0.403558	-3.015366	3.312618
30	1	0	1.450774	-1.676230	3.772320
31	1	0	-0.217872	-1.367247	3.291980
32	6	0	1.312082	-4.355620	1.154307
33	1	0	2.299887	-4.807559	0.996532
34	1	0	1.011196	-4.571100	2.181671
35	1	0	0.621742	-4.879297	0.480342

TS A-to-B

```
Zero-point correction=                0.278059 (Hartree/Particle)
 Thermal correction to Energy=          0.298119
 Thermal correction to Enthalpy=         0.299064
 Thermal correction to Gibbs Free Energy=     0.228803
 Sum of electronic and zero-point Energies=      -625.132581
 Sum of electronic and thermal Energies=       -625.112520
 Sum of electronic and thermal Enthalpies=      -625.111576
 Sum of electronic and thermal Free Energies=     -625.181837
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.232688	0.300967	-0.133807
2	6	0	0.018122	0.202068	1.233738
3	6	0	1.082490	0.038560	2.123463
4	6	0	2.392278	-0.025948	1.650738
5	6	0	2.620118	0.085527	0.274107
6	6	0	1.552958	0.238832	-0.609737
7	1	0	-0.577661	0.409547	-0.848837
8	1	0	3.224298	-0.151257	2.337332
9	1	0	3.636302	0.045928	-0.105821
10	1	0	1.736166	0.306484	-1.678168
11	7	0	0.688815	-0.032958	3.516121
12	6	0	1.566596	0.710242	4.437916
13	1	0	1.832083	1.658236	3.967237
14	1	0	1.046240	0.927319	5.371012
15	1	0	2.487994	0.158634	4.672499
16	6	0	0.134781	-1.292911	3.982753
17	6	0	-0.058525	-2.346573	3.150058
18	1	0	0.320647	-2.272362	2.135515
19	46	0	-1.579547	0.184683	2.456175
20	15	0	-2.889554	1.207633	0.773166
21	1	0	-3.097167	0.456639	-0.419527
22	1	0	-4.227839	1.569700	1.103812
23	1	0	-2.392990	2.433686	0.246120
24	15	0	-3.405144	0.056104	4.251627
25	1	0	-3.306658	0.897243	5.403521
26	1	0	-4.763712	0.331985	3.899534
27	1	0	-3.599229	-1.200563	4.903410
28	6	0	-0.185625	-1.317369	5.457795
29	1	0	-0.815782	-2.170993	5.708561
30	1	0	0.728858	-1.408739	6.056183
31	1	0	-0.693992	-0.404147	5.786721
32	6	0	-0.687907	-3.670654	3.485913
33	1	0	-1.402423	-3.966642	2.708370
34	1	0	0.076374	-4.458751	3.520356
35	1	0	-1.212320	-3.684071	4.444632

B

```
Zero-point correction=                0.279194 (Hartree/Particle)
 Thermal correction to Energy=          0.299569
 Thermal correction to Enthalpy=         0.300513
 Thermal correction to Gibbs Free Energy=     0.229859
 Sum of electronic and zero-point Energies=      -625.174041
 Sum of electronic and thermal Energies=       -625.153667
 Sum of electronic and thermal Enthalpies=      -625.152723
 Sum of electronic and thermal Free Energies=     -625.223376
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.839689	-0.102290	-2.194626
2	6	0	0.831799	-0.010727	-0.800067
3	6	0	2.074870	-0.041049	-0.132002
4	6	0	3.276226	-0.120791	-0.847576
5	6	0	3.258322	-0.159007	-2.241085
6	6	0	2.039519	-0.151958	-2.915898
7	1	0	-0.097220	-0.125982	-2.744044
8	1	0	4.223484	-0.193489	-0.321251
9	1	0	4.192939	-0.216718	-2.789841
10	1	0	2.014517	-0.185435	-4.001290
11	7	0	2.105582	-0.018401	1.303210
12	6	0	3.024793	0.921430	1.967988
13	1	0	3.775456	1.243181	1.250121
14	1	0	2.481426	1.808220	2.314365
15	1	0	3.524948	0.448216	2.815306
16	6	0	1.171390	-0.689298	1.989548
17	6	0	0.270097	-1.599394	1.320579
18	1	0	0.735907	-2.066809	0.451233
19	46	0	-0.901024	-0.093239	0.286566
20	15	0	-1.808455	1.820325	-1.042248
21	1	0	-1.874357	1.677904	-2.462607
22	1	0	-3.105781	2.379632	-0.809255
23	1	0	-1.030313	3.015563	-0.970715
24	15	0	-3.052626	-0.382077	1.607824
25	1	0	-4.174510	0.461565	1.329414
26	1	0	-3.708786	-1.648825	1.508717
27	1	0	-3.047563	-0.255218	3.033337
28	6	0	-0.509403	-2.625667	2.132973
29	1	0	-1.165522	-3.198020	1.471149
30	1	0	0.165373	-3.347508	2.614190
31	1	0	-1.131829	-2.189733	2.920430
32	6	0	1.117835	-0.486974	3.479108
33	1	0	1.954524	-1.014249	3.957007
34	1	0	1.193128	0.567571	3.758524
35	1	0	0.198810	-0.893144	3.898094

TS B-to-C

```
Zero-point correction=                0.276047 (Hartree/Particle)
 Thermal correction to Energy=          0.296965
 Thermal correction to Enthalpy=        0.297909
 Thermal correction to Gibbs Free Energy=     0.224604
 Sum of electronic and zero-point Energies=      -625.128492
 Sum of electronic and thermal Energies=       -625.107573
 Sum of electronic and thermal Enthalpies=      -625.106629
 Sum of electronic and thermal Free Energies=     -625.179934
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.065382	0.217955	0.140905
2	6	0	-0.050091	0.189216	1.536214
3	6	0	1.197621	0.120370	2.199459
4	6	0	2.398182	0.231719	1.506217
5	6	0	2.360184	0.377655	0.114140
6	6	0	1.140788	0.351817	-0.562367
7	1	0	-1.004752	0.181791	-0.401012
8	1	0	3.352382	0.170938	2.019351
9	1	0	3.289025	0.476434	-0.438061
10	1	0	1.118963	0.445481	-1.644149
11	7	0	1.092535	-0.174553	3.593026
12	6	0	2.165555	0.189074	4.514704
13	1	0	2.296574	1.277202	4.533270
14	1	0	1.940880	-0.171762	5.516575
15	1	0	3.100026	-0.275487	4.190235
16	6	0	-0.142812	-0.568454	3.948331
17	6	0	-0.986116	-0.959949	2.826858
18	1	0	-0.495525	-1.726578	2.220755
19	46	0	-1.533977	1.310291	2.593756
20	15	0	-2.715092	2.660432	0.711539
21	1	0	-1.992532	3.769915	0.157122
22	1	0	-3.035731	2.022015	-0.535024
23	1	0	-3.970599	3.336238	0.888396
24	15	0	-2.237018	2.735355	4.523221
25	1	0	-1.685751	4.057388	4.566455
26	1	0	-3.618249	3.100677	4.645452
27	1	0	-2.015689	2.398822	5.902979
28	6	0	-2.436067	-1.395192	3.023933
29	1	0	-2.948158	-1.423271	2.058334
30	1	0	-2.459574	-2.416235	3.430363
31	1	0	-3.008841	-0.741310	3.685799
32	6	0	-0.523660	-0.751820	5.385163
33	1	0	-0.033654	-1.650400	5.785305
34	1	0	-0.227341	0.094707	6.010708
35	1	0	-1.599745	-0.896111	5.480938

E

```
Zero-point correction=                0.264693 (Hartree/Particle)
 Thermal correction to Energy=          0.285293
 Thermal correction to Enthalpy=         0.286237
 Thermal correction to Gibbs Free Energy=     0.214782
 Sum of electronic and zero-point Energies=      -624.744098
 Sum of electronic and thermal Energies=       -624.723498
 Sum of electronic and thermal Enthalpies=      -624.722554
 Sum of electronic and thermal Free Energies=     -624.794009
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.425588	1.399062	-1.521779
2	6	0	-0.441527	1.119509	-0.563266
3	6	0	-0.261558	2.034777	0.497852
4	6	0	-1.147543	3.122610	0.633404
5	6	0	-2.151382	3.347795	-0.308021
6	6	0	-2.279838	2.502367	-1.408406
7	1	0	-1.544090	0.738264	-2.378165
8	1	0	-1.029523	3.824782	1.453020
9	1	0	-2.811301	4.204081	-0.190134
10	1	0	-3.037255	2.688843	-2.166142
11	7	0	0.820310	1.877125	1.381939
12	6	0	0.781724	2.542949	2.671081
13	1	0	-0.231236	2.476545	3.079265
14	1	0	1.450115	2.036867	3.372021
15	1	0	1.064809	3.608352	2.638298
16	6	0	2.052267	1.392194	0.856818
18	15	0	-1.777982	-1.890792	-0.882235
19	1	0	-2.473027	-1.712107	-2.126570
20	1	0	-2.033411	-3.303579	-0.746334
21	1	0	-2.831347	-1.437361	-0.023171
22	15	0	1.712968	-2.895565	-0.183910
23	1	0	2.797145	-2.897704	0.755437
24	1	0	1.029364	-4.048597	0.339267
25	1	0	2.398413	-3.583187	-1.247177
26	46	0	0.458947	-0.702678	-0.506219
27	6	0	3.280509	2.101306	1.396534
28	1	0	3.199768	3.190406	1.278092
29	1	0	3.432191	1.906235	2.465857
30	1	0	4.187518	1.772524	0.887819
31	6	0	3.309266	0.097380	-0.920156
32	1	0	4.118930	0.832199	-0.823129
33	1	0	3.737969	-0.882906	-0.658418
34	1	0	3.057859	0.048217	-1.986565

TS E-to-D

```
Zero-point correction=                0.263086 (Hartree/Particle)
 Thermal correction to Energy=            0.283575
 Thermal correction to Enthalpy=          0.284520
 Thermal correction to Gibbs Free Energy=     0.212585
 Sum of electronic and zero-point Energies=      -624.739166
 Sum of electronic and thermal Energies=       -624.718676
 Sum of electronic and thermal Enthalpies=      -624.717732
 Sum of electronic and thermal Free Energies=     -624.789666
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.256042	1.513188	-1.222152
2	6	0	0.956147	0.276267	-0.622554
3	6	0	1.972973	-0.358846	0.133422
4	6	0	3.165203	0.321089	0.438721
5	6	0	3.403634	1.580136	-0.110404
6	6	0	2.469231	2.161438	-0.974492
7	1	0	0.518797	1.994168	-1.861240
8	1	0	3.929352	-0.149158	1.050751
9	1	0	4.339663	2.088798	0.106473
10	1	0	2.674739	3.124821	-1.435546
11	7	0	1.770287	-1.708702	0.419263
12	6	0	2.690528	-2.425446	1.280185
13	1	0	2.871776	-1.844324	2.190373
14	1	0	2.254875	-3.379675	1.579786
15	1	0	3.663495	-2.622745	0.802991
16	6	0	0.884854	-2.358387	-0.465038
17	6	0	-0.033973	-1.602385	-1.125114
18	46	0	-1.019346	-0.076112	-0.153761
19	15	0	-1.467103	2.153920	1.000291
20	1	0	-1.400834	3.318682	0.159246
21	1	0	-2.569851	2.613878	1.814647
22	1	0	-0.424714	2.548074	1.905771
23	15	0	-3.295451	-1.128519	0.244378
24	1	0	-3.483737	-2.506676	-0.124959
25	1	0	-3.758121	-1.268147	1.601267
26	1	0	-4.547492	-0.650784	-0.291095
27	6	0	-0.721290	-2.008240	-2.406251
28	1	0	-0.220609	-2.844178	-2.914633
29	1	0	-1.774495	-2.290126	-2.259016
30	1	0	-0.724661	-1.168549	-3.111238
31	6	0	1.134546	-3.826716	-0.715044
32	1	0	2.178621	-4.032993	-0.988794
33	1	0	0.906495	-4.437205	0.169313
34	1	0	0.495103	-4.192606	-1.520452

System with terminal CO_2Me on enamine:

A, the **A→B** transition state structure, and **B** were recomputed using a reactant with a carbomethoxy group on the terminal alkene carbon of the enamine. Energies (kcal/mol) relative to that of **A:** +6.0 (**A→B**), -16.6 (**B**). Also, the predicted **E→D** barrier for this system is 4.1 kcal/mol. This suggests that the inherent electronic effect of a terminal ester actually favors reaction.

A

```
Zero-point correction=                0.265812 (Hartree/Particle)
 Thermal correction to Energy=           0.288038
 Thermal correction to Enthalpy=          0.288982
 Thermal correction to Gibbs Free Energy=     0.211222
 Sum of electronic and zero-point Energies=      -774.405341
 Sum of electronic and thermal Energies=       -774.383115
 Sum of electronic and thermal Enthalpies=      -774.382171
 Sum of electronic and thermal Free Energies=     -774.459931
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.177211	0.577623	-2.430272
2	6	0	0.842326	0.259894	-1.118287
3	6	0	1.810032	-0.218992	-0.248376
4	6	0	3.137586	-0.409042	-0.614432
5	6	0	3.475605	-0.091626	-1.935372
6	6	0	2.510715	0.392827	-2.825558
7	1	0	0.455960	0.959169	-3.146680
8	1	0	3.880584	-0.787371	0.081520
9	1	0	4.499256	-0.222266	-2.272122
10	1	0	2.798524	0.633076	-3.845181
11	7	0	1.200015	-0.438837	1.079040
12	6	0	1.716129	0.486350	2.128013
13	1	0	1.669327	1.509059	1.753625
14	1	0	1.099282	0.394544	3.025298
15	1	0	2.752496	0.235068	2.379451
16	6	0	1.088868	-1.786106	1.536914
17	6	0	1.321482	-2.901854	0.835150
18	1	0	0.750066	-1.871318	2.566470
19	1	0	1.675766	-2.904629	-0.189022
20	46	0	-0.720388	0.209635	0.142622
21	15	0	-2.310524	0.986809	-1.456265
22	1	0	-3.361877	0.091839	-1.812093
23	1	0	-3.055263	2.151637	-1.108655
24	1	0	-1.821597	1.352378	-2.741705
25	15	0	-2.387358	-0.091178	2.063813
26	1	0	-3.578406	0.695081	2.145517
27	1	0	-2.959483	-1.390075	2.226235
28	1	0	-1.902296	0.110810	3.392936
29	6	0	1.074770	-4.205451	1.504533
30	8	0	0.597629	-4.333313	2.616604
31	8	0	1.450853	-5.222235	0.712566
32	6	0	1.269818	-6.542674	1.263698
33	1	0	1.619256	-7.228428	0.492751
34	1	0	1.857471	-6.654778	2.177958
35	1	0	0.215213	-6.717363	1.490177

TS A-to-B

```
Zero-point correction=                0.265216 (Hartree/Particle)
 Thermal correction to Energy=           0.286677
 Thermal correction to Enthalpy=         0.287621
 Thermal correction to Gibbs Free Energy=     0.213111
 Sum of electronic and zero-point Energies=      -774.397662
 Sum of electronic and thermal Energies=       -774.376202
 Sum of electronic and thermal Enthalpies=      -774.375257
 Sum of electronic and thermal Free Energies=     -774.449767
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.321098	0.570909	-0.161858
2	6	0	0.104844	0.333853	1.189573
3	6	0	1.169761	-0.000709	2.028006
4	6	0	2.470144	-0.111225	1.543710
5	6	0	2.691924	0.129002	0.183246
6	6	0	1.629653	0.461126	-0.658989
7	1	0	-0.481660	0.825775	-0.847659
8	1	0	3.291910	-0.370935	2.205034
9	1	0	3.697377	0.052630	-0.218481
10	1	0	1.811030	0.633296	-1.715987
11	7	0	0.778749	-0.186248	3.415625
12	6	0	1.515383	0.567086	4.443313
13	1	0	1.639374	1.598480	4.109317
14	1	0	0.944627	0.557807	5.375683
15	1	0	2.501891	0.127095	4.633933
16	6	0	0.146482	-1.373217	3.798447
17	6	0	-0.160641	-2.444419	3.026579
18	1	0	0.193265	-2.567280	2.010118
19	46	0	-1.468352	0.268534	2.449099
20	15	0	-2.863921	1.338258	0.880068
21	1	0	-3.059880	0.663628	-0.358541
22	1	0	-4.206712	1.601053	1.274161
23	1	0	-2.440067	2.623932	0.439625
24	15	0	-3.167640	-0.171006	4.307814
25	1	0	-4.573662	-0.066230	4.079961
26	1	0	-3.061591	-1.518237	4.774453
27	1	0	-3.078569	0.545622	5.540195
28	1	0	-0.153554	-1.387259	4.844178
29	6	0	-1.003864	-3.495147	3.624178
30	8	0	-1.628677	-3.377314	4.671336
31	8	0	-1.013109	-4.602579	2.867087
32	6	0	-1.794018	-5.705272	3.369958
33	1	0	-2.843155	-5.415827	3.469917
34	1	0	-1.681353	-6.498657	2.632024
35	1	0	-1.414899	-6.025586	4.343154

B

```
Zero-point correction=                0.266502 (Hartree/Particle)
 Thermal correction to Energy=          0.288309
 Thermal correction to Enthalpy=         0.289253
 Thermal correction to Gibbs Free Energy=     0.214341
 Sum of electronic and zero-point Energies=      -774.434925
 Sum of electronic and thermal Energies=       -774.413119
 Sum of electronic and thermal Enthalpies=      -774.412175
 Sum of electronic and thermal Free Energies=     -774.487087
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.908021	-0.298477	-2.216977
2	6	0	0.853724	-0.136242	-0.832052
3	6	0	2.078644	-0.025447	-0.135392
4	6	0	3.300887	-0.003650	-0.815187
5	6	0	3.323213	-0.113761	-2.205615
6	6	0	2.129423	-0.272537	-2.905249
7	1	0	-0.007021	-0.434101	-2.786684
8	1	0	4.234481	0.062234	-0.265043
9	1	0	4.272455	-0.096149	-2.731341
10	1	0	2.138357	-0.367844	-3.987162
11	7	0	2.058255	0.046828	1.297644
12	6	0	2.976298	0.961826	1.990597
13	1	0	2.938713	1.945242	1.515458
14	1	0	2.678505	1.043057	3.037129
15	1	0	4.000304	0.580459	1.947997
16	6	0	1.142207	-0.638742	1.959720
17	6	0	0.285286	-1.623333	1.381674
18	1	0	0.703941	-2.217567	0.571193
19	46	0	-0.899856	-0.193667	0.241560
20	15	0	-1.807046	1.573077	-1.218232
21	1	0	-1.875190	1.288191	-2.615186
22	1	0	-3.115573	2.111931	-1.016257
23	1	0	-1.049806	2.781496	-1.255261
24	15	0	-2.960936	-0.281530	1.717887
25	1	0	-2.832527	0.285422	3.020104
26	1	0	-4.161239	0.367984	1.290674
27	1	0	-3.499477	-1.555100	2.068439
28	1	0	1.043630	-0.428504	3.022565
29	6	0	-0.514045	-2.403162	2.370614
30	8	0	-0.877034	-1.980656	3.456127
31	8	0	-0.787092	-3.630979	1.906794
32	6	0	-1.520006	-4.498625	2.798691
33	1	0	-1.625204	-5.440129	2.261551
34	1	0	-0.964036	-4.641361	3.727853
35	1	0	-2.500292	-4.073126	3.027667

E

```
Zero-point correction=                0.253494 (Hartree/Particle)
 Thermal correction to Energy=          0.274805
 Thermal correction to Enthalpy=         0.275749
 Thermal correction to Gibbs Free Energy=     0.202548
 Sum of electronic and zero-point Energies=      -774.018981
 Sum of electronic and thermal Energies=       -773.997671
 Sum of electronic and thermal Enthalpies=      -773.996727
 Sum of electronic and thermal Free Energies=     -774.069927
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.526829	1.369537	-1.449611
2	6	0	-0.501574	1.113374	-0.524585
3	6	0	-0.306909	2.056973	0.509067
4	6	0	-1.213335	3.126280	0.663649
5	6	0	-2.253557	3.318561	-0.241980
6	6	0	-2.398292	2.455077	-1.325482
7	1	0	-1.655049	0.704255	-2.300290
8	1	0	-1.094864	3.836634	1.473921
9	1	0	-2.930780	4.158015	-0.107221
10	1	0	-3.182764	2.613622	-2.061373
11	7	0	0.826585	1.984634	1.349553
12	6	0	0.946985	2.900743	2.476048
13	1	0	0.076953	2.811553	3.134949
14	1	0	1.835769	2.637289	3.051229
15	1	0	1.035265	3.948544	2.155477
16	6	0	1.961944	1.334689	0.928034
17	6	0	2.054784	0.373277	-0.026111
18	1	0	2.875423	1.682953	1.407016
19	15	0	-1.776348	-1.892548	-0.998056
20	1	0	-2.464067	-1.810214	-2.257140
21	1	0	-1.952754	-3.306099	-0.794441
22	1	0	-2.855881	-1.448202	-0.169111
23	15	0	1.675641	-2.906007	-0.547898
24	1	0	2.850492	-2.993340	0.263358
25	1	0	1.028904	-4.099163	-0.064305
26	1	0	2.217961	-3.472652	-1.748243
27	46	0	0.435352	-0.691057	-0.601969
28	6	0	3.432677	0.069161	-0.432126
29	8	0	4.457914	0.538928	0.044386
30	8	0	3.504815	-0.829030	-1.473072
31	6	0	4.830762	-1.097054	-1.940052
32	1	0	5.442957	-1.552360	-1.154966
33	1	0	4.715007	-1.784361	-2.780719
34	1	0	5.319856	-0.175711	-2.267989

TS E-to-D

```
Zero-point correction=                0.250640 (Hartree/Particle)
 Thermal correction to Energy=          0.272426
 Thermal correction to Enthalpy=         0.273370
 Thermal correction to Gibbs Free Energy=     0.197580
 Sum of electronic and zero-point Energies=      -774.007462
 Sum of electronic and thermal Energies=       -773.985676
 Sum of electronic and thermal Enthalpies=      -773.984732
 Sum of electronic and thermal Free Energies=     -774.060521
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.180593	1.491601	-1.240696
2	6	0	0.914876	0.267793	-0.593003
3	6	0	1.975716	-0.331308	0.133421
4	6	0	3.171138	0.363209	0.379538
5	6	0	3.367329	1.614031	-0.199835
6	6	0	2.389266	2.159419	-1.042506
7	1	0	0.418313	1.940489	-1.871915
8	1	0	3.960368	-0.086967	0.974446
9	1	0	4.299522	2.145085	-0.027232
10	1	0	2.562676	3.116665	-1.528520
11	7	0	1.813127	-1.691680	0.415699
12	6	0	2.820875	-2.457990	1.127175
13	1	0	2.964967	-2.061566	2.138197
14	1	0	2.484941	-3.493292	1.208716
15	1	0	3.786127	-2.439614	0.603820
16	6	0	0.850936	-2.297607	-0.345832
17	6	0	-0.063362	-1.535012	-1.025724
18	1	0	0.935205	-3.371716	-0.484965
19	46	0	-1.058320	-0.009772	-0.053762
20	15	0	-1.419550	2.126935	1.260113
21	1	0	-1.571778	3.356953	0.528239
22	1	0	-2.428384	2.410690	2.252611
23	1	0	-0.293877	2.545633	2.047758
24	15	0	-3.417040	-0.949535	0.042569
25	1	0	-3.575474	-2.299431	-0.423221
26	1	0	-4.214522	-1.093780	1.235225
27	1	0	-4.456265	-0.372231	-0.769422
28	6	0	-0.728920	-2.185449	-2.163369
29	8	0	-0.539087	-3.331854	-2.546129
30	8	0	-1.616992	-1.363240	-2.803012
31	6	0	-2.226623	-1.929705	-3.967522
32	1	0	-2.857109	-1.141446	-4.382879
33	1	0	-1.468646	-2.234447	-4.694934
34	1	0	-2.830247	-2.805679	-3.709605

System with internal CO_2Me on enamine:

A

```
Zero-point correction=              0.266540 (Hartree/Particle)
 Thermal correction to Energy=          0.288017
 Thermal correction to Enthalpy=         0.288962
 Thermal correction to Gibbs Free Energy=     0.215323
 Sum of electronic and zero-point Energies=      -774.403370
 Sum of electronic and thermal Energies=       -774.381893
 Sum of electronic and thermal Enthalpies=      -774.380949
 Sum of electronic and thermal Free Energies=     -774.454588
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.117188	0.481918	-2.409994
2	6	0	0.778782	0.165158	-1.097620
3	6	0	1.759223	-0.241102	-0.205459
4	6	0	3.105402	-0.329674	-0.547759
5	6	0	3.445491	-0.014623	-1.868542
6	6	0	2.464356	0.377592	-2.785486
7	1	0	0.385022	0.809049	-3.142332
8	1	0	3.865116	-0.631363	0.167273
9	1	0	4.482770	-0.074295	-2.183213
10	1	0	2.751175	0.615741	-3.805905
11	7	0	1.145444	-0.485893	1.117150
12	6	0	1.705930	0.428739	2.160981
13	1	0	1.691135	1.445438	1.767215
14	1	0	1.095356	0.371456	3.059850
15	1	0	2.738836	0.146093	2.394603
16	6	0	1.121081	-1.880524	1.526567
17	6	0	1.615223	-2.889832	0.797080
18	1	0	1.527621	-3.904368	1.163924
19	1	0	2.089775	-2.739679	-0.164468
20	46	0	-0.774972	0.220147	0.170176
21	15	0	-2.344902	0.947582	-1.464740
22	1	0	-3.510896	0.144661	-1.635126
23	1	0	-2.932954	2.231604	-1.267933
24	1	0	-1.898415	1.060500	-2.811649
25	15	0	-2.445978	0.345510	2.093989
26	1	0	-3.656183	1.094411	1.935822
27	1	0	-2.988986	-0.865638	2.610664
28	1	0	-1.966957	0.934004	3.299078
29	6	0	0.395957	-2.158166	2.812642
30	8	0	-0.397033	-1.387249	3.328811
31	8	0	0.707322	-3.351586	3.318815
32	6	0	0.016140	-3.734632	4.529396
33	1	0	0.424999	-4.708370	4.794243
34	1	0	0.207653	-3.004169	5.318069
35	1	0	-1.058485	-3.802761	4.344935

TS A-to-B

```
Zero-point correction=                0.264998 (Hartree/Particle)
 Thermal correction to Energy=           0.286304
 Thermal correction to Enthalpy=         0.287248
 Thermal correction to Gibbs Free Energy=     0.213585
 Sum of electronic and zero-point Energies=      -774.384101
 Sum of electronic and thermal Energies=       -774.362795
 Sum of electronic and thermal Enthalpies=      -774.361851
 Sum of electronic and thermal Free Energies=     -774.435514
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.226725	0.365334	-0.118339
2	6	0	0.011827	0.206994	1.243974
3	6	0	1.083942	-0.015933	2.117809
4	6	0	2.389606	-0.061565	1.630438
5	6	0	2.613468	0.121854	0.261241
6	6	0	1.542745	0.320474	-0.607757
7	1	0	-0.586875	0.510483	-0.823174
8	1	0	3.222807	-0.235623	2.304737
9	1	0	3.628022	0.095683	-0.124025
10	1	0	1.718551	0.439579	-1.672853
11	7	0	0.724640	-0.193237	3.504416
12	6	0	1.626619	0.409664	4.502639
13	1	0	1.933956	1.390192	4.135756
14	1	0	1.092797	0.542354	5.443288
15	1	0	2.519947	-0.205648	4.675031
16	6	0	0.092097	-1.424612	3.831843
17	6	0	-0.157656	-2.439142	2.970955
18	1	0	0.182292	-2.431474	1.942948
19	46	0	-1.615619	0.187244	2.437231
20	15	0	-2.768974	1.500233	0.849363
21	1	0	-3.013828	0.897312	-0.417384
22	1	0	-4.073996	1.950737	1.200640
23	1	0	-2.140490	2.718548	0.467084
24	15	0	-3.461717	0.172568	4.209559
25	1	0	-4.803599	0.498939	3.835108
26	1	0	-3.712313	-1.035879	4.923289
27	1	0	-3.293565	1.069401	5.304073
28	1	0	-0.701127	-3.309014	3.316890
29	6	0	-0.424922	-1.528843	5.251054
30	8	0	-0.964286	-0.611929	5.844935
31	8	0	-0.238820	-2.749012	5.751809
32	6	0	-0.733689	-2.971936	7.093641
33	1	0	-0.455291	-3.996852	7.332877
34	1	0	-0.267376	-2.267930	7.785695
35	1	0	-1.818731	-2.847688	7.121927

B

```
Zero-point correction=                0.266043 (Hartree/Particle)
 Thermal correction to Energy=          0.287827
 Thermal correction to Enthalpy=         0.288771
 Thermal correction to Gibbs Free Energy=     0.213582
 Sum of electronic and zero-point Energies=      -774.421496
 Sum of electronic and thermal Energies=       -774.399711
 Sum of electronic and thermal Enthalpies=      -774.398767
 Sum of electronic and thermal Free Energies=     -774.473956
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.010860	0.116646	-0.519017
2	6	0	-1.675041	0.354817	-0.185525
3	6	0	-1.281641	1.698162	0.005425
4	6	0	-2.208742	2.746302	-0.079275
5	6	0	-3.544323	2.472932	-0.367230
6	6	0	-3.945622	1.157692	-0.591210
7	1	0	-3.348840	-0.896725	-0.715717
8	1	0	-1.882684	3.775066	0.038453
9	1	0	-4.257915	3.287862	-0.434073
10	1	0	-4.984174	0.933438	-0.816797
11	7	0	0.091060	2.015111	0.285374
12	6	0	0.358055	3.062779	1.296878
13	1	0	-0.510903	3.117601	1.950974
14	1	0	1.240599	2.812010	1.881507
15	1	0	0.528705	4.027741	0.813672
16	6	0	1.035333	1.305327	-0.322470
17	6	0	0.745393	0.333466	-1.342039
18	1	0	1.632136	-0.071138	-1.819515
19	1	0	-0.023305	0.634838	-2.055597
20	46	0	-0.275756	-1.143938	-0.204123
21	15	0	-1.674155	-2.533403	1.318973
22	1	0	-3.027458	-2.781465	0.934688
23	1	0	-1.301261	-3.857077	1.713743
24	1	0	-1.901448	-1.965776	2.609231
25	15	0	1.553347	-2.863045	-0.456338
26	1	0	2.380563	-3.170666	0.669647
27	1	0	1.225557	-4.196917	-0.855673
28	1	0	2.578019	-2.591412	-1.414759
29	6	0	2.486798	1.588913	0.014515
30	8	0	2.920961	2.707464	0.171492
31	8	0	3.210518	0.465616	0.052305
32	6	0	4.632246	0.655517	0.282314
33	1	0	5.056444	-0.347027	0.292802
34	1	0	5.061921	1.254411	-0.523074
35	1	0	4.792126	1.157377	1.238437

System with internal methyl group and terminal CO_2Me group on the enamine:

A

```
Zero-point correction=                0.294122 (Hartree/Particle)
 Thermal correction to Energy=          0.317628
 Thermal correction to Enthalpy=         0.318572
 Thermal correction to Gibbs Free Energy=     0.238311
 Sum of electronic and zero-point Energies=      -813.690035
 Sum of electronic and thermal Energies=       -813.666529
 Sum of electronic and thermal Enthalpies=      -813.665584
 Sum of electronic and thermal Free Energies=     -813.745845
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.181019	0.342899	-2.360793
2	6	0	0.832064	0.117157	-1.032831
3	6	0	1.783232	-0.316743	-0.123980
4	6	0	3.112558	-0.541478	-0.467374
5	6	0	3.466089	-0.316144	-1.802250
6	6	0	2.514453	0.117663	-2.732191
7	1	0	0.470988	0.686672	-3.106777
8	1	0	3.844740	-0.884873	0.257482
9	1	0	4.491284	-0.479593	-2.119519
10	1	0	2.813236	0.286954	-3.762830
11	7	0	1.169541	-0.422461	1.218456
12	6	0	1.723622	0.618467	2.134943
13	1	0	1.751635	1.564791	1.595210
14	1	0	1.093612	0.727821	3.016813
15	1	0	2.739973	0.352037	2.447377
16	6	0	1.053333	-1.756423	1.794007
17	6	0	1.237673	-2.843129	1.016553
18	1	0	1.518786	-2.730523	-0.022861
19	46	0	-0.740873	0.203865	0.209288
20	15	0	-2.289627	0.866946	-1.480602
21	1	0	-3.378768	-0.016776	-1.738335
22	1	0	-2.985899	2.093816	-1.272480
23	1	0	-1.786642	1.063278	-2.797206
24	15	0	-2.483721	0.169384	2.089880
25	1	0	-3.798130	0.685259	1.862855
26	1	0	-2.837903	-1.103991	2.632851
27	1	0	-2.190503	0.864298	3.304167
28	6	0	1.076143	-4.252641	1.452316
29	8	0	0.699216	-4.659451	2.536864
30	8	0	1.412714	-5.066471	0.432126
31	6	0	1.315726	-6.478336	0.702966
32	1	0	1.632482	-6.971234	-0.215612
33	1	0	1.969430	-6.751468	1.534844
34	1	0	0.286600	-6.748229	0.952656
35	6	0	0.691379	-1.799412	3.253105
36	1	0	0.437753	-2.821039	3.532350
37	1	0	1.529778	-1.472106	3.879680
38	1	0	-0.155583	-1.140288	3.477482

TS A-to-B

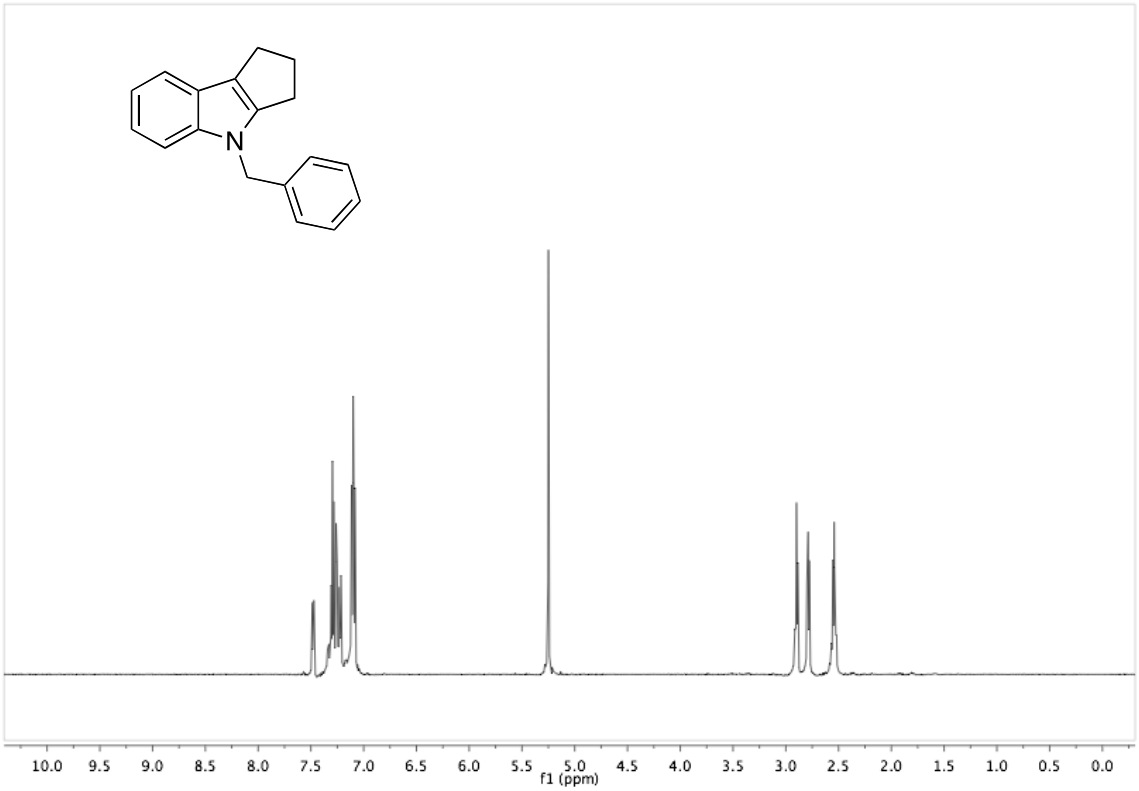
Zero-point correction= 0.293579 (Hartree/Particle)
Thermal correction to Energy= 0.316325
Thermal correction to Enthalpy= 0.317270
Thermal correction to Gibbs Free Energy= 0.240271
Sum of electronic and zero-point Energies= -813.681369
Sum of electronic and thermal Energies= -813.658622
Sum of electronic and thermal Enthalpies= -813.657678
Sum of electronic and thermal Free Energies= -813.734676

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.744160	-0.791698	-1.333204
2	6	0	1.787127	-0.494209	-0.370367
3	6	0	1.349423	-1.470656	0.522640
4	6	0	1.840996	-2.773017	0.466733
5	6	0	2.803446	-3.079517	-0.500606
6	6	0	3.248663	-2.100010	-1.390238
7	1	0	3.104765	-0.057746	-2.048056
8	1	0	1.491523	-3.529372	1.163998
9	1	0	3.205506	-4.086103	-0.558639
10	1	0	3.989995	-2.350049	-2.143709
11	7	0	0.391534	-0.988547	1.510900
12	6	0	0.806988	-1.205084	2.911703
13	1	0	1.883795	-1.043940	2.972501
14	1	0	0.312943	-0.496807	3.576146
15	1	0	0.580680	-2.224738	3.248993
16	6	0	-0.991187	-0.937336	1.179194
17	6	0	-1.420031	-1.212481	-0.087495
18	1	0	-0.746863	-1.666663	-0.804268
19	46	0	0.600039	1.060015	0.090456
20	15	0	1.894956	2.527611	-1.224743
21	1	0	1.872494	2.305866	-2.631657
22	1	0	1.579526	3.914541	-1.154141
23	1	0	3.294308	2.542088	-0.963509
24	15	0	-1.324699	2.644213	0.677877
25	1	0	-1.509710	3.857895	-0.052797
26	1	0	-2.579920	2.000700	0.443686
27	1	0	-1.524514	3.144281	2.000977
28	6	0	-2.774592	-0.928249	-0.591352
29	8	0	-3.586786	-0.142465	-0.116432
30	8	0	-3.005649	-1.628793	-1.716594
31	6	0	-4.292685	-1.428695	-2.332289
32	1	0	-4.423295	-0.381083	-2.615258
33	1	0	-4.293056	-2.069038	-3.213748
34	1	0	-5.091970	-1.716923	-1.645495
35	6	0	-1.912933	-0.568199	2.313064
36	1	0	-2.921884	-0.412680	1.937465
37	1	0	-1.932208	-1.378949	3.051648
38	1	0	-1.585283	0.335487	2.839094

B

```
Zero-point correction=                0.294951 (Hartree/Particle)
 Thermal correction to Energy=          0.318050
 Thermal correction to Enthalpy=         0.318994
 Thermal correction to Gibbs Free Energy=     0.241926
 Sum of electronic and zero-point Energies=      -813.722558
 Sum of electronic and thermal Energies=       -813.699459
 Sum of electronic and thermal Enthalpies=      -813.698515
 Sum of electronic and thermal Free Energies=     -813.775583
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.821507	-0.335013	-2.143500
2	6	0	0.805207	-0.117228	-0.764361
3	6	0	2.042290	-0.079265	-0.085607
4	6	0	3.248920	-0.220728	-0.781032
5	6	0	3.241028	-0.389810	-2.165440
6	6	0	2.027849	-0.449517	-2.847204
7	1	0	-0.111512	-0.413015	-2.694473
8	1	0	4.192395	-0.238148	-0.243357
9	1	0	4.179935	-0.495638	-2.699398
10	1	0	2.011533	-0.586624	-3.924533
11	7	0	2.061135	0.076206	1.345360
12	6	0	2.978668	1.071381	1.929804
13	1	0	3.710273	1.355138	1.177354
14	1	0	2.426950	1.969532	2.228323
15	1	0	3.498497	0.661366	2.797798
16	6	0	1.135370	-0.535938	2.091079
17	6	0	0.274919	-1.523086	1.475074
18	1	0	0.754929	-2.076744	0.671310
19	46	0	-0.918841	-0.094609	0.340881
20	15	0	-1.808980	1.678285	-1.122974
21	1	0	-1.848125	1.406337	-2.523733
22	1	0	-3.123247	2.212016	-0.943517
23	1	0	-1.057538	2.891299	-1.137222
24	15	0	-2.980002	-0.148636	1.820713
25	1	0	-2.833020	0.298626	3.166382
26	1	0	-4.122180	0.625536	1.441042
27	1	0	-3.615279	-1.402500	2.057685
28	6	0	-0.568453	-2.433737	2.307907
29	8	0	-1.215634	-2.139212	3.302116
30	8	0	-0.554103	-3.667151	1.779028
31	6	0	-1.340915	-4.665603	2.462948
32	1	0	-1.182776	-5.586882	1.904030
33	1	0	-1.000956	-4.774118	3.495133
34	1	0	-2.397798	-4.387859	2.457559
35	6	0	1.056209	-0.190873	3.551375
36	1	0	0.168401	-0.635016	3.996853
37	1	0	1.938284	-0.586925	4.072150
38	1	0	1.045103	0.891933	3.710460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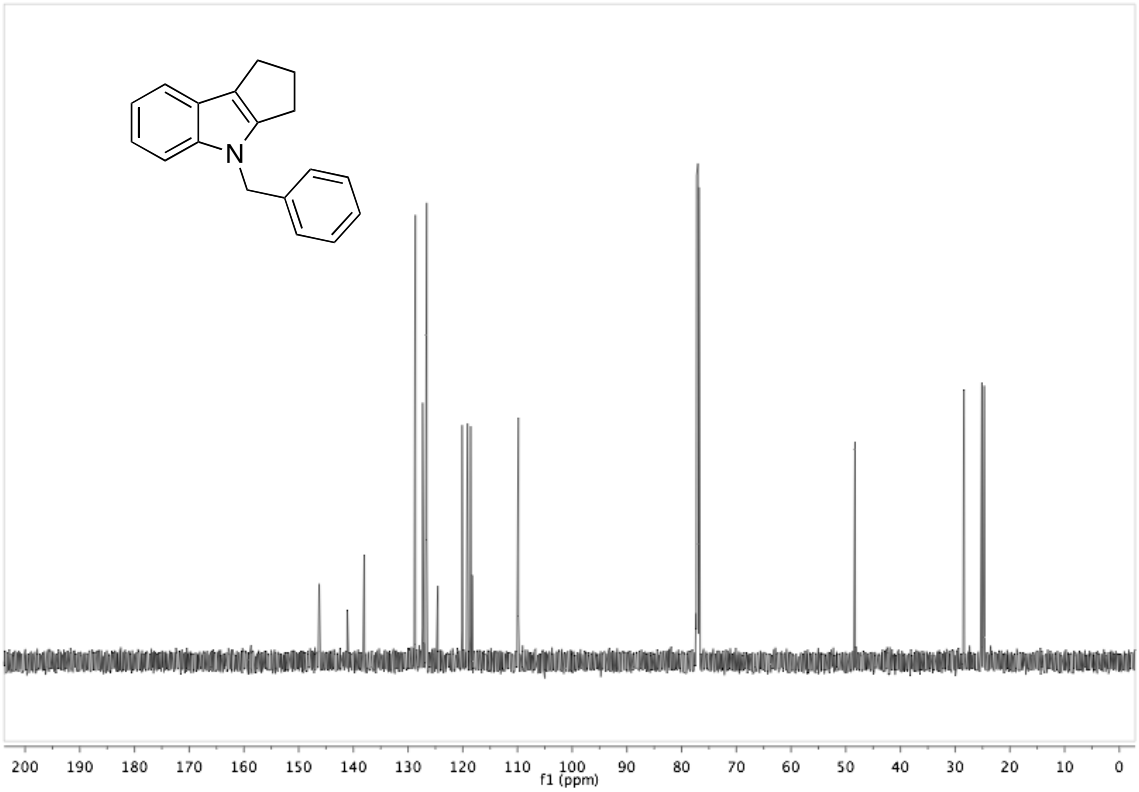
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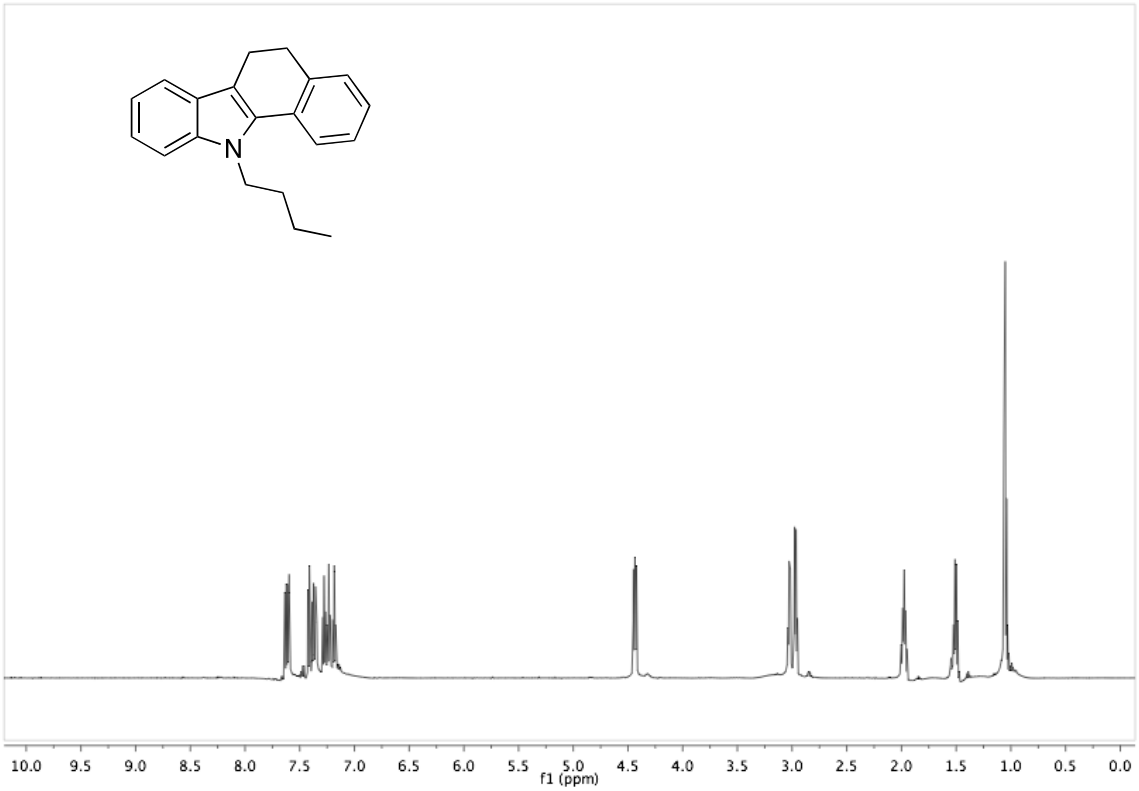
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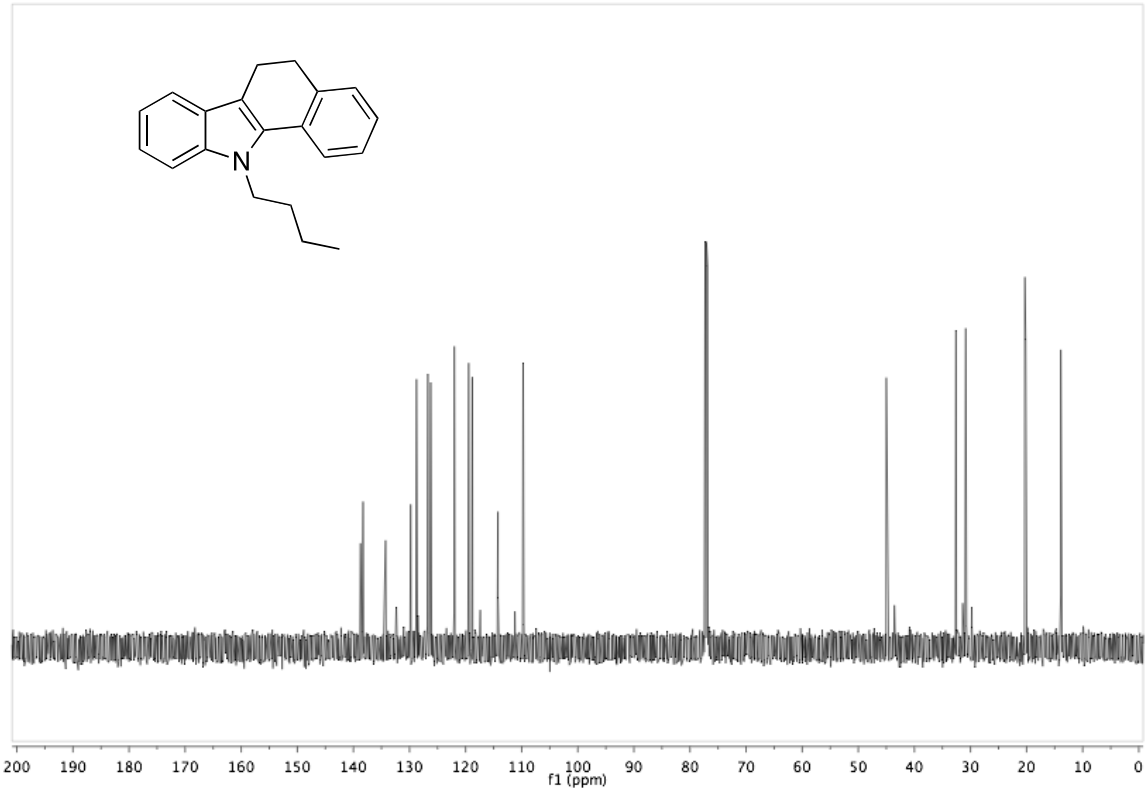
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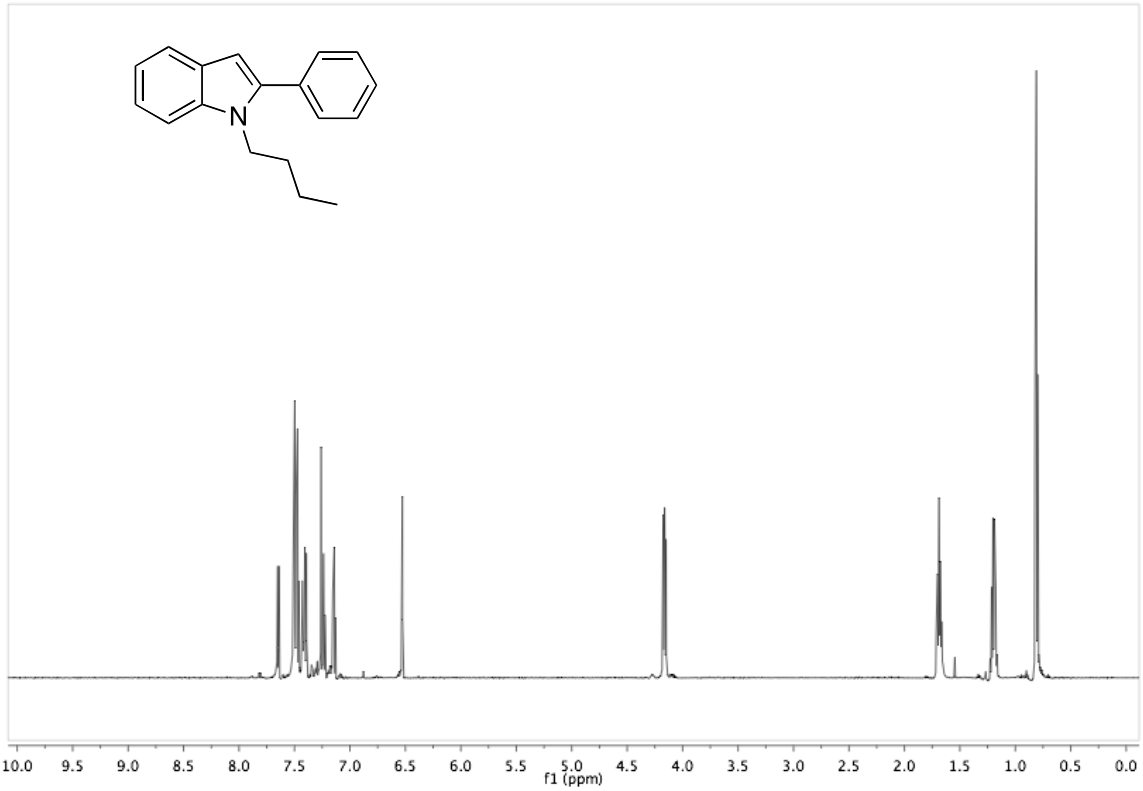
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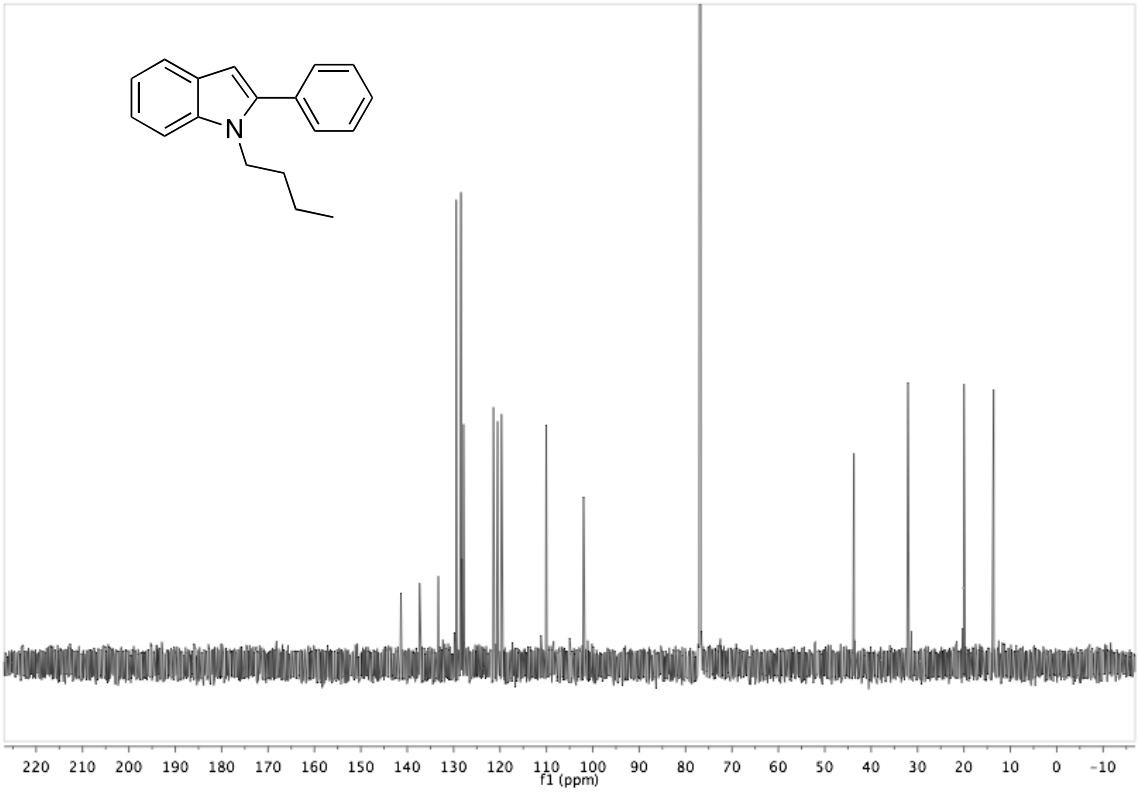
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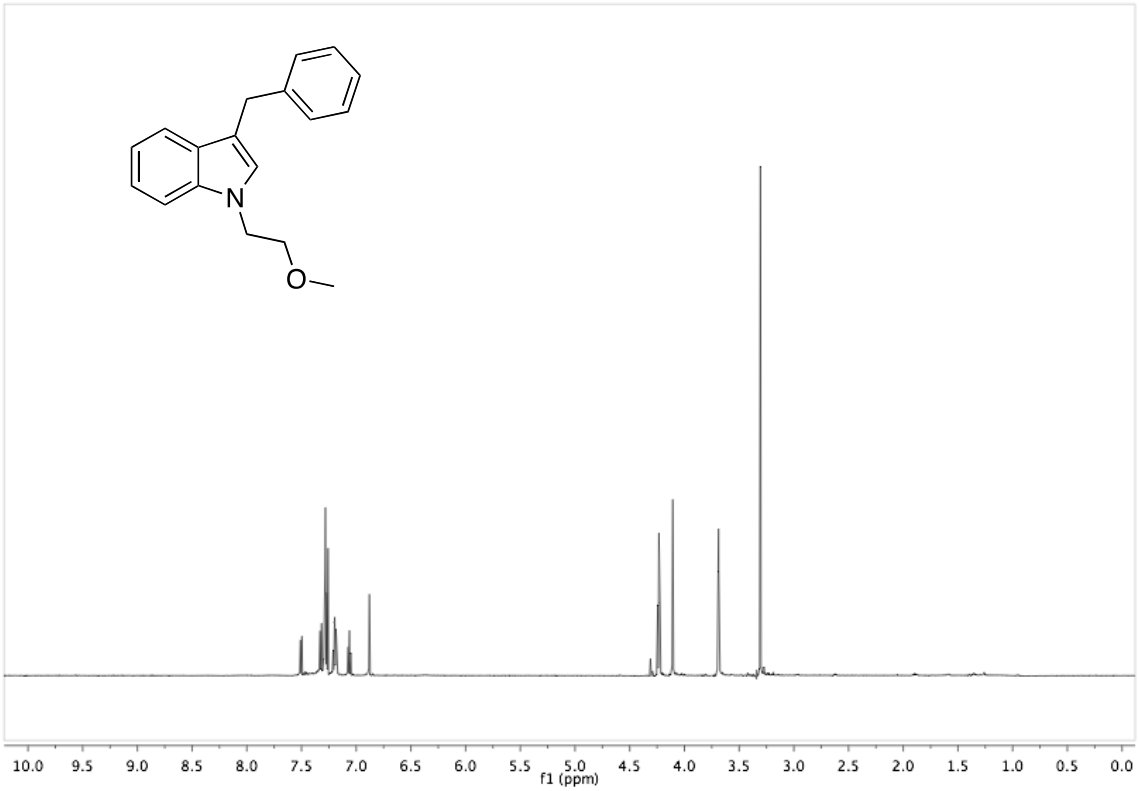
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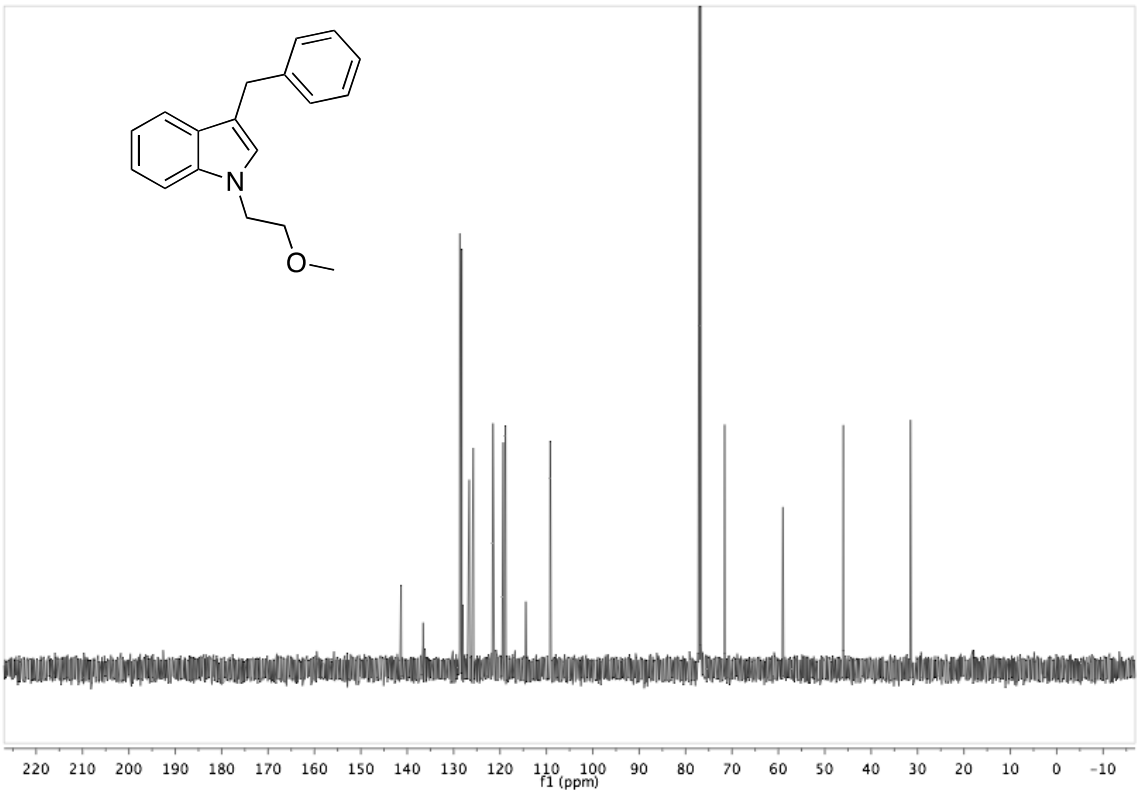
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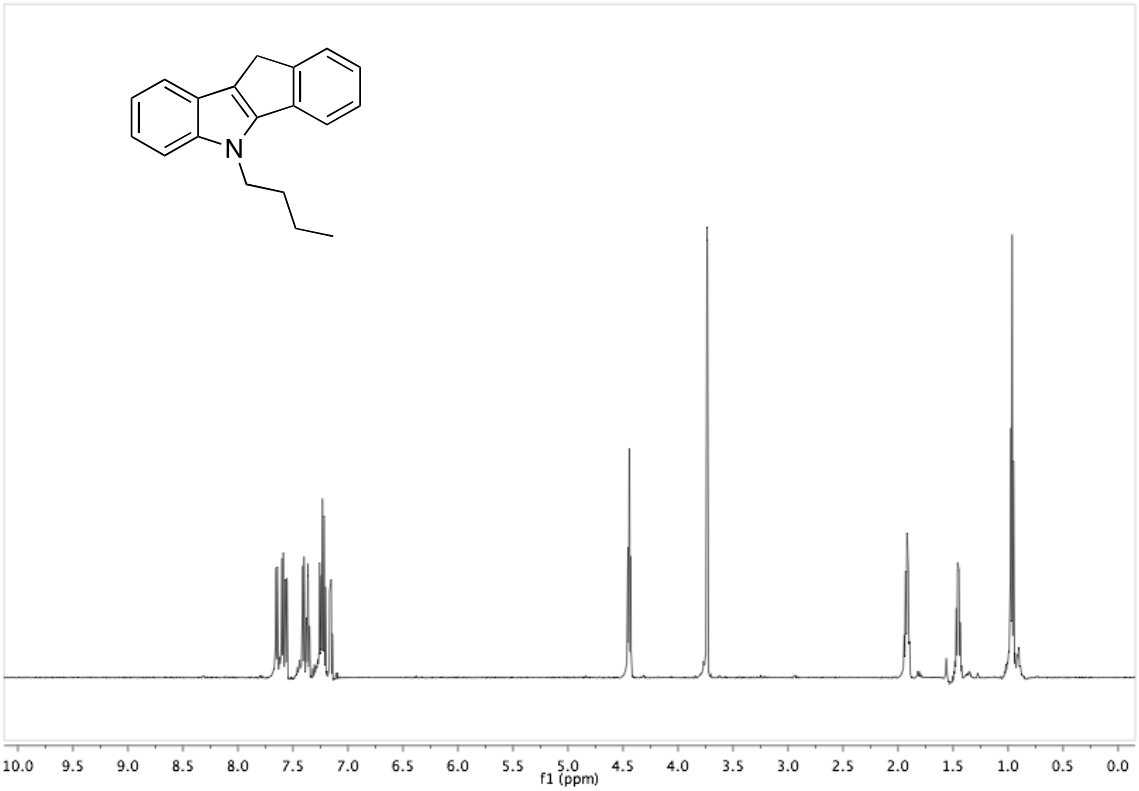
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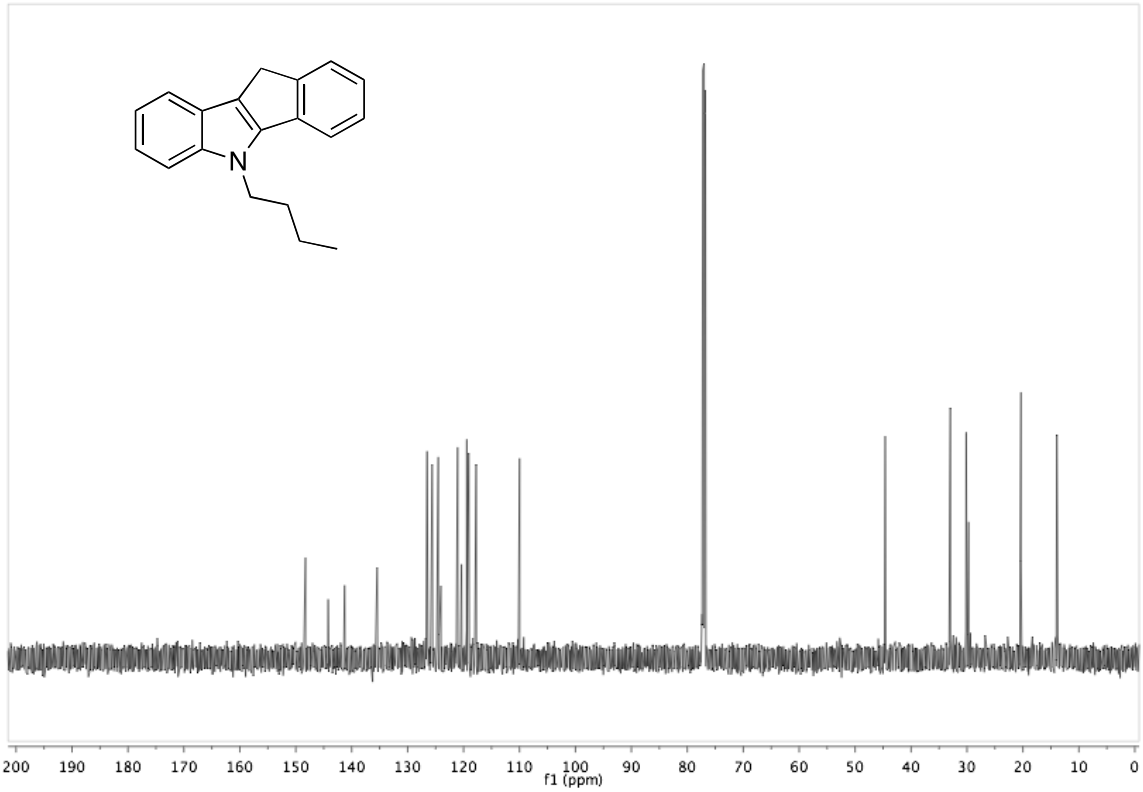
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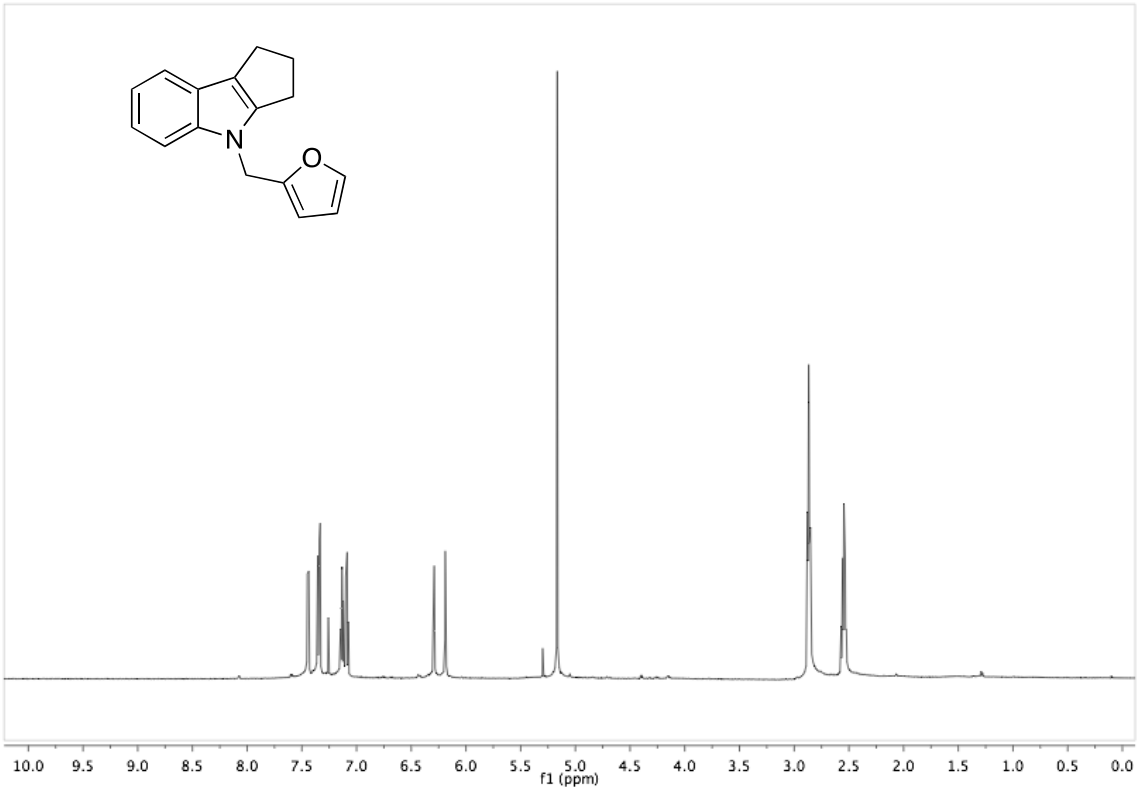
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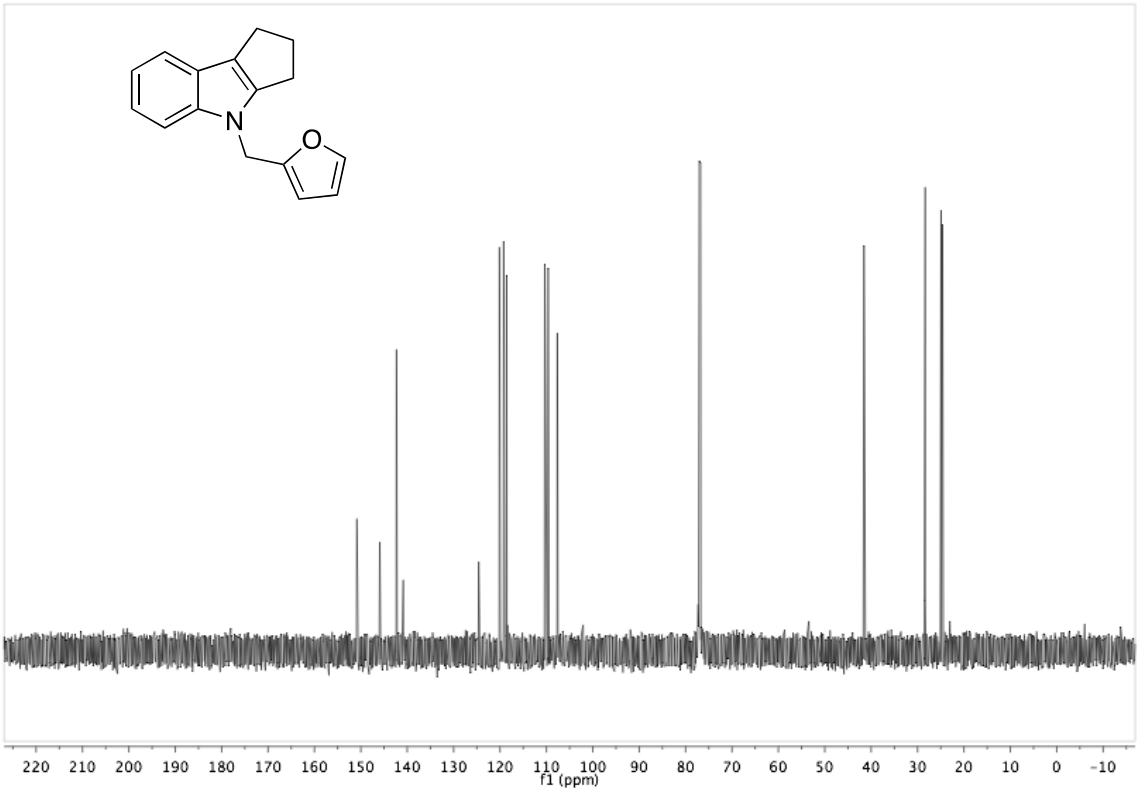
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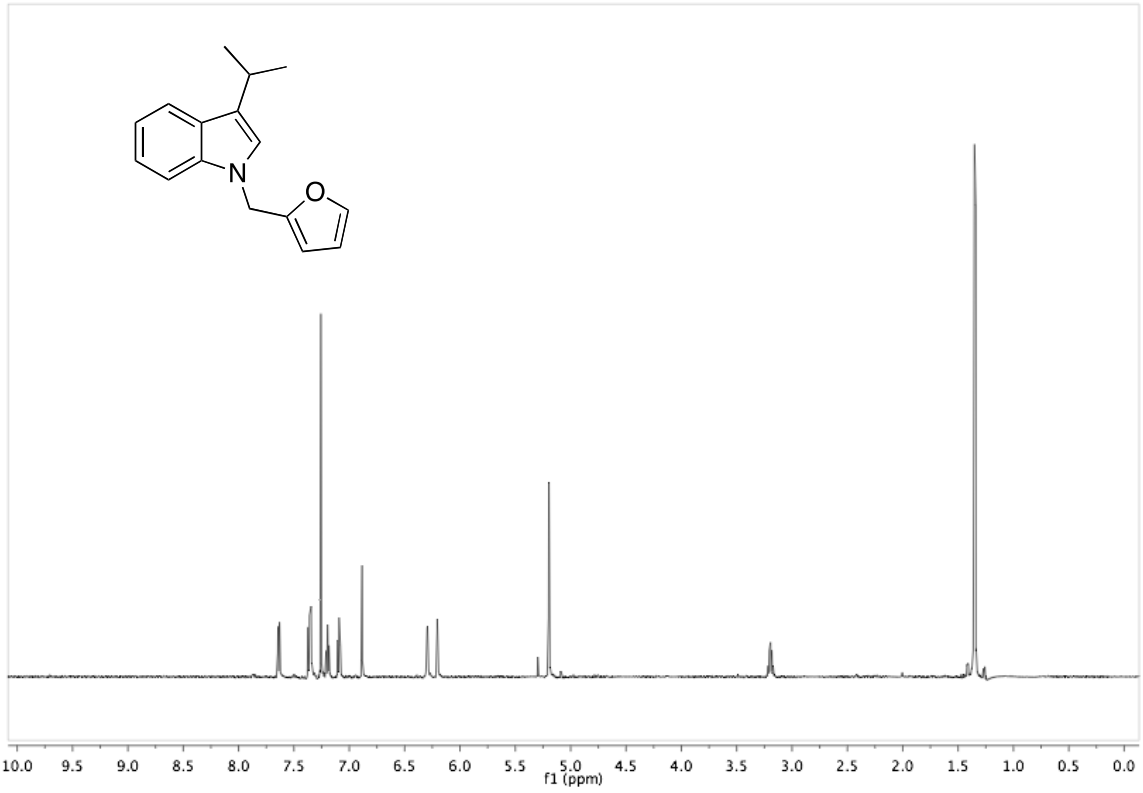
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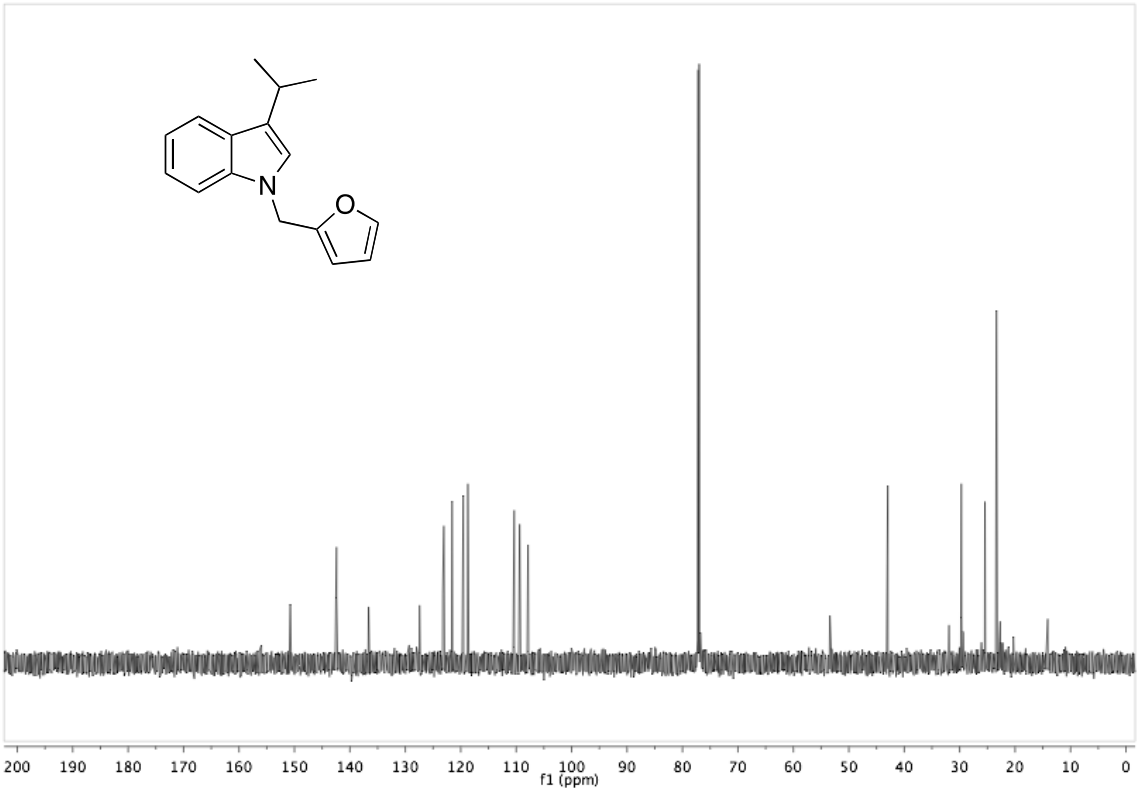
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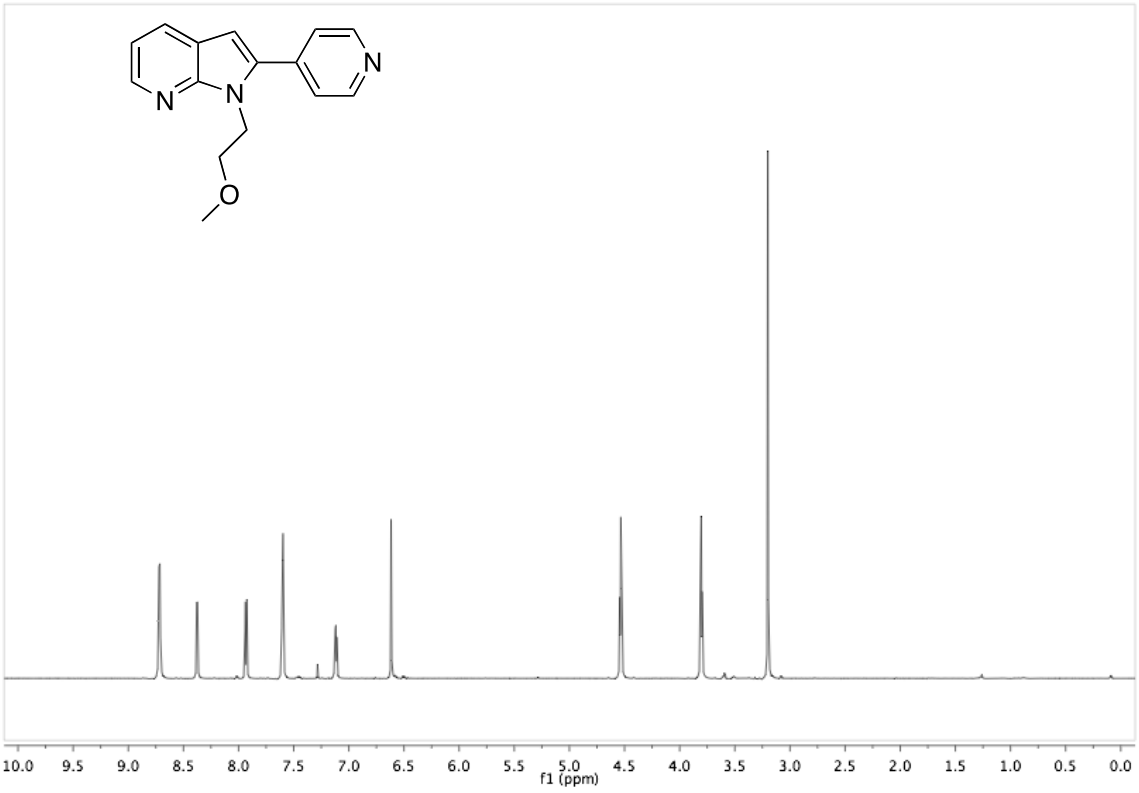
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N
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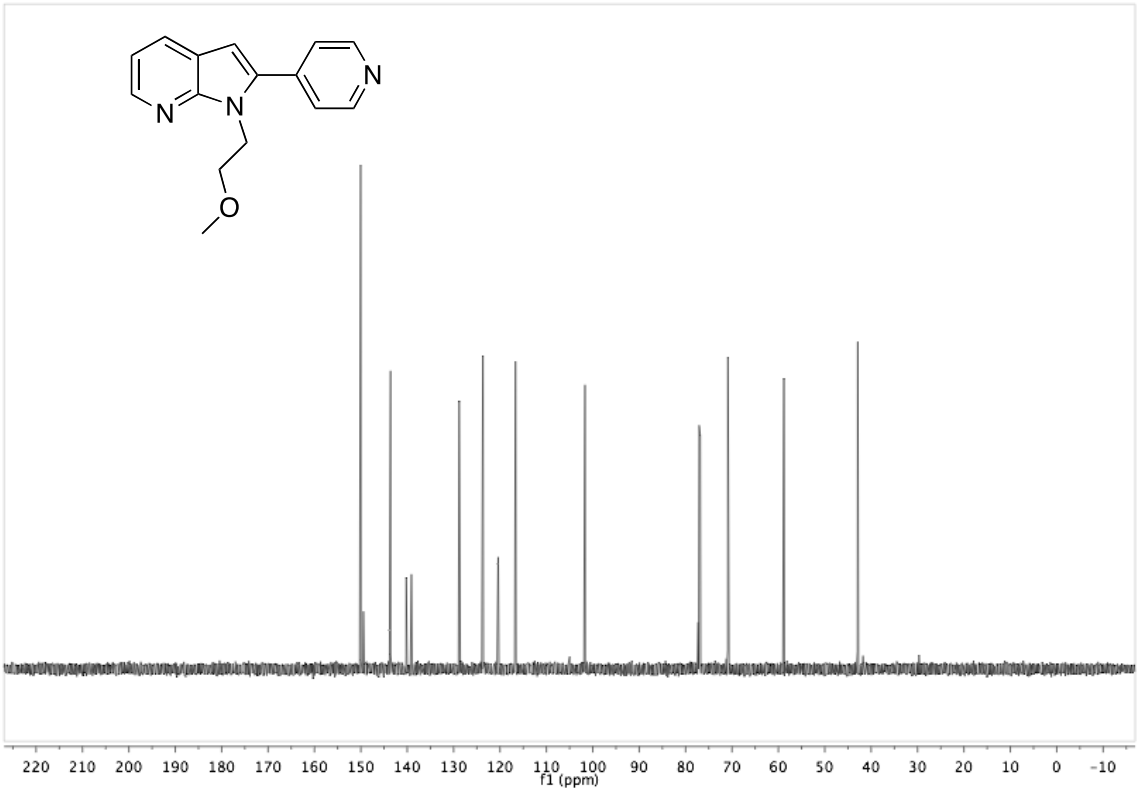
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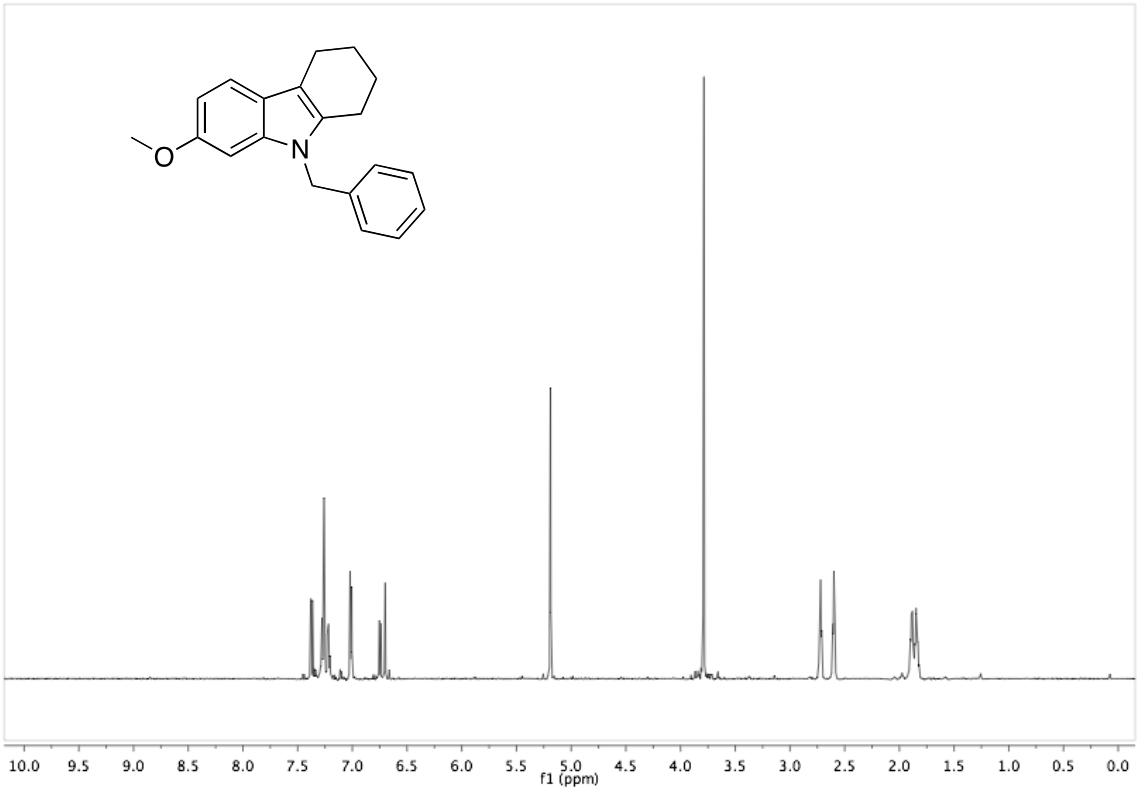
O
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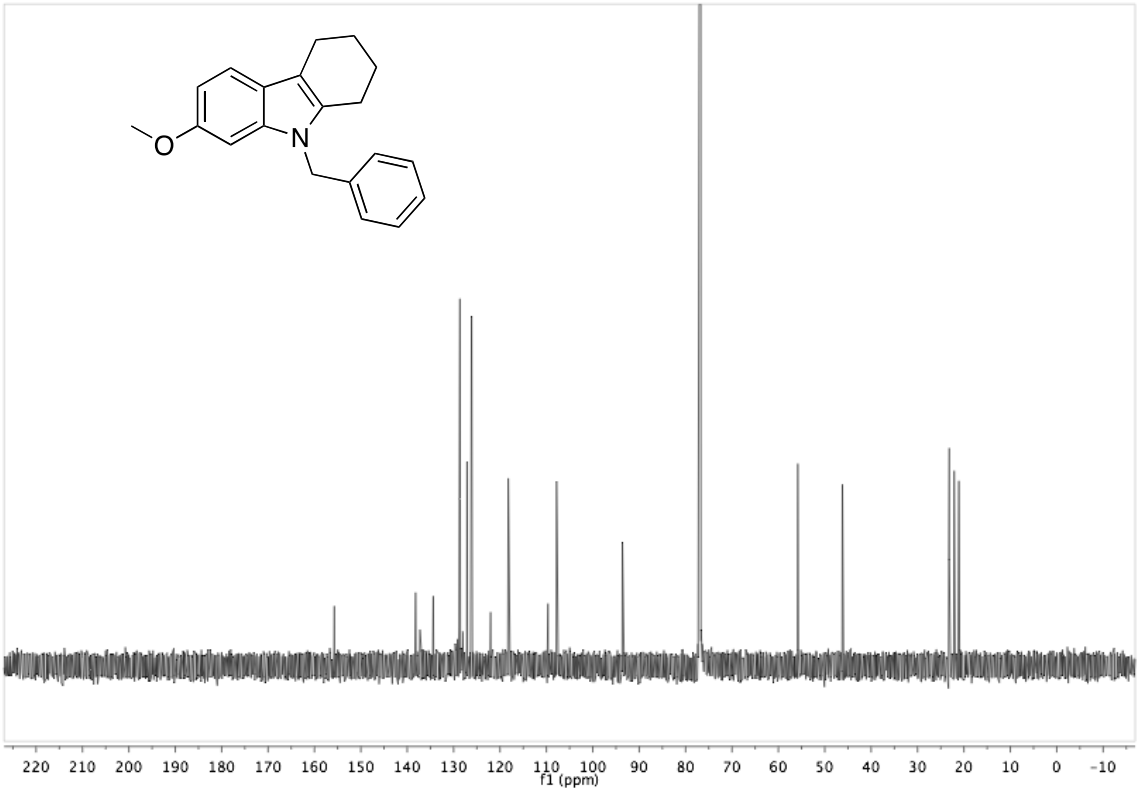
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N
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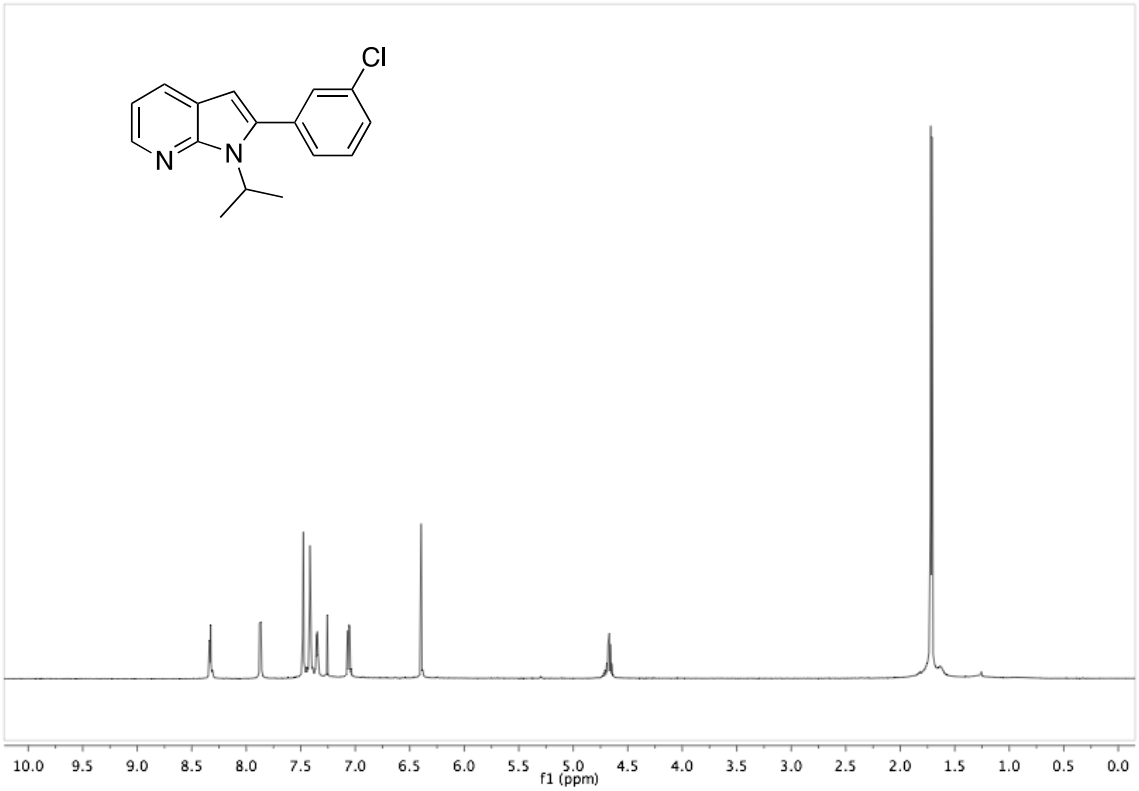
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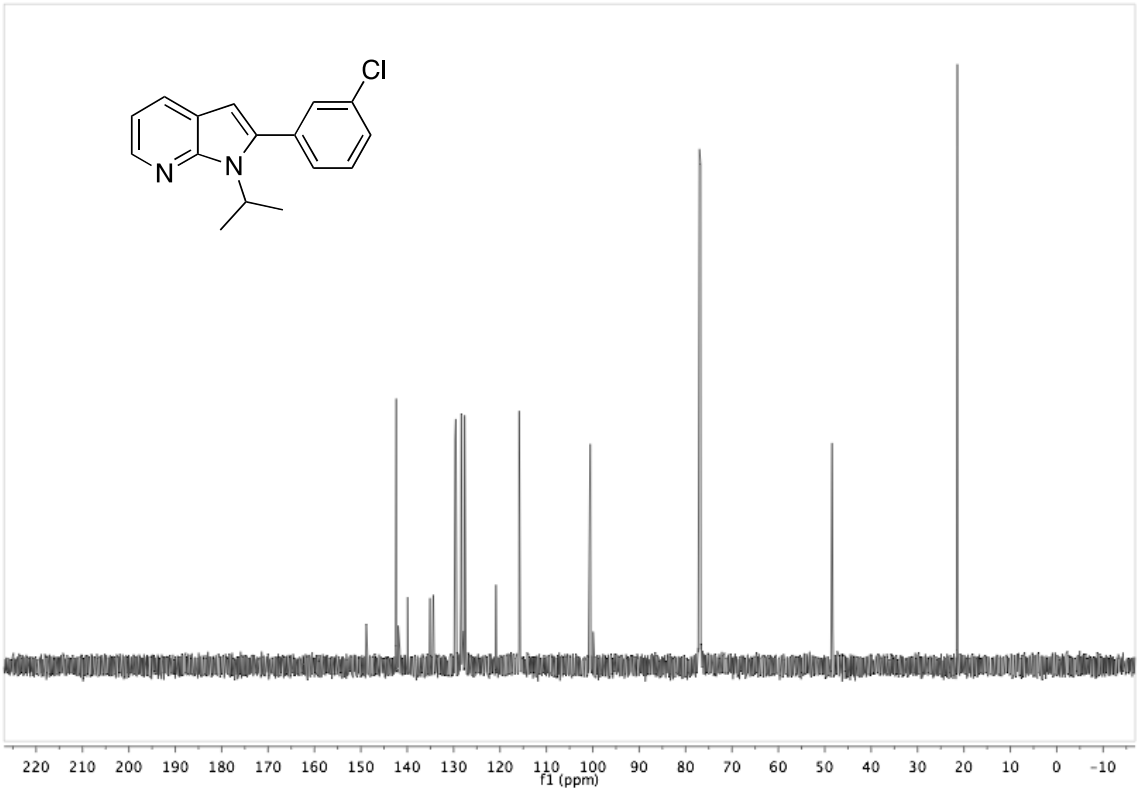
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N
N
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f1 (ppm)