Supporting Information

Ruthenium-Catalyzed Cascade C-H Activation/Annulation of *N*-Alkoxybenzamides: Reaction Development and Mechanistic Insight

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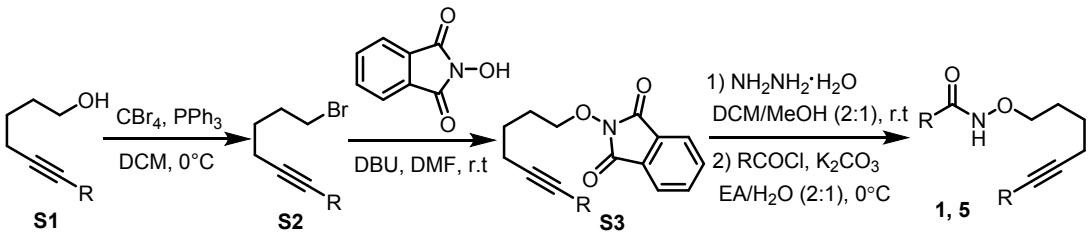
Contents

1. General Information

Commercially available reagents were used without additional purification. Column chromatography was performed with silica gel (70-230 mesh). ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AM (300 or 400 MHz) spectrometer at ambient temperature using $CDCl_3$ or DMSO-d_6 as solvent. HRMS (ESI) spectrometry data were acquired on a quadrupole orthogonal acceleration time-of-flight mass spectrometer [Synapt G2 high definition mass spectrometer (HDMS), Waters, Milford, MA]. Samples were infused at 3 μL min^{-1}, and spectra were obtained in the positive ionization mode with a resolution of 15000 [full width at half maximum (FWHM)] with leucine encephalin as lock mass. Melting points were recorded on a Reichert Thermovar apparatus and are uncorrected. IR spectra were recorded on Bruker Alpha FT-IR spectrometer.

2. Synthesis of the Substrates



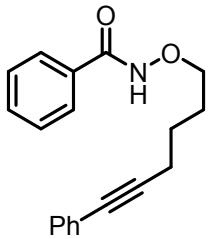
To a stirring solution of CBr_4 (7.2 mmol) in DCM (12 mL), a solution of alcohol **S1** (4.0 mmol) in DCM was added to the resulting mixture at 0 °C.[1] After stirring for another 5 minutes, a solution of PPh_3 (8.0 mmol) in DCM was added dropwise at 0 °C. The contents were then stirred at 0 °C for 1 h (judging by TLC analysis). The solution was concentrated in *vacuo*. The obtained crude product was purified by flash column chromatography on silica gel (*n*-heptane/ethyl acetate from 50:1 to 10:1) to give the desired product **S2**.

To a stirred mixture of *N*-hydroxyphthalimide (3.0 mmol) and **S2** (3.3 mmol) in DMF (6 mL) was added DBU (3.6 mmol) slowly at ambient temperature.[2] The contents were then stirred for 1 h (judging by TLC

analysis). The reaction mixture was extracted twice with DCM. The solvent from the combined organic layers were dried over Na_2SO_4, filtered, and removed under reduced pressure. The residue was purified by flash column chromatography on silica gel (*n*-heptane/ethyl acetate from 6:1 to 2:1) to give the product afford **S3**.

In a 100 mL round-bottom flask was charged **S3** (3.0 mmol),[3] solvent 15 mL [MeOH/DCM (1:2)], and then slowly added hydrazine monohydrate (3.3 mmol), then stirred at room temperature for 4 h. Upon completion (indicated by TLC), the solvent was then removed under reduce pressure. The residue was washed with DCM and filtered, collected the DCM part and removed the solvent to give the crude *O*-alkoxylamine, which was used in next step without further purification.

The crude *O*-alkoxylamine which was obtained in the previous step was added to a biphasic mixture of K_2CO_3 (3.6 mmol) in solvent 15 mL [EA/H_2O (2:1)].[3] The resulting solution was cooled to 0 °C followed by dropwise addition of the acid chloride (3.3 mmol) dissolved in a minimum amount of EtOAc. The reaction was allowed to stir at same temperature for 6 h. Upon completion (indicated by TLC), the phases were separated and the aqueous phase was extracted twice with EtOAc. The combined organic layers were dried over Na_2SO_4, filtered, and evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel (*n*-heptane/ethyl acetate from 4:1 to 1:1) to give the product **1**, **5**.



1a

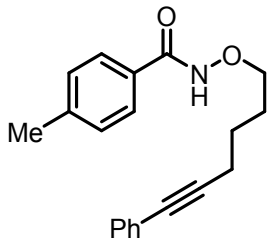
1a was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.22 (s, 1H), 7.79 – 7.68 (m, 2H), 7.50 (t, *J* = 7.3 Hz, 1H), 7.44 – 7.34 (m, 4H), 7.32 – 7.23 (m, 3H), 4.09 (t, *J* = 6.3 Hz, 2H), 2.49 (t, *J* = 6.8 Hz, 2H), 1.97 – 1.84 (m, 2H), 1.79 – 1.67 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 131.8, 131.5, 128.6, 128.2, 127.6, 127.0, 123.8, 89.7, 81.1, 76.2, 27.1, 25.0, 19.1.

IR (ATR-neat) *v* (cm^{-1}) 3192, 2946, 1645, 1578, 1516, 1488, 1309, 1041, 1022, 755, 690.

HRMS (ESI, m/z) calcd for $C_{19}H_{20}NO_2$ $(M+H)^+$: 294.1488, found: 294.1498.



1b

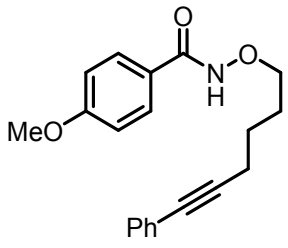
1b was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.21 (s, 1H), 7.64 (d, *J* = 7.9 Hz, 2H), 7.42 – 7.33 (m, 2H), 7.28 (dd, *J* = 4.1, 2.5 Hz, 3H), 7.18 (d, *J* = 7.9 Hz, 2H), 4.08 (t, *J* = 6.3 Hz, 2H), 2.48 (t, *J* = 6.8 Hz, 2H), 2.38 (s, 3H), 1.94 – 1.84 (m, 2H), 1.79 – 1.66 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 142.4, 131.5, 129.2, 129.0, 128.1, 127.5, 127.0, 123.8, 89.7, 81.0, 76.2, 27.0, 25.0, 21.4, 19.0.

IR (ATR-neat) *v* (cm^{-1}) 3207, 2948, 1644, 1489, 1154, 1034, 1018, 754, 691.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.1639.



1c

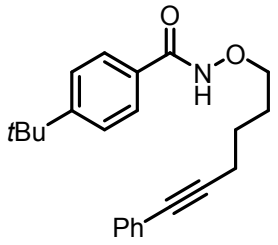
1c was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.10 (s, 1H), 7.76 – 7.66 (m, 2H), 7.39 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.30 – 7.26 (m, 3H), 6.93 – 6.79 (m, 2H), 4.07 (t, *J* = 6.3 Hz, 2H), 3.82 (s, 3H), 2.49 (t, *J* = 6.8 Hz, 2H), 1.90 – 1.78 (m, 2H), 1.76 – 1.64 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 162.3, 131.4, 128.9, 128.1, 127.5, 124.0, 123.7, 113.6, 89.7, 80.9, 76.0, 55.2, 27.0, 25.0, 19.0.

IR (ATR-neat) *v* (cm^{-1}) 3193, 2938, 1638, 1605, 1489, 1253, 1152, 1024, 841, 756, 691.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_3$ $(M+H)^+$: 324.1594, found: 324.1580.



1d

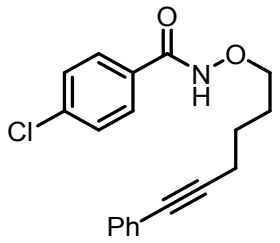
1d was obtained as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 7.67 (d, *J* = 8.1 Hz, 2H), 7.36 (d, *J* = 8.1 Hz, 4H), 7.25 (d, *J* = 5.8 Hz, 3H), 4.06 (t, *J* = 6.2 Hz, 2H), 2.46 (t, *J* = 6.9 Hz, 2H), 1.93 – 1.80 (m, 2H), 1.79 – 1.66 (m, 2H), 1.29 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 155.4, 131.5, 129.0, 128.1, 127.5, 126.9, 125.5, 123.8, 89.7, 81.0, 76.2, 34.8, 31.0, 27.0, 25.0, 19.0.

IR (ATR-neat) *v* (cm^{-1}) 3202, 2958, 1641, 1489, 1309, 1106, 1013, 849, 755, 691.

HRMS (ESI, m/z) calcd for $C_{23}H_{28}NO_2$ $(M+H)^+$: 350.2114, found: 350.2120.



1e

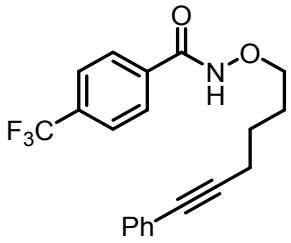
1e was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.31 (s, 1H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.39 – 7.32 (m, 3H), 7.30 (s, 1H), 7.26 (t, *J* = 3.3 Hz, 3H), 4.05 (t, *J* = 6.2 Hz, 2H), 2.47 (t, *J* = 6.8 Hz, 2H), 1.94 – 1.80 (m, 2H), 1.79 – 1.66 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 165.8, 138.3, 131.6, 130.6, 128.9, 128.6, 128.2, 127.6, 124.0, 89.7, 81.3, 76.5, 27.1, 25.2, 19.1.

IR (ATR-neat) *v* (cm^{-1}) 3207, 2943, 1645, 1482, 1246, 1152, 1091, 1013, 843, 754, 691.

HRMS (ESI, m/z) calcd for $C_{19}H_{19}ClNO_2$ $(M+H)^+$: 328.1099, found: 328.1099.



1f

1f was obtained as a yellow oil.

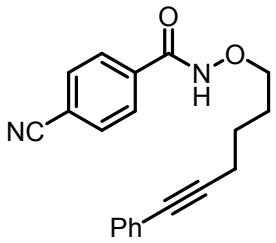
^{1}H NMR (300 MHz, $CDCl_3$) δ 9.24 (s, 1H), 7.79 (d, *J* = 8.1 Hz, 2H), 7.59 (d, *J* = 8.1 Hz, 2H), 7.36 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.27 – 7.23 (m, 3H), 4.09 (t, *J* = 6.2 Hz, 2H), 2.48 (t, *J* = 6.8 Hz, 2H), 1.97 – 1.83 (m, 2H), 1.79 – 1.69 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 165.1, 135.1, 133.5 (q, *J* = 32.7 Hz), 131.4, 128.2, 127.6, 127.6, 125.5 (q, *J* = 3.7 Hz), 125.2, 123.6, 121.6, 89.6, 81.1, 76.3, 26.9, 24.9, 19.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1.

IR (ATR-neat) *v* (cm^{-1}) 3195, 2943, 1651, 1490, 1324, 1126, 1066, 855, 755, 691.

HRMS (ESI, m/z) calcd for $C_{20}H_{19}F_3NO_2$ $(M+H)^+$: 362.1362, found: 362.1370.



1g

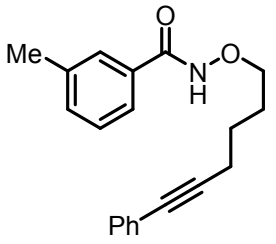
1g was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.70 (s, 1H), 7.82 (d, *J* = 7.3 Hz, 2H), 7.62 (d, *J* = 8.6 Hz, 2H), 7.40 – 7.31 (m, 2H), 7.27 – 7.23 (m, 3H), 4.07 (s, 2H), 2.46 (t, *J* = 6.8 Hz, 2H), 1.87 (d, *J* = 6.5 Hz, 2H), 1.79 – 1.66 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 164.4, 135.8, 132.2, 131.4, 128.1, 127.8, 127.6, 123.6, 117.7, 115.2, 89.5, 81.1, 76.3, 26.9, 24.9, 19.0.

IR (ATR-neat) *v* (cm^{-1}) 3199, 2946, 2231, 1651, 1489, 1282, 1017, 853, 755, 691.

HRMS (ESI, m/z) calcd for $C_{20}H_{19}N_2O_2$ $(M+H)^+$: 319.1441, found: 319.1437.



1h

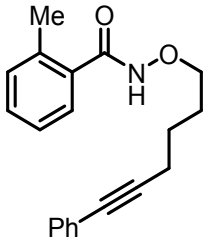
1h was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.08 (s, 1H), 7.55 (s, 1H), 7.48 (d, *J* = 7.1 Hz, 1H), 7.37 (dd, *J* = 6.2, 3.0 Hz, 2H), 7.27 – 7.23 (m, 5H), 4.06 (t, *J* = 6.3 Hz, 2H), 2.47 (t, *J* = 6.8 Hz, 2H), 2.33 (s, 3H), 1.94 – 1.81 (m, 2H), 1.80 – 1.67 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 138.6, 132.6, 132.3, 131.6, 128.5, 128.1, 127.8, 127.5, 124.1, 89.7, 81.2, 76.4, 27.3, 25.3, 21.2, 19.2.

IR (ATR-neat) *v* (cm^{-1}) 3193, 2945, 1644, 1488, 1304, 1040, 807, 755, 689.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.1634.



1i

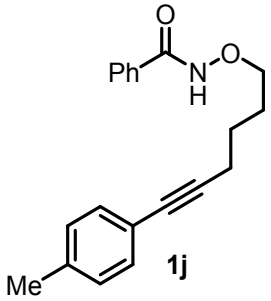
1i was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (s, 1H), 7.39 – 7.32 (m, 2H), 7.31 – 7.22 (m, 5H), 7.22 – 7.09 (m, 2H), 4.06 (s, 2H), 2.46 (d, *J* = 6.9 Hz, 2H), 2.40 (s, 3H), 1.89 – 1.72 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.9, 136.8, 132.7, 131.4, 131.0, 130.4, 128.1, 127.5, 127.0, 125.6, 123.7, 89.6, 81.1, 76.3, 27.0, 25.0, 19.5, 19.0.

IR (ATR-neat) *v* (cm^{-1}) 3172, 2945, 1646, 1489, 1026, 895, 755, 691.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.1633.



1j

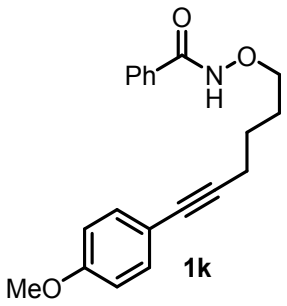
1j was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.30 (s, 1H), 7.83 – 7.73 (m, 2H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.32 (dd, *J* = 18.9, 7.7 Hz, 4H), 7.07 (d, *J* = 7.8 Hz, 2H), 4.03 (t, *J* = 6.4 Hz, 2H), 2.41 (t, *J* = 6.9 Hz, 2H), 2.32 (s, 3H), 1.93 – 1.79 (m, 2H), 1.77 – 1.64 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.4, 137.4, 131.8, 131.7, 131.3, 128.8, 128.4, 127.1, 120.6, 88.9, 81.0, 76.0, 27.0, 25.0, 21.2, 19.0.

IR (ATR-neat) *v* (cm^{-1}) 3201, 2946, 1646, 1509, 1309, 1022, 816, 710, 692.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.1632.



1k

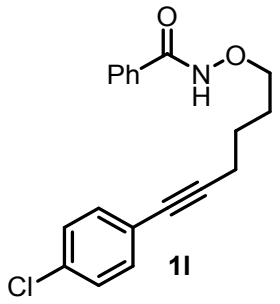
1k was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.05 (s, 1H), 7.71 (d, *J* = 7.3 Hz, 2H), 7.47 (t, *J* = 7.1 Hz, 1H), 7.36 (dd, *J* = 11.5, 4.3 Hz, 2H), 7.30 (d, *J* = 8.9 Hz, 2H), 6.79 (dd, *J* = 9.2, 2.4 Hz, 2H), 4.07 (t, *J* = 6.2 Hz, 2H), 3.78 (s, 3H), 2.45 (t, *J* = 6.8 Hz, 2H), 1.95 – 1.82 (m, 2H), 1.78 – 1.66 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.6, 159.1, 132.8, 132.0, 131.9, 128.6, 127.1, 116.0, 113.8, 88.1, 80.8, 76.4, 55.2, 27.0, 25.2, 19.1.

IR (ATR-neat) *v* (cm^{-1}) 3203, 2950, 1646, 1508, 1243, 1024, 831, 710, 692.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_3$ $(M+H)^+$: 324.1594, found: 324.1586.



1l

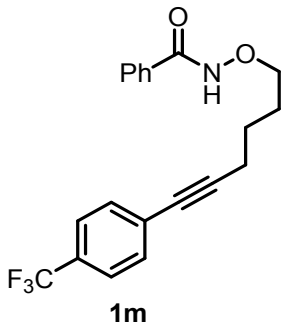
1l was obtained as a red solid. Melting point 49-51 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.98 (s, 1H), 7.77 – 7.69 (m, 2H), 7.56 – 7.47 (m, 1H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.33 – 7.22 (m, 4H), 4.09 (t, *J* = 6.3 Hz, 2H), 2.49 (t, *J* = 6.8 Hz, 2H), 1.94 – 1.81 (m, 2H), 1.80 – 1.67 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.5, 133.4, 132.7, 131.9, 131.8, 128.5, 128.4, 127.0, 122.2, 90.8, 79.9, 76.1, 27.0, 24.9, 19.0.

IR (ATR-neat) *v* (cm^{-1}) 3176, 2943, 1643, 1486, 1314, 1089, 1012, 825, 692.

HRMS (ESI, m/z) calcd for $C_{19}H_{19}ClNO_2$ $(M+H)^+$: 328.1099, found: 328.1103.



1m

1m was obtained as a red solid. Melting point 52-54 °C.

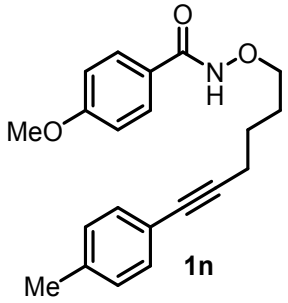
^{1}H NMR (300 MHz, $CDCl_3$) δ 9.01 (s, 1H), 7.72 (d, *J* = 7.3 Hz, 2H), 7.52 – 7.44 (m, 5H), 7.42 – 7.34 (m, 2H), 4.08 (t, *J* = 5.8 Hz, 2H), 2.50 (t, *J* = 6.8 Hz, 2H), 1.93 – 1.84 (m, 2H), 1.82 – 1.70 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.4, 131.8, 131.8, 131.6, 129.4, 128.9, 128.4, 127.6, 127.1, 125.7, 125.0 (q, *J* = 3.8 Hz), 122.1, 92.5, 79.8, 75.9, 27.0, 24.8, 19.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.8.

IR (ATR-neat) *v* (cm^{-1}) 3204, 2942, 1645, 1323, 1160, 1102, 842, 691.

HRMS (ESI, m/z) calcd for $C_{20}H_{19}F_3NO_2$ $(M+H)^+$: 362.1362, found: 362.1370.



1n

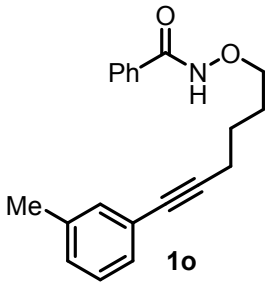
1n was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.24 (s, 1H), 7.76 – 7.64 (m, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.08 (d, *J* = 7.8 Hz, 2H), 6.89 – 6.79 (m, 2H), 4.06 (t, *J* = 6.3 Hz, 2H), 3.81 (s, 3H), 2.46 (t, *J* = 6.8 Hz, 2H), 2.34 (s, 3H), 1.92 – 1.79 (m, 2H), 1.78 – 1.64 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.1, 162.3, 137.4, 131.2, 128.9, 128.8, 124.0, 120.6, 113.6, 88.9, 80.9, 75.9, 55.1, 27.0, 25.0, 21.2, 18.9.

IR (ATR-neat) *v* (cm^{-1}) 3200, 2940, 1638, 1605, 1494, 1253, 1179, 1024, 816, 759.

HRMS (ESI, m/z) calcd for $C_{21}H_{24}NO_3$ $(M+H)^+$: 338.1751, found: 338.1737.



1o

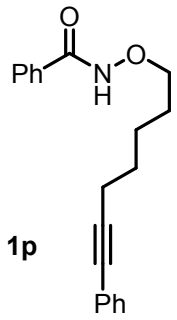
1o was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.58 (s, 1H), 7.80 – 7.71 (m, 2H), 7.53 – 7.43 (m, 1H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.25 – 7.13 (m, 3H), 7.12 – 7.06 (m, 1H), 4.07 (t, *J* = 6.3 Hz, 2H), 2.46 (t, *J* = 6.8 Hz, 2H), 2.31 (s, 3H), 1.95 – 1.85 (m, 2H), 1.81 – 1.70 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.4, 137.7, 132.0, 131.8, 128.5, 128.4, 128.0, 127.0, 123.5, 89.3, 81.1, 76.1, 27.0, 25.0, 21.1, 19.0.

IR (ATR-neat) *v* (cm^{-1}) 3207, 2946, 1647, 1483, 1152, 1022, 783, 711, 690.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.1632



1p

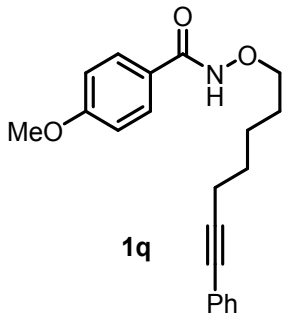
1p was obtained as a colorless oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.38 (s, 1H), 7.74 (d, *J* = 7.4 Hz, 2H), 7.46 (t, *J* = 7.2 Hz, 1H), 7.39 – 7.33 (m, 4H), 7.25 (d, *J* = 2.8 Hz, 3H), 4.00 (t, *J* = 6.3 Hz, 2H), 2.38 (t, *J* = 6.5 Hz, 2H), 1.70 (dd, *J* = 13.5, 6.8 Hz, 2H), 1.65 – 1.46 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 131.8, 131.4, 128.5, 128.1, 127.4, 127.1, 123.8, 90.0, 80.7, 76.5, 28.3, 27.5, 25.0, 19.2.

IR (ATR-neat) *v* (cm^{-1}) 3197, 2939, 1644, 1488, 1309, 1021, 891, 755, 690.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.1631.



1q

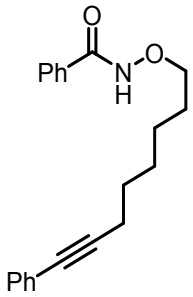
1q was obtained as a colorless oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.37 (s, 1H), 7.72 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 3.7 Hz, 2H), 7.25 (d, *J* = 4.8 Hz, 3H), 6.85 (d, *J* = 8.5 Hz, 2H), 3.99 (t, *J* = 6.3 Hz, 2H), 3.78 (s, 3H), 2.38 (t, *J* = 6.2 Hz, 2H), 1.70 (dd, *J* = 13.4, 6.9 Hz, 2H), 1.61 – 1.52 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 162.4, 131.4, 128.9, 128.1, 127.4, 124.1, 123.8, 113.7, 90.0, 80.7, 76.5, 55.2, 28.3, 27.5, 25.0, 19.2.

IR (ATR-neat) *v* (cm^{-1}) 3197, 2938, 1638, 1606, 1490, 1255, 1026, 843, 757, 692.

HRMS (ESI, m/z) calcd for $C_{21}H_{24}NO_3$ $(M+H)^+$: 338.1751, found: 338.1748.



1r

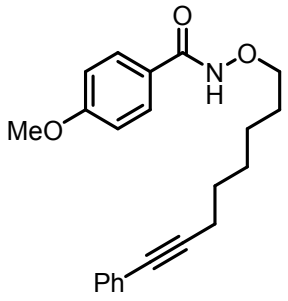
1r was obtained as a colorless oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.72 (s, 1H), 7.75 (d, *J* = 7.4 Hz, 2H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.40 – 7.30 (m, 4H), 7.24 (d, *J* = 4.5 Hz, 3H), 3.97 (t, *J* = 6.4 Hz, 2H), 2.36 (t, *J* = 6.8 Hz, 2H), 1.65 (dd, *J* = 13.3, 6.8 Hz, 2H), 1.60 – 1.50 (m, 2H), 1.49 – 1.30 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 131.8, 131.7, 131.4, 128.4, 128.0, 127.4, 127.1, 123.8, 90.1, 80.6, 76.5, 28.5, 28.4, 27.8, 25.2, 19.1.

IR (ATR-neat) *v* (cm^{-1}) 3201, 2934, 1646, 1488, 1311, 1022, 756, 711, 690.

HRMS (ESI, m/z) calcd for $C_{21}H_{24}NO_2$ $(M+H)^+$: 322.1801, found: 322.1812.



1s

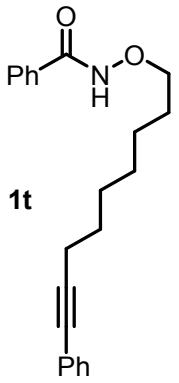
1s was obtained as a colorless oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.29 (s, 1H), 7.72 (d, *J* = 8.7 Hz, 2H), 7.37 (dd, *J* = 6.4, 3.0 Hz, 2H), 7.26 – 7.23 (m, 3H), 6.86 (d, *J* = 8.7 Hz, 2H), 3.98 (t, *J* = 6.6 Hz, 2H), 3.79 (s, 3H), 2.37 (t, *J* = 6.9 Hz, 2H), 1.74 – 1.63 (m, 2H), 1.62 – 1.52 (m, 2H), 1.51 – 1.31 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 162.3, 131.4, 128.9, 128.1, 127.4, 124.1, 123.9, 113.7, 90.2, 80.6, 76.6, 55.2, 28.5, 28.5, 27.8, 25.3, 19.2.

IR (ATR-neat) *v* (cm^{-1}) 3200, 2935, 1637, 1605, 1489, 1253, 1025, 842, 756, 691.

HRMS (ESI, m/z) calcd for $C_{22}H_{26}NO_3$ $(M+H)^+$: 352.1907, found: 352.1916.



1t

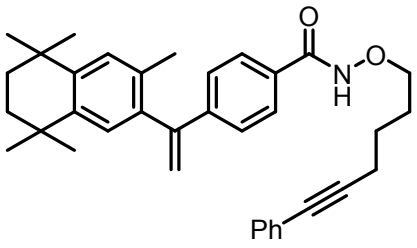
1t was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.12 (s, 1H), 7.73 (d, *J* = 7.3 Hz, 2H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.38 (dd, *J* = 7.8, 4.7 Hz, 4H), 7.25 (d, *J* = 2.2 Hz, 3H), 4.00 (t, *J* = 6.5 Hz, 2H), 2.38 (t, *J* = 6.9 Hz, 2H), 1.68 (dd, *J* = 13.7, 6.8 Hz, 2H), 1.58 (dd, *J* = 14.1, 6.9 Hz, 2H), 1.50 – 1.25 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 131.9, 131.8, 131.4, 128.5, 128.1, 127.4, 127.1, 123.9, 90.3, 80.6, 76.8, 28.8, 28.7, 28.5, 27.9, 25.6, 19.3.

IR (ATR-neat) *v* (cm^{-1}) 3207, 2931, 1645, 1488, 1310, 1021, 891, 755, 690.

HRMS (ESI, m/z) calcd for $C_{22}H_{26}NO_2$ $(M+H)^+$: 336.1958, found: 336.1964.



1u

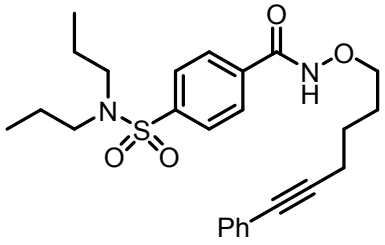
1u was obtained as a yellow solid. Melting point 84-86 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.91 (s, 1H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.40 – 7.31 (m, 2H), 7.28 (s, 1H), 7.22 (dd, *J* = 5.1, 1.7 Hz, 4H), 7.09 (d, *J* = 8.7 Hz, 2H), 5.75 (d, *J* = 1.1 Hz, 1H), 5.28 (d, *J* = 1.0 Hz, 1H), 4.07 (t, *J* = 6.1 Hz, 2H), 2.48 (t, *J* = 6.8 Hz, 2H), 1.93 (s, 3H), 1.91 – 1.83 (m, 2H), 1.80 – 1.71 (m, 2H), 1.70 (s, 4H), 1.30 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 148.9, 144.8, 144.4, 142.3, 137.9, 132.7, 131.5, 130.6, 128.2, 128.0, 127.6, 127.1, 126.8, 123.8, 116.6, 89.7, 81.2, 76.4, 35.2, 35.2, 34.1, 33.9, 31.9, 31.9, 26.9, 25.1, 19.9, 19.1.

IR (ATR-neat) *v* (cm^{-1}) 2955, 1640, 1490, 1311, 1041, 900, 856, 755, 691.

HRMS (ESI, m/z) calcd for $C_{36}H_{42}NO_2$ $(M+H)^+$: 520.3210, found: 520.3220.



1v

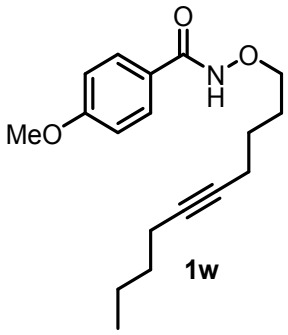
1v was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.32 (s, 1H), 7.81 – 7.69 (m, 4H), 7.42 – 7.33 (m, 2H), 7.26 (t, *J* = 3.1 Hz, 3H), 4.10 (t, *J* = 5.8 Hz, 2H), 3.13 – 2.99 (m, 4H), 2.49 (t, *J* = 6.8 Hz, 2H), 1.90 (dd, *J* = 13.6, 6.4 Hz, 2H), 1.77 (dd, *J* = 14.0, 6.8 Hz, 2H), 1.60 – 1.45 (m, 4H), 0.86 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 164.9, 142.9, 135.6, 131.5, 128.2, 127.9, 127.6, 127.1, 123.7, 89.6, 81.1, 76.3, 49.9, 27.0, 25.0, 21.8, 19.0, 11.1.

IR (ATR-neat) *v* (cm^{-1}) 3206, 2964, 1653, 1336, 1159, 1088, 991, 742, 692.

HRMS (ESI, m/z) calcd for $C_{25}H_{33}N_2O_4S$ $(M+H)^+$: 457.2155, found: 457.2167.



1w

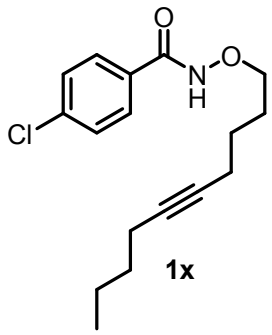
1w was obtained as a colorless oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.00 (s, 1H), 7.71 (d, *J* = 8.8 Hz, 2H), 6.89 (d, *J* = 8.9 Hz, 2H), 4.01 (t, *J* = 6.4 Hz, 2H), 3.83 (s, 3H), 2.25 – 2.07 (m, 4H), 1.90 – 1.73 (m, 2H), 1.66 – 1.54 (m, 2H), 1.51 – 1.30 (m, 4H), 0.89 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.4, 162.5, 128.9, 124.3, 113.8, 80.7, 79.5, 76.3, 55.3, 31.2, 27.0, 25.4, 21.9, 18.4, 18.4, 13.5.

IR (ATR-neat) *v* (cm^{-1}) 3198, 2932, 1638, 1606, 1493, 1253, 1152, 1025, 842, 755.

HRMS (ESI, m/z) calcd for $C_{18}H_{26}NO_3$ $(M+H)^+$: 304.1907, found: 304.1906.



1x

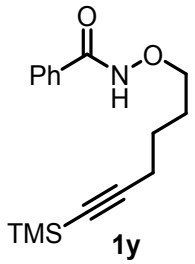
1x was obtained as a colorless solid. Melting point 58-60 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.22 (s, 1H), 7.69 (d, *J* = 8.3 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 4.02 (t, *J* = 6.1 Hz, 2H), 2.27 – 2.06 (m, 4H), 1.87 – 1.72 (m, 2H), 1.67 – 1.53 (m, 2H), 1.52 – 1.30 (m, 4H), 0.89 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 165.4, 138.1, 130.2, 128.7, 128.6, 80.7, 79.3, 76.2, 31.1, 26.9, 25.3, 21.8, 18.3, 18.3, 13.5.

IR (ATR-neat) *v* (cm^{-1}) 3197, 2930, 1643, 1479, 1314, 1092, 1012, 888, 844, 759.

HRMS (ESI, m/z) calcd for $C_{17}H_{23}ClNO_2$ $(M+H)^+$: 308.1412, found: 308.1416.



1y

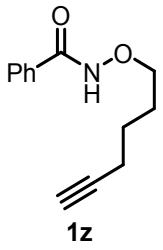
1y was obtained as a colorless oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.36 (s, 1H), 7.72 (d, *J* = 7.3 Hz, 2H), 7.47 (t, *J* = 7.0 Hz, 1H), 7.37 (t, *J* = 7.4 Hz, 2H), 4.00 (t, *J* = 6.1 Hz, 2H), 2.25 (t, *J* = 6.9 Hz, 2H), 1.76 (dd, *J* = 13.9, 6.5 Hz, 2H), 1.68 – 1.55 (m, 2H), 0.11 (s, 9H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.5, 132.0, 131.9, 128.5, 127.1, 106.9, 84.9, 76.2, 27.0, 24.9, 19.5, 0.1.

IR (ATR-neat) *v* (cm^{-1}) 3191, 2955, 2173, 1644, 1482, 1248, 1023, 841, 758, 692.

HRMS (ESI, m/z) calcd for $C_{16}H_{24}NO_2Si$ $(M+H)^+$: 290.1571, found: 290.1578.



1z

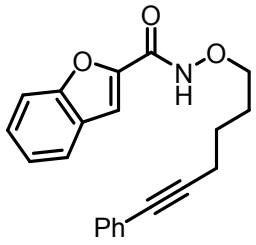
1z was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.19 (s, 1H), 7.74 (d, *J* = 7.7 Hz, 2H), 7.56 – 7.45 (m, 1H), 7.40 (t, *J* = 7.1 Hz, 2H), 4.04 (t, *J* = 5.5 Hz, 2H), 2.31 – 2.20 (m, 2H), 1.95 (d, *J* = 2.4 Hz, 1H), 1.81 (dd, *J* = 14.0, 6.4 Hz, 2H), 1.72 – 1.59 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.5, 131.9, 131.8, 128.6, 127.1, 84.1, 76.1, 68.7, 26.8, 24.7, 18.0.

IR (ATR-neat) *v* (cm^{-1}) 3198, 2949, 1644, 1483, 1311, 1023, 890, 711, 692.

HRMS (ESI, m/z) calcd for $C_{13}H_{16}NO_2$ $(M+H)^+$: 218.1175, found: 218.1174.



5

5 was obtained as a yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.28 (s, 1H), 7.64 (d, *J* = 7.7 Hz, 1H), 7.51 (s, 1H), 7.39 (dd, *J* = 9.3, 4.3 Hz, 4H), 7.30 – 7.23 (m, 4H), 4.14 (t, *J* = 6.3 Hz, 2H), 2.50 (t, *J* = 6.8 Hz, 2H), 2.00 – 1.87 (m, 2H), 1.85 – 1.71 (m, 2H).

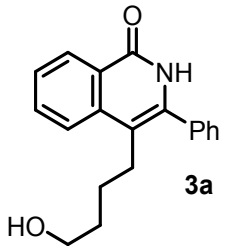
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.4, 154.7, 146.6, 131.5, 128.1, 127.5, 127.2, 127.0, 123.8, 122.6, 111.7, 111.6, 89.6, 81.1, 76.8, 27.0, 25.0, 19.0.

IR (ATR-neat) *v* (cm^{-1}) 3185, 2944, 1653, 1489, 1296, 1115, 1033, 858, 746, 691.

HRMS (ESI, m/z) calcd for $C_{21}H_{20}NO_3$ $(M+H)^+$: 334.1438, found: 334.1428.

3. Ruthenium-Catalyzed Annulations

To a Schlenk flask equipped with a stir bar were added **1** (0.3 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (0.03 mmol), NaOAc (0.6 mmol) and MeOH (3.0 mL). The reaction was stirred for 4 h at 60 °C, cooled to room temperature. The solvent was removed in *vacuo* and the remaining residue was purified by a silica gel column chromatography to afford the product **3** (*n*-heptane/ethyl acetate from 1:1 to 1:4) and **2** (DCM/MeOH from 50:1 to 20:1).



3a

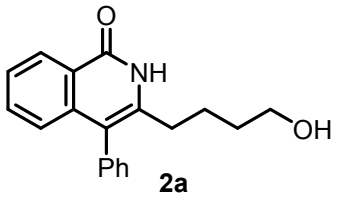
3a was obtained as a yellow solid (81%). Melting point 85-87 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.85 (s, 1H), 8.35 (d, *J* = 7.9 Hz, 1H), 7.78 – 7.63 (m, 2H), 7.49 – 7.36 (m, 6H), 3.49 (t, *J* = 6.3 Hz, 2H), 2.68 – 2.55 (m, 2H), 2.47 (s, 1H), 1.70 – 1.58 (m, 2H), 1.56 – 1.46 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 162.4, 137.8, 137.1, 135.3, 132.6, 129.1, 129.0, 128.7, 127.9, 126.2, 125.7, 123.6, 114.0, 62.1, 32.4, 26.9, 26.7.

IR (ATR-neat) *v* (cm^{-1}) 2931, 2853, 1650, 1606, 1492, 1360, 1053, 1036, 889, 844, 764, 687.

HRMS (ESI, m/z) calcd for $C_{19}H_{20}NO_2$ (M+H) $^+$: 294.1488, found: 294.1501.



2a

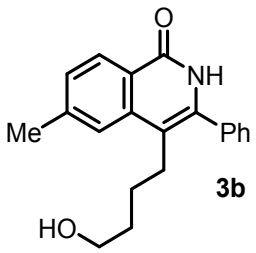
2a was obtained as a yellow solid (10%). Melting point 208-210 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 12.31 (s, 1H), 8.55 (d, *J* = 7.8 Hz, 1H), 7.62 – 7.42 (m, 5H), 7.31 (dd, *J* = 10.0, 3.5 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 1H), 3.89 – 3.72 (m, 3H), 2.65 – 2.48 (m, 2H), 1.97 – 1.82 (m, 2H), 1.68 – 1.55 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 164.8, 139.4, 139.1, 136.3, 132.5, 131.2, 128.7, 127.7, 127.3, 126.0, 125.3, 124.3, 117.4, 61.2, 31.7, 30.4, 25.6.

IR (ATR-neat) *v* (cm^{-1}) 2930, 2853, 1647, 1605, 1445, 1359, 1053, 890, 764, 701.

HRMS (ESI, m/z) calcd for $C_{19}H_{20}NO_2$ $(M+H)^+$: 294.1488, found: 294.1490.



3b

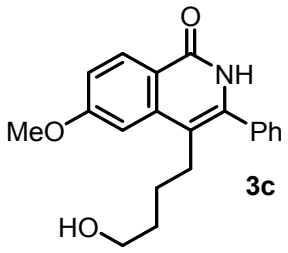
3b was obtained as a yellow solid (79%). Melting point 118-120 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.29 (s, 1H), 8.29 (d, *J* = 8.2 Hz, 1H), 7.52 (s, 1H), 7.49 – 7.37 (m, 5H), 7.31 (dd, *J* = 8.2, 1.5 Hz, 1H), 3.53 (t, *J* = 6.3 Hz, 2H), 2.70 – 2.58 (m, 2H), 2.53 (s, 3H), 2.01 (s, 1H), 1.66 – 1.58 (m, 2H), 1.56 – 1.44 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 143.2, 137.9, 137.0, 135.5, 129.1, 128.9, 128.8, 128.0, 127.9, 123.5, 123.5, 113.8, 62.3, 32.3, 26.8, 26.6, 22.3.

IR (ATR-neat) *v* (cm^{-1}) 2922, 2871, 1642, 1613, 1442, 1313, 1162, 1063, 978, 829, 773, 696.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.1656.



3c

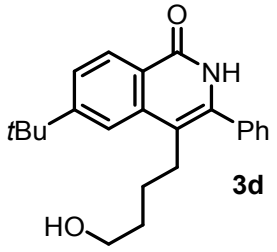
3c was obtained as a yellow solid (83%). Melting point 125-127 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.92 (s, 1H), 8.43 – 8.28 (m, 1H), 7.54 – 7.35 (m, 5H), 7.18 – 7.03 (m, 2H), 3.94 (s, 3H), 3.55 (d, *J* = 6.5 Hz, 2H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.71 – 1.62 (m, 2H), 1.58 – 1.44 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 163.4, 161.7, 140.1, 137.8, 135.8, 130.3, 129.3, 128.9, 120.0, 114.8, 113.5, 106.4, 62.3, 55.5, 32.5, 27.1, 26.4.

IR (ATR-neat) *v* (cm^{-1}) 2925, 2865, 1605, 1487, 1327, 1232, 1069, 1020, 844, 752, 699.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_3$ $(M+H)^+$: 324.1594, found: 324.1596.



3d

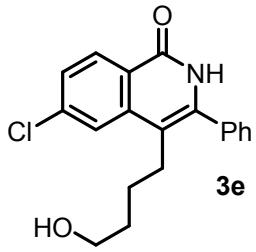
3d was obtained as a yellow solid (80%). Melting point 129-131 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.70 (s, 1H), 8.40 (d, *J* = 8.5 Hz, 1H), 7.75 (d, *J* = 1.8 Hz, 1H), 7.60 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.49 (dd, *J* = 5.3, 1.9 Hz, 3H), 7.43 (dd, *J* = 6.9, 2.9 Hz, 2H), 3.58 (t, *J* = 6.5 Hz, 2H), 2.76 – 2.64 (m, 2H), 1.69 – 1.61 (m, 2H), 1.59 – 1.48 (m, 2H), 1.44 (s, 9H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 162.0, 156.2, 137.8, 137.1, 136.0, 129.2, 129.0, 128.9, 128.0, 124.4, 123.9, 119.9, 114.1, 62.4, 35.4, 32.6 31.3, 27.0, 26.7.

IR (ATR-neat) v (cm^{-1}) 2953, 2867, 1626, 1610, 1418, 1316, 1063, 1025, 842, 768, 700.

HRMS (ESI, m/z) calcd for $C_{23}H_{28}NO_2$ $(M+H)^+$: 350.2114, found: 350.2119.



3e

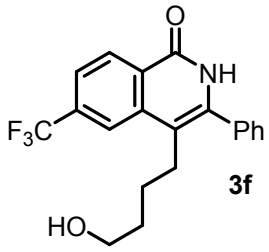
3e was obtained as a yellow solid (85%). Melting point 152-154 °C.

^1H NMR (300 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.36 (d, J = 8.6 Hz, 1H), 7.72 (d, J = 2.0 Hz, 1H), 7.51 (dt, J = 6.0, 2.5 Hz, 3H), 7.48 – 7.40 (m, 3H), 3.55 (d, J = 6.7 Hz, 2H), 2.69 – 2.57 (m, 2H), 1.66 – 1.58 (m, 2H), 1.58 – 1.47 (m, 2H), 1.42 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.6, 139.5, 139.3, 138.4, 135.0, 129.8, 129.5, 129.0, 128.8, 126.9, 124.2, 123.3, 113.2, 62.2, 32.2, 26.8, 26.5.

IR (ATR-neat) v (cm^{-1}) 2926, 2866, 1648, 1598, 1442, 1334, 1060, 1023, 870, 840, 765, 693.

HRMS (ESI, m/z) calcd for $C_{19}H_{19}ClNO_2$ $(M+H)^+$: 328.1099, found: 328.1091.



3f

3f was obtained as a yellow solid (72%). Melting point 168-170 °C.

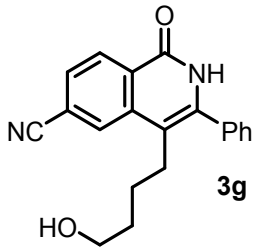
^1H NMR (300 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.56 (d, J = 8.3 Hz, 1H), 8.04 (s, 1H), 7.73 (dd, J = 8.3, 1.7 Hz, 1H), 7.53 (dt, J = 5.8, 2.4 Hz, 3H), 7.46 (dd, J = 6.7, 2.9 Hz, 2H), 3.65 – 3.53 (m, 2H), 2.77 – 2.66 (m, 2H), 1.68 – 1.63 (m, 2H), 1.58 – 1.47 (m, 2H), 1.29 (d, J = 8.4 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3, 138.5, 138.0, 134.9, 134.3 (d, J = 32.4 Hz), 129.4 (d, J = 48.0 Hz), 128.9 (d, J = 22.8 Hz), 128.1, 122.4 (d, J = 3.3 Hz), 121.1 (d, J = 4.1 Hz), 113.8, 62.1, 32.1, 26.7, 26.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.0.

IR (ATR-neat) v (cm^{-1}) 2942, 1655, 1286, 1159, 1124, 1060, 897, 843, 770, 697.

HRMS (ESI, m/z) calcd for $C_{20}H_{19}F_3NO_2$ $(M+H)^+$: 362.1362, found: 362.1366.



3g

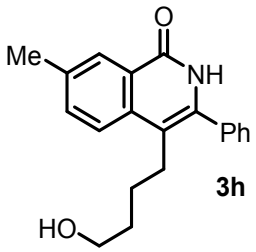
3g was obtained as a yellow solid (67%). Melting point 188-190 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.61 (s, 1H), 8.40 (d, J = 8.2 Hz, 1H), 8.32 (d, J = 7.3 Hz, 1H), 7.99 (dd, J = 30.3, 8.2 Hz, 1H), 7.87 (d, J = 8.2 Hz, 1H), 7.52 (d, J = 4.8 Hz, 2H), 7.44 (d, J = 7.3 Hz, 2H), 4.34 (t, J = 5.1 Hz, 1H), 3.28 (dd, J = 11.6, 6.1 Hz, 2H), 2.56 – 2.51 (m, 2H), 1.56 – 1.43 (m, 2H), 1.33 (dt, J = 12.7, 6.1 Hz, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 166.9, 160.8, 140.7, 138.1, 134.9, 132.8, 129.7, 129.5, 129.5, 128.8, 128.7, 128.4, 119.1, 115.5, 112.4, 60.7, 32.6, 27.0, 26.5.

IR (ATR-neat) v (cm^{-1}) 2927, 2231, 1653, 1548, 1441, 1315, 1026, 841, 766, 731, 693.

HRMS (ESI, m/z) calcd for $C_{20}H_{19}N_2O_2$ $(M+H)^+$: 319.1441, found: 319.1439.



3h

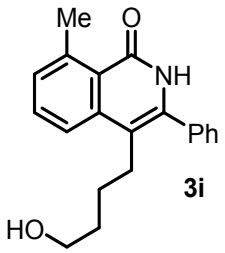
3h was obtained as a red solid (63%). Melting point 109-111 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63 (s, 1H), 8.28 (s, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.57 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.53 – 7.40 (m, 5H), 3.61 – 3.49 (m, 2H), 2.72 – 2.62 (m, 2H), 2.52 (s, 3H), 1.71 – 1.59 (m, 2H), 1.56 – 1.46 (m, 2H), 1.44 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 136.4, 136.0, 135.5, 134.2, 129.0, 128.9, 128.7, 127.5, 125.6, 123.7, 114.0, 62.2, 32.4, 26.9, 26.7, 21.2.

IR (ATR-neat) *v* (cm^{-1}) 2921, 2860, 1651, 1495, 1349, 1064, 909, 826, 776, 702.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.1649.



3i

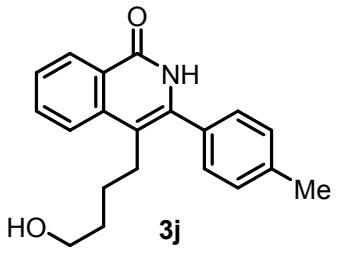
3i was obtained as a red solid (61%). Melting point 112-114 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.67 (s, 1H), 7.63 – 7.52 (m, 2H), 7.47 (q, *J* = 3.9, 3.2 Hz, 5H), 7.23 (d, *J* = 6.9 Hz, 1H), 3.54 (t, *J* = 6.4 Hz, 2H), 2.83 (s, 3H), 2.69 – 2.59 (m, 2H), 1.66 – 1.57 (m, 2H), 1.57 – 1.48 (m, 2H), 1.44 (s, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 163.2, 142.6, 139.7, 137.4, 135.8, 131.8, 129.5, 129.1, 129.0, 128.8, 121.7, 113.7, 62.4, 32.6, 27.4, 26.6, 23.7.

IR (ATR-neat) *v* (cm^{-1}) 2924, 2866, 1645, 1471, 1305, 1071, 1027, 776, 761, 697.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.1653.



3j

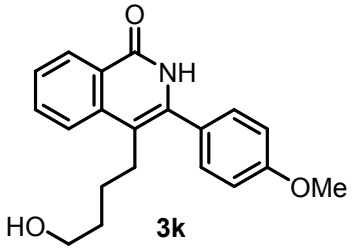
3j was obtained as a yellow solid (79%). Melting point 125-127 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (s, 1H), 8.52 – 8.44 (m, 1H), 7.80 – 7.72 (m, 2H), 7.52 (ddd, *J* = 8.1, 6.3, 1.9 Hz, 1H), 7.37 – 7.29 (m, 4H), 3.59 (t, *J* = 7.3 Hz, 2H), 2.75 – 2.65 (m, 2H), 2.45 (s, 3H), 1.70 – 1.63 (m, 2H), 1.60 – 1.51 (m, 2H), 1.39 (s, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 162.2, 139.2, 137.9, 137.0, 132.7, 132.5, 129.5, 128.7, 128.0, 126.2, 125.7, 123.7, 113.9, 62.3, 32.4, 26.9, 26.7, 21.3.

IR (ATR-neat) *v* (cm^{-1}) 2930, 2864, 1738, 1643, 1468, 1353, 1217, 1058, 812, 766, .

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.1647.



3k

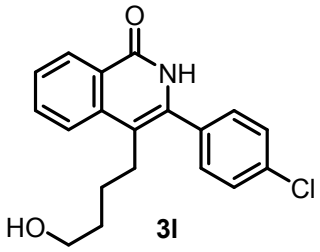
3k was obtained as a yellow solid (82%). Melting point 118-120 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.97 (s, 1H), 8.42 (d, *J* = 8.2 Hz, 1H), 7.78 – 7.66 (m, 2H), 7.53 – 7.42 (m, 1H), 7.33 (d, *J* = 8.8 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 3.86 (s, 3H), 3.55 (t, *J* = 6.2 Hz, 2H), 2.73 – 2.60 (m, 2H), 1.69 – 1.59 (m, 2H), 1.57 – 1.46 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 162.3, 160.1, 138.0, 136.9, 132.6, 130.2, 128.0, 127.7, 126.1, 125.7, 123.6, 114.2, 114.0, 62.3, 55.3, 32.5, 27.0, 26.7.

IR (ATR-neat) v (cm^{-1}) 2928, 1644, 1605, 1511, 1246, 1292, 1181, 1032, 888, 839, 770.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_3$ $(M+H)^+$: 324.1594, found: 324.1604.



3l

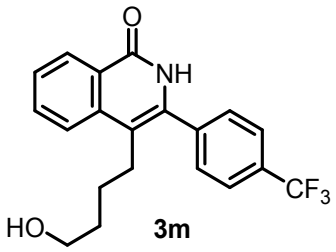
3l was obtained as a yellow solid (83%). Melting point 120-122 °C.

^1H NMR (300 MHz, $CDCl_3$) δ 8.81 (s, 1H), 8.52 – 8.39 (m, 1H), 7.77 (s, 2H), 7.59 – 7.47 (m, 3H), 7.40 (d, J = 7.4 Hz, 2H), 3.60 (s, 2H), 2.66 (d, J = 5.9 Hz, 2H), 1.74 – 1.64 (m, 2H), 1.59 – 1.48 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 137.7, 135.7, 135.4, 133.8, 132.9, 130.4, 129.2, 128.1, 126.7, 125.9, 123.8, 114.4, 62.3, 32.4, 27.0, 26.7.

IR (ATR-neat) v (cm^{-1}) 2922, 2862, 1645, 1486, 1320, 1088, 1013, 813, 772, 722.

HRMS (ESI, m/z) calcd for $C_{19}H_{19}ClNO_2$ $(M+H)^+$: 328.1099, found: 328.1094.



3m

3m was obtained as a yellow solid (80%). Melting point 161-163 °C.

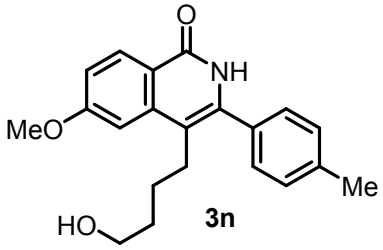
^1H NMR (300 MHz, $CDCl_3$) δ 9.97 (s, 1H), 8.35 (d, J = 8.3 Hz, 1H), 7.75 (dd, J = 4.1, 2.9 Hz, 4H), 7.59 – 7.48 (m, 3H), 3.55 (t, J = 6.1 Hz, 2H), 2.71 – 2.58 (m, 2H), 1.69 – 1.59 (m, 2H), 1.57 – 1.45 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 162.5, 138.8, 137.6, 135.6, 132.9, 132.0, 129.7, 128.0, 127.3, 126.8, 125.8 (d, J = 3.7 Hz), 123.8, 114.6, 62.2, 32.4, 27.0, 26.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.8.

IR (ATR-neat) *v* (cm^{-1}) 2922, 2868, 1643, 1321, 1156, 1121, 1067, 1016, 822, 775.

HRMS (ESI, m/z) calcd for $C_{20}H_{19}F_3NO_2$ $(M+H)^+$: 362.1362, found: 362.1360.



3n

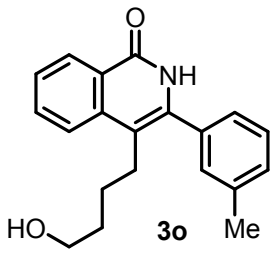
3n was obtained as a yellow solid (67%). Melting point 76-78 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.14 (s, 1H), 8.30 (d, *J* = 8.8 Hz, 1H), 7.27 – 7.19 (m, 4H), 7.08 (d, *J* = 2.1 Hz, 1H), 7.02 (dd, *J* = 8.8, 2.3 Hz, 1H), 3.90 (s, 3H), 3.53 (t, *J* = 6.3 Hz, 2H), 2.65 – 2.52 (m, 2H), 2.39 (s, 3H), 1.68 – 1.56 (m, 2H), 1.55 – 1.43 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 163.0, 162.0, 140.0, 138.9, 137.8, 132.5, 129.9, 129.3, 128.7, 119.4, 114.6, 113.5, 105.8, 62.0, 55.3, 32.3, 27.0, 26.4, 21.2.

IR (ATR-neat) *v* (cm^{-1}) 2928, 2870, 1603, 1494, 1456, 1229, 1066, 1026, 845, 818, 784.

HRMS (ESI, m/z) calcd for $C_{21}H_{24}NO_3$ $(M+H)^+$: 338.1751, found: 338.1756.



3o

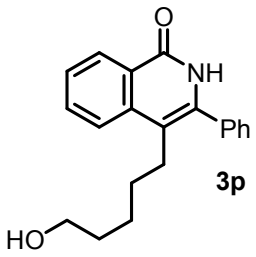
3o was obtained as a yellow oil (71%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.42 (d, *J* = 8.0 Hz, 1H), 7.81 – 7.68 (m, 2H), 7.52 – 7.40 (m, 1H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.24 (dd, *J* = 12.4, 9.5 Hz, 3H), 3.55 (t, *J* = 6.3 Hz, 2H), 2.73 – 2.60 (m, 2H), 2.42 (s, 3H), 1.85 (s, 1H), 1.72 – 1.59 (m, 2H), 1.56 – 1.43 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 138.4, 137.8, 137.2, 135.2, 132.6, 129.8, 129.5, 128.5, 127.8, 126.1, 126.0, 125.6, 123.6, 114.0, 62.1, 32.4, 26.9, 26.7, 21.4.

IR (ATR-neat) *v* (cm^{-1}) 2925, 2861, 1643, 1483, 1347, 1153, 1033, 768, 728, 705.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.1654.



3p

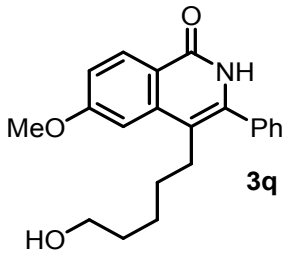
3p was obtained as a yellow solid (87%). Melting point 88-90 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.60 (d, *J* = 25.7 Hz, 1H), 8.42 – 8.33 (m, 1H), 7.74 – 7.67 (m, 2H), 7.51 – 7.38 (m, 6H), 3.57 – 3.47 (m, 2H), 2.68 – 2.55 (m, 2H), 1.64 – 1.52 (m, 2H), 1.44 (dt, *J* = 13.4, 6.6 Hz, 2H), 1.36 – 1.25 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 137.8, 137.0, 135.3, 132.6, 129.0, 129.0, 128.6, 127.9, 126.2, 125.7, 123.6, 114.1, 62.5, 32.2, 30.3, 27.1, 25.7.

IR (ATR-neat) *v* (cm^{-1}) 2930, 2866, 1650, 1605, 1551, 1469, 1360, 1159, 1037, 892, 763, 704.

HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ $(M+H)^+$: 308.1645, found: 308.16440.



3q

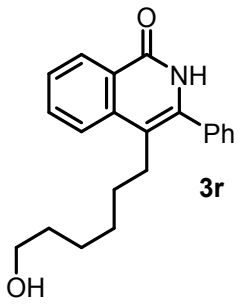
3q was obtained as a yellow solid (76%). Melting point 109-111 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 8.36 – 8.27 (m, 1H), 7.49 – 7.43 (m, 3H), 7.43 – 7.38 (m, 2H), 7.06 (dd, *J* = 7.8, 2.1 Hz, 2H), 3.92 (s, 3H), 3.54 (t, *J* = 6.5 Hz, 2H), 2.62 – 2.53 (m, 2H), 1.58 (dt, *J* = 15.7, 7.8 Hz, 2H), 1.50 – 1.41 (m, 2H), 1.36 – 1.27 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 162.0, 139.9, 137.7, 135.4, 130.0, 129.0, 128.9, 128.7, 119.5, 114.6, 113.7, 106.0, 62.5, 55.4, 32.2, 29.9, 27.2, 25.7.

IR (ATR-neat) *v* (cm^{-1}) 2932, 2862, 1637, 1609, 1452, 1372, 1228, 1074, 1026, 837, 777, 700.

HRMS (ESI, m/z) calcd for $C_{21}H_{24}NO_3$ $(M+H)^+$: 338.1751, found: 338.1754.



3r

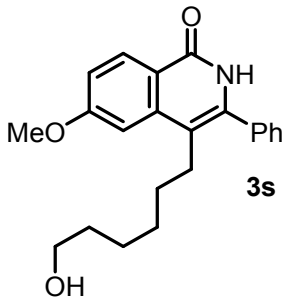
3r was obtained as a yellow solid (84%). Melting point 126-128 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.25 (s, 1H), 8.41 (d, *J* = 8.0 Hz, 1H), 7.75 – 7.69 (m, 2H), 7.53 – 7.45 (m, 4H), 7.45 – 7.40 (m, 2H), 3.56 (t, *J* = 6.6 Hz, 2H), 2.62 (dd, *J* = 9.2, 6.9 Hz, 2H), 1.62 – 1.52 (m, 2H), 1.51 – 1.42 (m, 2H), 1.26 (dd, *J* = 8.8, 5.4 Hz, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 137.9, 136.8, 135.5, 132.7, 129.2, 128.9, 128.8, 128.0, 126.3, 125.8, 123.7, 114.3, 62.8, 32.6, 30.4, 29.4, 27.1, 25.3.

IR (ATR-neat) *v* (cm^{-1}) 2928, 2854, 1651, 1606, 1447, 1361, 1161, 1054, 894, 844, 764, 704.

HRMS (ESI, m/z) calcd for $C_{21}H_{24}NO_2$ $(M+H)^+$: 322.1801, found: 322.1798.



3s

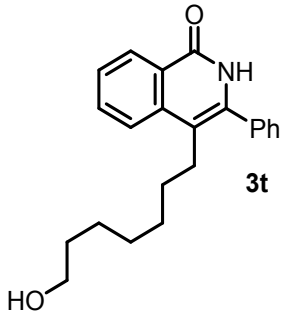
3s was obtained as a yellow solid (80%). Melting point 88-90 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 9.44 (s, 1H), 8.31 (d, *J* = 9.3 Hz, 1H), 7.50 – 7.43 (m, 3H), 7.43 – 7.37 (m, 2H), 7.09 – 7.02 (m, 2H), 3.92 (s, 3H), 3.53 (t, *J* = 6.5 Hz, 2H), 2.60 – 2.51 (m, 2H), 1.54 (dd, *J* = 14.7, 7.1 Hz, 2H), 1.49 – 1.41 (m, 2H), 1.24 (dd, *J* = 9.9, 6.6 Hz, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 162.0, 139.9, 137.7, 135.4, 130.0, 128.9, 128.6, 119.5, 114.5, 113.8, 105.9, 62.5, 55.3, 32.5, 30.0, 29.3, 27.1, 25.2.

IR (ATR-neat) *v* (cm^{-1}) 2928, 2856, 1649, 1606, 1458, 1336, 1228, 1033, 941, 832, 775, 704.

HRMS (ESI, m/z) calcd for $C_{22}H_{26}NO_3$ $(M+H)^+$: 352.1907, found: 352.1910.



3t

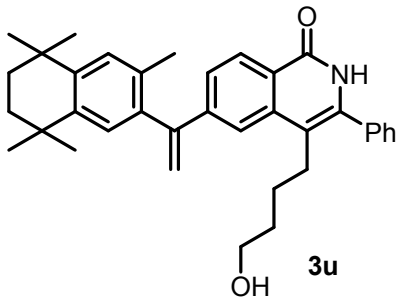
3t was obtained as a yellow solid (80%). Melting point 103-105 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (s, 1H), 8.45 (d, *J* = 7.9 Hz, 1H), 7.77 – 7.70 (m, 2H), 7.54 – 7.46 (m, 4H), 7.45 – 7.41 (m, 2H), 3.59 (t, *J* = 6.6 Hz, 2H), 2.68 – 2.57 (m, 2H), 1.58 (dd, *J* = 14.5, 7.3 Hz, 2H), 1.49 (dd, *J* = 13.8, 7.0 Hz, 2H), 1.33 – 1.17 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 137.9, 136.8, 135.5, 132.7, 129.1, 128.9, 128.8, 128.0, 126.3, 125.8, 123.7, 114.3, 62.9, 32.6, 30.4, 29.5, 28.9, 27.2, 25.6.

IR (ATR-neat) *v* (cm^{-1}) 2926, 2851, 1650, 1614, 1445, 1359, 1035, 889, 842, 763, 718.

HRMS (ESI, m/z) calcd for $C_{22}H_{26}NO_2$ $(M+H)^+$: 336.1958, found: 336.1967.



3u

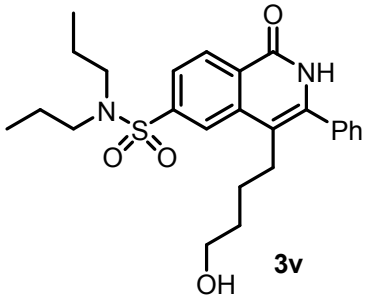
3u was obtained as a yellow solid (64%). Melting point 101-103 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.40 (d, *J* = 8.4 Hz, 1H), 7.63 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.48 (dd, *J* = 5.1, 1.9 Hz, 4H), 7.41 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.20 (s, 1H), 7.11 (d, *J* = 14.5 Hz, 1H), 6.00 – 5.93 (m, 1H), 5.46 – 5.37 (m, 1H), 3.41 (d, *J* = 7.0 Hz, 2H), 2.59 – 2.43 (m, 2H), 2.02 (s, 3H), 1.73 (s, 4H), 1.46 (q, *J* = 8.2 Hz, 2H), 1.32 (d, *J* = 6.5 Hz, 14H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.1, 149.3, 145.0, 144.4, 142.5, 138.2, 137.9, 137.1, 135.4, 132.9, 129.2, 128.9, 128.9, 128.1, 128.1, 128.0, 124.8, 124.5, 122.1, 117.0, 114.3, 62.3, 35.2, 35.2, 34.0, 33.9, 32.1, 32. 0, 31.9, 26.9, 26.7, 20.0.

IR (ATR-neat) *v* (cm^{-1}) 2951, 2910, 2864, 1650, 1625, 1493, 1454, 1361, 1268, 1024, 896, 766, 699.

HRMS (ESI, m/z) calcd for $C_{36}H_{42}NO_2$ $(M+H)^+$: 520.3210, found: 520.3210.



3v

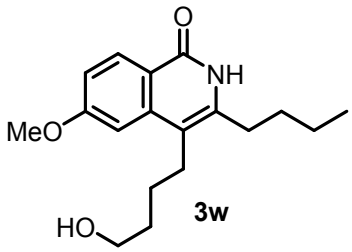
3v was obtained as a yellow solid (56%). Melting point 106-108 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.97 (s, 1H), 8.46 (d, *J* = 8.4 Hz, 1H), 8.26 (d, *J* = 1.7 Hz, 1H), 7.93 – 7.78 (m, 1H), 7.48 (dtt, *J* = 9.9, 6.3, 2.9 Hz, 5H), 3.57 (t, *J* = 6.3 Hz, 2H), 3.21 – 3.06 (m, 4H), 2.77 – 2.65 (m, 2H), 1.90 (s, 1H), 1.71 – 1.49 (m, 8H), 0.88 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.7, 144.0, 139.1, 138.2, 134.7, 129.5, 129.3, 128.9, 128.9, 127.9, 123.3, 123.1, 114.2, 61.9, 50.0, 31.9, 26.7, 22.0, 11.2.

IR (ATR-neat) *v* (cm^{-1}) 2963, 2929, 2872, 1660, 1415, 1337, 1148, 1056, 986, 869, 772, 700.

HRMS (ESI, m/z) calcd for $C_{25}H_{33}N_2O_4S$ $(M+H)^+$: 457.2155, found: 457.2162.



3w

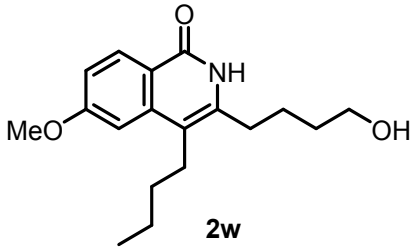
3w was obtained as a yellow solid (27%). Melting point 84-86 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.56 (s, 1H), 8.39 – 8.32 (m, 1H), 7.06 – 7.00 (m, 2H), 3.93 (s, 3H), 3.72 (t, *J* = 6.1 Hz, 2H), 2.75 – 2.67 (m, 2H), 2.64 – 2.56 (m, 2H), 1.75 – 1.63 (m, 6H), 1.45 (dd, *J* = 14.9, 7.4 Hz, 2H), 0.97 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 162.8, 140.3, 138.3, 129.9, 119.0, 113.9, 112.2, 105.3, 62.6, 55.4, 32.7, 31.3, 31.0, 26.3, 26.2, 22.6, 13.9.

IR (ATR-neat) v (cm^{-1}) 2923, 2855, 1651, 1606, 1463, 1337, 1239, 1218, 1064, 1028, 838, 749.

HRMS (ESI, m/z) calcd for $C_{18}H_{26}NO_3$ $(M+H)^+$: 304.1907, found: 304.1902.



2w

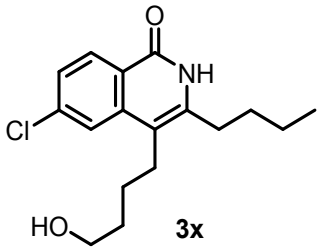
2w was obtained as a yellow solid (59%). Melting point 118-120 °C.

^1H NMR (300 MHz, $CDCl_3$) δ 11.97 (s, 1H), 8.45 (d, J = 8.8 Hz, 1H), 7.08 (dd, J = 11.6, 2.7 Hz, 2H), 4.13 (s, 1H), 3.93 (s, 3H), 3.87 (s, 2H), 2.81 – 2.62 (m, 4H), 1.96 – 1.82 (m, 2H), 1.81 – 1.69 (m, 2H), 1.63 – 1.40 (m, 4H), 0.99 (t, J = 7.1 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 164.2, 163.0, 140.8, 139.1, 129.8, 118.6, 114.4, 113.4, 105.1, 60.5, 55.3, 32.3, 31.6, 29.6, 26.3, 25.5, 22.9, 14.0.

IR (ATR-neat) v (cm^{-1}) 2929, 2866, 1645, 1610, 1500, 1464, 1376, 1237, 1056, 841, 750.

HRMS (ESI, m/z) calcd for $C_{18}H_{26}NO_3$ $(M+H)^+$: 304.1907, found: 304.1915.



3x

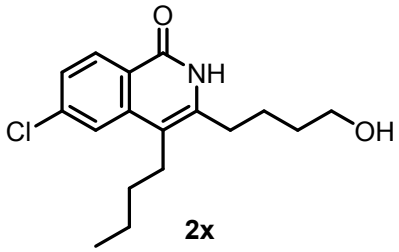
3x was obtained as a yellow solid (31%). Melting point 125-127 °C.

^1H NMR (400 MHz, $CDCl_3$) δ 10.08 (s, 1H), 8.34 (d, J = 8.6 Hz, 1H), 7.63 (d, J = 1.8 Hz, 1H), 7.38 (dd, J = 8.5, 1.8 Hz, 1H), 3.73 (t, J = 6.2 Hz, 2H), 2.74 – 2.67 (m, 2H), 2.67 – 2.60 (m, 2H), 1.75 – 1.61 (m, 6H), 1.46 (dd, J = 14.9, 7.4 Hz, 2H), 0.98 (t, J = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7, 139.7, 139.4, 139.3, 129.6, 126.0, 122.6, 112.0, 62.6, 32.6, 31.3, 30.9, 26.5, 26.2, 22.6, 13.8.

IR (ATR-neat) *v* (cm^{-1}) 2926, 2869, 1671, 1599, 1456, 1333, 1056, 909, 829, 775, 727.

HRMS (ESI, m/z) calcd for $C_{17}H_{23}ClNO_2$ $(M+H)^+$: 308.1412, found: 308.1422.



2x

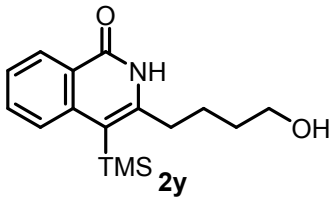
2x was obtained as a yellow solid (65%). Melting point 170-172 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 12.06 (s, 1H), 8.42 (d, *J* = 8.6 Hz, 1H), 7.64 (d, *J* = 1.5 Hz, 1H), 7.42 (dd, *J* = 8.6, 1.7 Hz, 1H), 3.85 (s, 2H), 3.74 (s, 1H), 2.85 – 2.58 (m, 4H), 1.85 (d, *J* = 15.7 Hz, 2H), 1.81 – 1.68 (m, 2H), 1.63 – 1.40 (m, 4H), 0.99 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 164.0, 140.0, 139.9, 139.4, 129.5, 126.3, 122.9, 122.6, 113.2, 60.8, 32.5, 31.6, 29.8, 26.2, 25.5, 22.9, 13.9.

IR (ATR-neat) *v* (cm^{-1}) 2922, 2856, 1668, 1628, 1599, 1460, 1312, 1056, 910, 860, 775.

HRMS (ESI, m/z) calcd for $C_{17}H_{23}ClNO_2$ $(M+H)^+$: 308.1412, found: 308.1417.



2y

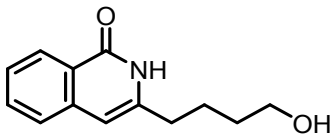
2y was obtained as a yellow solid (89%). Melting point 153-155 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 11.60 (s, 1H), 8.49 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 3.84 (s, 2H), 3.56 (s, 1H), 2.92 – 2.75 (m, 2H), 1.89 (dt, *J* = 14.5, 7.4 Hz, 2H), 1.79 – 1.68 (m, 2H), 0.49 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.2, 148.1, 142.3, 131.8, 127.6, 127.1, 125.6, 124.5, 109.5, 60.6, 32.8, 31.5, 27.1, 3.3.

IR (ATR-neat) *v* (cm^{-1}) 3432, 2931, 2892, 1647, 1586, 1465, 1355, 1275, 1251, 1077, 1030, 839, 778.

HRMS (ESI, m/z) calcd for $C_{16}H_{24}NO_2Si$ $(M+H)^+$: 290.1571, found: 290.1568.



2z

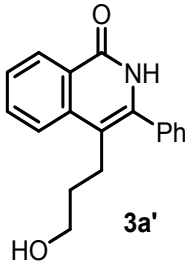
2z was obtained as a yellow solid (68%). Melting point 115-117 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 11.63 (s, 1H), 8.40 (d, *J* = 8.0 Hz, 1H), 7.68 – 7.57 (m, 1H), 7.50 – 7.40 (m, 2H), 6.38 (s, 1H), 3.80 (t, *J* = 5.9 Hz, 2H), 2.74 – 2.62 (m, 2H), 1.97 – 1.85 (m, 2H), 1.71 (dt, *J* = 12.6, 6.3 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 165.3, 142.0, 138.9, 132.7, 127.3, 126.1, 125.7, 104.7, 61.3, 32.6, 31.5, 25.3.

IR (ATR-neat) *v* (cm^{-1}) 3410, 2924, 2880, 1631, 1548, 1346, 1264, 1064, 944, 819, 758.

HRMS (ESI, m/z) calcd for $C_{13}H_{16}NO_2$ $(M+H)^+$: 218.1175, found: 218.1177.

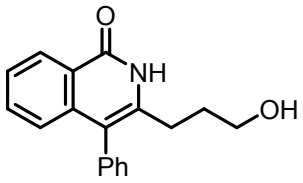


3a'

3a' was obtained as a yellow solid (31%).[3]

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (s, 1H), 8.49 (d, *J* = 8.0 Hz, 1H), 7.87 – 7.72 (m, 2H), 7.60 – 7.42 (m, 6H), 3.60 (q, *J* = 5.7 Hz, 2H), 2.83 – 2.71 (m, 2H), 1.87 – 1.78 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.1, 137.7, 137.0, 135.3, 132.8, 129.3, 129.0, 128.9, 128.1, 126.5, 125.9, 123.7, 113.5, 62.2, 33.2, 23.5.



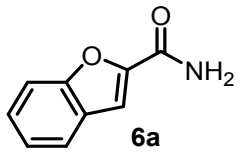
2a'

2a' was obtained as a yellow solid (58%).[3]

^{1}H NMR (300 MHz, $CDCl_3$) δ 12.40 (s, 1H), 8.41 (d, *J* = 7.9 Hz, 1H), 7.59 – 7.41 (m, 5H), 7.31 – 7.25 (m, 2H), 7.13 (d, *J* = 8.1 Hz, 1H), 4.06 (s, 1H), 3.71 (s, 2H), 2.73 (t, *J* = 7.2 Hz, 2H), 1.93 (d, *J* = 5.9 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 164.8, 139.4, 138.9, 136.0, 132.7, 131.0, 128.8, 127.8, 127.0, 126.2, 125.3, 123.7, 118.1, 60.9, 32.7, 27.1.

To a Schlenk flask equipped with a stir bar were added **5** (0.3 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (0.03 mmol), NaOAc (0.6 mmol) and MeOH (3.0 mL). The reaction was stirred for 4 h at 60 °C, cooled to room temperature. The solvent was removed in *vacuo* and the remaining residue was purified by a silica gel column chromatography to afford the product **4b** (*n*-heptane/ethyl acetate from 6:1 to 2:1), **6a** (*n*-heptane/ethyl acetate from 2:1 to 1:2), **6b** (*n*-heptane/ethyl acetate from 1:1 to 1:4) and **6c** (DCM/MeOH from 50:1 to 20:1).



6a

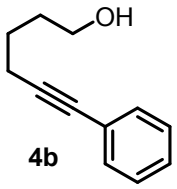
6a was obtained as a yellow solid (33%). Melting point 135-137 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.7 Hz, 1H), 7.51 (d, *J* = 3.9 Hz, 2H), 7.43 (t, *J* = 7.7 Hz, 1H), 7.29 (dd, *J* = 14.1, 6.3 Hz, 1H), 6.53 (s, 1H), 6.08 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.7, 154.9, 148.1, 127.5, 127.2, 123.8, 122.8, 111.8, 111.3.

IR (ATR-neat) *v* (cm^{-1}) 3425, 3153, 2880, 1658, 1591, 1398, 986, 785, 740.

HRMS (ESI, m/z) calcd for $C_9H_8NO_2$ $(M+H)^+$: 162.0550, found: 162.0552.



4b

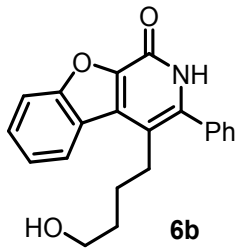
4b was obtained as a yellow oil (31%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 (dd, *J* = 6.4, 3.0 Hz, 2H), 7.31 – 7.21 (m, 3H), 3.70 (t, *J* = 6.0 Hz, 2H), 2.45 (t, *J* = 6.4 Hz, 2H), 1.82 – 1.63 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 131.5, 128.2, 127.5, 123.8, 89.8, 80.9, 62.4, 31.9, 25.0, 19.2.

IR (ATR-neat) *v* (cm^{-1}) 3322, 2937, 1489, 1062, 754, 690.

HRMS (ESI, m/z) calcd for $C_{12}H_{15}O$ $(M+H)^+$: 175.1117, found: 175.1115.



6b

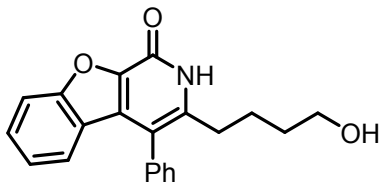
6b was obtained as a yellow oil (20%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.75 (s, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 8.3 Hz, 1H), 7.63 – 7.36 (m, 7H), 3.55 (d, *J* = 6.8 Hz, 2H), 2.83 (d, *J* = 8.1 Hz, 2H), 1.87 (s, 1H), 1.73 (q, *J* = 7.7 Hz, 2H), 1.58 (t, *J* = 7.2 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0, 153.8, 143.5, 138.1, 134.2, 130.5, 129.4, 129.2, 128.9, 128.7, 123.8, 123.3, 123.1, 113.6, 113.1, 62.2, 32.2, 27.9, 26.6.

IR (ATR-neat) *v* (cm^{-1}) 2921, 2854, 1652, 1441, 1226, 1111, 1037, 840, 752, 695.

HRMS (ESI, m/z) calcd for $C_{21}H_{20}NO_3$ $(M+H)^+$: 334.1438, found: 334.1447.



6c

6c was obtained as a yellow solid (29%). Melting point 237-239 °C.

^{1}H NMR (300 MHz, DMSO-d_6) δ 11.98 (s, 1H), 7.83 – 7.71 (m, 1H), 7.63 – 7.46 (m, 4H), 7.41 (d, *J* = 6.4 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 1H), 6.66 – 6.54 (m, 1H), 4.32 (d, *J* = 4.6 Hz, 1H), 3.26 (d, *J* = 6.4 Hz, 2H), 2.40 (d, *J* = 7.4 Hz, 2H), 1.54 (s, 2H), 1.30 (s, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 156.5, 154.1, 142.1, 141.5, 135.7, 130.8, 129.7, 129.3, 129.1, 128.6, 123.8, 123.4, 122.7, 113.1, 112.6, 60.8, 32.4, 29.8, 26.5.

IR (ATR-neat) *v* (cm^{-1}) 2856, 1659, 1462, 1443, 1192, 1030, 903, 749, 705.

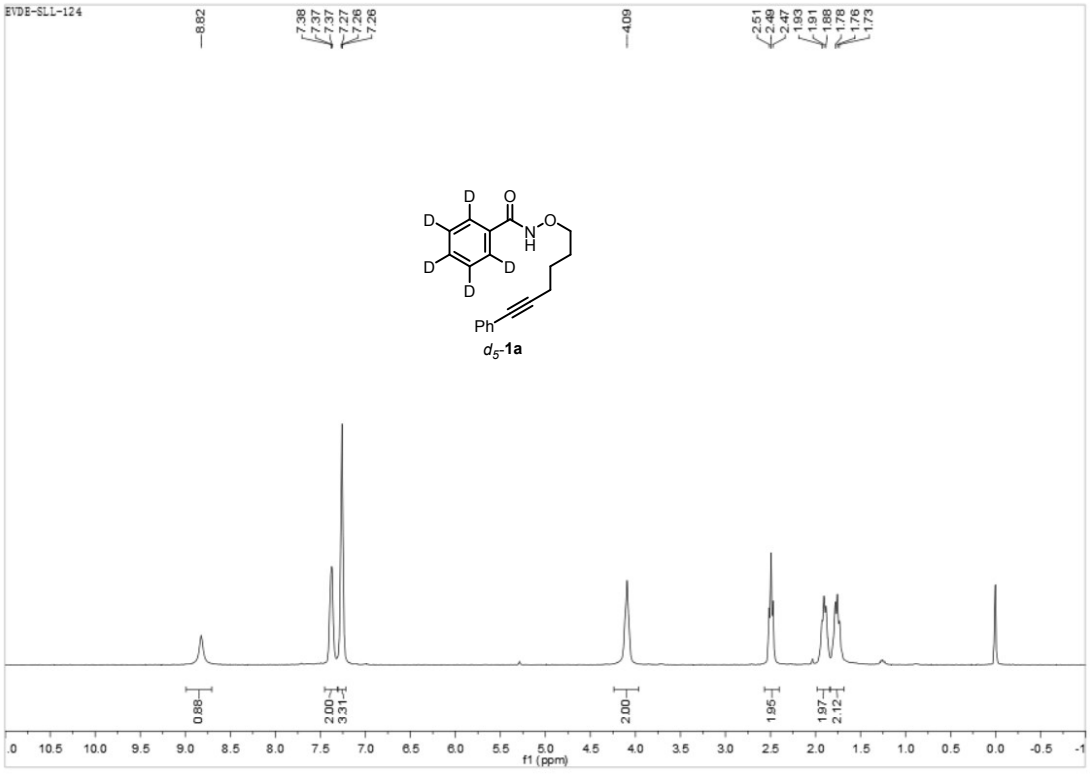
HRMS (ESI, m/z) calcd for $C_{21}H_{20}NO_3$ $(M+H)^+$: 334.1438, found: 334.1447.

4. Additional Experiments

Irreversible C-H bond metalation:

To a Schlenk flask equipped with a stir bar were added **1a** (0.3 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (0.03 mmol), NaOAc (0.6 mmol) and CD_3OD (3.0 mL). The reaction was stirred for 30 min at 60 °C, cooled to room temperature. The solvent was removed in *vacuo* and the remaining residue was purified by a silica gel column chromatography (*n*-heptane/ethyl acetate or DCM/MeOH). **1a**, **2a** and **3a** were isolated and no deuterium incorporation was found.

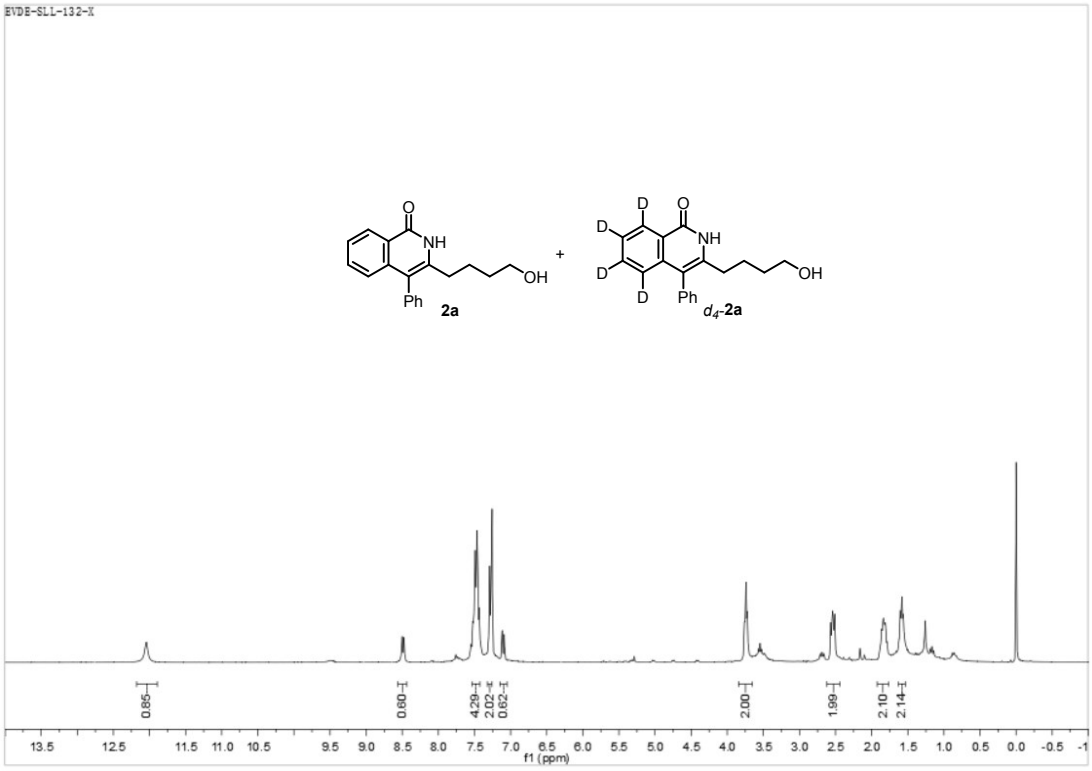
KIE experiments:

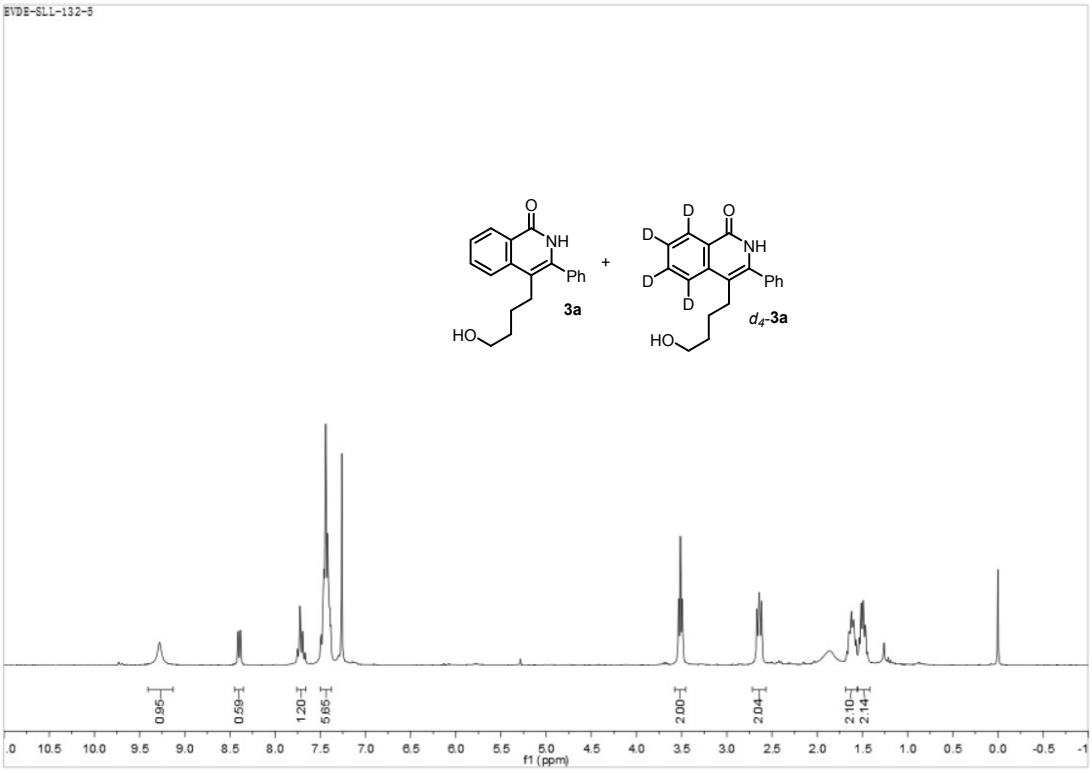


To one Schlenk flask equipped with a stir bar were added **1a** (0.15 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (0.015 mmol), NaOAc (0.3 mmol) and MeOH (1.5 mL). The reaction was stirred for 30 min at 60 °C, cooled to room temperature.

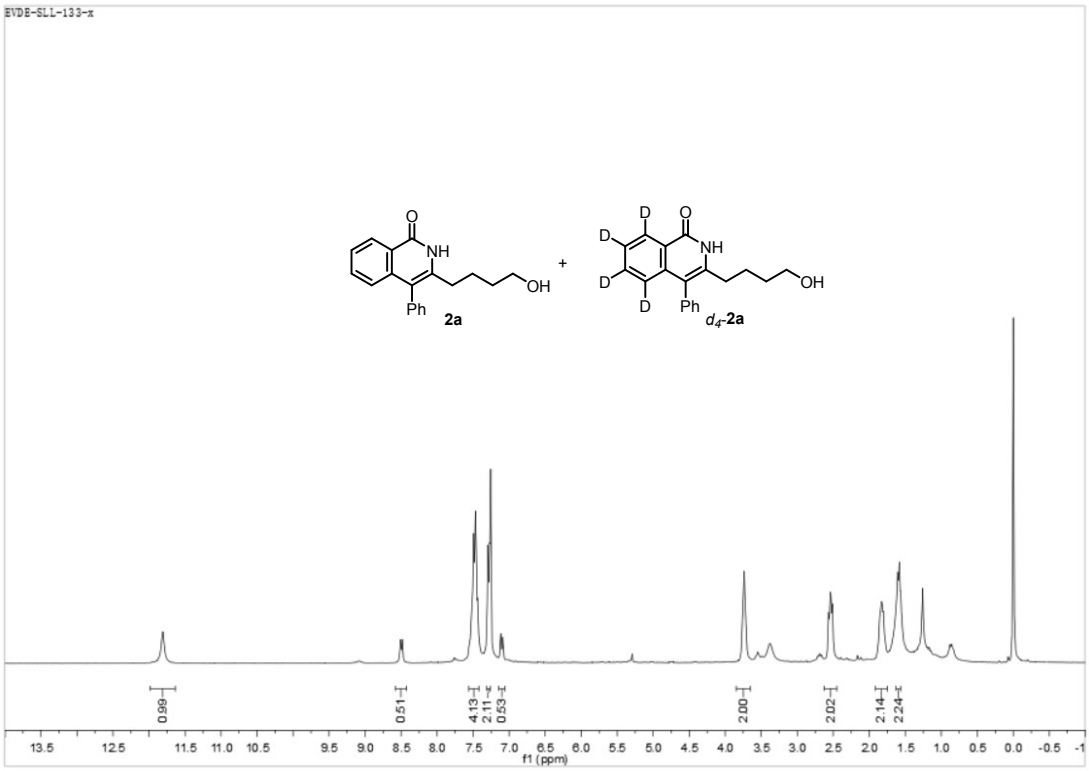
To another Schlenk flask equipped with a stir bar were added d_5-**1a** (0.15 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (0.015 mmol), NaOAc (0.3 mmol) and MeOH (1.5 mL). The reaction was stirred for 30 min at 60 °C, cooled to room temperature.

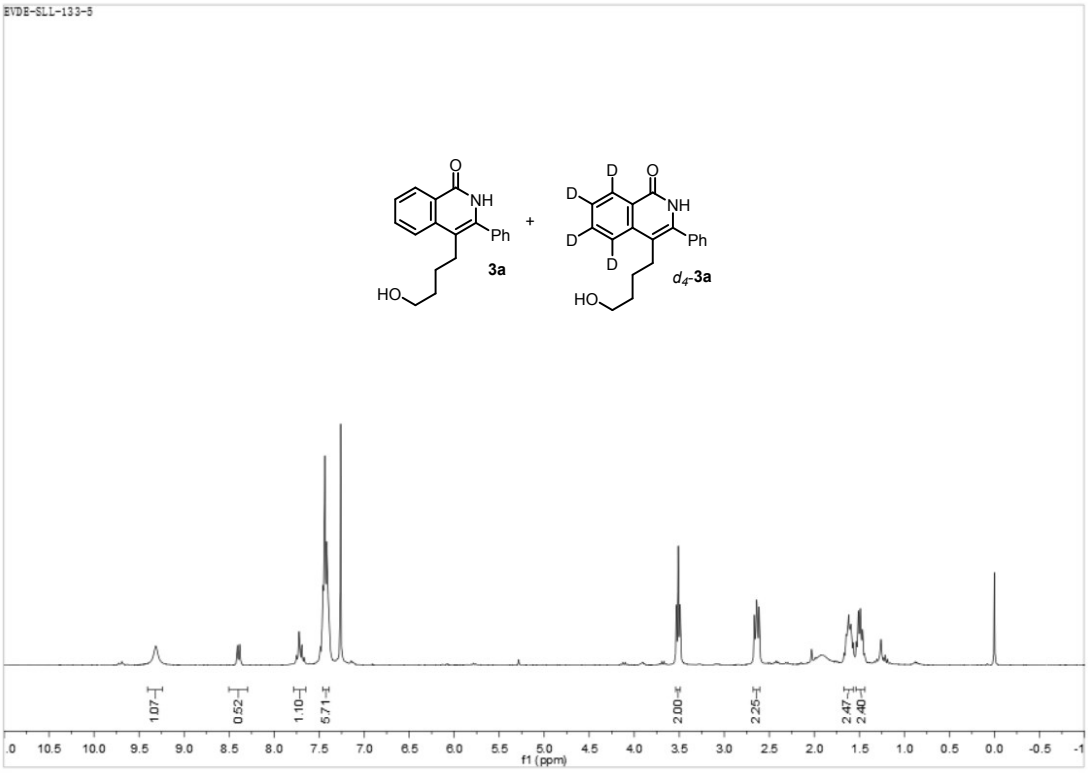
Then these two reaction mixture were combined and the solvent was removed in *vacuo* and the remaining residue was purified by a silica gel column chromatography (*n*-heptane/ethyl acetate or DCM/MeOH) to afford the product **2a**, **3a**, d_4-**2a** and d_4-**3a**. The ratio of **2a** and d_4-**2a** was determined by ^{1}H NMR to be 0.60:0.40 (see below). The ratio of **3a** and d_4-**3a** was determined by ^{1}H NMR to be 0.59:0.41 (see below).





To a Schlenk flask equipped with a stir bar were added **1a** (0.15 mmol), d_5-**1a** (0.15 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (0.03 mmol), NaOAc (0.6 mmol) and MeOH (3.0 mL). The reaction was stirred for 30 min at 60 °C, cooled to room temperature. The solvent was removed in *vacuo* and the remaining residue was purified by a silica gel column chromatography (*n*-heptane/ethyl acetate or DCM/MeOH) to afford the product **2a**, **3a**, d_4-**2a** and d_4-**3a**. The ratio of **2a** and d_4-**2a** was determined by ^{1}H NMR to be 0.51:0.49 (see below). The ratio of **3a** and d_4-**3a** was determined by ^{1}H NMR to be 0.52:0.48 (see below).





Control experiment:

To a Schlenk flask equipped with a stir bar were added **1a** (0.1 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (0.005 mmol), NaOAc (0.2 mmol) and MeOH (1.0 mL). The reaction was stirred for 30 min at r.t. The solvent was removed in *vacuo* and the remaining residue was purified by a silica gel column chromatography to afford the product **2a**, **3a**, **4a**, **4b** and **4c**.

Reaction of benzamide and alcohol:

To a Schlenk flask equipped with a stir bar were added **4a** (0.1 mmol), **4b** (0.15 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (0.01 mmol), NaOAc (0.2 mmol), $Cu(OAc)_2$ (0.2 mmol) and MeOH (1.0 mL). The reaction was stirred for 4 h at 60 °C, cooled to room temperature. The solvent was removed in *vacuo* and the remaining residue was purified by a silica gel column chromatography to afford the product **2a** and **3a**.

Crossing experiment:

To a Schlenk flask equipped with a stir bar were added **1c** (0.1 mmol), **1j** (0.1 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (0.02 mmol), NaOAc (0.4 mmol) and MeOH (2.0 mL). The reaction was stirred for 4 h at 60 °C, cooled to room temperature. The solvent was removed in *vacuo* and the remaining residue was purified by a silica gel column chromatography to afford the product **3a**, **3c**, **3j** and **3n**.

5. Single Crystal X-Ray Diffraction

A single crystal of **3c** was obtained by slow diffusion from a solution of the compound in DCM layered with heptane at room temperature for several days. X-ray intensity data were collected at 293(2) K on an Agilent SuperNova diffractometer with Eos CCD detector using MoKα radiation. The images were processed (unit cell determination, intensity data integration, correction for Lorentz and polarization effects, and empirical absorption correction) using CrysAlisPRO[4]. Using Olex2[5], the structure was solved with the ShelXT[6] structure solution program using Intrinsic Phasing and refined with the ShelXL[7] refinement package using full-matrix least-squares minimization on F^2. The asymmetric unit contains one molecule **3c** and one molecule DCM. All H atoms were placed in idealized positions and refined in the riding mode. Non-hydrogen atoms were refined anisotropically and hydrogen atoms in the riding mode with isotropic temperature factors fixed at 1.2 times U_{eq} of the parent atoms (1.5 for -OH and methyl groups). Crystal data, data collection and structure refinement details are summarized in Table S1. Crystallographic data for **3c** has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 1959807.

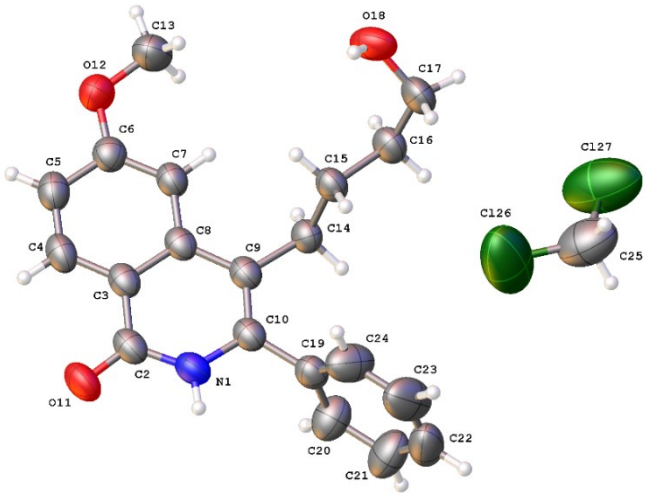


Figure S1. Molecular structure of **3c** showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small circles of arbitrary radii.

Table S1. Crystal data, data collection and structure refinement details of compound **3c**

	3c
Empirical formula	$C_{20}H_{21}NO_3$, CH_2Cl_2
Formula weight	408.30
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.9486(5)
b/Å	9.5948(4)
c/Å	12.8823(6)
α/°	82.687(4)
β/°	71.563(4)
γ/°	87.665(4)
Volume/Å^3	1040.77(9)
Z	2
ρ_{calc}g/cm^3	1.303
μ/mm^{-1}	0.332
F(000)	428.0
Crystal size/mm^3	0.4 × 0.15 × 0.15

Radiation	MoKα (λ = 0.71073 Å)
2Θ range for data collection/°	4.798 to 52.742
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -16 ≤ l ≤ 16
Reflections collected	21373
Independent reflections	4239 [R_{int} = 0.0220, R_{sigma} = 0.0185]
Data/restraints/parameters	4239/0/250
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0650, wR_2 = 0.1713
Final R indexes [all data]	R_1 = 0.0866, wR_2 = 0.1897
Largest diff. peak/hole / e $Å^{-3}$	0.34/-0.43

6. DFT Calculation Details

Computational Details. All the density functional theory (DFT) calculations were carried out using Gaussian 16 software[8] with B3LYP-D3/def2-TZVP method[9]. Vibrational frequency calculations were performed at the same level of theory to examine if the optimized structure is an intermediate or transition state. Both the singlet and triplet electronic states were considered for those crucial structures. Intrinsic reaction coordinate (IRC) calculations were performed for those key transition states to verify that they connect the right intermediates. The solvent effect of methanol was considered in the single point calculations with the implicit solvation model (SMD)[10]. All energies presented in the main text and here are Gibbs free energies relative to the substrate and the $Ru(OAc)_2$(*p*-cymene) catalyst, unless otherwise stated, and are calculated in each case using a standard state for the translational component of the partition function corresponding to a concentration of 1 mol dm^{-3}. The default free energies obtained from Gaussian are therefore corrected for all species by adding a term RT ln (24.5) = 2.12 kcal mol^{-1}. So as to give insight into the effects of solvation, relative Gibbs free energies are provided calculated in the

gas phase and while taking into account solvation effects for methanol solvent using the SMD model, and these are referred to as ΔG_{gas} and ΔG_{soln}, respectively. In every case, these numbers are presented with main, solution phase number first, and the gas phase value second, in parentheses.

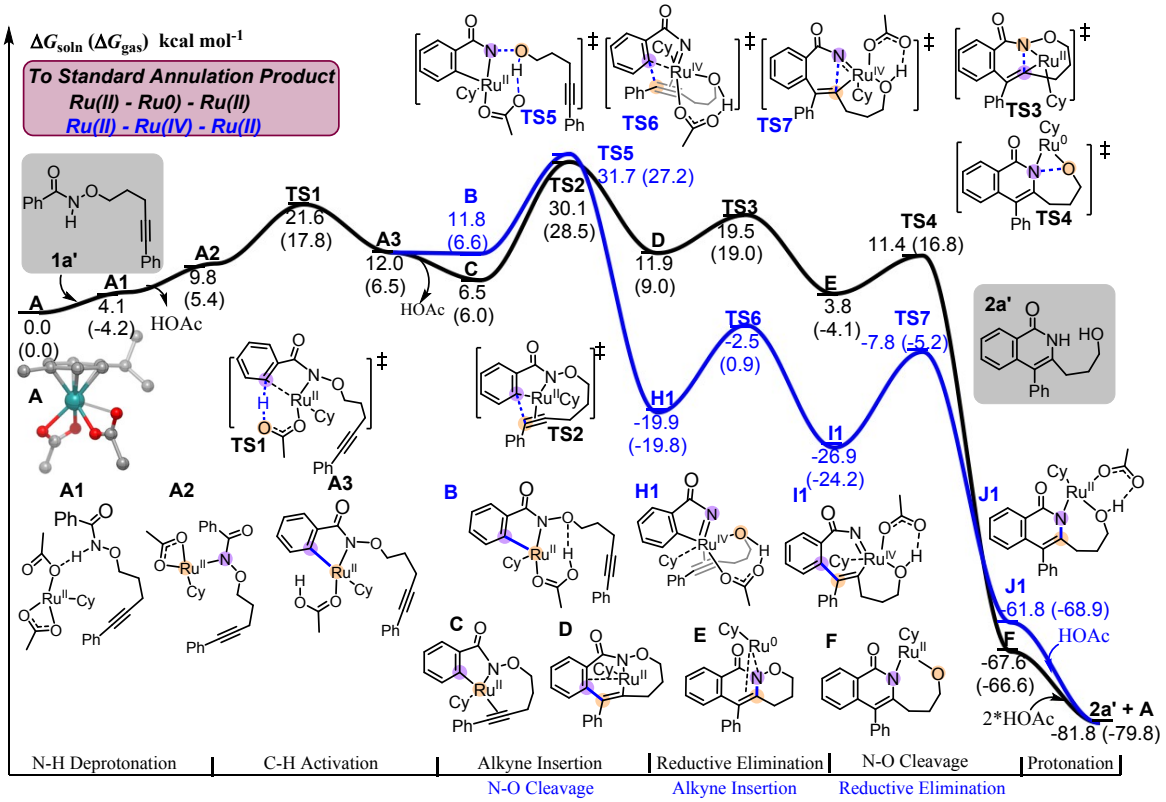


Figure S2. Two possible routes leading to the **standard annulation** product. Both the solution phase and gas phase (in parentheses) Gibbs free energies (in kcal mol^{-1}) calculated at the B3LYP-D3/def2-TZVP (SMD: methanol) level are shown.

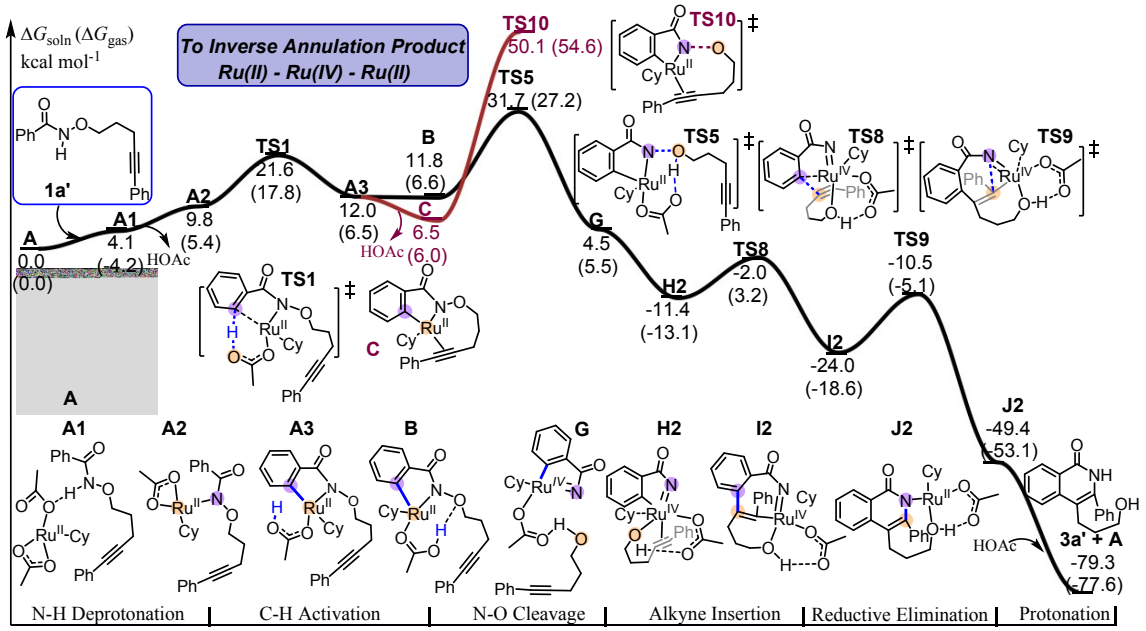
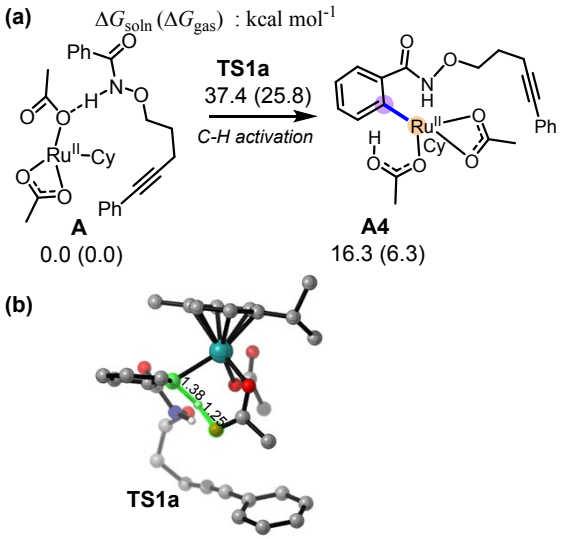


Figure S3. Calculated Gibbs free energy profile in gas phase (in parentheses) and solution phase for Ru-catalyzed **inverse annulation** reaction at the B3LYP-D3/def2-TZVP (SMD) level.

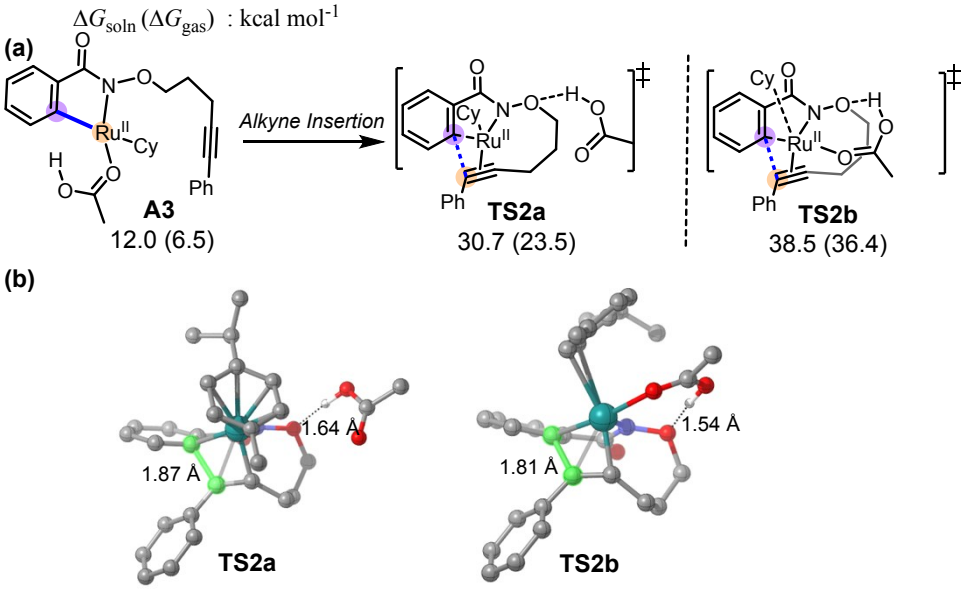
High Energy Routes. Our calculations support the mechanism initiated with the deprotonation of N-H occuring prior to C-H activation, since the pathway involving C-H activation occurring first involves a higher energy transition state (**TS1a** in **Scheme S1**).

We have considered several other possible reaction routes (below, Scheme **S3** –**S4**) leading to the standard annulation product. In the traditional annulation mechanism with alkyne insertion occurring prior to N-O cleavage, alkyne insertion into the Ru-N bond preceding C-C reductive elimination (**Scheme S3**) is less facile and requires a higher barrier (35.4 kcal mol^{-1}, **TS12**) than that for alkyne insertion into the Ru-C bond (30.1 kcal mol^{-1}, **TS2** in **Figure S2**). In addition, once the alkyne insertion into Ru-C bond is completed, the path with N-O oxidative cleavage prior to reductive elimination (**Scheme S4**) is calculated to be less favorable (**TS13**, 23.2 kcal mol^{-1} *vs* 19.5 kcal mol^{-1}, **TS3**).

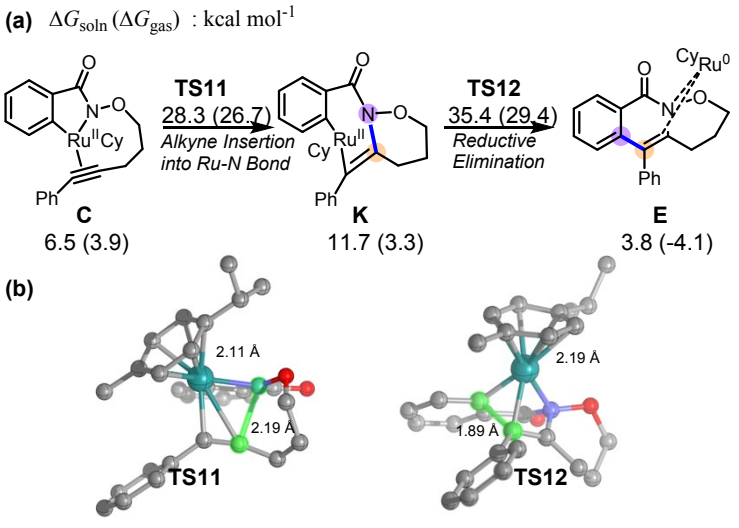
In the newly proposed mechanism consisting of N-O cleavage occurring before alkyne insertion, we also examined the route involving N-O cleavage occurring prior to C-H activation (**Scheme S5**), and this route is found to be highly unfavorable due to a high-energy C-H activation transition state (**TS16**, 58.7 kcal mol^{-1}). After N-O cleavage, alkyne insertion into Ru=N site is also found to be less favorable (10.7 kcal mol^{-1}, **TS17** in **Scheme S6**) than insertion into Ru-C bond (**TS6** and **TS8**, -2.0 - -2.5 kcal mol^{-1}).



Scheme S1. (a) Schematic mechanism involving C-H activation prior to N-H deprotonation, with calculated Gibbs free energies (kcal mol^{-1}) relative to overall reactants (values in parentheses are gas phase free energies). (b) Geometries of singlet **TS1a.** The barrier here is higher than the common pathway with N-H deprotonation occurring first.

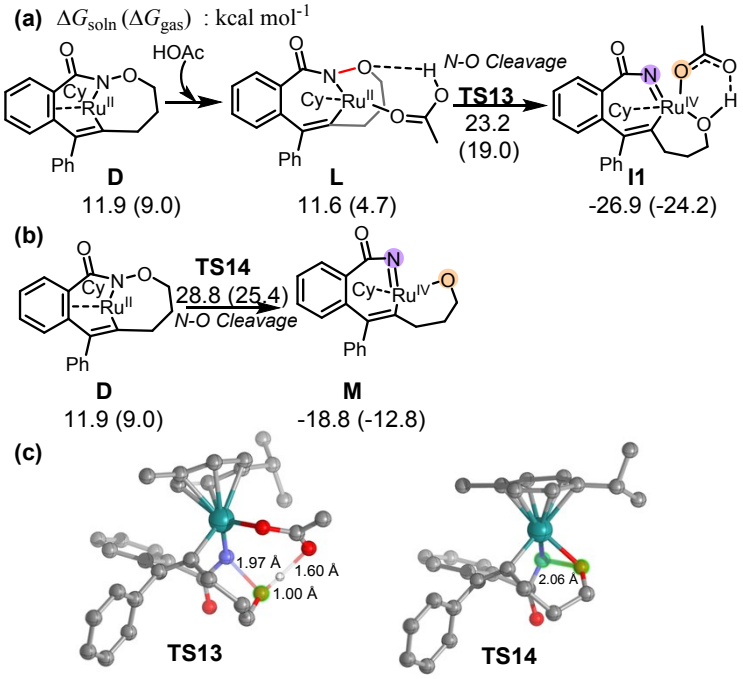


Scheme S2. (a) Schematic mechanism of the rate determining alkyne insertion step in presence of acetic acid, with calculated Gibbs free energies (kcal mol^{-1}) relative to overall reactants (values in parentheses are gas phase free energies). The acetic acid is either coordinated (**TS2b**) or not coordinated to the metal (**TS2a**); (b) Geometries of singlet **TS2a** and **TS2b.** Our calculation shows that in the presence of acetic acid, alkyne insertion has a comparable barrier (**TS2a**; 30.7 kcal/mol) to the one in absence of acetic acid (**TS2**; 30.1 kcal/mol). Thus, alkyne insertion step is not sensitive to the presence of acetic acid.

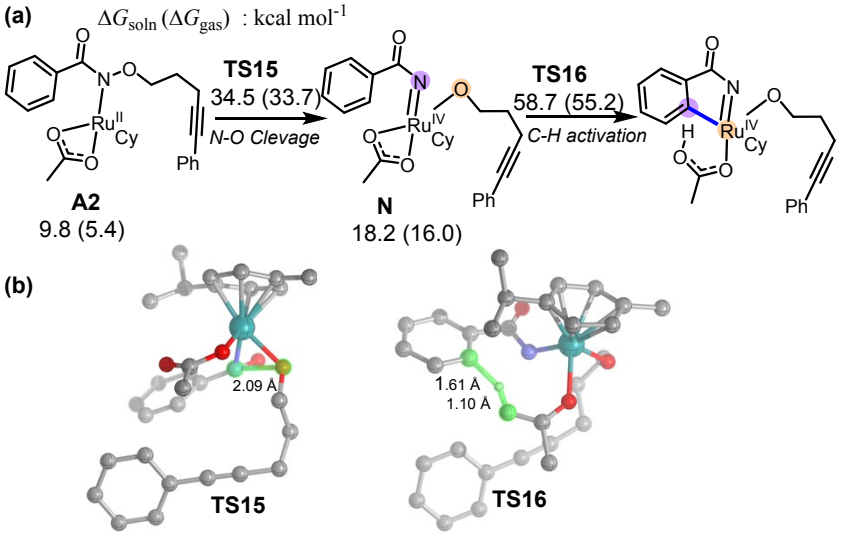


Scheme S3. (a) Schematic mechanism involving alkyne insertion into the Ru-N bond prior to the reductive elimination leading to the standard annulation product, with calculated Gibbs free energies

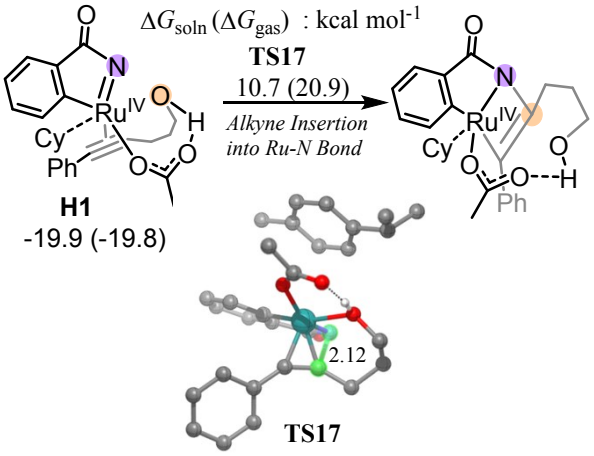
(kcal mol^{-1}) relative to overall reactants (values in parentheses are gas phase free energies). (b) Geometries of singlet **TS11** and **TS12.**



Scheme S4. Schematic mechanism involving N-O cleavage following alkyne insertion into the Ru-C bond in the (a) presence and (b) absence of metal-coordinated acetic acid, with calculated Gibbs free energies (kcal mol^{-1}) relative to overall reactants (values in parentheses are gas phase free energies). (c) Geometries of singlet state **TS13** and **TS14.**



Scheme S5. (a) Schematic mechanism involving N-O cleavage prior to C-H activation, with calculated Gibbs free energies (kcal mol^{-1}) relative to overall reactants (values in parentheses are gas phase free energies). (b) Geometries of singlet **TS15** and **TS16.**

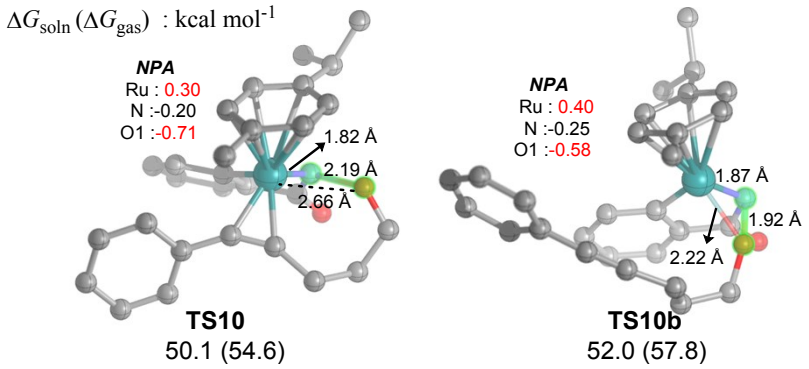


Scheme S6. Schematic mechanism involving alkyne insertion into the Ru=N bond after N-O cleavage, with calculated Gibbs free energies (kcal mol^{-1}) relative to overall reactants (values in parentheses are gas phase free energies).

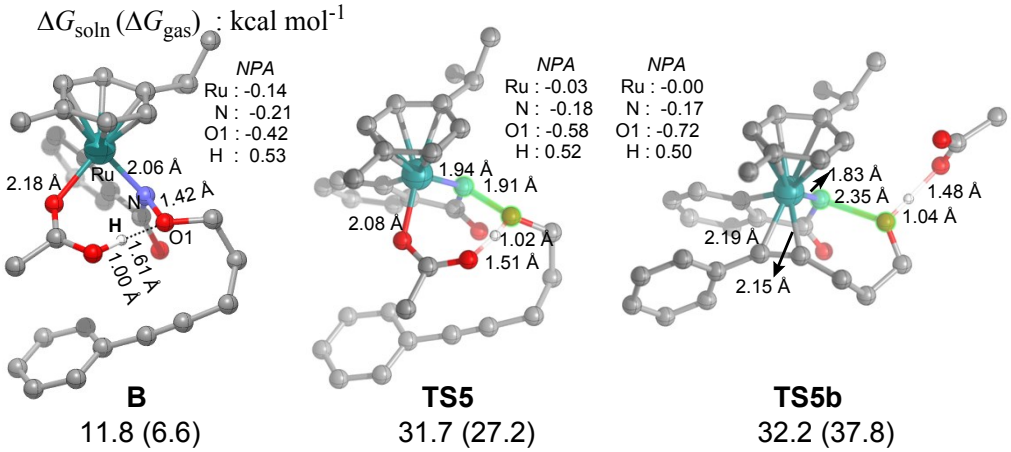
Routes to the Inverse Annulation Product. As discussed in the main text, N-O cleavage in the absence of HOAc assistance (direct cleavage) is significantly more unfavorable (>50.1 kcal mol^{-1}, **TS10** in **Figure S3**) compared to the HOAc assisted process. In the direct cleavage process, two transition state isomers (**Scheme S7**) were located, one TS with alkyne coordination to the metal (**TS10,** 50.1 kcal mol^{-1}) while the other does not have this interaction (**TS10b,** 52.0 kcal mol^{-1}). Both of them show very high energies (>50.1 kcal mol^{-1}), and their alkoxyl oxygen atom displays considerable negative charge. However, with the assistance of the *in situ* generated HOAc, the barrier for N-O cleavage can be decreased to 31.7 kcal mol^{-1} in solution (**TS5**, **Scheme S8**). The HOAc can either coordinate to the metal center and form a O-H···O hydrogen bond with the internal oxidizing N-O group (**TS5**), or dissociate from the metal center, but still preserve the hydrogen bond (**TS5b**). **TS5** is slightly favored by 0.5 kcal mol^{-1} in energy over **TS5b**. In both TSs, the proton transfer to the N-O oxidizing site is almost complete and the negatively charged oxygen atom is largely neutralized.

We have considered the effect of one explicit methanol molecule in the N-O cleavage step. In absence of acetic acid, the methanol could also transfer its hydrogen to neutralize alkoxyl oxygen atom of the substrate, and result into a negative methoxyl group (**TS5d**, **TS5e** in **Scheme 9**). However, the calculated barrier is much higher (>51.0 kcal/mol) than the acetic acid assisted mechanism, which could be explained by the facile deprotonation of more acidic acetic acid, and stabilization of negative charge in the acetate. The methanol mediated proton transfer barrier is comparable to the barrier of direct N-O cleavage process (**TS10**), and experiments also found the reaction proceeds smoothly to the desired product with alcohol-free solvents (e.g., Acetone). Thus, the role of methanol could be excluded in the reaction.

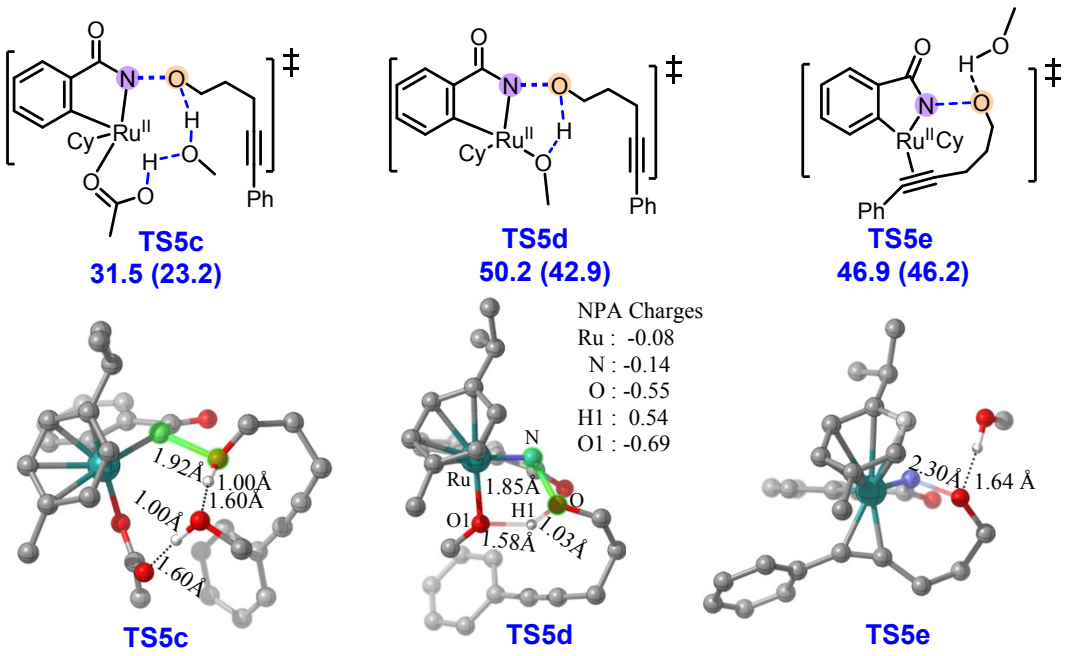
Once N-O cleavage is finished, the subsequent reaction steps leading to the annulation product (alkyne insertion, reductive elimination and protonation) become much more facile, and their barriers are much lower than the N-O cleavage step. It can be noted that N-O cleavage (**TS5**) and alkyne insertion (**TS8**) TSs occur preferentially in the singlet state (**Scheme S10**), while the reductive elimination (**TS9**) step prefers the triplet state. In the main text and here, the presented Gbbs free energies refer to the lower spin state for that species or transition state. We assume that spin-state change, where needed, occurs faster than steps involving changes in chemical connectivity.



Scheme S7. Geometries and Gibbs free energies (kcal mol^{-1}) of direct N-O cleavage transition states prior to alkyne insertion. NPA charge on key atoms are shown. Both the gas phase (in parentheses) and solution phase Gibbs free energies are shown.

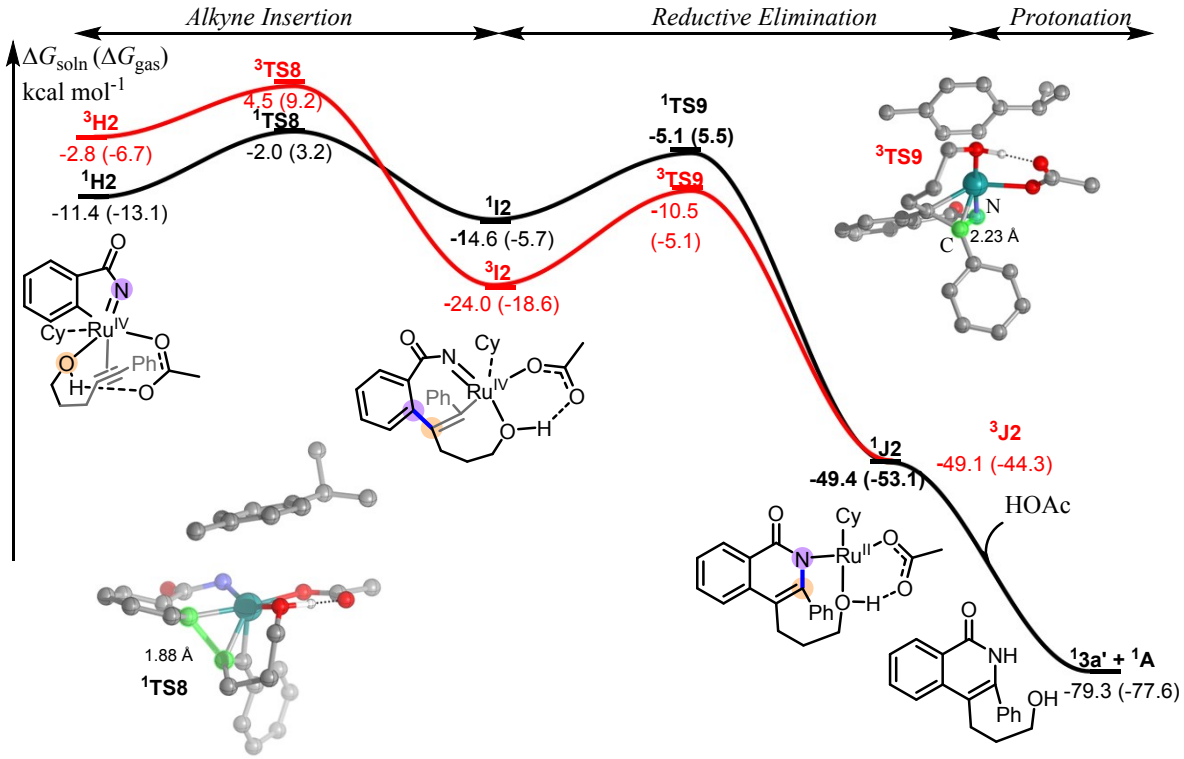


Scheme S8. Geometries and Gibbs free energies (kcal mol^{-1}) of HOAc-assisted N-O cleavage transition states prior to alkyne insertion. Both the gas phase (in parentheses) and solution phase Gibbs free energies are shown.

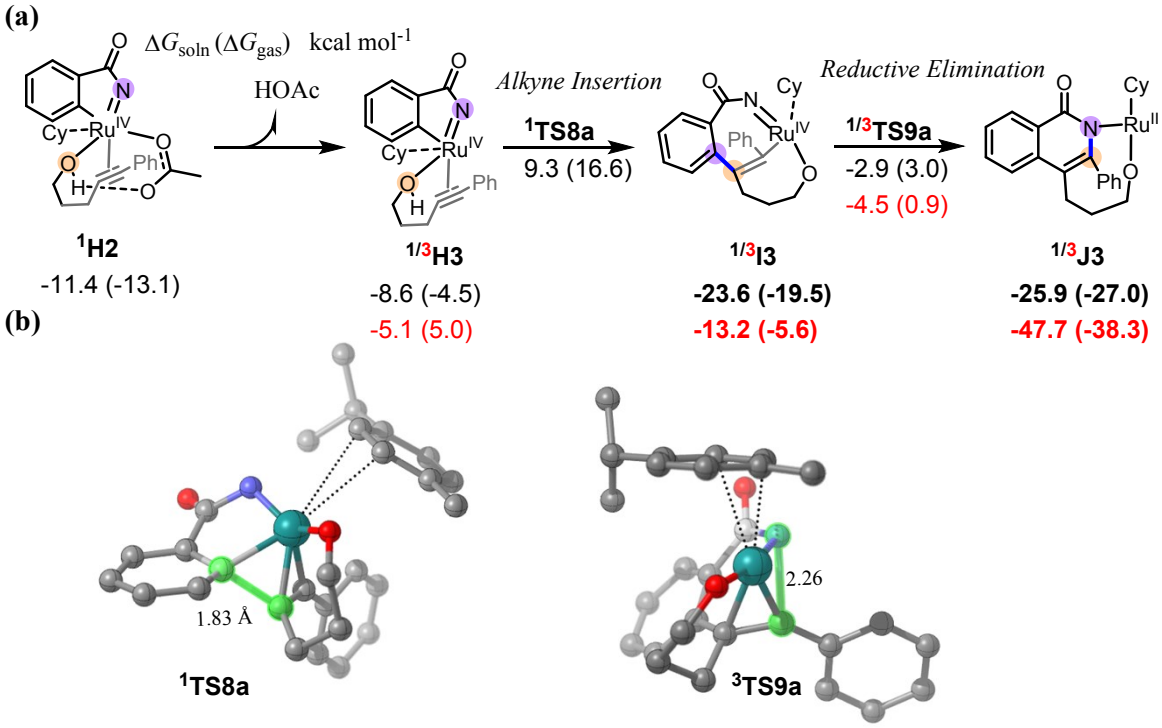


Scheme S9. The explicit effect of solvent (methanol) on the N-O cleavage transition state (**TS5**) in presence (**TS5c**) and absence (**TS5d** and **TS5e**) of acetic acid. Both the gas phase (in parentheses) and solution phase Gibbs free energies are shown. **TS5c** is the methanol mediated transition state of **TS5,** and **TS5c** has a comparable energy to **TS5**, indicating methanol plays a minor role in modulating the reaction mechanism**.** In absence of acetic acid, methanol is not efficient to enhance N-O bond cleavage,

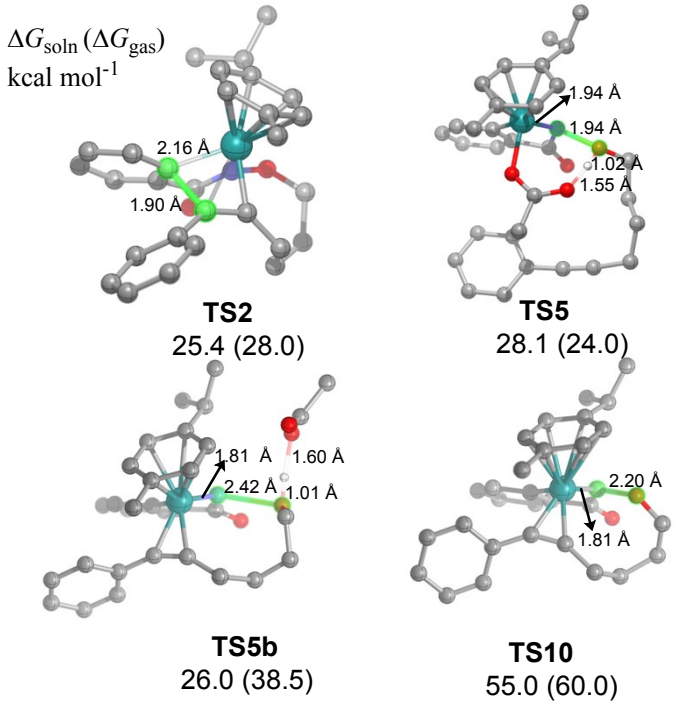
and the barrier (**TS5d** and **TS5e**) is much higher than that of the acetic acid-mediated proton transfer mechanism.



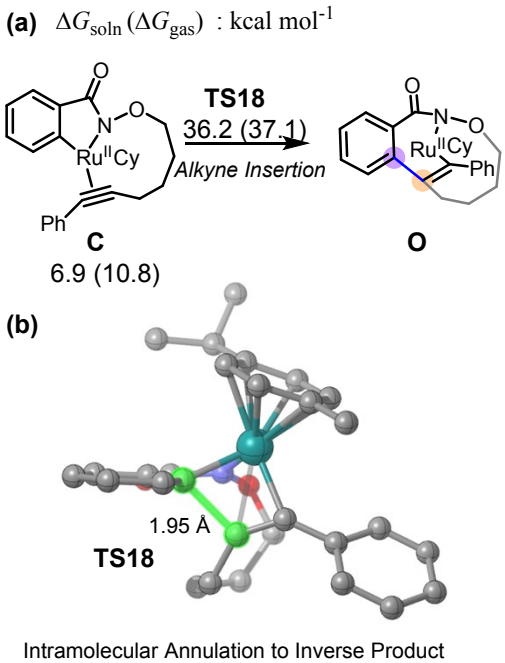
Scheme S10. Free energetic profile (kcal mol^{-1}) of alkyne insertion followed by C-N reductive elimination and protonation to give the **inverse annulation product** at singlet and triplet state. Geometries of ^{1}**TS8** and ^{3}**TS9** are shown with the key bond lengths provided in Å. Both the gas phase (in parentheses) and solution phase Gibbs free energies are shown.



Scheme S11. Free energetic profile (kcal mol^{-1}) of alkyne insertion followed by C-N reductive elimination and protonation to give the **inverse annulation product in absence of acetic acid** at singlet and triplet state. Geometries of **^{1}TS8a** and **^{3}TS9a** are shown with the key bond lengths provided in Å. Both the gas phase (in parentheses) and solution phase Gibbs free energies are shown.



Scheme S12. Key transition states involved by using the **four-carbon-atom tethered substrate**. Note that the energy refers to the energy sum of the catalyst and substrate, and both the solution phase and gas phase (in parentheses) free energies are provided.



Intramolecular Annulation to Inverse Product

Scheme S13. Alkyne insertion transition state corresponding to the intramolecular annulation to inverse annulation product. The **four-carbon-atom tethered substrate** is used**.** Both the solution phase and gas

phase (in parentheses) free energies are provided. The barrier here is much higher than that of **TS2** (25.4 kcal/mol in **Scheme S12**) leading to the standard annulation product.

Effect of DFT functionals. To assess how DFT functionals affects the relative energies of different reaction mechanism, a series of DFT functionals including BP86-D3, BLYP-D3, B3LYP-D3, B3LYP*-D3 (15 % HF), B3PW91-D3, PBE0-D3, TPSSh-D3, ωb97xd, M06-D3, M06L-D3 and M11-L (**Table S2**), were applied in the SMD single point energy calculation of **TS2 (**Alkyne insertion step in the traditional annulation mechanism) and **TS5/TS5b** (N-O cleavage step in the newly proposed reaction mechanism). Note that for B3LYP*, we have used the dispersion correction with parameters optimized for B3LYP. The current results show that BP86-D3, BLYP-D3, B3LYP-D3, B3LYP*-D3 and M06L-D3 predicted somewhat comparable reaction barriers for **TS2** and **TS5**, while B3PW91-D3, PBE0-D3, ωb97xd, TPSSh-D3, M06-D3 predict that **TS2** is much lower in energy than **TS5**. The sensitivity of the computed relative energies of **TS5** to the functional seems to be associated with the change in oxidation state of the metal associated with the N-O bond cleavage occurring in this step.

In the absence of a through benchmarking exercise, it is not immediately obvious which functional gives the most accurate values. However, here we can rely on a key experimental observation to rule out some functionals. Experiments clearly show formation of the inverse annulation product, which cannot be formed following the traditional mechanism. Hence the new **TS5** must be competitive with **TS2**, unlike what is calculated with B3PW91-D3, PBE0-D3, ωb97xd, TPSSh-D3, and M06-D3. For these reasons, we prefer to trust the B3LYP-D3 results, which yield comparable barrier heights for **TS2** and **TS5**.

Table S2. Solution phase Gibbs free energies in kcal mol^{-1} of **TS2** (alkyne insertion in the traditional mechanism), **TS5** and **TS5b** (HOAc assisted N-O cleavage). The SMD solvation energies are calculated with different DFT methods with def2-TZVP basis set, while the free energy correction calculated at the B3LYP-D3/def2-TZVP level.

	B3LYP-D3	B3LYP*-D3[a]	BLYP-D3	M06L-D3	M11L	BP86-D3
TS2	30.0	27.0	25.1	33.7	32.3	11.5
TS5	31.7	28.3	19.1	36.8	37.9	17.1
TS5b	32.0	28.5	17.3	40.0	45.4	14.9
	B3PW91-D3	M06-D3	TPSSh-D3	ωb97xd	PBE0-D3	
TS2	16.7	23.6	22.6	25.5	20.0	
TS5	29.9	33.5	31.9	42.2	36.5	
TS5b	28.9	35.4	33.6	39.2	37.5	

a. 15% HF exchange

Table S3. Relative electronic energy and Gibbs free energies (kcal/mol) in gas phase and SMD solution (methanol). ΔG_{gas} and ΔG_{sol} denotes to the gas phase and solution phase Gibbs energies applied the standard state correction.

	ΔE	ΔE(SMD)	ΔG^*_{gas}	ΔG_{gas}	ΔG^*_{soln}	ΔG_{soln}
^{1}A	0.0	0.0	0.0	0.0	0.0	0.0
^{3}A	26.3	21.5	23.9	23.9	19.1	19.1
2a'	-85.2	-87.3	-79.8	-79.8	-81.8	-81.8
3a'	-83.2	-84.9	-77.6	-77.6	-79.3	-79.3

N-H/C-H Activation

^{1}A1	-20.8	-12.4	-2.1	-4.2	6.2	4.1
^{3}A1	5.6	8.7	22.3	20.2	25.4	23.3
^{1}A2	-1.3	3.1	5.4	5.4	9.8	9.8
^{3}A2	18.2	19.7	21.7	21.7	23.2	23.2
^{1}TS1	16.3	20.1	17.8	17.8	21.6	21.6
^{3}TS1	41.5	45.5	39.4	39.4	43.4	43.4
^{1}A3	1.7	7.2	6.5	6.5	12.0	12.0
^{1}B	2.4	7.6	6.6	6.6	11.8	11.8
^{1}C	10.5	11.0	3.9	6.0	4.4	6.5
^{3}C	25.8	23.4	14.8	16.9	12.4	14.5
		To Standard Annulation : Traditional Mechanism				
^{1}TS2	31.6	33.2	26.4	28.5	28.0	30.1
^{3}TS2	60.6	60.4	50.1	52.2	49.9	52.0
^{1}TS2a	17.4	24.6	23.5	23.5	30.7	30.7
^{1}TS2b	31.6	33.7	36.4	36.4	38.5	38.5
^{1}D	12.2	15.2	6.9	9.0	9.8	11.9

^{3}D	28.3	28.0	19.1	21.2	18.8	20.9
^{1}TS3	23.1	23.7	16.9	19.0	17.4	19.5
^{3}TS3	47.6	48.8	38.8	40.9	40.0	42.2
^{1}E	-1.6	6.3	-6.2	-4.1	1.7	3.8
^{3}E	11.6	12.9	4.5	6.6	5.8	7.9
^{1}TS4	23.1	17.8	14.7	16.8	9.3	11.4
^{1}F	-62.9	-64.0	-68.7	-66.6	-69.7	-67.6
^{3}F	-45.8	-46.7	-53.8	-51.7	-54.6	-52.5
			Novel Mechanism: HOAc assisted N-O Cleavage			
^{1}TS5	24.9	29.4	27.2	27.2	31.7	31.7
^{1}TS5b	36.7	31.1	37.8	37.8	32.2	32.2
^{1}TS5c	8.8	17.1	25.3	23.2	33.6	31.5
^{1}G	4.3	3.3	5.5	5.5	4.5	4.5
			Higher Energy Route: Methanol assisted N-O Cleavage			
^{1}TS5d	41.3	48.7	42.9	42.9	50.2	50.2
^{1}TS5e	46.2	46.9	46.2	46.2	46.9	46.9

			Novel Mechanism: To Standard Annulation			
^{1}H1	-21.1	-21.2	-19.8	-19.8	-19.9	-19.9
^{1}TS6	-0.9	-4.3	0.9	0.9	-2.5	-2.5
^{3}TS6	3.1	3.6	4.7	4.7	5.1	5.1
^{1}I1	-27.7	-30.4	-24.2	-24.2	-26.9	-26.9
^{3}I1	-26.5	-27.7	-23.3	-23.3	-24.6	-24.6
^{1}TS7	-1.7	-5.0	1.2	1.2	-2.0	-2.0
^{3}TS7	-6.7	-9.3	-5.2	-5.2	-7.8	-7.8
^{1}J1	-78.9	-71.8	-68.9	-68.9	-61.8	-61.8
			Novel Mechanism: To Inverse Annulation			
^{1}H2	-14.2	-12.5	-13.1	-13.1	-11.4	-11.4
^{3}H2	-9.2	-5.3	-6.7	-6.7	-2.8	-2.8
^{1}TS8	0.4	-4.8	3.2	3.2	-2.0	-2.0
^{3}TS8	7.2	2.5	9.2	9.2	4.5	4.5
^{1}I2	-9.8	-18.8	-5.7	-5.7	-14.6	-14.6
^{3}I2	-21.0	-26.4	-18.6	-18.6	-24.0	-24.0

^{1}TS9	0.8	-9.8	5.5	5.5	-5.1	-5.1
^{3}TS9	-6.6	-12.0	-5.1	-5.1	-10.5	-10.5
^{1}J2	-63.1	-59.3	-53.1	-53.1	-49.4	-49.4
^{3}J2	-49.5	-54.3	-44.3	-44.3	-49.1	-49.1
^{1}H3	4.26	0.13	-6.60	-4.49	-10.74	-8.62
^{3}H3	16.41	6.31	2.90	5.02	-7.20	-5.08
^{1}TS8a	25.85	18.51	14.47	16.58	7.13	9.25
^{1}I3	-11.10	-15.28	-21.57	-19.46	-25.76	-23.64
^{3}I3	4.79	-2.87	-7.70	-5.58	-15.35	-13.23
^{1}TS9a	11.81	5.88	0.88	2.99	-5.05	-2.93
^{3}TS9a	11.10	5.75	-1.22	0.89	-6.57	-4.45
^{1}J3	-22.98	-21.87	-29.16	-27.04	-28.05	-25.93
^{3}J3	-32.62	-42.03	-40.41	-38.29	-49.82	-47.70
			High Energy Routes			
^{1}TS10	65.1	60.6	52.5	54.6	48.0	50.1
^{1}TS10b	66.5	60.7	55.7	57.8	49.9	52.0

^{1}TS11	31.6	33.1	24.6	26.7	26.2	28.3
^{3}TS11	65.4	68.3	54.2	56.3	57.2	59.3
^{1}K	7.7	16.1	1.2	3.3	9.6	11.7
^{3}K	34.1	35.0	24.3	26.4	25.2	27.4
^{1}TS12	34.2	40.3	27.3	29.4	33.3	35.4
^{3}TS12	59.3	64.2	50.3	52.4	55.2	57.3
^{1}L	-3.9	3.0	4.7	4.7	11.6	11.6
^{1}TS13	10.7	14.9	19.0	19.0	23.2	23.2
^{1}TS14	32.1	35.5	23.3	25.4	26.7	28.8
^{1}M	-4.1	-10.1	-14.9	-12.8	-20.9	-18.8
^{3}M	5.1	-4.7	-6.8	-4.7	-16.7	-14.5
^{1}TS15	31.2	32.0	33.7	33.7	34.5	34.5
^{1}N	12.8	15.1	16.0	16.0	18.2	18.2
^{1}TS16	56.3	59.8	55.2	55.2	58.7	58.7
^{1}TS17	18.5	8.3	20.9	20.9	10.7	10.7

Four Carbon Tethered Substrate

2a	-89.1	-89.9	-83.9	-83.9	-84.7	-84.7
3a	-83.5	-85.1	-77.7	-77.7	-79.4	-79.4
^{1}A1	-23.3	-17.7	-3.8	-5.9	1.8	-0.3
^{1}TS2	32.9	30.2	25.9	28.0	23.3	25.4
^{1}TS5	20.0	24.1	24.0	24.0	28.1	28.1
^{1}TS5b	37.1	24.5	38.5	38.5	26.0	26.0
^{1}TS10	70.0	65.0	57.9	60.0	52.9	55.0
^{1}TS18	41.4	40.4	35.0	37.1	34.0	36.1

Table S4. Absolute electronic energy (au) and Gibbs free energies in gas phase and SMD solution phase (methanol).

	E	*E*(SMD)	G^*_{gas}	G^*_{soln}
1a'	-901.6250692	-901.653414	-901.369214	-901.397559
HOAc	-229.1923909	-229.20254	-229.158117	-229.168266
^{1}A	-941.8698302	-941.902918	-941.605096	-941.638184
^{3}A	-941.8278435	-941.868566	-941.566907	-941.60763
2a'	-901.7609146	-901.792521	-901.496382	-901.527989

3a'	-901.7576685	-901.788703	-901.492876	-901.52391
^{1}A1	-1843.527981	-1843.57608	-1842.977724	-1843.02583
^{3}A1	-1843.485928	-1843.54244	-1842.938724	-1842.99523
^{1}A2	-1614.304571	-1614.34892	-1613.807541	-1613.85189
^{3}A2	-1614.273455	-1614.32247	-1613.781567	-1613.83058
^{1}TS1	-1614.276591	-1614.3218	-1613.787804	-1613.83301
^{3}TS1	-1614.236352	-1614.28131	-1613.753343	-1613.7983
^{1}A3	-1614.299793	-1614.34231	-1613.805914	-1613.84843
^{1}B	-1614.298729	-1614.3417	-1613.805662	-1613.84863
^{1}C	-1385.093345	-1385.13374	-1384.651845	-1384.69224
^{3}C	-1385.068946	-1385.11396	-1384.634463	-1384.67947
^{1}TS2	-1385.059701	-1385.09837	-1384.61596	-1384.65463
^{3}TS2	-1385.013494	-1385.05498	-1384.57818	-1384.61966
^{1}TS2a	-1614.274738	-1614.314669	-1613.778669	-1613.8186
^{1}TS2b	-1614.252111	-1614.300051	-1613.758185	-1613.806125
^{1}D	-1385.090616	-1385.1271	-1384.647099	-1384.68359
^{3}D	-1385.064973	-1385.10661	-1384.627583	-1384.66922
^{1}TS3	-1385.07328	-1385.11355	-1384.631204	-1384.67147
^{3}TS3	-1385.034217	-1385.07343	-1384.596177	-1384.63539
^{1}E	-1385.112676	-1385.14125	-1384.667974	-1384.69655

^{3}E	-1385.091626	-1385.13075	-1384.650847	-1384.68997
^{1}TS4	-1385.0733	-1385.12296	-1384.634717	-1384.68438
^{1}F	-1385.210402	-1385.25328	-1384.767481	-1384.81036
^{3}F	-1385.183054	-1385.22562	-1384.743735	-1384.7863
^{1}TS5	-1614.262876	-1614.30698	-1613.772912	-1613.81701
^{1}TS5b	-1614.244079	-1614.30431	-1613.755899	-1613.81613
^{1}TS5c	-1730.065302	-1730.1113	-1729.524472	-1729.57047
^{1}TS5d	-1500.82102	-1500.85842	-1500.338302	-1500.37571
^{1}TS5e	-1500.813236	-1500.86126	-1500.333025	-1500.38105
^{1}G	-1614.295685	-1614.34855	-1613.807496	-1613.86036
^{1}H1	-1614.33608	-1614.38763	-1613.847708	-1613.89926
^{1}TS6	-1614.304018	-1614.36071	-1613.814747	-1613.87144
^{3}TS6	-1614.297565	-1614.34812	-1613.808748	-1613.8593
^{1}I1	-1614.346674	-1614.40219	-1613.854823	-1613.91034
^{3}I1	-1614.344664	-1614.39797	-1613.853314	-1613.90662
^{1}TS7	-1614.305289	-1614.36175	-1613.814234	-1613.8707
^{3}TS7	-1614.313185	-1614.36861	-1613.824469	-1613.8799
^{1}J1	-1614.428307	-1614.46825	-1613.92596	-1613.96591
^{1}H2	-1614.325066	-1614.37363	-1613.837003	-1613.88557
^{3}H2	-1614.317092	-1614.36224	-1613.826822	-1613.87197

^{1}TS8	-1614.301842	-1614.36139	-1613.811047	-1613.8706
^{3}TS8	-1614.291068	-1614.34982	-1613.801494	-1613.86024
^{1}I2	-1614.318185	-1614.38379	-1613.825198	-1613.8908
^{3}I2	-1614.336011	-1614.39587	-1613.845795	-1613.90565
^{1}TS9	-1614.301213	-1614.36943	-1613.807413	-1613.87563
^{3}TS9	-1614.312991	-1614.37292	-1613.824356	-1613.88428
^{1}J2	-1614.402991	-1614.44836	-1613.900859	-1613.94623
^{3}J2	-1614.381361	-1614.44037	-1613.886738	-1613.94575
^{1}H3	-1385.103331	-1385.151052	-1384.6686	-1384.71632
^{3}H3	-1385.083965	-1385.141198	-1384.65346	-1384.71069
^{1}TS8a	-1385.068926	-1385.121748	-1384.63502	-1384.68785
^{1}I3	-1385.127805	-1385.17561	-1384.69245	-1384.74026
^{3}I3	-1385.102484	-1385.155819	-1384.67034	-1384.72367
^{1}TS9a	-1385.091302	-1385.141876	-1384.65668	-1384.70725
^{3}TS9a	-1385.092436	-1385.142088	-1384.66003	-1384.70968
^{1}J3	-1385.146745	-1385.186106	-1384.70455	-1384.74391
^{3}J3	-1385.162099	-1385.218229	-1384.72248	-1384.77861
^{1}TS10	-1385.006388	-1385.05471	-1384.57442	-1384.62274
^{1}TS10b	-1385.004194	-1385.05458	-1384.569295	-1384.61968
^{1}TS11	-1385.059802	-1385.09849	-1384.618812	-1384.6575

^{3}TS11	-1385.005887	-1385.04235	-1384.57166	-1384.60812
^{1}K	-1385.09791	-1385.12564	-1384.656155	-1384.68388
^{3}K	-1385.055829	-1385.09553	-1384.619286	-1384.65898
^{1}TS12	-1385.055537	-1385.08706	-1384.614604	-1384.64612
^{3}TS12	-1385.015626	-1385.04901	-1384.577886	-1384.61127
^{1}L	-1614.308692	-1614.34908	-1613.808665	-1613.84906
^{1}TS13	-1614.285499	-1614.33002	-1613.785914	-1613.83044
^{1}TS14	-1385.059035	-1385.09471	-1384.620963	-1384.65664
^{1}M	-1385.116705	-1385.16739	-1384.681875	-1384.73256
^{3}M	-1385.101975	-1385.15877	-1384.668972	-1384.72577
^{1}TS15	-1614.252824	-1614.30278	-1613.762547	-1613.81251
^{1}N	-1614.282041	-1614.32978	-1613.790696	-1613.83844
^{1}TS16	-1614.212802	-1614.25855	-1613.728156	-1613.77391
^{1}TS17	-1614.273018	-1614.34058	-1613.782918	-1613.85048
Four-carbon-atom tether substrate				
1a	-940.9560841	-940.98261	-940.672712	-940.699238
2a	-941.0980123	-941.125892	-940.806347	-940.834227
3a	-941.0891028	-941.11829	-940.796603	-940.82579
^{1}A1	-1882.862993	-1882.91367	-1882.283858	-1882.33453
^{1}TS2	-1424.388711	-1424.43225	-1423.92028	-1423.96382

^{1}TS5	-1653.601672	-1653.64452	-1653.081452	-1653.1243
^{1}TS5b	-1653.574376	-1653.6439	-1653.058273	-1653.12779
^{1}TS10	-1424.329657	-1424.37692	-1423.869293	-1423.91655
^{1}TS18	-1424.37519	-1424.416	-1423.905822	-1423.94663

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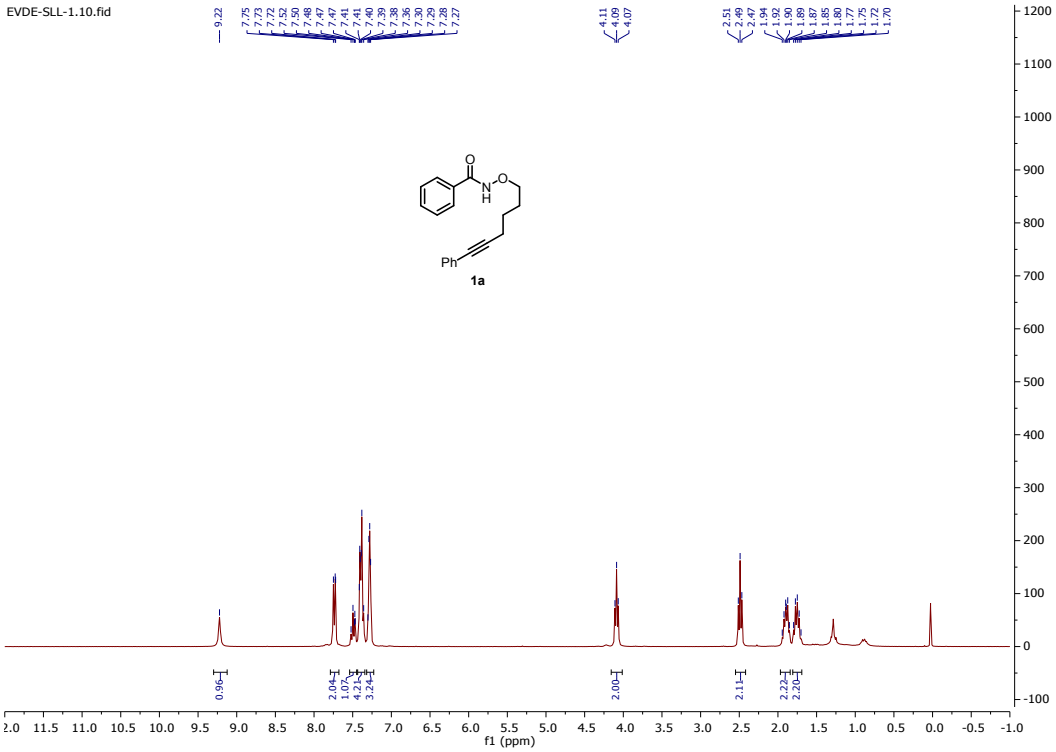
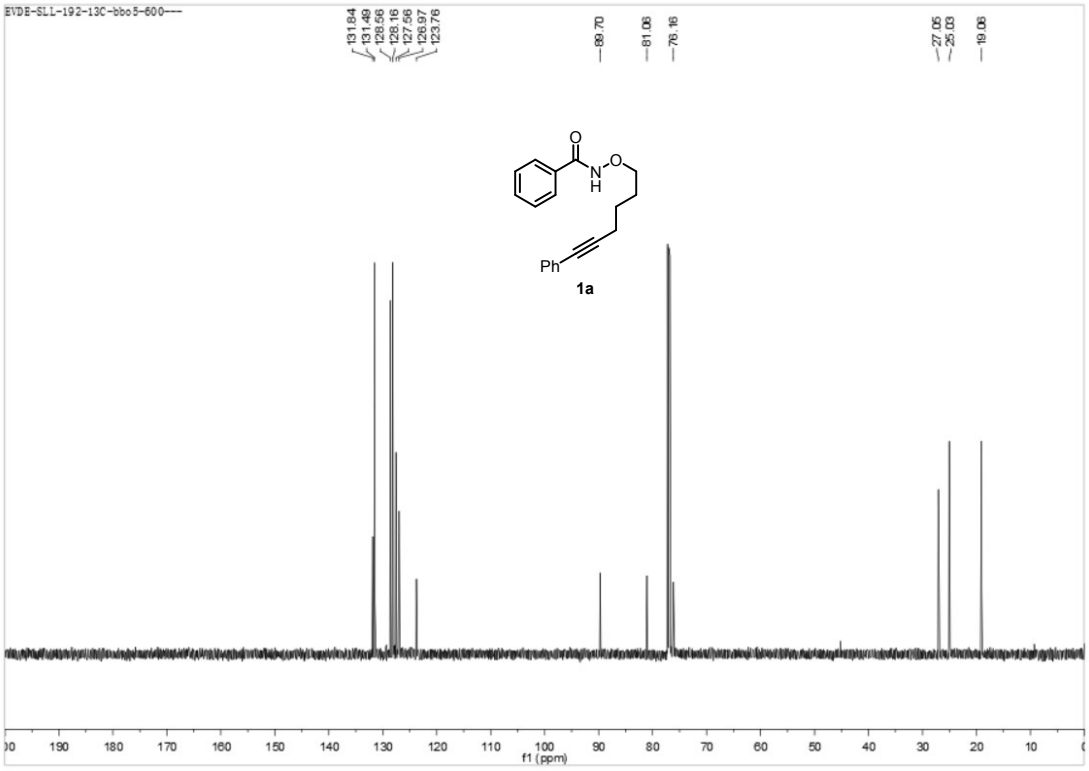
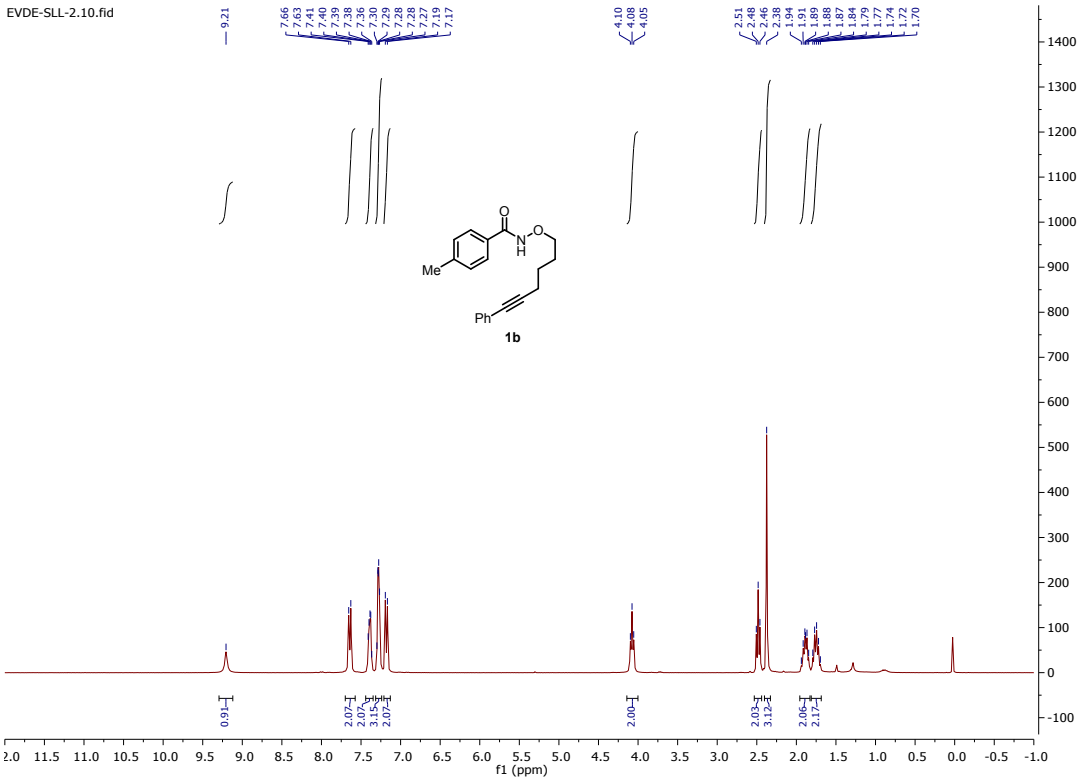
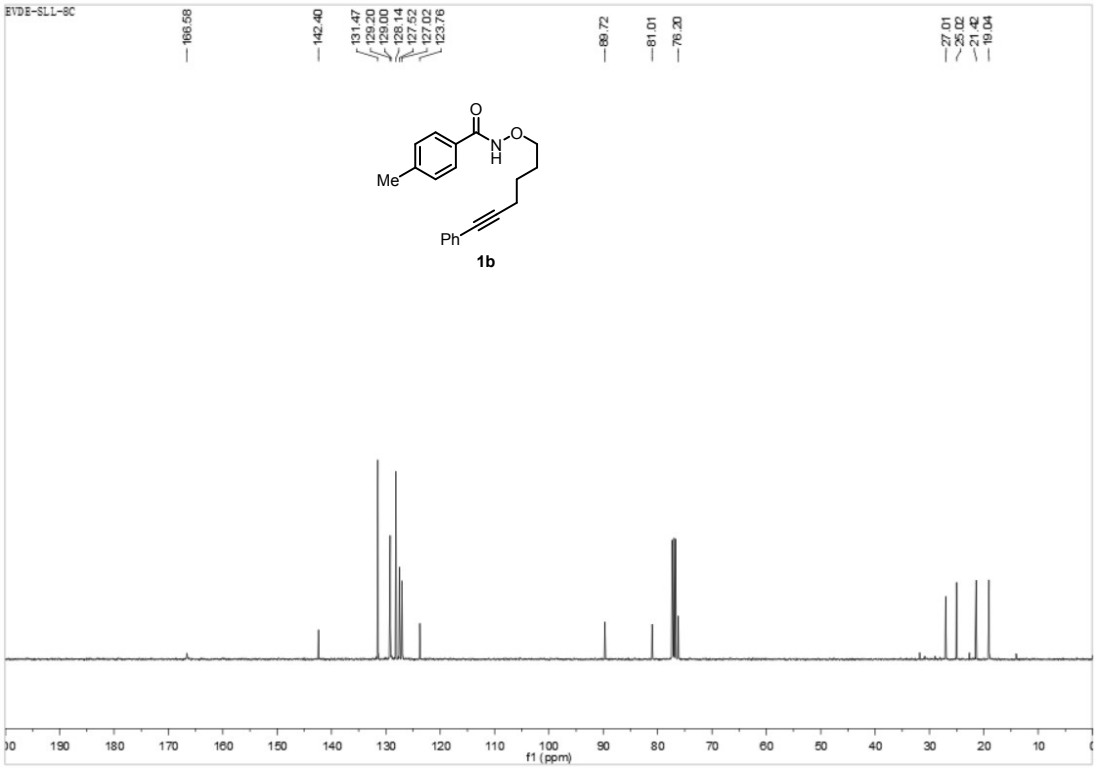
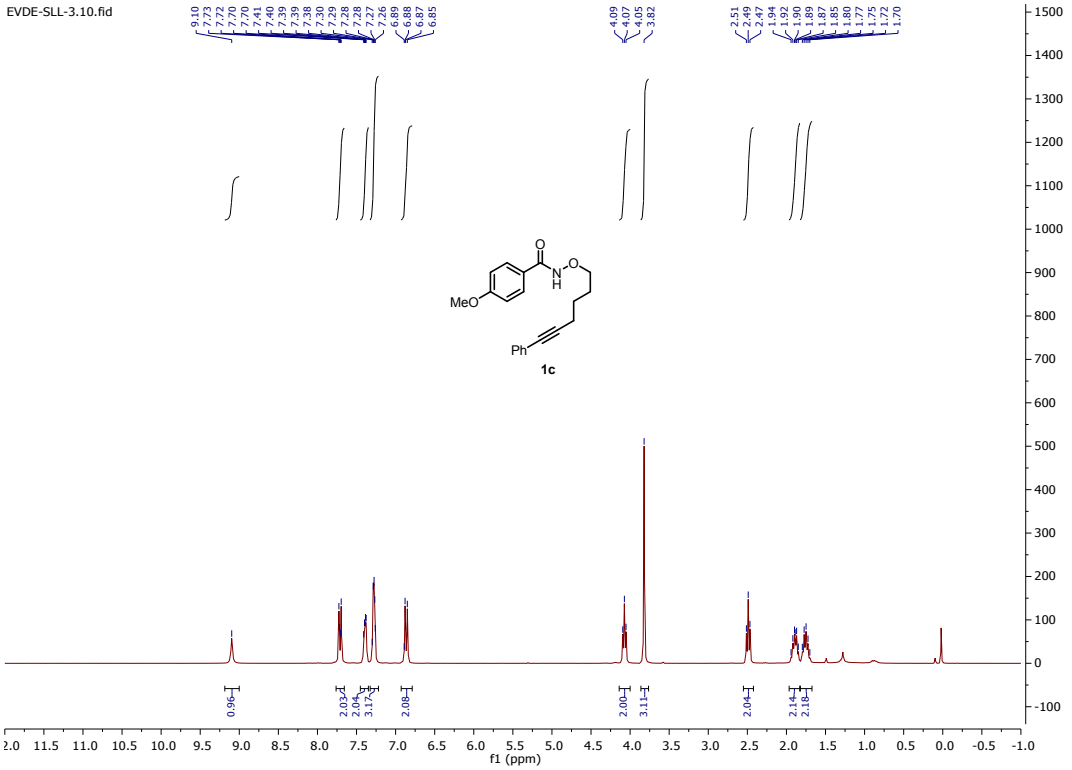
8. NMR Spectra

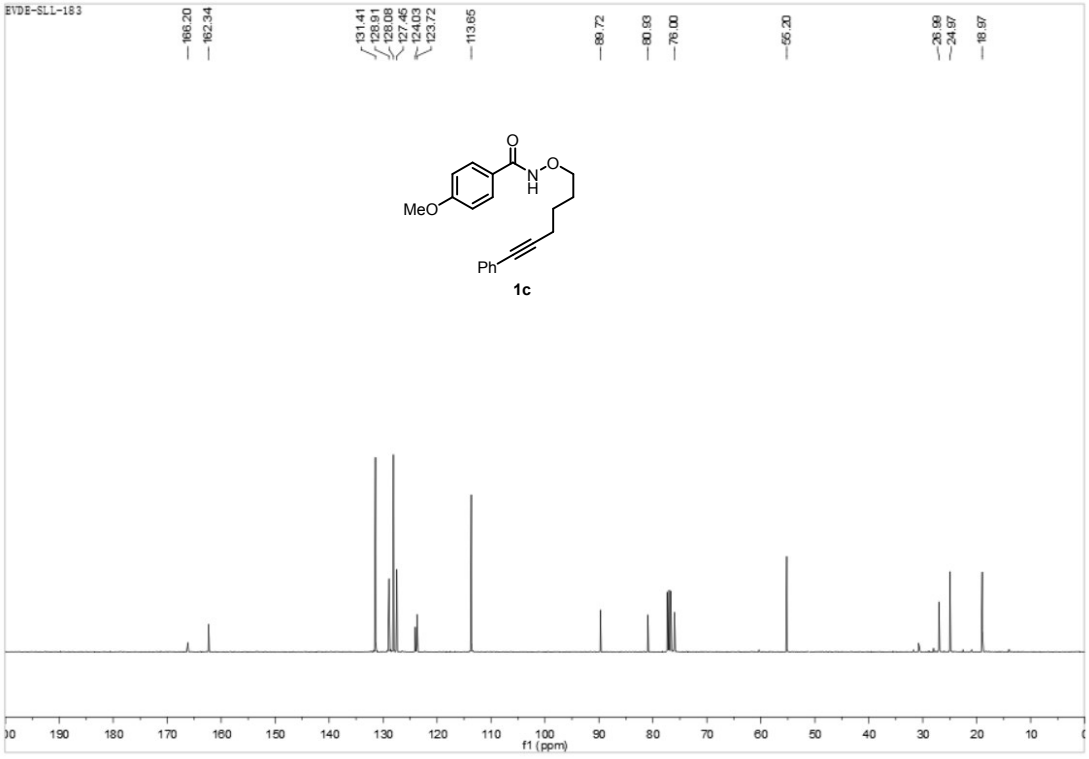


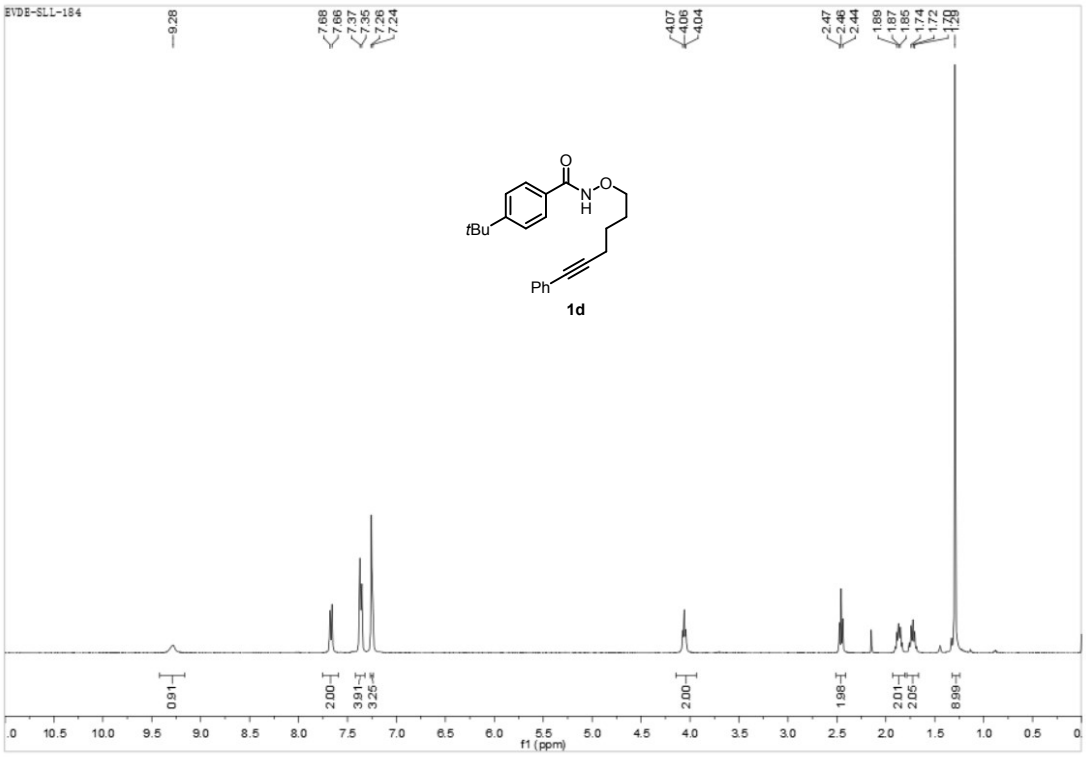


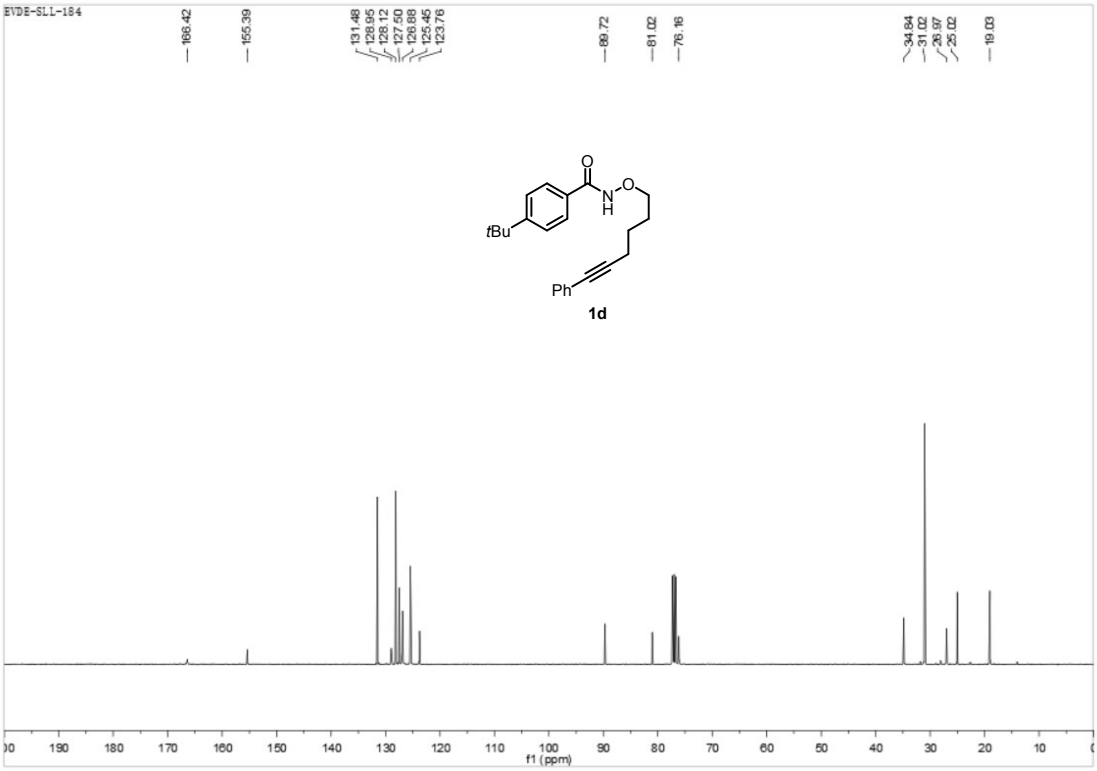

EVDE-SLL-2.10.fid
Me
Ph
1b
f1 (ppm)

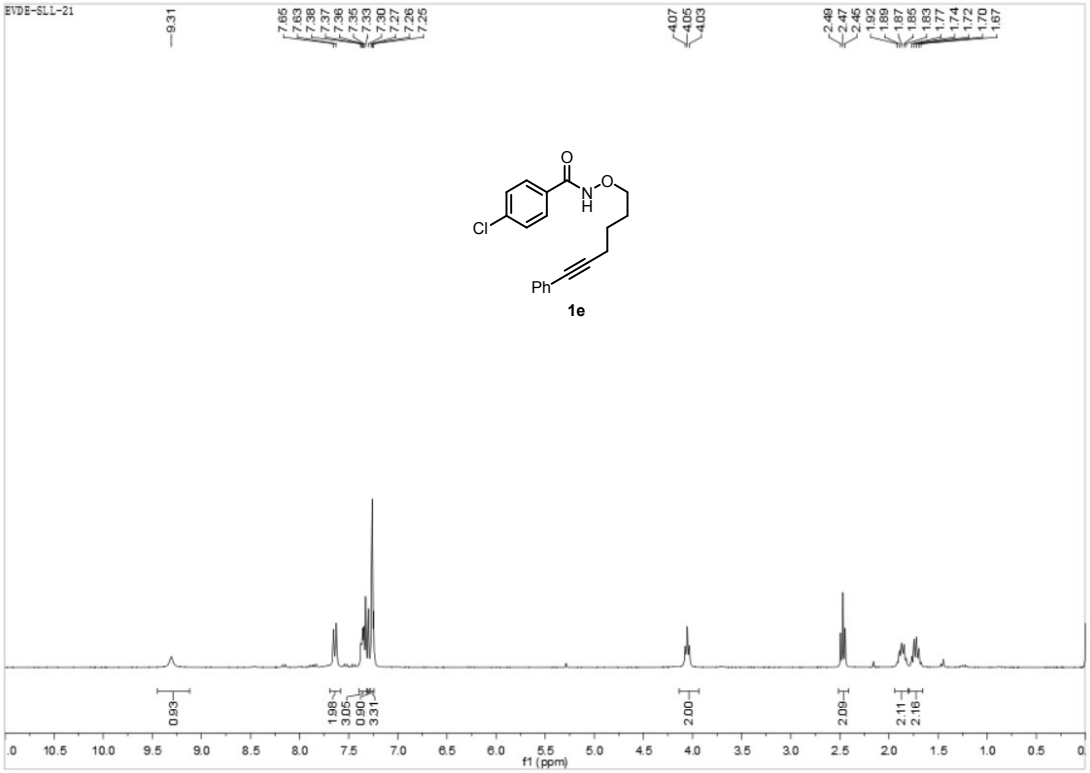

EVDE-SLL-BC
Me
Ph
1b
f1 (ppm)

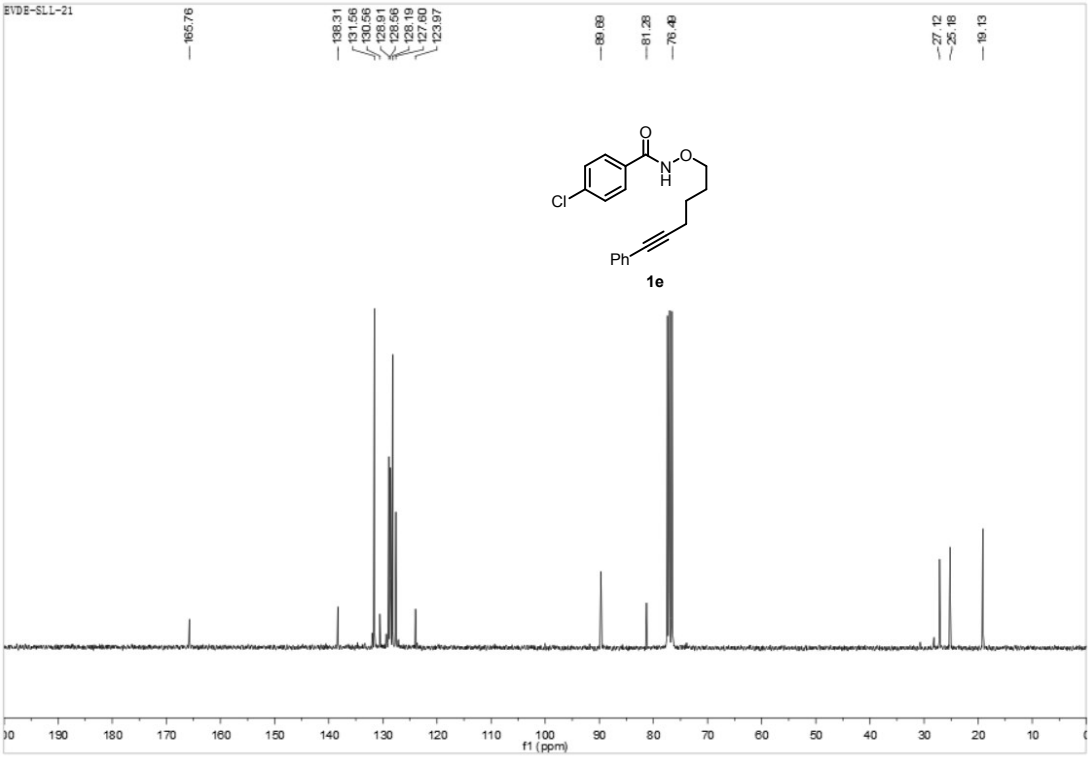

EVDE-SLL-3.10.fid
9.10
7.73
7.72
7.70
7.41
7.40
7.39
7.39
7.38
7.30
7.29
7.28
7.28
7.27
7.26
6.89
6.88
6.87
6.85
4.09
4.07
4.05
3.82
2.51
2.49
2.47
1.94
1.92
1.90
1.89
1.87
1.85
1.80
1.77
1.75
1.72
1.70
MeO
Ph
1c
0.96
2.03
2.04
3.17
2.08
2.00
3.11
2.04
2.14
2.18
f1 (ppm)

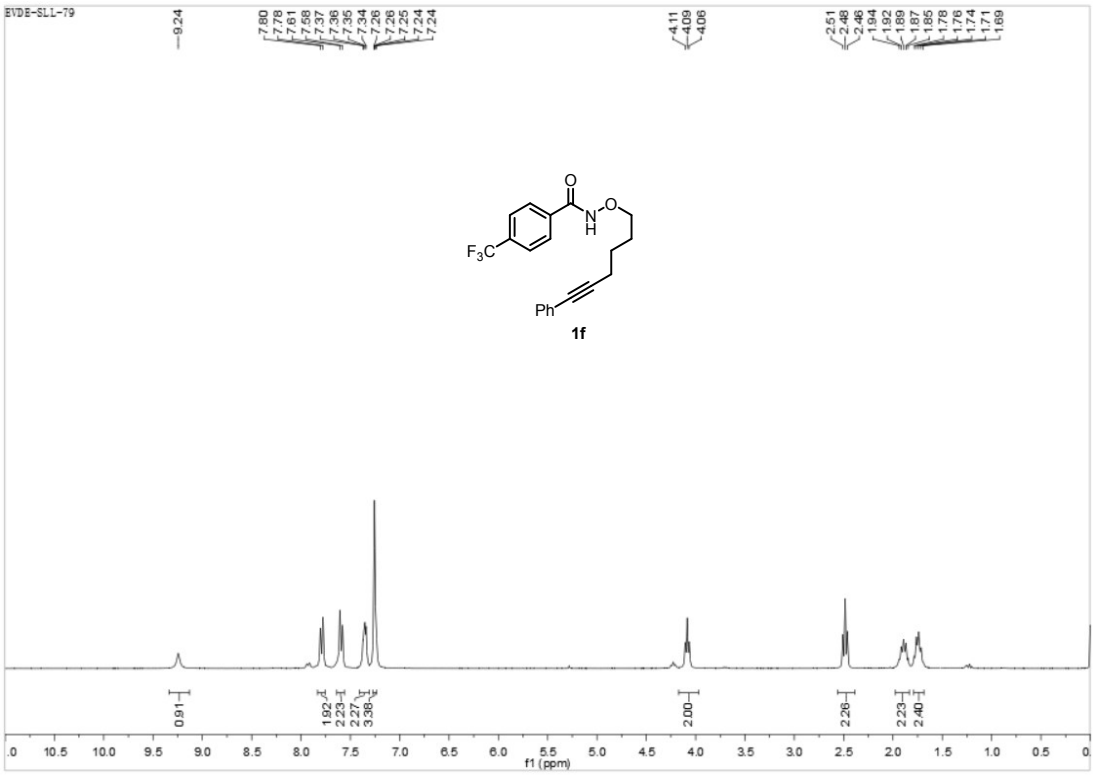

EVDE-SLL-183
166.20
162.34
131.41
128.91
128.08
127.45
124.03
123.72
113.65
89.72
80.93
76.00
55.20
28.99
24.97
18.97
MeO
Ph
1c
f1 (ppm)

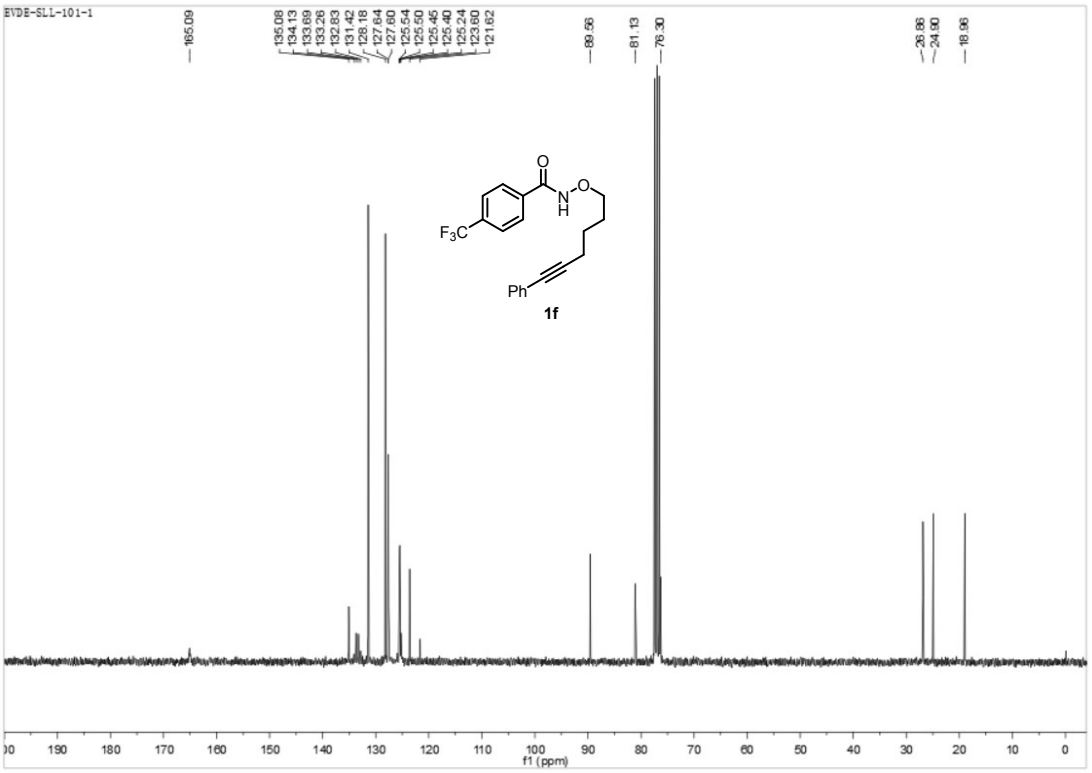

EVDE-SLL-184
9.28
7.68
7.66
7.37
7.35
7.26
7.24
4.07
4.06
4.04
2.47
2.46
2.44
1.89
1.87
1.85
1.74
1.72
1.29
O
N
H
O
tBu
Ph
1d
0.91
2.00
3.91
3.25
2.00
1.98
2.01
2.05
8.99
f1 (ppm)

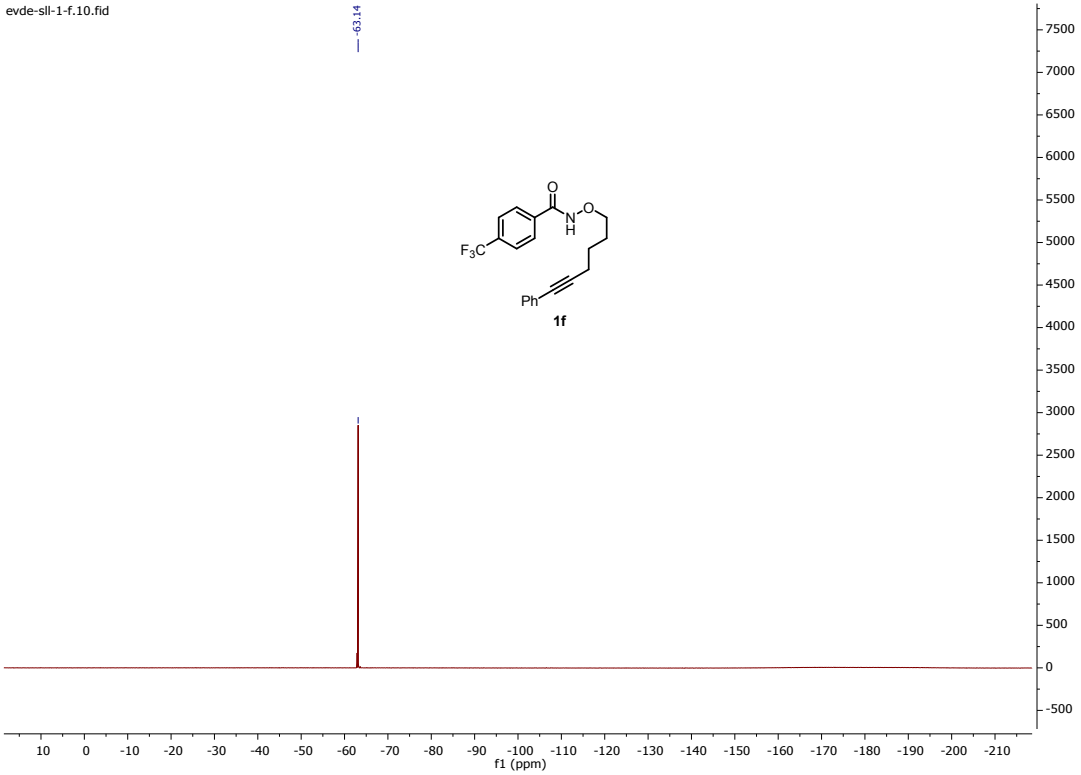

EVDE-SLL-184
166.42
155.39
131.48
128.95
128.12
127.50
126.88
125.45
123.76
89.72
81.02
76.16
34.84
31.02
26.97
25.02
19.03
O
N
H
O
tBu
Ph
1d
f1 (ppm)

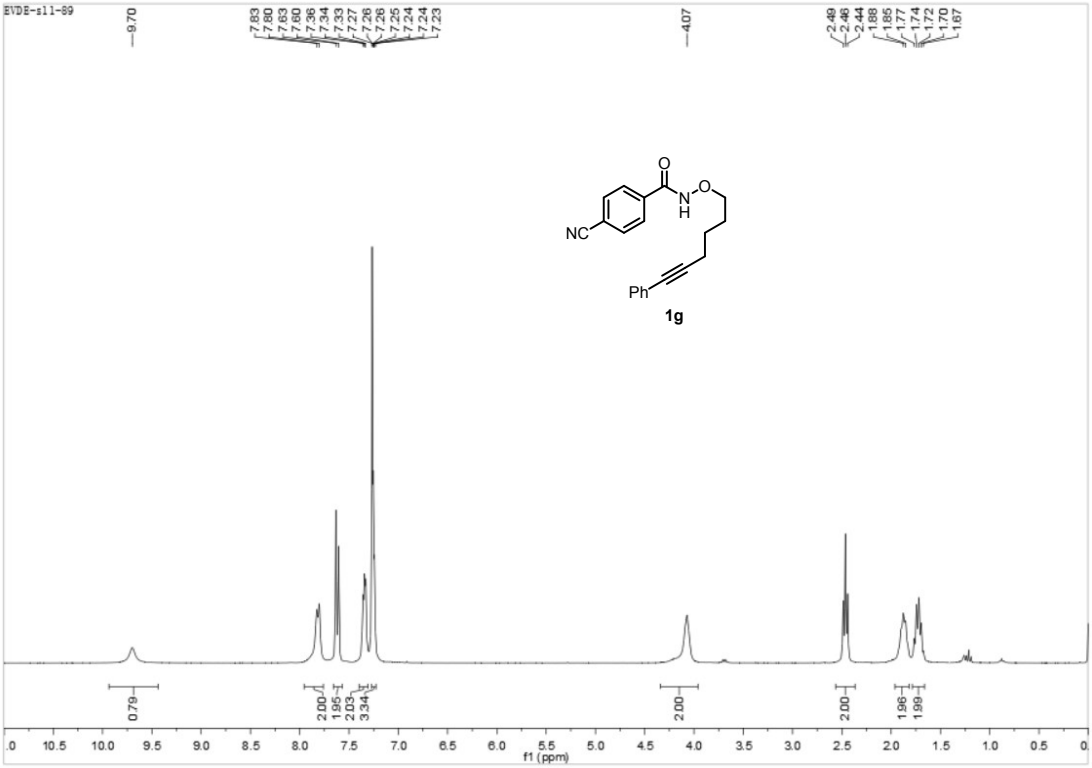

EVDE-SLL-21
9.31
7.65
7.63
7.38
7.37
7.36
7.35
7.33
7.30
7.27
7.26
7.25
4.07
4.05
4.03
2.49
2.47
2.45
1.92
1.89
1.87
1.85
1.83
1.77
1.74
1.72
1.70
1.67
O
N
H
O
Cl
Ph
1e
0.93
1.98
3.05
0.90
3.31
2.00
2.09
2.11
2.16
f1 (ppm)

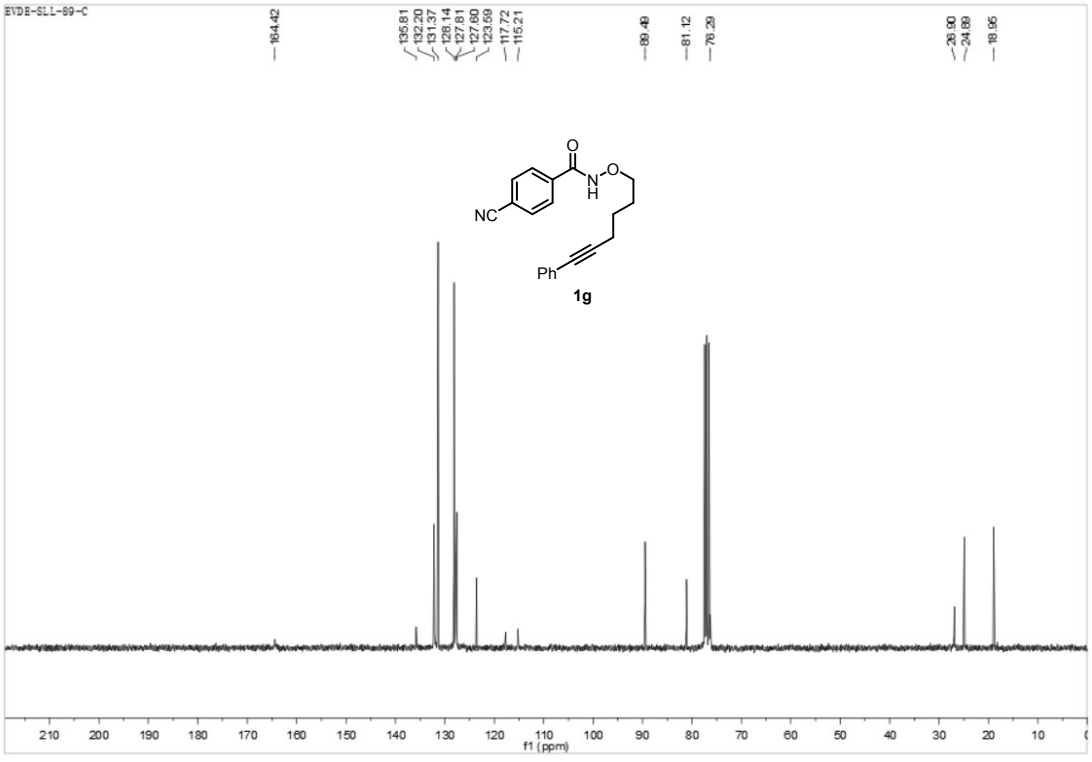

EVDE-SLL-21
165.76
138.31
131.56
130.56
128.91
128.56
128.19
127.60
123.97
89.69
81.28
76.49
27.12
25.18
19.13
O
N
H
O
Cl
Ph
1e
f1 (ppm)

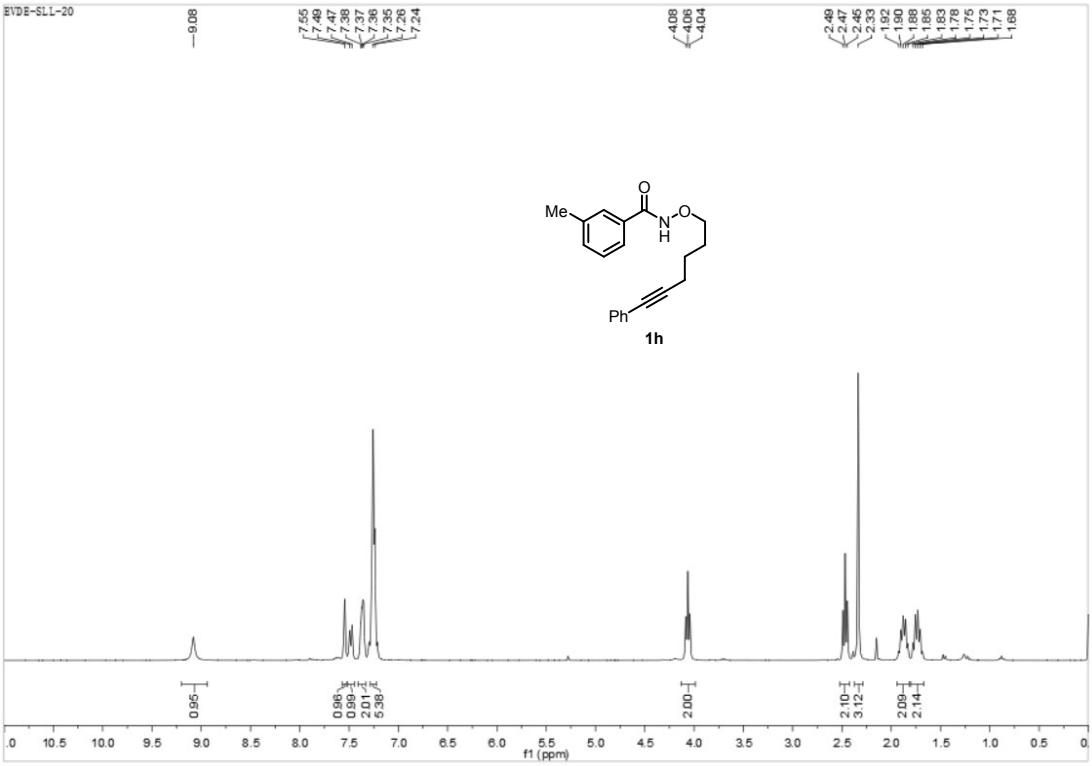

EVDE-SLL-79
9.24
7.80
7.78
7.61
7.58
7.37
7.36
7.35
7.34
7.26
7.26
7.25
7.24
7.24
4.11
4.09
4.06
2.51
2.48
2.46
1.94
1.92
1.89
1.87
1.85
1.78
1.76
1.74
1.71
1.69
O
N
H
O
F3C
Ph
1f
0.91
1.92
2.23
2.27
3.38
2.00
2.26
2.23
2.40
f1 (ppm)

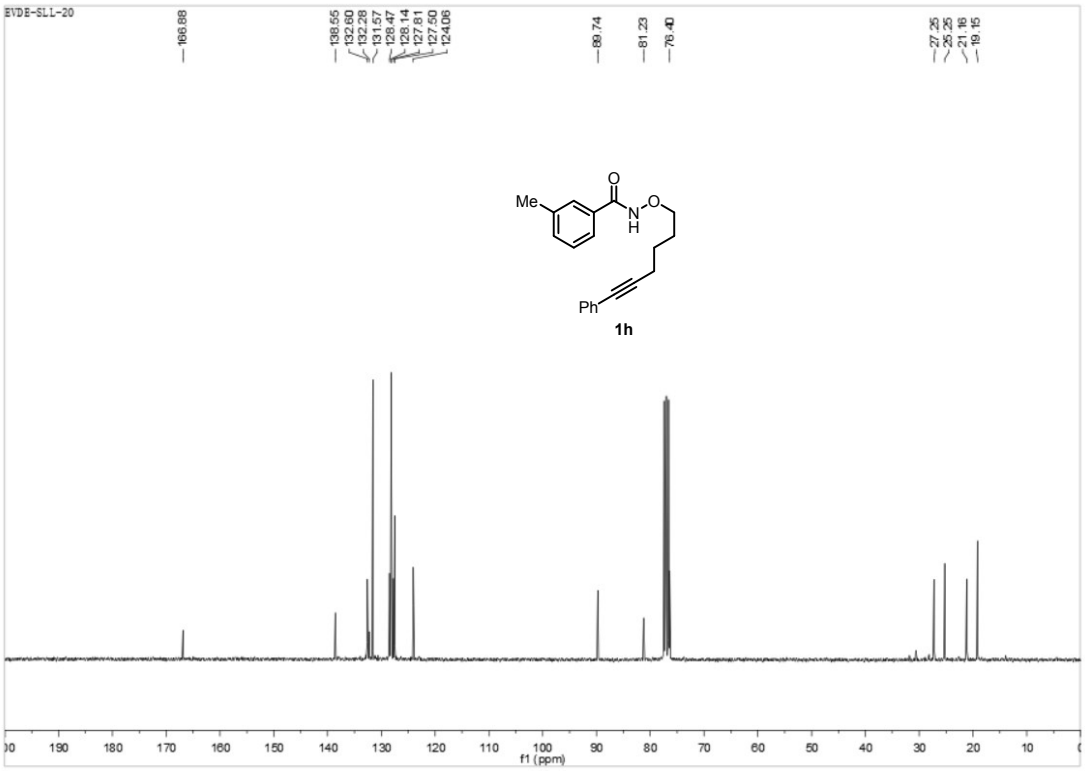

EVDE-SLL-101-1
165.09
135.08
134.13
133.69
133.26
132.83
131.42
128.18
127.64
127.60
125.54
125.50
125.45
125.40
125.24
123.60
121.62
89.56
81.13
76.30
26.86
24.90
18.96
O
N
H
O
F3C
Ph
1f
f1 (ppm)

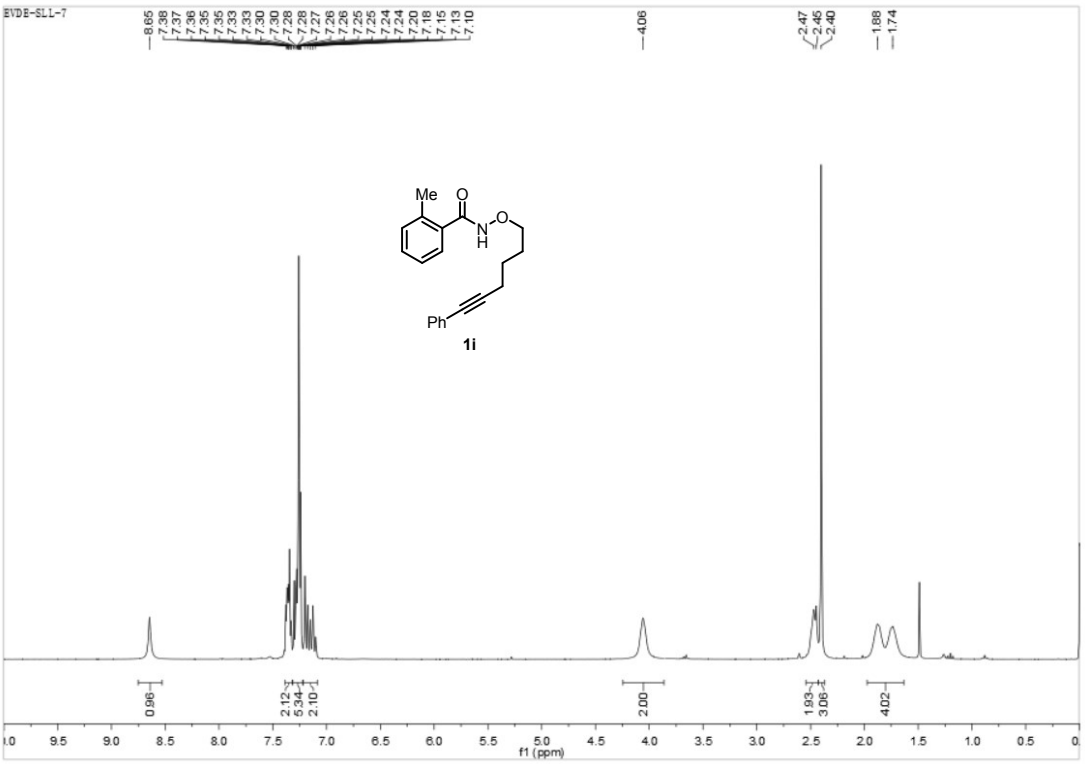

evde-sll-1-f.10.fid
-63.14
O
N
H
O
F3C
Ph
1f
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

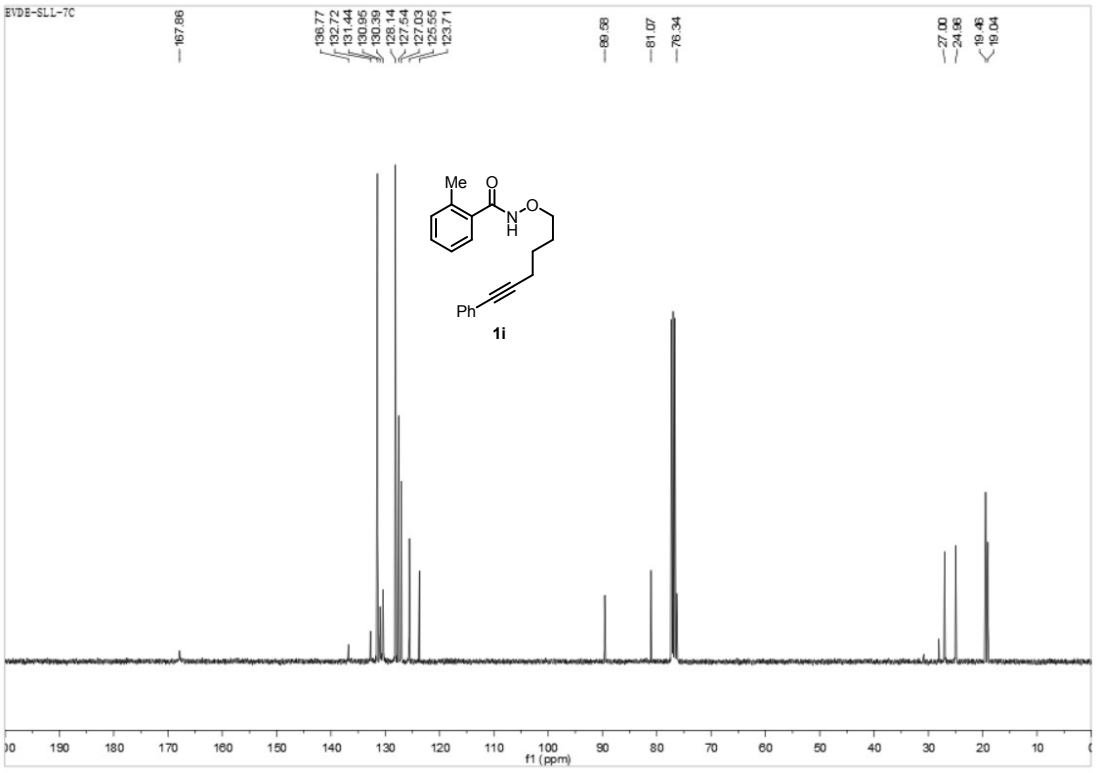

EVDE-s11-89
9.70
7.83
7.80
7.63
7.60
7.36
7.34
7.33
7.27
7.26
7.26
7.25
7.24
7.24
7.23
4.07
2.49
2.46
2.44
1.88
1.85
1.77
1.74
1.72
1.70
1.67
0.79
2.00
1.95
2.03
3.34
2.00
2.00
1.96
1.99
f1 (ppm)
NC
O
N
H
O
Ph
1g

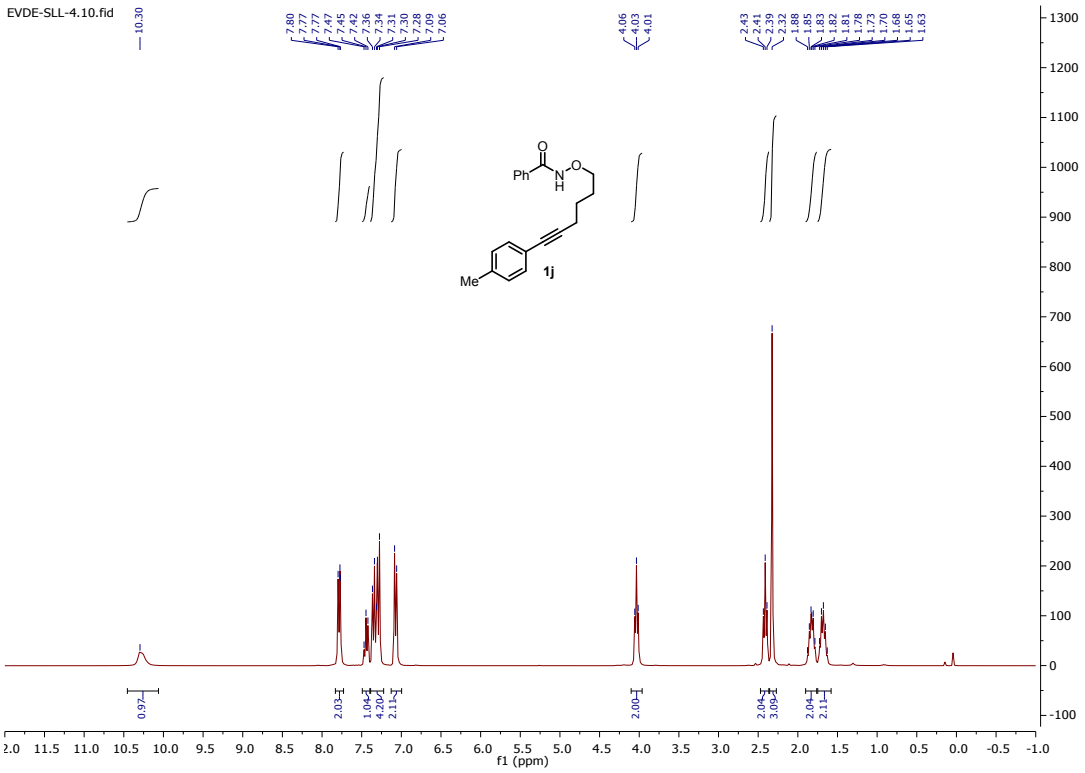

EVDE-SLL-89-C
164.42
135.81
132.20
131.37
128.14
127.81
127.60
123.59
117.72
115.21
89.49
81.12
76.29
26.90
24.89
18.95
f1 (ppm)
NC
O
N
H
O
Ph
1g

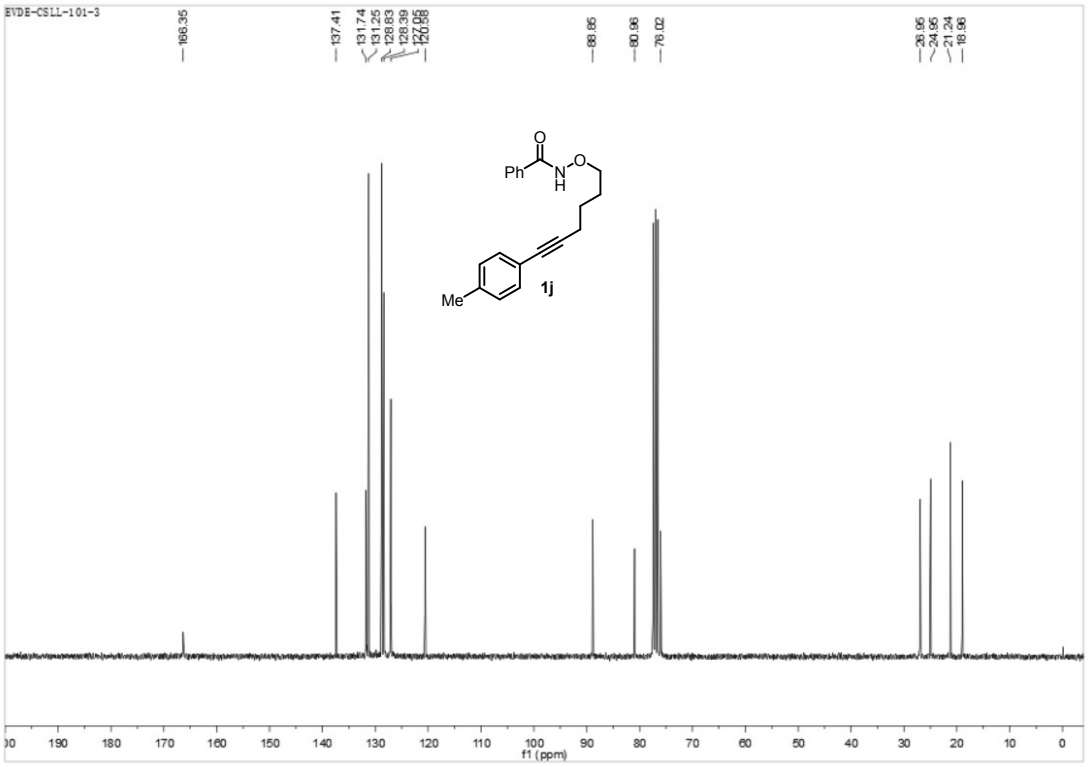

EVDE-SLL-20
Me
O
N
H
O
Ph
1h
f1 (ppm)

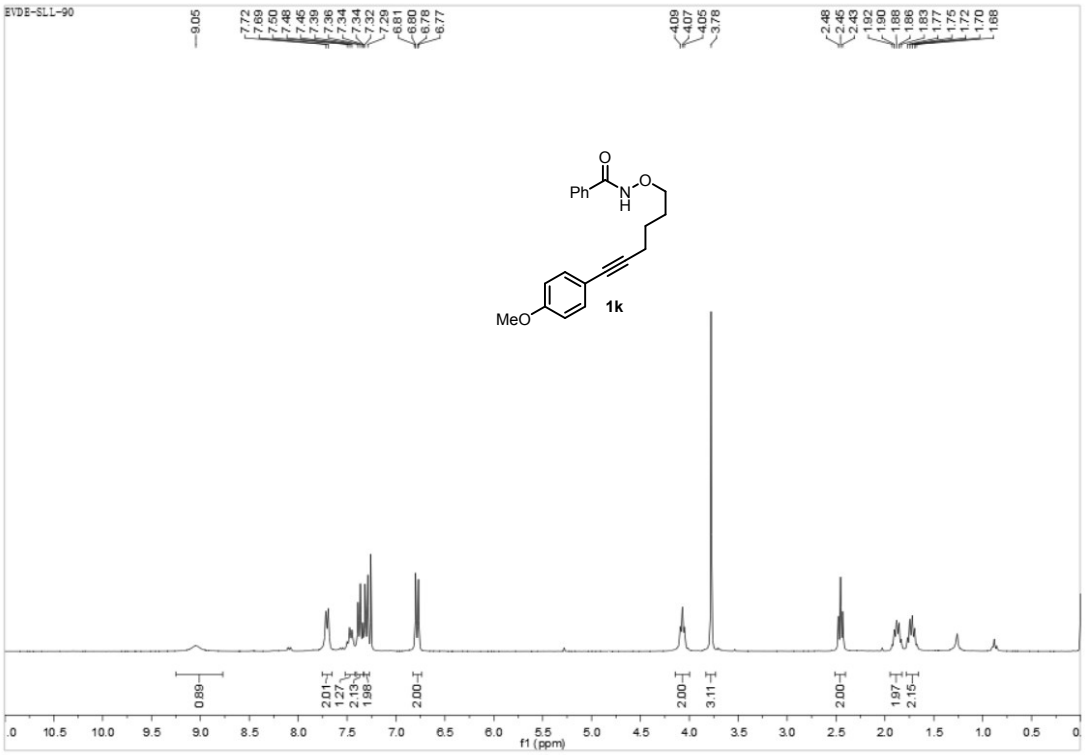

EVDE-SLL-20
Me
O
N
H
O
Ph
1h
f1 (ppm)

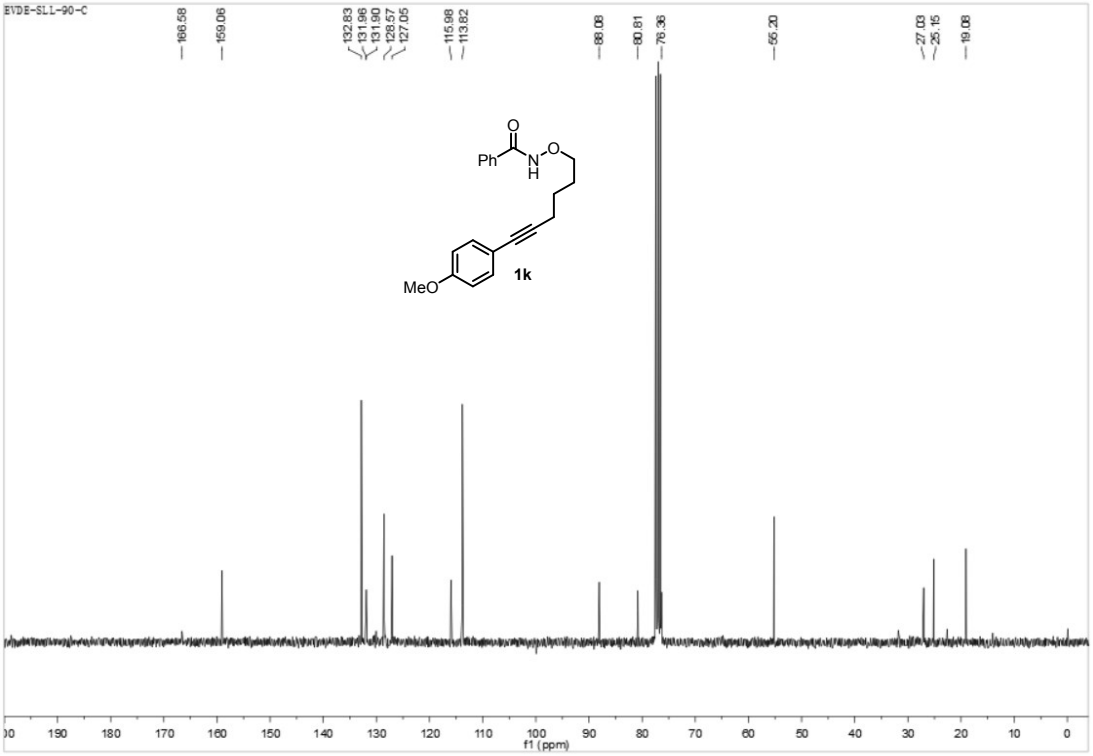

EVDE-SLL-7
8.65
7.38
7.37
7.36
7.35
7.35
7.33
7.33
7.30
7.30
7.28
7.28
7.27
7.26
7.26
7.25
7.25
7.24
7.24
7.20
7.18
7.15
7.13
7.10
4.06
2.47
2.45
2.40
1.88
1.74
Me
O
N
H
O
Ph
1i
0.96
2.12
5.34
2.10
2.00
1.93
3.06
4.02
f1 (ppm)

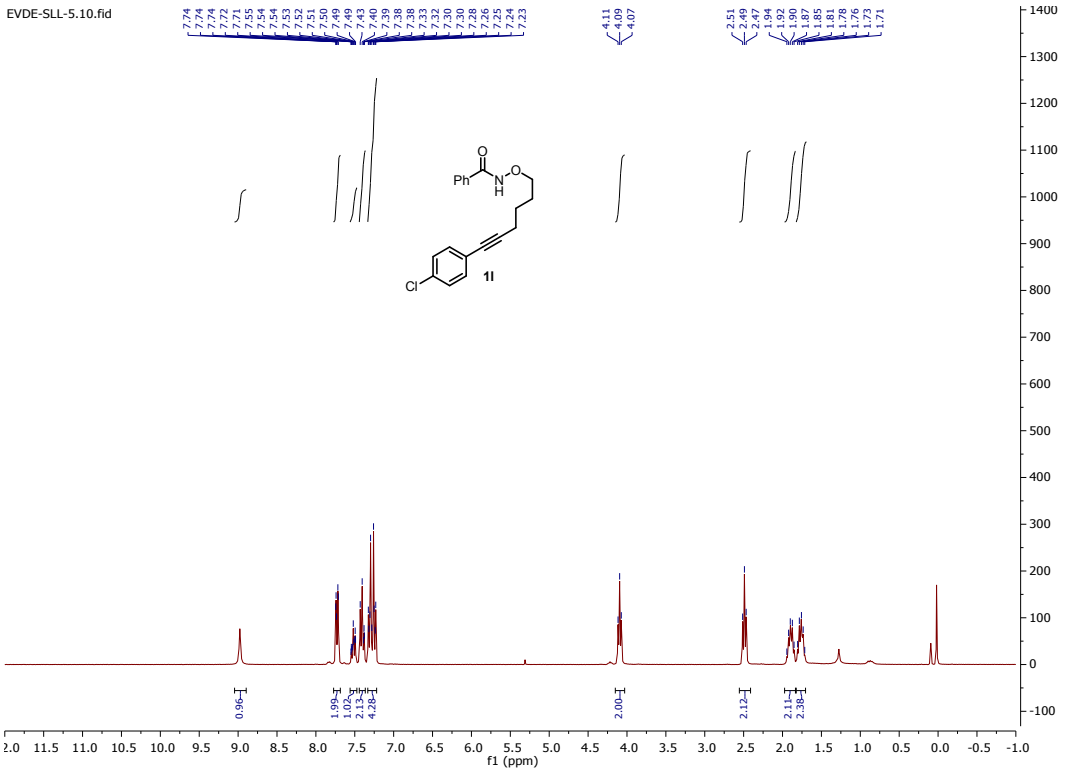

EVDE-SLL-7C
167.86
136.77
132.72
131.44
130.95
130.39
128.14
127.54
127.03
125.55
123.71
89.58
81.07
76.34
27.00
24.96
19.46
19.04
Me
O
N
H
O
Ph
1i
f1 (ppm)

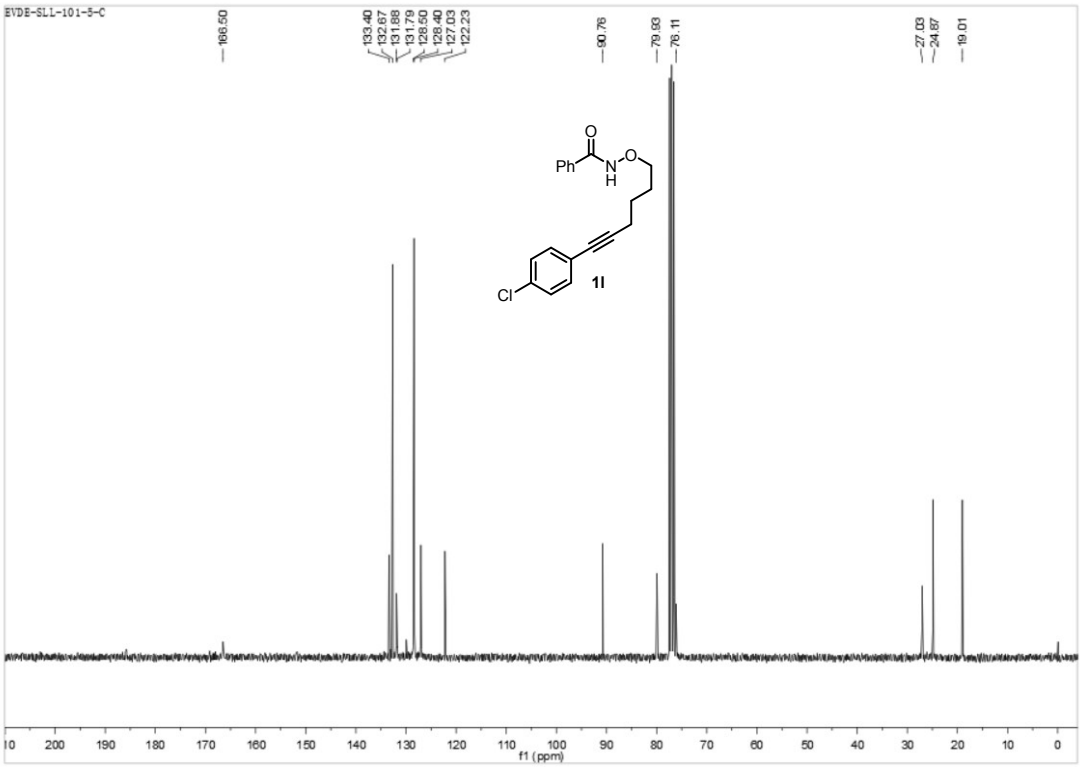

EVDE-SLL-4.10.fid
10.30
7.80
7.77
7.77
7.47
7.45
7.42
7.36
7.34
7.31
7.30
7.28
7.09
7.06
4.06
4.03
4.01
2.43
2.41
2.39
2.32
1.88
1.85
1.83
1.82
1.81
1.78
1.73
1.70
1.68
1.65
1.63
Ph
O
N
H
O
Me
1j
0.97
2.03
1.04
4.20
2.11
2.00
2.04
3.09
2.04
2.11
f1 (ppm)

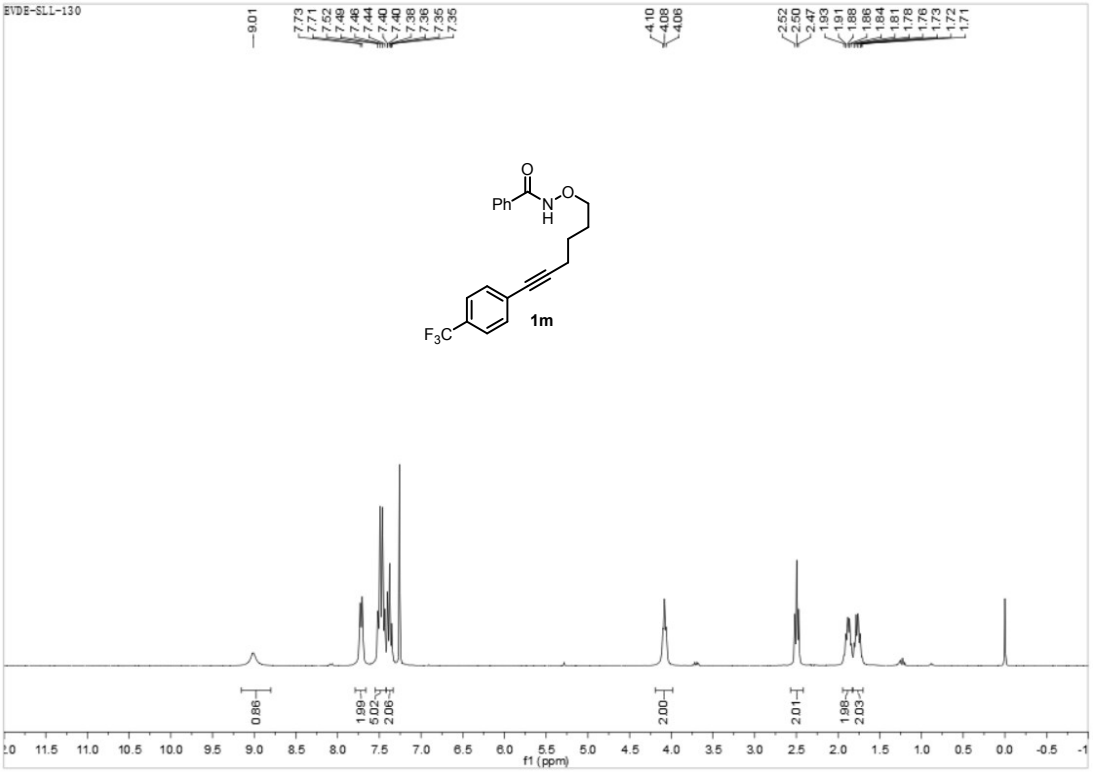

EVDE-CSLL-101-3
166.35
137.41
131.74
131.25
128.83
128.39
127.05
120.58
86.85
80.96
76.02
26.95
24.95
21.24
18.96
Ph
O
N
H
O
Me
1j
f1 (ppm)

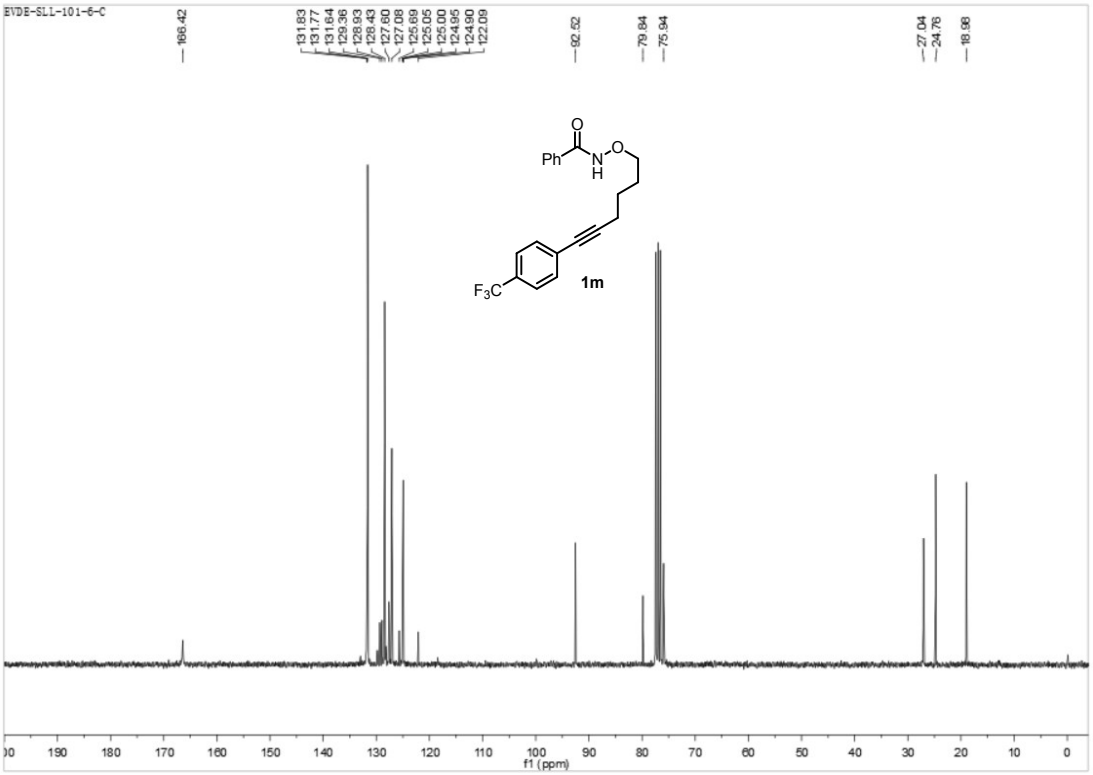

EVDE-SLL-90
9.05
7.72
7.69
7.50
7.48
7.45
7.39
7.36
7.34
7.34
7.32
7.29
6.81
6.80
6.78
6.77
4.09
4.07
4.06
3.78
2.48
2.45
2.43
1.92
1.90
1.88
1.86
1.83
1.77
1.75
1.72
1.70
1.68
Ph
O
N
H
O
MeO
1k
0.89
2.01
1.27
2.13
1.98
2.00
2.00
3.11
2.00
1.97
2.15
f1 (ppm)

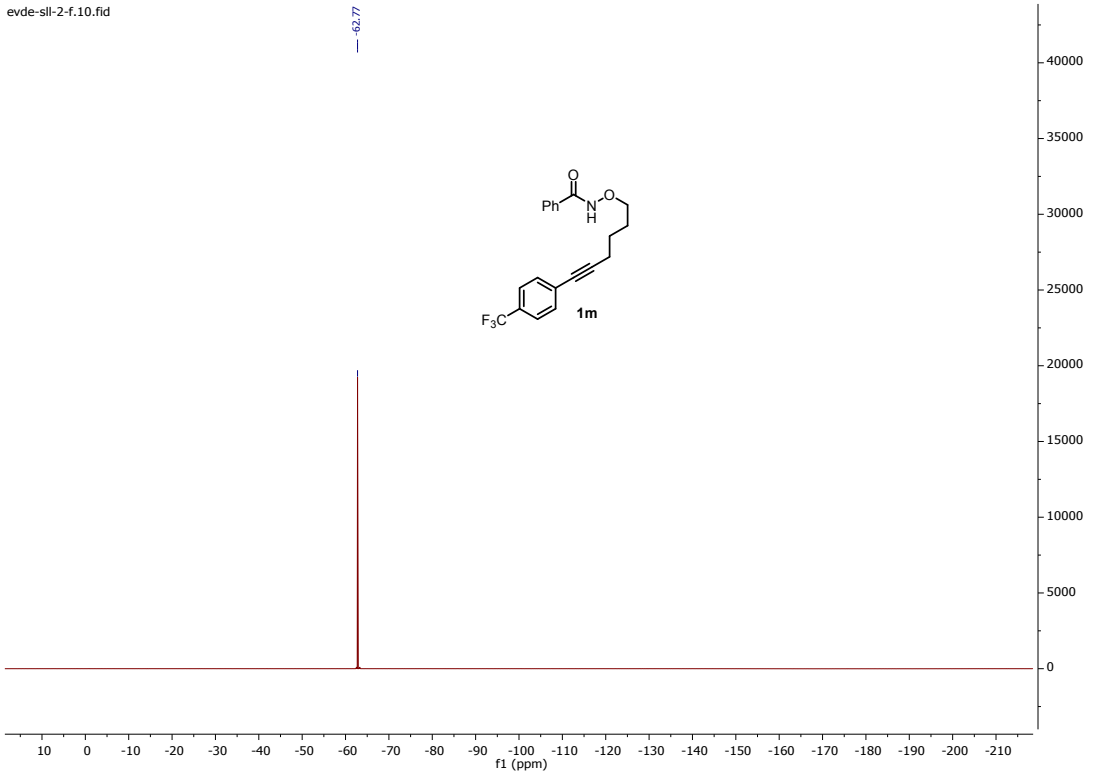

EVDE-SLL-90-C
166.58
159.06
132.83
131.96
131.90
128.57
127.05
115.98
113.82
88.08
80.81
76.36
55.20
27.03
25.15
19.08
Ph
O
N
H
O
MeO
1k
f1 (ppm)

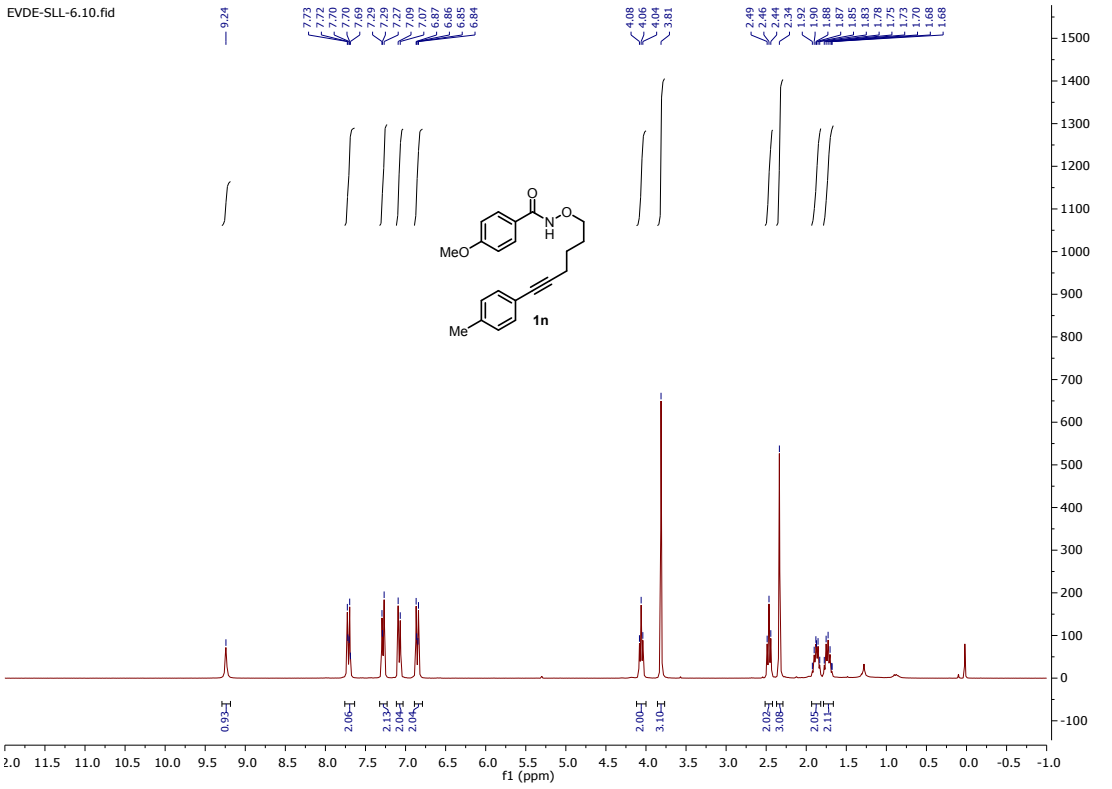

EVDE-SLL-5.10.fid
7.74 7.74 7.74 7.72 7.71 7.55 7.54 7.54 7.53 7.52 7.51 7.50 7.49 7.49 7.43 7.40 7.39 7.38 7.33 7.32 7.30 7.30 7.28 7.26 7.25 7.24 7.23
4.11 4.09 4.07
2.51 2.49 2.47 1.94 1.92 1.90 1.87 1.85 1.81 1.78 1.76 1.73 1.71
Ph
O
N
H
O
Cl
1l
0.96 1.99 1.02 2.13 4.28 2.00 2.12 2.11 2.38
f1 (ppm)

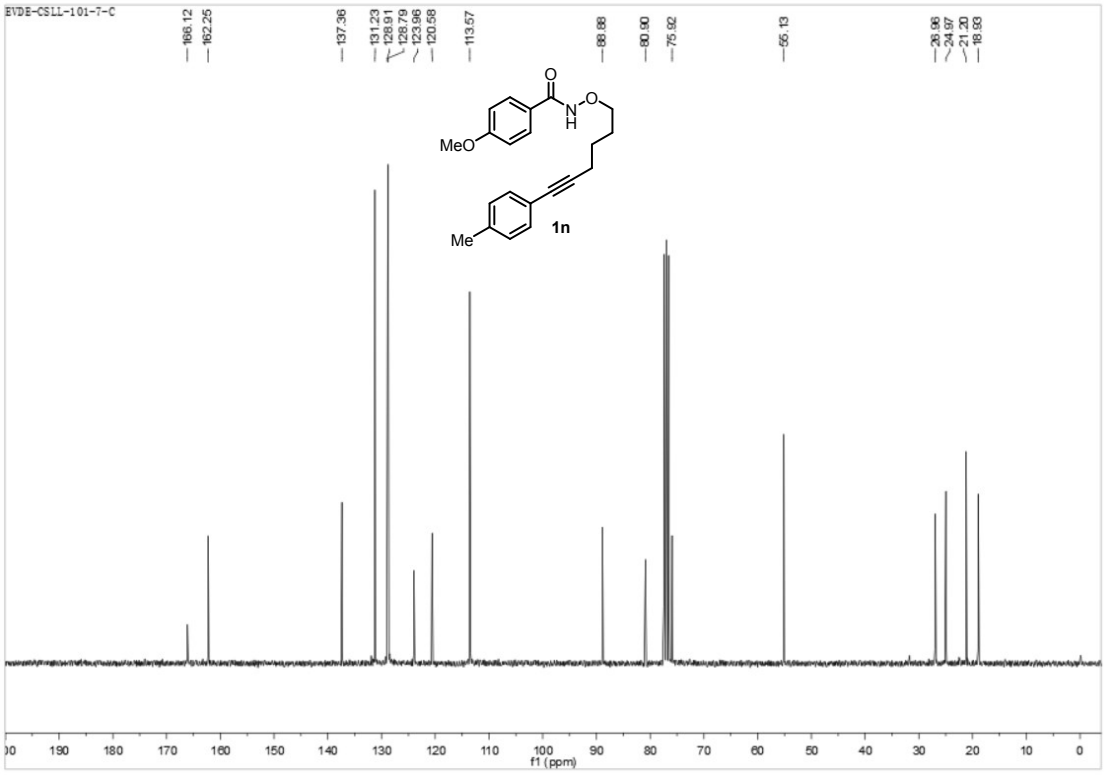

EVDE-SLL-101-5-C
166.50
133.40 132.67 131.88 131.79 128.50 128.40 127.03 122.23
90.76
79.93
76.11
27.03
24.87
19.01
Ph
O
N
H
O
Cl
1l
f1 (ppm)

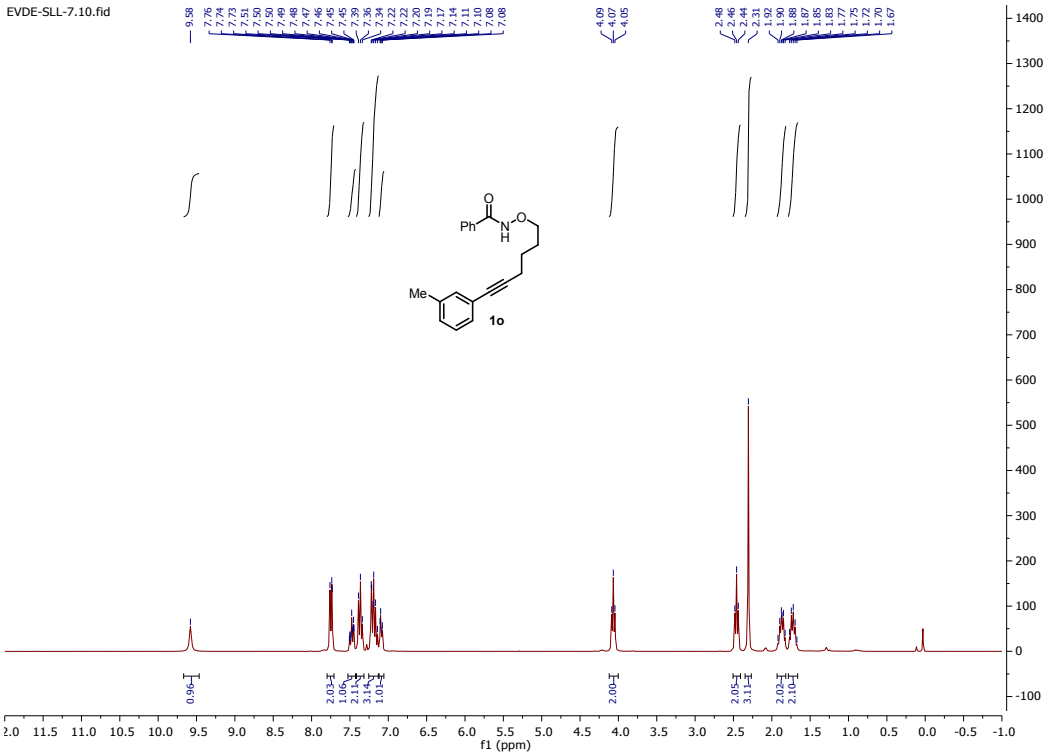

EVDE-SLL-130
9.01
7.73
7.71
7.52
7.49
7.46
7.44
7.40
7.40
7.38
7.36
7.35
7.35
4.10
4.08
4.06
2.52
2.50
2.47
1.93
1.91
1.88
1.86
1.84
1.81
1.78
1.76
1.73
1.72
1.71
Ph
O
N
H
O
F3C
1m
0.86
1.99
5.02
2.06
2.00
2.01
1.98
2.03
f1 (ppm)

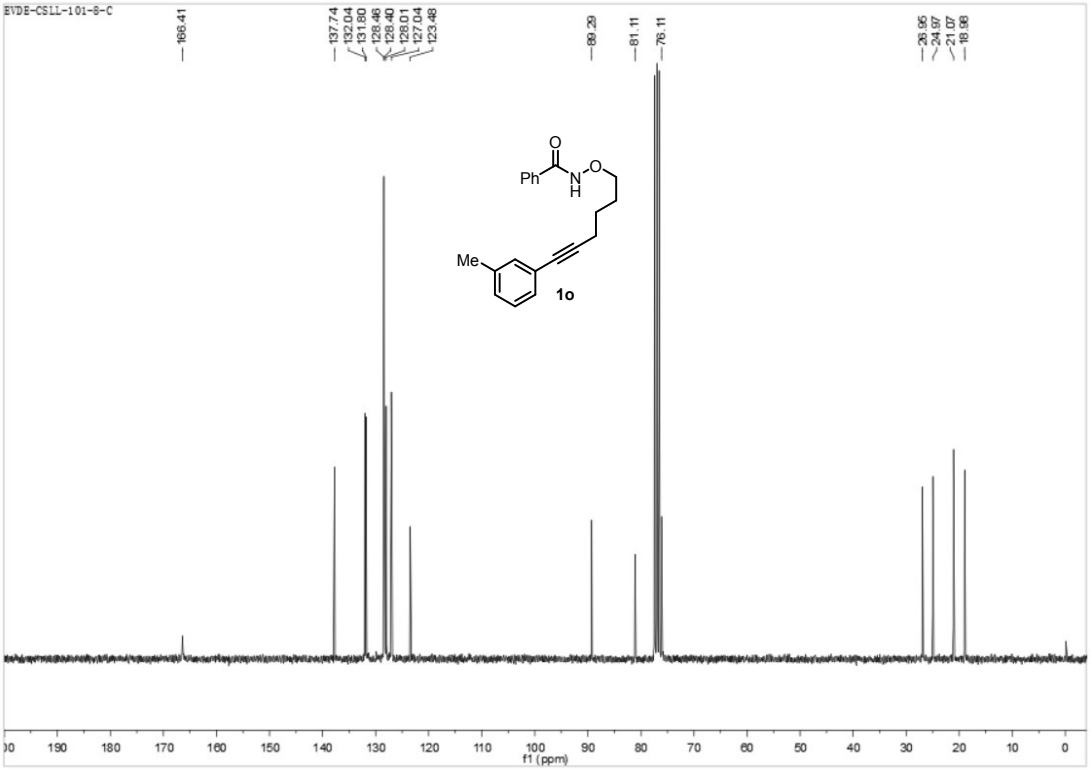

EVDE-SLL-101-6-C
166.42
131.83
131.77
131.64
129.36
128.93
128.43
127.60
127.08
125.69
125.05
125.00
124.95
124.90
122.09
92.52
79.84
75.94
27.04
24.76
18.98
Ph
O
N
H
O
F3C
1m
f1 (ppm)

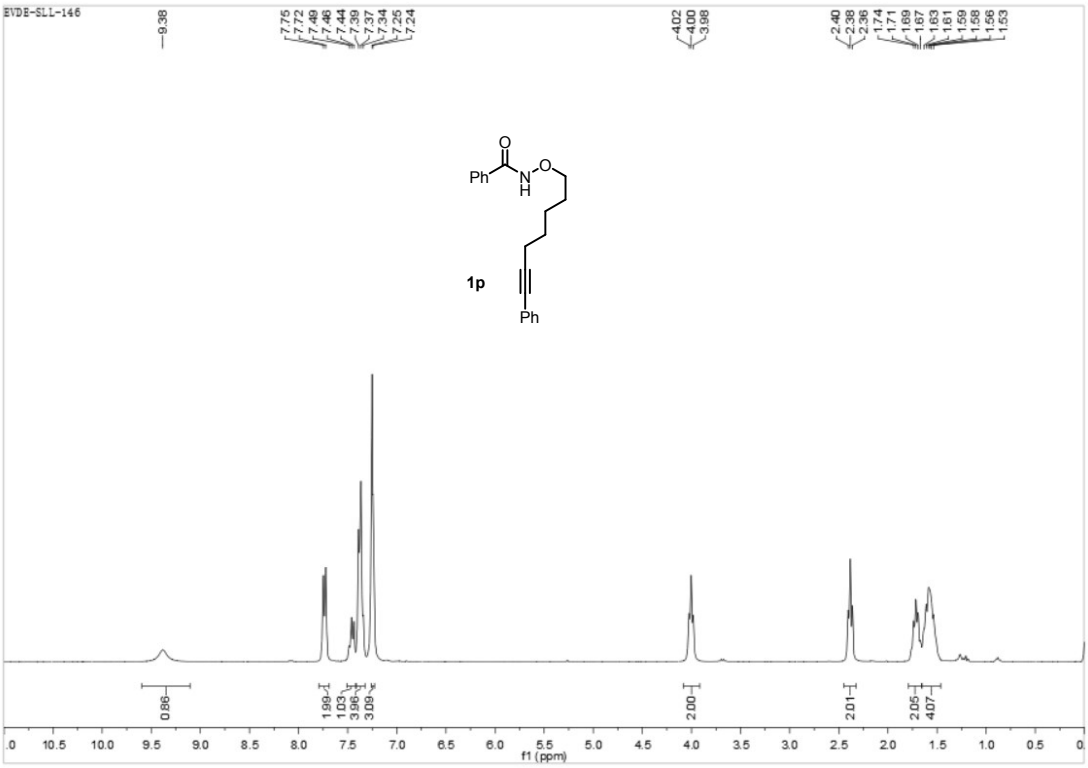

evde-sll-2-f.10.fid
-62.77
40000
35000
30000
25000
20000
15000
10000
5000
0
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
O
Ph
N
H
O
F3C
1m

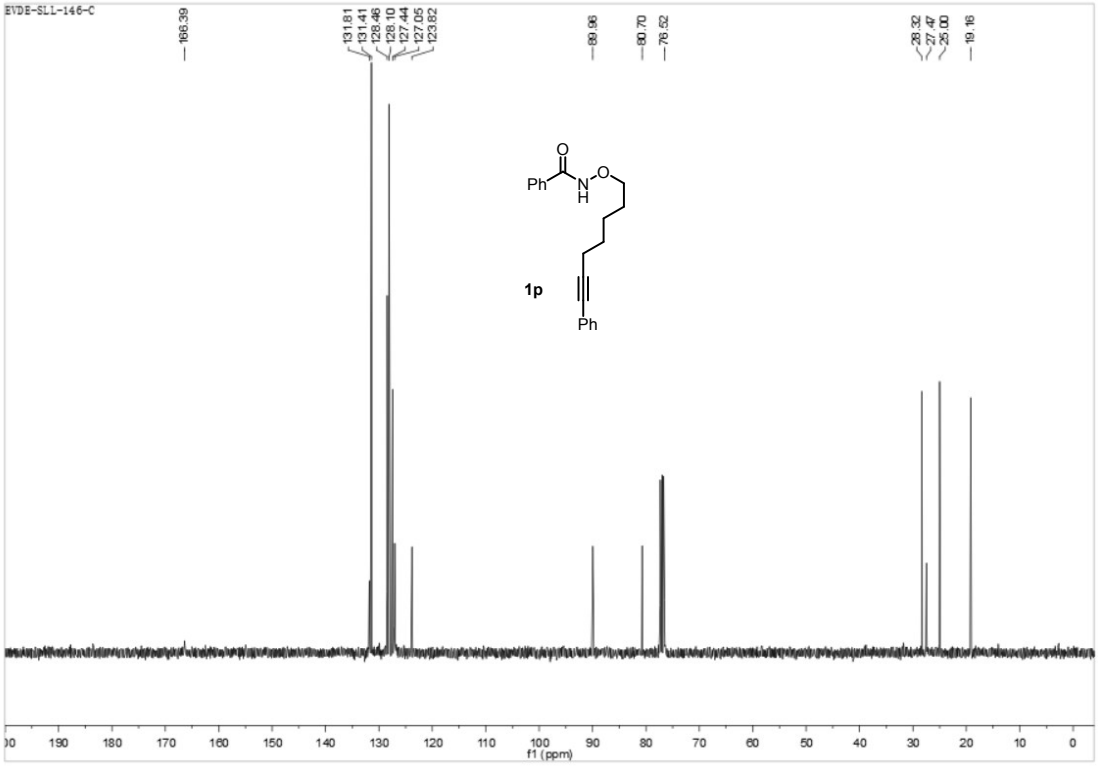

EVDE-SLL-6.10.fid
MeO
Me
1n
f1 (ppm)

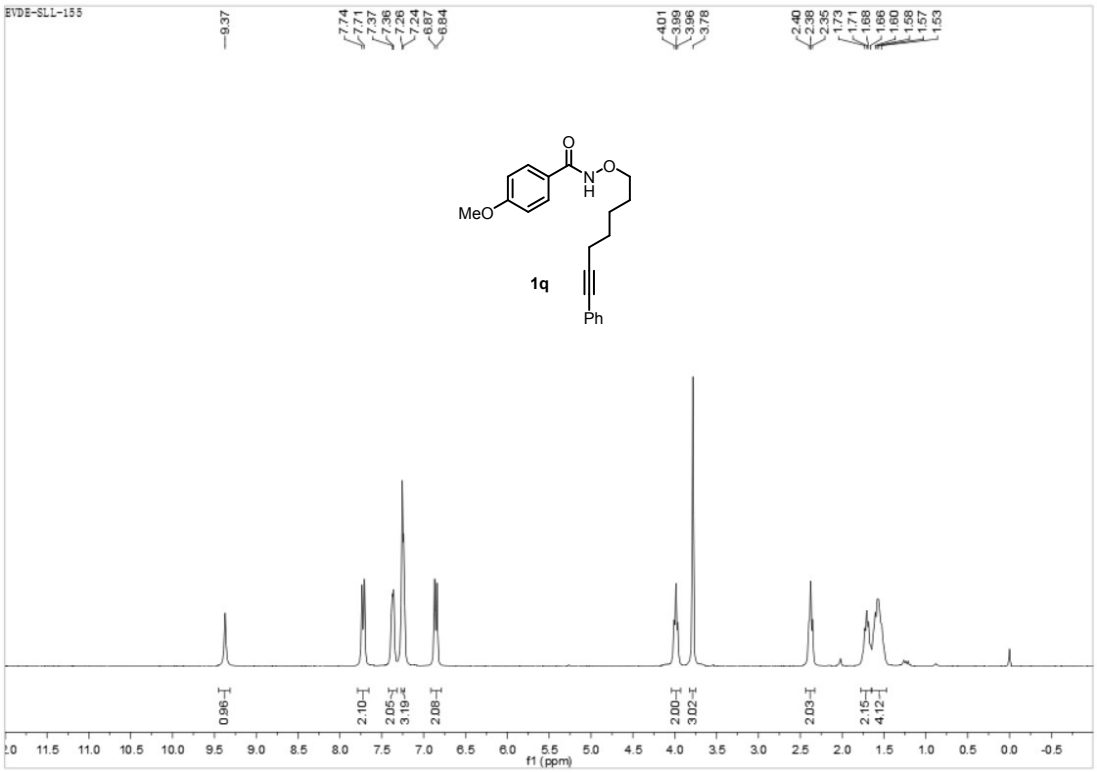

EVDE-CSLL-101-7-C
MeO
Me
1n
f1 (ppm)

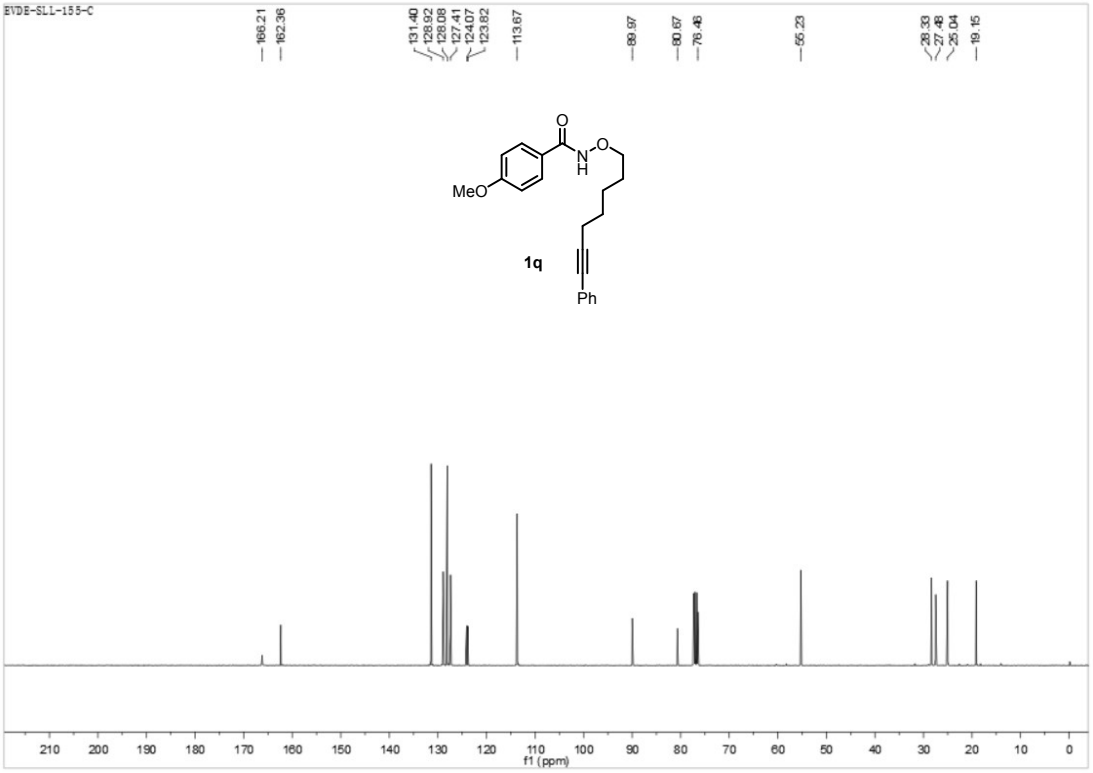

EVDE-SLL-7.10.fid
Ph
O
N
H
O
Me
1o
f1 (ppm)

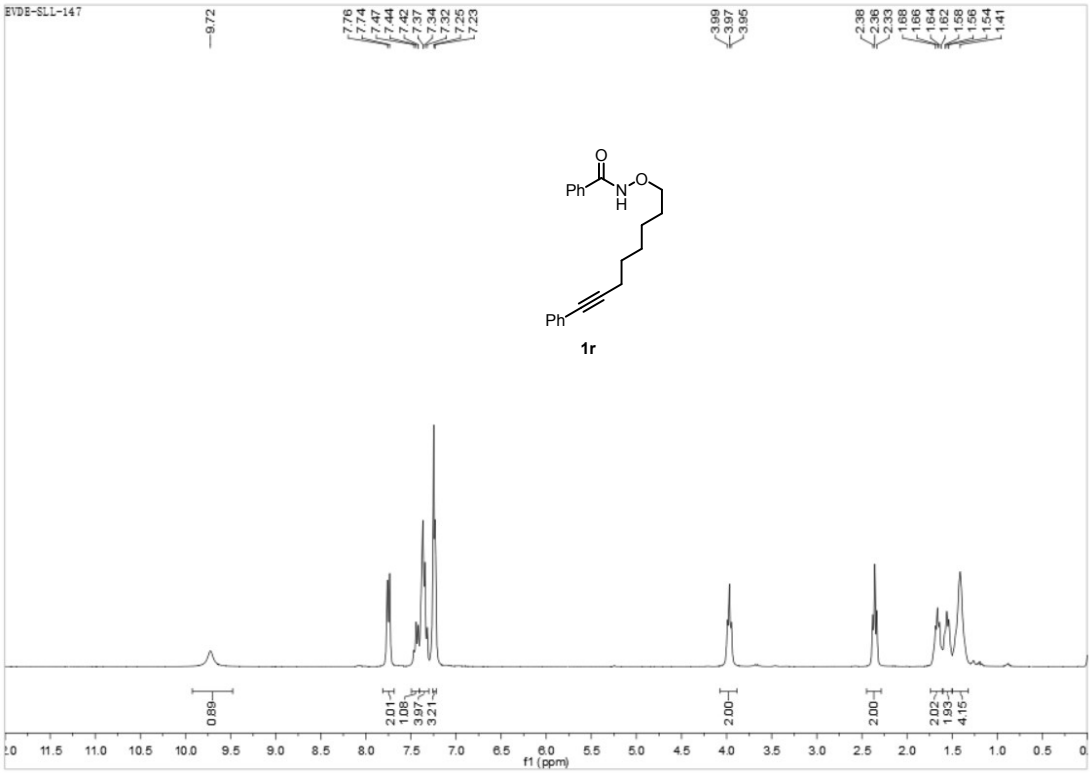

EVDE-CSLL-101-8-C
Ph
O
N
H
O
Me
1o
f1 (ppm)

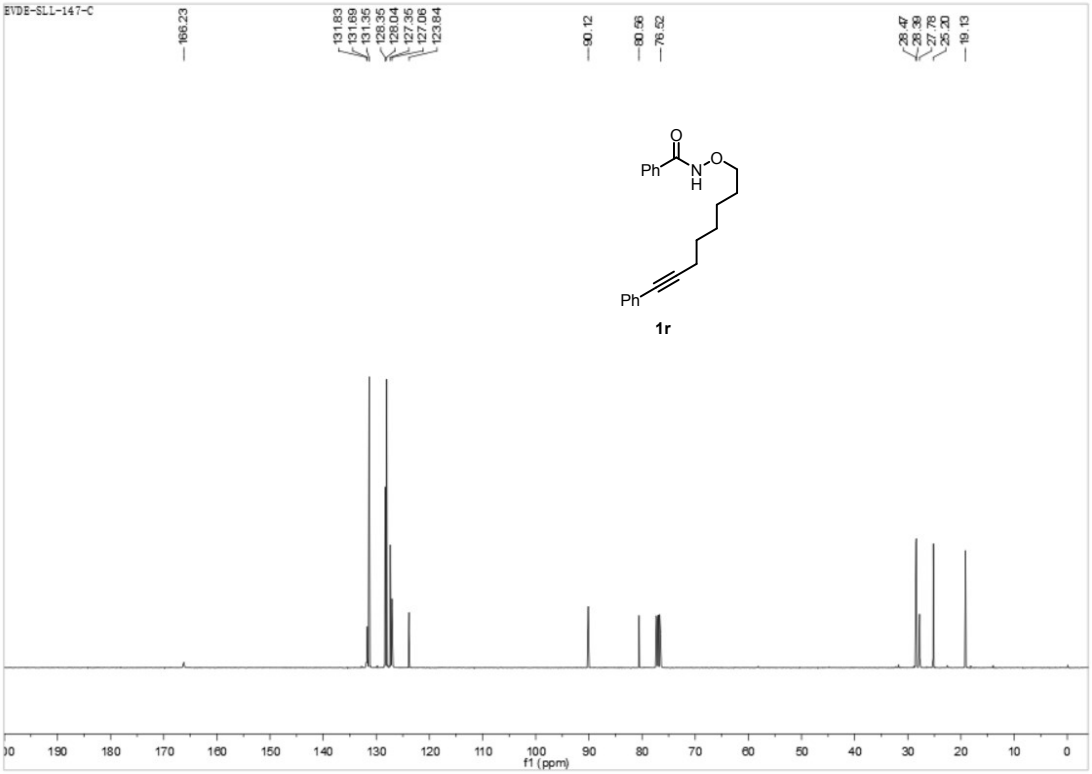

EVDE-SLL-146
9.38
7.75
7.72
7.49
7.46
7.44
7.39
7.37
7.34
7.25
7.24
4.02
4.00
3.98
2.40
2.38
2.36
1.74
1.71
1.69
1.67
1.63
1.61
1.59
1.58
1.56
1.53
Ph
O
N
H
O
1p
Ph
0.86
1.99
1.03
3.96
3.09
2.00
2.01
2.05
4.07
f1 (ppm)

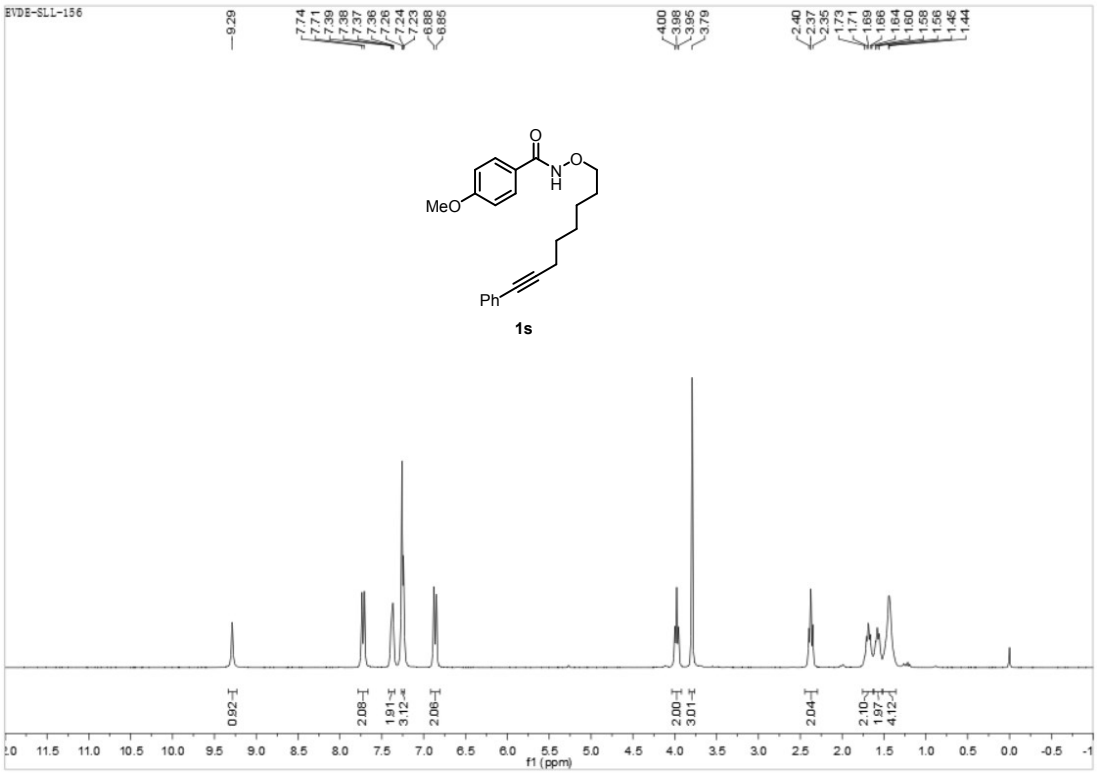

EVDE-SLL-146-C
166.39
131.81
131.41
128.46
128.10
127.44
127.05
123.62
89.96
80.70
76.52
28.32
27.47
25.00
19.16
Ph
O
N
H
O
1p
Ph
f1 (ppm)

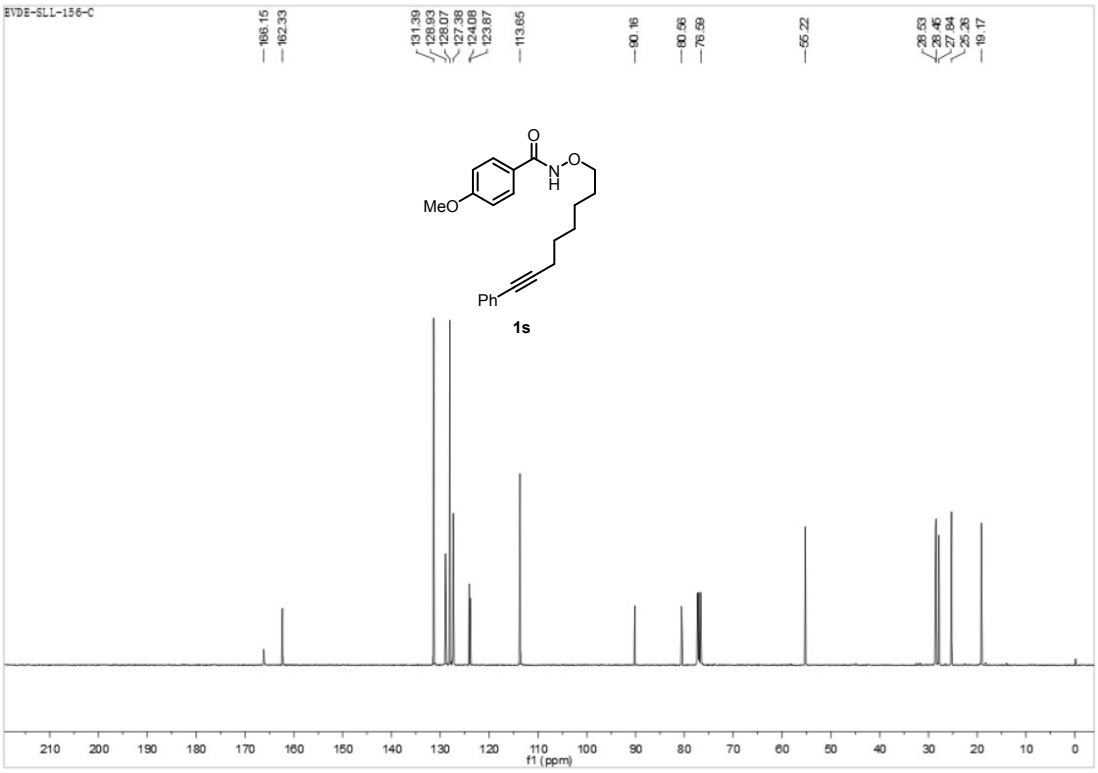

EVDE-SLL-155
9.37
7.74
7.71
7.37
7.36
7.26
7.24
6.87
6.84
4.01
3.99
3.96
3.78
2.40
2.38
2.35
1.73
1.71
1.68
1.66
1.60
1.58
1.57
1.53
O
N
H
O
MeO
1q
Ph
0.96
2.10
2.05
3.19
2.08
2.00
3.02
2.03
2.15
4.12
f1 (ppm)

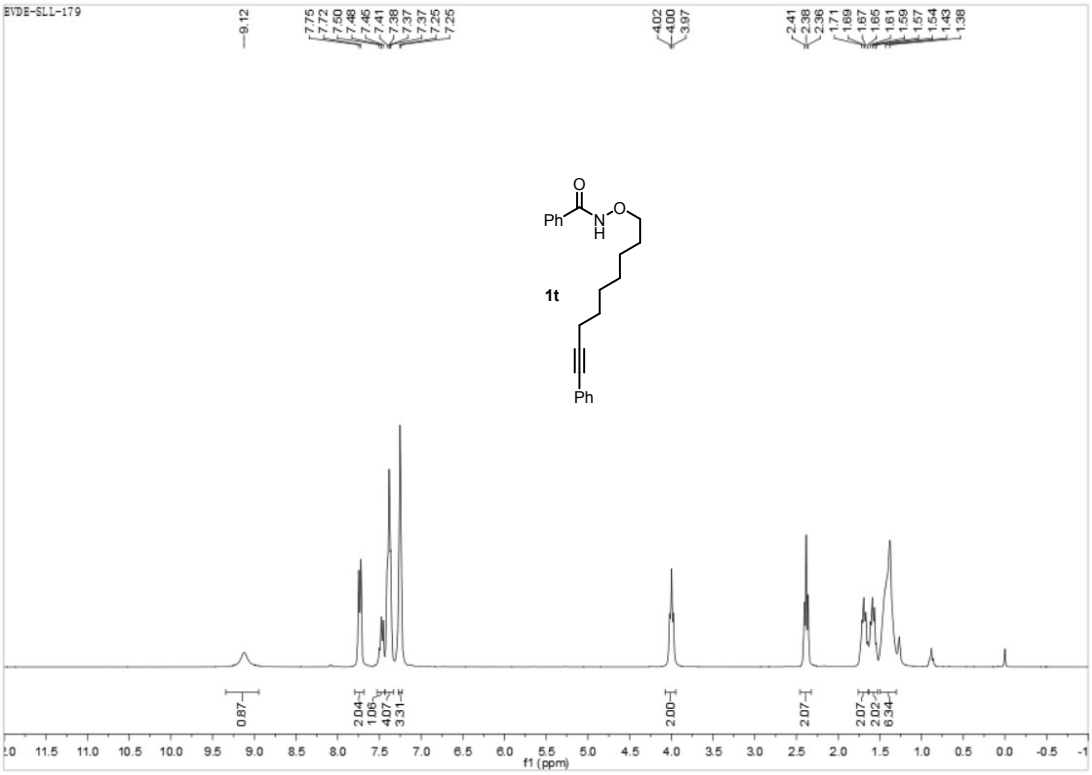

EVDE-SLL-155-C
166.21
162.36
131.40
128.92
128.08
127.41
124.07
123.62
113.67
89.97
80.67
76.48
55.23
29.33
27.48
25.04
19.15
O
N
H
O
MeO
1q
Ph
f1 (ppm)

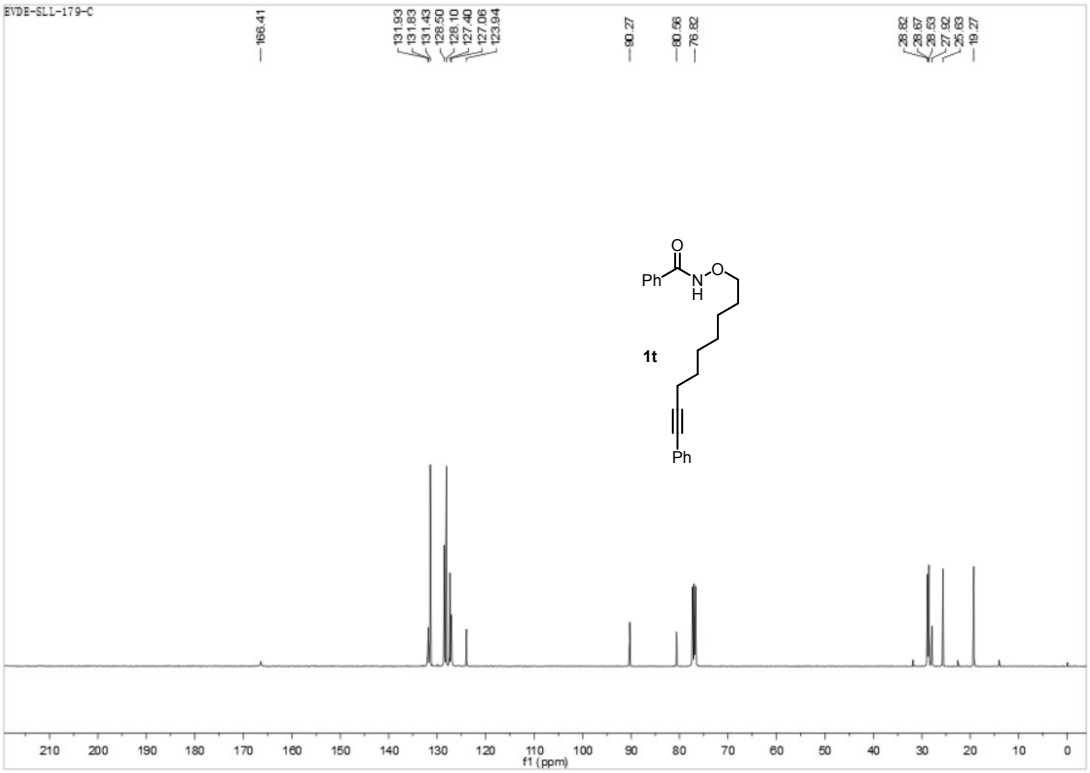

EVDE-SLL-147
9.72
7.76
7.74
7.47
7.44
7.42
7.37
7.34
7.32
7.25
7.23
3.99
3.97
3.95
2.38
2.36
2.33
1.68
1.66
1.64
1.62
1.58
1.56
1.54
1.41
Ph
O
N
H
O
Ph
1r
0.89
2.01
1.08
3.97
3.21
2.00
2.00
2.02
1.93
4.15
f1 (ppm)

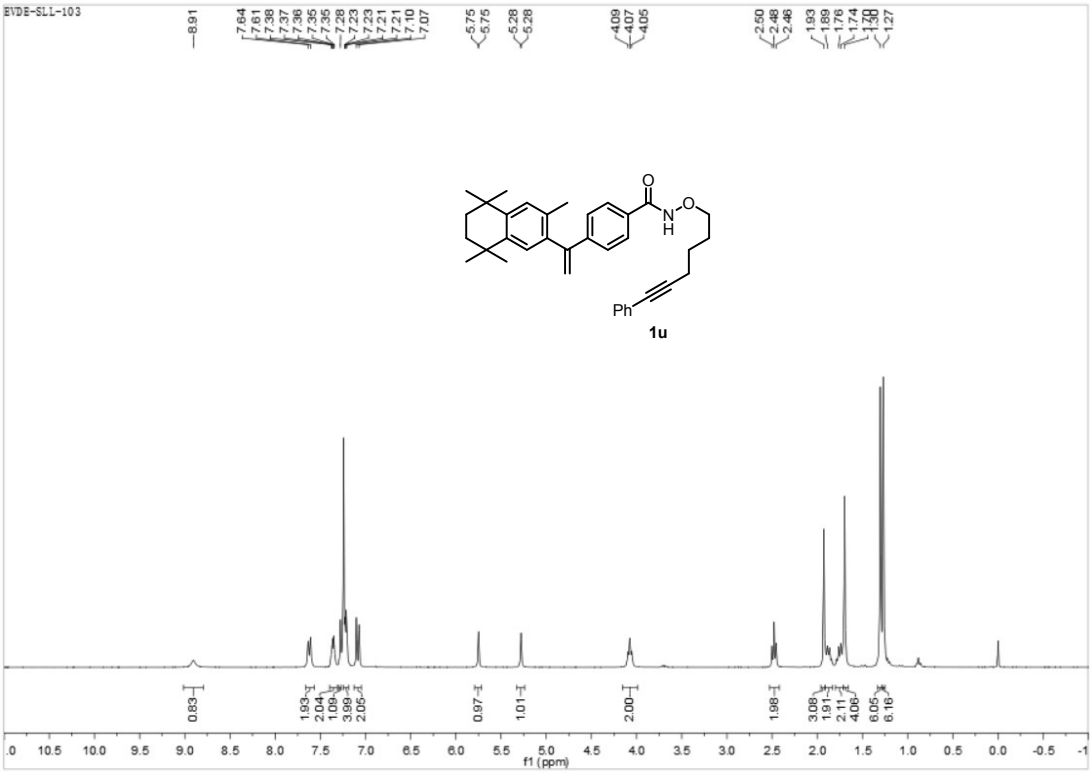

EVDE-SLL-147-C
166.23
131.83
131.69
131.35
128.35
128.04
127.35
127.06
123.84
90.12
80.66
76.52
28.47
28.39
27.78
25.20
19.13
Ph
O
N
H
O
Ph
1r
f1 (ppm)

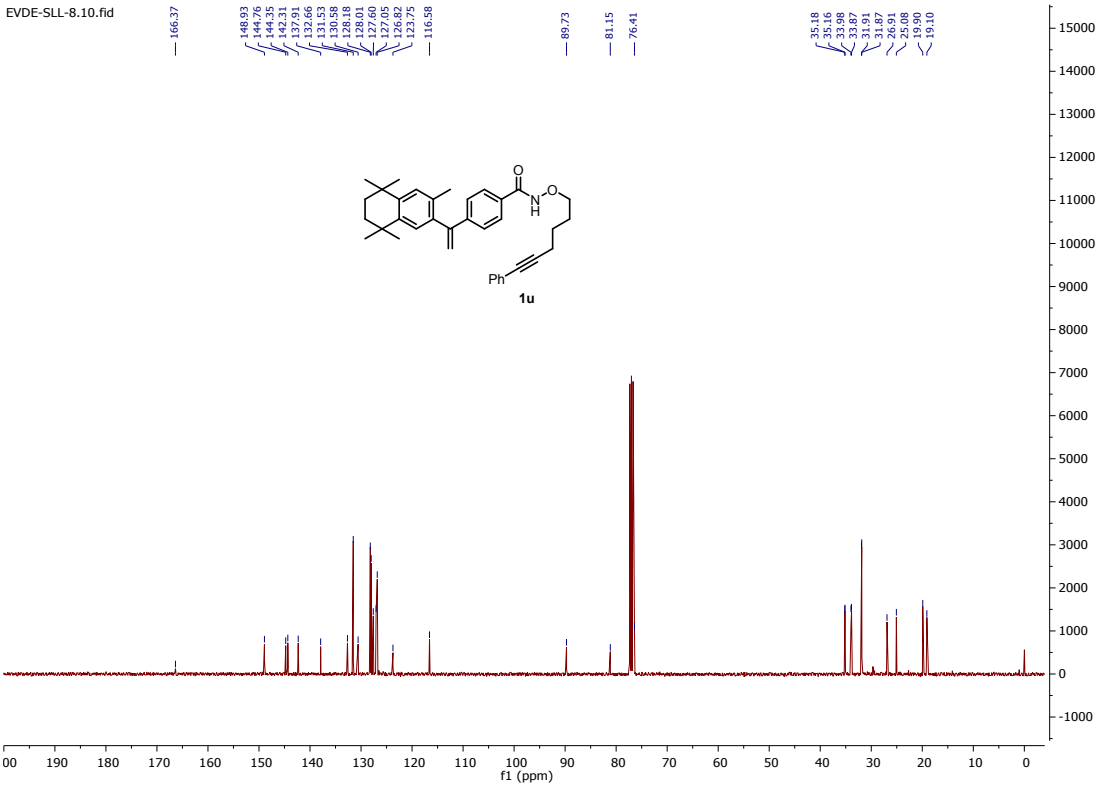

EVDE-SLL-156
9.29
7.74
7.71
7.39
7.38
7.37
7.36
7.26
7.24
7.23
6.88
6.85
4.00
3.98
3.95
3.79
2.40
2.37
2.35
1.73
1.71
1.69
1.66
1.64
1.60
1.58
1.56
1.45
1.44
O
N
H
O
MeO
Ph
1s
0.92
2.08
1.91
3.12
2.06
2.00
3.01
2.04
2.10
1.97
4.12
f1 (ppm)

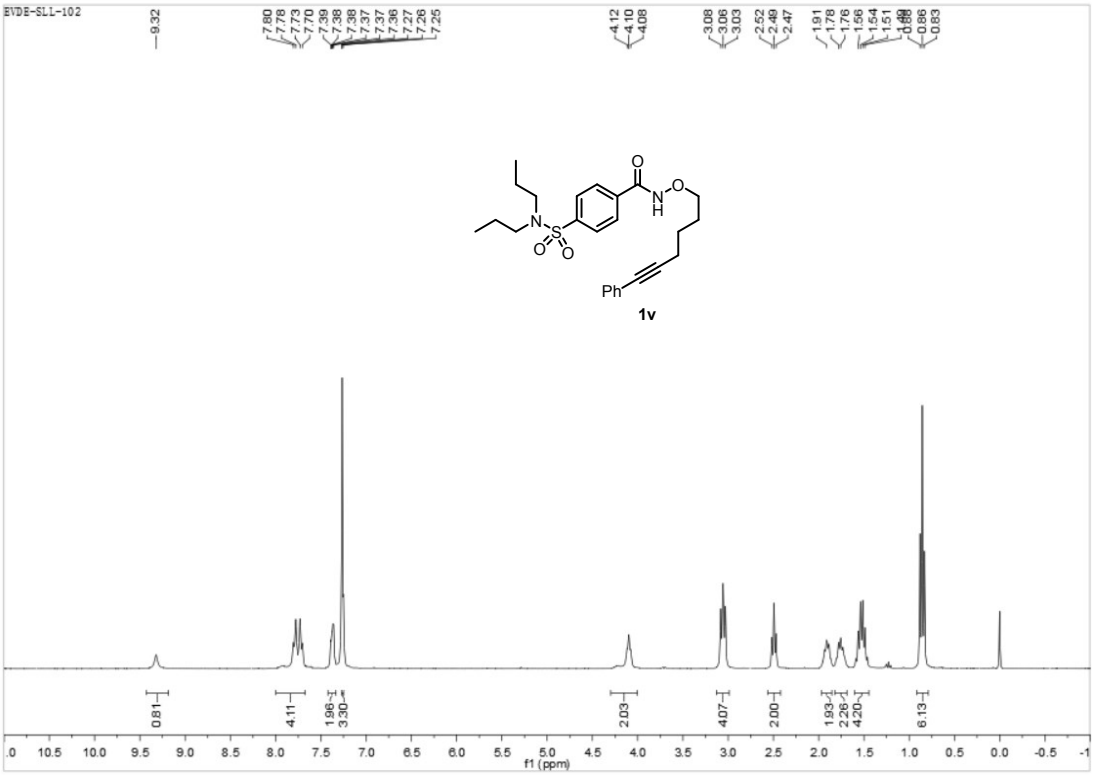

EVDE-SLL-156-C
166.15
162.33
131.39
128.93
128.07
127.38
124.08
123.87
113.65
90.16
80.56
76.59
55.22
28.53
28.45
27.84
25.28
19.17
O
N
H
O
MeO
Ph
1s
f1 (ppm)

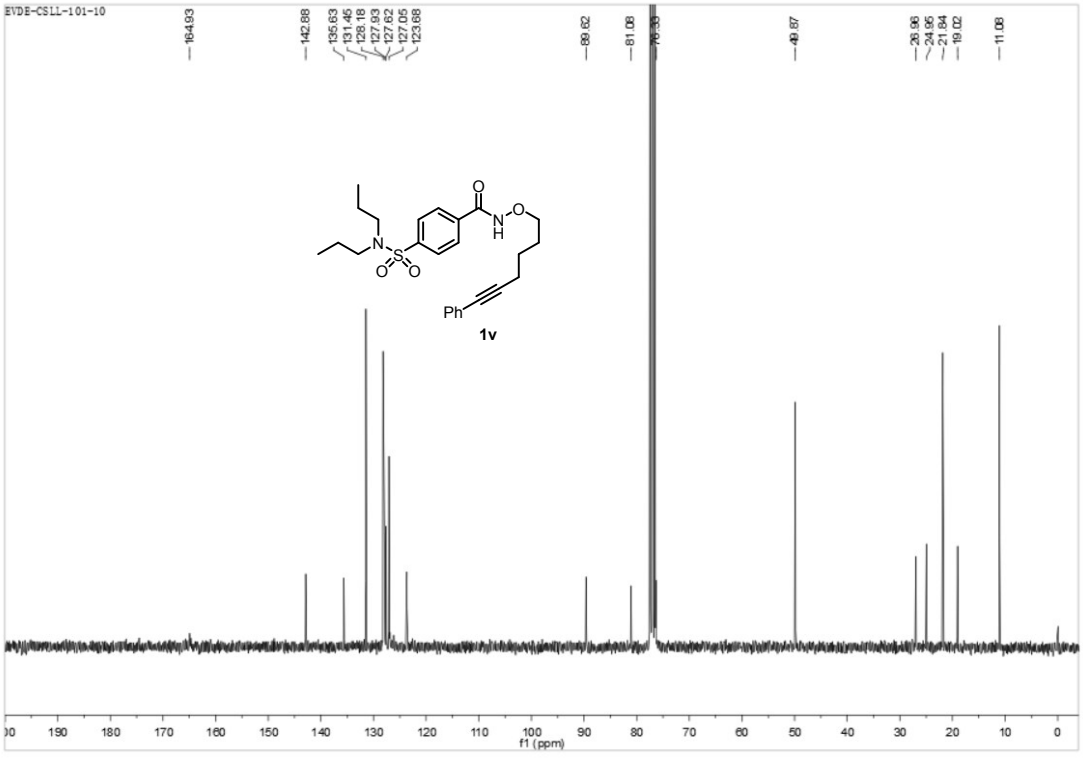

EVDE-SLL-179
9.12
7.75
7.72
7.50
7.48
7.45
7.41
7.38
7.37
7.37
7.25
7.25
4.02
4.00
3.97
2.41
2.38
2.36
1.71
1.69
1.67
1.65
1.61
1.59
1.57
1.54
1.43
1.38
Ph
O
N
H
O
1t
Ph
0.87
2.04
1.06
4.07
3.31
2.00
2.07
2.07
2.02
6.34
f1 (ppm)

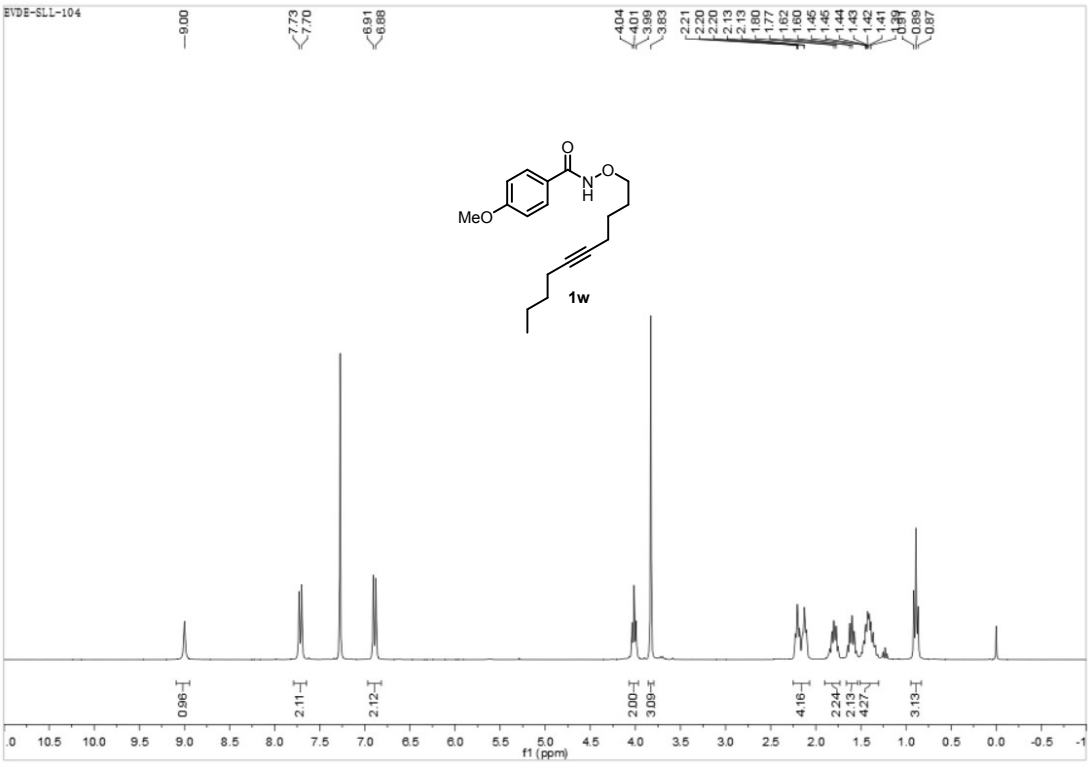

EVDE-SLL-179-C
166.41
131.93
131.63
131.43
128.50
128.10
127.40
127.06
123.94
90.27
80.56
76.82
28.82
28.67
28.53
27.92
25.63
19.27
Ph
O
N
H
O
1t
Ph
f1 (ppm)

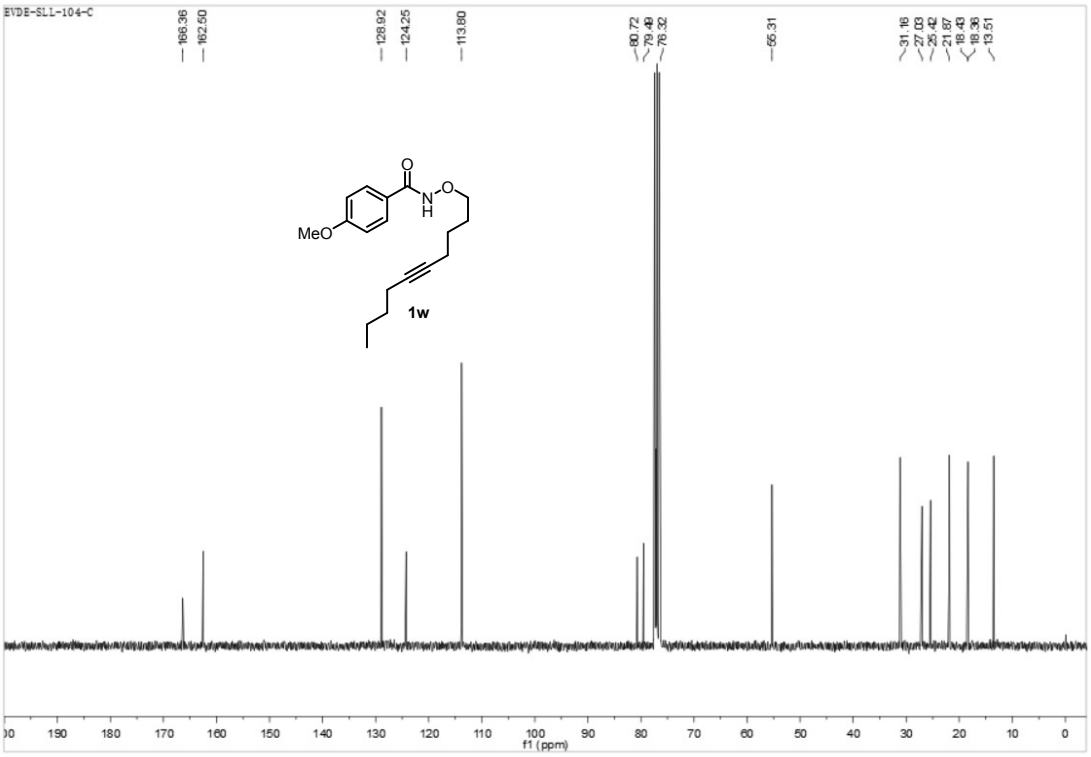

EVDE-SLL-103
8.91
7.64
7.61
7.38
7.37
7.36
7.35
7.35
7.28
7.23
7.23
7.21
7.21
7.10
7.07
5.75
5.75
5.28
5.28
4.09
4.07
4.05
2.50
2.48
2.46
1.93
1.89
1.76
1.74
1.30
1.27
O
N
H
O
Ph
1u
0.83
1.93
2.04
1.09
3.99
2.05
0.97
1.01
2.00
1.98
3.08
1.91
2.11
4.06
6.05
6.16
f1 (ppm)

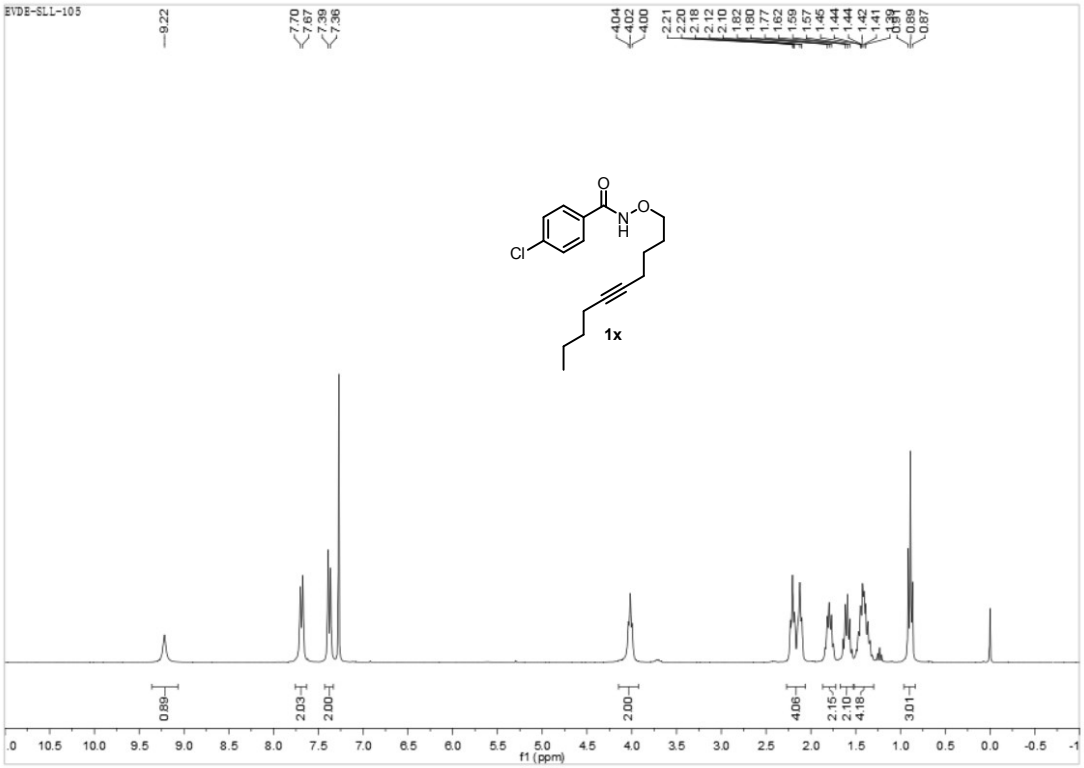

EVDE-SLL-8.10.fid
166.37
148.93
144.76
144.35
142.31
137.91
132.66
131.53
130.58
128.18
128.01
127.60
127.05
126.82
123.75
116.58
89.73
81.15
76.41
35.18
35.16
33.98
33.87
31.91
31.87
26.91
25.08
19.90
19.10
O
N
H
O
Ph
1u
f1 (ppm)

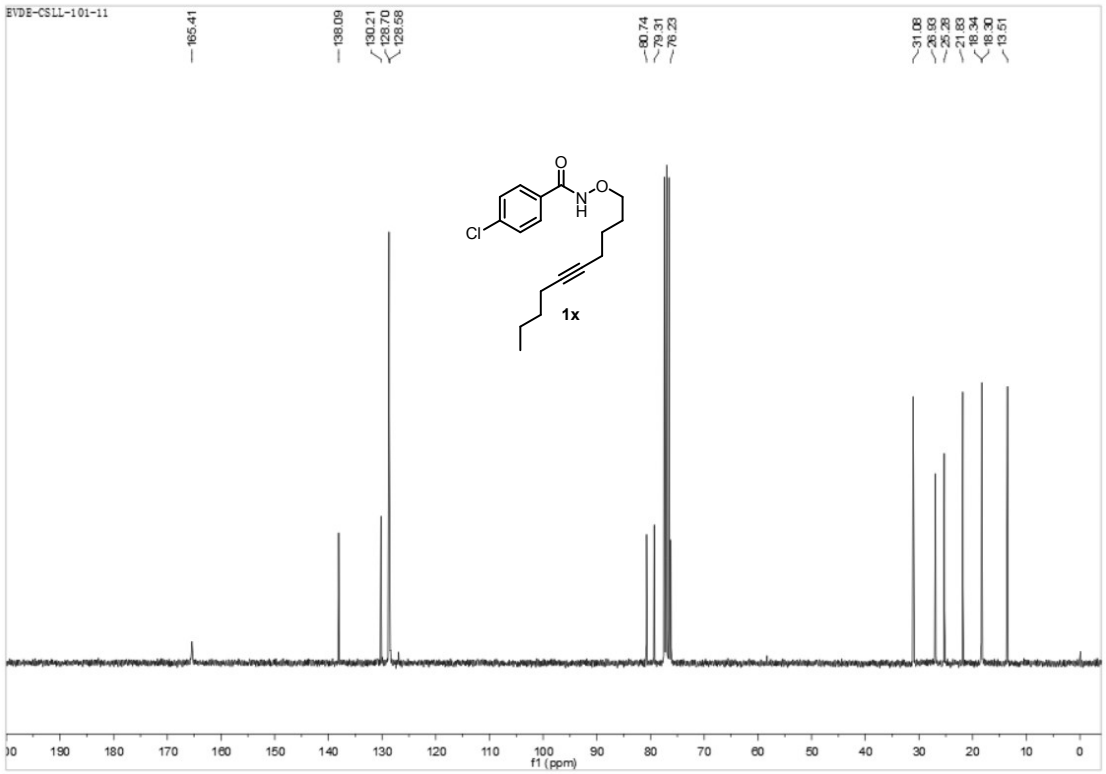

EVDE-SLL-102
1v
f1 (ppm)

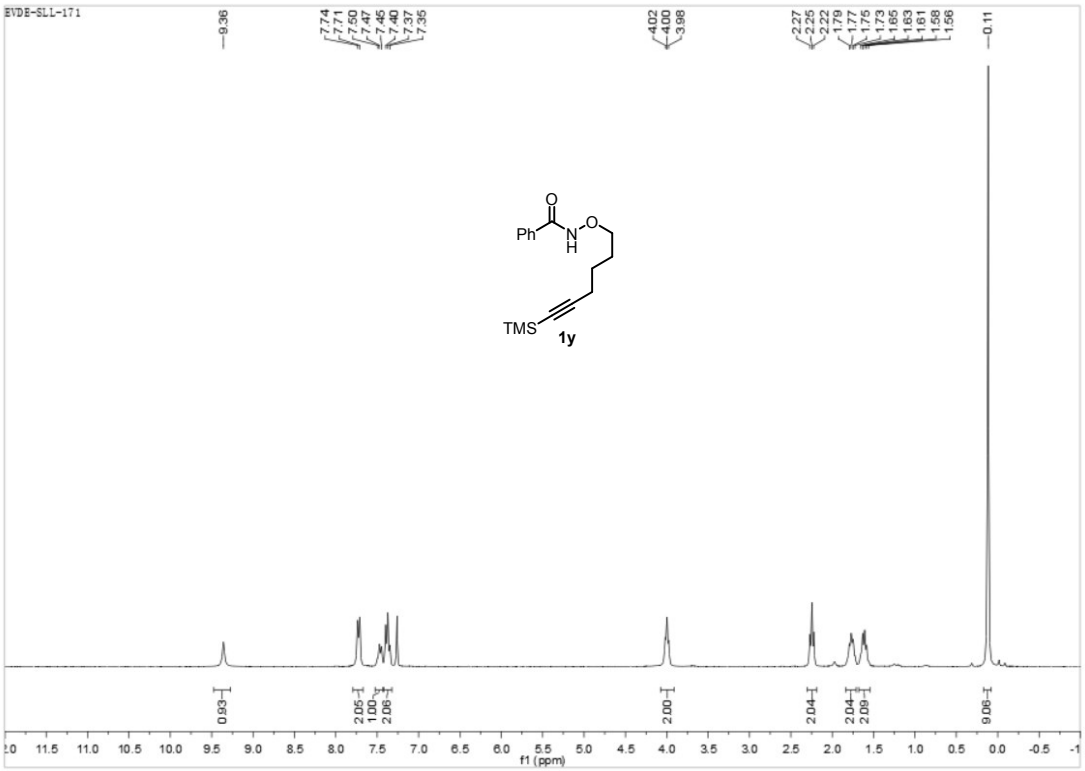

EVDE-CSLL-101-10
1v
f1 (ppm)

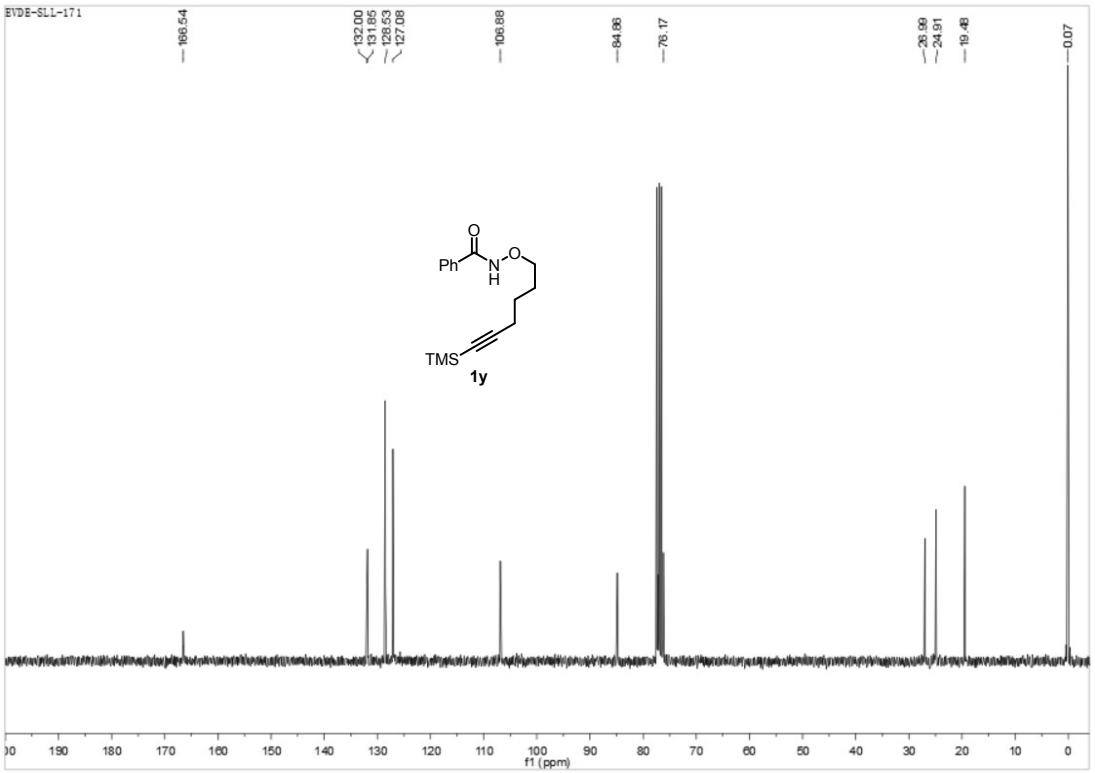

EVDE-SLL-104
MeO
1w
f1 (ppm)

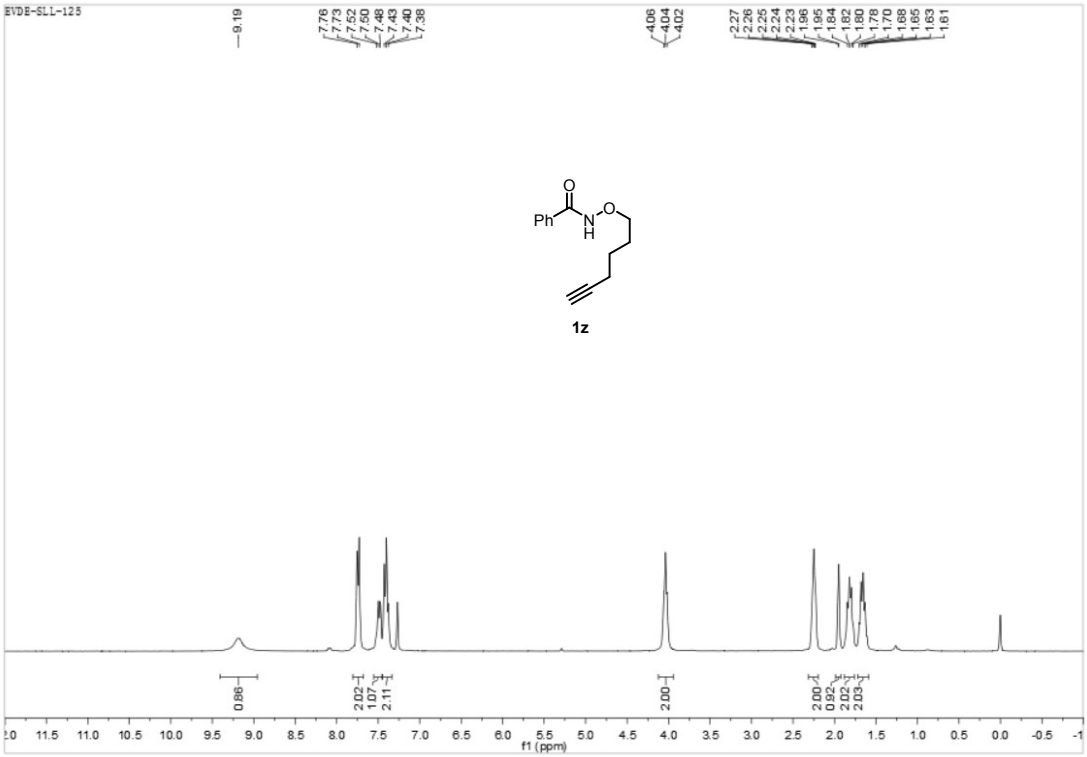

EVDE-SLL-104-C
MeO
1w
f1 (ppm)

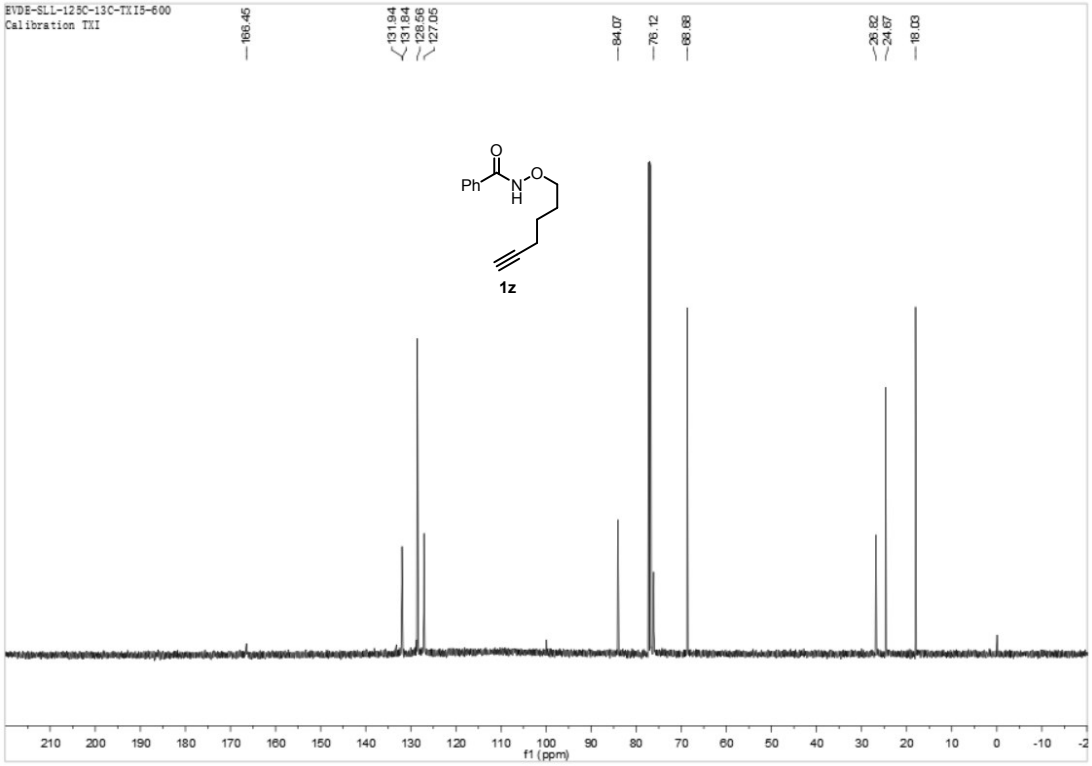

EVDE-SLL-105
9.22
7.70
7.67
7.39
7.36
4.04
4.02
4.00
2.21
2.20
2.18
2.12
2.10
1.82
1.80
1.77
1.62
1.59
1.57
1.45
1.44
1.44
1.42
1.41
0.89
0.87
O
N
H
O
Cl
1x
0.89
2.03
2.00
2.00
4.06
2.15
2.10
4.18
3.01
f1 (ppm)

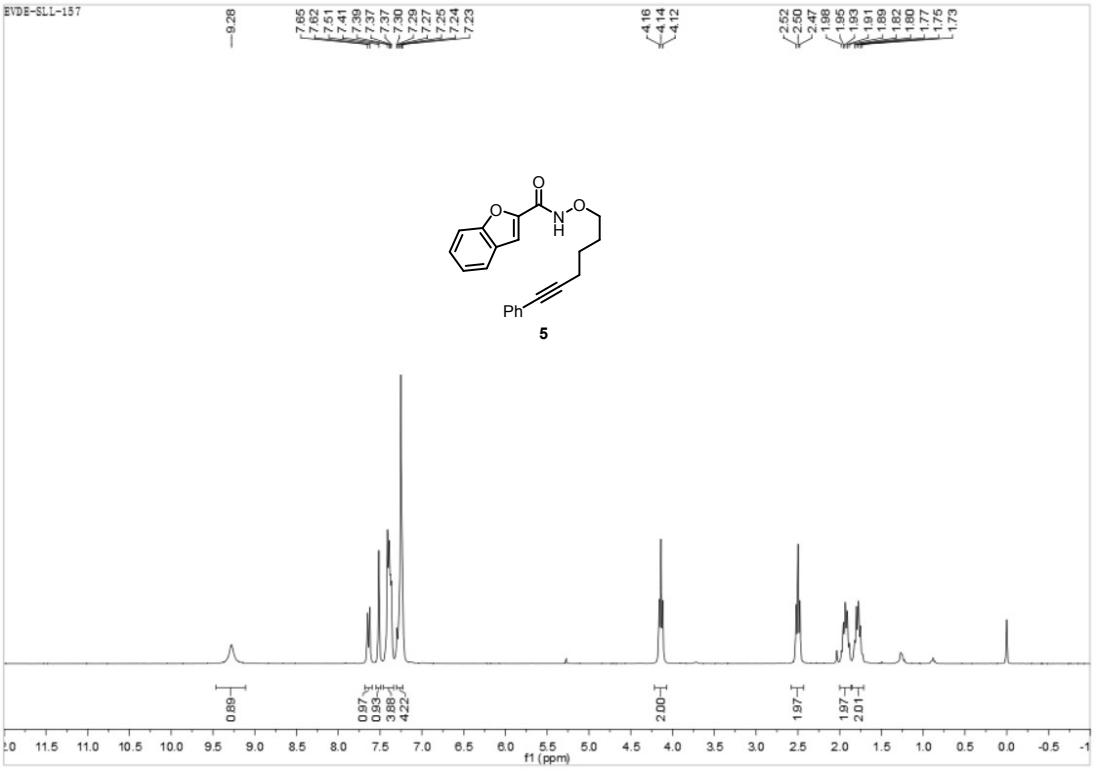

EVDE-CSLL-101-11
165.41
138.09
130.21
128.70
128.58
80.74
79.31
78.23
31.08
26.93
25.28
21.83
18.34
18.30
13.51
O
N
H
O
Cl
1x
f1 (ppm)


EVDE-SLL-171
9.36
7.74
7.71
7.50
7.47
7.45
7.40
7.37
7.35
4.02
4.00
3.98
2.27
2.25
2.22
1.79
1.77
1.75
1.73
1.65
1.63
1.61
1.58
1.56
0.11
Ph
O
N
H
O
TMS
1y
0.93
2.05
1.00
2.06
2.00
2.04
2.04
2.09
9.06
f1 (ppm)

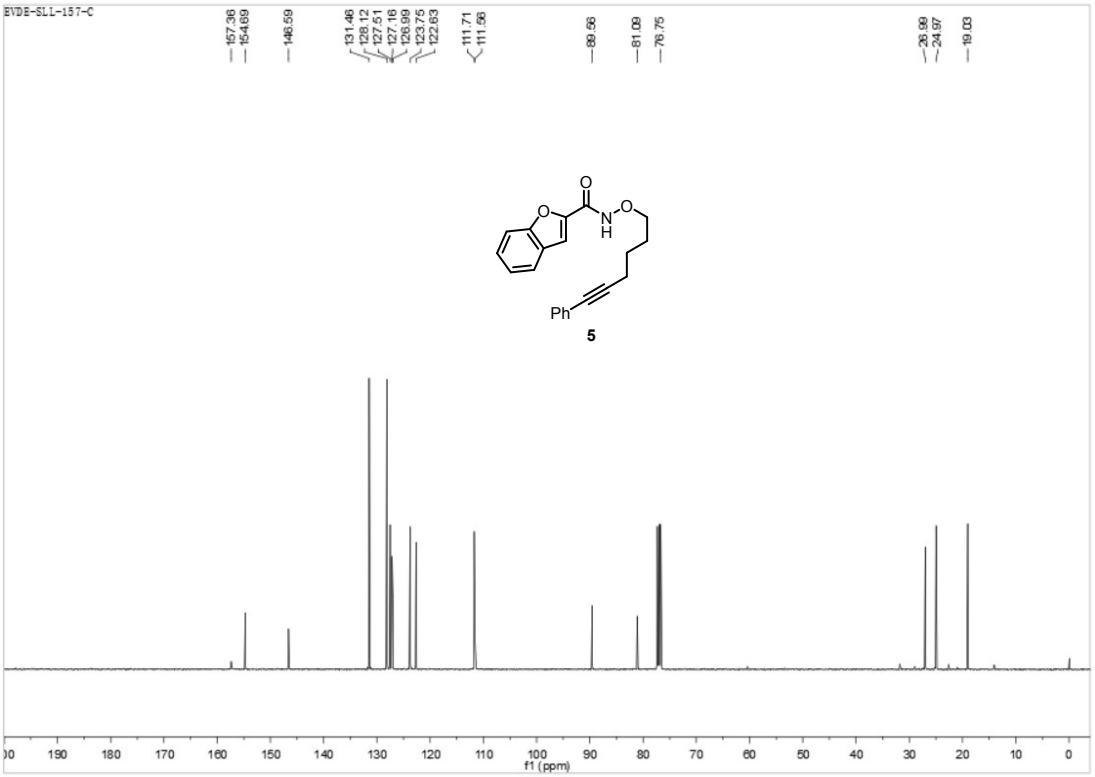

EVDE-SLL-171
166.54
132.00
131.65
128.53
127.08
106.88
84.86
76.17
26.99
24.91
19.48
0.07
Ph
O
N
H
O
TMS
1y
f1 (ppm)


EVDE-SLL-125
9.19
7.76
7.73
7.52
7.50
7.48
7.43
7.40
7.38
4.06
4.04
4.02
2.27
2.26
2.25
2.24
2.23
1.96
1.95
1.84
1.82
1.80
1.78
1.70
1.68
1.65
1.63
1.61
Ph
O
N
H
O
1z
0.86
2.02
1.07
2.11
2.00
2.00
0.92
2.02
2.03
f1 (ppm)

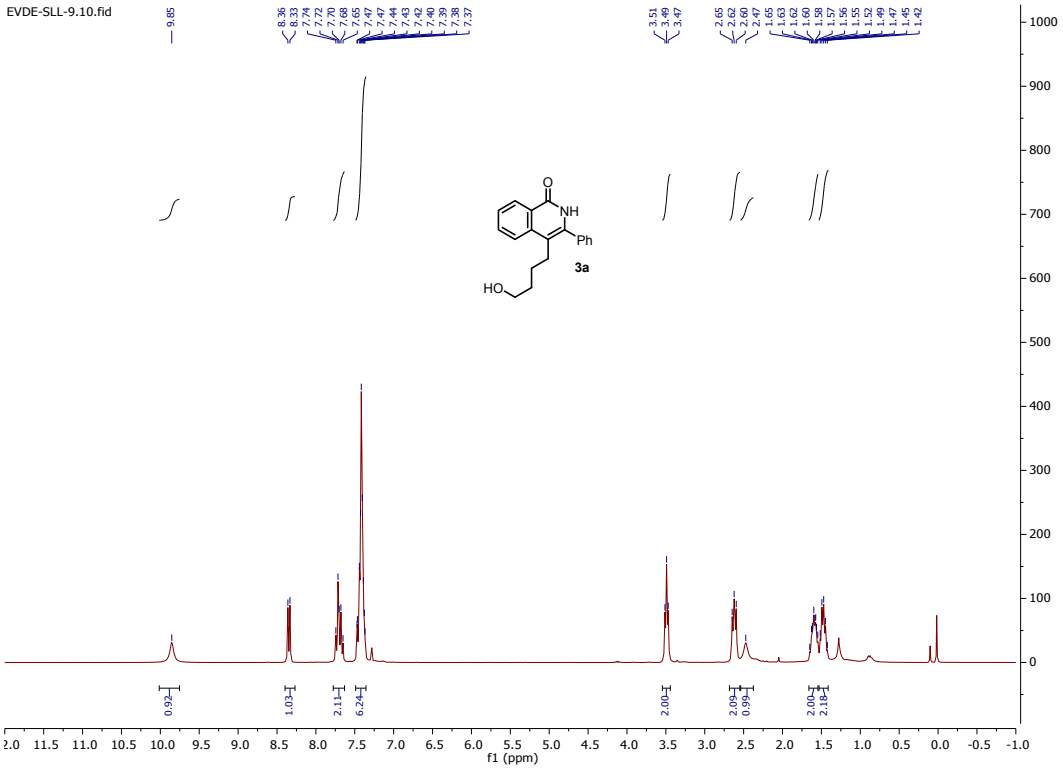

EVDE-SLL-125C-13C-TXI5-600
Calibration TXI
166.45
131.94
131.84
128.56
127.05
84.07
76.12
68.68
26.82
24.67
18.03
Ph
O
N
H
O
1z
f1 (ppm)

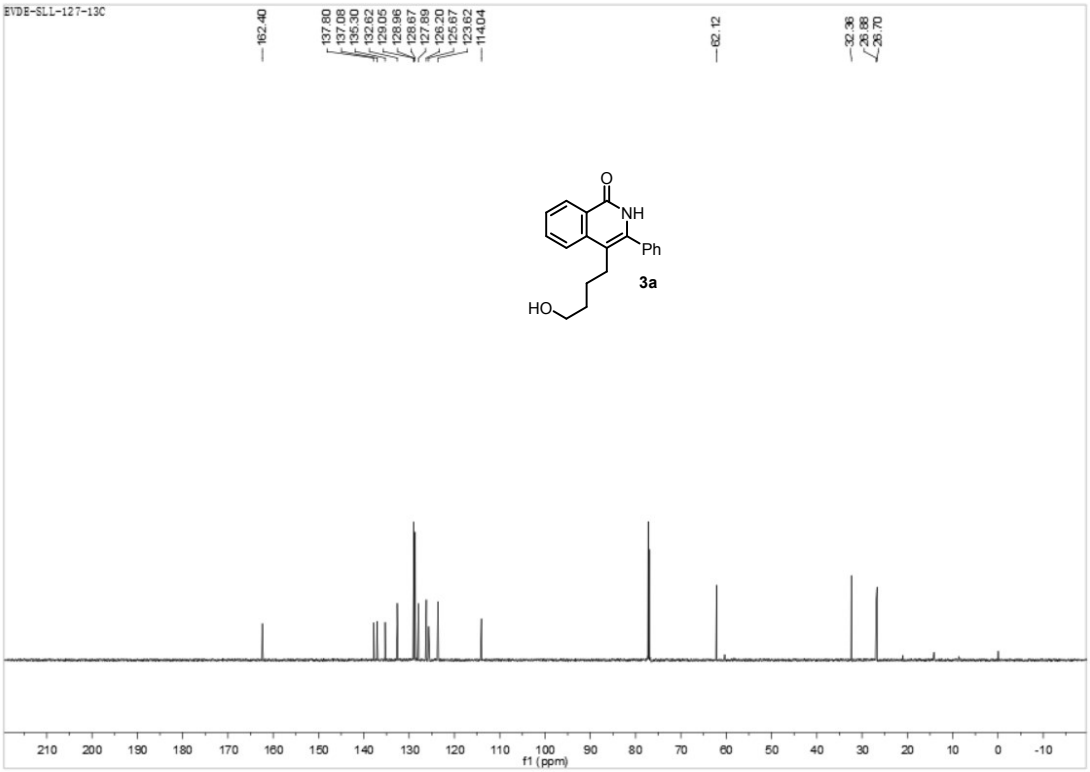

EVDE-SLL-157
9.28
7.65
7.62
7.51
7.41
7.39
7.37
7.37
7.30
7.29
7.27
7.25
7.24
7.23
4.16
4.14
4.12
2.52
2.50
2.47
1.98
1.95
1.93
1.91
1.89
1.82
1.80
1.77
1.75
1.73
O
O
N
H
O
Ph
0.89
0.97
0.93
3.88
4.22
2.00
1.97
1.97
2.01
f1 (ppm)

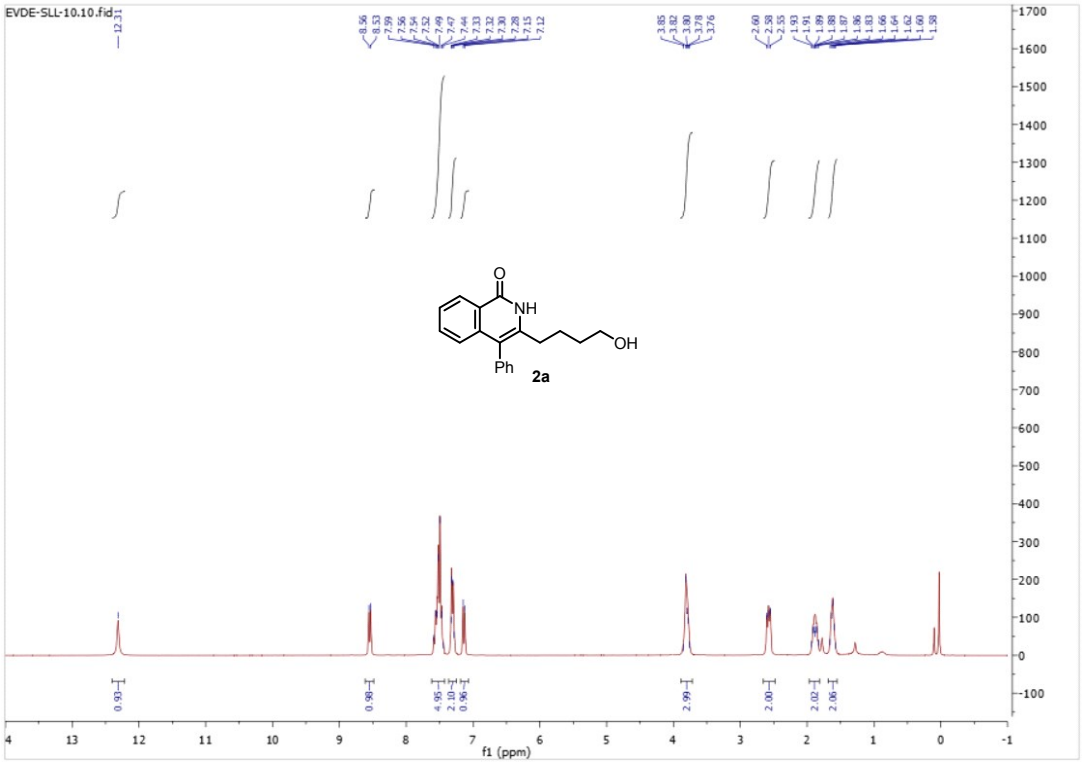
5

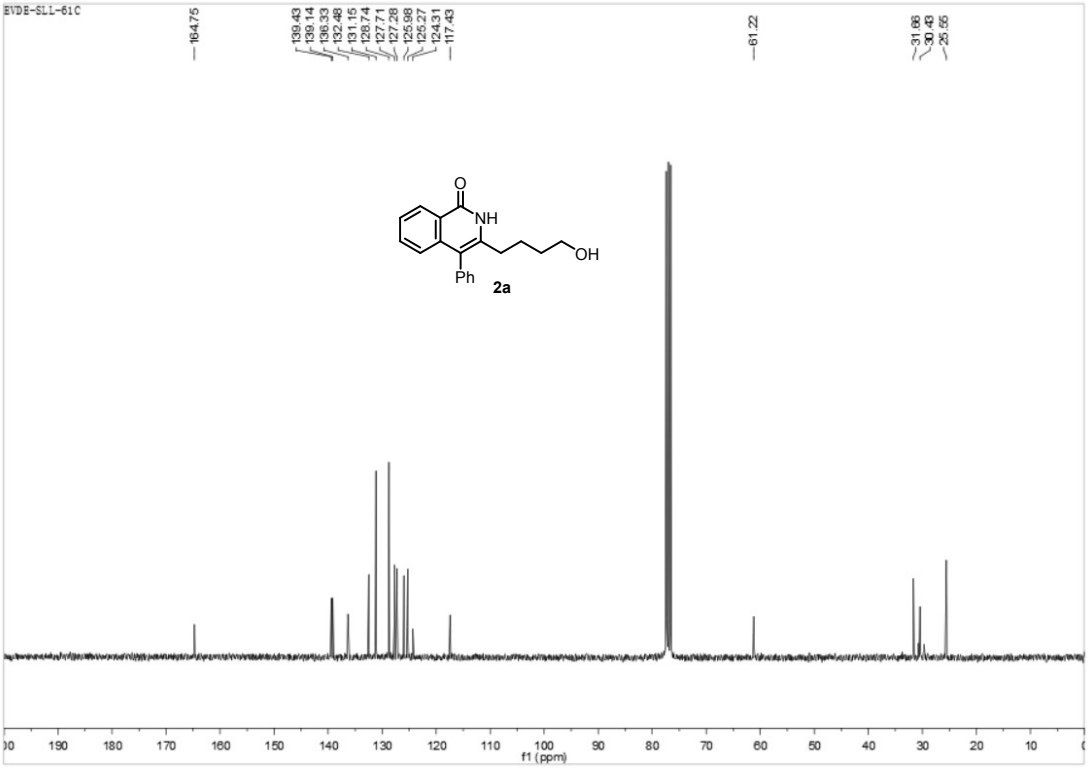

EVDE-SLL-157-C
157.36
154.69
146.59
131.46
128.12
127.51
127.16
126.99
123.75
122.63
111.71
111.66
89.56
81.09
76.75
26.99
24.97
19.03
O
O
N
H
O
Ph
f1 (ppm)

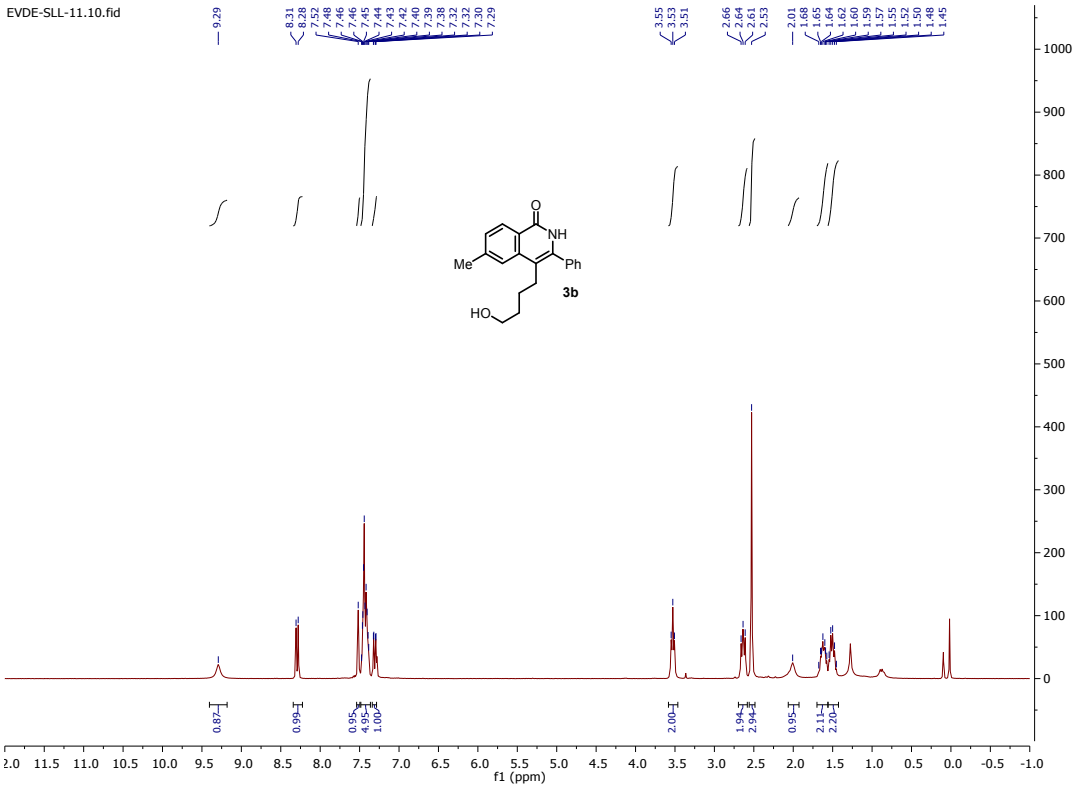
5

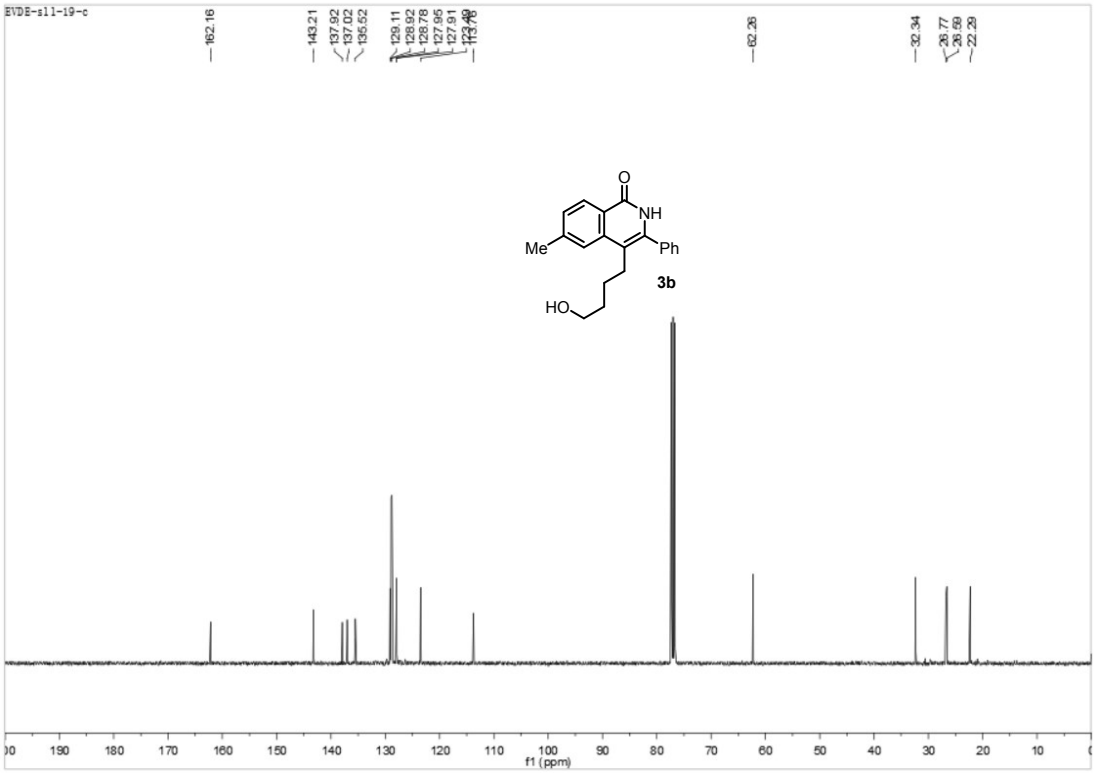

EVDE-SLL-9.10.fid
9.85
8.36
8.33
7.74
7.72
7.70
7.68
7.65
7.47
7.44
7.43
7.42
7.40
7.39
7.38
7.37
3.51
3.49
3.47
2.65
2.62
2.60
2.47
1.65
1.63
1.62
1.60
1.58
1.57
1.56
1.55
1.52
1.49
1.47
1.45
1.42
O
NH
Ph
HO
3a
0.92
1.03
2.11
6.24
2.00
2.09
0.99
2.00
2.18
f1 (ppm)

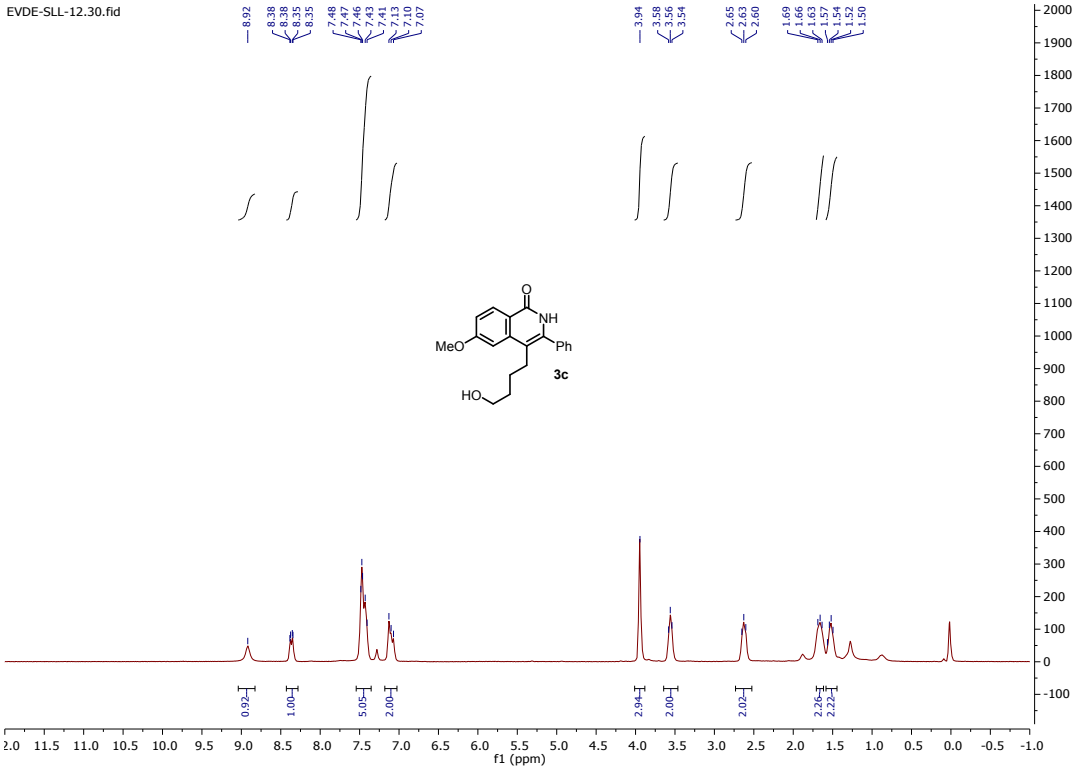

EVDE-SLL-127-13C
162.40
137.80
137.08
135.30
132.62
129.05
128.96
128.67
127.89
126.20
125.67
123.62
114.04
62.12
32.36
28.88
28.70
O
NH
Ph
HO
3a
f1 (ppm)

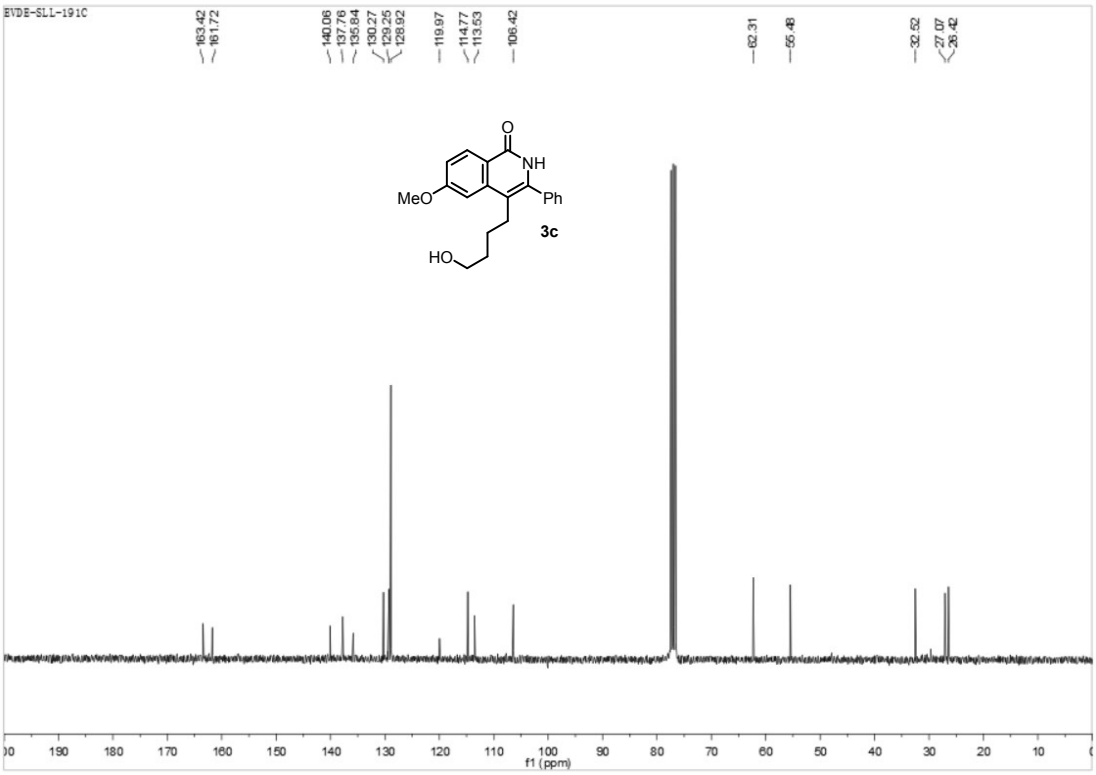

EVDE-SLL-10.10.fid
O
NH
OH
Ph
2a
f1 (ppm)

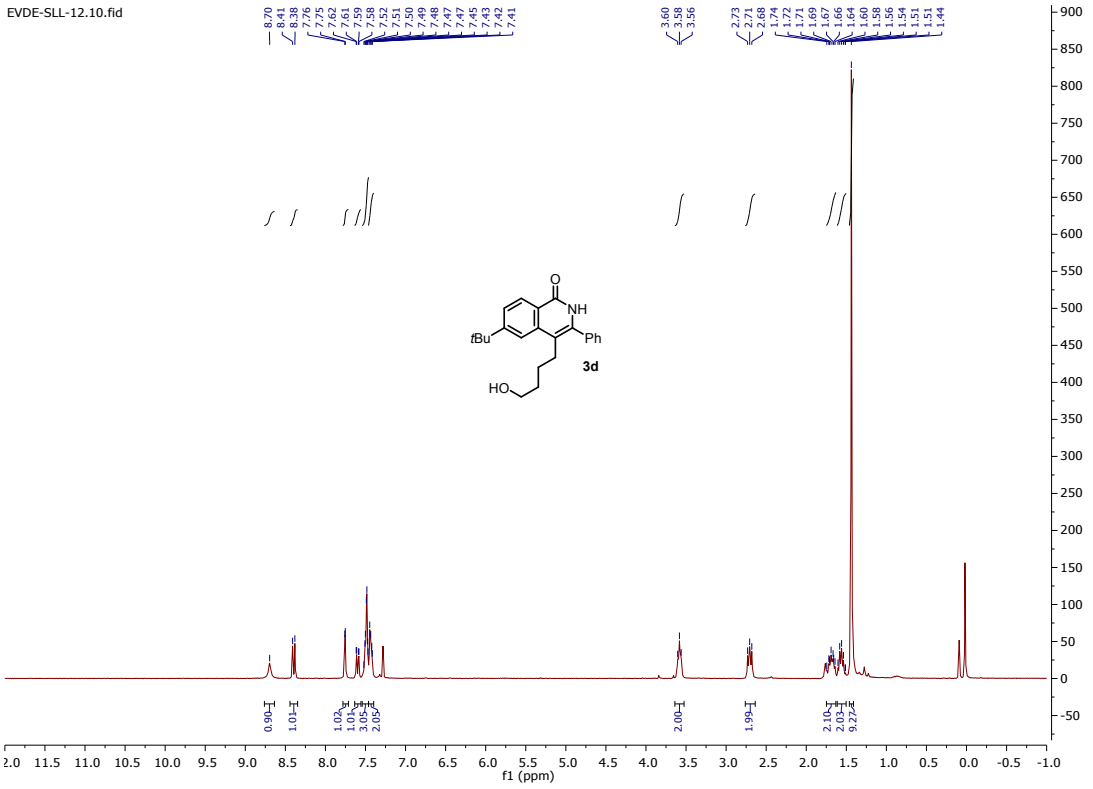

EVDE-SLL-61C
O
NH
OH
Ph
2a
f1 (ppm)

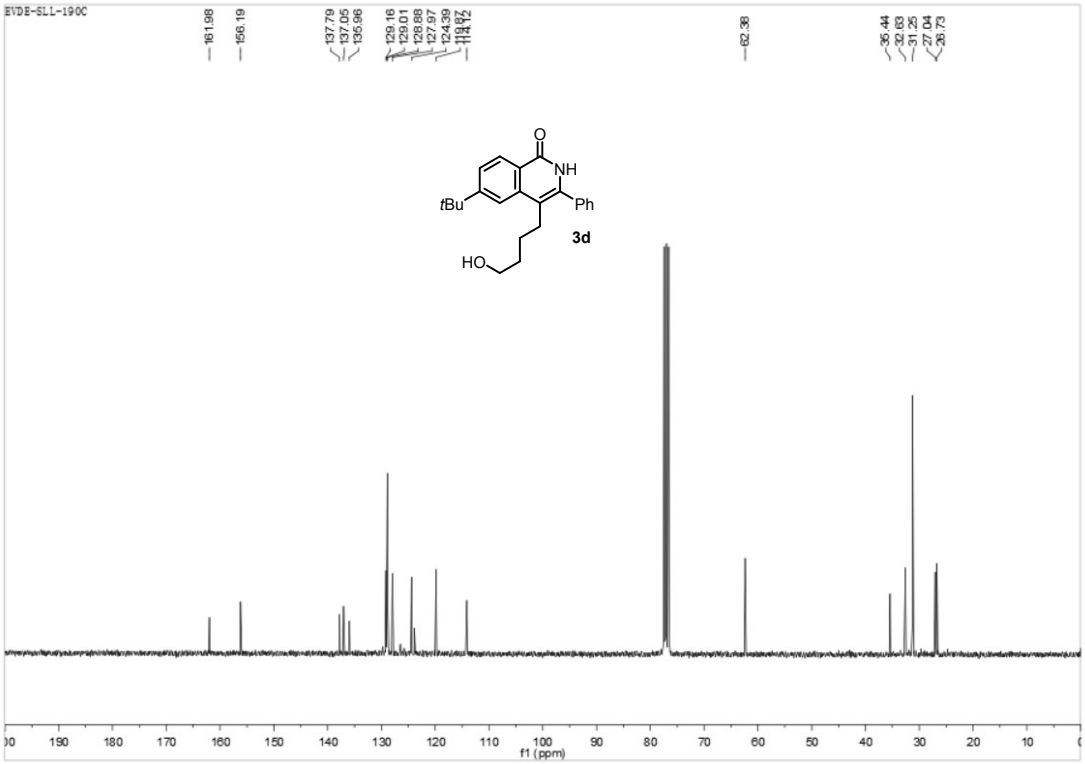

EVDE-SLL-11.10.fid
f1 (ppm)
3b

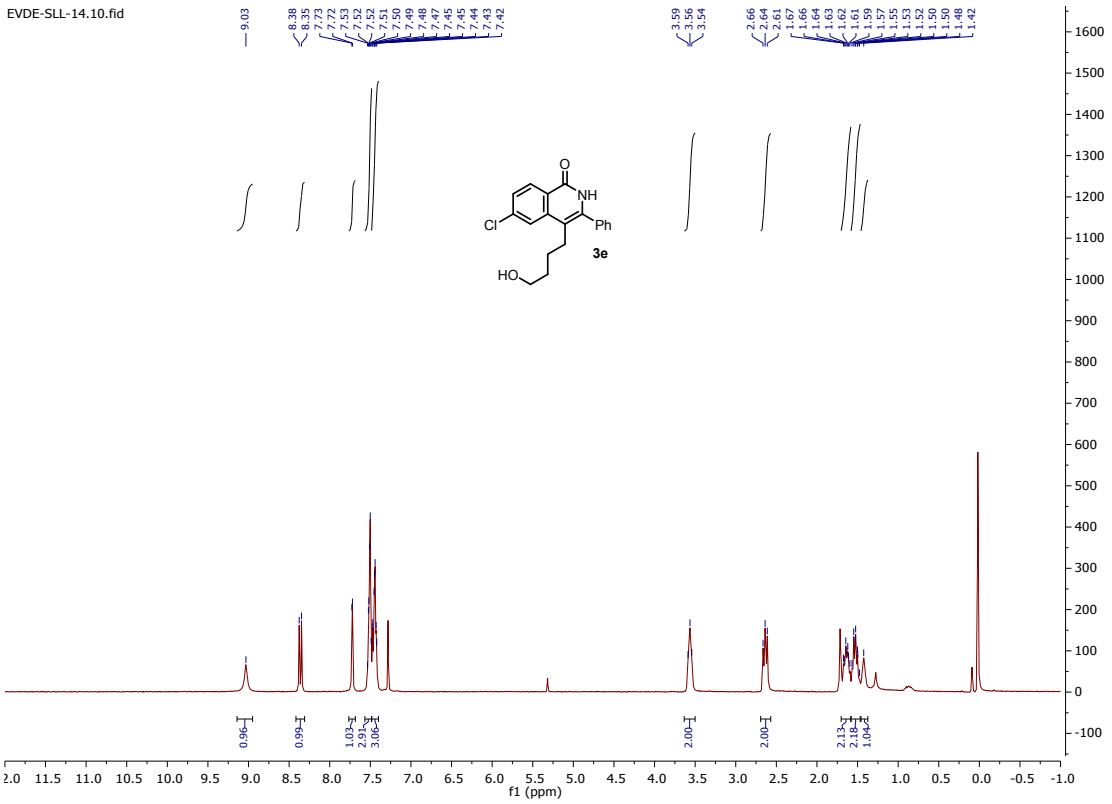

EVDE-sll-19-c
f1 (ppm)
3b

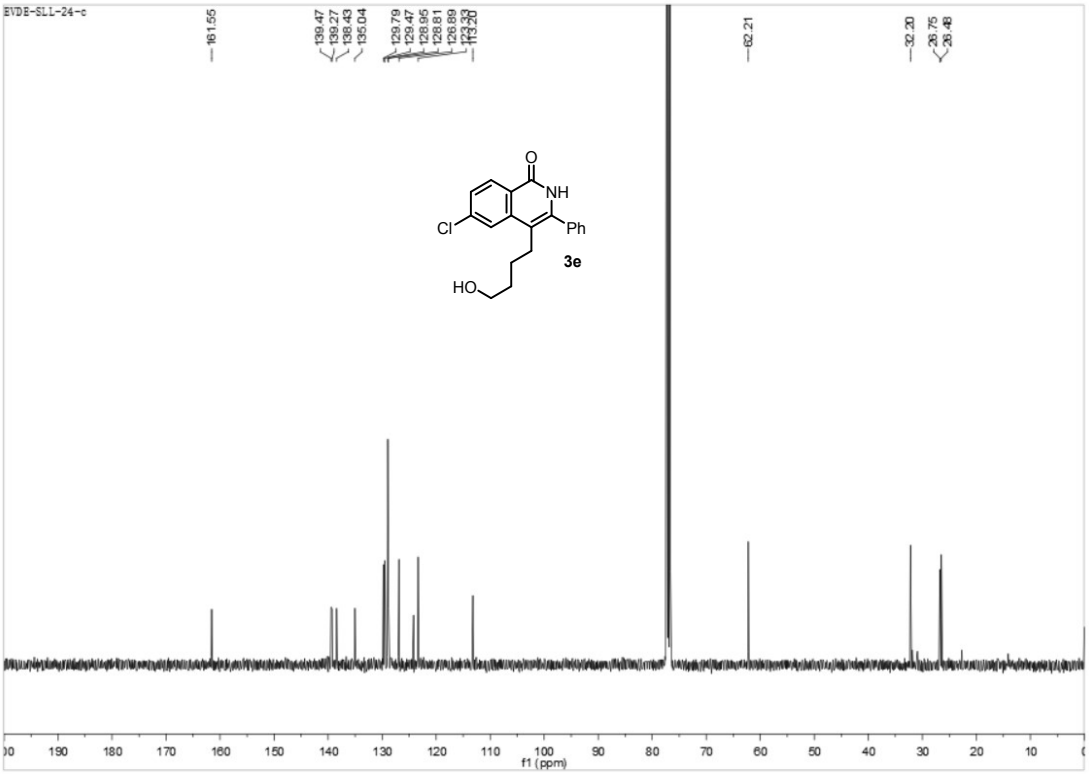

EVDE-SLL-12.30.fid
8.92
8.38
8.38
8.35
8.35
7.48
7.47
7.46
7.43
7.41
7.13
7.10
7.07
3.94
3.58
3.56
3.54
2.65
2.63
2.60
1.69
1.66
1.65
1.57
1.54
1.52
1.50
O
NH
MeO
Ph
HO
3c
0.92
1.00
5.05
2.00
2.94
2.00
2.02
2.26
2.22
f1 (ppm)

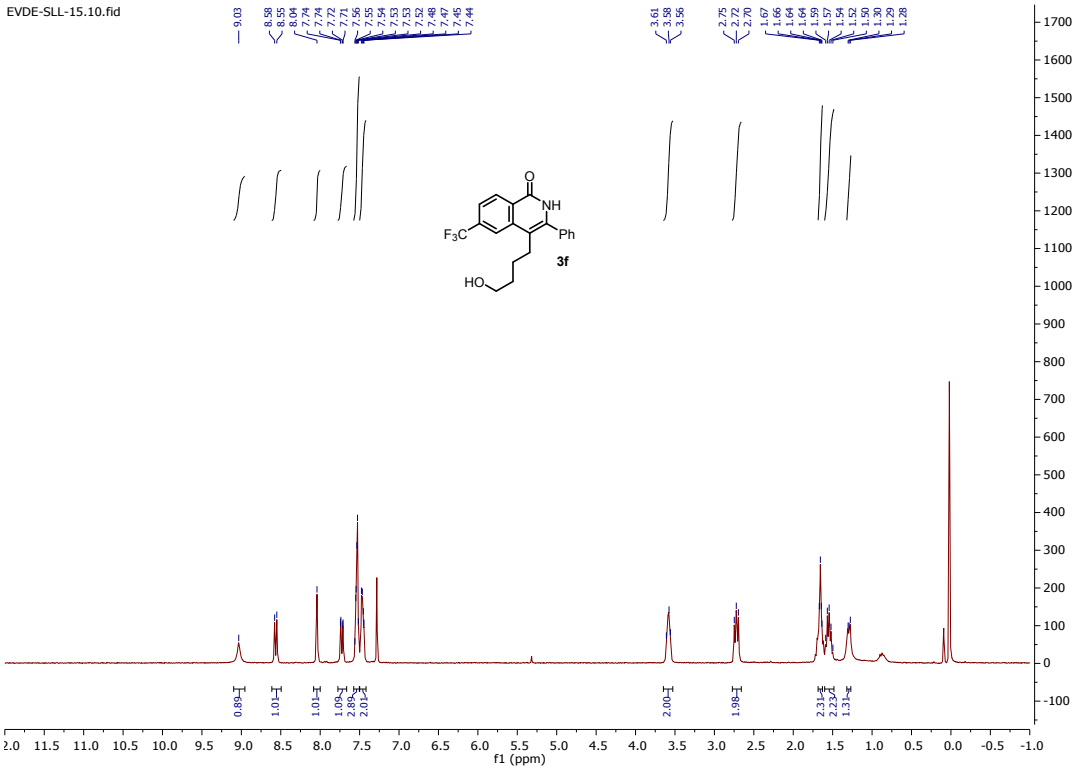

EVDE-SLL-191C
163.42
161.72
140.06
137.76
135.84
130.27
129.25
128.92
119.97
114.77
113.53
106.42
62.31
55.48
32.52
27.07
26.42
O
NH
MeO
Ph
HO
3c
f1 (ppm)

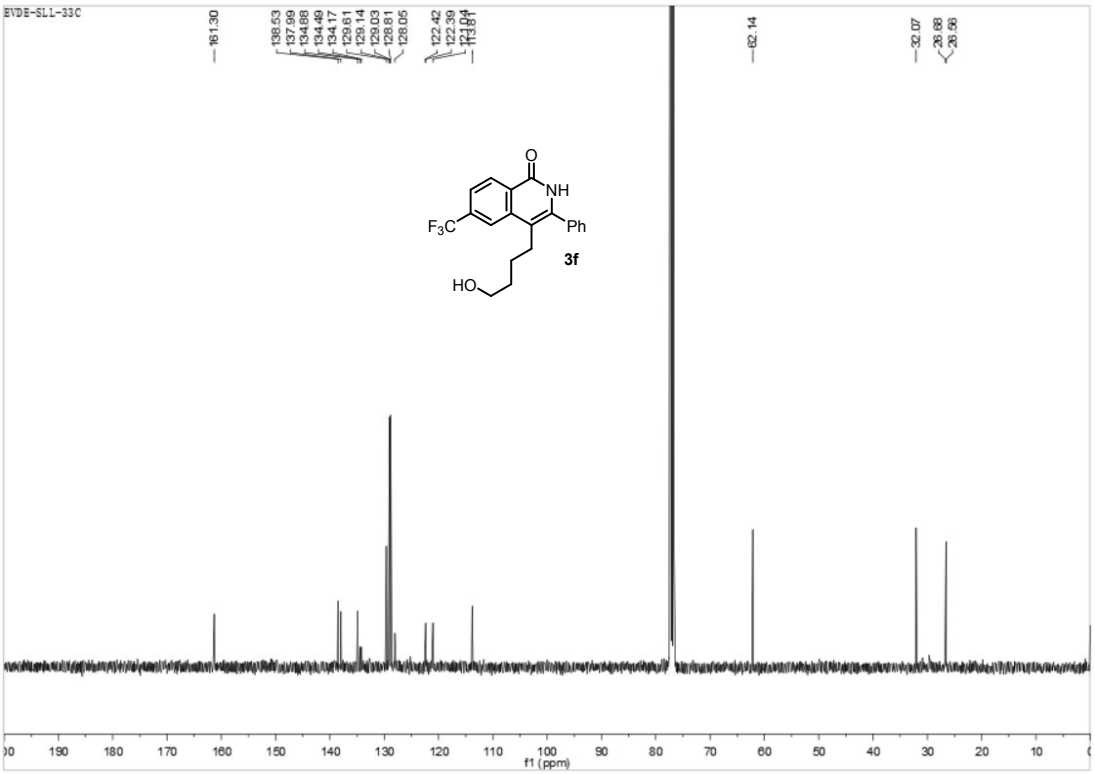

EVDE-SLL-12.10.fid
f1 (ppm)
O
NH
tBu
Ph
HO
3d

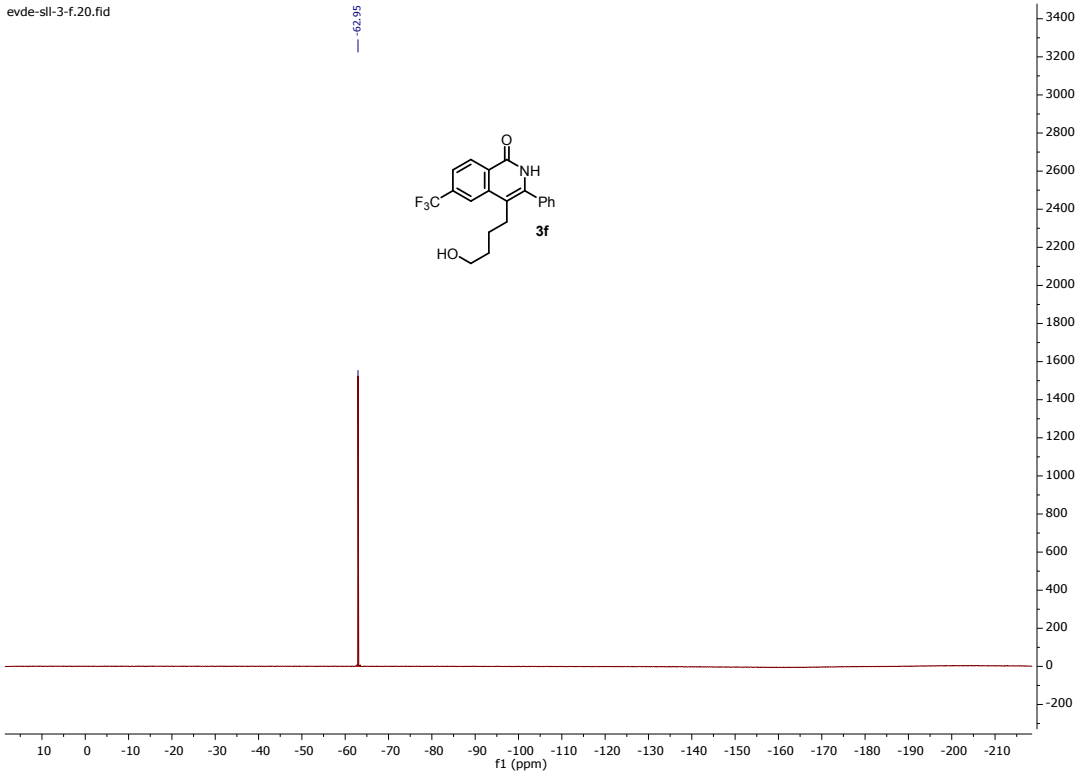

EVDE-SLL-190C
f1 (ppm)
O
NH
tBu
Ph
HO
3d

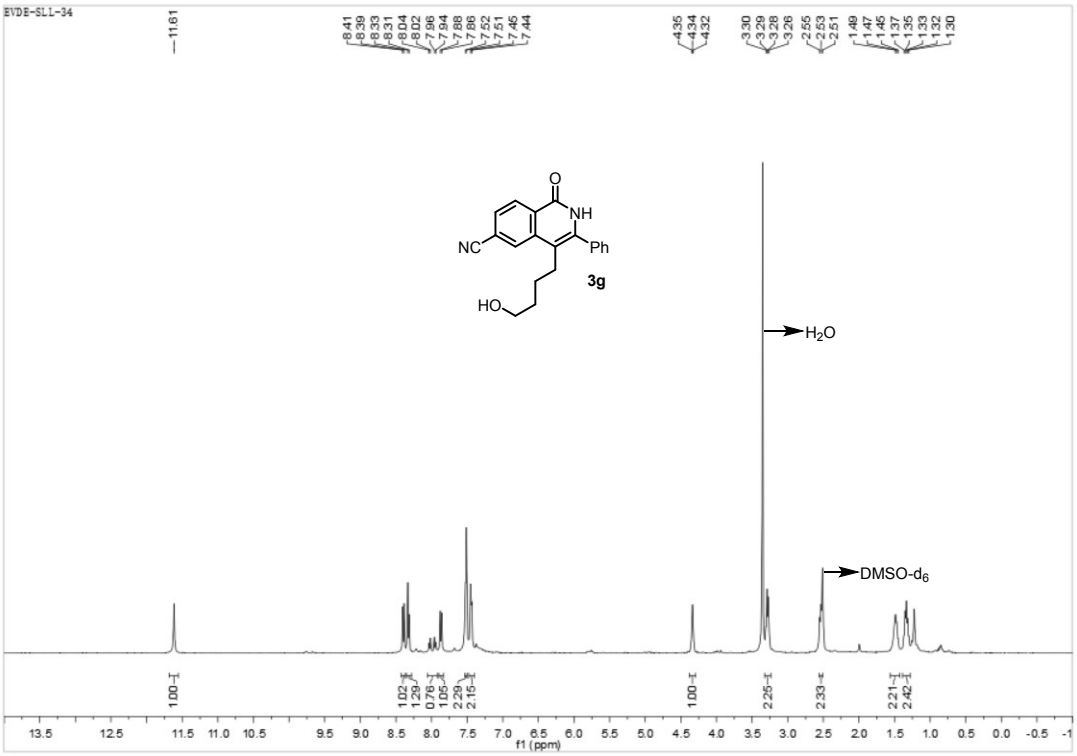

EVDE-SLL-14.10.fid
9.03
8.38
8.35
7.73
7.72
7.53
7.52
7.52
7.51
7.50
7.49
7.48
7.47
7.45
7.45
7.44
7.43
7.42
3.59
3.56
3.54
2.66
2.64
2.61
1.67
1.66
1.64
1.63
1.62
1.61
1.59
1.57
1.55
1.53
1.52
1.50
1.50
1.48
1.42
O
NH
Cl
Ph
HO
3e
0.96
0.99
1.03
2.91
3.06
2.00
2.00
2.13
2.18
1.04
f1 (ppm)

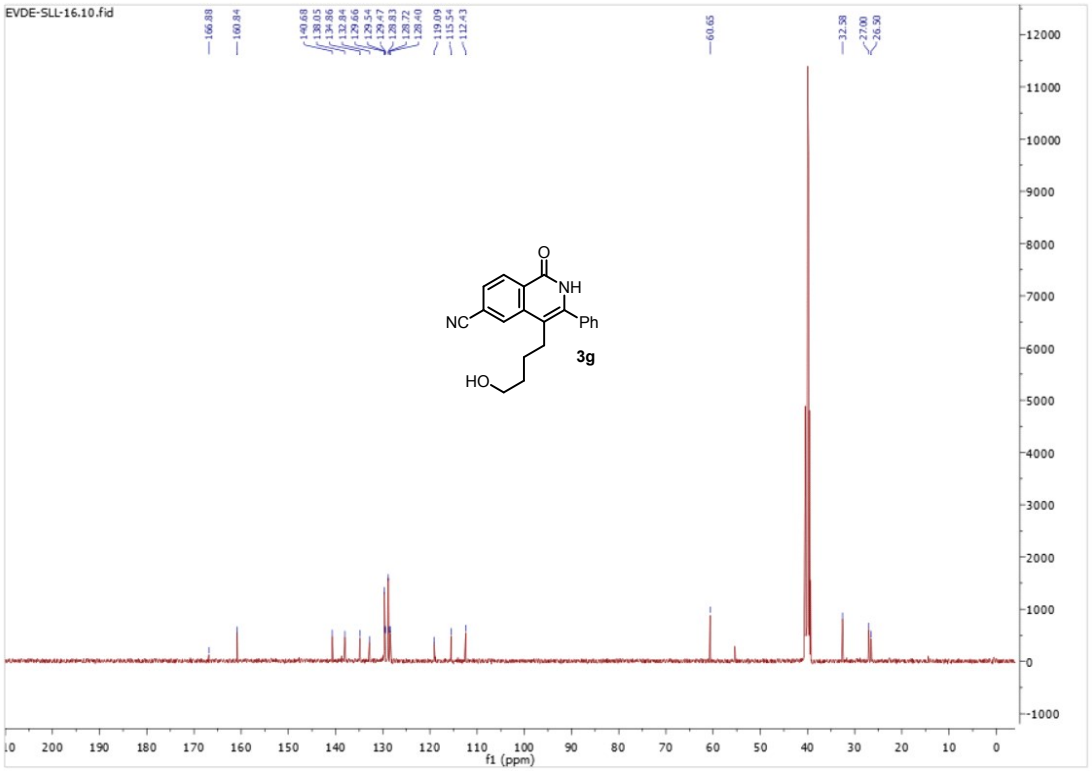

EVDE-SLL-24-c
161.55
139.47
139.27
138.43
135.04
129.79
129.47
128.95
128.81
126.89
123.33
123.20
62.21
32.20
28.75
28.48
O
NH
Cl
Ph
HO
3e
f1 (ppm)

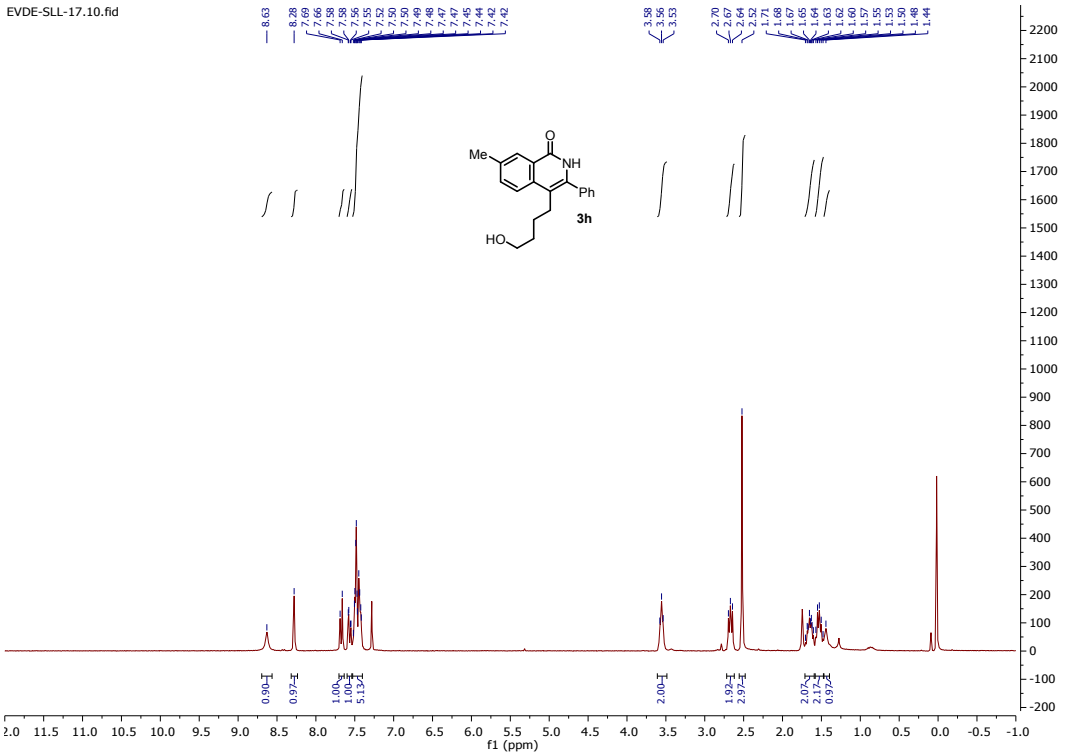

EVDE-SLL-15.10.fid
O
NH
F3C
Ph
HO
3f
f1 (ppm)

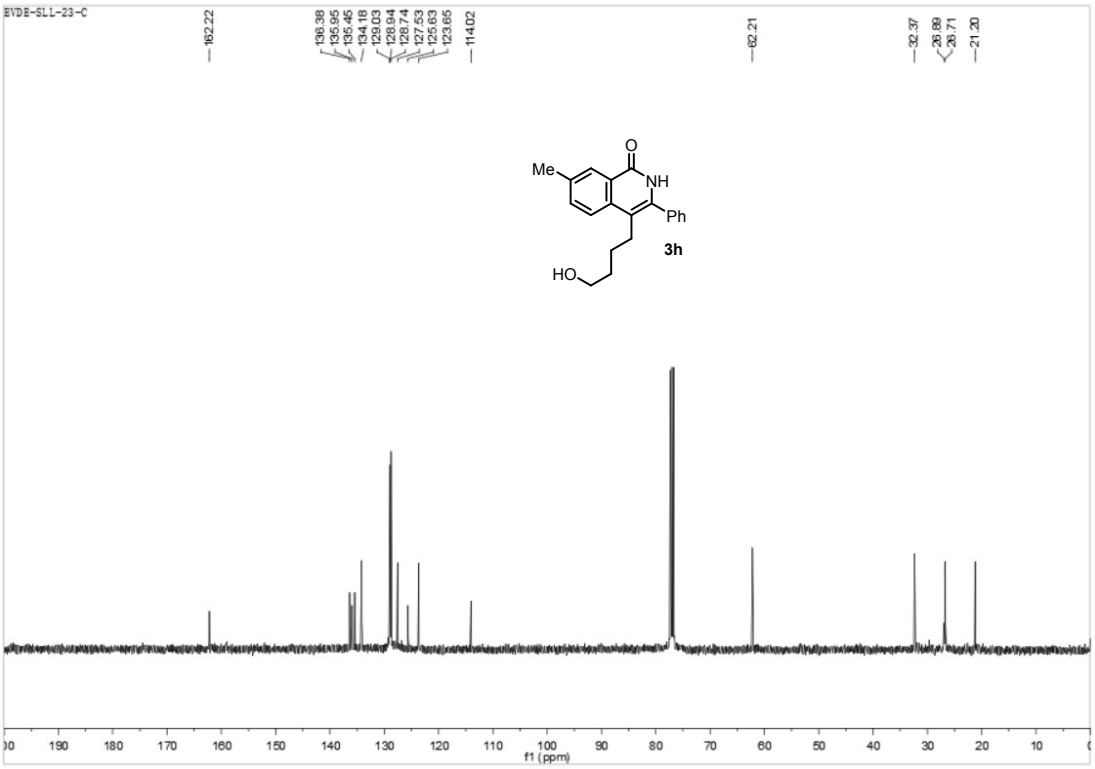

EVDE-SLL-33C
O
NH
F3C
Ph
HO
3f
f1 (ppm)

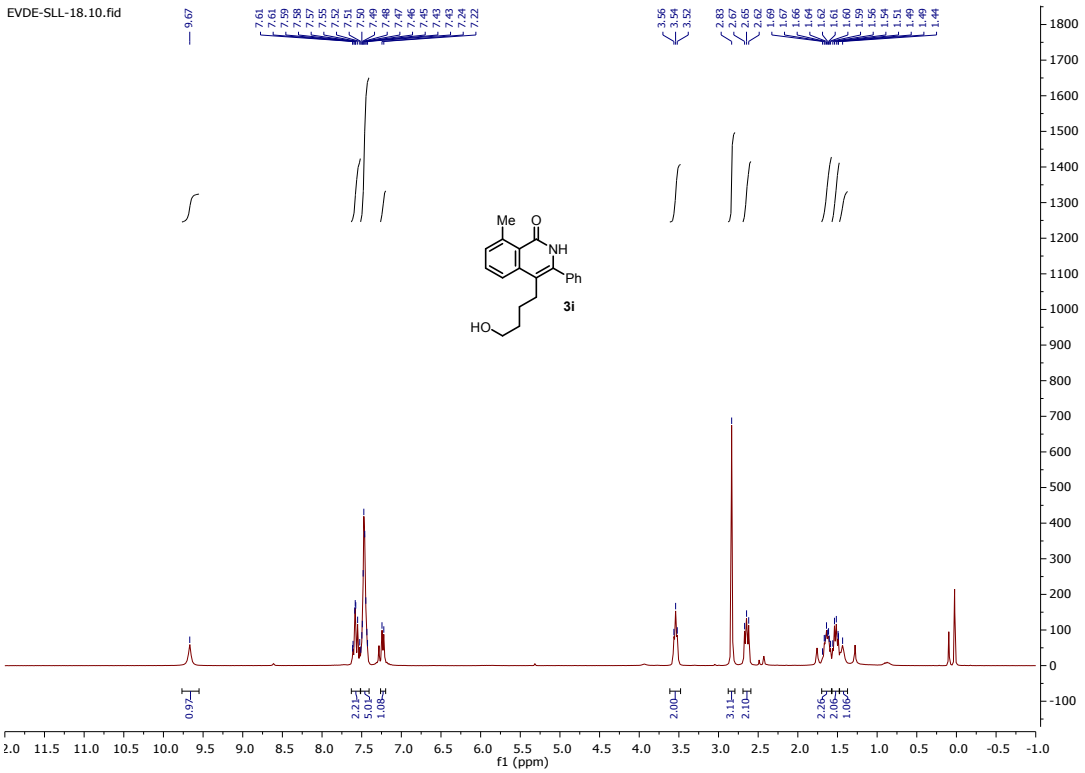

evde-sll-3-f.20.fid
-62.95
O
NH
F3C
Ph
HO
3f
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

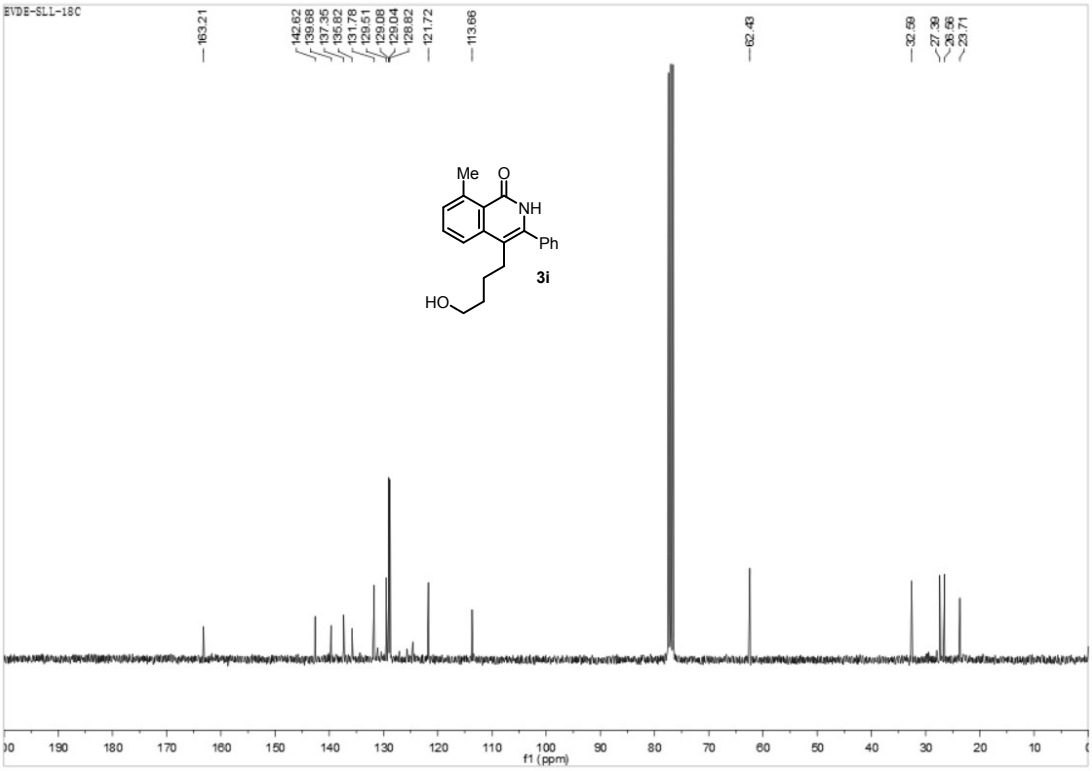

EVDE-SLL-34
11.61
8.41
8.39
8.33
8.31
8.04
8.02
7.96
7.94
7.88
7.86
7.52
7.51
7.45
7.44
4.35
4.34
4.32
3.30
3.29
3.28
3.26
2.55
2.53
2.51
1.49
1.47
1.45
1.37
1.35
1.33
1.32
1.30
O
NH
NC
Ph
HO
3g
H2O
DMSO-d6
1.00
1.02
1.29
0.76
1.05
2.29
2.15
1.00
2.25
2.33
2.21
2.42
f1 (ppm)

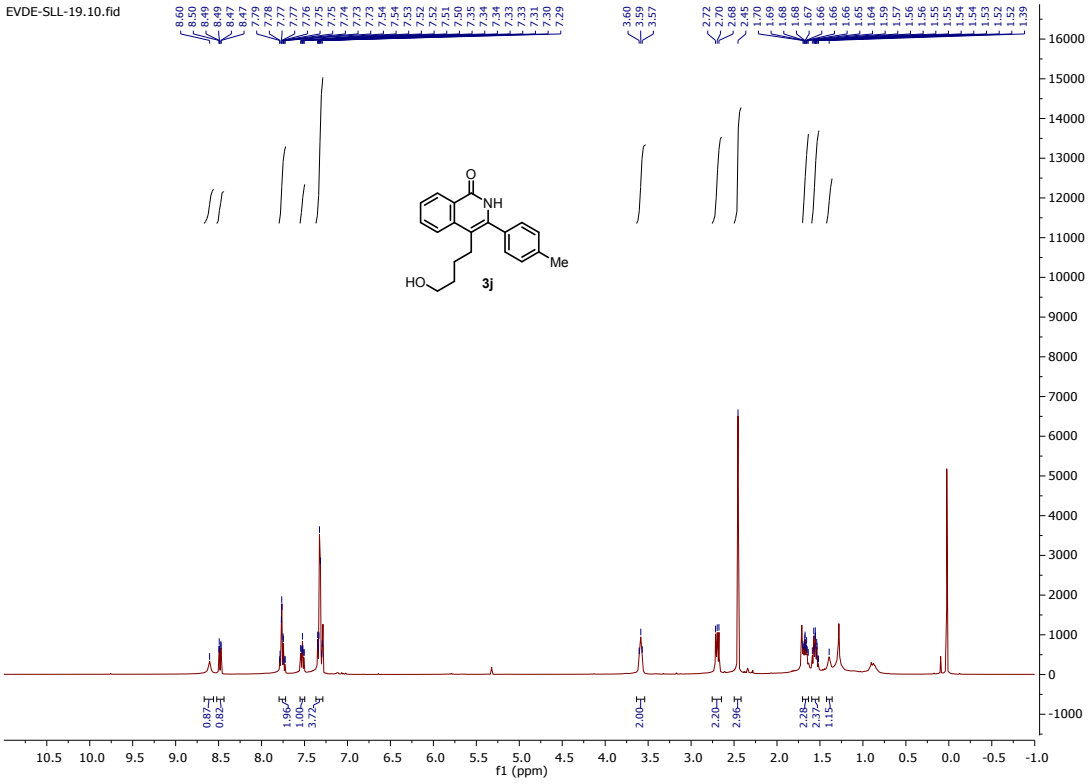

EVDE-SLL-16.10.fid
166.88
160.84
140.68
138.05
134.86
132.84
132.66
129.54
129.47
128.83
128.72
128.40
119.09
115.54
112.43
60.65
32.58
27.00
26.50
O
NH
NC
Ph
HO
3g
f1 (ppm)

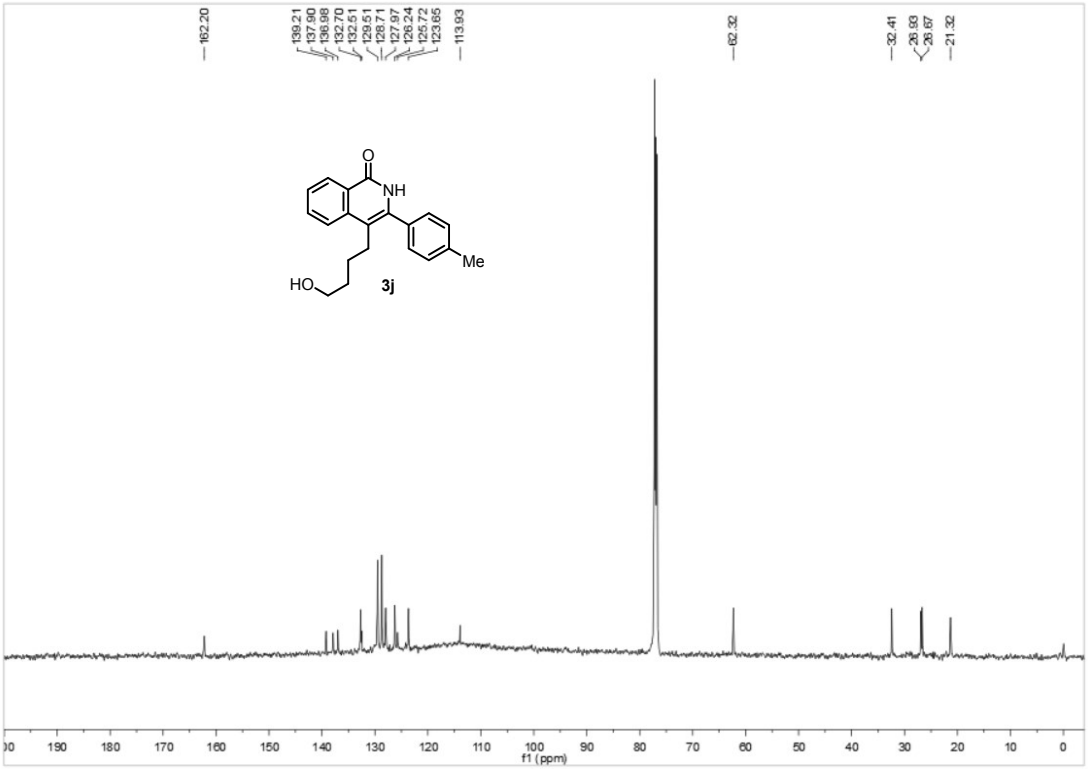

EVDE-SLL-17.10.fid
Me
NH
Ph
HO
3h
f1 (ppm)

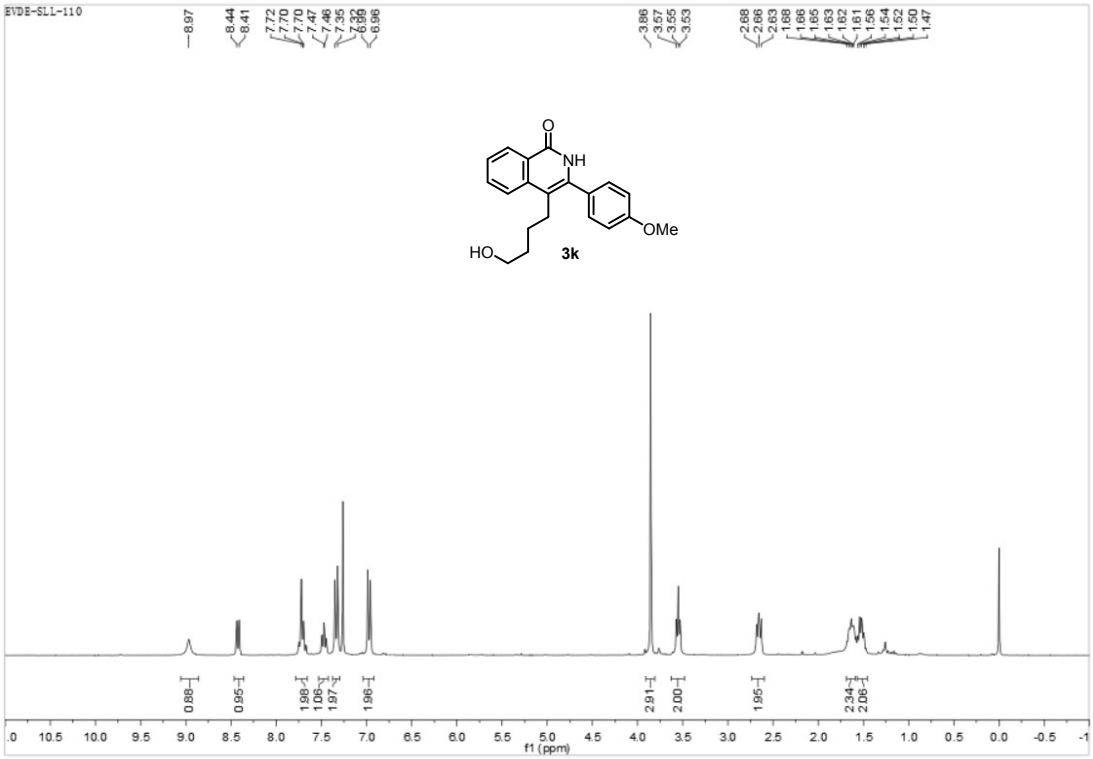

EVDE-SLL-23-C
Me
NH
Ph
HO
3h
f1 (ppm)

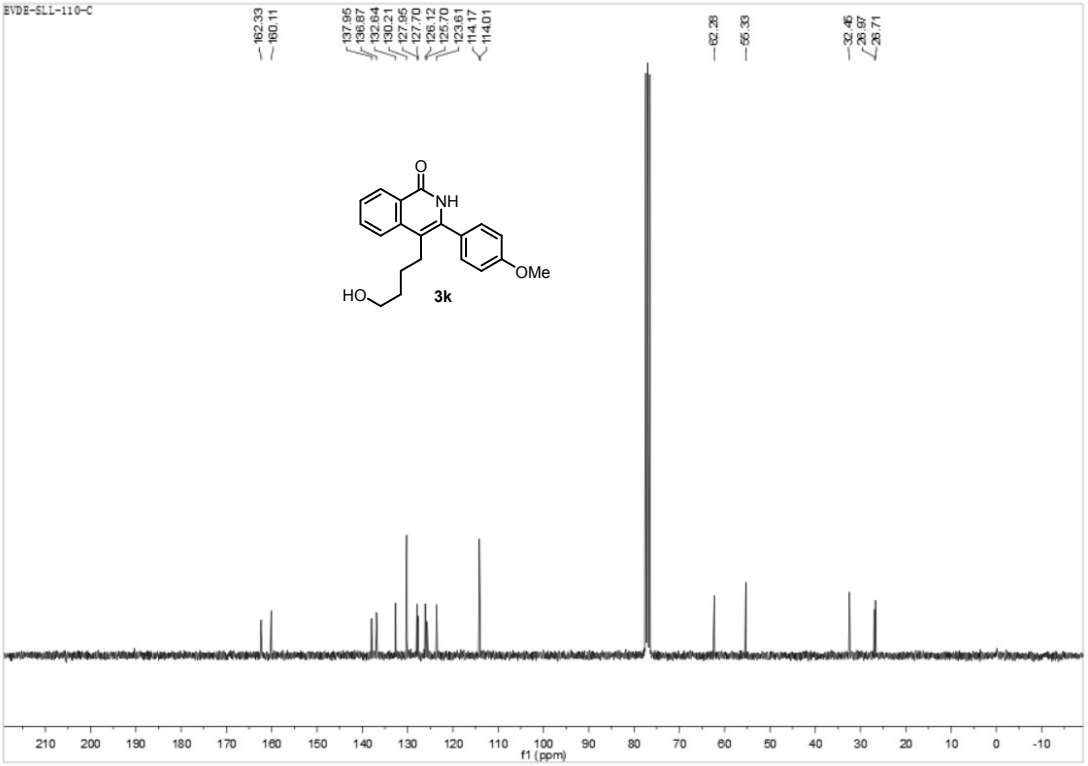

EVDE-SLL-18.10.fid
Me
O
NH
Ph
HO
3i
f1 (ppm)

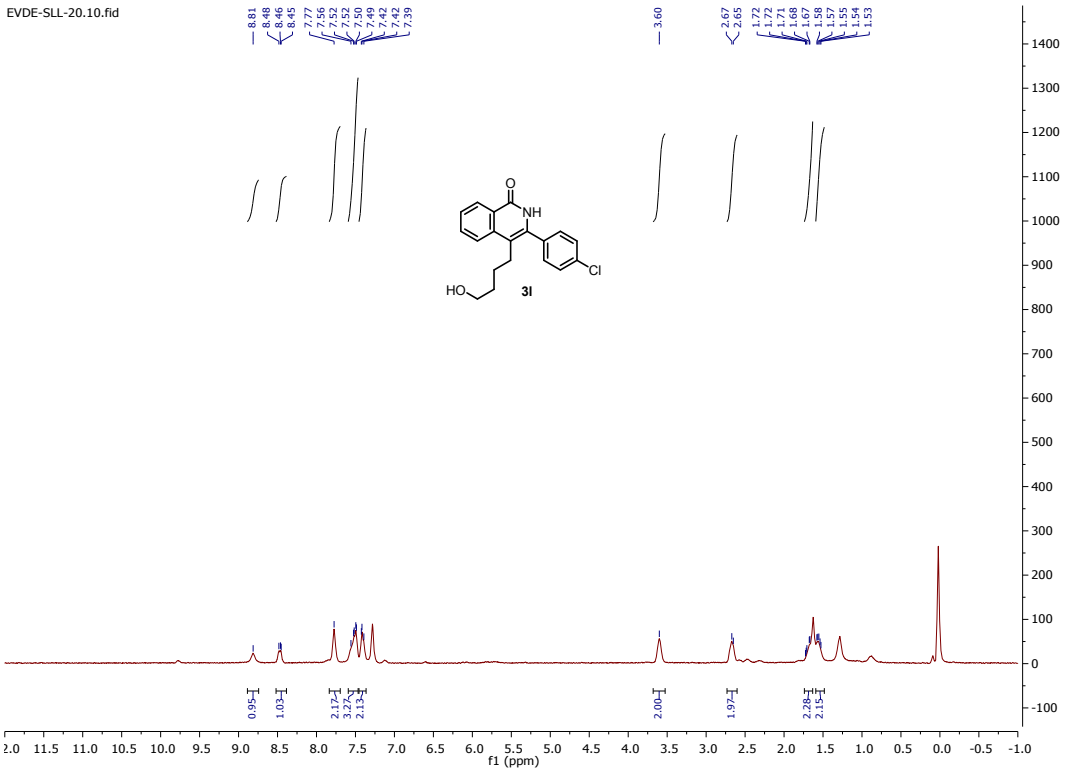

EVDE-SLL-18C
Me
O
NH
Ph
HO
3i
f1 (ppm)

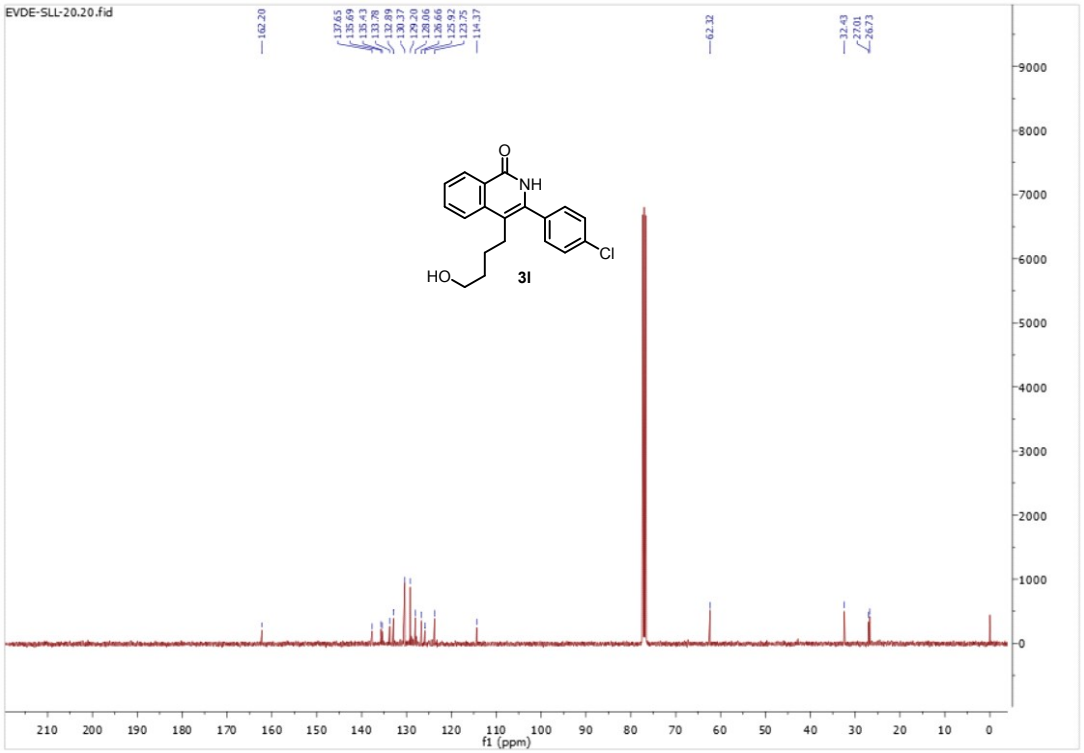

EVDE-SLL-19.10.fid
O
NH
Me
HO
3j
f1 (ppm)

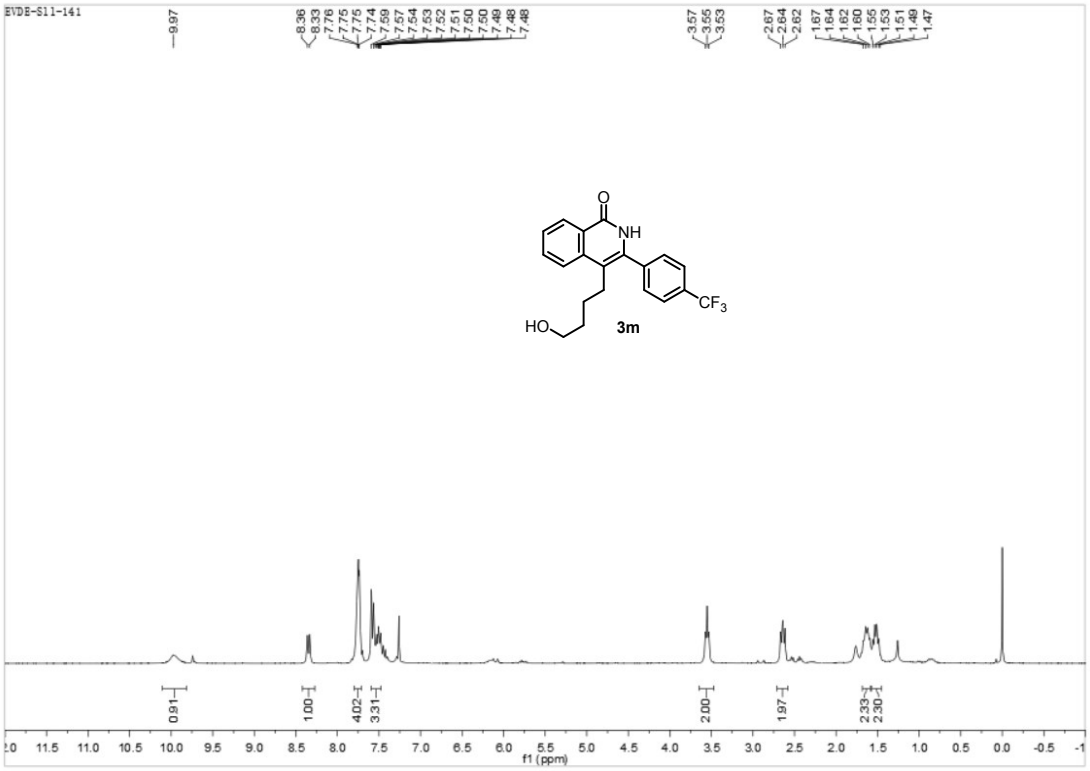

162.20
139.21
137.90
136.98
132.70
132.51
129.51
128.71
127.97
126.24
125.72
123.65
113.93
62.32
32.41
28.93
28.67
21.32
O
NH
Me
HO
3j
f1 (ppm)

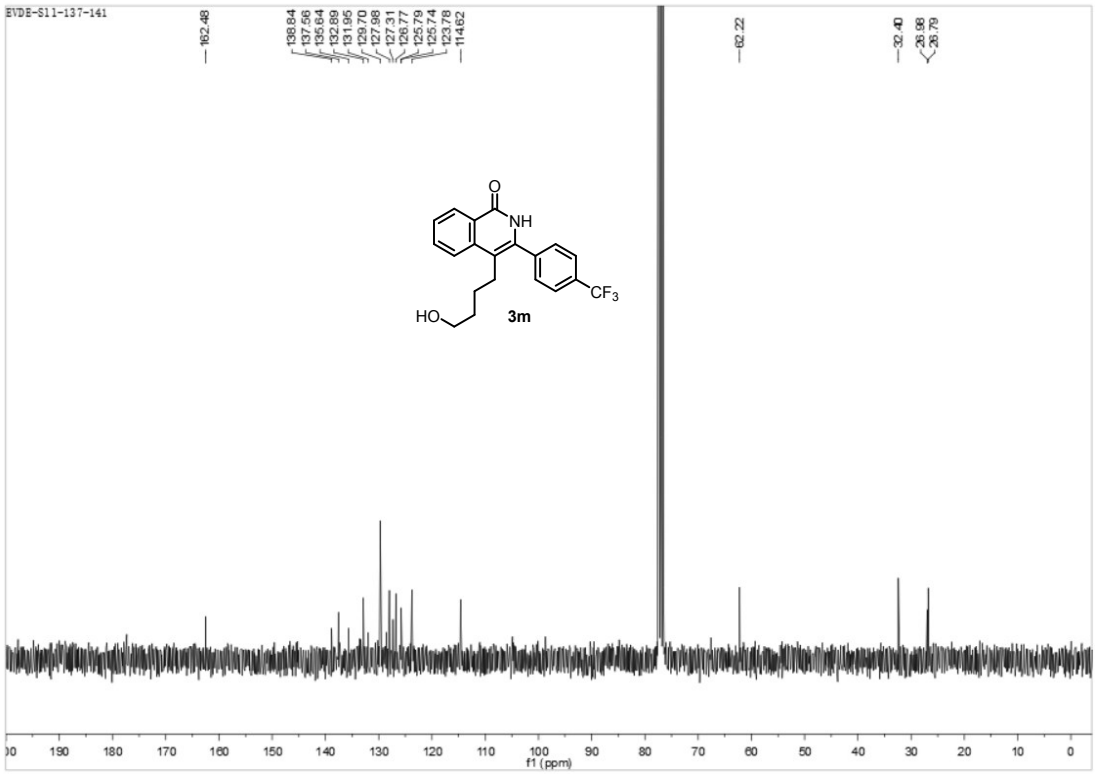

EVDE-SLL-110
8.97
8.44
8.41
7.72
7.70
7.70
7.47
7.46
7.35
7.32
6.99
6.96
3.86
3.57
3.55
3.53
2.68
2.66
2.63
1.88
1.86
1.85
1.83
1.62
1.61
1.56
1.54
1.52
1.50
1.47
O
NH
OMe
HO
3k
0.88
0.95
1.98
1.06
1.97
1.96
2.91
2.00
1.95
2.34
2.06
f1 (ppm)

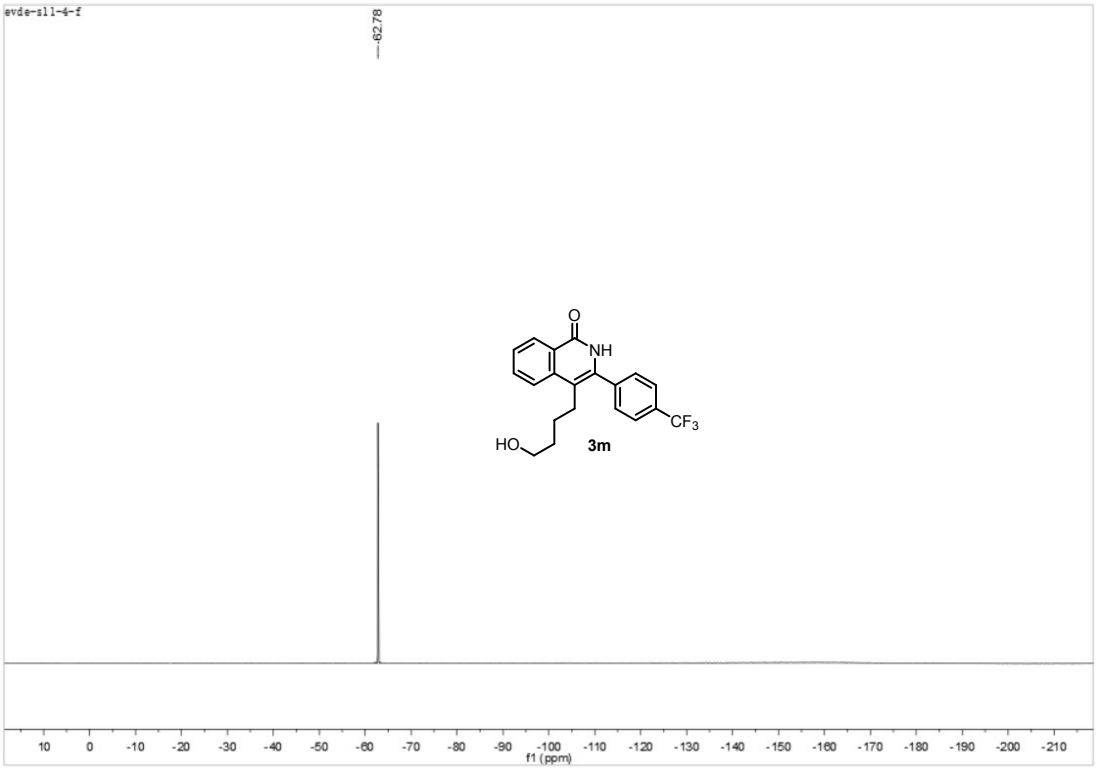

EVDE-SLL-110-C
162.33
160.11
137.95
136.87
132.64
130.21
127.95
127.70
126.12
125.70
123.81
114.17
114.01
62.28
55.33
32.45
28.97
28.71
O
NH
OMe
HO
3k
f1 (ppm)

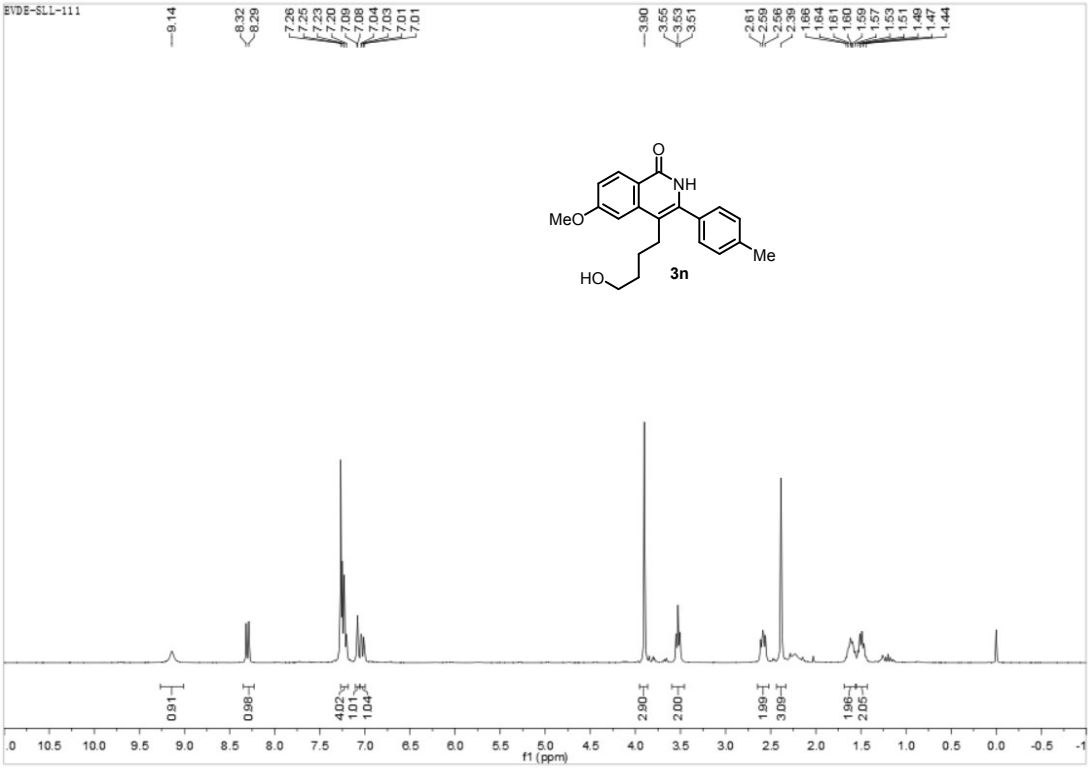

EVDE-SLL-20.10.fid
8.81
8.48
8.46
8.45
7.77
7.55
7.52
7.52
7.50
7.49
7.42
7.42
7.39
3.60
2.67
2.65
1.72
1.72
1.71
1.68
1.67
1.58
1.57
1.55
1.54
1.53
O
NH
Cl
HO
3l
0.95
1.03
2.17
3.22
2.13
2.00
1.97
2.28
2.15
f1 (ppm)

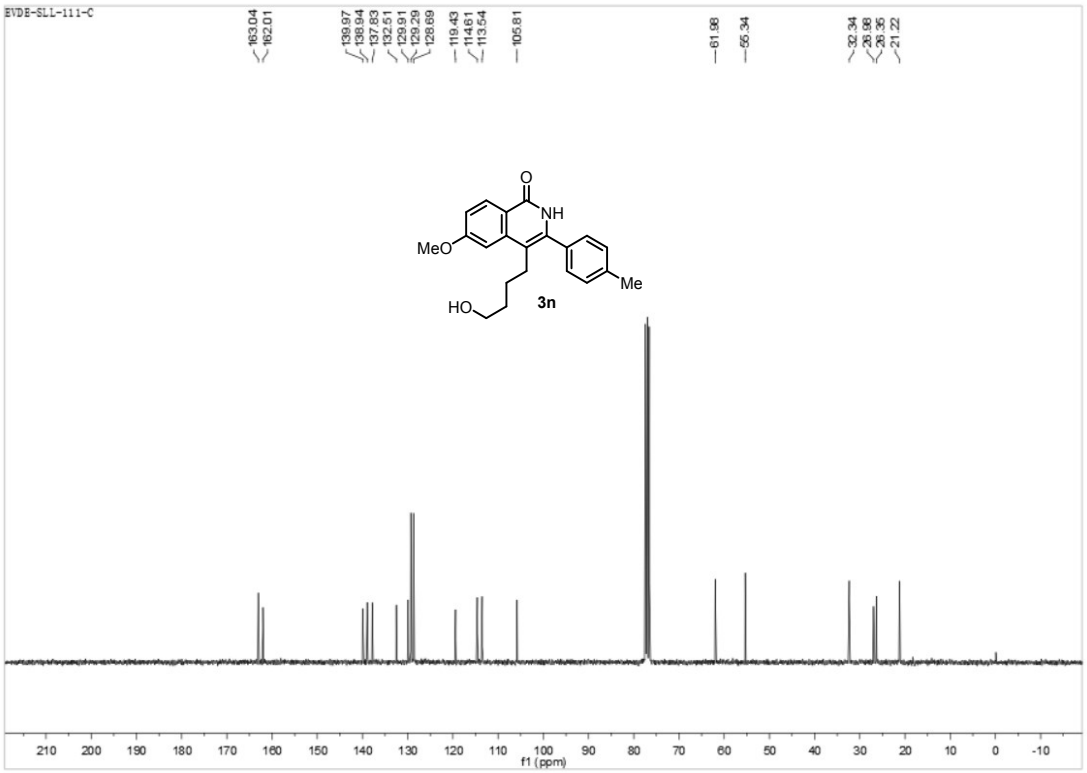

EVDE-SLL-20.20.fid
162.20
137.65
135.69
135.43
133.78
132.89
130.37
129.30
128.06
126.66
125.92
123.75
114.37
62.32
32.43
27.01
26.73
O
NH
Cl
HO
3l
f1 (ppm)

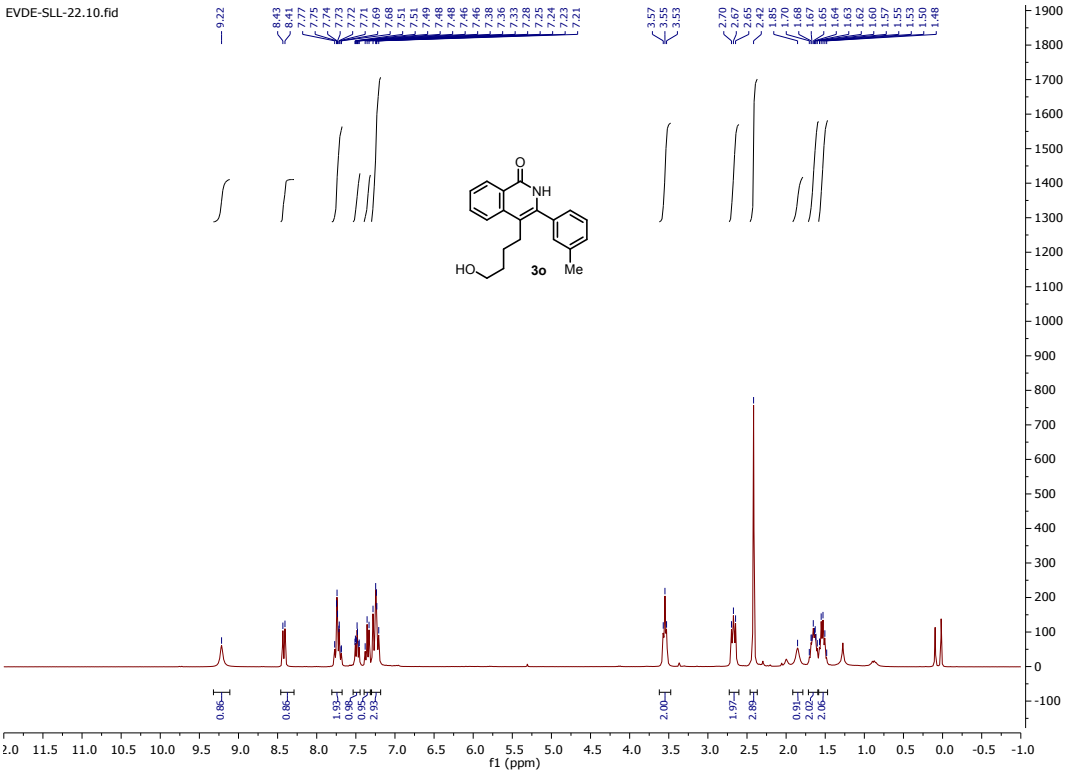

EVDE-S11-141
9.97
8.36
8.33
7.76
7.75
7.75
7.74
7.59
7.57
7.54
7.53
7.52
7.51
7.50
7.50
7.49
7.48
7.48
3.57
3.55
3.53
2.67
2.64
2.62
1.67
1.64
1.62
1.60
1.55
1.53
1.51
1.49
1.47
O
NH
CF3
HO
3m
0.91
1.00
4.02
3.31
2.00
1.97
2.33
2.30
f1 (ppm)

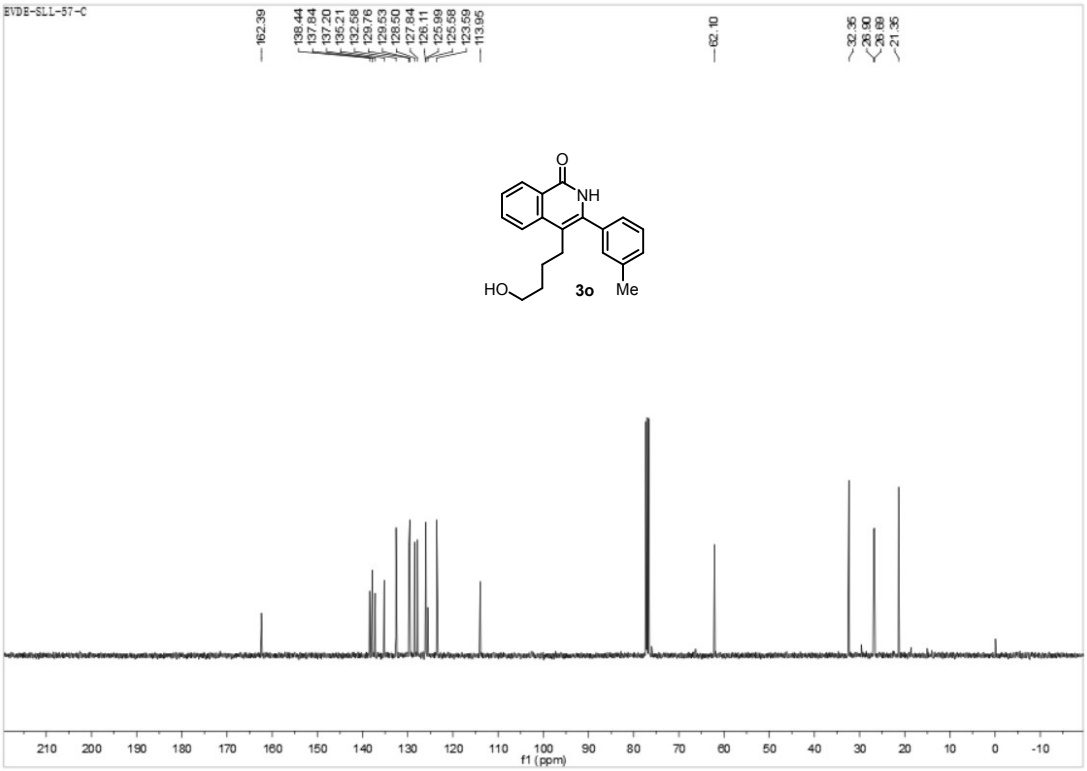

EVDE-S11-137-141
162.48
138.84
137.56
135.64
132.89
131.95
129.70
127.98
127.31
126.77
125.79
125.74
123.78
114.62
62.22
32.40
28.98
28.79
O
NH
CF3
HO
3m
f1 (ppm)

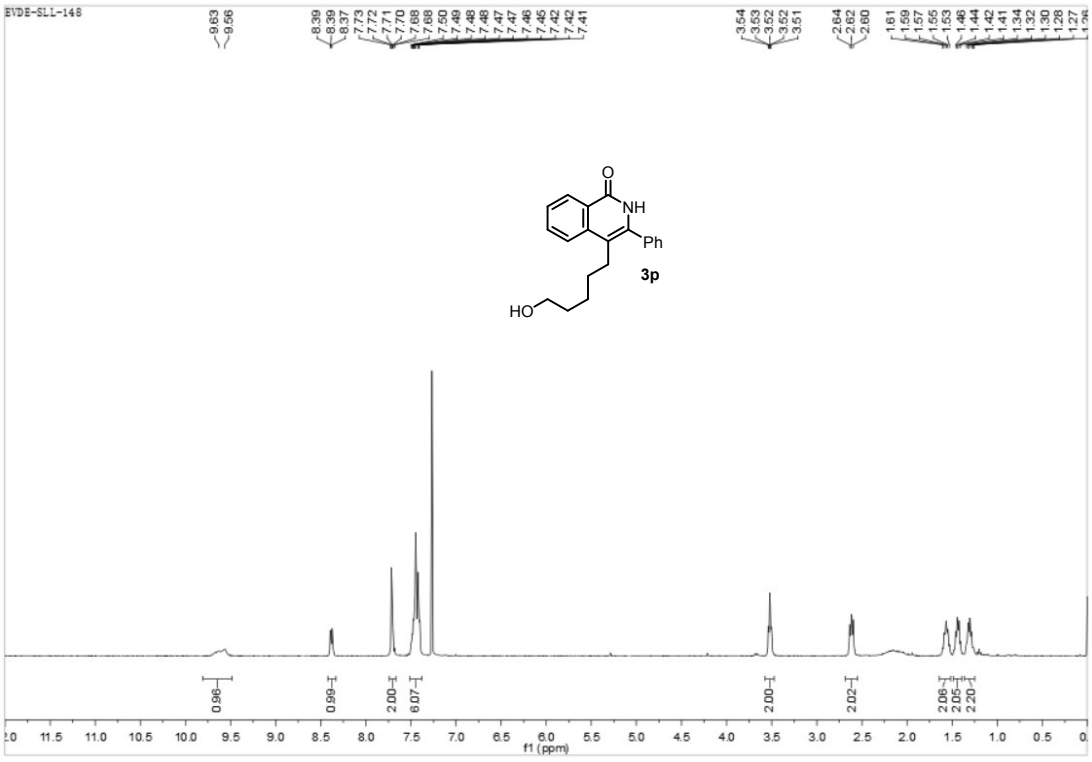

evde-s11-6-f
-62.78
O
NH
HO
CF3
3m
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

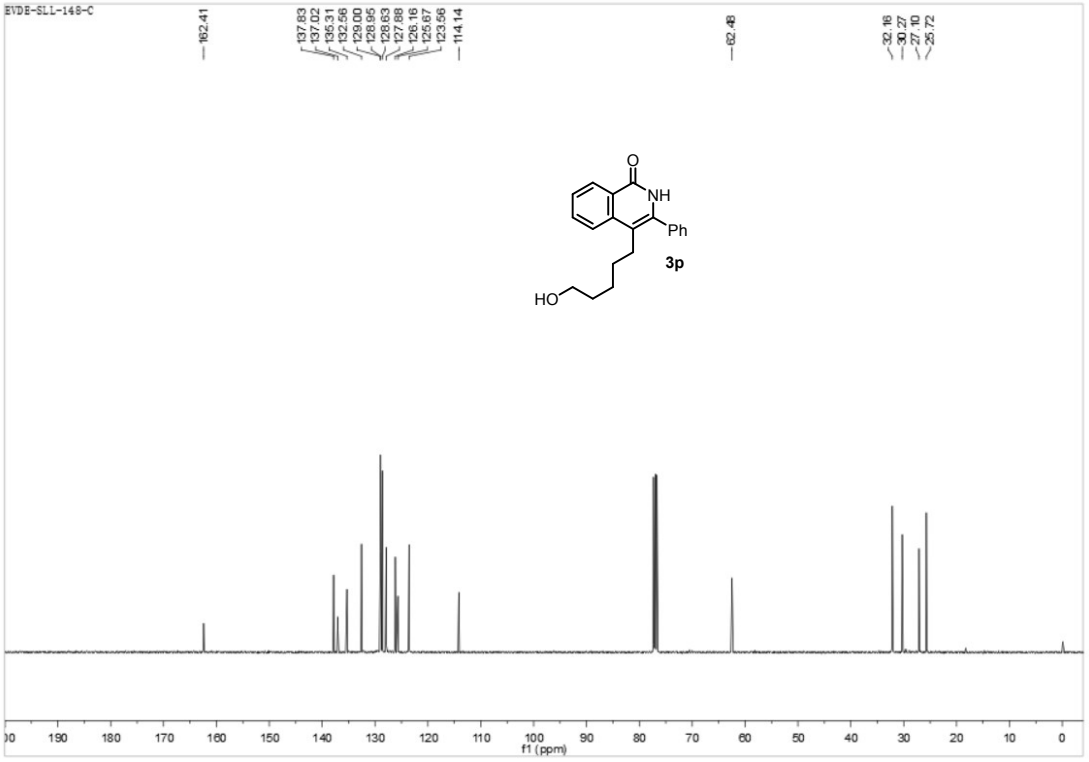

EVDE-SLL-111
9.14
8.32
8.29
7.26
7.25
7.23
7.20
7.09
7.08
7.04
7.03
7.01
7.01
3.90
3.55
3.53
3.51
2.61
2.59
2.56
2.39
2.38
1.64
1.61
1.60
1.59
1.57
1.53
1.51
1.49
1.47
1.44
O
NH
MeO
Me
HO
3n
0.91
0.98
4.02
1.01
1.04
2.90
2.00
1.99
3.09
1.96
2.05
f1 (ppm)

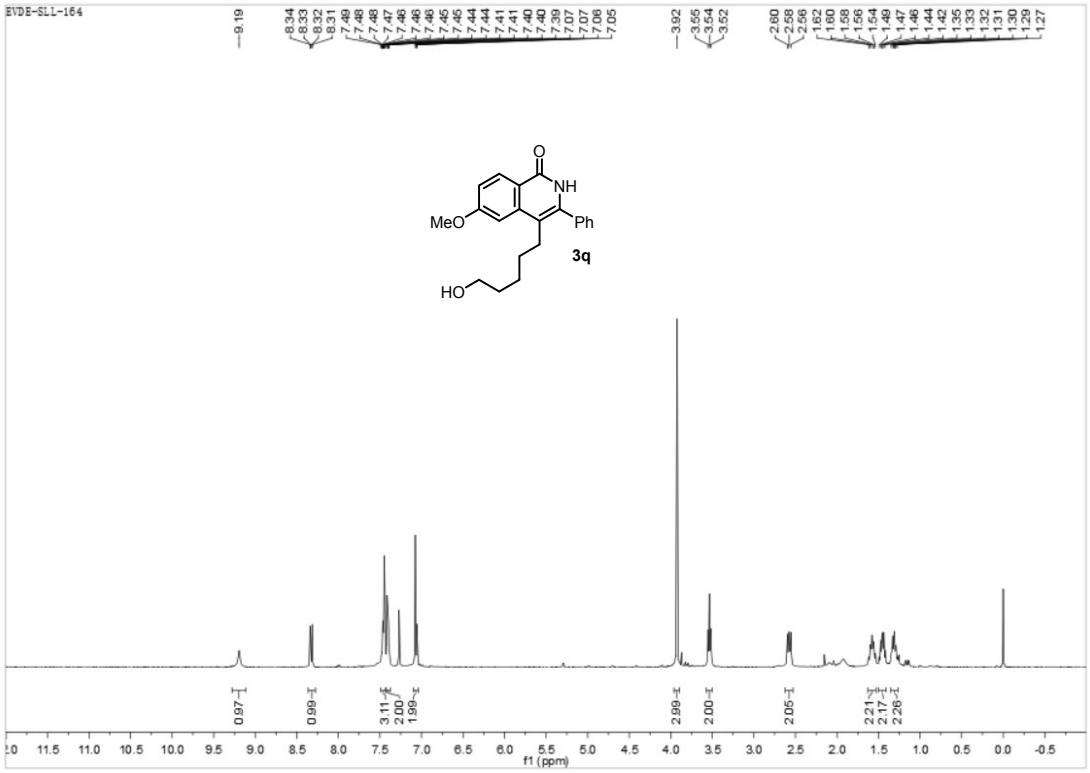

EVDE-SLL-111-C
163.04
162.01
139.97
138.94
137.83
132.51
129.91
129.29
128.69
119.43
114.61
113.54
105.81
61.98
55.34
32.34
28.98
26.35
21.22
O
NH
MeO
Me
HO
3n
f1 (ppm)

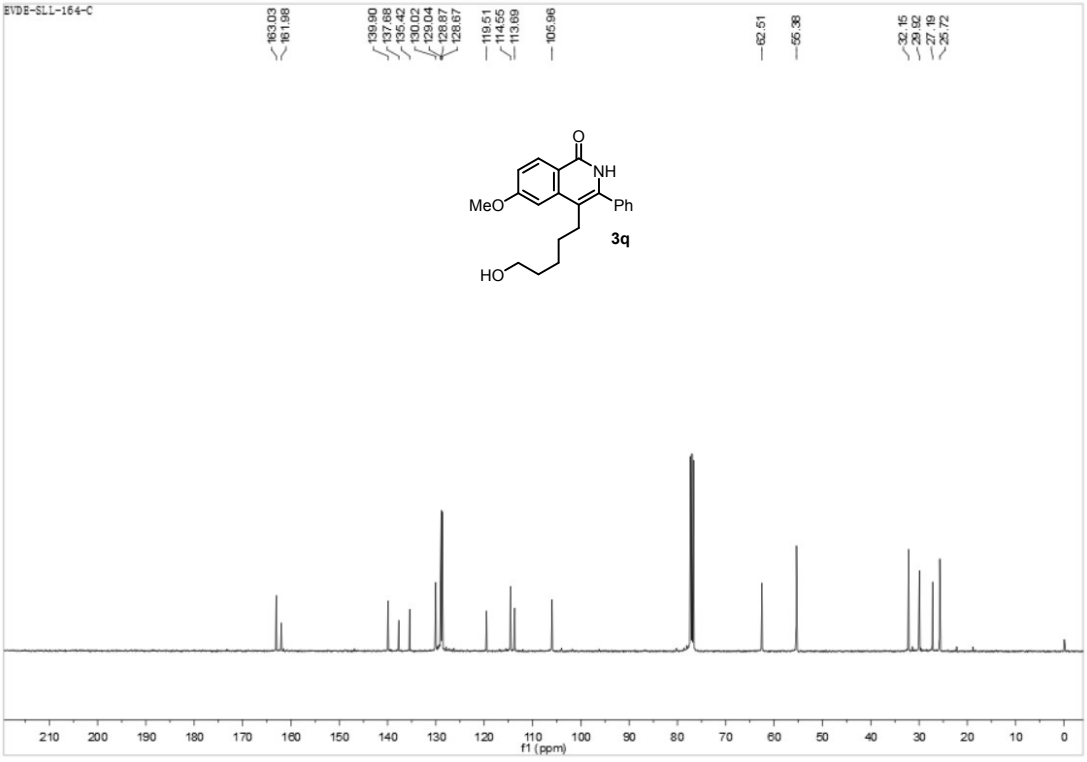

EVDE-SLL-22.10.fid
O
NH
HO
3o
Me
f1 (ppm)

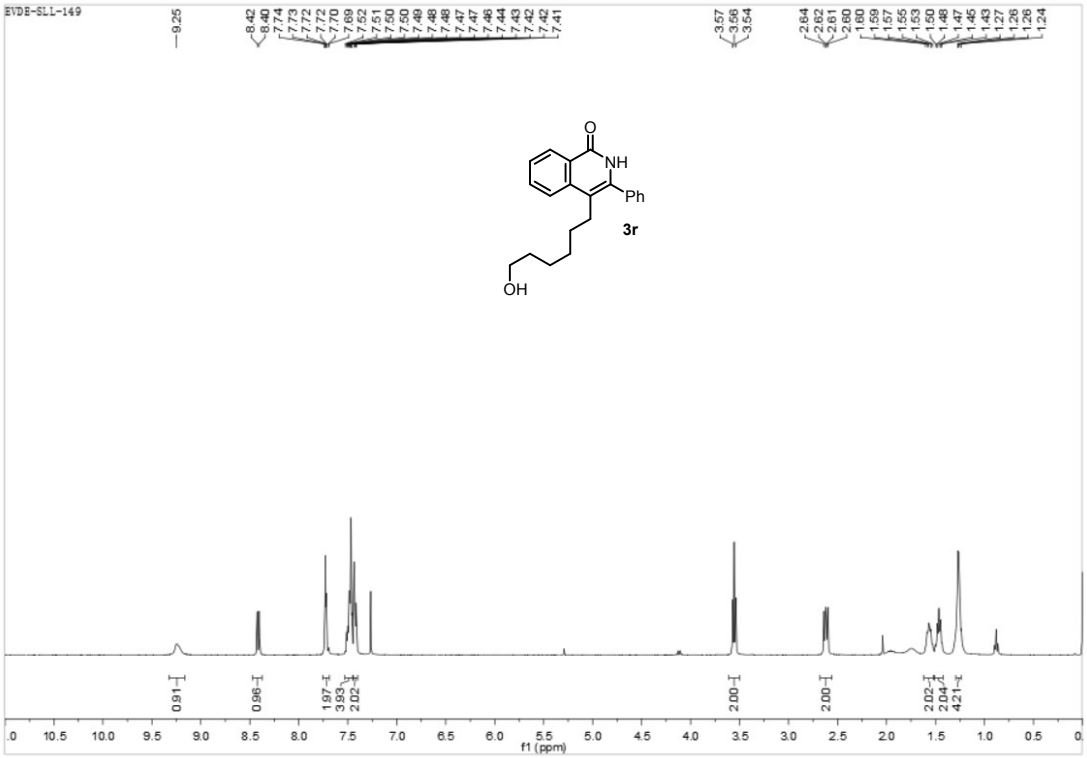

EVDE-SLL-57-C
O
NH
HO
3o
Me
f1 (ppm)

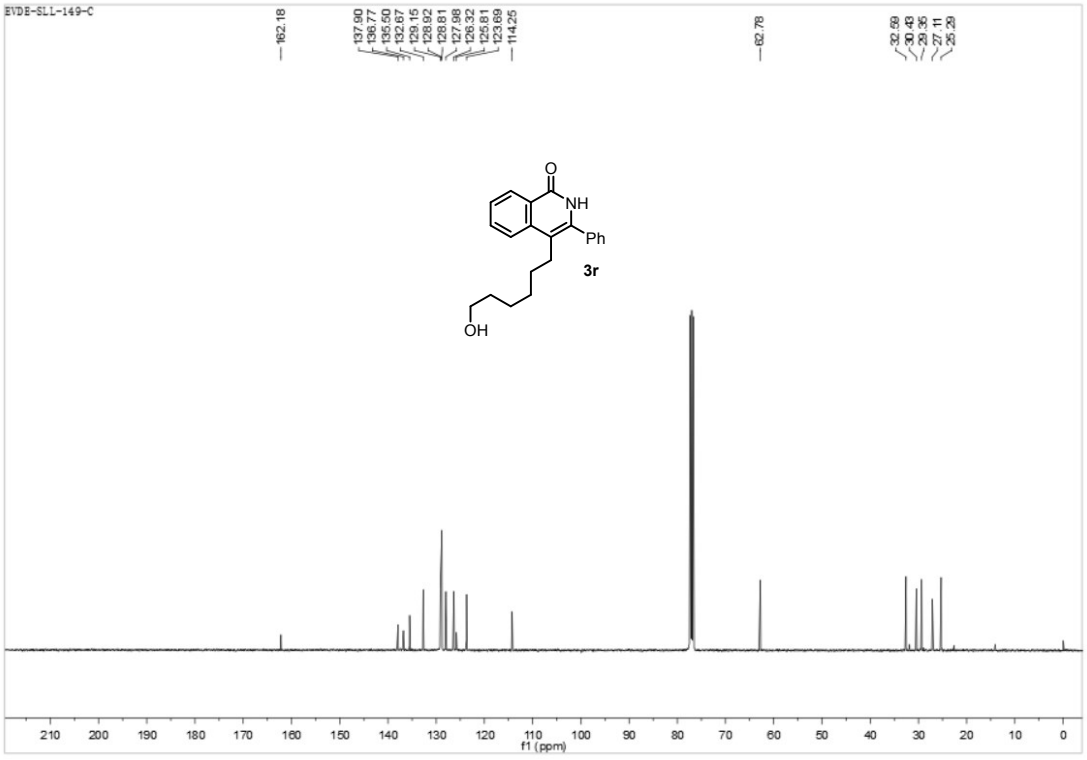

EVDE-SLL-148
O
NH
Ph
HO
3p
f1 (ppm)

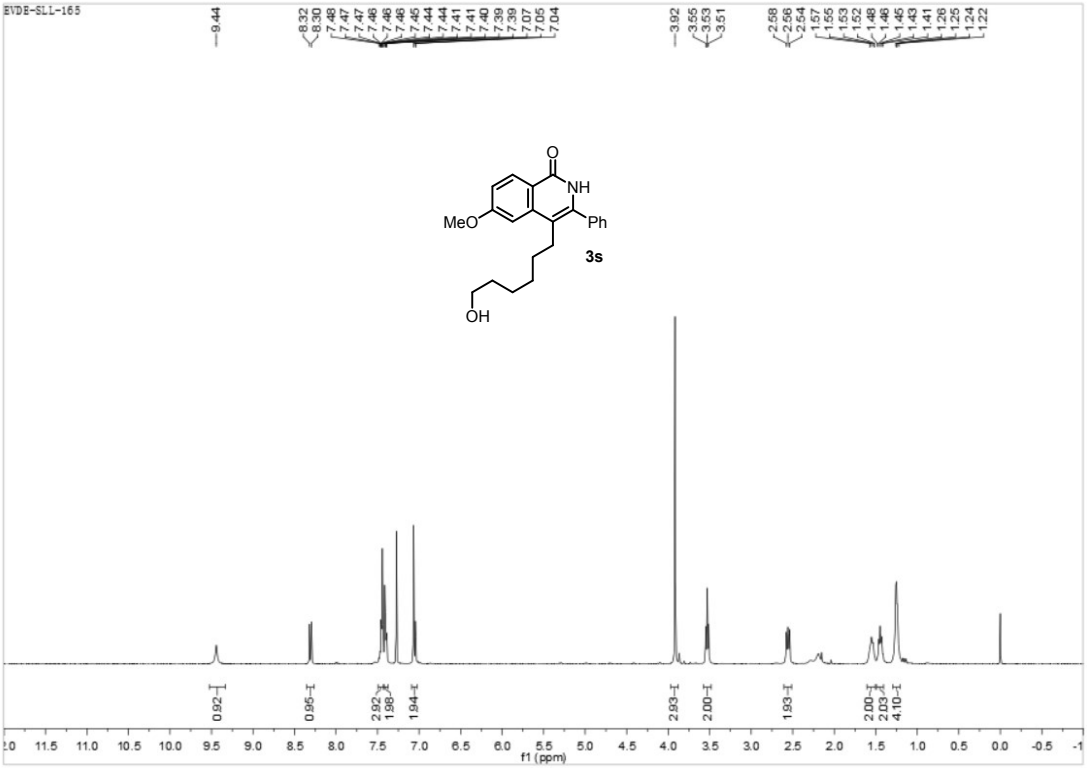

EVDE-SLL-148-C
O
NH
Ph
HO
3p
f1 (ppm)

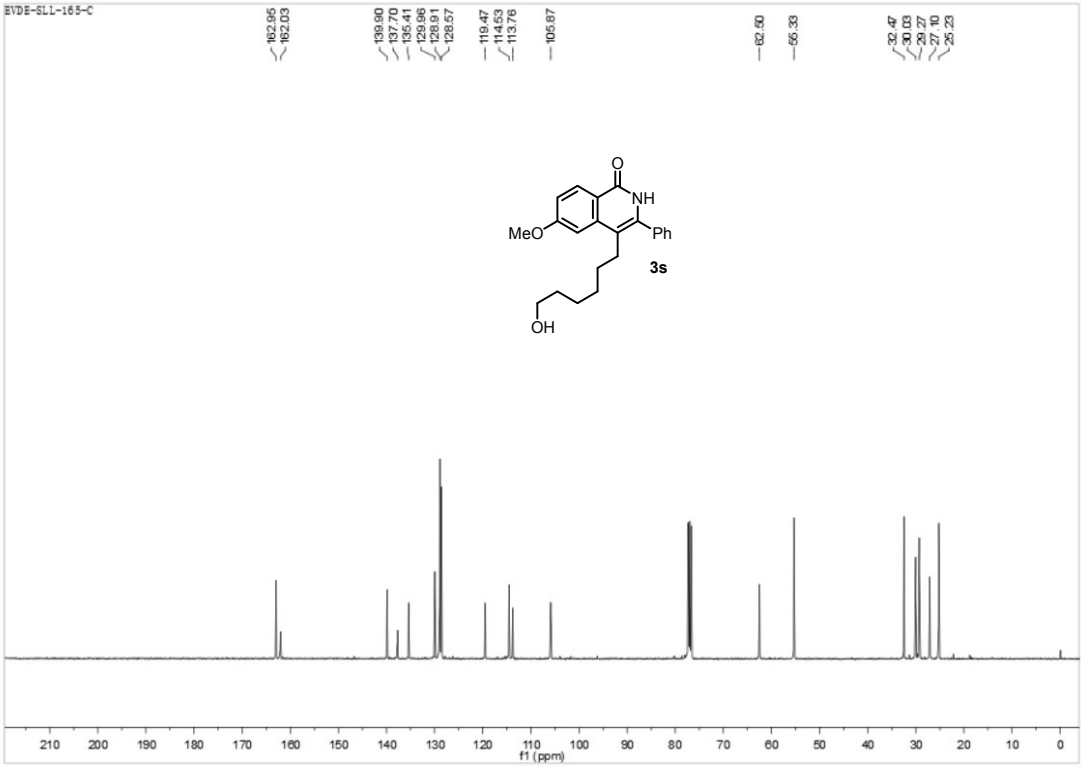

EVDE-SLL-164
O
NH
MeO
Ph
HO
3q
f1 (ppm)

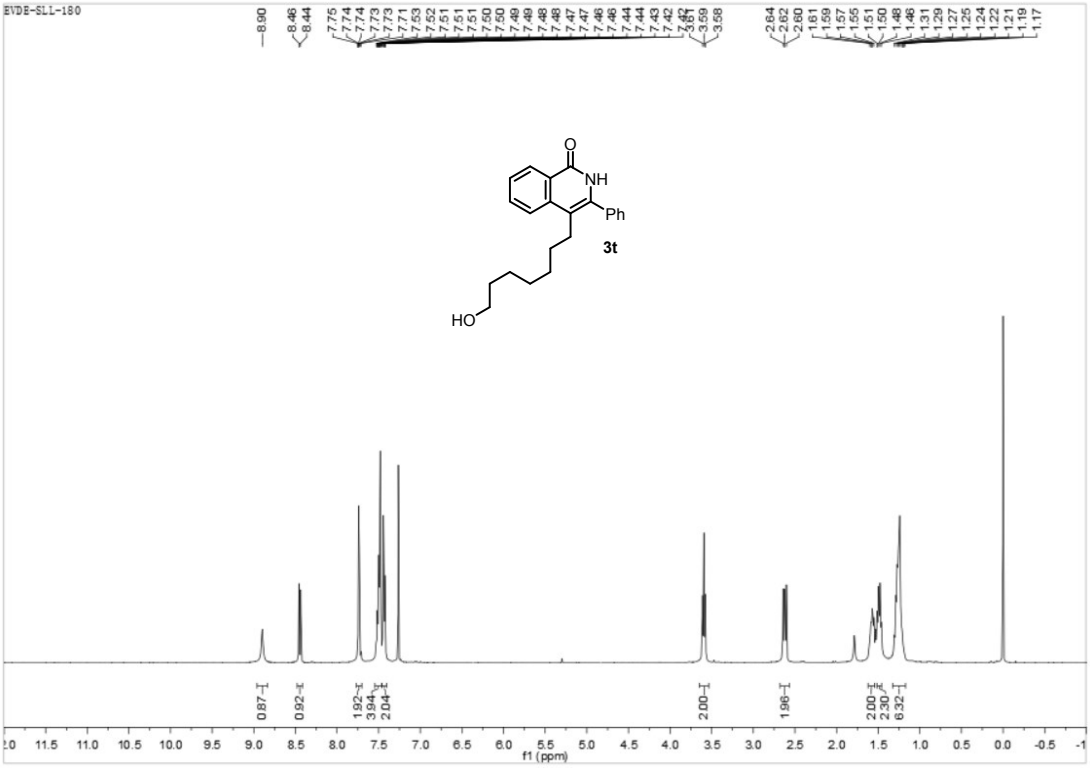

EVDE-SLL-164-C
O
NH
MeO
Ph
HO
3q
f1 (ppm)

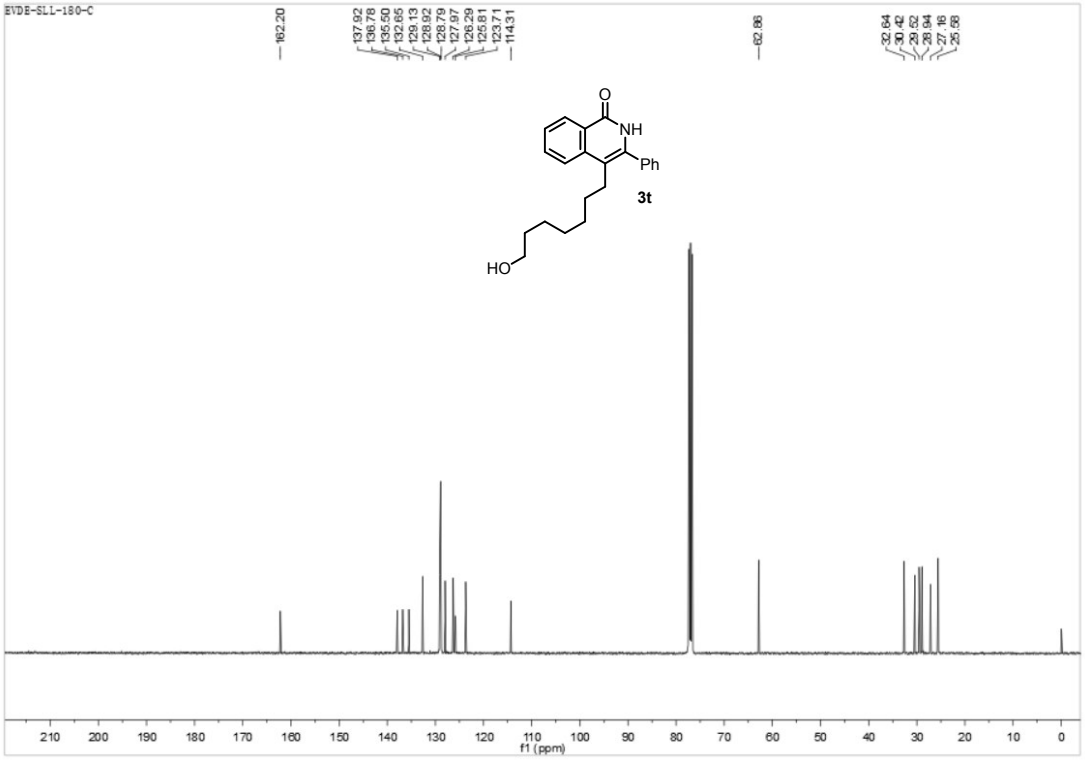

EVDB-SLL-149
O
NH
Ph
3r
OH
f1 (ppm)

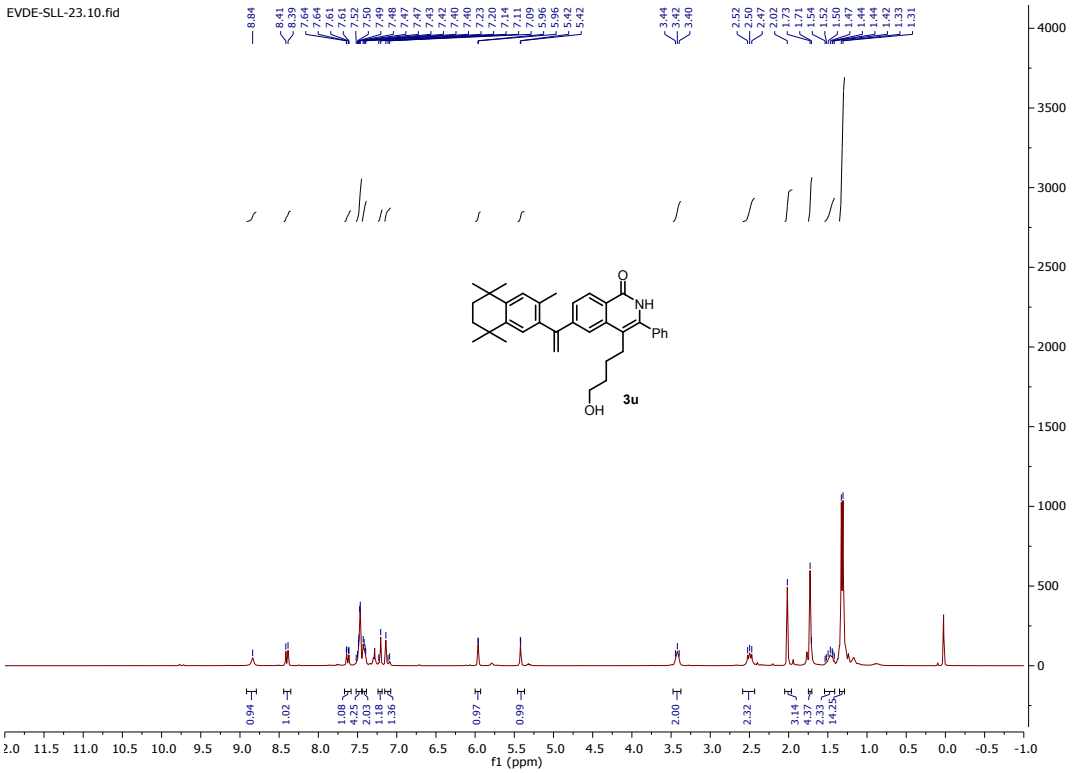

EVDB-SLL-149-C
O
NH
Ph
3r
OH
f1 (ppm)

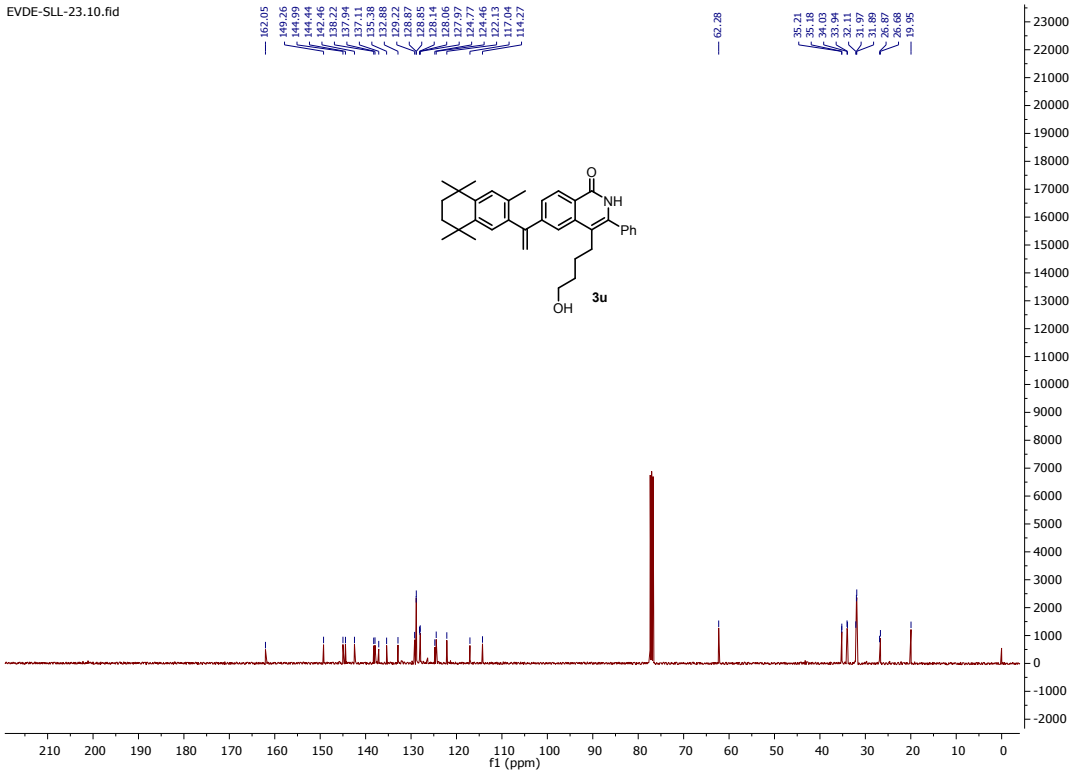

EVDE-SLL-165
9.44
8.32
8.30
7.48
7.47
7.47
7.46
7.46
7.46
7.45
7.44
7.44
7.41
7.41
7.40
7.39
7.07
7.05
7.04
3.92
3.55
3.53
3.51
2.58
2.56
2.54
1.57
1.55
1.53
1.52
1.48
1.46
1.45
1.43
1.41
1.26
1.25
1.24
1.22
O
NH
MeO
Ph
3s
OH
0.92
0.95
2.92
1.98
1.94
2.93
2.00
1.93
2.00
2.03
4.10
f1 (ppm)

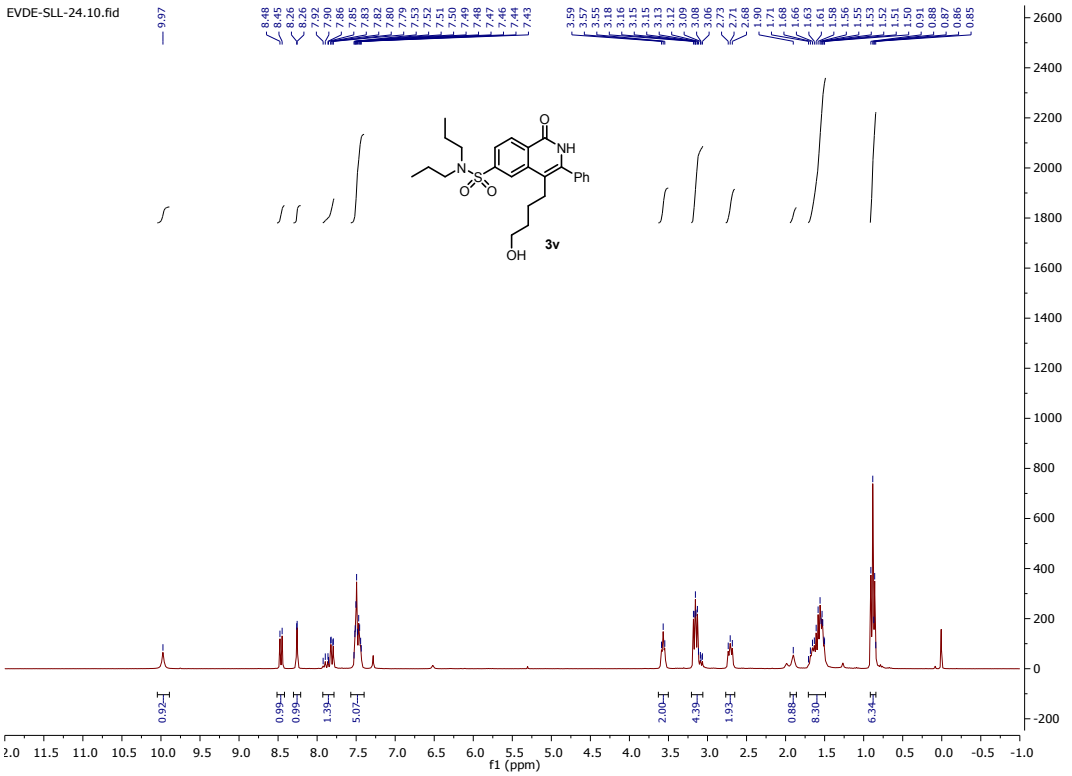

EVDE-SLL-165-C
162.95
162.03
139.90
137.70
135.41
129.96
128.91
128.57
119.47
114.53
113.76
105.87
62.50
55.33
32.47
30.03
29.27
27.10
25.23
O
NH
MeO
Ph
3s
OH
f1 (ppm)

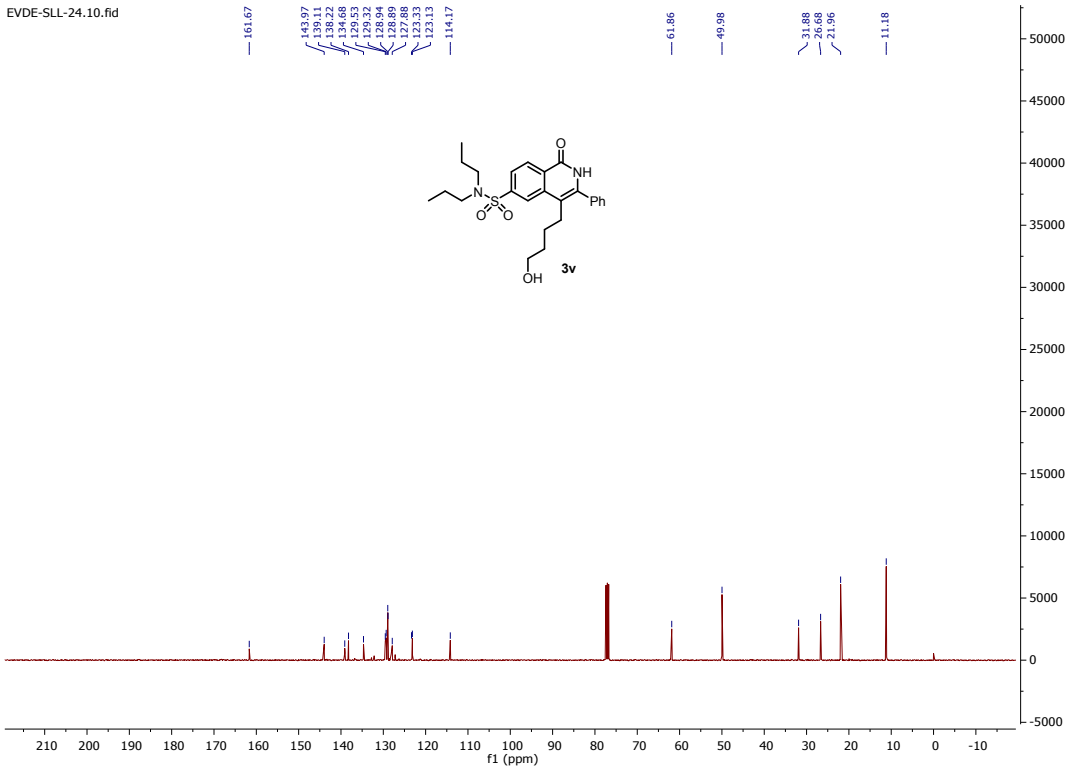

EVDE-SLL-180
O
NH
Ph
3t
HO
f1 (ppm)

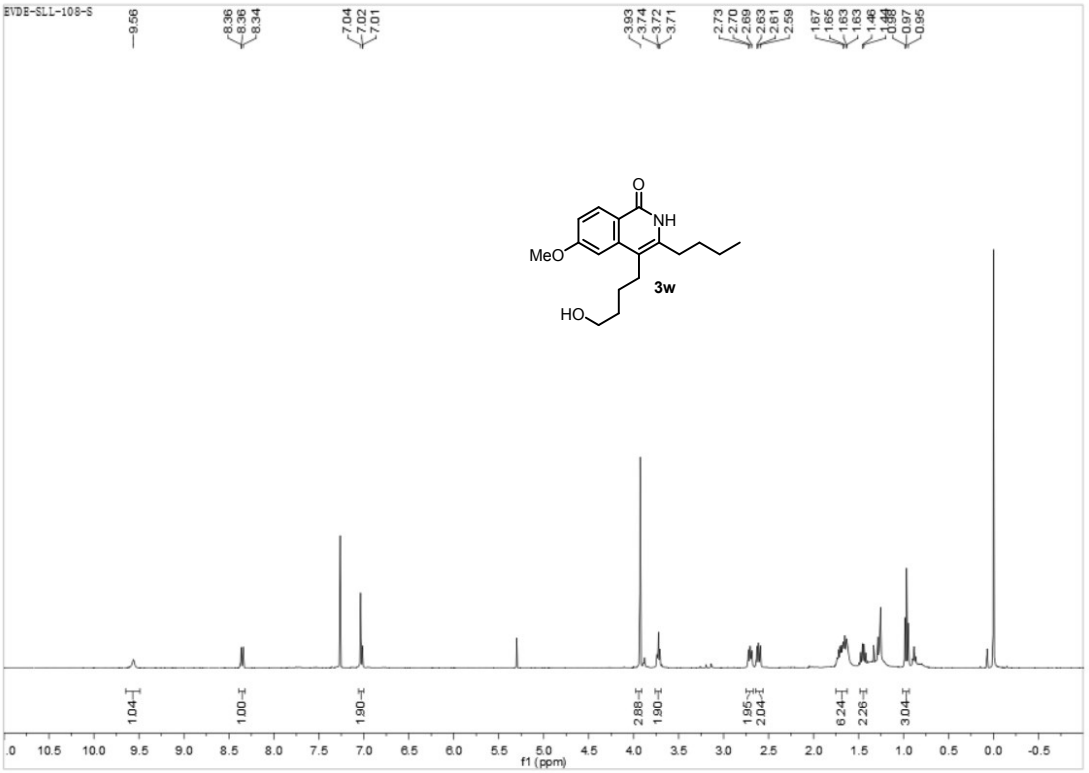

EVDE-SLL-180-C
O
NH
Ph
3t
HO
f1 (ppm)

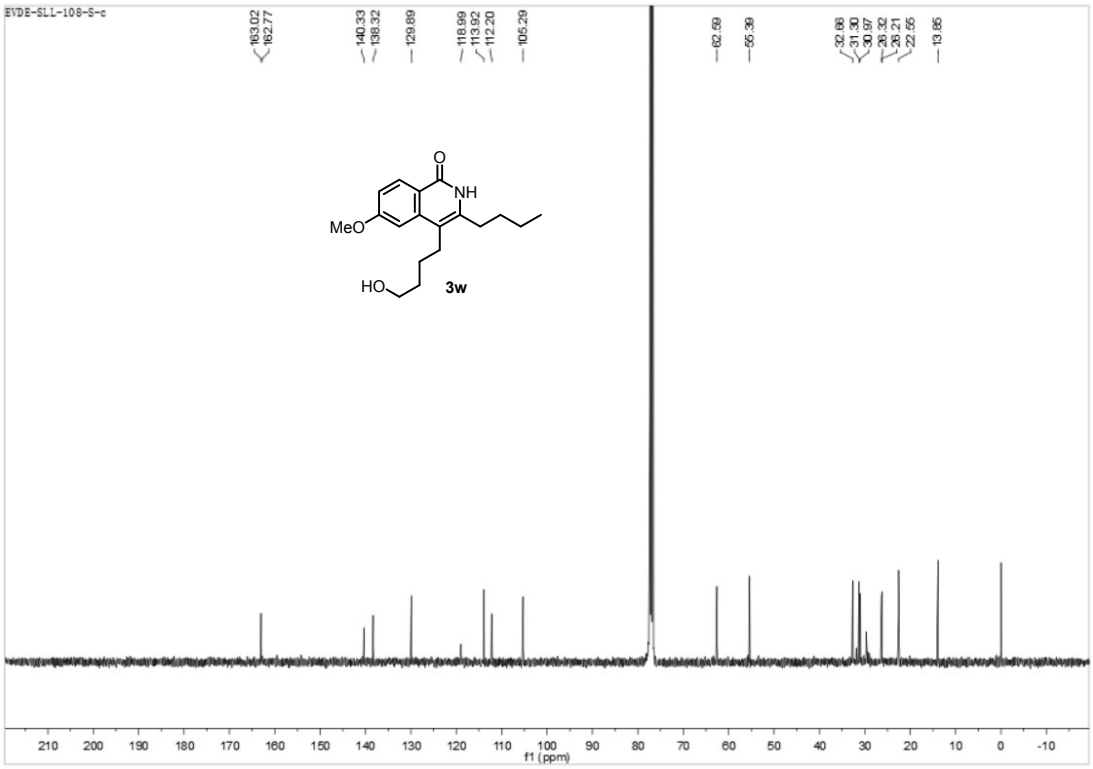

EVDE-SLL-23.10.fid
8.84
8.41
8.39
7.64
7.64
7.61
7.61
7.52
7.50
7.49
7.48
7.47
7.47
7.43
7.42
7.40
7.40
7.23
7.20
7.14
7.11
7.09
5.96
5.42
5.42
3.44
3.42
3.40
2.52
2.50
2.47
2.02
1.73
1.71
1.54
1.52
1.50
1.47
1.44
1.44
1.42
1.33
1.31
O
NH
Ph
OH
3u
0.94
1.02
1.08
4.25
2.03
1.18
1.36
0.97
0.99
2.00
2.32
3.14
4.37
2.33
14.25
f1 (ppm)

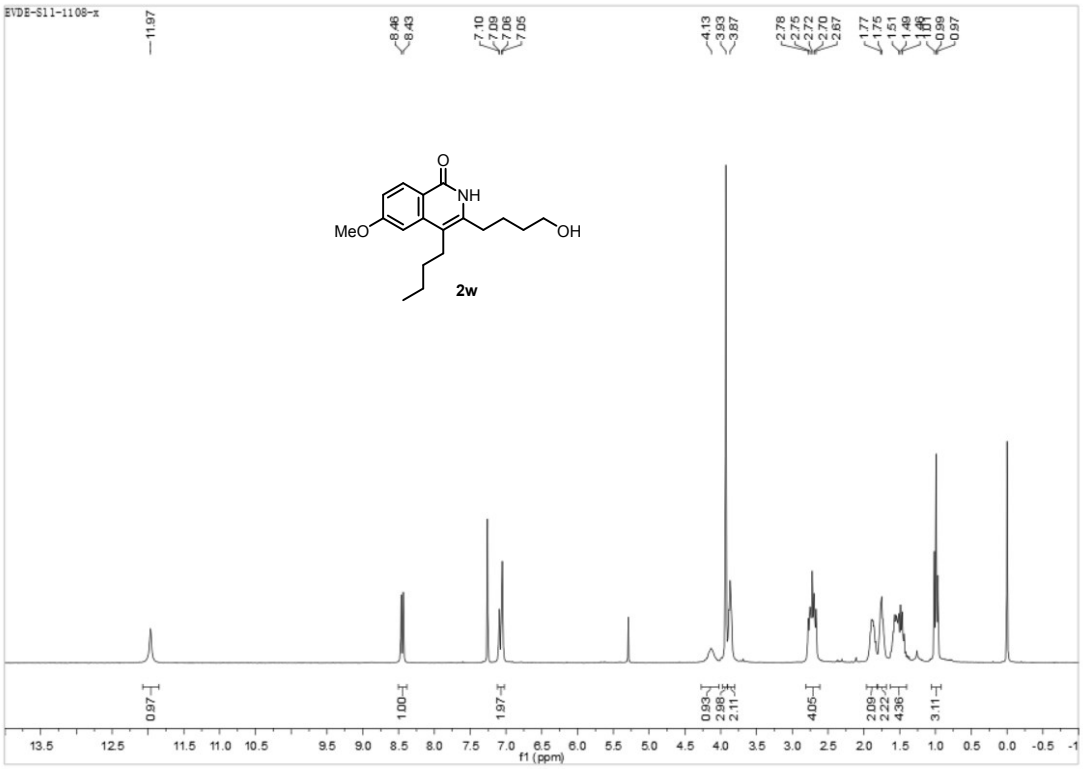

EVDE-SLL-23.10.fid
162.05
149.26
144.99
143.44
142.46
138.22
137.94
137.11
135.38
132.88
129.22
128.87
128.85
128.14
128.06
127.97
124.77
124.46
122.13
117.04
114.27
62.28
35.21
35.18
34.03
33.94
32.11
31.97
31.89
26.87
26.68
19.95
O
NH
Ph
OH
3u
f1 (ppm)

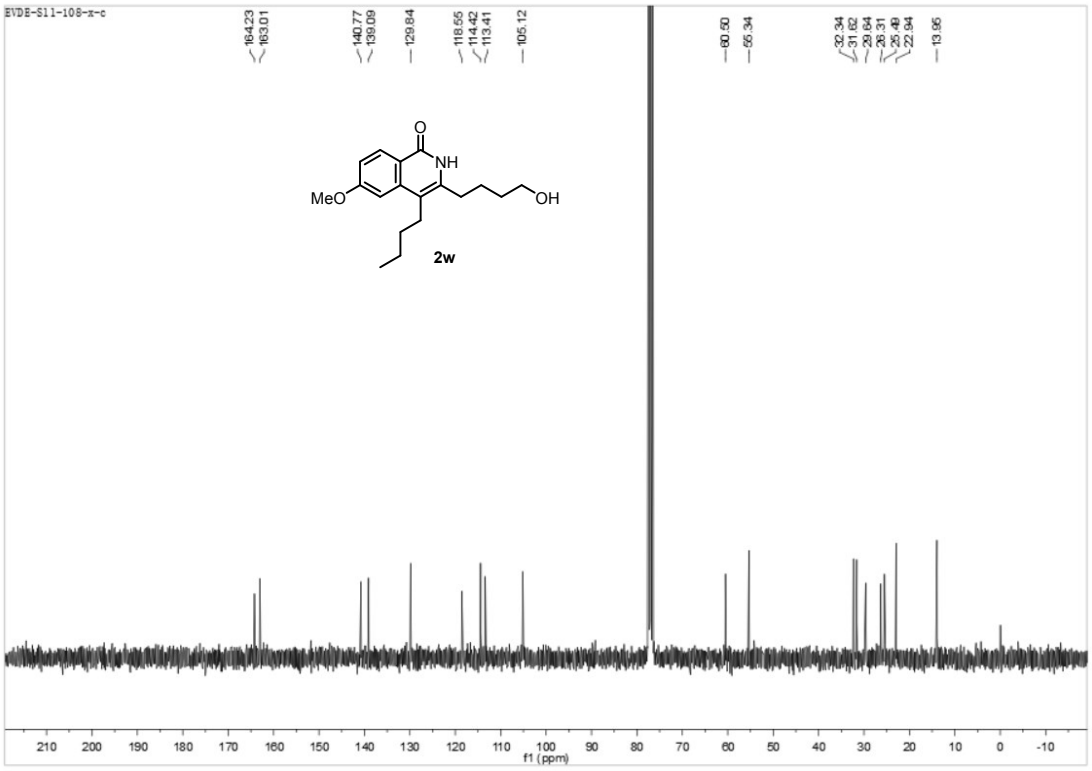

EVDE-SLL-24.10.fid
3v
f1 (ppm)

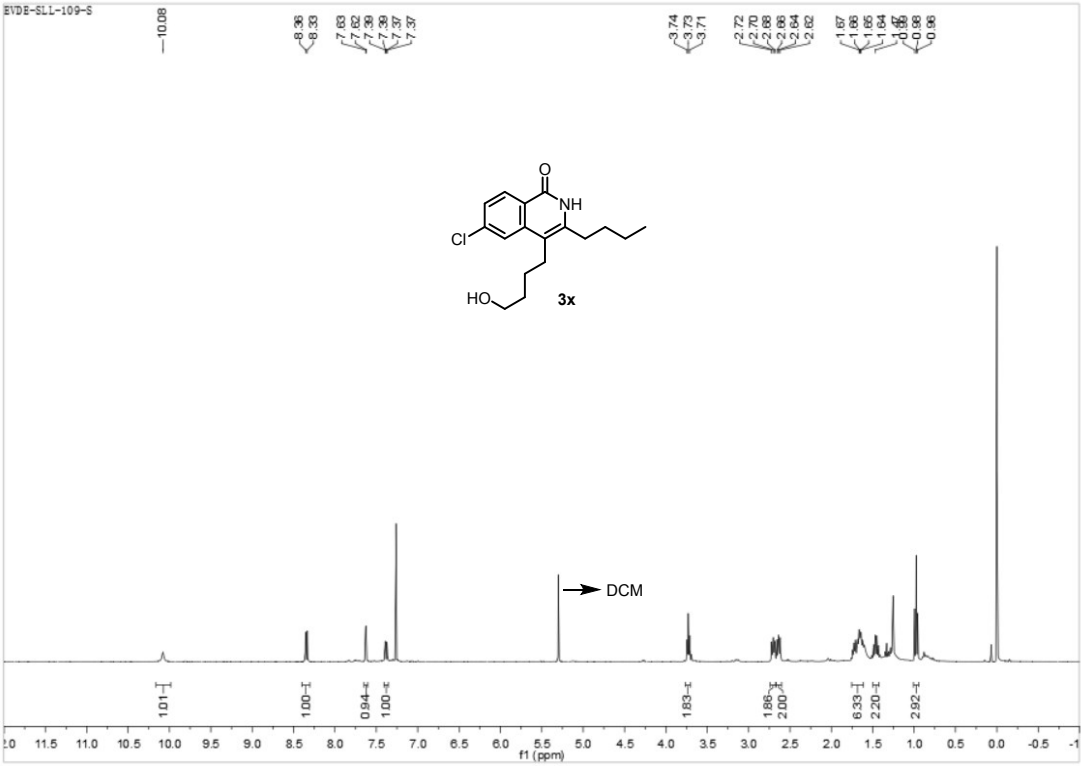

EVDE-SLL-24.10.fid
3v
f1 (ppm)

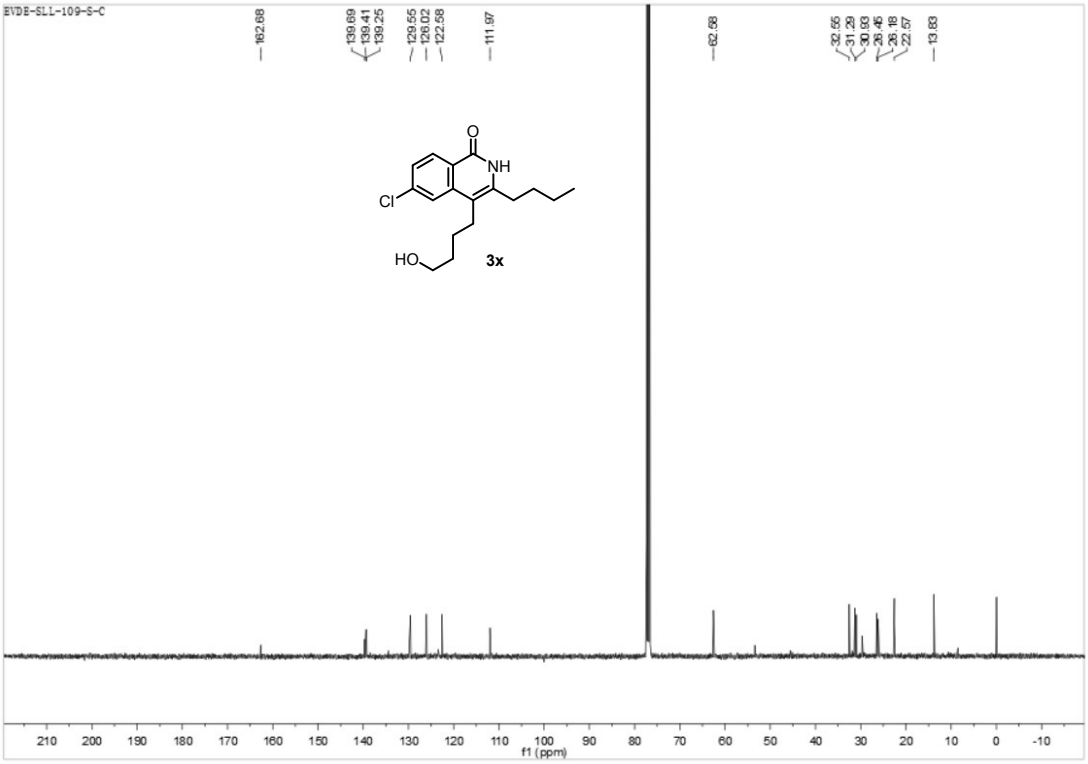

EVDE-SLL-108-S
9.56
8.36
8.36
8.34
7.04
7.02
7.01
3.93
3.74
3.72
3.71
2.73
2.70
2.69
2.63
2.61
2.59
1.67
1.65
1.63
1.63
1.46
1.44
0.98
0.97
0.95
O
NH
MeO
HO
3w
1.04
1.00
1.90
2.88
1.90
1.95
2.04
6.24
2.26
3.04
f1 (ppm)

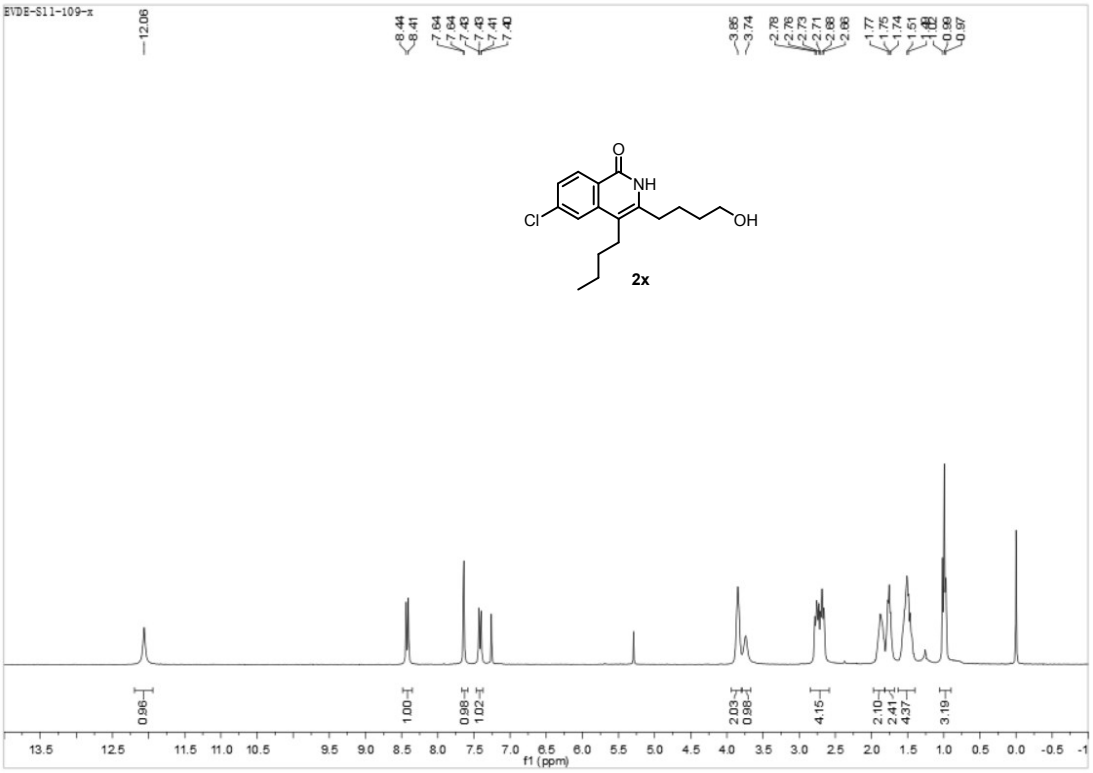

EVDE-SLL-108-S-c
163.02
162.77
140.33
138.32
129.89
118.99
113.92
112.20
105.29
62.59
55.39
32.66
31.30
30.97
26.32
26.21
22.55
13.85
O
NH
MeO
HO
3w
f1 (ppm)

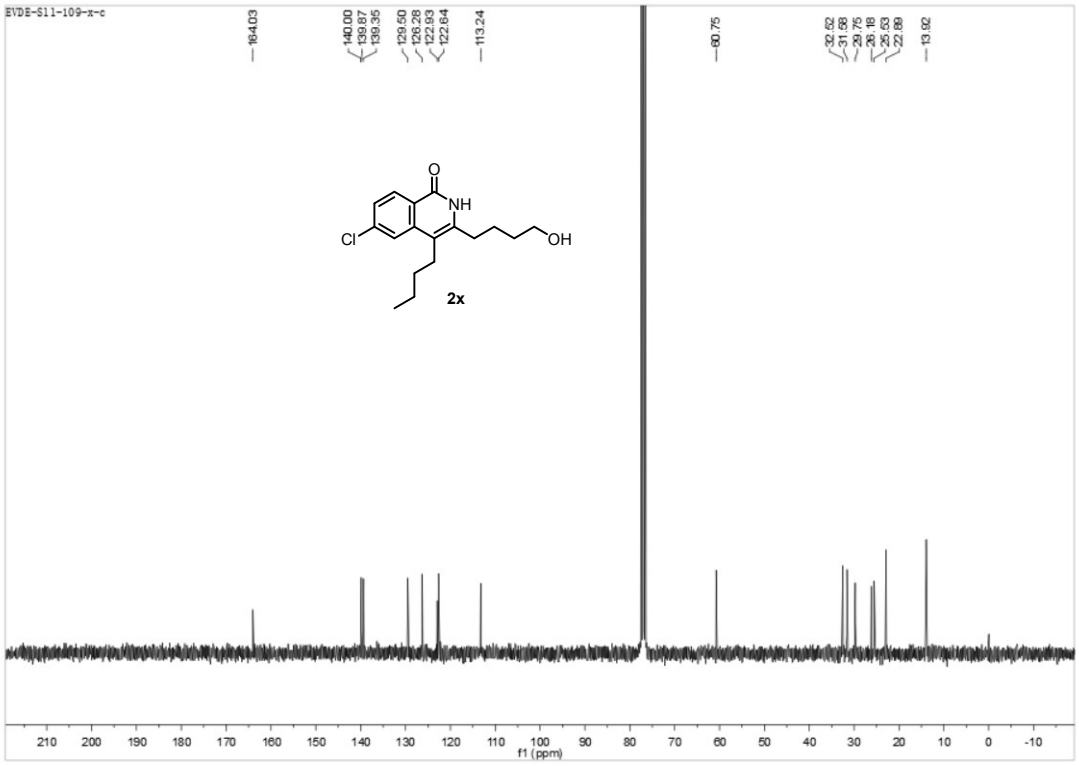

EVDE-S11-1108-x
11.97
8.46
8.43
7.10
7.09
7.08
7.05
4.13
3.93
3.87
2.78
2.75
2.72
2.70
2.67
1.77
1.75
1.51
1.49
1.00
0.99
0.97
O
NH
MeO
OH
2w
0.97
1.00
1.97
0.93
2.98
2.11
4.05
2.09
2.22
4.36
3.11
f1 (ppm)

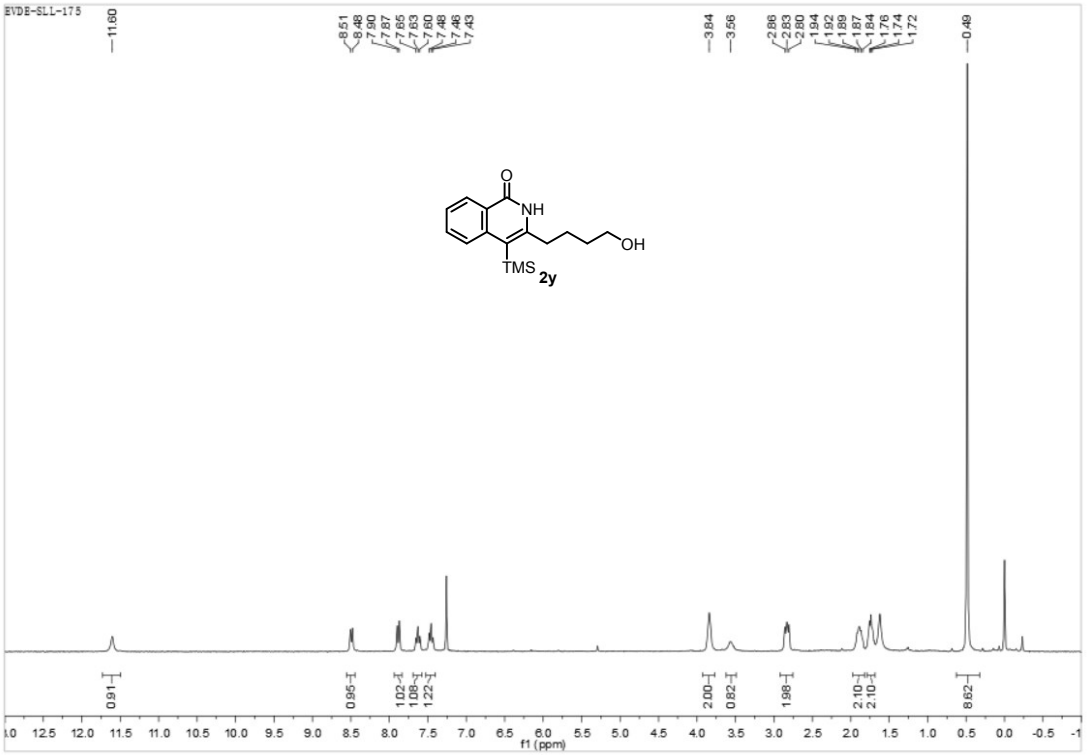

EVDE-S11-108-x-c
164.23
163.01
140.77
139.09
129.84
118.55
114.42
113.41
105.12
60.50
55.34
32.34
31.62
29.64
26.31
25.49
22.94
13.95
O
NH
MeO
OH
2w
f1 (ppm)

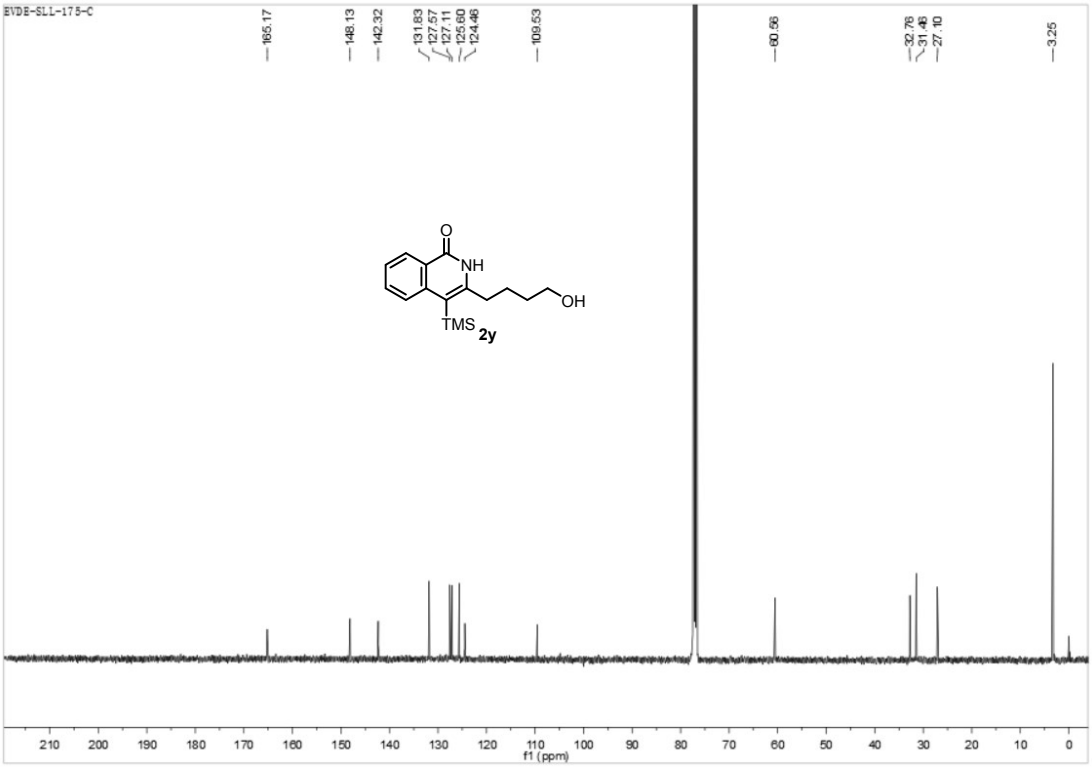

EVDE-SLL-109-S
10.08
8.36
8.33
7.63
7.62
7.39
7.38
7.37
7.37
3.74
3.73
3.71
2.72
2.70
2.68
2.66
2.64
2.62
1.67
1.66
1.65
1.64
0.98
0.98
0.96
O
NH
Cl
HO
3x
DCM
1.01
1.00
0.94
1.00
1.83
1.86
2.00
6.33
2.20
2.92
f1 (ppm)

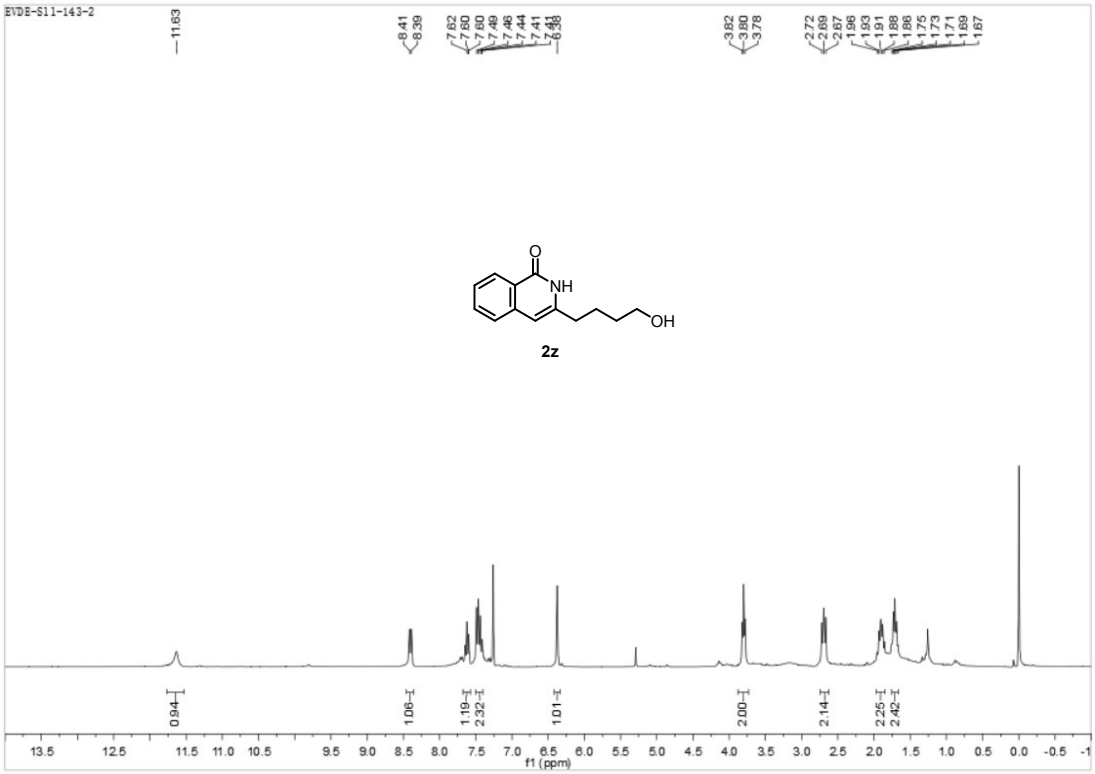

EVDE-SLL-109-S-C
162.68
139.89
139.41
139.25
129.55
126.02
122.58
111.97
62.59
32.55
31.29
30.93
26.45
26.18
22.57
13.83
O
NH
Cl
HO
3x
f1 (ppm)

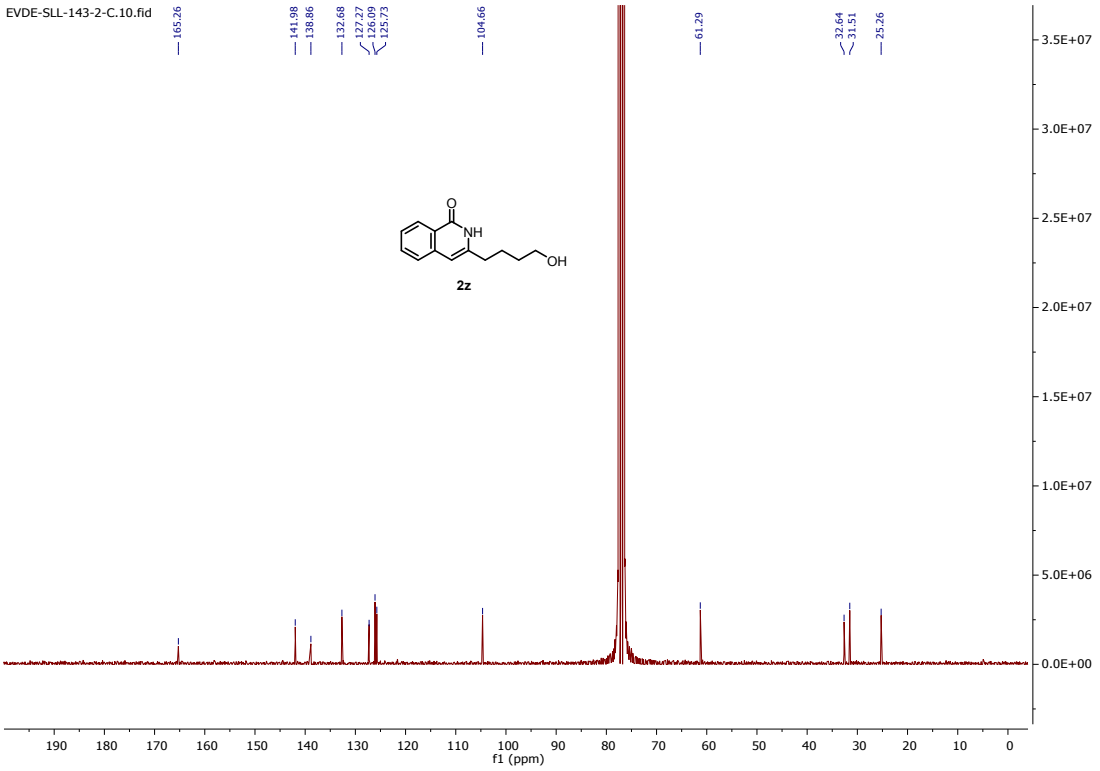

EVDE-S11-109-x
12.06
8.44
8.41
7.64
7.64
7.43
7.43
7.41
7.40
3.85
3.74
2.78
2.76
2.73
2.71
2.68
2.66
1.77
1.75
1.74
1.51
0.99
0.97
O
NH
Cl
OH
2x
0.96
1.00
0.98
1.02
2.03
0.98
4.15
2.10
2.41
4.37
3.19
f1 (ppm)

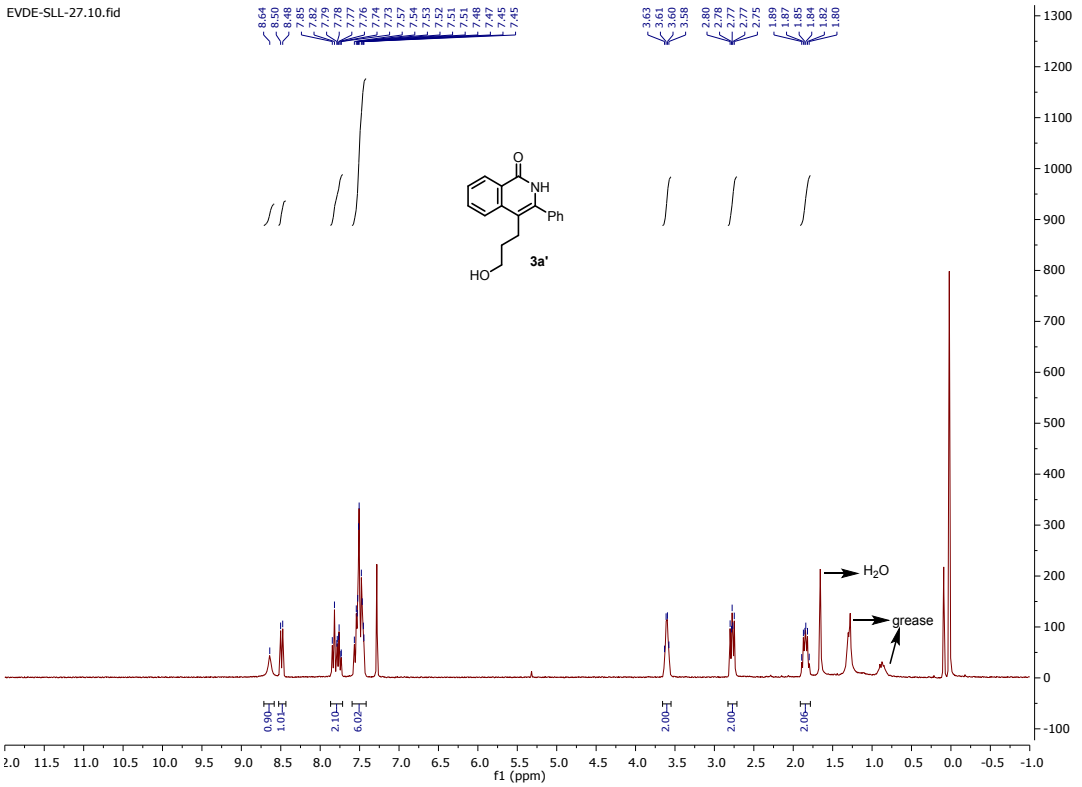

EVDE-S11-109-x-c
164.03
140.00
139.87
139.35
129.50
126.28
122.93
122.64
113.24
60.75
32.62
31.66
29.75
26.18
25.53
22.89
13.92
O
NH
Cl
OH
2x
f1 (ppm)

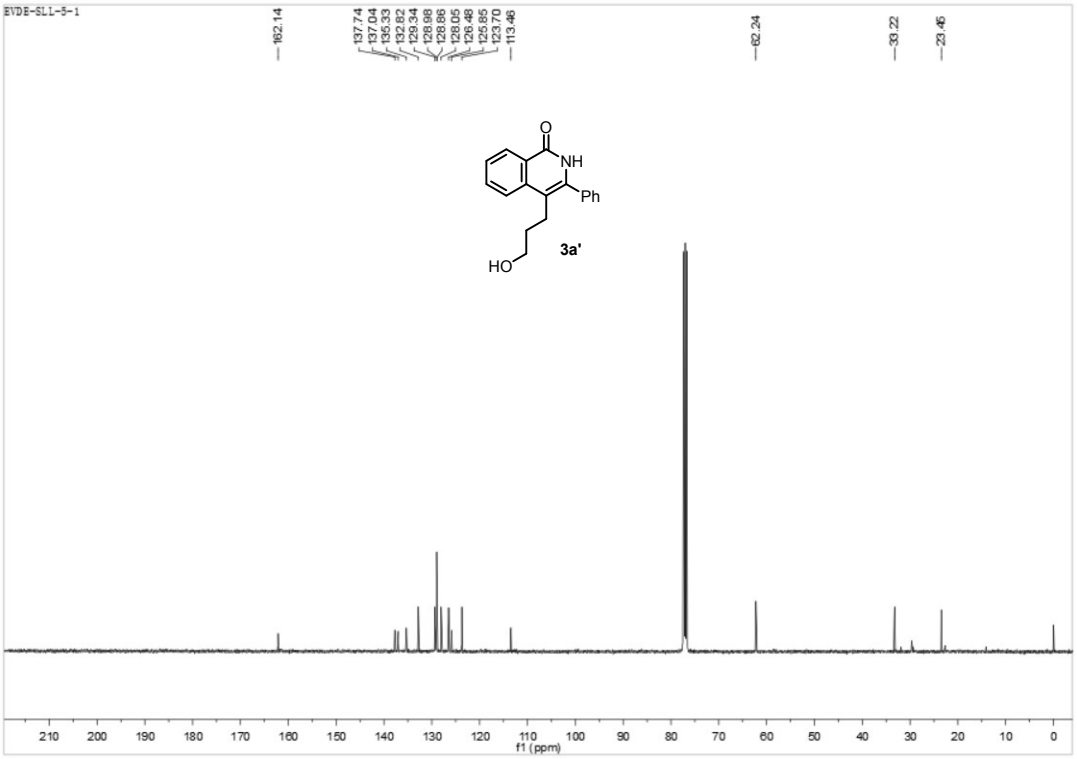

EVDE-SLL-175
11.60
8.51
8.48
7.90
7.87
7.65
7.63
7.60
7.48
7.46
7.43
3.84
3.56
2.86
2.83
2.80
1.94
1.92
1.89
1.87
1.84
1.76
1.74
1.72
0.49
O
NH
OH
TMS
2y
0.91
0.95
1.02
1.08
1.22
2.00
0.82
1.98
2.10
2.10
8.62
f1 (ppm)

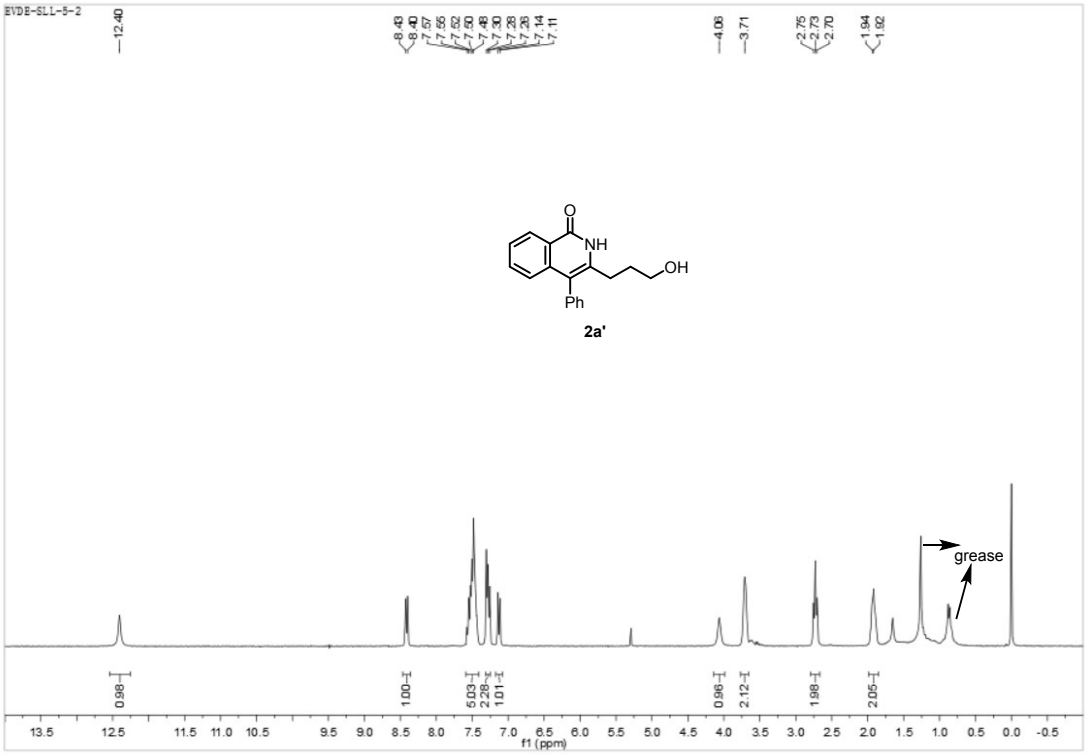

EVDE-SLL-175-C
165.17
148.13
142.32
131.83
127.57
127.11
125.60
124.46
109.53
60.56
32.76
31.46
27.10
3.25
O
NH
OH
TMS
2y
f1 (ppm)

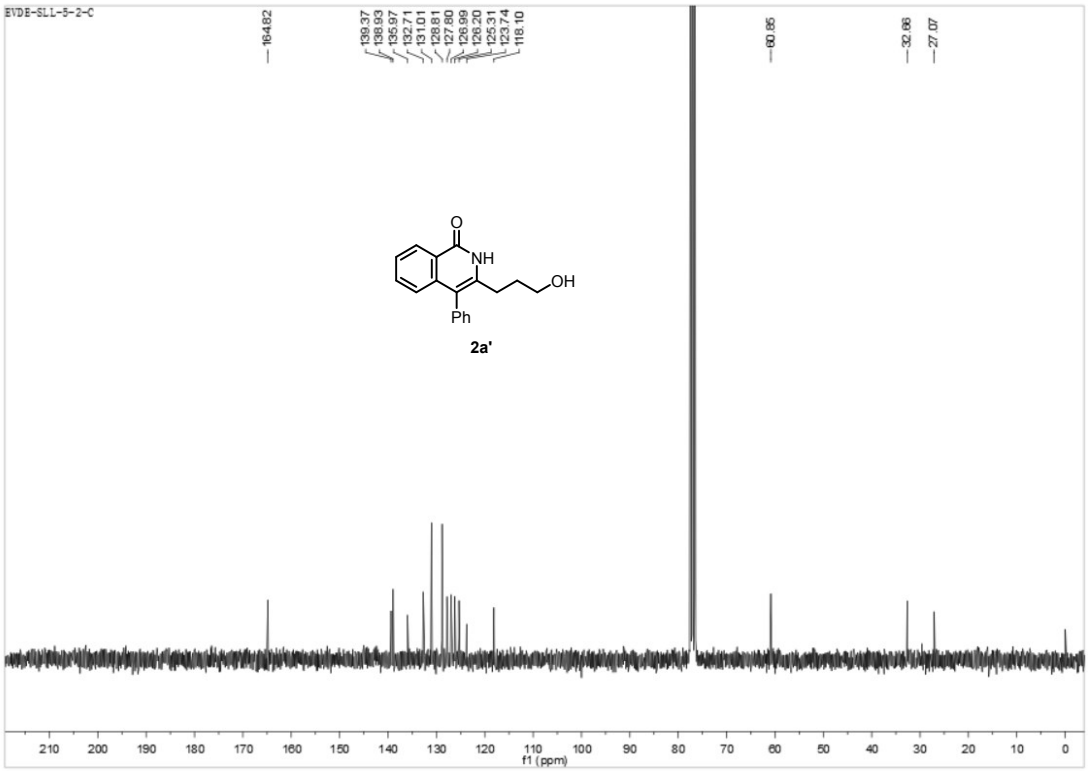

EVDE-S11-143-2
11.63
8.41
8.39
7.62
7.60
7.60
7.49
7.46
7.44
7.41
7.41
6.38
3.82
3.80
3.78
2.72
2.69
2.67
1.96
1.93
1.91
1.88
1.86
1.75
1.73
1.71
1.69
1.67
O
NH
OH
2z
0.94
1.06
1.19
2.32
1.01
2.00
2.14
2.25
2.42
f1 (ppm)

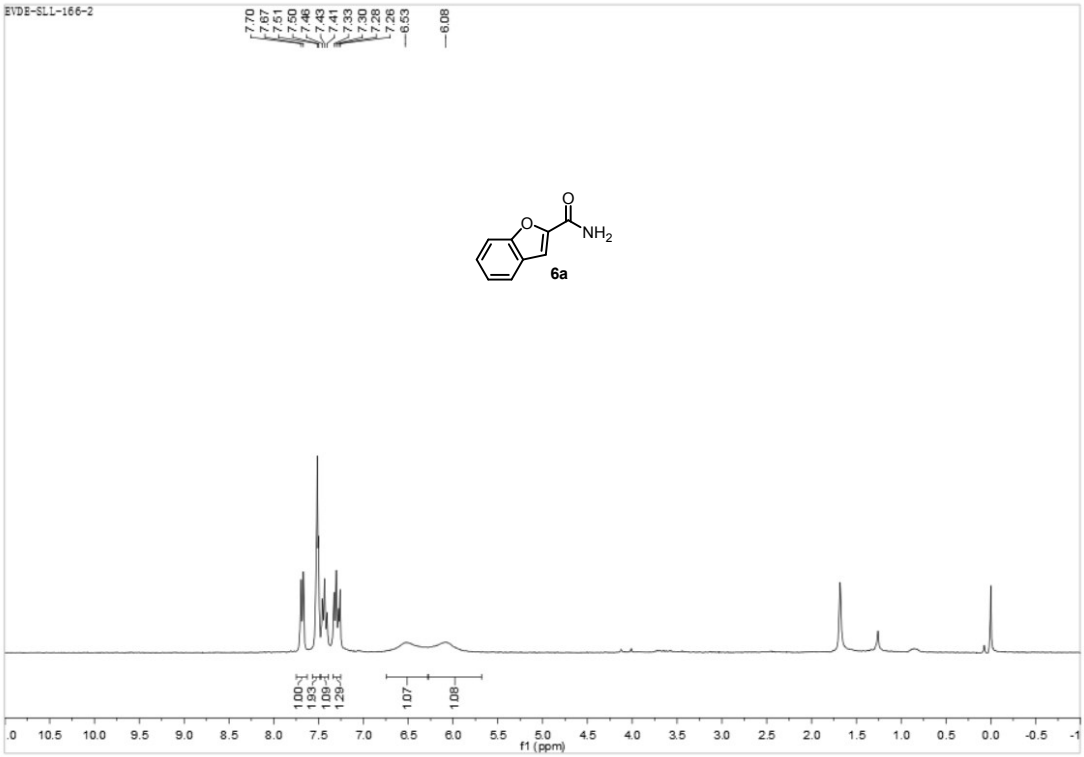

EVDE-SLL-143-2-C.10.fid
165.26
141.98
138.86
132.68
127.27
126.09
125.73
104.66
61.29
32.64
31.51
25.26
O
NH
OH
2z
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
f1 (ppm)

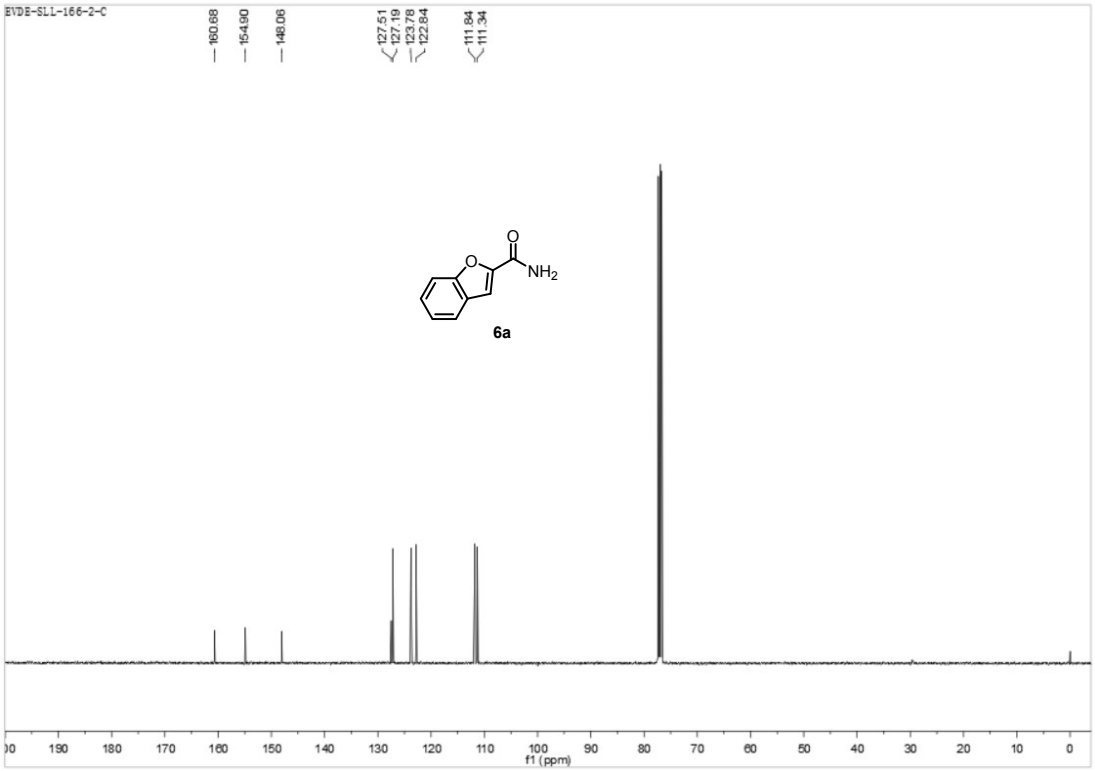

EVDE-SLL-27.10.fid
8.64
8.50
8.48
7.85
7.82
7.79
7.78
7.77
7.76
7.74
7.73
7.57
7.54
7.53
7.52
7.51
7.51
7.48
7.47
7.45
7.45
3.63
3.61
3.60
3.58
2.80
2.78
2.77
2.77
2.75
1.89
1.87
1.85
1.84
1.82
1.80
O
NH
Ph
HO
3a'
H2O
grease
0.90
1.04
2.10
6.02
2.00
2.00
2.06
f1 (ppm)

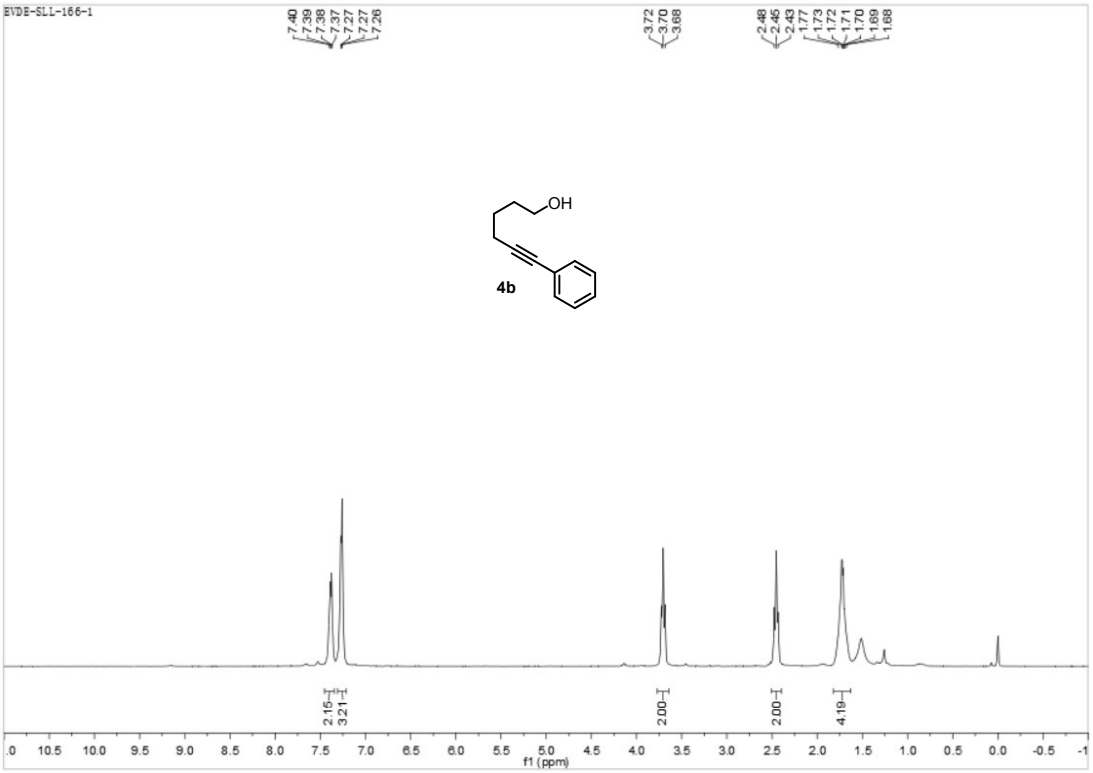

EVDE-SLL-5-1
162.14
137.74
137.04
135.53
132.82
129.34
128.98
128.86
128.05
128.48
125.65
123.70
113.46
62.24
33.22
23.46
O
NH
Ph
HO
3a'
f1 (ppm)

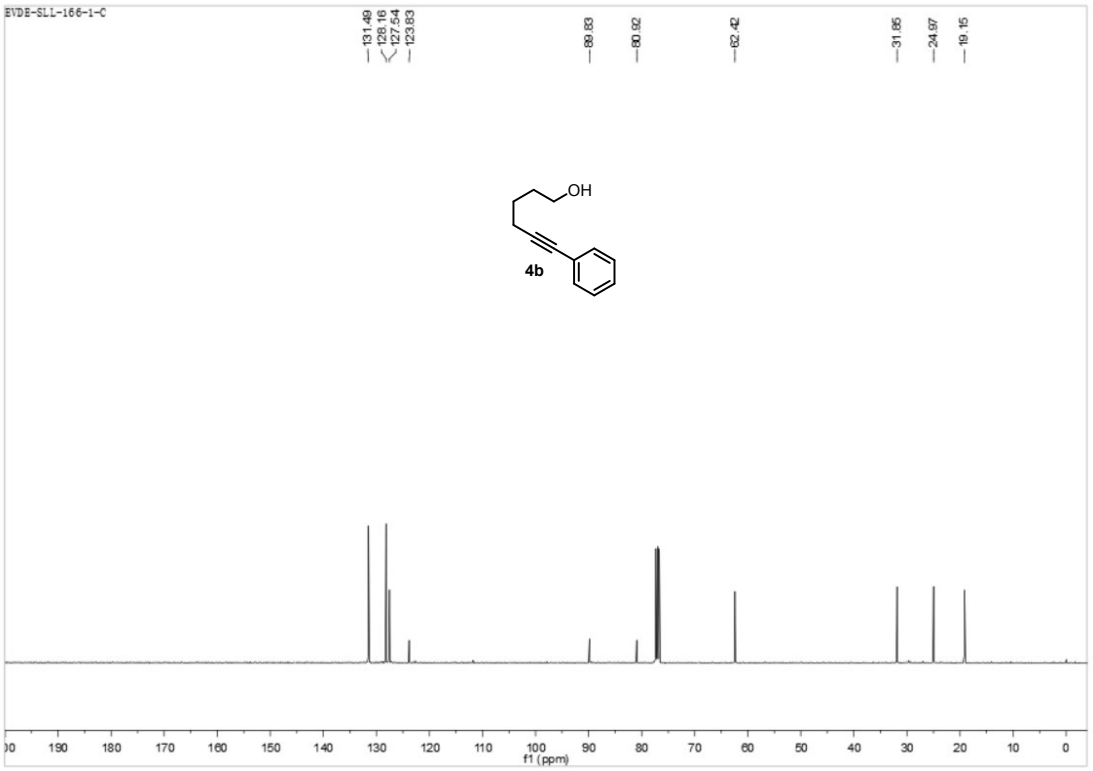

EVDE-SLL-5-2
12.40
8.43
8.40
7.57
7.55
7.52
7.50
7.48
7.30
7.28
7.26
7.14
7.11
4.06
3.71
2.75
2.73
2.70
1.94
1.92
O
NH
OH
Ph
2a'
grease
0.98
1.00
5.03
2.28
1.01
0.96
2.12
1.98
2.05
f1 (ppm)

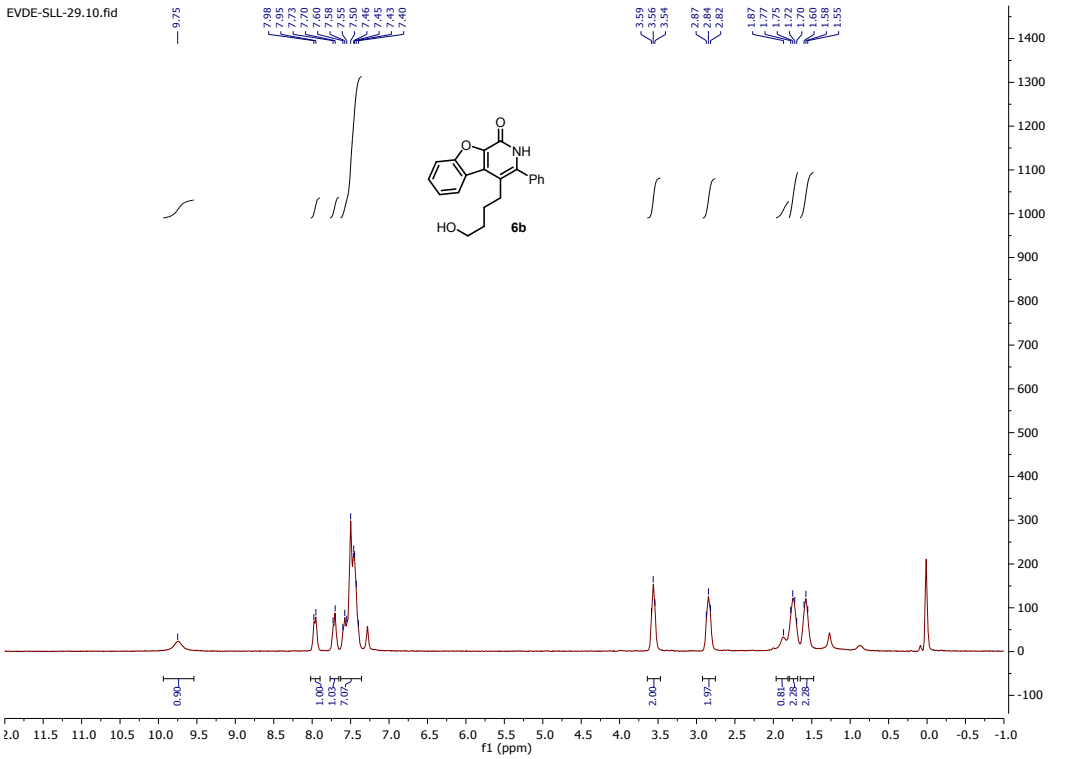

EVDE-SLL-5-2-C
164.82
139.37
138.93
135.97
132.71
131.01
128.81
127.80
126.99
126.20
125.31
123.74
118.10
60.85
32.66
27.07
O
NH
OH
Ph
2a'
f1 (ppm)

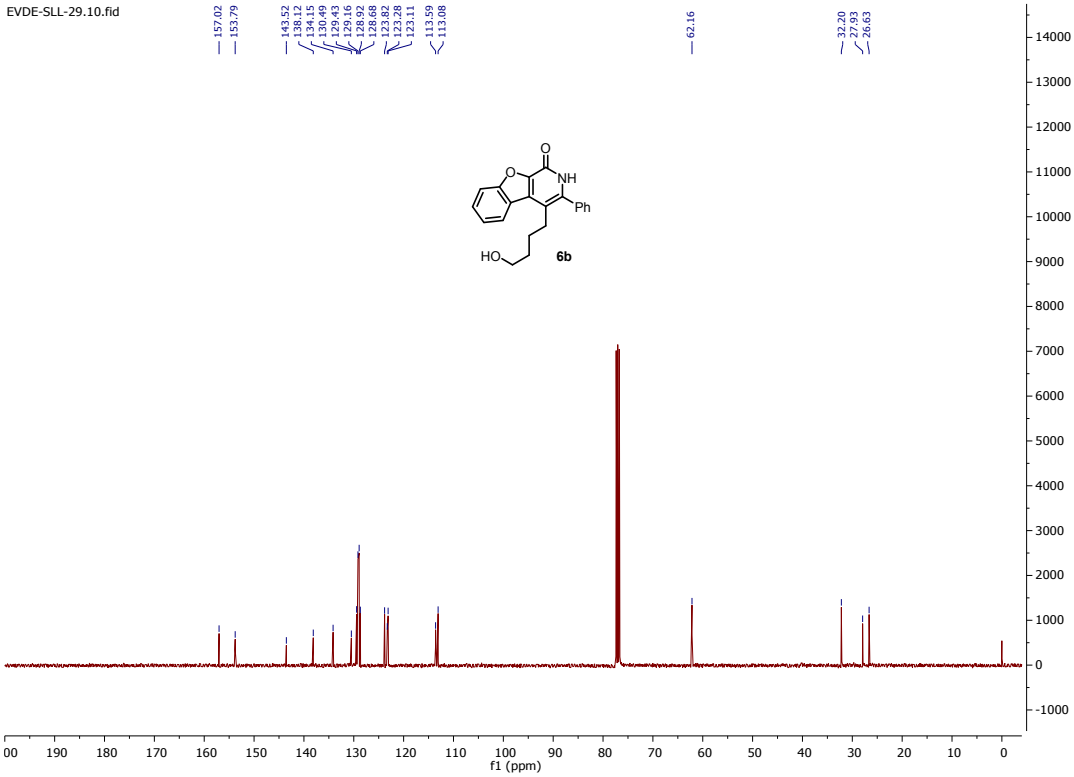

EVDE-SLL-166-2
7.70
7.67
7.51
7.50
7.46
7.43
7.41
7.33
7.30
7.28
7.26
6.53
6.08
O
O
NH2
6a
1.00
1.93
1.09
1.29
1.07
1.08
f1 (ppm)

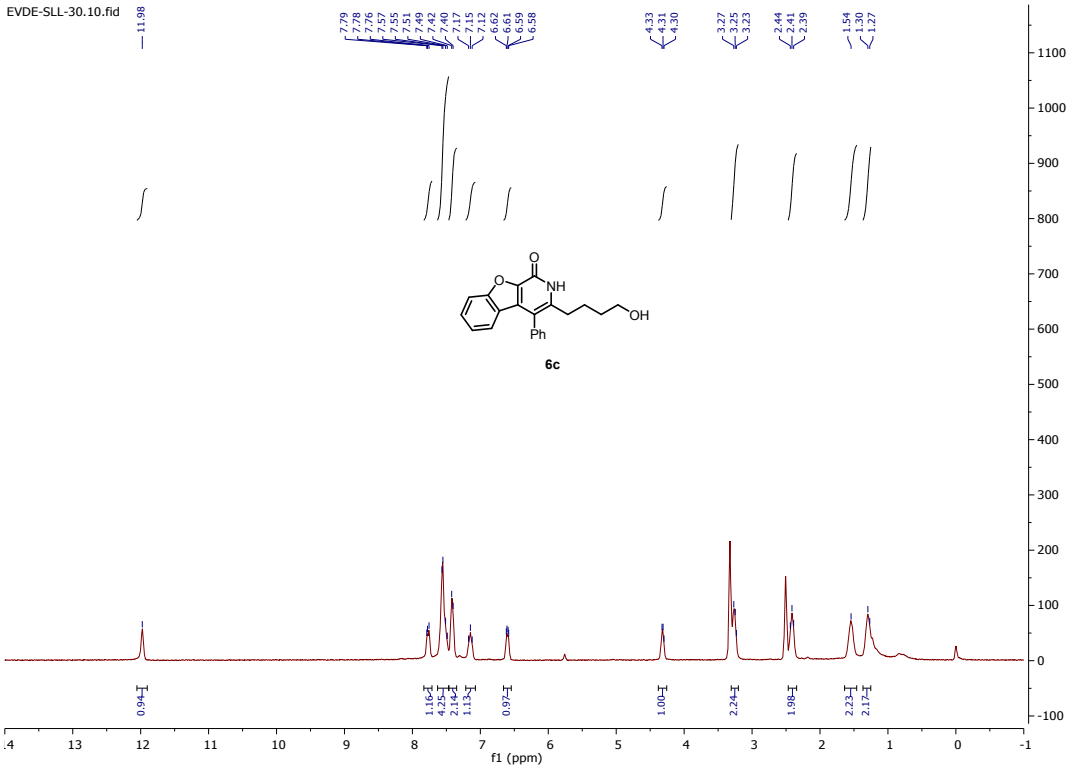

EVDE-SLL-166-2-C
160.68
154.90
148.06
127.51
127.19
123.78
122.84
111.84
111.34
O
O
NH2
6a
f1 (ppm)

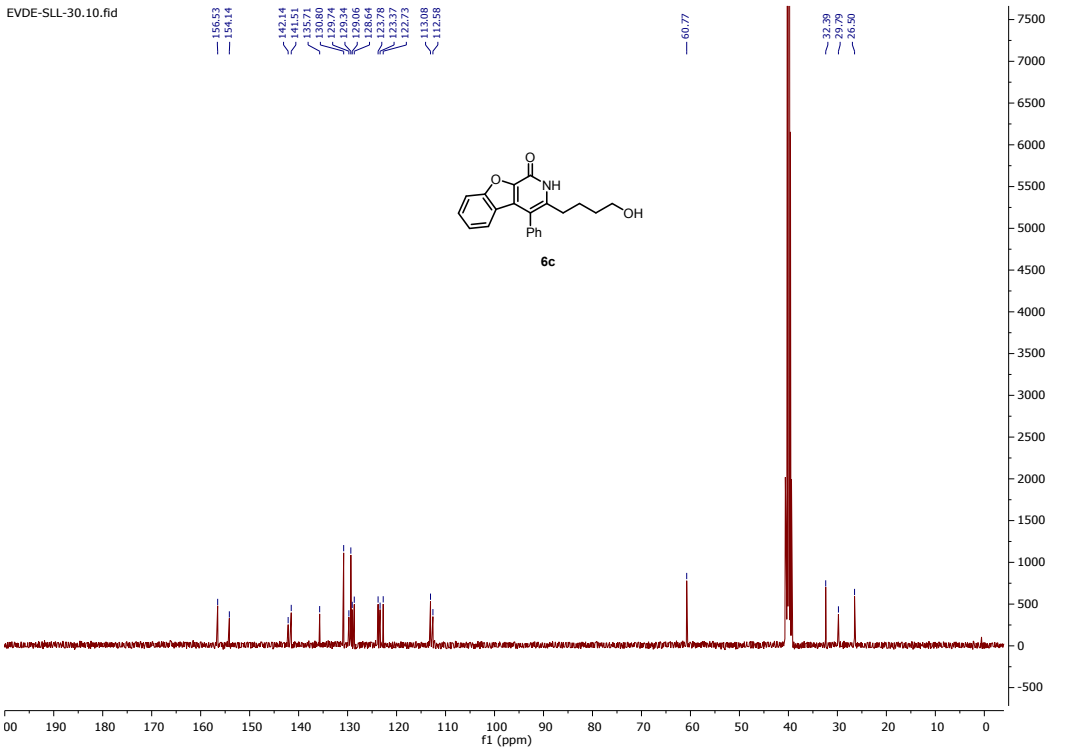

EVDE-SLL-166-1
7.40
7.39
7.38
7.37
7.27
7.27
7.26
3.72
3.70
3.68
2.48
2.46
2.43
1.77
1.73
1.72
1.71
1.70
1.69
1.68
OH
4b
2.15
3.21
2.00
2.00
4.19
f1 (ppm)


EVDE-SLL-166-1-C
131.49
128.16
127.54
123.83
89.83
80.92
62.42
31.85
24.97
19.15
OH
4b
f1 (ppm)


EVDE-SLL-29.10.fid
9.75
7.98
7.95
7.73
7.70
7.60
7.58
7.55
7.50
7.46
7.45
7.43
7.40
3.59
3.56
3.54
2.87
2.84
2.82
1.87
1.77
1.75
1.72
1.70
1.60
1.58
1.55
O
NH
Ph
HO
6b
0.90
1.00
1.03
7.07
2.00
1.97
0.81
2.28
2.28
f1 (ppm)


EVDE-SLL-29.10.fid
157.02
153.79
143.52
138.12
134.15
130.49
129.43
129.16
128.92
128.68
123.82
123.28
123.11
113.59
113.08
62.16
32.20
27.93
26.63
O
NH
Ph
HO
6b
f1 (ppm)


EVDE-SLL-30.10.fid
11.98
7.79
7.78
7.76
7.57
7.55
7.51
7.49
7.42
7.40
7.17
7.15
7.12
6.62
6.61
6.59
6.58
4.33
4.31
4.30
3.27
3.25
3.23
2.44
2.41
2.39
1.54
1.30
1.27
O
NH
OH
Ph
6c
0.94
1.16
4.25
2.14
1.13
0.97
1.00
2.24
1.98
2.23
2.17
f1 (ppm)


EVDE-SLL-30.10.fid
156.53
154.14
142.14
141.51
135.71
130.80
129.74
129.34
129.06
128.64
123.78
123.37
122.73
113.08
112.58
60.77
32.39
29.29
26.50
O
NH
OH
Ph
6c
f1 (ppm)

9. Cartesian Coordinates of DFT Optimized Structures

Coordinates

Three-Carbon Tethered Substrate

1a'

C,0,-2.7134183547,0.5633345313,1.7171696684

C,0,-4.095011623,0.6879939055,1.7098922075

C,0,-4.8417466208,0.1198850659,0.6818196454

C,0,-4.2004543798,-0.5694668287,-0.3412563422

C,0,-2.8173223472,-0.703108427,-0.3317618094

C,0,-2.0644734722,-0.1431201672,0.7032641752

H,0,-2.1158211766,1.0107264333,2.4998991115

H,0,-4.5908517216,1.2316910049,2.5039219847

H,0,-5.9196006287,0.22164368,0.6735427221

H,0,-4.7761647966,-0.9960760482,-1.1527515072

H,0,-2.3270623452,-1.2124789053,-1.1513852335

C,0,-0.5717025958,-0.247673908,0.7877208905

O,0,0.1143988387,0.5687826656,1.3696291326

N,0,-0.0339255211,-1.3257931191,0.1133130181

H,0,-0.5911288472,-2.1625123062,0.0216906049

O,0,1.288285854,-1.6620463861,0.38366835

C,0,2.1898821399,-0.9742513017,-0.5005430917

H,0,2.064900358,0.1044214786,-0.3727449716

H,0,1.9439903627,-1.2420810565,-1.5336010394

C,0,3.6015058667,-1.4150810857,-0.1522531382

H,0,4.2434320635,-1.172281571,-1.003634782

H,0,3.6126407749,-2.5020795124,-0.0419782063

C,0,4.2074355568,-0.7526022737,1.1014202358

H,0,5.2492032075,-1.074483647,1.1951148121

H,0,4.2339214258,0.3321387815,0.9490101817

C,0,3.4939383845,-1.0356593938,2.3380597652

C,0,2.8433225154,-1.2528262212,3.3266895962

C,0,1.9744293525,-1.4684419661,4.4342999274

C,0,0.7302031696,-0.81859031,4.4691539112

C,0,2.3229278379,-2.3250735596,5.4874530786

C,0,-0.1372280446,-1.0286739973,5.5312486545

H,0,0.4655405018,-0.1583844289,3.6538249614

C,0,1.448441032,-2.527967645,6.5461950291

H,0,3.2810157848,-2.8278440878,5.4646556693

C,0,0.216008303,-1.8825734318,6.5725072871

H,0,-1.0949385203,-0.522881187,5.5472454968

H,0,1.7295181911,-3.1927439775,7.3535908089

H,0,-0.4639861055,-2.0433074368,7.3996812251

^{1}A

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C,0,-1.3204529844,2.2943034096,-0.4327293118

C,0,-1.9886052173,1.028034894,-0.5182682413

C,0,-1.1905168478,-0.1169115846,-0.7073571937

C,0,0.2300184756,-0.0294861771,-0.7594832693

C,0,0.8808485202,1.216756706,-0.6309969548

H,0,0.5567590995,3.3512626716,-0.3416529277

H,0,-1.9018995819,3.1794458555,-0.208143472

H,0,-1.6281407428,-1.101538011,-0.6755897582

H,0,0.8009776962,-0.945276976,-0.7701647705

C,0,2.3760763128,1.3133314116,-0.5652188588

H,0,2.7730923322,1.6204653552,-1.5366530455

H,0,2.6833404939,2.0497290157,0.1776364843

H,0,2.8180192469,0.3536615905,-0.3014866362

C,0,-3.4934579495,0.95819374,-0.366568793

H,0,-3.7905993134,1.8532827277,0.1882553317

C,0,-4.1535968223,1.0140515713,-1.7525796513

H,0,-5.2406973604,1.0372324397,-1.6564661216

H,0,-3.8426029179,1.8999244818,-2.3100000871

H,0,-3.8845206782,0.1338107706,-2.3410824013

C,0,-3.9671266008,-0.2572577174,0.4345059528

H,0,-3.4650504466,-0.3085419113,1.4010132786

H,0,-5.0429318256,-0.1908485678,0.6050200207

H,0,-3.7780108286,-1.1914843099,-0.0973589633

Ru,0,-0.4730976405,0.9568816322,1.0583656411

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C,0,-0.2481091832,2.0736442578,3.2953519621

C,0,-0.5923910822,-2.748763637,3.3241341047

H,0,-0.5578845021,-3.8005035116,3.0500367092

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O,0,-0.5703297763,-0.6098387436,2.3636657799

O,0,0.7751295351,1.7482533627,2.6207994083

O,0,-1.3816509831,1.9383970007,2.7444975373

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C,0,-1.8773798875,0.5197244825,-0.5228476052

C,0,-0.5551532178,0.1720295087,-0.8488019264

C,0,0.4885702762,1.0623967464,-0.5578005322

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H,0,-1.3348817406,3.825349486,0.3071885922

H,0,-3.139010497,2.1241467573,0.1982970622

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H,0,-4.2989132765,-1.1062817204,-2.3508932682

H,0,-3.6583443717,0.5245217304,-2.5800439863

H,0,-2.6085447379,-0.8784702606,-2.8118300048

C,0,-2.7539023009,-1.8423930818,-0.1777659438

H,0,-2.4580649448,-1.8050792756,0.8707377311

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H,0,-3.5273718675,-1.4485121045,4.1144627106

H,0,-3.222569667,0.02700572,5.0173785792

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H,0,3.9180015323,0.3776804461,3.6614632765

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O,0,-1.9197930151,0.120055641,2.7476001101

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H,0,-2.1878846117,0.2727634655,1.8947904346

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C,0,-3.7798872067,-3.4424133141,-0.4884119439

H,0,-3.5019329392,-3.7126088622,-1.5070977783

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H,0,-1.5254123732,2.5676975941,-1.4604224811

H,0,-3.1675554416,3.1287931579,-1.7851870324

C,0,-4.1491826836,2.9806640495,0.7952562902

H,0,-4.4573253235,2.5022697371,1.7265662294

H,0,-3.9790077903,4.0394986961,0.9985789704

H,0,-4.9734737489,2.901879448,0.0812298987

Ru,0,-1.8816320395,-0.7801150675,-0.8601495776

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C,0,0.6783215354,2.3439882732,1.1289194071

H,0,0.3757342389,4.0692392121,2.3547439265

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H,0,-0.348175132,-1.6522924678,4.6806807099

H,0,-0.0278589411,0.0918821073,4.7806268843

C,0,1.7426495765,-1.125196317,4.502083495

H,0,1.8718098737,-1.3114397377,5.5717998877

H,0,2.3329270222,-0.240345898,4.2639050523

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H,0,2.9921312387,-2.8923894371,4.3124212141

H,0,1.4588655887,-3.0252526478,3.4768124244

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C,0,3.5509365284,-1.5812166099,1.4829068598

C,0,4.2671726279,-1.1226795202,0.3366854439

C,0,3.5812246555,-0.6704169922,-0.797495834

C,0,5.6703362975,-1.1123242952,0.328131597

C,0,4.2756689334,-0.2247200998,-1.9120815822

H,0,2.503696182,-0.6760603908,-0.8188465968

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H,0,7.4427774052,-0.6568821768,-0.7820674401

H,0,6.2102580577,0.1309664497,-2.7809690965

C,0,0.1107335257,-2.3080722337,-1.0607790264

C,0,1.3121486257,-3.1652554841,-1.2569331171

H,0,1.0102067039,-4.1720386965,-1.5409593135

H,0,1.8922952214,-2.7278710153,-2.070950509

H,0,1.9248326819,-3.1787029558,-0.3578630548

O,0,-0.938046228,-2.4716938293,-1.7541248998

O,0,0.0786577514,-1.3746986692,-0.1979231636

C,0,1.0972852199,1.8699560242,-0.1143345981

H,0,1.0113360491,0.8264122549,-0.3766148913

C,0,0.0444782454,1.3023719747,-4.2125665414

H,0,1.0150508175,1.2931034139,-4.7037142195

H,0,-0.1917775125,2.3134688652,-3.8759119706

H,0,-0.7319235103,1.0040835971,-4.918255193

C,0,0.0467002511,0.3596519423,-3.0178894237

O,0,-1.1014538166,0.3339102657,-2.4167934439

O,0,1.0606656838,-0.2533588511,-2.7013083563

N,0,0.5686196605,0.17652704,2.1921234586

H,0,1.0164223583,-0.247428357,1.3912942194

^{3}A1

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C,0,3.1442904356,-0.2028473501,0.8217395676

C,0,2.610646739,1.0993352241,0.812221334

C,0,2.8101262917,1.9610839205,-0.301389278

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H,0,4.4955510842,-0.1383684919,-2.3438165228

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H,0,2.3771186702,2.9519575984,-0.2655271905

C,0,3.9053566267,2.5517991223,-2.5075428562

H,0,4.6464194619,2.1526576784,-3.1991780714

H,0,2.9830446748,2.736491811,-3.0619717957

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C,0,3.0078252379,-1.097715617,2.0330216591

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C,0,-1.5332480168,-2.7606116348,1.0696209317

C,0,-0.662805652,-0.8974195926,2.335145437

H,0,-0.1113669489,-1.3173985252,4.354686818

H,0,-0.7549947791,-3.7141453973,4.2278332349

H,0,-1.6707071721,-4.6313722239,2.1152519826

H,0,-1.9418718722,-3.1445331089,0.1447186176

C,0,-0.239577224,0.5324538028,2.5000018142

O,0,0.4459714784,0.908618251,3.4450121369

O,0,-0.1955027106,2.6765496486,1.492121087

C,0,-0.8474787675,3.5691249512,2.4148184623

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H,0,-2.7096010402,4.3926173823,2.9646968367

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H,0,-3.8289315221,4.3487427012,0.9527148957

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C,0,-3.3771197653,-0.6537316062,-1.4634331104

C,0,-5.2986176285,-0.5733958094,-0.0034492233

C,0,-3.7598739667,-1.9160074475,-1.8927491476

H,0,-2.4669286528,-0.2217143267,-1.8476893957

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H,0,-5.8922681246,-0.0487192073,0.7336738344

C,0,-4.9073980021,-2.5132868286,-1.3813054715

H,0,-3.1443962469,-2.4194374327,-2.6267461905

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C,0,-1.3859588313,2.0667598664,-2.9303343318

H,0,-1.1049527771,2.9385462634,-3.5186065199

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H,0,-2.1146803719,2.3263164069,-2.1652525556

O,0,0.9326585122,1.4460106306,-2.919165322

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H,0,-1.2771438986,-0.8145627988,0.2597098466

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H,0,-0.9932688627,-3.8772367313,-2.9511748031

H,0,-0.1217279674,-3.9742686977,-1.3933588825

H,0,0.7743588233,-4.0785554661,-2.9020149378

C,0,0.1015754456,-2.0991829285,-2.4238328255

O,0,1.1444786016,-1.738114189,-1.7124076826

O,0,-0.6431393156,-1.3582845896,-3.0393624371

N,0,-0.7113957184,1.3876326695,1.5583949097

H,0,-1.0049810999,1.0938946021,0.6346269178

[1]A2

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C,0,2.9980406449,-0.5231512827,-1.8236022276

C,0,2.5554511122,-1.4959543625,-0.8648771425

C,0,2.8826848222,-1.278372785,0.4906282197

C,0,3.5276675566,-0.0838998199,0.9165459181

C,0,3.8812541584,0.9130079005,-0.0163444911

H,0,3.8628588008,1.4175342168,-2.135115902

H,0,2.7367022873,-0.6374203852,-2.8657283162

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^{3}A2

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^{1}A3

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C,0,-1.5870560442,0.6174390654,0.9376763668

C,0,-2.9362930713,0.4436498653,0.4670152264

C,0,-3.7717152016,1.5550238273,0.2881384451

C,0,-3.4470272512,-0.8340123004,0.200512799

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H,0,-5.7130601753,2.2618024966,-0.2775281484

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^{3}C

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^{3}D

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^{1}E

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^{3}E

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C,0,5.7759126523,1.0892813761,1.180969569

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H,0,5.3867983648,0.8055148136,2.1600262761

H,0,6.6170808978,0.4303948067,0.9511733673

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H,0,4.4733069032,1.3307315673,-2.0382787881

H,0,5.5125324844,2.4965780684,-1.2028900392

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Ru,0,-0.1838056155,0.1599531105,0.0785191707

C,0,-1.116075531,-2.8940298011,0.7793454386

C,0,-1.5184921462,-3.6495105406,-0.2896711055

C,0,-2.3451473651,-3.0814462089,-1.275075697

C,0,-2.7505593578,-1.7760631757,-1.170950237

C,0,-2.3393027921,-0.9582112191,-0.0884547861

C,0,-1.5055181701,-1.5375046202,0.9112877677

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H,0,-2.6662592876,-3.6795980452,-2.1184978681

H,0,-3.3975038295,-1.3435122155,-1.922901923

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O,0,-1.6566876232,-0.9220224914,3.2530813318

N,0,0.0035905169,-0.0105627395,1.8976972548

O,0,1.1961826507,1.7444490346,-0.0626985594

C,0,0.8146898433,3.1313572213,-0.0063908197

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H,0,1.6452581831,3.6725781156,0.4532218291

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C,0,-1.728799948,2.8139689454,0.1273084154

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H,0,-1.810319557,3.2657436503,-0.8689839073

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C,0,-2.8155709277,0.4643168127,-0.0550694661

C,0,-4.2552995878,0.7517181353,-0.1164818244

C,0,-5.1650180958,-0.1394907784,0.4706006021

C,0,-4.7564981951,1.9030954471,-0.738163367

C,0,-6.52676774,0.1218136283,0.4511366196

H,0,-4.7941088812,-1.030510781,0.9605292984

C,0,-6.1206620604,2.1577947193,-0.7642902539

H,0,-4.0768703524,2.5870261881,-1.2267010692

C,0,-7.0104280775,1.2712459844,-0.1666201993

H,0,-7.2126165431,-0.5713083533,0.9215157471

H,0,-6.490867895,3.048111382,-1.2568733528

H,0,-8.0739125123,1.4726495556,-0.1849705777

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H,0,2.1999096099,-2.2296127023,-2.9848655343

H,0,1.0247205746,-1.4816894098,-4.0642535139

H,0,2.7015532296,-0.8693804497,-4.0269502797

C,0,1.5007128299,-0.3301901105,-2.3353691334

O,0,2.0235686539,0.7898996502,-2.2522880539

O,0,0.5809875618,-0.7861129727,-1.5432099189

H,0,1.639608179,1.5134145961,-0.9467500806

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C,0,-2.505963309,1.7203288107,0.8424593929

C,0,-2.9965025894,0.4805643413,1.2436165061

C,0,-3.878503339,-0.2503531713,0.435849677

C,0,-4.2607842336,0.3205936837,-0.7724418356

C,0,-3.7741940576,1.5645000936,-1.1686976353

C,0,-2.8789712913,2.2796900779,-0.3828557882

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C,0,-5.5444281902,-1.4046737,1.9137274044

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Ru,0,-0.303357733,-0.3887089115,0.3837854485

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C,0,1.805156279,2.2752034493,-0.4738792787

C,0,1.7170778424,1.1704279573,0.4060452979

C,0,1.1861445945,1.3975725153,1.7032596303

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H,0,-1.3374338402,-4.0510170673,0.7350861287

C,0,0.7241936716,-3.4739178351,0.4856007922

H,0,1.0569367357,-4.5143403592,0.4348154792

H,0,0.7998456405,-3.1598716418,1.5278839277

C,0,1.6432285728,-2.5999650923,-0.3824683438

H,0,2.6865729092,-2.8699364718,-0.1949171951

H,0,1.4478002145,-2.8124638248,-1.4407741427

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H,0,3.6353063779,-1.5241341236,-1.9845129635

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H,0,6.6919721482,1.2054754884,0.775343845

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H,0,7.6004586078,-0.2093867923,-1.0465087203

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H,0,-2.0931547771,1.2164914249,-3.6705928118

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C,0,-1.3620971941,-0.3988111194,-2.4989074032

O,0,-1.8502540683,-1.5441164224,-2.3346325288

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H,0,5.4185121447,-1.8029995872,-2.022118144

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H,0,3.2073494833,-2.6868766289,1.6029934695

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H,0,4.9624998284,-2.4871222439,1.6383862554

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C,0,-0.5136914267,1.6794553507,-1.2977531711

O,0,0.2590174955,2.5255383452,-1.752859436

N,0,-0.1298856803,0.3624003477,-1.0934399089

O,0,0.9083526938,-1.4763520036,1.1101627382

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H,0,-0.3763386362,-3.0752654674,0.9851559627

H,0,1.3422106105,-3.4650131091,0.8572701243

C,0,0.4731892797,-2.6944866182,-0.9581786949

H,0,0.4838421635,-3.7159662225,-1.3505676271

H,0,1.3606543524,-2.1995185966,-1.3508614687

C,0,-0.7883264642,-1.9974135783,-1.4526990204

H,0,-0.7233992851,-1.9128005769,-2.5439060387

H,0,-1.6380070078,-2.6461122575,-1.2484329245

C,0,-1.1186440448,-0.6034057463,-0.9559176783

C,0,-2.407059581,-0.3070030507,-0.610634625

C,0,-3.4313922798,-1.3619018257,-0.3767060029

C,0,-4.393360846,-1.6747453637,-1.3389412566

C,0,-3.4618615329,-2.0372848652,0.8464029191

C,0,-5.347969703,-2.6562811113,-1.0976544289

H,0,-4.3848650193,-1.1454233638,-2.2840573813

C,0,-4.4177861892,-3.0179899101,1.0902519397

H,0,-2.7355365003,-1.7718122199,1.6053887447

C,0,-5.3609923218,-3.3332381416,0.1178602096

H,0,-6.0821205694,-2.8926741123,-1.8581884618

H,0,-4.4286611305,-3.5329758105,2.0432462855

H,0,-6.1048776038,-4.0970905801,0.3073403012

C,0,-1.3815778119,2.0167934882,2.7998883185

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H,0,-2.0498111947,2.397539205,2.0250907254

H,0,-1.9759295853,1.6184170042,3.6187099642

C,0,-0.5264657949,0.93198712,2.192515502

O,0,-0.8029575539,-0.2676276573,2.4177928712

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H,0,0.139267708,-1.0800723253,1.6901726689

^{1}H2

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C,0,-2.6892807517,0.59188792,-1.3403281317

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C,0,-3.7647254416,1.7021353914,0.4747376521

C,0,-4.1884041272,0.4720003475,0.9671790579

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H,0,-4.7788657508,0.4407690024,1.8769034579

C,0,-4.2984638425,-2.049031145,0.8794212738

H,0,-4.1780730171,-2.8473319019,0.147242536

H,0,-3.6988968818,-2.3211962732,1.7532862587

H,0,-5.3429089266,-2.0287849846,1.1977185785

C,0,-2.5267665237,3.1020048589,-1.2865000654

H,0,-1.4653989799,2.9649234875,-1.5250660564

C,0,-3.2589376154,3.3940054494,-2.6075211346

H,0,-2.87072079,4.3042169139,-3.0707684558

H,0,-3.1451724598,2.5763100628,-3.3199724118

H,0,-4.3274452418,3.5339281599,-2.4254938673

C,0,-2.6401270987,4.3004893221,-0.3431103372

H,0,-2.1319529393,4.1155645007,0.6028047239

H,0,-2.1912086989,5.1818432924,-0.8061942621

H,0,-3.6852670999,4.5438615977,-0.1355029283

Ru,0,0.4874612065,-0.1495673559,-0.0030616641

C,0,-0.432003324,-3.9048035498,-1.891264317

C,0,-1.0085976993,-4.7486446562,-0.9517490796

C,0,-1.169107818,-4.2981505658,0.3550042467

C,0,-0.7450513875,-3.0243167754,0.7381357678

C,0,-0.1664146393,-2.1604884133,-0.1859056238

C,0,-0.0314728156,-2.6358080265,-1.4925323784

H,0,-0.2978243651,-4.2034641733,-2.9237485534

H,0,-1.3365826816,-5.741356661,-1.2318601279

H,0,-1.6363282834,-4.9423586761,1.0908073359

H,0,-0.9087612003,-2.7295264994,1.7626118349

C,0,0.4985890891,-1.6201484064,-2.4252303987

O,0,0.8598095962,-1.7557850742,-3.57147982

N,0,0.4930907408,-0.3893362448,-1.7452122773

O,0,-0.8388749981,0.4178640527,1.5023409889

C,0,-1.0888555945,-0.166452103,2.7767753009

H,0,-1.6377630216,-1.0932377632,2.6160198328

H,0,-1.7513975375,0.513832042,3.3180470422

C,0,0.1865235448,-0.3929888617,3.5828583922

H,0,-0.0875459818,-0.7686971444,4.5722603009

H,0,0.6797224617,0.5713758683,3.7264165595

C,0,1.1829091711,-1.3762514762,2.9342604911

H,0,2.0920680828,-1.4240018993,3.5416738278

H,0,0.7668108124,-2.3847459756,2.9184216589

C,0,1.5609525324,-0.9649348462,1.5755366788

C,0,2.3607438228,-0.5033661317,0.7008136361

C,0,3.6747266304,-0.1366482294,0.2440066859

C,0,4.7894731876,-0.5147945177,1.0089782135

C,0,3.866149306,0.5744287066,-0.9458250817

C,0,6.0675471923,-0.1842680489,0.5888973287

H,0,4.6430010616,-1.0752915485,1.9234684359

C,0,5.150074575,0.8995114325,-1.3591080307

H,0,3.0058983389,0.8747820109,-1.5261872467

C,0,6.2509460338,0.5241389374,-0.5963700508

H,0,6.9227284383,-0.4815087481,1.1824430018

H,0,5.2909548867,1.4479644784,-2.2815166058

H,0,7.2506154274,0.7799227651,-0.9239997523

C,0,1.1397306904,4.2962013643,0.3275511506

H,0,0.5124157058,4.7198692087,-0.4603687477

H,0,1.0572033112,4.9327505646,1.2060665429

H,0,2.1645163072,4.2589168849,-0.0357290935

C,0,0.6309670417,2.9087672144,0.6294161572

O,0,1.100662839,1.9574784041,-0.0608410736

O,0,-0.2480215009,2.7802246414,1.5272191918

H,0,-0.6557180458,1.4844181018,1.5747931456

^{3}H2

C,0,-2.4122110318,-0.3434836963,-1.9555838676

C,0,-2.0463754772,0.8944572673,-1.4171380193

C,0,-2.7922104265,1.4808398112,-0.3775862462

C,0,-3.8663085256,0.7541435705,0.1257266173

C,0,-4.2084573701,-0.4867673721,-0.4040286906

C,0,-3.4969531635,-1.0582539374,-1.4559570653

H,0,-1.8281352323,-0.7523034901,-2.7695220643

H,0,-1.2567994162,1.4662453698,-1.8895739093

H,0,-4.4622779148,1.1575120027,0.933307238

H,0,-5.0521162155,-1.023878851,0.0153466509

C,0,-3.8531801814,-2.417485971,-1.9892605865

H,0,-3.4644426653,-3.1961037971,-1.3293830564

H,0,-4.934942396,-2.54777572,-2.0558367206

H,0,-3.4258280884,-2.5820671882,-2.9785622335

C,0,-2.4568793372,2.8864684195,0.0772085057

H,0,-1.3693634186,2.9668027852,0.076236554

C,0,-2.9928522095,3.9078764914,-0.9416067217

H,0,-2.7033510723,4.9211998835,-0.6542909503

H,0,-2.6029242645,3.7132766518,-1.9417537873

H,0,-4.083658451,3.8662842023,-0.991945523

C,0,-2.9445112461,3.2242353941,1.4858603957

H,0,-2.6161149511,2.4733359963,2.2036531761

H,0,-2.5430296467,4.1903051555,1.7959290022

H,0,-4.0341151246,3.2934345823,1.5309776311

Ru,0,0.1314398183,-0.1810428257,-0.0930197881

C,0,-0.9499942293,-4.2953875937,-0.4759712568

C,0,-1.8661443086,-4.591791682,0.5269466516

C,0,-2.2825760931,-3.5825863249,1.3914405979

C,0,-1.7570543359,-2.2920397288,1.2985866379

C,0,-0.8036424202,-1.9903607919,0.3315686349

C,0,-0.4458524376,-3.0048683675,-0.5640916067

H,0,-0.6370394647,-5.0361663321,-1.2015070249

H,0,-2.2734362065,-5.5904606653,0.6199682897

H,0,-3.0279788351,-3.798021488,2.1483828264

H,0,-2.1280831897,-1.5322256469,1.9713523059

C,0,0.415248498,-2.5236874368,-1.6819078337

O,0,0.8546880214,-3.1937809308,-2.5994904829

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O,0,-0.5449740763,0.9496079695,1.7450017093

C,0,-0.6185712065,0.5299433605,3.1070456548

H,0,-1.4520207456,-0.166860116,3.1837801013

H,0,-0.8641327008,1.4023322187,3.720188774

C,0,0.6635338694,-0.1124557003,3.6298395915

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[1]I3

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^{3}I3

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H,0,1.2871784816,4.1955209456,-2.111984586

H,0,2.2145295834,5.6716455846,-0.3182455636

H,0,2.929547555,4.6528913094,1.8258493756

H,0,2.7618418655,2.2479170772,2.1792668251

C,0,0.8766038253,1.5715539973,-2.0137908152

O,0,0.2281284073,2.0251975387,-2.9336839665

N,0,0.9643074126,0.1906389062,-1.7854141655

O,0,-0.7525574986,-0.4065473603,1.4913908227

C,0,-0.0042380216,-0.8288085232,2.6189777073

H,0,0.2062051193,-1.9034049345,2.5434173916

H,0,-0.6422272738,-0.6730415847,3.4955579631

C,0,1.300384429,-0.0655612516,2.8163560079

H,0,1.7390645423,-0.400324834,3.7610159253

H,0,1.0675479347,0.9949970304,2.9253731234

C,0,2.3240689987,-0.2846083599,1.683633802

H,0,3.2922715097,0.12291061,1.993349076

H,0,2.4655425758,-1.3574304669,1.5475712685

C,0,1.8807126938,0.3322421528,0.3787602694

C,0,1.8511414194,-0.3931545061,-0.8520780436

C,0,2.6710660254,-1.5490577279,-1.268550989

C,0,2.2171048654,-2.4267519979,-2.2603241564

C,0,3.9403820773,-1.7568584481,-0.7209215875

C,0,3.0008782525,-3.4937231692,-2.6714056301

H,0,1.2463118854,-2.2592712414,-2.705544511

C,0,4.7232712031,-2.8289098761,-1.1315236116

H,0,4.3266672714,-1.0637289719,0.0138038501

C,0,4.2548690057,-3.7045660196,-2.103714433

H,0,2.6335579405,-4.1649097803,-3.4376131607

H,0,5.705409089,-2.972428841,-0.698713087

H,0,4.8651289667,-4.5390461263,-2.4250558396

^{3}J3

C,0,1.3534825368,2.4008057936,-1.0134863876

C,0,2.0555707791,1.1930966201,-1.1959250944

C,0,3.1896651106,0.899745361,-0.4079904756

C,0,3.5745926291,1.8436087367,0.5329536075

C,0,2.8804048751,3.0411515844,0.7060221762

C,0,1.7623815694,3.344001618,-0.0557029338

H,0,0.5583532393,2.6544233184,-1.7058874034

H,0,1.798083848,0.5615305275,-2.0373818993

H,0,4.4388691277,1.6434494386,1.1557807528

H,0,3.2211696145,3.7466131199,1.4545975494

C,0,0.9805105271,4.6116533509,0.1450040354

H,0,0.6896808476,5.0568354601,-0.8087509555

H,0,0.0609891581,4.4117945898,0.7030896347

H,0,1.5537363224,5.3504375394,0.7054172121

C,0,3.9394870654,-0.4125766747,-0.5300278504

H,0,4.956094977,-0.2211929466,-0.1708176494

C,0,3.3193963471,-1.4738689531,0.3960301535

H,0,3.9376694551,-2.3741557272,0.4146946589

H,0,3.2099930247,-1.099002206,1.4141172154

H,0,2.3294598858,-1.7652457901,0.0400652759

C,0,4.0375755521,-0.9375154376,-1.9661198381

H,0,4.4532657084,-0.1834607276,-2.6375295117

H,0,4.6885259026,-1.813661497,-1.9970115679

H,0,3.0631892133,-1.2403130107,-2.3533873243

Ru,0,0.1196585326,0.4551644756,0.1514649084

C,0,0.4492150113,-3.8811616641,-1.2106925818

C,0,0.5385283041,-4.904751547,-0.2784218068

C,0,0.0632976126,-4.6942146068,1.0124341968

C,0,-0.5012164142,-3.4762523357,1.3708558359

C,0,-0.6097930478,-2.4379377652,0.4411010967

C,0,-0.1182669004,-2.6619630898,-0.8604964203

H,0,0.8325408684,-3.9961744488,-2.215729829

H,0,0.9822159833,-5.853975865,-0.5493524938

H,0,0.133008166,-5.4844256719,1.749770127

H,0,-0.8644650196,-3.3457614861,2.3797681998

C,0,-0.107202403,-1.5305740035,-1.835129183

O,0,0.6105405874,-1.5432835009,-2.8224944355

N,0,-0.895348058,-0.4220220076,-1.5374238699

O,0,0.8697795711,0.7722221491,1.8940778215

C,0,0.0367549891,0.7206780742,3.0293315337

H,0,-0.7028257622,1.5372503773,3.0094871225

H,0,0.6731462644,0.8866283827,3.9066305656

C,0,-0.6900572022,-0.6167786133,3.2008034635

H,0,-1.1589339954,-0.6210309749,4.1899406889

H,0,0.0583666341,-1.4118979819,3.1943778981

C,0,-1.7819527975,-0.8830327312,2.1433569601

H,0,-2.3932425309,-1.73279323,2.4649040396

H,0,-2.446389926,-0.0190251739,2.127819705

C,0,-1.2406615081,-1.1300235314,0.7488409481

C,0,-1.6878418964,-0.3805486466,-0.4010078441

C,0,-2.9193642475,0.4489778613,-0.4826477406

C,0,-2.9328491448,1.63402128,-1.2261046488

C,0,-4.1036163348,0.0217160324,0.1218596161

C,0,-4.0925742316,2.3874914776,-1.3308903142

H,0,-2.0301851619,1.9466546046,-1.7325320141

C,0,-5.2677752409,0.7717016804,0.007585016

H,0,-4.1190664132,-0.9131511618,0.6658894137

C,0,-5.2638271566,1.9616134307,-0.7107530199

H,0,-4.0858757044,3.306070146,-1.9040174966

H,0,-6.1797034099,0.4215372877,0.4745014882

H,0,-6.1697143334,2.54810869,-0.7970393271

[1]TS8a

C,0,-1.9162288996,-0.367658179,-2.2068465847

C,0,-2.4936874229,0.7833012749,-1.6830390981

C,0,-3.6109090478,0.7179014629,-0.8485029631

C,0,-4.1406445201,-0.5434873924,-0.5833004414

C,0,-3.558365885,-1.69978597,-1.0963920888

C,0,-2.4310982378,-1.6365828255,-1.9109095548

H,0,-1.0751646949,-0.2901578278,-2.887764863

H,0,-2.0390516037,1.7396984528,-1.8998875586

H,0,-5.0113952639,-0.6284419806,0.0577992742

H,0,-3.9847092313,-2.6655257508,-0.8499770498

C,0,-1.7970395567,-2.8729144194,-2.4868126222

H,0,-0.7161204521,-2.7475073042,-2.5583572524

H,0,-2.0137365548,-3.7514750724,-1.8770062181

H,0,-2.175197409,-3.0701889748,-3.4942841392

C,0,-4.1830150417,1.9669917874,-0.2073341724

H,0,-5.102626713,1.6723337529,0.3093447968

C,0,-3.2112140399,2.5321824933,0.8411481781

H,0,-3.6327393383,3.4208892848,1.3162247948

H,0,-3.0006493826,1.7984820157,1.6210465703

H,0,-2.2558279729,2.8107235282,0.3919624509

C,0,-4.5568291862,3.0352955405,-1.243067506

H,0,-5.2471370189,2.6389407926,-1.9901343996

H,0,-5.0319378709,3.8888482322,-0.754866061

H,0,-3.6721144546,3.4063043668,-1.7642855119

Ru,0,0.7651053325,0.0374266568,-0.7667772776

C,0,3.5288076298,2.72535102,0.8222160976

C,0,4.8173044378,2.3632759659,0.4597949108

C,0,5.0166175119,1.182015094,-0.2567219732

C,0,3.9643741108,0.321369975,-0.5165213568

C,0,2.6661511613,0.5913616509,-0.0313296268

C,0,2.4636867197,1.876990709,0.5479327546

H,0,3.3137569207,3.6889401118,1.2678594868

H,0,5.6541675509,3.0116808489,0.6850435826

H,0,6.0068951942,0.9266580024,-0.6130689295

H,0,4.1693139222,-0.5836490888,-1.0648775186

C,0,1.0834612118,2.4284298072,0.4955721974

O,0,0.6365515886,3.3300105439,1.1772842349

N,0,0.3603927828,1.7766311081,-0.4996988373

O,0,1.2131907719,-1.2518015174,-2.1712074029

C,0,2.2779325405,-2.1649503832,-2.1394228404

H,0,3.2370676932,-1.6690495906,-2.3424263719

H,0,2.1207901334,-2.8701343189,-2.9657915964

C,0,2.3474633466,-2.9838521777,-0.8412999248

H,0,3.0558499012,-3.8066339412,-0.9751524217

H,0,1.3604010422,-3.4270892548,-0.6861868872

C,0,2.7386849399,-2.2021351963,0.4392000575

H,0,2.5386636814,-2.8353545633,1.3073707075

H,0,3.8042730252,-1.9799715152,0.4481805584

C,0,1.9209780614,-0.95842546,0.5901423865

C,0,0.665485473,-0.7804800275,1.0021609539

C,0,-0.2533040338,-1.0565682641,2.0584131001

C,0,-1.6302253403,-0.875145494,1.868154534

C,0,0.2139266538,-1.5073729872,3.3063479503

C,0,-2.5188462412,-1.1527368985,2.8924600735

H,0,-1.9868759405,-0.5212425149,0.9131306952

C,0,-0.6817797708,-1.7793834749,4.327092319

H,0,1.2784678682,-1.6226957724,3.4651613323

C,0,-2.0495723169,-1.6056538414,4.1230292188

H,0,-3.5797948622,-1.0104980773,2.7317400211

H,0,-0.3163709367,-2.1206633,5.287278278

H,0,-2.7458239134,-1.8166393984,4.9247429649

[1]TS9a

C,0,1.3534825368,2.4008057936,-1.0134863876

C,0,2.0555707791,1.1930966201,-1.1959250944

C,0,3.1896651106,0.899745361,-0.4079904756

C,0,3.5745926291,1.8436087367,0.5329536075

C,0,2.8804048751,3.0411515844,0.7060221762

C,0,1.7623815694,3.344001618,-0.0557029338

H,0,0.5583532393,2.6544233184,-1.7058874034

H,0,1.798083848,0.5615305275,-2.0373818993

H,0,4.4388691277,1.6434494386,1.1557807528

H,0,3.2211696145,3.7466131199,1.4545975494

C,0,0.9805105271,4.6116533509,0.1450040354

H,0,0.6896808476,5.0568354601,-0.8087509555

H,0,0.0609891581,4.4117945898,0.7030896347

H,0,1.5537363224,5.3504375394,0.7054172121

C,0,3.9394870654,-0.4125766747,-0.5300278504

H,0,4.956094977,-0.2211929466,-0.1708176494

C,0,3.3193963471,-1.4738689531,0.3960301535

H,0,3.9376694551,-2.3741557272,0.4146946589

H,0,3.2099930247,-1.099002206,1.4141172154

H,0,2.3294598858,-1.7652457901,0.0400652759

C,0,4.0375755521,-0.9375154376,-1.9661198381

H,0,4.4532657084,-0.1834607276,-2.6375295117

H,0,4.6885259026,-1.813661497,-1.9970115679

H,0,3.0631892133,-1.2403130107,-2.3533873243

Ru,0,0.1196585326,0.4551644756,0.1514649084

C,0,0.4492150113,-3.8811616641,-1.2106925818

C,0,0.5385283041,-4.904751547,-0.2784218068

C,0,0.0632976126,-4.6942146068,1.0124341968

C,0,-0.5012164142,-3.4762523357,1.3708558359

C,0,-0.6097930478,-2.4379377652,0.4411010967

C,0,-0.1182669004,-2.6619630898,-0.8604964203

H,0,0.8325408684,-3.9961744488,-2.215729829

H,0,0.9822159833,-5.853975865,-0.5493524938

H,0,0.133008166,-5.4844256719,1.749770127

H,0,-0.8644650196,-3.3457614861,2.3797681998

C,0,-0.107202403,-1.5305740035,-1.835129183

O,0,0.6105405874,-1.5432835009,-2.8224944355

N,0,-0.895348058,-0.4220220076,-1.5374238699

O,0,0.8697795711,0.7722221491,1.8940778215

C,0,0.0367549891,0.7206780742,3.0293315337

H,0,-0.7028257622,1.5372503773,3.0094871225

H,0,0.6731462644,0.8866283827,3.9066305656

C,0,-0.6900572022,-0.6167786133,3.2008034635

H,0,-1.1589339954,-0.6210309749,4.1899406889

H,0,0.0583666341,-1.4118979819,3.1943778981

C,0,-1.7819527975,-0.8830327312,2.1433569601

H,0,-2.3932425309,-1.73279323,2.4649040396

H,0,-2.446389926,-0.0190251739,2.127819705

C,0,-1.2406615081,-1.1300235314,0.7488409481

C,0,-1.6878418964,-0.3805486466,-0.4010078441

C,0,-2.9193642475,0.4489778613,-0.4826477406

C,0,-2.9328491448,1.63402128,-1.2261046488

C,0,-4.1036163348,0.0217160324,0.1218596161

C,0,-4.0925742316,2.3874914776,-1.3308903142

H,0,-2.0301851619,1.9466546046,-1.7325320141

C,0,-5.2677752409,0.7717016804,0.007585016

H,0,-4.1190664132,-0.9131511618,0.6658894137

C,0,-5.2638271566,1.9616134307,-0.7107530199

H,0,-4.0858757044,3.306070146,-1.9040174966

H,0,-6.1797034099,0.4215372877,0.4745014882

H,0,-6.1697143334,2.54810869,-0.7970393271

^{3}TS9a

C,0,2.4122354412,1.6443448837,-1.3763590969

C,0,2.5373003643,0.2484846738,-1.3933754809

C,0,3.4252885948,-0.4042599251,-0.5318961396

C,0,4.1873918899,0.3876368578,0.3240769507

C,0,4.0708049324,1.7719917337,0.3337737018

C,0,3.1800795698,2.4295033194,-0.5096742781

H,0,1.7515320674,2.1192479046,-2.0932479407

H,0,1.9662777242,-0.3168169567,-2.1194332497

H,0,4.8821071576,-0.0893153512,1.0061535308

H,0,4.6726349605,2.3507067255,1.0248552445

C,0,3.0064785674,3.9211807705,-0.4444706528

H,0,2.5230795384,4.3084489036,-1.3421653154

H,0,2.384413388,4.1916990782,0.4132111434

H,0,3.9653883398,4.4289856344,-0.3265421634

C,0,3.5566791961,-1.9133552394,-0.5382141784

H,0,4.2413149304,-2.1782120976,0.2738722857

C,0,2.2137134755,-2.605655204,-0.26876552

H,0,2.3527164647,-3.6839461145,-0.1668985167

H,0,1.7498085167,-2.2301963373,0.6440882632

H,0,1.514571006,-2.4413111242,-1.0890624845

C,0,4.1719054201,-2.4140650216,-1.8535510629

H,0,5.1422702379,-1.9498742165,-2.0388664974

H,0,4.3090166808,-3.4972991197,-1.8247251358

H,0,3.5189938896,-2.1829724205,-2.6978454268

Ru,0,0.2696763449,0.8408625,0.1393183314

C,0,-1.6658846794,-3.2271438903,-1.3675037639

C,0,-2.0601586992,-4.2598958864,-0.5290070911

C,0,-2.0914106502,-4.0393627518,0.8395361802

C,0,-1.7728636807,-2.7869592675,1.3496043712

C,0,-1.4176537492,-1.7170603265,0.5190802661

C,0,-1.3261316994,-1.9717375454,-0.8701383542

H,0,-1.572912511,-3.3831931013,-2.4334391122

H,0,-2.3132433109,-5.2293113824,-0.9387138996

H,0,-2.3640182543,-4.8374968695,1.5189464986

H,0,-1.8088969709,-2.6517700576,2.4198308237

C,0,-0.7452388587,-1.002337725,-1.8877725886

O,0,-0.3957006666,-1.4189644093,-2.9959035496

N,0,-0.5518607602,0.280788605,-1.5384819263

O,0,1.3314895431,1.1764201951,1.7003543828

C,0,1.1887696894,0.7617857821,3.0283017768

H,0,0.7897943626,1.5960439478,3.6261156496

H,0,2.1833754534,0.5248962713,3.4278391707

C,0,0.2709272947,-0.4501414376,3.2156814901

H,0,0.1995887591,-0.6605199821,4.2873517643

H,0,0.7163719527,-1.3284101706,2.7408391119

C,0,-1.1280019528,-0.2017218564,2.6342808996

H,0,-1.8585311812,-0.863234927,3.1015307311

H,0,-1.4395131975,0.8135604337,2.8939512768

C,0,-1.1842365603,-0.3598804592,1.1154525026

C,0,-1.5876879219,0.8007367479,0.4009429729

C,0,-2.8204902,1.432054788,0.0612278441

C,0,-2.8443705099,2.6149107159,-0.6971354002

C,0,-4.0316863932,0.8671671615,0.4975907033

C,0,-4.0502060273,3.2157295837,-1.0069674675

H,0,-1.9065920721,3.0304272047,-1.0393076026

C,0,-5.2361327633,1.4783889422,0.1898518485

H,0,-4.0083554822,-0.0538284266,1.0653814087

C,0,-5.2458013431,2.6507080521,-0.5616137552

H,0,-4.0680385547,4.1233766333,-1.5961445277

H,0,-6.1675054735,1.041273905,0.5257392443

H,0,-6.1880636296,3.1251436465,-0.805612191

^{1}I2

C,0,-3.0750316472,-0.5504879406,-0.9183177925

C,0,-2.6416848186,0.6690385852,-1.4203899697

C,0,-2.9648531276,1.8729677404,-0.7841733844

C,0,-3.7285073061,1.7997076678,0.3769562942

C,0,-4.1551111762,0.5750129601,0.8832735532

C,0,-3.8361139696,-0.6206207292,0.2497327787

H,0,-2.812659126,-1.4628254357,-1.4382212035

H,0,-2.042807453,0.6888236465,-2.3233308911

H,0,-3.9969389722,2.7029112515,0.9079253593

H,0,-4.7452712879,0.555400454,1.7930450561

C,0,-4.2531443896,-1.9476555433,0.8245803956

H,0,-4.4733445665,-2.6722587162,0.0387916951

H,0,-3.4527543141,-2.373986099,1.4361252171

H,0,-5.1373297995,-1.8500064174,1.4561952825

C,0,-2.5106132254,3.1824518631,-1.4036553408

H,0,-1.4752127638,3.0276660106,-1.7232987227

C,0,-3.3369548755,3.4953082124,-2.6627819223

H,0,-2.9725492463,4.4042284632,-3.1474470949

H,0,-3.2847157354,2.6804343301,-3.3859117806

H,0,-4.3874948955,3.6460446813,-2.4017447868

C,0,-2.5358816167,4.3715799256,-0.4410913441

H,0,-1.9977333411,4.1536030702,0.4817101545

H,0,-2.0737736911,5.2421547035,-0.9104832853

H,0,-3.5602536443,4.6503162822,-0.1816911802

Ru,0,0.332627835,-0.2857719333,-0.2552504452

C,0,-0.868593208,-3.3467492571,-1.509594544

C,0,-1.6042451111,-4.1826211761,-0.715840236

C,0,-1.3306332692,-4.2306174426,0.6601523178

C,0,-0.3598901039,-3.4342424212,1.2004694499

C,0,0.4455912435,-2.5533581596,0.4122748404

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C,0,4.4566592046,-0.8007641092,0.8673173431

C,0,3.6229396225,0.9852815422,-0.5455791447

C,0,5.7433489297,-0.3161673688,0.719783409

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^{1}J2

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^{3}J2

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C,0,-5.0890033583,1.6084452243,1.3510395457

H,0,-4.3579845858,2.6471723029,3.0835234709

H,0,-5.5171200259,0.4499242541,-0.4078469955

H,0,-6.0870567412,2.0218487144,1.4221772389

^{3}K

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C,0,-1.928962526,-2.0305854689,0.267130649

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H,0,-5.4112758797,-1.5342600437,-0.2339637163

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C,0,1.82204922,4.4684654293,-0.5841877822

C,0,3.1120121939,4.6403015299,-1.0566936887

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C,0,3.5325188677,2.2992580685,-0.6880903329
C,0,2.2211694008,2.0962611987,-0.2394393809
C,0,1.3596281409,3.211306798,-0.1870480922
H,0,1.1392786877,5.3043710895,-0.5153135482
H,0,3.4469299839,5.6161877674,-1.3838419015
H,0,4.9894362178,3.6672449728,-1.4526299997
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O,0,-0.5706987713,4.1454947052,0.8312814512
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^{3}M

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H,0,0.6063120819,-0.8786600408,2.3510374367

C,0,0.5144787285,-3.0040019593,1.9962205316

H,0,0.5167319403,-3.9001792539,2.6235523945

H,0,-0.2665494315,-3.1322282219,1.2426903497

C,0,1.7897413645,-2.8535138405,1.3112395546

C,0,2.8076093543,-2.611288175,0.7111460615

C,0,3.9752687838,-2.294337773,-0.0419219257

C,0,3.8858105639,-1.443760621,-1.1559585509

C,0,5.2297290249,-2.8134030574,0.3109827017

C,0,5.0211113549,-1.126186373,-1.8883936716

H,0,2.9271711977,-1.0265517323,-1.4356134212

C,0,6.3591038867,-2.4905364841,-0.4277170131

H,0,5.3058797256,-3.4679837987,1.1692758899

C,0,6.2609545418,-1.646266047,-1.5297048012

H,0,4.9349935403,-0.4655792522,-2.7422791254

H,0,7.3205733284,-2.8982003529,-0.1410667576

H,0,7.1441340619,-1.3957309247,-2.1036802288

C,0,0.0966521733,-1.3683421086,-1.4788713516

C,0,0.5639496398,-2.6715407095,-2.092264903

H,0,-0.2933709543,-3.2713437013,-2.3992851067

H,0,1.2112060301,-2.4690539349,-2.9417921069

H,0,1.1137625125,-3.2375958095,-1.3401843946

O,0,-0.8081220369,-1.5638759281,-0.5463150998

O,0,0.5283837192,-0.2819765738,-1.8248779471

C,0,1.8917878018,1.4702856083,0.6279384781

H,0,1.5743445262,0.4407484023,0.5554755033

2a'

C,0,0.9192930751,3.1455558206,-0.5512714479

C,0,0.2005667042,3.9840684525,0.2763811431

C,0,-1.0795821727,3.6050360514,0.6968487078

C,0,-1.6299973929,2.4057185177,0.291508696

C,0,-0.9187050101,1.5335800002,-0.5566498482

C,0,0.3749128571,1.92726056,-0.9701302577

H,0,1.9125558785,3.4018326501,-0.8948673558

H,0,0.6229600934,4.9265357226,0.60001012

H,0,-1.6466185994,4.2580560692,1.349081528

H,0,-2.6188607962,2.1264326456,0.6279718791

C,0,1.1729692555,1.0612293069,-1.8448190603

O,0,2.297448462,1.3070844879,-2.2580212321

C,0,-0.4201147331,-3.4172753474,-0.4140275595

H,0,-1.4788592949,-3.4983469818,-0.1338565551

H,0,0.0523252167,-4.3905933827,-0.2345792193

C,0,-0.3031542965,-3.0714476916,-1.8885512019

H,0,-0.6280212833,-3.9420969357,-2.4647875456

H,0,0.7546517626,-2.9205718684,-2.1218236538

C,0,-1.1446683358,-1.8643598035,-2.3433207793

H,0,-1.1028911006,-1.8124440894,-3.4373534767

H,0,-2.18751128,-2.0349231755,-2.0807976816

C,0,-0.7156212484,-0.5295591211,-1.7997955067

C,0,-1.46563351,0.2661013797,-0.9948369316

C,0,-2.8117444038,-0.1614877381,-0.5224701901

C,0,-2.9371277898,-0.9911573524,0.5934516163

C,0,-3.9711094411,0.2717592836,-1.1680871488

C,0,-4.1902871929,-1.3896638879,1.0452212617

H,0,-2.0367664401,-1.3231468495,1.0939147131

C,0,-5.2257550715,-0.1249972524,-0.7183373238

H,0,-3.8833442478,0.9225498135,-2.0294373893

C,0,-5.3385216789,-0.9581641521,0.3895739461

H,0,-4.2711793102,-2.0357551591,1.9108094474

H,0,-6.1150686759,0.2158782225,-1.2337501288

H,0,-6.314942094,-1.2677133891,0.7404196094

O,0,0.2266387388,-2.3997690198,0.349168411

H,0,0.2644795835,-2.6695372817,1.2721443034

N,0,0.5357181129,-0.115112271,-2.2000578427

H,0,1.0874178695,-0.7165829734,-2.7939558657

3a'

C,0,0.8388413459,-3.8585221657,-1.1477263217

C,0,1.277754081,-4.6817926661,-0.1317198739

C,0,0.7742812178,-4.501115133,1.1606908607

C,0,-0.1488097178,-3.5098912071,1.426941154

C,0,-0.6165654346,-2.652085217,0.4097471201

C,0,-0.097512779,-2.8516658471,-0.8914282208

H,0,1.2005504906,-3.9659229953,-2.1615500577

H,0,2.0027371018,-5.4602007633,-0.3310597936

H,0,1.1110109118,-5.144423824,1.964503155

H,0,-0.5164899472,-3.3994383296,2.4366611377

C,0,-0.5356957474,-2.0099765837,-2.0100460544

O,0,-0.1472634033,-2.100273039,-3.1664643617

C,0,-0.6978336499,0.8800496051,2.507315201

H,0,-1.6458929534,1.4090878675,2.3407222191

H,0,-0.1628108031,1.3945342986,3.3151796279

C,0,-0.9698525602,-0.5564130846,2.9268682784

H,0,-1.3262858044,-0.5368511328,3.9614993119

H,0,-0.0202669637,-1.0959852466,2.9263541007

C,0,-2.0192432584,-1.2961530398,2.0740803177

H,0,-2.2869471502,-2.22664913,2.5816428217

H,0,-2.9273008688,-0.6956843102,2.0656476372

C,0,-1.5845728448,-1.6005360376,0.6611043355

C,0,-1.9960082057,-0.8476312499,-0.3930193655

C,0,-2.9491835685,0.2878925057,-0.3271322934

C,0,-2.5196829633,1.5729207224,-0.6690698333

C,0,-4.2837283864,0.0963852612,0.035104441

C,0,-3.4009238194,2.6460117333,-0.6277541803

H,0,-1.4841188265,1.72519627,-0.9440735073

C,0,-5.164966091,1.170007499,0.0763482003

H,0,-4.6279698687,-0.9006949358,0.2783092952

C,0,-4.7253968481,2.448025059,-0.2513840316

H,0,-3.0530788785,3.6381495317,-0.88692571

H,0,-6.1976253635,1.006544953,0.3575468035

H,0,-5.4124696988,3.2839948169,-0.2198026977

N,0,-1.4811794726,-1.0658122265,-1.6569738415

H,0,-1.8252000126,-0.5048196384,-2.4227121906

O,0,0.092298016,0.8832967325,1.3162983005

H,0,0.3214771947,1.792806237,1.101153556

^{1}TS1

C,0,-1.9162277071,-2.0920422558,-0.980890301

C,0,-2.9398270684,-1.1167593663,-0.7623490812

C,0,-2.9997281251,-0.3536266974,0.4199239163

C,0,-1.9766936578,-0.5923865824,1.3988655304

C,0,-0.9663120593,-1.5360756545,1.1864965648

C,0,-0.9068858678,-2.2966345367,-0.0301095682

H,0,-1.877724505,-2.6174435654,-1.9255742004

H,0,-3.6395220754,-0.9203838505,-1.5607900764

H,0,-1.9353037247,0.0423277529,2.2734326544

H,0,-0.1560053235,-1.6241924761,1.8984855976

C,0,0.2433711811,-3.2283451415,-0.2650339368

H,0,0.2905274004,-3.5460114401,-1.3060775382

H,0,1.1802863709,-2.7317918153,-0.0100898208

H,0,0.1494822053,-4.1173725826,0.3637786466

C,0,-4.0468706813,0.7041011656,0.700471673

H,0,-3.5020741277,1.5751388676,1.0771731152

C,0,-4.8380750121,1.1397867929,-0.5312195158

H,0,-5.4854009771,1.9783241154,-0.2726626422

H,0,-4.1844299744,1.4640673844,-1.3393109581

H,0,-5.4768918885,0.334032065,-0.9026091545

C,0,-4.9907338372,0.211498853,1.8094620069

H,0,-4.445935448,-0.0601089135,2.7153178923

H,0,-5.7056244509,0.9937365571,2.070015965

H,0,-5.5532725011,-0.6650629564,1.4780730436

Ru,0,-1.0096460105,-0.1026639901,-0.5109463245

C,0,-2.5662206772,2.8123139828,-3.2282827009

C,0,-2.9387704298,2.1497313821,-4.3923630628

C,0,-2.5164345762,0.8404276262,-4.6194491793

C,0,-1.7118191019,0.2016029217,-3.6856096511

C,0,-1.7766613751,2.1633911029,-2.2888964236

H,0,-2.8963485665,3.8212971654,-3.0156586702

H,0,-3.5595365119,2.651066947,-5.1246784528

H,0,-2.8010098865,0.3298662964,-5.5314880999

H,0,-1.3407343322,-0.7962740503,-3.8899767055

C,0,-1.5109693171,2.8135095331,-0.9638434506

O,0,-1.8188681265,3.9735576023,-0.710113665

N,0,-0.9322637312,1.9246123376,-0.1122322552

O,0,-0.951461972,2.3405862118,1.2378418723

C,0,0.1558029864,3.1892906126,1.5681685048

H,0,-0.1054970823,3.5747019522,2.5575270367

H,0,0.1911209586,4.0284459443,0.8715946602

C,0,1.4796667231,2.4403047717,1.6063522523

H,0,2.275120148,3.133505265,1.8923078671

H,0,1.7079593268,2.0738582305,0.6082759227

C,0,1.4316913411,1.2534245589,2.5836056917

H,0,1.3317365219,1.6241097548,3.6093022583

H,0,0.5275083488,0.6814852851,2.3666866204

C,0,2.5765224142,0.3612157063,2.490464565

C,0,3.5067171414,-0.3959077442,2.37303199

C,0,4.5810457873,-1.3113507595,2.1793059712

C,0,4.4826936681,-2.3160939568,1.2042864554

C,0,5.7540215303,-1.2292295584,2.9434082457

C,0,5.5250500427,-3.2087493662,1.002661489

H,0,3.5819134455,-2.3806717354,0.6086151481

C,0,6.7929487906,-2.1256818451,2.7368489516

H,0,5.8386896251,-0.4567920022,3.6963295476

C,0,6.6841681829,-3.117931134,1.767425331

H,0,5.4337520035,-3.9781094676,0.2460100737

H,0,7.6924458141,-2.0491365634,3.3347469685

H,0,7.4969725026,-3.8150465255,1.6086301802

C,0,1.7943576376,0.2938537625,-1.4725968385

C,0,3.2926717037,0.2127287808,-1.3437415555

H,0,3.588493067,0.3027863898,-0.301540973

H,0,3.6198073681,-0.7621807474,-1.7120883691

H,0,3.7624124518,0.9801912283,-1.9550425663

O,0,1.1024309373,-0.0679513562,-0.4747610305

O,0,1.2939745802,0.6915337685,-2.5549560054

C,0,-1.328022975,0.8464062243,-2.5003575589

H,0,-0.0418228619,0.6649082883,-2.3577523876

^{3}TS1

C,0,0.4860419069,0.3573904756,2.7460507806

C,0,1.420227029,-0.6403533599,2.3819878468

C,0,1.0043525653,-1.7474846675,1.594217424

C,0,-0.3631583787,-1.8016120583,1.2192318471

C,0,-1.2983694844,-0.8678973782,1.6850422248

C,0,-0.8804672634,0.2432072196,2.4316543737

H,0,0.8323293269,1.2122498545,3.3116570356

H,0,2.4417220124,-0.5551453209,2.7214619799

H,0,-0.7013665458,-2.6259783105,0.6070333902

H,0,-2.3301098422,-0.9536565682,1.3767123116

C,0,-1.8440489094,1.3357241392,2.7876595184

H,0,-1.5367064016,1.8643616281,3.6905200374

H,0,-1.8932772813,2.0586269243,1.9692633407

H,0,-2.8494466427,0.9418952316,2.9339044273

C,0,1.9263262943,-2.891006101,1.2128386171

H,0,1.6433895837,-3.1836077821,0.1983765702

C,0,3.4096293732,-2.5197491361,1.188368321

H,0,3.9902633743,-3.3549866771,0.7954477045

H,0,3.5987398932,-1.6556661589,0.5528285433

H,0,3.788122362,-2.3032630367,2.19035882

C,0,1.6755652514,-4.0820164496,2.15232048

H,0,0.6289775011,-4.3910159409,2.1386173514

H,0,2.2862584919,-4.9356605118,1.8525302945

H,0,1.9371844448,-3.8242847575,3.1817186662

Ru,0,0.8737154706,0.1265837779,0.3420663222

C,0,4.7003918406,1.6036769291,-0.7442520215

C,0,5.0609425326,2.584172751,0.1734143941

C,0,4.1080733666,3.1070857478,1.0470923252

C,0,2.7958301386,2.6543243431,1.0006083721

C,0,3.3889714762,1.1510216023,-0.7794564352

H,0,5.4226950206,1.1668047402,-1.4223154437

H,0,6.0825748383,2.9410645354,0.2111286296

H,0,4.3903142747,3.8778606454,1.7542941258

H,0,2.0522034648,3.0979961366,1.6530418608

C,0,3.0084343052,0.0114913874,-1.6628705464

O,0,3.7087260095,-0.4455718657,-2.5493762514

N,0,1.7716551266,-0.4913949044,-1.2858919972

O,0,1.4587444472,-1.7195362747,-1.8906829558

C,0,0.8356176292,-1.5360700252,-3.1754139127

H,0,0.9347750126,-2.5117335725,-3.6576157144

H,0,1.40991758,-0.811132279,-3.7533690591

C,0,-0.621085391,-1.1262889852,-3.0370731886

H,0,-1.0277730745,-0.8721910319,-4.0191315725

H,0,-0.6762632779,-0.2274128488,-2.4243958551

C,0,-1.4665302309,-2.24018797,-2.3866675394

H,0,-1.7215219127,-3.0028563243,-3.1286642345

H,0,-0.8498938431,-2.7386418982,-1.6332243931

C,0,-2.6670234247,-1.7302779948,-1.7436511417

C,0,-3.6000050114,-1.2240898056,-1.1741434981

C,0,-4.6296724623,-0.5522221736,-0.4545349651

C,0,-4.3450231555,0.6775685866,0.1604326818

C,0,-5.9182335627,-1.0901305907,-0.3314394694

C,0,-5.3267916245,1.3450627951,0.8780111644

H,0,-3.3468438607,1.0834529894,0.0643693003

C,0,-6.8940531146,-0.4142877414,0.3878874785

H,0,-6.1430469242,-2.0375351328,-0.8034594078

C,0,-6.6038646701,0.8039471055,0.9951006381

H,0,-5.0948694178,2.2928111034,1.3485583105

H,0,-7.885816714,-0.8399668322,0.4752072194

H,0,-7.3682730753,1.3277582921,1.5548386029

C,0,-0.7327586855,2.3325038267,-1.0630710398

C,0,-1.9092968083,3.0326560303,-1.7002702013

H,0,-2.5304862754,2.3034308917,-2.2191064401

H,0,-2.5191460845,3.4828544795,-0.9142245435

H,0,-1.5753069962,3.8105921812,-2.381893792

O,0,-0.9510091654,1.2564652181,-0.4438657801

O,0,0.4114380844,2.8583723775,-1.1744861462

C,0,2.405265376,1.6632324279,0.0879420552

H,0,1.2780321083,2.0923430924,-0.5095828416

[1]TS2

C,0,-0.8834056796,1.9617766503,1.8332105465

C,0,-2.0010815603,1.0936130821,1.8844883164

C,0,-2.7846935359,0.8954012439,0.735876093

C,0,-2.5063007005,1.7022742936,-0.4166831684

C,0,-1.4625110707,2.6471944203,-0.4113707683

C,0,-0.6093972937,2.7869459634,0.7114700611

H,0,-0.2157688027,2.0039654872,2.6844588801

H,0,-2.1573619183,0.4868861385,2.7633671846

H,0,-3.0875283548,1.5490912324,-1.315575337

H,0,-1.2662207478,3.2286962344,-1.3038700464

C,0,0.5331212509,3.7602894144,0.714985838

H,0,1.3570471493,3.3963700335,1.3292812054

H,0,0.9111555716,3.9228130959,-0.2948790251

H,0,0.2171414198,4.7283590846,1.1137342964

C,0,-3.9047107803,-0.1203531168,0.659526056

H,0,-3.8987148671,-0.4929833847,-0.3681333177

C,0,-3.7075689355,-1.3228053254,1.5828678001

H,0,-4.4720704587,-2.0734835715,1.377826619

H,0,-2.7321253672,-1.7815302884,1.4236055301

H,0,-3.7993480723,-1.045572294,2.6360594776

C,0,-5.2513644114,0.5731260579,0.918145458

H,0,-5.4112314169,1.4073689847,0.2322306945

H,0,-6.0728225763,-0.1339054133,0.7887047798

H,0,-5.2971698199,0.9620048707,1.9384960619

Ru,0,-0.6451186797,0.6001720795,0.0629288033

C,0,0.7318893193,-3.2012778308,1.4159611089

C,0,1.4363328818,-2.9658232613,2.5899522742

C,0,1.7771900216,-1.6573437786,2.9396515466

C,0,1.4572659172,-0.6024242353,2.1019983593

C,0,0.7559750431,-0.8184667641,0.9024715444

C,0,0.3646124661,-2.1409932176,0.5969554703

H,0,0.4275459525,-4.1990565833,1.1243472278

H,0,1.7102818814,-3.7898534659,3.2363877045

H,0,2.3139632841,-1.4658949948,3.8610360528

H,0,1.7840783519,0.399388877,2.3510550954

C,0,-0.5149347959,-2.3579379962,-0.5881561144

O,0,-0.6370672909,-3.4262622977,-1.1883748266

N,0,-1.1298541086,-1.1880715804,-0.8655539697

O,0,-1.9473814269,-1.1146443614,-1.9990025089

C,0,-1.309533704,-1.4165766876,-3.2598696788

H,0,-1.9384245894,-0.8855932798,-3.9794442786

H,0,-1.3821019276,-2.4911940134,-3.438655028

C,0,0.148678396,-0.9973449301,-3.4214239457

H,0,0.367580066,-1.0802353368,-4.4906645563

H,0,0.7940512496,-1.7146109377,-2.9141084062

C,0,0.526952269,0.4272309152,-2.9462527076

H,0,1.4796897626,0.7106423474,-3.4073025038

H,0,-0.2273501909,1.146285066,-3.2748166952

C,0,0.6610486105,0.4338838805,-1.4753528682

C,0,1.4851997724,0.1263748169,-0.5247602731

C,0,2.9265580039,0.3084404378,-0.3277357158

C,0,3.5081302865,1.5514654679,-0.5976978675

C,0,3.7535092846,-0.7565617677,0.0466993986

C,0,4.8834162808,1.7273881633,-0.4988239823

H,0,2.8686178538,2.3764252918,-0.8829176117

C,0,5.1267899742,-0.5818452268,0.1342726372

H,0,3.3113040282,-1.7207488112,0.2580062747

C,0,5.6962731702,0.6605659629,-0.1337139683

H,0,5.3189101218,2.6966554002,-0.7078451356

H,0,5.7565844382,-1.4180710883,0.4107441022

H,0,6.7681130048,0.794458847,-0.0589831933

^{3}TS2

C,0,-1.6148798468,-1.6150943189,-2.2784971995

C,0,-2.7589330286,-0.9449393434,-1.8009359186

C,0,-3.1368942841,-1.0332632673,-0.4704599865

C,0,-2.3188843272,-1.8153655175,0.3877559454

C,0,-1.2621842489,-2.6097437359,-0.1182306176

C,0,-0.881456384,-2.5029604129,-1.4805518446

H,0,-1.3063048239,-1.4631811544,-3.3050518562

H,0,-3.3000820429,-0.3011660484,-2.4791681775

H,0,-2.5953254202,-1.9098815251,1.4299366045

H,0,-0.7716920811,-3.330832393,0.5236140235

C,0,0.2108146185,-3.3622073034,-2.0565719993

H,0,0.7052494227,-2.8607708061,-2.8885660771

H,0,0.9649349336,-3.601867185,-1.3066337156

H,0,-0.2015571056,-4.3031863615,-2.4318340796

C,0,-4.3124109065,-0.2848394167,0.114999731

H,0,-4.0631727304,-0.0998603585,1.1633899235

C,0,-4.5511813145,1.0802924966,-0.5345294088

H,0,-5.3336952635,1.6150587735,0.006546203

H,0,-3.6448615046,1.6844501963,-0.5070745058

H,0,-4.8821080916,0.9829240097,-1.5713459687

C,0,-5.5776061499,-1.1581071466,0.0669484505

H,0,-5.4226665818,-2.116015972,0.5675034855

H,0,-6.4105896656,-0.6486045134,0.5563226836

H,0,-5.8653010207,-1.3619648799,-0.9672297486

Ru,0,-0.3086442486,-0.5621175209,-0.067241973

C,0,1.2923728052,2.9015922473,-1.8875893416

C,0,2.1142223827,2.4697675056,-2.9179960738

C,0,2.4357620967,1.1131155504,-3.0251057062

C,0,1.9815470395,0.2077649852,-2.0827501929

C,0,1.1570271268,0.628431832,-1.0240928193

C,0,0.7872427003,1.9906368508,-0.9632438073

H,0,0.9978441673,3.9395022829,-1.7929344826

H,0,2.4959454425,3.176635926,-3.6435567277

H,0,3.0676151665,0.7695685867,-3.8352855078

H,0,2.2946564485,-0.8273699275,-2.1330805284

C,0,-0.2323273534,2.423791815,0.03889493

O,0,-0.342297936,3.5722305475,0.4614186812

N,0,-0.9857304108,1.3437712158,0.3967526522

O,0,-1.8619319614,1.4964245899,1.4834383886

C,0,-1.2868742733,1.9829727197,2.7148690812

H,0,-1.9906274581,1.6153847447,3.4662495245

H,0,-1.3062120847,3.0744557466,2.7067240163

C,0,0.1330324258,1.5350444004,3.0629879768

H,0,0.2881136851,1.8385905678,4.1027769494

H,0,0.8531026452,2.0984868521,2.4688775723

C,0,0.4557221907,0.0249864644,2.9404536802

H,0,1.3348758299,-0.2020088166,3.5526990363

H,0,-0.3770035528,-0.5727547451,3.3184506022

C,0,0.743405561,-0.3079810697,1.5274768199

C,0,1.6994712419,-0.1916563243,0.6248245662

C,0,3.1509048025,-0.3613533319,0.6554175292

C,0,3.6802489015,-1.5309823426,1.2171951694

C,0,4.0331634719,0.6226144603,0.1943369485

C,0,5.0535101841,-1.7102142125,1.3172777668

H,0,3.0016024901,-2.3001108901,1.5640475959

C,0,5.4049465076,0.4413010482,0.3014174338

H,0,3.6369170863,1.5318478917,-0.2356178847

C,0,5.9213973794,-0.7243072477,0.8593377173

H,0,5.4457934244,-2.6221121763,1.7501646529

H,0,6.0743542792,1.2159931042,-0.05102863

H,0,6.9923136441,-0.8632541463,0.9360984377

^{1}TS2a

C,0,-0.1575818109,0.8396847183,-2.7061932956

C,0,-0.6454943891,1.9621962397,-1.9850817087

C,0,-1.7591447411,1.8569018334,-1.1394813301

C,0,-2.4049732483,0.5825966486,-1.0799544322

C,0,-1.966647076,-0.5236990431,-1.8281447939

C,0,-0.7964249013,-0.418162243,-2.6365051383

H,0,0.7453231823,0.9420661005,-3.2940391003

H,0,-0.0760094583,2.8796365451,-2.0160873034

H,0,-3.2450140866,0.4605717152,-0.4104767431

H,0,-2.464131509,-1.477061021,-1.715083945

C,0,-0.2804300756,-1.6030240767,-3.3984641569

H,0,0.775942838,-1.4838699205,-3.6379503052

H,0,-0.4023384184,-2.5188070292,-2.8193724409

H,0,-0.8288211036,-1.7226025703,-4.3364343962

C,0,-2.2811662827,2.9959502045,-0.2898962523

H,0,-2.6590248582,2.5368595303,0.6287536142

C,0,-1.2013183489,4.0021877843,0.1116593517

H,0,-1.6116600129,4.7214806188,0.8219415161

H,0,-0.3509499692,3.5068847901,0.5809794551

H,0,-0.8380856816,4.5692395168,-0.7488375917

C,0,-3.4576075965,3.687499458,-0.9953802263

H,0,-4.2477582401,2.9766120193,-1.2446125318

H,0,-3.8867008618,4.460477098,-0.3548910058

H,0,-3.125472189,4.1613080713,-1.9225703407

Ru,0,-0.2707731565,0.2117280368,-0.5444968012

C,0,1.9683410934,2.3536257831,2.3633323356

C,0,2.8588809191,3.1482956457,1.6545251537

C,0,3.0601291423,2.9126246691,0.2919499238

C,0,2.409024648,1.8697843248,-0.3430923891

C,0,1.5032262432,1.0515533219,0.3554803534

C,0,1.2731437533,1.3377183607,1.717566656

H,0,1.7722758641,2.5166842758,3.4159283126

H,0,3.3888275891,3.951027313,2.1511049545

H,0,3.7459682306,3.5362695863,-0.2687142847

H,0,2.6198222772,1.6592605633,-1.384269208

C,0,0.2201436564,0.5599901975,2.4321022029

O,0,0.1852358753,0.3856650301,3.6492067451

N,0,-0.6478143191,0.0872533549,1.508081117

O,0,-1.6288865017,-0.8095500365,1.9742997576

C,0,-1.1858955565,-2.0191593247,2.6461069679

H,0,-2.0413180347,-2.6842336968,2.5156812008

H,0,-1.0496221982,-1.7856090015,3.7017918757

C,0,0.0737663129,-2.685406713,2.1084866159

H,0,0.0805626925,-3.6928035091,2.5357162225

H,0,0.9567106408,-2.1745207964,2.4934791698

C,0,0.1874035526,-2.7925152312,0.5678493626

H,0,0.9083525455,-3.5793450204,0.320478864

H,0,-0.7797418235,-3.0624318414,0.141490045

C,0,0.6577605041,-1.4936237159,0.0460201512

C,0,1.7205764004,-0.7625381662,-0.0497518148

C,0,3.122208447,-1.0239008635,-0.3895576728

C,0,3.4237612358,-1.8353869816,-1.4881900298

C,0,4.1704513809,-0.5478064478,0.4058485569

C,0,4.7409087963,-2.1637565486,-1.7866155722

H,0,2.6135112118,-2.2045385019,-2.1035025121

C,0,5.4834405624,-0.8854320679,0.1127307663

H,0,3.9455333124,0.080584144,1.2569132094

C,0,5.7740747898,-1.6896109947,-0.9865983346

H,0,4.9591294458,-2.7897935775,-2.6428743056

H,0,6.2838805913,-0.5213904489,0.7445024267

H,0,6.8008055114,-1.9455681667,-1.2159958476

C,0,-5.7292909131,-2.4881883726,0.143158987

H,0,-5.8119173862,-3.3912525432,-0.4549070312

H,0,-6.1559228661,-1.6408129597,-0.396433159

H,0,-6.2935059872,-2.5968783487,1.0703931998

C,0,-4.2828630522,-2.2113698631,0.4575079247

O,0,-3.3584383112,-2.8931159312,0.0694395435

O,0,-4.1351533313,-1.1174114451,1.206219461

H,0,-3.1709791882,-0.9671308636,1.4266074386

^{1}TS2b

C,0,-0.8182538628,-0.5068273135,-2.6264680809

C,0,-1.4112411606,0.6085658974,-2.0156950496

C,0,-2.7928081752,0.6500468644,-1.7761749665

C,0,-3.5462320896,-0.4478480287,-2.1784049969

C,0,-2.9604604651,-1.5514901543,-2.7999085862

C,0,-1.5948732148,-1.6052454382,-3.0342664168

H,0,0.2238564851,-0.4535889199,-2.9220527791

H,0,-0.8051907039,1.4796007926,-1.8230679615

H,0,-4.61986631,-0.4362808637,-2.0240646271

H,0,-3.5870510053,-2.3800289912,-3.1107636765

C,0,-0.9483825482,-2.8114379274,-3.6556136839

H,0,-0.5651714671,-3.4815791765,-2.8797253201

H,0,-1.6563881034,-3.379258062,-4.2606678203

H,0,-0.1051387003,-2.5322233522,-4.2902524535

C,0,-3.4759451077,1.8345231348,-1.1140374832

H,0,-4.4254235904,1.9779413806,-1.6422213041

C,0,-3.8062898093,1.5242517226,0.3555371537

H,0,-4.3963751763,2.3335435088,0.7913072962

H,0,-4.3742692473,0.5977564698,0.4505333261

H,0,-2.8910471089,1.4215774201,0.9381912118

C,0,-2.6868598146,3.1420814109,-1.2146259511

H,0,-2.4234991446,3.3776535342,-2.2476595081

H,0,-3.2821641013,3.9668815248,-0.8193138869

H,0,-1.7659039598,3.0976378509,-0.6302559989

Ru,0,-0.0064989625,-0.7739391455,-0.142625158

C,0,1.2477271944,3.2406984567,0.0168296666

C,0,1.942110351,3.4937531826,-1.1613311821

C,0,2.3505982807,2.4282875242,-1.9649019866

C,0,2.0990787586,1.1218148397,-1.5792366018

C,0,1.3918198953,0.8371620565,-0.3963215031

C,0,0.9591370755,1.93415615,0.383586354

H,0,0.8955722108,4.0443139763,0.6515236133

H,0,2.1571981578,4.5121008765,-1.4584953214

H,0,2.8844243418,2.6209278944,-2.8873838887

H,0,2.4789526439,0.30414552,-2.1793283137

C,0,0.0802493219,1.6452256044,1.5588250642

O,0,-0.0371967881,2.3680726568,2.5447099906

N,0,-0.5618918225,0.478150136,1.3243973515

O,0,-1.3228539152,-0.0327179373,2.3996060618

C,0,-0.635629971,-0.3494997875,3.6464415493

H,0,-1.2487462597,-1.1542435193,4.0595960759

H,0,-0.7149050046,0.5327981703,4.2814872681

C,0,0.8259899471,-0.7740046398,3.5741511826

H,0,1.0694904872,-1.1036466328,4.5896550758

H,0,1.4501471242,0.0970797146,3.3742914153

C,0,1.2040339415,-1.8963013482,2.5797774259

H,0,2.1820615998,-2.2975351164,2.8655372575

H,0,0.4823439849,-2.7155235065,2.6357263225

C,0,1.2633686941,-1.3312656278,1.2100408976

C,0,2.081610263,-0.558102018,0.521844211

C,0,3.5491704322,-0.5077478344,0.4678920065

C,0,4.2582087136,-1.7151714321,0.4128179124

C,0,4.2737946875,0.6864998283,0.5707884576

C,0,5.646737104,-1.729276445,0.4652610488

H,0,3.7056072314,-2.6411185125,0.3172534855

C,0,5.6596134149,0.6690219352,0.6237265661

H,0,3.7445745959,1.6275668804,0.6267918

C,0,6.3536526321,-0.5370412878,0.5692988129

H,0,6.1758442321,-2.6729940103,0.415166326

H,0,6.2017774936,1.6020826362,0.7144125037

H,0,7.4356843625,-0.5454943768,0.6057847728

C,0,-3.5753044393,-3.4982481115,0.1362096791

H,0,-3.1399416746,-4.0726772213,-0.6757249086

H,0,-4.5234682512,-3.0641850086,-0.1841314357

H,0,-3.7815838832,-4.1411055636,0.992954103

C,0,-2.6494738663,-2.3932114244,0.5428561371

O,0,-1.5762856623,-2.2160265503,-0.0342675618

O,0,-3.0859172886,-1.6687856969,1.5372221268

H,0,-2.3966076826,-0.9854844088,1.8396910228

^{1}TS3

C,0,1.7909955063,-2.0717918994,-1.2007877756

C,0,2.7494114305,-1.2863161243,-0.5695942677

C,0,2.8999481395,0.0874138179,-0.9259565951

C,0,2.1703716419,0.5890048913,-2.047654925

C,0,1.2490447641,-0.2435344357,-2.733709362

C,0,0.9955747084,-1.555252534,-2.2744995026

H,0,1.5947476375,-3.0730631759,-0.8406341927

H,0,3.2935416561,-1.6864273314,0.2723518993

H,0,2.326878706,1.6110037565,-2.3664847136

H,0,0.6809740849,0.1498624349,-3.5672754024

C,0,-0.0358338288,-2.4328619776,-2.9261548517

H,0,-0.6270121525,-2.9618432531,-2.177755839

H,0,-0.7192414892,-1.853079539,-3.545226684

H,0,0.445862606,-3.1804754045,-3.5626091555

C,0,3.8928668027,0.9957035369,-0.2295612273

H,0,3.4785082939,2.0040452207,-0.2900446076

C,0,4.0962385501,0.6767791325,1.2523337324

H,0,4.7168789338,1.4477138514,1.7111761303

H,0,3.1454700938,0.6496053403,1.782015254

H,0,4.6082177745,-0.278170456,1.3949446346

C,0,5.2283229216,0.9661878641,-0.9909724714

H,0,5.1002256245,1.2468905808,-2.0382412042

H,0,5.9385326199,1.6603144213,-0.5373498617

H,0,5.6694501244,-0.0334254477,-0.9622082123

Ru,0,0.717338905,-0.088460906,-0.5855581082

C,0,-0.2345535821,-0.9643600699,3.5883670581

C,0,-0.7030560438,-2.2631861938,3.711862039

C,0,-1.34120887,-2.8562891877,2.6226247767

C,0,-1.5316482695,-2.1504618432,1.4490471529

C,0,-1.0795075179,-0.8210286662,1.3020669406

C,0,-0.3813534693,-0.2534355961,2.4015491801

H,0,0.2713256516,-0.4700305326,4.407958343

H,0,-0.5673670612,-2.8101997629,4.6356587499

H,0,-1.701353827,-3.8755957117,2.6935267629

H,0,-2.0526744067,-2.6196894569,0.6252632026

C,0,0.232885793,1.0976759427,2.30708333

O,0,0.2477703592,1.919830489,3.2219795269

N,0,0.7667797712,1.2732861107,1.070212264

O,0,1.2879878614,2.5381844347,0.7761545758

C,0,0.3336299719,3.6249962886,0.8165164701

H,0,0.771576385,4.3573336862,0.1338474538

H,0,0.3139810637,4.0355263413,1.8276060096

C,0,-1.0943906145,3.289360426,0.3920292263

H,0,-1.5916601847,4.2417766189,0.1901300206

H,0,-1.627516514,2.8267376131,1.2237011219

C,0,-1.2431729397,2.3788910174,-0.853653554

H,0,-2.292576532,2.3739598833,-1.1613798566

H,0,-0.64049618,2.7606177643,-1.6802002144

C,0,-0.8188086312,1.0163048909,-0.461443424

C,0,-1.5238419805,-0.0384086602,0.1147222561

C,0,-2.8623958098,-0.3355852221,-0.4651080398

C,0,-3.04875743,-0.3693849085,-1.8503162964

C,0,-3.980493545,-0.5149319561,0.3595297956

C,0,-4.3108185504,-0.5672356633,-2.3994583595

H,0,-2.1890799369,-0.2465638936,-2.4959146941

C,0,-5.2395467656,-0.7138485236,-0.1870688423

H,0,-3.8542259435,-0.4919278885,1.4340390715

C,0,-5.4111978216,-0.7414649508,-1.5695341821

H,0,-4.4319705228,-0.5927714938,-3.4754477216

H,0,-6.0931639808,-0.8418668474,0.4669584242

H,0,-6.3947938317,-0.9001857423,-1.9931105881

^{3}TS3

C,0,-1.2508315332,1.3877951202,2.1490220593

C,0,-2.4198434181,0.8300520334,1.5870836261

C,0,-2.8391798127,1.1633152489,0.2755761269

C,0,-2.0166609472,2.0227599931,-0.4804743076

C,0,-0.821975343,2.5557865417,0.0784761026

C,0,-0.4440531689,2.2853355136,1.4157173944

H,0,-0.9592136224,1.1081457806,3.1529778501

H,0,-2.9897069393,0.12272108,2.170057167

H,0,-2.2935499228,2.2772162283,-1.4946465039

H,0,-0.204285583,3.2094436342,-0.5237415115

C,0,0.7887281989,2.8941136189,2.0209104985

H,0,1.2352984012,2.219884987,2.7522828799

H,0,1.5390826203,3.1120083769,1.2611315439

H,0,0.5431504899,3.829457982,2.5317365675

C,0,-4.0887919831,0.5842786141,-0.3555412006

H,0,-3.8528047328,0.4375918371,-1.4129795551

C,0,-4.4989332292,-0.7767606378,0.2088559666

H,0,-5.3201767234,-1.1849359692,-0.3822074453

H,0,-3.6715125134,-1.4837336023,0.1698429101

H,0,-4.8519449748,-0.695362919,1.2400064532

C,0,-5.2380145571,1.6003613861,-0.2486144304

H,0,-4.9701122524,2.5590620546,-0.6965502512

H,0,-6.1267449291,1.2224083246,-0.7580910065

H,0,-5.498785918,1.7787959992,0.7975371641

Ru,0,-0.625734148,0.32518077,0.1576104768

C,0,0.5111924752,-3.1613772966,1.937269612

C,0,1.2268606818,-2.9085939975,3.0975209787

C,0,2.0126856687,-1.7572060461,3.176760661

C,0,2.1021355121,-0.9020216128,2.098690569

C,0,1.3906340829,-1.1359758103,0.8939881139

C,0,0.5485327238,-2.2912384948,0.8513864751

H,0,-0.1083870421,-4.0446205943,1.8500542826

H,0,1.1696812475,-3.5927474448,3.9342801578

H,0,2.5655213573,-1.5370685715,4.0819171424

H,0,2.7311613932,-0.025246995,2.1663854882

C,0,-0.365794885,-2.6222202653,-0.3041961102

O,0,-0.4002281839,-3.7398624993,-0.8172713534

N,0,-1.1317017782,-1.5555869093,-0.6073644951

O,0,-1.9114380199,-1.6089735323,-1.7687569494

C,0,-1.2431762269,-1.9948534332,-2.9957381672

H,0,-1.8491009815,-1.4948536274,-3.7560146153

H,0,-1.3363930129,-3.0760276029,-3.1136236432

C,0,0.2292662625,-1.6191742758,-3.1688233015

H,0,0.4429877762,-1.7447973643,-4.2356276278

H,0,0.8536265402,-2.3398956593,-2.6409009398

C,0,0.6442922043,-0.191859978,-2.7420909788

H,0,1.6357377513,0.0250825354,-3.1609631529

H,0,-0.055893363,0.5368832491,-3.1592780091

C,0,0.6833202278,-0.0953853961,-1.2709687906

C,0,1.6219013519,-0.2363979042,-0.2654365748

C,0,2.9239866257,0.480212264,-0.4024260347

C,0,2.9527362181,1.783164779,-0.9086337318

C,0,4.1428681253,-0.1594686245,-0.147125023

C,0,4.1569002745,2.4350214829,-1.1408827225

H,0,2.0145706423,2.2787907966,-1.1209489292

C,0,5.3475676802,0.4870998737,-0.3894880833

H,0,4.1419778533,-1.1738218899,0.2294660019

C,0,5.3606000322,1.7888567482,-0.8813520123

H,0,4.1558655315,3.4475362147,-1.5253225649

H,0,6.2800290637,-0.0290642346,-0.1975048599

H,0,6.3010607317,2.2931121206,-1.0637173867

^{1}TS4

C,0,-2.7697244447,-0.1884545511,-1.2119025982

C,0,-3.691908423,-0.0970224865,-0.1312122974

C,0,-3.707807521,-1.0872232499,0.8714233943

C,0,-2.8119738714,-2.1874816595,0.7254918024

C,0,-1.945073125,-2.3191085261,-0.3781397024

C,0,-1.8900236557,-1.3016824961,-1.3654743833

H,0,-2.6942402856,0.6438054282,-1.8995721284

H,0,-4.3138346103,0.7819950263,-0.0506456398

H,0,-2.7676159622,-2.9274141549,1.5147373889

H,0,-1.2716378055,-3.1638283993,-0.4350082473

C,0,-0.9371286445,-1.3768710642,-2.5229563466

H,0,-0.6391760433,-0.3807665877,-2.848517185

H,0,-0.0360879696,-1.927919792,-2.2535239077

H,0,-1.4083935056,-1.8851255425,-3.3691101034

C,0,-4.628313194,-1.0188974233,2.0727735328

H,0,-4.1467343376,-1.5978575006,2.8674851484

C,0,-4.8445994509,0.4022572705,2.5990788237

H,0,-5.3961542399,0.3712485834,3.5402677562

H,0,-3.8957211988,0.9136068395,2.7657414985

H,0,-5.4299084983,1.004416222,1.9014275627

C,0,-5.9659174149,-1.6994149639,1.7409621579

H,0,-5.818614065,-2.7276661616,1.4056078657

H,0,-6.6156727682,-1.7161277203,2.6182718902

H,0,-6.4839613035,-1.1571544297,0.946503991

Ru,0,-1.5881935527,-0.2867140742,0.5699737197

C,0,1.0655081426,2.4629739345,-2.7038760514

C,0,2.2402886422,2.307192989,-3.398057576

C,0,3.2639642447,1.5151937743,-2.8435442478

C,0,3.1043912373,0.9073963717,-1.6229593289

C,0,1.9093909048,1.0566878049,-0.8686056377

C,0,0.8769102998,1.8580926227,-1.4457036761

H,0,0.2538051925,3.0589388076,-3.0992478866

H,0,2.3788846662,2.7846044286,-4.3592540962

H,0,4.1890688859,1.3750481532,-3.3899650579

H,0,3.8976728064,0.2873636213,-1.2299577929

C,0,-0.4089225767,2.0543754203,-0.7998308718

O,0,-1.3581892047,2.6666077073,-1.2543125392

N,0,-0.5518369899,1.3837778209,0.4645260084

O,0,-0.9889960903,2.705107624,1.6210470157

C,0,0.0313478928,2.687570249,2.5683912255

H,0,-0.1650605101,3.5061298365,3.2732455438

H,0,1.010869988,2.896684042,2.1097748856

C,0,0.1010480729,1.3565031695,3.3371504151

H,0,-0.7297621329,1.2918648606,4.0425290336

H,0,1.0308267176,1.3213089368,3.910811597

C,0,0.0716182553,0.1442959936,2.3791544759

H,0,0.6834996847,-0.6788935657,2.7337627188

H,0,-1.000386124,-0.2445594414,2.4245459047

C,0,0.4498495172,0.5332775226,0.9704362646

C,0,1.7041486565,0.4016818205,0.3785743922

C,0,2.7365971705,-0.4417385311,1.0191667779

C,0,2.5026744763,-1.8011581096,1.2607979085

C,0,3.9671476903,0.0927092847,1.4204756456

C,0,3.4542172936,-2.5940769167,1.8920898779

H,0,1.563478488,-2.2341170853,0.9373435861

C,0,4.9234026116,-0.6991952969,2.0429011396

H,0,4.1639779228,1.1430126448,1.2454354102

C,0,4.670053209,-2.0462056352,2.2850330908

H,0,3.2498376704,-3.6432279432,2.0680573285

H,0,5.8658853131,-0.261804533,2.3487261909

H,0,5.4145110481,-2.6623247311,2.7731714647

^{1}TS5

C,0,-2.6300731388,-1.650926424,1.7991963842

C,0,-3.1615102996,-1.4129514669,0.4909236244

C,0,-3.4774745184,-0.108558109,0.051589001

C,0,-3.1739599113,0.969127794,0.9353915091

C,0,-2.5588583085,0.7472690464,2.1689889217

C,0,-2.2952659949,-0.5856857369,2.6318200841

H,0,-2.4194304129,-2.6646280654,2.1114160329

H,0,-3.333818916,-2.2591642238,-0.157110128

H,0,-3.3318931823,1.9850123511,0.5974558242

H,0,-2.2474309468,1.5883843199,2.772580327

C,0,-1.6095390751,-0.7881140849,3.9486624735

H,0,-1.4068602405,-1.8413039167,4.13627189

H,0,-0.6593246365,-0.2515267075,3.9581095619

H,0,-2.2245489595,-0.3991274482,4.7635207738

C,0,-4.0774793186,0.1946641561,-1.3035820058

H,0,-3.5715925941,1.0989521811,-1.6545826034

C,0,-3.8338607126,-0.896419365,-2.3456774653

H,0,-4.1789367477,-0.5551218691,-3.3226622348

H,0,-2.774031165,-1.1378206545,-2.4249713333

H,0,-4.3833895189,-1.8111684538,-2.1102473701

C,0,-5.5754774438,0.500651882,-1.1527498983

H,0,-5.7520472817,1.3097667277,-0.4413561317

H,0,-6.0015093113,0.7963768345,-2.1132122285

H,0,-6.1161687909,-0.3812012277,-0.8001189655

Ru,0,-1.2844651398,-0.2711803775,0.5238615989

C,0,0.8682093458,-2.169877351,-2.6315236515

C,0,1.0188726081,-3.5018286668,-2.2788139704

C,0,0.5403684305,-3.9451046918,-1.0433412163

C,0,-0.1074822437,-3.0773805014,-0.1687676405

C,0,0.2282558517,-1.3104353943,-1.7424335374

H,0,1.2595653197,-1.7771029498,-3.5619259034

H,0,1.5187321003,-4.1919130529,-2.9467983683

H,0,0.6797775178,-4.982001105,-0.7592069228

H,0,-0.4529196616,-3.454267955,0.7862949879

C,0,0.1653412047,0.1642914286,-1.9561778505

O,0,0.8613680389,0.7931652495,-2.7321731213

N,0,-0.8522701762,0.6222583664,-1.1414593365

O,0,-0.5263067361,2.4678398553,-0.7959540347

C,0,-0.168369529,3.5486348407,-1.6636075043

H,0,-0.572465928,4.4496069454,-1.1831202633

H,0,-0.7241329254,3.3838351679,-2.5869965212

C,0,1.3070515576,3.7459501738,-1.9794651382

H,0,1.3602717955,4.6719786192,-2.5610570662

H,0,1.6506341646,2.9358866886,-2.6167052875

C,0,2.923463876,2.6290395337,-0.427913444

C,0,3.4734864342,1.5780094044,-0.2224198461

C,0,4.0398553577,0.2928463698,0.0134986442

C,0,3.6252876564,-0.7986378607,-0.7622076593

C,0,4.9800594946,0.0830034372,1.0316502475

C,0,4.1238033959,-2.0674875843,-0.5111156092

H,0,2.904106887,-0.635225695,-1.5491882998

C,0,5.4805668352,-1.1888112557,1.2726683813

H,0,5.3052647817,0.922280691,1.6325366354

C,0,5.0515738632,-2.2688558085,0.5066936228

H,0,3.7746598291,-2.9008612753,-1.1071087856

H,0,6.2054391691,-1.3384297106,2.0634081729

H,0,5.4383304244,-3.2611371108,0.7027070953

C,0,0.9346178674,1.2154426307,1.8665474171

C,0,2.073721427,1.1963657266,2.8597876233

H,0,2.582352232,0.2362887408,2.8573592572

H,0,2.771238585,1.9970994867,2.6239712015

H,0,1.6632207972,1.386628289,3.8550174535

O,0,0.5433060986,0.0679053366,1.4625468023

O,0,0.4318373458,2.313449449,1.5458939396

C,0,-0.2950566048,-1.7366947562,-0.514182023

H,0,-0.0845894566,2.4446056732,0.1285279488

C,0,2.2382592513,3.8728400096,-0.7480538208

H,0,2.9901716402,4.6434442475,-0.9420998486

H,0,1.6769636429,4.208621202,0.1305225985

^{1}TS5b

C,0,-0.5664071702,-2.497532351,-0.0771452806

C,0,-1.4497702069,-1.7927166583,-0.9353332388

C,0,-2.4140747048,-0.8984823851,-0.4303083029

C,0,-2.4183620845,-0.6577457942,0.9682544238

C,0,-1.502303348,-1.309307632,1.7932681489

C,0,-0.5886137469,-2.2790104901,1.3009490752

H,0,0.1308088404,-3.207489571,-0.501760954

H,0,-1.38033023,-1.9685109894,-1.999100407

H,0,-3.1247820313,0.0660566637,1.3906381769

H,0,-1.5017227853,-1.0799299429,2.8519519837

C,0,0.3194173021,-3.0051947819,2.2470785862

H,0,1.0194610496,-3.6498931739,1.7174774418

H,0,0.8852888722,-2.2983028514,2.8569065964

H,0,-0.2674724776,-3.6266816968,2.9272697449

C,0,-3.3945918657,-0.144293215,-1.2947780044

H,0,-3.3783181646,0.8875175732,-0.9318384434

C,0,-3.038917502,-0.1370521666,-2.7791620888

H,0,-3.7268037226,0.5198194563,-3.3118739954

H,0,-2.0275045121,0.2362288665,-2.9468427276

H,0,-3.1255065952,-1.1311659193,-3.2274509996

C,0,-4.81297047,-0.691909785,-1.0524199155

H,0,-5.0876182044,-0.6210850583,-0.0000868817

H,0,-5.530091431,-0.1019628139,-1.6250196978

H,0,-4.893166837,-1.7334035612,-1.3760683613

Ru,0,-0.1462287483,-0.0937840037,0.0714382298

C,0,1.993475075,1.6081253584,-3.1902417586

C,0,2.7995350426,0.6128253397,-3.7257808167

C,0,2.7815758436,-0.6663771597,-3.1689440884

C,0,1.977392533,-0.9649969558,-2.0700559086

C,0,1.1601766968,0.0225561525,-1.5313070588

C,0,1.1780050319,1.2928606238,-2.1092278742

H,0,1.9833765022,2.6138418255,-3.5921481817

H,0,3.440382528,0.8249873585,-4.5717989611

H,0,3.4140648162,-1.4400575112,-3.5876299191

H,0,2.0251146032,-1.9533741504,-1.6314059422

C,0,0.2772006614,2.2361904921,-1.3997784159

O,0,0.3392967247,3.4454961294,-1.369898285

N,0,-0.687459456,1.4572683878,-0.7318151705

O,0,-1.7196889717,2.4769153649,1.1108417529

C,0,-1.2177240174,3.5401230071,1.8669619396

H,0,-1.7940630352,3.6353414964,2.8017173476

H,0,-1.2943327877,4.4954504813,1.333486541

C,0,0.2417521796,3.2512959494,2.1986849946

H,0,0.5866201888,3.9585667243,2.9567136884

H,0,0.8527197526,3.4080401265,1.3083493663

C,0,0.4490877153,1.8092176518,2.7278844071

H,0,1.228428985,1.7989863276,3.4967797653

H,0,-0.4741247024,1.4540026146,3.1887723238

C,0,0.900329896,0.8610379287,1.6913706976

C,0,1.7715405607,0.2080737774,1.0766782228

C,0,3.1231295716,-0.176232568,0.7512108847

C,0,3.5854288214,-1.4758321929,0.9763841479

C,0,3.9802538088,0.7622301871,0.1648147621

C,0,4.8822736921,-1.8279727432,0.6303177752

H,0,2.9250929761,-2.2063840602,1.4219689967

C,0,5.2730940818,0.4027195375,-0.1853100942

H,0,3.6150889726,1.760549664,-0.0338113525

C,0,5.7282219556,-0.8915600876,0.0448106156

H,0,5.2327817784,-2.8355515485,0.8149317921

H,0,5.9243677572,1.133997467,-0.6463272122

H,0,6.7371168121,-1.1696953795,-0.2316269304

C,0,-6.4339748515,2.3997856145,1.1031682678

H,0,-7.0396372656,1.8581205005,1.8273996337

H,0,-6.5515555184,3.4756709016,1.2375208887

H,0,-6.7803067248,2.1618578205,0.0942976039

C,0,-4.961480063,2.0153067902,1.2216204131

O,0,-4.6513729951,1.0429880639,1.9407396415

O,0,-4.1564315763,2.7194141002,0.533424669

H,0,-2.7216798148,2.5950954037,0.8591128521

[1]TS5c

C,0,-3.1663815611,-1.5053683603,1.633096695

C,0,-3.5198709265,-1.1019046035,0.306377698

C,0,-3.4329111906,0.2470247983,-0.1016823699

C,0,-2.9003236467,1.1738425983,0.8379656226

C,0,-2.4731337268,0.7694648883,2.1042372062

C,0,-2.616414125,-0.5886005086,2.5287257805

H,0,-3.2705360408,-2.5426883585,1.9197734031

H,0,-3.8759490338,-1.8534819203,-0.3822233838

H,0,-2.7422654791,2.2027928899,0.541301012

H,0,-2.0021177038,1.4817792343,2.7633808344

C,0,-2.1528405009,-0.9918871892,3.8956112906

H,0,-2.0272941295,-2.0711485349,3.9713874556

H,0,-1.2065403668,-0.5050748545,4.1304439385

H,0,-2.8865148912,-0.6779702072,4.6434335168

C,0,-3.8334966169,0.7311050339,-1.4777126881

H,0,-3.074725914,1.4654052826,-1.7652134861

C,0,-3.8318003429,-0.3651402769,-2.5424978015

H,0,-3.9986877217,0.0756852546,-3.5263649521

H,0,-2.8791154709,-0.8937936804,-2.5628201041

H,0,-4.6301035765,-1.0920559822,-2.374549199

C,0,-5.1932499768,1.4422427351,-1.4065177872

H,0,-5.1837843581,2.2557354407,-0.6786708346

H,0,-5.4551182756,1.861027861,-2.3800158668

H,0,-5.9804510959,0.7416381213,-1.1174163217

Ru,0,-1.4004880375,-0.5598547305,0.479023595

C,0,0.2894543372,-2.998947949,-2.5887188903

C,0,-0.0102209264,-4.3145910998,-2.2724025627

C,0,-0.7263703616,-4.5954015521,-1.1063346858

C,0,-1.1550834489,-3.5753911566,-0.2612887353

C,0,-0.144425194,-1.9877231832,-1.7349227421

H,0,0.8664908452,-2.7378157438,-3.4672631986

H,0,0.3196948404,-5.121641738,-2.9142508017

H,0,-0.9450203438,-5.6259540374,-0.8501327633

H,0,-1.6875157011,-3.8345545367,0.6455672868

C,0,0.2275905548,-0.5629075887,-1.924576379

O,0,1.1003305732,-0.153871686,-2.6702966437

N,0,-0.6406819872,0.1884106465,-1.1372648758

O,0,0.4021683664,1.7934772126,-0.9902134842

C,0,0.0409338312,2.758137459,-1.9847928203

H,0,-0.386295496,3.6306966123,-1.4777883701

H,0,-0.734414995,2.3175281208,-2.615410049

C,0,1.2443517603,3.1499922542,-2.8245869079

H,0,0.8957963851,3.8553261955,-3.5857071503

H,0,1.6160989382,2.2595948474,-3.3315016723

C,0,3.142968835,2.8371514447,-1.2394984709

C,0,3.7146978416,1.9420926722,-0.6730792477

C,0,4.3005385793,0.7846830274,-0.0852870106

C,0,3.8591722104,-0.4830876712,-0.4984186843

C,0,5.3067386934,0.8734110185,0.8863072497

C,0,4.422802406,-1.627175115,0.0456617337

H,0,3.0754392239,-0.5490732412,-1.2414041406

C,0,5.8634536639,-0.2788425248,1.4251313234

H,0,5.6462440909,1.8488144015,1.2097542642

C,0,5.4265146955,-1.5314339567,1.005231817

H,0,4.067789342,-2.5981950304,-0.275635192

H,0,6.639981373,-0.1984969967,2.1756183385

H,0,5.8617135391,-2.4278325104,1.4288594598

C,0,1.0009033458,-0.254362873,2.29683328

C,0,2.3014532558,-0.824354213,2.8147692064

H,0,3.1230235549,-0.2509548649,2.3830657492

H,0,2.3443008449,-0.7067900212,3.8971653927

H,0,2.422790072,-1.8658550321,2.5300474934

O,0,0.4498577011,-0.9285414128,1.3602597174

O,0,0.565981705,0.8030059408,2.7960259458

C,0,-0.8811009376,-2.241724576,-0.5714865217

H,0,0.1301846269,2.1371221897,-0.0844366612

C,0,2.3863730531,3.8058906208,-2.0211299165

H,0,3.0648798533,4.3114750751,-2.7154281248

H,0,1.9819447367,4.5894735709,-1.369346578

C,0,0.8508946685,3.8211781411,1.595149306

H,0,0.5628470727,4.7289465371,1.0636644741

H,0,0.8995492489,4.040674077,2.6641474926

H,0,1.8383478966,3.5029747554,1.2486937054

O,0,-0.1385872228,2.8242845711,1.3291637163

H,0,0.0647807619,2.0328189881,1.9077050747

[1]TS5d

C,0,-2.5438100809,-1.141707508,2.0268036353

C,0,-3.127075544,-1.3274612312,0.7328064044

C,0,-3.6175915487,-0.2448692622,-0.0395946023

C,0,-3.4323944889,1.0614517662,0.5132139454

C,0,-2.8980133593,1.267357725,1.8079743372

C,0,-2.4158791684,0.1644262719,2.5664645114

H,0,-2.1767783912,-2.00325568,2.5869361647

H,0,-3.1643881381,-2.338111105,0.3240076444

H,0,-3.7066166093,1.9299159475,-0.0913041351

H,0,-2.7602388371,2.2827318112,2.1838662648

C,0,-1.6773000575,0.4159056611,3.850641849

H,0,-1.3996035817,-0.5212694709,4.3523060224

H,0,-0.7544296485,0.971554404,3.6157844453

H,0,-2.2819587577,1.0242086669,4.5413727773

C,0,-4.272687825,-0.4082344088,-1.4001829326

H,0,-3.9870834166,0.485717891,-1.9807733066

C,0,-3.7833921637,-1.6344495786,-2.1781885226

H,0,-4.1990256705,-1.6224558281,-3.1975874675

H,0,-2.6862750189,-1.6519042378,-2.2511992166

H,0,-4.1117492514,-2.5755016229,-1.7068580434

C,0,-5.8042822691,-0.4104701098,-1.2478326109

H,0,-6.1620640176,0.4949084538,-0.7321768258

H,0,-6.2936360232,-0.4574911899,-2.2339104999

H,0,-6.1362208516,-1.2841921077,-0.6623691972

Ru,0,-1.4111975664,0.0644234037,0.4456746257

C,0,0.7800532072,-1.7481579374,-2.7323792344

C,0,0.8414963004,-3.114450245,-2.4672565401

C,0,0.3104600999,-3.6087586417,-1.2627681274

C,0,-0.3076474847,-2.7582597049,-0.3408333408

C,0,0.1661138467,-0.9059164265,-1.7970961473

H,0,1.2132878832,-1.3158915435,-3.6382642535

H,0,1.3127076766,-3.796881392,-3.1792524005

H,0,0.3814625393,-4.6785156367,-1.0437159849

H,0,-0.7068653907,-3.1801871701,0.5861724395

C,0,0.194269482,0.5788249745,-1.890757874

O,0,1.0168136364,1.2301663447,-2.5140602252

N,0,-0.883968024,1.0622328105,-1.1416320426

O,0,-0.174790519,2.616926382,-0.3149144679

C,0,0.1828212776,3.8658237315,-0.8835952193

H,0,-0.0616179421,4.6311759349,-0.1192291044

H,0,-0.5161423543,4.0119860836,-1.7226277247

C,0,1.608792271,4.0754361365,-1.3733115482

H,0,1.6203972101,5.0892190178,-1.8110521127

H,0,1.8277384625,3.3599933986,-2.1768111806

C,0,3.219814917,2.6521057581,-0.0768669026

C,0,3.6673066228,1.5236476947,-0.0347597163

C,0,4.116410824,0.1665305326,-0.0450258375

C,0,3.670866865,-0.6955709008,-1.0689230411

C,0,4.9604744083,-0.3429979996,0.9618200006

C,0,4.0518176605,-2.0368183061,-1.071594933

H,0,3.0073344814,-0.2956555999,-1.8375326385

C,0,5.3405834828,-1.6857288369,0.947976112

H,0,5.3042274476,0.3215889082,1.7575409039

C,0,4.88614216,-2.5372475688,-0.0654327026

H,0,3.6781732263,-2.697449345,-1.8568481458

H,0,5.9923161634,-2.0720429782,1.7361973349

H,0,5.179408296,-3.590328676,-0.0687936461

C,0,-0.4187136585,-1.3790112165,-0.6008922329

C,0,2.7027212792,4.0021889941,-0.2833829211

H,0,3.547292222,4.6500327727,-0.5794157244

H,0,2.3261293585,4.4261050017,0.6667913521

C,0,1.3126176023,-0.0886934741,1.7600591736

H,0,0.9215147613,-0.6890346171,2.6094595311

H,0,2.16955183,0.5004209178,2.1334809361

H,0,1.7026486725,-0.796292004,1.0073835938

O,0,0.3390287672,0.7767863387,1.2506863314

H,0,0.3929394478,2.0770817163,0.3513702346

^{1}TS5e

C,0,0.3501983018,-2.549599583,0.8108337117

C,0,-0.3704970036,-2.4058083317,-0.3968987968

C,0,-1.7111233345,-1.9557626065,-0.3925406509

C,0,-2.3129623744,-1.6976531414,0.86720729

C,0,-1.6006240714,-1.8391157898,2.0566528426

C,0,-0.247135059,-2.2476059974,2.0541718976

H,0,1.3791293709,-2.9127900436,0.7755680457

H,0,0.1218147882,-2.6518633076,-1.3377681664

H,0,-3.3364492807,-1.3197491979,0.8839920998

H,0,-2.0842252701,-1.5855513809,3.0020174642

C,0,0.5384552352,-2.3152751703,3.3362378794

H,0,1.3218052182,-3.0866263762,3.2941204043

H,0,1.0318270224,-1.3460495497,3.5260210856

H,0,-0.114119522,-2.5295739374,4.1949967043

C,0,-2.5356952321,-1.7474849737,-1.6498416586

H,0,-3.0525969473,-0.7873878489,-1.4804861086

C,0,-1.7073117977,-1.650769324,-2.932483752

H,0,-2.3586889824,-1.3785133299,-3.7768602844

H,0,-0.9213275679,-0.8856364553,-2.854089458

H,0,-1.2277243892,-2.6109659113,-3.1895183877

C,0,-3.6156890717,-2.8396948258,-1.7617468833

H,0,-4.2514089746,-2.8733005151,-0.8639102251

H,0,-4.2686723739,-2.6396526693,-2.625834646

H,0,-3.1624455325,-3.836168927,-1.8998965094

Ru,0,-0.0016279893,-0.0660855123,0.3320186976

C,0,1.31357258,1.7839423219,-3.2530399552

C,0,2.3905567288,1.0412494036,-3.7443040615

C,0,2.8328977797,-0.0882470731,-3.0415031559

C,0,2.2231892646,-0.4817029787,-1.8408250234

C,0,1.1368976008,0.2456500582,-1.3451751997

C,0,0.6980840626,1.3710268773,-2.0686190505

H,0,0.9364403562,2.6705190675,-3.7695529773

H,0,2.8855036566,1.3359552944,-4.6729385208

H,0,3.674121203,-0.670383454,-3.4287026908

H,0,2.6135757463,-1.3457813805,-1.2981143849

C,0,-0.4795192682,2.0529702923,-1.446786413

O,0,-0.9198029768,3.1565102189,-1.6992214654

N,0,-1.0285926437,1.1354867243,-0.5329279835

O,0,-2.068909424,1.3852117489,1.4640222024

C,0,-2.0030687071,2.6236556866,2.0469922675

H,0,-2.2554948225,2.5499299253,3.1378615753

H,0,-2.7528436991,3.3312072323,1.6236248223

C,0,-0.6161978767,3.2727320248,1.9406721089

H,0,-0.6148696127,4.2233536343,2.5017756741

H,0,-0.4150214972,3.5217020333,0.8860398526

C,0,0.5018610261,2.3785934913,2.4999757481

H,0,1.4082420748,2.9759337733,2.704139988

H,0,0.1749246052,1.9672288586,3.4735288481

C,0,0.9262781938,1.2389420874,1.6494486073

C,0,1.840261302,0.4362260617,1.2620399679

C,0,3.2326495037,0.0591309375,1.1156518108

C,0,3.7240160438,-1.1743336063,1.5826969563

C,0,4.1184429565,0.9391871256,0.4616839418

C,0,5.0654690955,-1.516844449,1.40483086

H,0,3.0505483514,-1.8577335817,2.0997635409

C,0,5.4570748851,0.5908687242,0.2823235207

H,0,3.7357959957,1.8866110138,0.0777749695

C,0,5.9353428046,-0.6379510052,0.7505380041

H,0,5.4344982066,-2.4748508689,1.7798239433

H,0,6.1301471528,1.280712843,-0.2328362021

H,0,6.9838947734,-0.9100598813,0.6065095521

C,0,-4.3818019375,1.7767956434,-0.8572634524

H,0,-4.9254304659,1.4407991509,-1.7589074508

H,0,-5.029107827,2.5232093355,-0.3476563698

H,0,-3.4677504689,2.3053622195,-1.1920445322

H,0,-3.3649136668,0.9437416378,0.5753108571

O,0,-4.0943704978,0.6673095074,-0.0463006655

^{1}TS6

C,0,-1.8001506337,-2.827849381,-0.3931973086

C,0,-2.536318424,-1.7357355931,-0.8257627873

C,0,-3.4012155916,-1.0478795884,0.0320229049

C,0,-3.5272287448,-1.5319726979,1.3325756918

C,0,-2.7977474165,-2.6362185163,1.7629673919

C,0,-1.9061953064,-3.2910537811,0.9177718671

H,0,-1.1173666265,-3.3146919059,-1.0794445743

H,0,-2.4246358565,-1.3908061102,-1.8451965494

H,0,-4.1871770834,-1.0392331836,2.0334372216

H,0,-2.9151346336,-2.9818277465,2.7841783329

C,0,-1.0443492691,-4.4214165545,1.4119539524

H,0,-0.8428163539,-5.1466215332,0.6217282699

H,0,-0.0772693105,-4.0436131545,1.7588888002

H,0,-1.5100339595,-4.9480916531,2.2466058075

C,0,-4.1478839805,0.1685378958,-0.4892683052

H,0,-3.4088600829,0.7737761732,-1.0242272341

C,0,-5.226237263,-0.2480731061,-1.5027727596

H,0,-5.7168450549,0.6319560833,-1.9253682337

H,0,-4.7996646723,-0.8235776139,-2.3251729037

H,0,-5.9889630646,-0.8647750346,-1.0199807871

C,0,-4.7549816855,1.044328653,0.6079598509

H,0,-4.0170857612,1.3171292785,1.3629817839

H,0,-5.1512090751,1.9631722514,0.171647044

H,0,-5.5839589697,0.5386701231,1.1106937728

Ru,0,-0.0600026115,0.709534749,-0.254029108

C,0,1.1358684593,-2.2122396159,-2.939173262

C,0,1.6749955266,-3.2718664341,-2.2277329599

C,0,1.9350285171,-3.1366711233,-0.8595702183

C,0,1.7273164447,-1.92774718,-0.2247076917

C,0,1.2454744967,-0.8217424014,-0.9457237972

C,0,0.9030546017,-0.9964149906,-2.2986747316

H,0,0.8480361529,-2.313684967,-3.978137298

H,0,1.8651616578,-4.2163969011,-2.7219556579

H,0,2.2997635769,-3.984253902,-0.2932494972

H,0,1.9359787344,-1.8257589698,0.8309332838

C,0,-0.0144526886,0.0084993353,-2.9053300836

O,0,-0.1517855322,0.1896717427,-4.1014523671

N,0,-0.7435188515,0.6994185482,-1.9429787544

O,0,-1.4328622438,2.3626596783,0.2401265816

C,0,-0.9069814492,3.7008115599,0.2723395465

H,0,-0.4243349043,3.8782287579,1.2406435477

H,0,-1.7531416453,4.3868709223,0.1851117825

C,0,0.0727936725,3.9586867627,-0.8676028284

H,0,0.1810742016,5.0399834571,-0.9807126292

H,0,-0.3642936472,3.5745055789,-1.7911305998

C,0,1.4746839718,3.3474457651,-0.6718769842

H,0,2.0972541485,3.5678444208,-1.5451028713

H,0,1.973897523,3.8075921941,0.1889270768

C,0,1.4220577002,1.8851417605,-0.4825669737

C,0,2.028857949,0.7319092529,-0.2636157754

C,0,3.2816378012,0.4115719677,0.4381985679

C,0,4.3374368712,-0.2333540986,-0.2085985915

C,0,3.4327522593,0.8139859989,1.767517421

C,0,5.5317330911,-0.4583931539,0.4615620043

H,0,4.2138178258,-0.556268328,-1.2337907704

C,0,4.6244588327,0.5723175135,2.4395687064

H,0,2.6051730688,1.2969966069,2.2707135798

C,0,5.6771922412,-0.0601305561,1.787268008

H,0,6.3493103117,-0.949840789,-0.0502248041

H,0,4.7291308471,0.8766541417,3.473250934

H,0,6.6068328023,-0.2450995737,2.3101103188

C,0,-0.9130840592,-0.5972735602,3.8184125228

H,0,-0.7292355964,-1.6420794087,3.581711368

H,0,-0.0762179927,-0.2242638133,4.4143691215

H,0,-1.8256160254,-0.4858681337,4.3996189323

C,0,-0.9997069136,0.230282966,2.5578156944

O,0,-1.6967065644,1.2539708574,2.5384050668

O,0,-0.2678263009,-0.2018681828,1.5824644778

H,0,-1.6682574708,2.0628706209,1.1715399036

^{3}TS6

C,0,2.1059912943,-1.9163360725,0.6946073633

C,0,2.8599021722,-0.7582486059,0.8940712129

C,0,3.7241675556,-0.2719443566,-0.0962462004

C,0,3.7879712331,-0.9802906823,-1.2914701441

C,0,3.0341565375,-2.1341884974,-1.4890647376

C,0,2.1851503827,-2.6282060045,-0.5052272465

H,0,1.4716703056,-2.2801986229,1.4930994495

H,0,2.8035042712,-0.2485032246,1.8481143329

H,0,4.4252618225,-0.6304123739,-2.0922512083

H,0,3.1094653816,-2.6583740255,-2.435696521

C,0,1.374728116,-3.8744508372,-0.7346288542

H,0,0.7586694057,-4.1140923929,0.1310807815

H,0,0.7066432535,-3.7510600926,-1.5900759715

H,0,2.0195287101,-4.7317500108,-0.9433409565

C,0,4.5671574025,0.9549299027,0.1944634973

H,0,3.9358916093,1.6248710787,0.784420802

C,0,5.7825804829,0.5697921065,1.0546172967

H,0,6.3610125336,1.4572391156,1.3224118044

H,0,5.4761736848,0.0721125172,1.9762456143

H,0,6.4393682025,-0.1116132006,0.5079184668

C,0,5.0070912014,1.7193780392,-1.0557488003

H,0,4.1601863459,1.9509659119,-1.7019950684

H,0,5.489705753,2.6554512594,-0.767826711

H,0,5.7348856086,1.1485664213,-1.6385417029

Ru,0,0.1957103463,0.3882949253,0.3652153331

C,0,-2.0063075938,-2.6650250122,2.2946340033

C,0,-2.3962642906,-3.5788855657,1.3194764582

C,0,-2.1924488159,-3.3049805936,-0.0366613699

C,0,-1.6279581794,-2.1035470266,-0.4311287663

C,0,-1.261539221,-1.15695387,0.536161548

C,0,-1.4505064488,-1.4571900257,1.9020926262

H,0,-2.115254038,-2.8770615555,3.3509672092

H,0,-2.8496728181,-4.5176198414,1.6128681272

H,0,-2.4801047265,-4.0370848942,-0.7809698625

H,0,-1.4758376929,-1.8728334584,-1.47733874

C,0,-0.8450349626,-0.4670411042,2.8615067163

O,0,-1.0649961135,-0.4586231524,4.0639242984

N,0,0.0041646526,0.3592735628,2.1729718867

O,0,1.5594230183,2.217679998,0.0836326267

C,0,1.0683848853,3.5589679795,0.2261860008

H,0,1.1166736258,4.0425867282,-0.7550792513

H,0,1.7503374008,4.0874292413,0.8973647942

C,0,-0.3500956669,3.6573499192,0.7786024865

H,0,-0.5819728148,4.7225186602,0.8669579945

H,0,-0.383871174,3.2366209247,1.7856993265

C,0,-1.4266287787,2.9907011028,-0.0949992396

H,0,-2.4148755348,3.380907124,0.1627047693

H,0,-1.2473912909,3.2353354829,-1.1474750596

C,0,-1.4482278351,1.5040783127,0.0372938203

C,0,-2.3143325794,0.5625469055,0.0595955198

C,0,-3.6731573032,0.1385843125,-0.1542485958

C,0,-4.4689274201,-0.3410845567,0.8934169442

C,0,-4.2172338179,0.2481118264,-1.4414548874

C,0,-5.7884620415,-0.6913200003,0.6555997672

H,0,-4.0427576901,-0.4376639502,1.8822363584

C,0,-5.5404799901,-0.1008183005,-1.6694507614

H,0,-3.5920397356,0.6046070798,-2.2492784203

C,0,-6.3268777727,-0.5731745203,-0.623481257

H,0,-6.4006239647,-1.0571610997,1.4698052927

H,0,-5.9567014748,-0.0089581279,-2.6645204311

H,0,-7.3574713576,-0.8510312023,-0.8041420001

C,0,1.1632737795,0.049214691,-4.0147588755

H,0,1.8278071239,-0.8168533838,-3.9838467821

H,0,0.1755521335,-0.3031932198,-4.3099624431

H,0,1.5485353357,0.7668758669,-4.7352489714

C,0,1.1181867703,0.6503140579,-2.6277091592

O,0,1.7752873472,1.6859030752,-2.3927472653

O,0,0.4075075929,0.0189798884,-1.7744265885

H,0,1.742102925,2.0524394064,-0.9055767418

^{1}TS7

C,0,-2.710789391,1.6502483477,1.5026452239

C,0,-2.9708647388,0.2897907243,1.5781529541

C,0,-3.8507503011,-0.3359788351,0.6917877881

C,0,-4.4631406638,0.4607226067,-0.2734680072

C,0,-4.1980383381,1.8245562936,-0.352781959

C,0,-3.3124563831,2.4433608151,0.5256865537

H,0,-2.0183735318,2.0876316003,2.2111719142

H,0,-2.4621431853,-0.2979356958,2.3330061433

H,0,-5.1458996975,0.021067566,-0.9879084394

H,0,-4.6902945268,2.4163974981,-1.116951968

C,0,-2.9740655192,3.9041751436,0.393373365

H,0,-2.7196228088,4.3444180445,1.3591639171

H,0,-2.1124014764,4.0399950385,-0.2673837514

H,0,-3.8044833773,4.4723107958,-0.0292084204

C,0,-4.1121792888,-1.8251128957,0.8367356367

H,0,-3.1380456045,-2.2855820509,1.029381006

C,0,-5.0090836438,-2.098473461,2.055388761

H,0,-5.1469337688,-3.1727303089,2.2022956689

H,0,-4.578597443,-1.6819621822,2.9671323206

H,0,-5.993799281,-1.6459076068,1.913610654

C,0,-4.6945790212,-2.4842959819,-0.4149400571

H,0,-4.1059784303,-2.2564837257,-1.3037332581

H,0,-4.725362174,-3.5685047773,-0.2868181643

H,0,-5.7200046239,-2.1531157475,-0.598247774

Ru,0,0.0238558395,-0.2275553082,-0.3696586322

C,0,0.6147303671,2.8341801948,0.5863194847

C,0,1.025453463,3.6263251675,-0.4516179279

C,0,1.9465745458,3.1268819092,-1.394553461

C,0,2.4605204213,1.860416043,-1.2753364291

C,0,2.0589216824,1.0026534777,-0.216435332

C,0,1.082374164,1.5027370363,0.7025917273

H,0,-0.077297361,3.193742285,1.3340176385

H,0,0.6485842641,4.6360376219,-0.5482668125

H,0,2.2654294643,3.7574111196,-2.2150302718

H,0,3.200209705,1.5002167306,-1.9777083358

C,0,0.6336233079,0.6344888465,1.8302938622

O,0,0.2243450789,1.0142625462,2.9067997389

N,0,0.4685425704,-0.6977726152,1.3776708565

O,0,-1.133123961,-1.9562223837,-0.6380524428

C,0,-0.5414596599,-3.2582629661,-0.7520072537

H,0,-0.1049095292,-3.3797315361,-1.7504878746

H,0,-1.3516177578,-3.9842782266,-0.643364018

C,0,0.5054567454,-3.4921913686,0.326181512

H,0,0.7070013999,-4.5660029761,0.3554479694

H,0,0.0874741811,-3.2105672033,1.2922439964

C,0,1.841820828,-2.7693318122,0.0999554227

H,0,2.552927465,-3.0736201618,0.8748073524

H,0,2.2579910098,-3.1145077158,-0.8540170695

C,0,1.7760528117,-1.2805269873,0.0417895378

C,0,2.7326853538,-0.3178203218,-0.0106243366

C,0,4.1917353499,-0.4262336078,0.0226605012

C,0,4.9621136662,0.6767129327,0.4306973244

C,0,4.8732005128,-1.6034214323,-0.3267934157

C,0,6.3447107644,0.6016821161,0.4960723278

H,0,4.4662694642,1.5959039748,0.7138960592

C,0,6.2574823568,-1.6748118749,-0.2618484434

H,0,4.3214863792,-2.4642053125,-0.6723567088

C,0,7.002073549,-0.575207963,0.1507931746

H,0,6.9118684993,1.4637854081,0.8241110115

H,0,6.7577174929,-2.5935873796,-0.5417444309

H,0,8.0817257735,-0.6335889898,0.2009396092

C,0,-2.5690793781,1.1841759799,-3.603616785

H,0,-3.0808299832,1.9638823793,-3.0383699045

H,0,-1.7743504735,1.6628223178,-4.176800859

H,0,-3.2700282794,0.6849622011,-4.2675153946

C,0,-1.9710121425,0.2072980034,-2.6247046438

O,0,-2.3575192865,-0.9733286012,-2.60212328

O,0,-1.0617804678,0.7020700096,-1.8527297928

H,0,-1.6992900581,-1.7141872828,-1.4546314683

^{3}TS7

C,0,2.515673579,1.4149654473,-1.2315019789

C,0,2.8401026559,0.1120604462,-1.5911618723

C,0,3.7219091167,-0.6553691432,-0.820897707

C,0,4.275355333,-0.05755006,0.3039162759

C,0,3.9447873845,1.2472758447,0.6686883905

C,0,3.0518319781,2.0036542862,-0.0786437409

H,0,1.864063621,1.9898680824,-1.8733215542

H,0,2.3980234208,-0.3119661588,-2.4849308653

H,0,4.9540039071,-0.6128142974,0.9368101552

H,0,4.3811354605,1.6697981139,1.5665561573

C,0,2.6167804961,3.3749740797,0.3563400435

H,0,2.5057955535,4.0491128772,-0.4946371425

H,0,1.6458336877,3.3142510244,0.8554210068

H,0,3.3293372826,3.818534451,1.0531309742

C,0,4.0144163943,-2.0823928727,-1.2418127218

H,0,3.0599850934,-2.4949447923,-1.584909168

C,0,4.9892817821,-2.1119521028,-2.429905849

H,0,5.1456725434,-3.1357689259,-2.7778554926

H,0,4.6123086738,-1.5222786779,-3.2667424713

H,0,5.9584370371,-1.6994972055,-2.138404574

C,0,4.5204133551,-2.9724353793,-0.1057299192

H,0,3.8684261896,-2.9152883856,0.7669205454

H,0,4.5672313324,-4.0124542805,-0.4345753402

H,0,5.5273290967,-2.6876736105,0.2085251837

Ru,0,0.116465314,-0.0955757731,-0.0745152915

C,0,-0.6218588745,2.833637024,-1.6607980515

C,0,-0.9585305048,3.8330418742,-0.7900553482

C,0,-1.7475140459,3.5418155379,0.3400706769

C,0,-2.205240819,2.2698618875,0.5498169659

C,0,-1.8679131802,1.2029058457,-0.3285199326

C,0,-1.0255948543,1.4903697602,-1.4433582363

H,0,-0.0557337665,3.0382540675,-2.5590006161

H,0,-0.6287061124,4.8477702957,-0.9724969056

H,0,-2.0078839753,4.3302826852,1.0347960274

H,0,-2.8411645793,2.0513261828,1.3969508922

C,0,-0.6014487451,0.4668783888,-2.4870639825

O,0,-0.3131880797,0.8018226791,-3.6329213542

N,0,-0.3663735222,-0.758611091,-1.953865634

O,0,1.2815385146,-1.754920038,0.4927475437

C,0,0.7831870472,-3.0963147895,0.6269659135

H,0,0.5143240876,-3.2630401596,1.6761231018

H,0,1.6059819492,-3.7697854084,0.373826697

C,0,-0.4052329654,-3.3682830882,-0.2751730045

H,0,-0.6235197183,-4.437653741,-0.2136395389

H,0,-0.1429867843,-3.1407723769,-1.3080963869

C,0,-1.6616878635,-2.5861055329,0.1213472185

H,0,-2.5171660827,-2.9334601467,-0.4658597112

H,0,-1.894107812,-2.8095624942,1.169712408

C,0,-1.544168914,-1.1075682088,-0.0308225654

C,0,-2.4978046095,-0.1330673808,-0.0917601641

C,0,-3.9436891007,-0.240068426,0.1161135596

C,0,-4.8020313004,0.6751253399,-0.5168165136

C,0,-4.5196749555,-1.2429976029,0.910705409

C,0,-6.1773072854,0.5773739416,-0.3765036613

H,0,-4.3814766485,1.4560973593,-1.1363252202

C,0,-5.8962095701,-1.3331483568,1.0562258915

H,0,-3.8863029872,-1.9397400498,1.4391022664

C,0,-6.7319777448,-0.4273539518,0.4108604567

H,0,-6.8193786449,1.2850415003,-0.8854910368

H,0,-6.3185337742,-2.1104322058,1.680532

H,0,-7.806045954,-0.50140173,0.5231951495

C,0,1.6304287606,1.4013702536,3.7755405709

H,0,2.2827391264,2.1860578632,3.3862566141

H,0,0.7037990676,1.8770567635,4.0957497773

H,0,2.1190103032,0.9073538279,4.6116257091

C,0,1.3537447351,0.4214569074,2.6608051172

O,0,1.8685248459,-0.7132206628,2.694361391

O,0,0.5974097248,0.862681651,1.7235682835

H,0,1.6161183239,-1.422890182,1.4086661794

^{1}TS8

C,0,-2.9576503047,-0.9710910617,-0.69196139

C,0,-2.7442265284,0.3130291815,-1.1818789043

C,0,-3.2282606582,1.438673624,-0.509080843

C,0,-3.9148937886,1.226407708,0.6847341757

C,0,-4.1236727534,-0.0574852146,1.1755669295

C,0,-3.6583603119,-1.1801618014,0.4953108376

H,0,-2.567320261,-1.8199061491,-1.2404092797

H,0,-2.1923957652,0.4414393775,-2.1049209209

H,0,-4.2934915388,2.0668726718,1.2502819336

H,0,-4.666474665,-0.1863607803,2.106071962

C,0,-3.9057913176,-2.5653223815,1.0324145806

H,0,-3.5597999944,-3.3284713025,0.3362947232

H,0,-3.3852496022,-2.7235155418,1.9816278739

H,0,-4.9690308579,-2.732305235,1.2197878028

C,0,-3.0199825296,2.8133422597,-1.1201156399

H,0,-1.9835612074,2.8405165558,-1.4717317978

C,0,-3.925739672,2.9934711134,-2.3505788282

H,0,-3.7355901808,3.9559805321,-2.8313793125

H,0,-3.7590869039,2.207180325,-3.0878215606

H,0,-4.9780127932,2.9614596088,-2.0569619008

C,0,-3.2175710885,3.9724844123,-0.1411718958

H,0,-2.610590297,3.8489792195,0.7557636273

H,0,-2.9369589795,4.9137906104,-0.6177855624

H,0,-4.2643143365,4.0629733389,0.1601212435

Ru,0,0.3564387382,-0.1026349318,-0.1068417158

C,0,0.2603815681,-3.9019433763,-1.8765778072

C,0,-0.3978485123,-4.7984157385,-1.0506828886

C,0,-0.78311214,-4.3956811757,0.2303902265

C,0,-0.4455021069,-3.1421800626,0.7071278903

C,0,0.3013935381,-2.2423442588,-0.0762440821

C,0,0.5832208575,-2.6336071933,-1.4038908569

H,0,0.4995094873,-4.1450323589,-2.9044927892

H,0,-0.6444791684,-5.791114453,-1.4051210933

H,0,-1.3580608886,-5.0657435227,0.8573313527

H,0,-0.7725500509,-2.8663912125,1.6971256945

C,0,0.9441545434,-1.5542653888,-2.3584078359

O,0,1.5302139442,-1.712905087,-3.4122639278

N,0,0.4913259412,-0.3163198048,-1.9113043068

O,0,-0.7548061261,0.2949474125,1.637101337

C,0,-0.6773266974,-0.3532262324,2.902906799

H,0,-1.2886764112,-1.2566438383,2.8493988484

H,0,-1.1400215302,0.3076254013,3.6405027391

C,0,0.7542046051,-0.6675001791,3.3335673341

H,0,0.7341573945,-1.0187300747,4.3692381134

H,0,1.3239021758,0.2650223853,3.3191261517

C,0,1.4927396357,-1.7186916966,2.472914506

H,0,2.5307311038,-1.7708146074,2.8102751992

H,0,1.0655120245,-2.7075647423,2.6235770483

C,0,1.5146121084,-1.3290178921,1.0256645206

C,0,2.2087201594,-0.3841812828,0.3984137701

C,0,3.4901016237,0.2012833284,0.1786895688

C,0,4.6432754373,-0.408491946,0.7072148805

C,0,3.6202972938,1.3789491317,-0.5762736991

C,0,5.8886234859,0.1588700485,0.5012381222

H,0,4.5491171718,-1.3317199242,1.2644251091

C,0,4.8730134973,1.9370888895,-0.7764071726

H,0,2.7316780055,1.8302153747,-0.9957732089

C,0,6.0067198424,1.3350575958,-0.237627592

H,0,6.7717397038,-0.3165517105,0.9087564349

H,0,4.9682545383,2.8419127771,-1.3629267679

H,0,6.982735136,1.7743578981,-0.4003046261

C,0,0.4032395957,4.3512051383,-0.0166544107

H,0,0.1856135867,4.5020392833,-1.0728628947

H,0,-0.1581847278,5.051061852,0.5970995489

H,0,1.4715102087,4.5264552781,0.1303354721

C,0,0.0958278896,2.9257325597,0.3769169441

O,0,0.4227631036,2.0318105997,-0.4608691887

O,0,-0.4421941118,2.7147921675,1.4969577154

H,0,-0.685146138,1.3616914987,1.6843966838

^{3}TS8

C,0,-2.9270965856,-0.9718318844,-0.6898392459

C,0,-2.6773184204,0.2960947146,-1.2078842483

C,0,-3.1560244642,1.4483731242,-0.5734933362

C,0,-3.8571379197,1.2795775471,0.6177219792

C,0,-4.09908163,0.0128599181,1.1370340882

C,0,-3.6538333672,-1.1360631126,0.4896167367

H,0,-2.552921721,-1.8418711796,-1.2147231854

H,0,-2.1275373702,0.3888700946,-2.1371597413

H,0,-4.2285078598,2.1409966295,1.1558911688

H,0,-4.6566658172,-0.080934715,2.0627919419

C,0,-3.9582064034,-2.5009557919,1.0486701634

H,0,-3.6191983142,-3.2898193761,0.378662756

H,0,-3.4702952117,-2.6536164706,2.0157556531

H,0,-5.0312068408,-2.6287359683,1.209047983

C,0,-2.9415509803,2.8001590406,-1.2286174193

H,0,-1.9136008385,2.8017299221,-1.6011310624

C,0,-3.8762835317,2.9582427764,-2.4401881948

H,0,-3.6853064378,3.9041673735,-2.9525556816

H,0,-3.7375185048,2.1494374846,-3.1587841309

H,0,-4.9215332923,2.9486579788,-2.1211839542

C,0,-3.1011288069,3.9875145093,-0.2767284561

H,0,-2.4984183963,3.8698388781,0.6243745925

H,0,-2.7955793213,4.909724433,-0.7741792518

H,0,-4.1425390226,4.1153976039,0.0289010369

Ru,0,0.2273823584,-0.0838146052,-0.1190215493

C,0,0.2724764502,-3.9671569799,-1.8305779953

C,0,-0.4437079211,-4.8371996842,-1.0176572392

C,0,-0.8955286035,-4.3993657123,0.226153064

C,0,-0.5872771706,-3.1264474438,0.6810149879

C,0,0.1856512308,-2.2515343179,-0.0945345485

C,0,0.5645224436,-2.6871148859,-1.3851697651

H,0,0.5804134099,-4.2427096138,-2.8314871825

H,0,-0.6774597028,-5.8372492705,-1.3597981333

H,0,-1.4984582923,-5.0526848743,0.8445254525

H,0,-0.9605114245,-2.8144245253,1.6439624845

C,0,1.0706201741,-1.6374763378,-2.3383511634

O,0,1.634917641,-1.8815083396,-3.3914171343

N,0,0.682066275,-0.4187082283,-1.8667242576

O,0,-0.7198426553,0.2611286743,1.8374798196

C,0,-0.5336388504,-0.4314467991,3.0712121264

H,0,-1.1792566686,-1.3120678756,3.0468137518

H,0,-0.8958419386,0.2116263973,3.8774648242

C,0,0.9167175157,-0.8222975026,3.3466682095

H,0,0.9722309627,-1.229810471,4.3606396017

H,0,1.5268325264,0.0839526602,3.327609196

C,0,1.517624817,-1.854552932,2.3691925905

H,0,2.5705382696,-1.9994432486,2.6244085324

H,0,1.0306301978,-2.8210766378,2.4779525414

C,0,1.4769909518,-1.3505971539,0.958859121

C,0,2.1123558202,-0.3503641826,0.3868739381

C,0,3.365138612,0.2911550379,0.1600150035

C,0,4.5539131001,-0.306232671,0.6189815547

C,0,3.4350054152,1.5214558408,-0.5138800135

C,0,5.7714841337,0.3235898253,0.4280920003

H,0,4.5092763023,-1.2680751289,1.113488677

C,0,4.6594766418,2.1421921378,-0.7012890949

H,0,2.5230468142,1.9605317865,-0.893559951

C,0,5.8283705203,1.5514657139,-0.2287983496

H,0,6.6809233213,-0.143927357,0.7835717907

H,0,4.7058399509,3.0873888673,-1.2270048759

H,0,6.7826571501,2.0393113908,-0.3811212889

C,0,0.4182932048,4.3010127566,0.063306057

H,0,0.0520013331,4.4708923512,-0.9474711771

H,0,0.0160130791,5.0409225454,0.750757026

H,0,1.5070230658,4.3928417992,0.0444432234

C,0,0.073418877,2.9049417899,0.5247610427

O,0,0.1370301415,2.0004779019,-0.3785818585

O,0,-0.2248009435,2.7100827512,1.7208230352

H,0,-0.5662744778,1.2748900216,1.9327187344

^{1}TS9

C,0,2.8234328722,1.134616194,-0.3016034848

C,0,2.4475562774,0.0955455267,-1.1491572927

C,0,2.7988090032,-1.2407195259,-0.8753458544

C,0,3.5315850254,-1.4732173619,0.2825637618

C,0,3.8957085072,-0.4300654288,1.1344202625

C,0,3.5459896528,0.8869415892,0.8669882758

H,0,2.5468671137,2.1498102211,-0.5569135185

H,0,1.9334225002,0.3224608246,-2.071807037

H,0,3.8217256531,-2.479470974,0.5504148939

H,0,4.448191231,-0.6598597196,2.0381877384

C,0,3.8718327865,2.0112027312,1.8088350145

H,0,4.395561126,2.8222826622,1.2971910114

H,0,2.949557091,2.4255526218,2.223567405

H,0,4.4954049822,1.6748175464,2.6374226585

C,0,2.3367389577,-2.3300837476,-1.8235467335

H,0,1.2494964495,-2.2152145556,-1.8927292851

C,0,2.9165241372,-2.1268060398,-3.232986575

H,0,2.5327084101,-2.8904325783,-3.9125185207

H,0,2.6465586876,-1.1555152083,-3.6469941809

H,0,4.0072768637,-2.2003651984,-3.2173421768

C,0,2.6318849658,-3.7456041638,-1.3298493292

H,0,2.2262376312,-3.9105499189,-0.3320587293

H,0,2.1788233903,-4.4761279871,-2.0020933814

H,0,3.7063359694,-3.946832541,-1.2996299519

Ru,0,-0.050734334,0.1641144498,0.1336684617

C,0,0.4196718833,2.8846081244,-2.2141076562

C,0,0.8508447021,4.0508480716,-1.6421929652

C,0,0.418280235,4.3941531866,-0.3462210979

C,0,-0.4176889038,3.5615423045,0.3408386049

C,0,-0.8800501995,2.3284227936,-0.218245789

C,0,-0.444032414,1.9845694809,-1.5422296938

H,0,0.6971949664,2.6234272327,-3.2261660347

H,0,1.5088126628,4.7161214322,-2.1869944385

H,0,0.740011585,5.3246461799,0.1039972459

H,0,-0.7529745532,3.8575522932,1.3227569159

C,0,-0.8222530255,0.7529829707,-2.3901304146

O,0,-1.1546477284,0.9422202839,-3.56677237

N,0,-0.6174597591,-0.3926508733,-1.7546682561

O,0,0.848445219,0.6523248736,2.1414354337

C,0,0.1183211762,1.4042505464,3.1127962913

H,0,0.3146612644,2.4598024651,2.9135652386

H,0,0.5360360333,1.1718818607,4.0962579118

C,0,-1.3832479844,1.1147109223,3.125954396

H,0,-1.7953122023,1.4613052067,4.0778161745

H,0,-1.5179699842,0.0306491306,3.0993156911

C,0,-2.1899018326,1.7687287986,1.9882278155

H,0,-3.2259720386,1.4363763557,2.0717029555

H,0,-2.2060340941,2.8494271263,2.1234965021

C,0,-1.6843600983,1.4182458065,0.5986414149

C,0,-1.8949400635,0.110424337,0.0966118906

C,0,-3.0051475597,-0.7632871744,-0.0757443756

C,0,-4.3142025058,-0.2585065795,0.031648673

C,0,-2.8088008467,-2.1233684439,-0.3790676821

C,0,-5.4011573233,-1.1002915201,-0.127185849

H,0,-4.4646478228,0.795956394,0.220811908

C,0,-3.9017466627,-2.956863619,-0.5308741546

H,0,-1.7986391614,-2.4779901453,-0.5100040948

C,0,-5.1943647788,-2.4504052357,-0.4016759229

H,0,-6.4070454944,-0.7089153287,-0.0495091759

H,0,-3.7528291994,-4.002253083,-0.7678243212

H,0,-6.045296215,-3.1077443585,-0.5305792223

C,0,0.3181911732,-3.897435044,1.7418038371

H,0,0.2128926892,-4.3047847204,0.7397148682

H,0,1.1776572503,-4.3369161279,2.2462636861

H,0,-0.5718162047,-4.1474577001,2.323678507

C,0,0.4515619811,-2.3907048121,1.7127216927

O,0,0.1257528523,-1.8417983127,0.6031300863

O,0,0.8284557632,-1.7963713158,2.7398600116

H,0,0.9270870487,-0.3087656013,2.4768649099

^{3}TS9

C,0,-1.5595554387,-2.3148109777,-0.261967496

C,0,-2.3289924175,-1.3478552219,-0.9141977573

C,0,-3.4190044153,-0.7373814831,-0.2731421146

C,0,-3.7241911767,-1.1630234071,1.0170774504

C,0,-2.9628892092,-2.1361242232,1.6599731754

C,0,-1.8618860135,-2.7209250988,1.0447725904

H,0,-0.747203244,-2.7905170256,-0.7961446313

H,0,-2.0902681266,-1.0958630141,-1.9416493537

H,0,-4.5515173509,-0.7160135851,1.5510700448

H,0,-3.2226047619,-2.4255348308,2.6718918778

C,0,-1.0056842305,-3.7484432534,1.7319640645

H,0,-1.1722924593,-4.7436301602,1.3113138429

H,0,0.0547966031,-3.5210596507,1.6008017303

H,0,-1.219732434,-3.7985563237,2.8001938919

C,0,-4.2048003847,0.3283392192,-1.012262272

H,0,-3.47137918,0.89845065,-1.5902635323

C,0,-5.1855441958,-0.3202054011,-2.0027312113

H,0,-5.7051055393,0.4435717028,-2.5856666377

H,0,-4.6679224321,-0.9837717552,-2.6970277578

H,0,-5.9351936864,-0.9091859325,-1.4683117358

C,0,-4.9297000787,1.3123761754,-0.0915588487

H,0,-4.2576320691,1.7338857087,0.6567879035

H,0,-5.3455093087,2.1335151435,-0.6782555468

H,0,-5.7628737851,0.8358443558,0.4307234358

Ru,0,-0.3064381167,0.1993951289,0.075260334

C,0,2.4899546642,-3.0868383057,-1.9591959915

C,0,3.3484340634,-3.9438459634,-1.2861733051

C,0,3.5846230243,-3.7335396385,0.0644474523

C,0,2.9811061778,-2.6683279785,0.7215667755

C,0,2.1324772037,-1.7729209402,0.0548134735

C,0,1.8806943198,-2.0131409576,-1.3146399458

H,0,2.2508738485,-3.2433878295,-3.0022961728

H,0,3.8153724585,-4.7701341155,-1.8066340734

H,0,4.2412049196,-4.3952642773,0.6160073406

H,0,3.195444285,-2.5353003116,1.7711200479

C,0,0.8925149136,-1.2194309787,-2.1498172707

O,0,0.4334647828,-1.7072808139,-3.1855188833

N,0,0.5393876201,0.0127730871,-1.7410897584

O,0,-1.2079665177,0.5010358463,1.9902559769

C,0,-0.5413379731,0.1861847252,3.2103980633

H,0,-0.75519709,-0.863130655,3.430229244

H,0,-0.9854042377,0.7958882047,4.0013749823

C,0,0.9639298765,0.4185359694,3.1480443624

H,0,1.347249453,0.3815233233,4.1718473325

H,0,1.1529321843,1.4315629218,2.782071191

C,0,1.72914199,-0.6251958524,2.3260690337

H,0,2.7969614377,-0.5101877198,2.5459213128

H,0,1.4479297862,-1.615741002,2.6934223576

C,0,1.543702574,-0.6109660146,0.8064619974

C,0,1.5073856205,0.6571573909,0.1599320616

C,0,2.4053153923,1.7080892621,-0.1867492256

C,0,3.7547651787,1.6142653537,0.1948368318

C,0,1.9575977346,2.8395547769,-0.8923031802

C,0,4.6343154119,2.6418269606,-0.1045423879

H,0,4.0964573453,0.7293803709,0.7154251089

C,0,2.8455827064,3.8551552974,-1.194476272

H,0,0.9227143594,2.8781110328,-1.2033757448

C,0,4.1801571634,3.7608052447,-0.7978715983

H,0,5.673080017,2.5702427644,0.1907271453

H,0,2.5063728316,4.7233316116,-1.7445479111

H,0,4.8699920621,4.5603621514,-1.0375458009

C,0,-2.2948154569,4.1785985288,-0.4474624145

H,0,-2.8983836071,4.7784529718,0.2292134404

H,0,-1.4420633396,4.7686448758,-0.7904284426

H,0,-2.869859187,3.8956892375,-1.3285996034

C,0,-1.7791213695,2.9399493081,0.2497593722

O,0,-1.2621816387,2.0559579709,-0.5135840432

O,0,-1.8744182525,2.8549719904,1.4942013686

H,0,-1.4793302849,1.4947524353,1.9338653066

^{1}TS10

C,0,-0.5602039333,-0.7487943333,-2.4453856625

C,0,-1.4266493049,0.3248857774,-2.1588365641

C,0,-2.5956572473,0.1249222474,-1.4152386188

C,0,-2.9027416728,-1.1981667792,-1.0224248162

C,0,-2.0656948733,-2.2532960206,-1.3294794544

C,0,-0.8619898485,-2.0506460657,-2.0293487273

H,0,0.3295846567,-0.5611528398,-3.032015219

H,0,-1.1654025617,1.3103382886,-2.5149925952

H,0,-3.777284804,-1.3725495358,-0.4134526267

H,0,-2.3166101986,-3.249250766,-0.9869597738

C,0,0.0621560769,-3.2045944178,-2.2994554879

H,0,0.7415518285,-2.9928468539,-3.1248442293

H,0,0.6682214516,-3.4249353585,-1.4168613992

H,0,-0.5022985506,-4.1053164733,-2.5441235674

C,0,-3.5222055101,1.246360351,-0.9943265825

H,0,-3.6368329875,1.1208827495,0.0877125834

C,0,-2.9605228808,2.6450389938,-1.2435727044

H,0,-3.6341063636,3.3912415167,-0.8205080373

H,0,-1.9848693905,2.7751394919,-0.7758145254

H,0,-2.8669605631,2.8581334887,-2.3121946998

C,0,-4.9021249697,1.0890896536,-1.6543896298

H,0,-5.3454136804,0.113995606,-1.4487943094

H,0,-5.5856913734,1.8525356197,-1.2788570747

H,0,-4.8286228088,1.2044739641,-2.7387871885

Ru,0,-0.358673021,-0.1613559871,0.0652763172

C,0,1.2817353393,3.6277478605,0.9574867732

C,0,2.2203260978,3.9356246384,-0.0195729594

C,0,2.4620428955,3.0306609978,-1.0515273296

C,0,1.7878160056,1.8104432477,-1.1136742729

C,0,0.8359930396,1.4944112116,-0.1505774302

C,0,0.599611204,2.4200838254,0.87370309

H,0,1.0677570876,4.3021715854,1.7776346913

H,0,2.7610827378,4.8726315302,0.0182422282

H,0,3.1915710442,3.2722821447,-1.8157908778

H,0,2.0247089492,1.1181558979,-1.9105166071

C,0,-0.4425711692,1.9833240672,1.8546360416

O,0,-0.6377278518,2.4266098832,2.9661492495

N,0,-1.1841681851,0.9941656098,1.1971912231

O,0,-2.2891784749,-0.7971623512,1.7825901893

C,0,-2.1349019371,-1.2656988668,3.0663799495

H,0,-2.4034106027,-2.3442490718,3.0960783025

H,0,-2.8275330208,-0.7662416713,3.7652273144

C,0,-0.7141600832,-1.1250334878,3.6245029423

H,0,-0.6904692537,-1.540208421,4.6370796126

H,0,-0.4682505454,-0.0640975817,3.7036836084

C,0,0.3429779139,-1.8544816385,2.7858861989

H,0,1.2741642268,-1.951839655,3.3540593479

H,0,-0.0066705132,-2.8756769545,2.5885471956

C,0,0.6819191885,-1.240838021,1.4854744559

C,0,1.4874018647,-1.0498361389,0.5235577336

C,0,2.8333998863,-1.1136250251,0.0057099102

C,0,3.1006217111,-1.3398669376,-1.3484542336

C,0,3.9137889903,-0.945651397,0.8835137935

C,0,4.4056220987,-1.4089432288,-1.8126198246

H,0,2.2748377839,-1.4603957707,-2.0338738763

C,0,5.2184484253,-1.0106909626,0.4165002829

H,0,3.7161764068,-0.7486023659,1.9288791018

C,0,5.4703352929,-1.243317765,-0.9321458932

H,0,4.5941106254,-1.5890268217,-2.8636300523

H,0,6.041723145,-0.8727170347,1.1060255497

H,0,6.4890239464,-1.2909237255,-1.2950959766

^{1}TS10b

C,0,-0.6597717759,0.8643139545,1.2311683269

C,0,0.0498674705,1.3895141263,0.1219719293

C,0,1.246596423,2.11640537,0.2897296085

C,0,1.7094150635,2.3160780695,1.6230959911

C,0,1.0459805612,1.7584559423,2.7009662477

C,0,-0.1433904504,0.9955167238,2.5206784986

H,0,-1.5756922355,0.3131304221,1.0673587194

H,0,-0.3588114699,1.251269166,-0.8680992163

H,0,2.6223692921,2.8755803295,1.7817841385

H,0,1.4447757155,1.8816526913,3.6996237346

C,0,-0.8481604626,0.4108787158,3.7105915973

H,0,-1.4820181778,-0.4244485643,3.420755779

H,0,-0.1336366512,0.0593409727,4.4559518876

H,0,-1.4734897447,1.1706512781,4.1881699325

C,0,1.9741308116,2.7911937131,-0.8570679364

H,0,3.0392313783,2.7508935635,-0.6106078169

C,0,1.785125913,2.1031260017,-2.2090041053

H,0,2.4275818665,2.5737949491,-2.9543827639

H,0,2.036811141,1.0446075093,-2.1556498537

H,0,0.7567017257,2.1911122924,-2.5667034898

C,0,1.5574556039,4.2702637486,-0.9261991152

H,0,1.7360049946,4.7833111484,0.0205756671

H,0,2.1213098732,4.7877533539,-1.7044727662

H,0,0.4941367906,4.3589121652,-1.1621852407

Ru,0,1.6441933517,-0.2455785601,0.8473660821

C,0,2.4541196231,-2.6208062938,-2.5453049226

C,0,1.2368857528,-2.8970256414,-3.1413521169

C,0,0.0623450143,-2.3846876131,-2.5744147218

C,0,0.0935989633,-1.6019988196,-1.4288457477

C,0,1.3159978167,-1.3086855317,-0.8021901827

C,0,2.4851371879,-1.8342753036,-1.3918383802

H,0,3.3850000174,-2.9996245071,-2.9502058811

H,0,1.186802147,-3.5048832515,-4.0355561284

H,0,-0.892114759,-2.6071397937,-3.0390701476

H,0,-0.8378218411,-1.2408969437,-1.0102722142

C,0,3.7047808257,-1.507690234,-0.6540072069

O,0,4.8359526859,-1.8726275432,-0.8843113241

N,0,3.4343317066,-0.6185281352,0.476317524

O,0,2.8234072089,-1.8697627801,1.7995667445

C,0,2.6964987177,-3.2691703732,1.6222660067

H,0,3.1926778213,-3.7220554644,2.4911730037

H,0,3.2503934125,-3.6048265013,0.7372774183

C,0,1.2494510324,-3.7357085627,1.5128475048

H,0,1.2240417517,-4.827436442,1.4707437932

H,0,0.8416381343,-3.3731915685,0.5720884826

C,0,0.3653468676,-3.2233137324,2.6746268958

H,0,0.3421632264,-3.9462585498,3.4951582476

H,0,0.8133647118,-2.3117024348,3.0839305093

C,0,-0.982424751,-2.9037497621,2.2296306702

C,0,-2.0405452501,-2.5670853782,1.7613960444

C,0,-3.2407791729,-2.0989992635,1.155345968

C,0,-4.1848873469,-1.3660907496,1.8899440628

C,0,-3.478488296,-2.3281207263,-0.2091581876

C,0,-5.3270837074,-0.8731023675,1.274812262

H,0,-4.012929042,-1.189852456,2.9437780686

C,0,-4.6229117804,-1.8324811326,-0.8165501057

H,0,-2.7548571122,-2.8955770775,-0.778997043

C,0,-5.5504056778,-1.1019641119,-0.0792817329

H,0,-6.0467520518,-0.3092842324,1.8550017985

H,0,-4.7927328082,-2.0175665226,-1.8698125448

H,0,-6.4424502264,-0.7164263743,-0.5560818653

^{1}TS11

C,0,-0.6181098744,-2.2001443371,-1.3693243726

C,0,-1.8916558672,-1.8442314262,-0.846461026

C,0,-2.0726955298,-1.7242117983,0.5474887786

C,0,-0.9888170332,-2.0768760507,1.4116761253

C,0,0.2570167786,-2.4183784988,0.8749506664

C,0,0.4771112596,-2.5047706202,-0.534231021

H,0,-0.4803449222,-2.2128955052,-2.4423003631

H,0,-2.6895767937,-1.588274435,-1.5262915264

H,0,-1.1175028836,-2.0068014123,2.4829123441

H,0,1.0943358573,-2.5903808742,1.5402128061

C,0,1.7958826128,-2.9502862258,-1.0947336018

H,0,1.9635874201,-2.5275112489,-2.0850738614

H,0,2.624000169,-2.6461095612,-0.4567573329

H,0,1.8203285308,-4.0402366389,-1.1845578317

C,0,-3.3958633754,-1.3101063284,1.1574675868

H,0,-3.1565300824,-0.7755411043,2.079014407

C,0,-4.2152839041,-0.3609268455,0.2832175965

H,0,-5.0833567117,-0.0063373331,0.8406177701

H,0,-3.630434946,0.5074748961,-0.0138407281

H,0,-4.587474456,-0.8588368182,-0.6151491135

C,0,-4.1999936666,-2.5693382442,1.5203183006

H,0,-3.6373147182,-3.2291308807,2.1836559806

H,0,-5.1291105813,-2.2932071797,2.0226506033

H,0,-4.4570454214,-3.1354420575,0.6217535865

Ru,0,-0.3301604733,-0.4427425962,-0.086317703

C,0,-0.7664881721,3.0309404981,-2.5784611736

C,0,-0.1724244184,2.7265658341,-3.7940989038

C,0,0.4098920799,1.4725523304,-3.9732303417

C,0,0.390774289,0.5284208282,-2.949753517

C,0,-0.2072164069,0.8088379285,-1.7163992929

C,0,-0.7761749038,2.0825712684,-1.5573495034

H,0,-1.2296296863,3.993077974,-2.3960301696

H,0,-0.1575078871,3.4549145807,-4.595101212

H,0,0.8831721862,1.2285978633,-4.9179039851

H,0,0.8672438448,-0.4303732227,-3.1205666841

C,0,-1.3907403916,2.4018627219,-0.2455907777

O,0,-1.9748868928,3.4385754239,0.0353279459

N,0,-1.1548423351,1.3574301135,0.6289605159

O,0,-1.9230438981,1.4481004837,1.8145256833

C,0,-1.1259788104,1.3346693954,2.9842416024

H,0,-0.5752316224,0.3861749913,2.9618389131

H,0,-1.848482816,1.2879272553,3.8002114674

C,0,-0.1604201994,2.4931617745,3.1928564409

H,0,0.4619207253,2.2543863291,4.0594468218

H,0,-0.7149769,3.4039038712,3.4199075886

C,0,0.7350579911,2.7578571537,1.9560741981

H,0,0.2892233234,3.5385951608,1.337177206

H,0,1.7242894238,3.1183252334,2.263584662

C,0,0.9651103371,1.5712345004,1.1481651348

C,0,1.4808312751,0.591646272,0.5601927432

C,0,2.8094725982,0.0437549065,0.3165545467

C,0,3.4886142266,-0.6533999343,1.3201500628

C,0,3.4007822404,0.173888214,-0.9433016676

C,0,4.736200946,-1.2111115407,1.066336264

H,0,3.0314155922,-0.7585245051,2.2958144748

C,0,4.6519311644,-0.376084093,-1.1861550437

H,0,2.8657452284,0.6979190172,-1.7234169376

C,0,5.3229023605,-1.0755365535,-0.1871543036

H,0,5.2511038352,-1.7505420296,1.8516061951

H,0,5.1022217396,-0.2637732589,-2.1645650704

H,0,6.2945486755,-1.5100483513,-0.3837212634

^{3}TS11

C,0,-0.3735177931,-2.3152042182,-1.0910855688

C,0,-1.7040818265,-1.9189348266,-0.760785648

C,0,-2.2406904863,-2.1226422175,0.5462298378

C,0,-1.3524097711,-2.4878611075,1.5426535731

C,0,0.0197601715,-2.7270135541,1.260568381

C,0,0.5157026579,-2.7110029348,-0.0576943676

H,0,-0.0680817174,-2.3779271868,-2.1270654454

H,0,-2.359384391,-1.6107213479,-1.5635353321

H,0,-1.6974833865,-2.566472544,2.5657327932

H,0,0.6940515556,-2.9722352504,2.070621657

C,0,1.9108612293,-3.1711189547,-0.3756462312

H,0,2.3095563486,-2.6527521877,-1.2472389546

H,0,2.5881590773,-2.9861431503,0.457368207

H,0,1.9135807544,-4.2444616361,-0.584632629

C,0,-3.6940188579,-1.8266446985,0.8341762723

H,0,-3.8581309553,-2.0368430946,1.8954243536

C,0,-4.0296434853,-0.3459255695,0.5938645046

H,0,-5.0809843956,-0.157265081,0.8211578269

H,0,-3.4195323215,0.3040052202,1.2195083522

H,0,-3.8592827458,-0.0663111402,-0.4477952405

C,0,-4.6230343277,-2.744660213,0.0254817306

H,0,-4.3990222481,-3.7975085401,0.2070914796

H,0,-5.6649574856,-2.5640208026,0.2974600122

H,0,-4.5243145861,-2.5590891309,-1.0463225107

Ru,0,-0.103183532,-0.4504975808,0.0071073082

C,0,-1.1629368985,3.0218661263,-2.2190132655

C,0,-0.7769505471,2.7684439932,-3.5246477857

C,0,-0.1812265437,1.5451135234,-3.8383417906

C,0,0.0220494891,0.5814913763,-2.8574597633

C,0,-0.3487801787,0.8203660381,-1.5275687238

C,0,-0.9405919001,2.0608283272,-1.2317674046

H,0,-1.641504564,3.9522846727,-1.9392506523

H,0,-0.9364244062,3.5101707147,-4.2968588222

H,0,0.1243095778,1.3423642674,-4.8585824982

H,0,0.4885068871,-0.3567898501,-3.1329014704

C,0,-1.3782717418,2.3025740231,0.1550815578

O,0,-2.1088112838,3.2074352217,0.5235212406

N,0,-0.8561365134,1.3100390051,1.0015934001

O,0,-1.4089989131,1.2625078504,2.2890872829

C,0,-1.1803624459,2.4413784995,3.1036130482

H,0,-1.1966682441,2.043552257,4.1213226712

H,0,-2.003186696,3.1410771551,2.9655925094

C,0,0.1560066448,3.1024614304,2.8093589392

H,0,0.4230523839,3.733093029,3.6601554271

H,0,0.0724401192,3.7526453213,1.938820287

C,0,1.2483685995,2.0583880374,2.5766330751

H,0,2.2386301086,2.5273923013,2.5708236044

H,0,1.2493263367,1.3361933645,3.4006128337

C,0,1.1598149187,1.3298905459,1.294766038

C,0,1.7248483084,0.5810139481,0.4433368252

C,0,3.0490410163,0.1390459406,0.0462333032

C,0,3.9422010369,-0.3940020077,0.9851103553

C,0,3.4376082706,0.1936362984,-1.2980352935

C,0,5.1867294177,-0.8643563553,0.5869296025

H,0,3.6462730943,-0.4477402303,2.0252316476

C,0,4.6910303802,-0.2578833786,-1.6868341659

H,0,2.7434329661,0.5917635882,-2.026229507

C,0,5.5681945869,-0.796223671,-0.7492769904

H,0,5.8631305442,-1.2804801852,1.3234255162

H,0,4.9808315393,-0.2001603216,-2.7287600971

H,0,6.5405072952,-1.1588738167,-1.0572945883

^{1}TS12

C,0,-0.906562131,-2.2733320103,-1.5567774882

C,0,-2.1097506741,-1.9589863177,-0.8759379556

C,0,-2.1110563683,-1.9170004753,0.5385714817

C,0,-0.9657572418,-2.3982994099,1.2534908155

C,0,0.2077105724,-2.7054762222,0.5757260169

C,0,0.2797264342,-2.6092329156,-0.8532840318

H,0,-0.8757216865,-2.2070015703,-2.6370574419

H,0,-2.9828411803,-1.6667012463,-1.438855836

H,0,-0.986335054,-2.4092320964,2.3349708587

H,0,1.0955973933,-2.9853603524,1.1292490462

C,0,1.5442372155,-2.9681793547,-1.5803063845

H,0,1.5384307612,-2.5743703202,-2.5963391686

H,0,2.4211876464,-2.5686692268,-1.0709139914

H,0,1.6537529969,-4.0548554452,-1.6432727153

C,0,-3.3274641184,-1.4838874222,1.3356204576

H,0,-2.9439062134,-1.0294979681,2.2536198096

C,0,-4.1926275354,-0.4329513111,0.6391452179

H,0,-4.9814164892,-0.0990318383,1.3153604471

H,0,-3.6093286584,0.4403393906,0.3518515166

H,0,-4.6797741951,-0.8350972063,-0.2519066255

C,0,-4.1573003766,-2.7195198683,1.7191912989

H,0,-3.555223484,-3.4566992639,2.253843238

H,0,-4.9945317713,-2.4344997119,2.3596045541

H,0,-4.5633281919,-3.201594163,0.8264997909

Ru,0,-0.4412376205,-0.6206558271,-0.2236505946

C,0,-1.0429553926,2.8664001082,-2.6165757282

C,0,-0.4317490935,2.6095705842,-3.8243346965

C,0,0.3574169657,1.4458377467,-3.9549798537

C,0,0.5451123496,0.5755422239,-2.9090358675

C,0,-0.0492726265,0.8078079085,-1.6290435239

C,0,-0.8786967922,1.9851410364,-1.5403034257

H,0,-1.6699580317,3.7389720377,-2.4764377474

H,0,-0.5593235553,3.2795676787,-4.6637205745

H,0,0.8265577918,1.2307459961,-4.9089782198

H,0,1.1757148142,-0.293618706,-3.0438828928

C,0,-1.4749931901,2.2384346864,-0.2683173275

O,0,-2.3151514083,3.0298358191,0.0979193872

N,0,-0.8614369002,1.3002537069,0.7389576138

O,0,-1.4867935724,1.3238664081,1.9955255673

C,0,-1.2166986638,2.5255745759,2.7720263545

H,0,-1.331523423,2.1729983157,3.7981334399

H,0,-1.9770338514,3.2707380372,2.5464719052

C,0,0.1947808289,3.0552964785,2.5265499932

H,0,0.5565771938,3.5560611304,3.4259080398

H,0,0.1824229398,3.7972305685,1.7255854779

C,0,1.1194734334,1.898925914,2.1270836352

H,0,2.1436689938,2.2292737844,1.952419578

H,0,1.1511245149,1.1515146094,2.9260919276

C,0,0.5968487096,1.2908999377,0.8661001131

C,0,1.1975271109,0.7688864288,-0.2136985567

C,0,2.6340454033,0.6010371741,-0.4145446824

C,0,3.3544753446,-0.3578959562,0.3095365814

C,0,3.3167171352,1.3824066126,-1.3538925693

C,0,4.7172867908,-0.5241549973,0.1091891729

H,0,2.8277734746,-0.9719039828,1.0295261638

C,0,4.6826552141,1.2145135291,-1.5524196559

H,0,2.7662754599,2.1172385761,-1.9258529876

C,0,5.3874488666,0.2618007987,-0.8254865137

H,0,5.259532703,-1.266403778,0.6822798662

H,0,5.1969509223,1.8294546131,-2.2806350507

H,0,6.4503609002,0.1311258386,-0.9844236491

^{3}TS12

C,0,-0.0651812743,-2.6561043058,-0.6306974235

C,0,-1.3908360015,-2.1989688076,-0.8342406763

C,0,-2.2409167404,-1.8505156497,0.2437425528

C,0,-1.6706881865,-1.9334155384,1.5384313346

C,0,-0.3659182193,-2.4281877642,1.7685420477

C,0,0.4747561244,-2.7577047555,0.6823152979

H,0,0.5463045027,-2.9103703355,-1.4853508003

H,0,-1.7371469393,-2.0715615052,-1.8502806552

H,0,-2.2462052362,-1.5777965569,2.3836649417

H,0,0.0231840937,-2.4572249333,2.7771019581

C,0,1.8728522372,-3.2553383728,0.9090628484

H,0,2.5396037959,-2.9487386937,0.104887249

H,0,2.2763200669,-2.8734828419,1.8464572333

H,0,1.8785430199,-4.3479723594,0.9560999714

C,0,-3.6735130117,-1.3968652022,0.0609059986

H,0,-3.8957158259,-0.7325210611,0.9017660312

C,0,-3.9077074845,-0.60468564,-1.227536837

H,0,-4.9226201562,-0.2041218084,-1.2367366846

H,0,-3.209177136,0.2265539143,-1.3167381037

H,0,-3.8025644499,-1.2358634449,-2.1129521106

C,0,-4.6203026936,-2.6045929337,0.1489091034

H,0,-4.4918803663,-3.1450765064,1.0886128486

H,0,-5.6612722545,-2.2820478325,0.0799164085

H,0,-4.4282622979,-3.3029170721,-0.6696996203

Ru,0,-0.2857822333,-0.6480916543,0.2998300698

C,0,-1.5613802315,2.810364705,-1.9192175743

C,0,-1.3614862047,2.4982598813,-3.2448557087

C,0,-0.6432213933,1.3358602834,-3.593305006

C,0,-0.1487978254,0.4956588482,-2.6147639405

C,0,-0.3598346478,0.7679349157,-1.2538410896

C,0,-1.0662632714,1.959160748,-0.9139538986

H,0,-2.1033337211,3.6999483601,-1.6228587274

H,0,-1.743291614,3.1491017288,-4.0210552912

H,0,-0.4727323732,1.102290772,-4.6371935133

H,0,0.4223270388,-0.3786680937,-2.9004254979

C,0,-1.2571850282,2.2526290164,0.4792437689

O,0,-1.8397125579,3.1596435525,1.0379733977

N,0,-0.4831710295,1.2208701256,1.282981138

O,0,-0.8378705309,1.1636250731,2.6493032306

C,0,-0.4234307105,2.3122321057,3.444079553

H,0,-0.2163220433,1.8664805484,4.4192905163

H,0,-1.2627893146,3.0013975357,3.5209607768

C,0,0.8165387586,3.0088622919,2.8909886997

H,0,1.3509442661,3.4855469293,3.7147104458

H,0,0.5156374819,3.7921570777,2.194161679

C,0,1.7202686652,2.0067356516,2.1631845006

H,0,2.627383848,2.4845032122,1.7927876252

H,0,2.0483052689,1.2255844802,2.8658110112

C,0,0.9418208922,1.4111583501,1.0430899258

C,0,1.2894357001,0.5908410489,-0.0602849282

C,0,2.516295146,0.6067858376,-0.8073586833

C,0,2.9368623916,-0.5152362792,-1.5492728429

C,0,3.3271944741,1.7618820576,-0.8666441782

C,0,4.1090336489,-0.4961091614,-2.2843977307

H,0,2.3188991281,-1.4012062327,-1.5378996683

C,0,4.502175153,1.7751262617,-1.5995411256

H,0,3.0049091427,2.659913775,-0.3575661434

C,0,4.9082183823,0.6466217172,-2.309511905

H,0,4.4069809133,-1.3760025771,-2.8419340044

H,0,5.1024761689,2.6764361419,-1.6293820107

H,0,5.8269160852,0.6604358222,-2.8814916535

^{1}TS13

C,0,0.4901479699,2.424772604,0.9266222686

C,0,1.395873897,2.6725272037,-0.1307867292

C,0,2.7229374631,2.1699323314,-0.1356704265

C,0,3.0253151255,1.279513318,0.8984703625

C,0,2.123192022,0.9967383769,1.9635737556

C,0,0.8529508014,1.5792112338,2.0130556571

H,0,-0.4863490333,2.8812529464,0.9079188029

H,0,1.0524008927,3.2809961653,-0.9561246965

H,0,3.9749278309,0.759901713,0.8829350227

H,0,2.4054282558,0.2671753485,2.7100038475

C,0,-0.1111951929,1.3220022615,3.1291108946

H,0,-1.1061283277,1.1278034858,2.7284674295

H,0,0.1963560957,0.4643154329,3.7260408686

H,0,-0.1713315532,2.1956996043,3.7827827829

C,0,3.7098729821,2.5118959002,-1.2298536785

H,0,4.6375895397,1.9812883945,-0.995337736

C,0,3.2347911766,2.0348371561,-2.6089905021

H,0,3.9706097435,2.3035435953,-3.3694678212

H,0,3.0933376611,0.9548925523,-2.6230992733

H,0,2.2838991245,2.4947266053,-2.8835564809

C,0,4.0155375197,4.0170712911,-1.2297460958

H,0,4.3725747072,4.3545274327,-0.2547977316

H,0,4.7806014045,4.2481910633,-1.9730558677

H,0,3.124094073,4.5962022609,-1.4818569517

Ru,0,1.0029527069,0.4509730685,-0.0213571523

C,0,-1.8827846869,3.1986869155,-1.7400137572

C,0,-2.6542732594,4.0405835015,-0.9469766508

C,0,-3.2427705996,3.5428541545,0.2126174739

C,0,-3.0405107041,2.2200744242,0.5855764592

C,0,-2.2131592462,1.3763128895,-0.1617600999

C,0,-1.6646695989,1.8828447487,-1.3514501868

H,0,-1.4658365954,3.5504389299,-2.6754599122

H,0,-2.8169511672,5.0686682563,-1.2444005556

H,0,-3.8651770919,4.1849590694,0.8232876584

H,0,-3.5166952613,1.8317175285,1.4773656142

C,0,-0.956292018,0.9128465289,-2.273774556

O,0,-1.4857075987,0.5898364675,-3.3254867191

N,0,0.2445222513,0.5574192906,-1.765196245

O,0,0.4577804132,-1.1325753239,-2.7497561609

C,0,-0.4816717447,-2.1437698135,-2.339638755

H,0,-0.4503857259,-2.9057242854,-3.1256571237

H,0,-1.4615692196,-1.6732927263,-2.3874661291

C,0,-0.238861619,-2.8328192165,-0.9952997944

H,0,0.7973705002,-3.1621680722,-0.962479127

H,0,-0.834823233,-3.7492711183,-1.0373001763

C,0,-0.6104811957,-2.113790259,0.3453930457

H,0,-1.5541658267,-2.5350805214,0.6897790471

H,0,0.1446936186,-2.3892916697,1.0814865819

C,0,-0.7467687125,-0.610591525,0.2684672528

C,0,-1.9697833679,-0.0337865968,0.2490034378

C,0,-3.2309709973,-0.7754952888,0.5633377467

C,0,-3.475665444,-1.2862393671,1.8402579738

C,0,-4.2161632742,-0.9339622527,-0.4161874498

C,0,-4.6615203211,-1.9524444179,2.1289606382

H,0,-2.7214199579,-1.1603164723,2.6077176186

C,0,-5.3995808633,-1.6033153853,-0.1320383685

H,0,-4.0444379733,-0.5303118713,-1.4069530498

C,0,-5.6271736764,-2.1155020011,1.1421311001

H,0,-4.8319185873,-2.3415748497,3.1254170676

H,0,-6.1465779432,-1.7254929661,-0.9066866282

H,0,-6.5512623591,-2.6342207307,1.3642179758

C,0,4.0083133623,-2.6700598493,-0.1776647181

H,0,4.5765768977,-3.1575415706,-0.9658193925

H,0,4.6804060246,-2.0541858752,0.4243860795

H,0,3.5639619638,-3.4107677558,0.4873854674

C,0,2.9259986316,-1.7901039075,-0.7684883499

O,0,2.0700730976,-1.3567244892,0.0840922615

O,0,2.9088831784,-1.5535990963,-1.9852073121

H,0,1.4034829549,-1.3222981153,-2.4677368017

^{1}TS14

C,0,2.6777706181,-1.0098073255,-0.7609504203

C,0,3.5729862934,0.0823912702,-0.6391918158

C,0,3.3629894714,1.235015685,-1.4157847008

C,0,2.3591145747,1.1987610788,-2.4379768936

C,0,1.5537527679,0.0653238822,-2.616544327

C,0,1.6735074489,-1.0684755559,-1.767247745

H,0,2.75942525,-1.8358945474,-0.0649369551

H,0,4.316348787,0.0742398352,0.1434103244

H,0,2.1933970338,2.0748145108,-3.0504706149

H,0,0.7654408833,0.0861911991,-3.3581825337

C,0,0.8021024199,-2.2761441358,-1.9460768887

H,0,0.7128327682,-2.8362220637,-1.0164844901

H,0,-0.2017058222,-1.9859594205,-2.2551123105

H,0,1.2183350127,-2.9399664402,-2.7093276957

C,0,4.1743729979,2.5014861429,-1.2381853637

H,0,3.5162208293,3.3270481389,-1.5268163313

C,0,4.6170647293,2.7521214444,0.2044435816

H,0,5.0853481941,3.7351678325,0.2798756397

H,0,3.7626261049,2.7192454828,0.8801705134

H,0,5.3571865371,2.0178603964,0.531045991

C,0,5.3692670263,2.4877319557,-2.2047953195

H,0,5.0489402142,2.3488978259,-3.2392421546

H,0,5.9195269073,3.4284407293,-2.141846025

H,0,6.0563151653,1.676366429,-1.9531918014

Ru,0,1.3417925132,0.7201864755,-0.487213637

C,0,-0.3032803379,-2.0315135746,2.6035603803

C,0,-0.8191774869,-3.289562587,2.3287557405

C,0,-1.6114597409,-3.4745056353,1.1957002015

C,0,-1.8761945957,-2.4166679621,0.3358461941

C,0,-1.3304741561,-1.149538902,0.5600464315

C,0,-0.5860141832,-0.9769026632,1.7413192578

H,0,0.2914786047,-1.8537196944,3.4900502573

H,0,-0.618718979,-4.117504713,2.9964909408

H,0,-2.0226799408,-4.4531401629,0.9811098582

H,0,-2.5030723822,-2.5698641515,-0.5335170391

C,0,-0.223683598,0.4881554914,2.0933052909

O,0,-0.8617127236,1.2123185841,2.8242299407

N,0,0.8924475998,0.5295808601,1.401026968

O,0,1.3056929152,2.4397919169,0.7531567998

C,0,0.4612476573,3.5301950761,0.4771800693

H,0,0.9550425796,4.1035517845,-0.329388119

H,0,0.4290287325,4.1626174817,1.3718882653

C,0,-0.9720862021,3.2407346863,0.0319852071

H,0,-1.4319863422,4.2015985174,-0.2202339775

H,0,-1.5304600995,2.8216468458,0.8718177131

C,0,-1.0888783984,2.2894005731,-1.1785426417

H,0,-2.120830436,2.3211624004,-1.5344532699

H,0,-0.4531026515,2.6507146332,-1.993118097

C,0,-0.695813224,0.9098715917,-0.723670786

C,0,-1.621872006,0.0072830428,-0.3288019962

C,0,-3.0771886738,0.1629205083,-0.6394623952

C,0,-3.5473152431,0.1244252452,-1.9542135002

C,0,-4.0036880447,0.3374243859,0.3937613313

C,0,-4.9021011756,0.2683229162,-2.2335747677

H,0,-2.8373130319,-0.0175200379,-2.7600731873

C,0,-5.3565055642,0.4853376454,0.1170849009

H,0,-3.6506055284,0.3713667986,1.4173811

C,0,-5.8116270491,0.4502893605,-1.1980351916

H,0,-5.2471556275,0.2349645457,-3.259849324

H,0,-6.0577174828,0.6316132721,0.929488424

H,0,-6.8669411699,0.5625259848,-1.4127837864

[1]TS15

C,0,3.8490257731,0.0141351806,1.5407758217

C,0,3.0162486318,1.1705420578,1.4773528736

C,0,2.747491913,1.8135935132,0.239432033

C,0,3.2762848134,1.2133666504,-0.9410590318

C,0,3.9543592177,-0.0119807256,-0.8800702203

C,0,4.2891976244,-0.6239566838,0.3791728103

H,0,4.0057933944,-0.4637756368,2.4988635492

H,0,2.5847265184,1.5581348501,2.3877349971

H,0,3.0151921736,1.6203872386,-1.9082182302

H,0,4.2063627755,-0.5225151972,-1.8000048976

C,0,5.0294600066,-1.9274251015,0.4020631162

H,0,4.9891322412,-2.3895018631,1.3874203556

H,0,4.5957157254,-2.6178638502,-0.3228008194

H,0,6.0780218284,-1.7739347054,0.1339089275

C,0,1.945627476,3.0914192837,0.1279527393

H,0,1.4123725909,3.037987062,-0.8244798102

C,0,0.9056190532,3.2767810686,1.232341574

H,0,0.2628436129,4.1222730395,0.9836414626

H,0,0.2827820868,2.3911150076,1.3526101259

H,0,1.378243124,3.4987377275,2.192739664

C,0,2.9151064778,4.2828911315,0.0527271658

H,0,3.6237556748,4.1768833158,-0.7711100578

H,0,2.3565696569,5.2083342789,-0.0968264985

H,0,3.4842192646,4.3776294502,0.9806700804

Ru,0,2.0494778684,-0.2960133311,0.1645266407

C,0,-0.900492226,2.780756966,-2.4206052731

C,0,-1.9512614919,3.6609230077,-2.2122865929

C,0,-2.9805607474,3.3218100414,-1.335326973

C,0,-2.9587598748,2.1008701808,-0.670570005

C,0,-0.8745773045,1.5556100641,-1.7490314585

H,0,-0.0984532284,3.0155655767,-3.1079475434

H,0,-1.9735923895,4.6087993664,-2.7354429794

H,0,-3.8022282261,4.0093023421,-1.1764294961

H,0,-3.7598407692,1.8268585872,0.0030770437

C,0,0.3080704628,0.6616248853,-1.9867681566

O,0,0.9915259814,0.7092063056,-3.0052165714

N,0,0.4999697788,-0.17961351,-0.9408673865

O,0,1.6028369033,-1.9411856846,-1.1024364831

C,0,0.5664712426,-2.8384104391,-0.8043294718

H,0,-0.0646434448,-2.4647037605,0.0042629354

H,0,1.0232697067,-3.7670707125,-0.4274844074

C,0,-0.2940133983,-3.1124137633,-2.0312710495

H,0,0.2676089842,-3.6963979781,-2.7642986936

H,0,-0.538811514,-2.1571811252,-2.4970046699

C,0,-1.5924844105,-3.8579022611,-1.6693620925

H,0,-2.1032969472,-4.1658320309,-2.586239536

H,0,-1.3508883405,-4.7820286065,-1.1310130209

C,0,-2.5116292195,-3.0572128028,-0.8653636545

C,0,-3.2625544124,-2.3683478978,-0.2209830138

C,0,-4.183476704,-1.5612944275,0.5116595329

C,0,-3.7399228945,-0.6693062027,1.4988413832

C,0,-5.5585596381,-1.6396290406,0.2415267381

C,0,-4.6493417832,0.1177435376,2.1918149439

H,0,-2.6846953266,-0.5716910186,1.709841055

C,0,-6.4602662646,-0.8492613048,0.9389569922

H,0,-5.9071033414,-2.3238522134,-0.5209011993

C,0,-6.0104732189,0.0328710704,1.917383058

H,0,-4.2855183758,0.8054796668,2.9449648778

H,0,-7.517803628,-0.9206975802,0.7171440803

H,0,-6.7160315977,0.6494346549,2.4600173175

C,0,0.0114942328,-0.843933192,2.2455331387

C,0,-0.6218122381,-1.8616984834,3.1782519492

H,0,0.1354105239,-2.4660831857,3.6752607754

H,0,-1.2551003932,-1.359865544,3.9065079434

H,0,-1.2432429261,-2.5310589174,2.5780374098

O,0,1.0701952728,-1.3064347415,1.6453721122

O,0,-0.4795973585,0.2652239332,2.0794883775

C,0,-1.9063288549,1.2177741147,-0.8718060703

H,0,-1.8833616042,0.2687951219,-0.3601877169

^{1}TS16

C,0,-3.6055163311,-1.4004080682,-1.5921751346

C,0,-2.9653004823,-0.1865771178,-2.0159183085

C,0,-2.9044137161,0.9477704608,-1.1904823318

C,0,-3.2481868834,0.7490198619,0.1784694904

C,0,-3.7486677303,-0.4882234475,0.6358443215

C,0,-4.0408614076,-1.5515605387,-0.2857574534

H,0,-3.7030802601,-2.2168057972,-2.2944893113

H,0,-2.5964458933,-0.1314818358,-3.0296706588

H,0,-3.0906212896,1.5450112063,0.8937667547

H,0,-3.9647852362,-0.6148696716,1.6873908679

C,0,-4.5770368704,-2.8458975909,0.2298509706

H,0,-4.8940542625,-3.5030084101,-0.5786150446

H,0,-3.7724616908,-3.3360722214,0.7876311455

H,0,-5.4154722833,-2.6810111878,0.9081612258

C,0,-2.3841293004,2.2908955187,-1.6451979014

H,0,-1.713635233,2.6474648311,-0.8591573788

C,0,-1.5792429459,2.2406638002,-2.9420561302

H,0,-1.1379694789,3.2187083257,-3.1341029612

H,0,-0.7649003863,1.5186205499,-2.8797878836

H,0,-2.2102006781,1.9893246575,-3.7984740038

C,0,-3.5565144602,3.2805336387,-1.750651631

H,0,-4.1056494067,3.3550242448,-0.8105364767

H,0,-3.1833212447,4.2743204959,-2.0026900648

H,0,-4.2578841114,2.9723540115,-2.5298060864

Ru,0,-1.7375198497,-0.7945757874,-0.1933675319

C,0,0.65154114,3.5695815711,1.5978768297

C,0,1.3437186364,4.5145027534,0.84693685

C,0,1.7130683242,4.2311795778,-0.4689905605

C,0,1.3928447483,3.0047012866,-1.062270523

C,0,0.3741772899,2.3455091297,1.0021600027

H,0,0.3245436187,3.7733750268,2.6104836276

H,0,1.5938060257,5.4755425941,1.2786467267

H,0,2.2637627189,4.9719771969,-1.0387422842

H,0,1.6903173449,2.8071244919,-2.0860808225

C,0,-0.4133628233,1.218351153,1.5212291217

O,0,-0.9999452262,1.0852472248,2.5881148178

N,0,-0.3677907831,0.2246664405,0.5672648177

O,0,-1.5390590366,-2.4364404503,0.9004039055

C,0,-1.1312161037,-2.4553318615,2.2444549051

H,0,-1.39698339,-3.4527741536,2.6258357907

H,0,-1.6748979539,-1.7157706166,2.8485608421

C,0,0.3687667061,-2.2170336605,2.4227244662

H,0,0.6390253391,-2.3818654077,3.4692100331

H,0,0.5847867171,-1.1752089169,2.2030258949

C,0,1.2191373622,-3.109277324,1.4894353031

H,0,1.4787595072,-4.0523970967,1.9792179434

H,0,0.6094751486,-3.3582196341,0.6157138638

C,0,2.4169874943,-2.4275348221,1.0235692225

C,0,3.3374122473,-1.7650351176,0.6142727079

C,0,4.3607383319,-0.9160964068,0.1024956874

C,0,4.0986169897,0.4502122482,-0.0834104619

C,0,5.6265370514,-1.4134488272,-0.2393151955

C,0,5.0752381125,1.2891718483,-0.5974749909

H,0,3.1231959511,0.8402457899,0.1702494322

C,0,6.599405819,-0.5665609482,-0.7525075784

H,0,5.8363196407,-2.4656953799,-0.0970834585

C,0,6.3289363703,0.7864649801,-0.9342258369

H,0,4.8518727862,2.339782281,-0.736081316

H,0,7.5730379012,-0.9641665532,-1.0112238104

H,0,7.0903320154,1.443898305,-1.3349409126

C,0,0.8147089097,-1.2688262803,-1.8685755306

C,0,1.7229928233,-2.201918121,-2.615409708

H,0,1.2251882388,-3.1474479925,-2.8137210669

H,0,2.0632875931,-1.7351257842,-3.5388671806

H,0,2.5965657833,-2.3782360707,-1.9848674815

O,0,-0.1978811482,-1.7363514712,-1.3142708842

O,0,1.1784973251,-0.0334511605,-1.8809502351

C,0,0.7458084791,2.0423845977,-0.2989011472

H,0,0.7993336467,0.6489073318,-1.1052051902

^{1}TS17

C,0,-1.93585448,-1.8348833389,-1.0358222702

C,0,-2.7268926348,-0.7005657324,-0.9077663193

C,0,-3.6115069397,-0.544495936,0.1640747174

C,0,-3.6559599444,-1.5660302051,1.1086160618

C,0,-2.854061902,-2.6995484431,0.9858707878

C,0,-1.9860111243,-2.8607474078,-0.0877536848

H,0,-1.27608525,-1.9222082288,-1.8882703178

H,0,-2.6383528128,0.0804821153,-1.6521695478

H,0,-4.3132185753,-1.4841945861,1.9644002462

H,0,-2.9093529875,-3.4716241903,1.7458380564

C,0,-1.1430270278,-4.0958973168,-0.2457593711

H,0,-0.2031785616,-3.8712794683,-0.7486710131

H,0,-0.9104676827,-4.5457779979,0.7206448176

H,0,-1.6658461336,-4.8486667006,-0.8433578461

C,0,-4.4940948037,0.6895878553,0.2218826266

H,0,-3.8687067697,1.5267936778,-0.1045541397

C,0,-5.6546121861,0.558792632,-0.7789988126

H,0,-6.2555040663,1.4713764911,-0.7971396001

H,0,-5.2885550181,0.3693944716,-1.7891680599

H,0,-6.3071390592,-0.2720491824,-0.4990268775

C,0,-5.0226898669,1.0245102347,1.6178312409

H,0,-4.2104577514,1.1201552956,2.3384286427

H,0,-5.5690315778,1.9698144131,1.5922156725

H,0,-5.7187192096,0.2613043306,1.9750993444

Ru,0,0.315217618,0.411488426,-0.0133730475

C,0,2.2807782539,-2.687262279,-2.0540052643

C,0,2.7255946386,-3.5838628889,-1.0882927016

C,0,2.4679060279,-3.3463608169,0.2625400413

C,0,1.7878041496,-2.1998522505,0.6607732198

C,0,1.367411998,-1.2886360836,-0.3048370288

C,0,1.6062219966,-1.5387254109,-1.6564963047

H,0,2.4310034278,-2.8621033017,-3.1120768752

H,0,3.2586913167,-4.4789678383,-1.3841605259

H,0,2.7906166657,-4.0649918774,1.0064610862

H,0,1.5514991878,-2.0378206134,1.7040984614

C,0,0.9974166963,-0.5676554831,-2.6214547698

O,0,1.0181274008,-0.7656938616,-3.8396905859

N,0,0.3032273237,0.4716753506,-2.0877618898

O,0,-1.3149478503,1.9274839504,0.156063251

C,0,-1.2612744547,3.2791447388,-0.3104138365

H,0,-0.7959654784,3.9127070758,0.4544398903

H,0,-2.288816386,3.6237018486,-0.4589818756

C,0,-0.4983277008,3.3660178072,-1.6210830146

H,0,-0.6246470041,4.369999637,-2.0322082536

H,0,-0.9131424593,2.64931993,-2.3277835569

C,0,1.0053340984,3.0890574347,-1.4624788736

H,0,1.4790640232,3.0617955207,-2.4478575795

H,0,1.4954530949,3.8860913212,-0.8899879901

C,0,1.29854897,1.8172017514,-0.7902228118

C,0,2.0298877361,1.2039146239,0.1741787712

C,0,3.3492442862,1.0805826851,0.6981193137

C,0,4.4244187498,1.7071756844,0.0419370402

C,0,3.5896174739,0.3539918391,1.8754970745

C,0,5.7083398218,1.591563078,0.5459073099

H,0,4.2388865566,2.2628325423,-0.8682878662

C,0,4.8742283047,0.2541504925,2.3798192006

H,0,2.7548496729,-0.1116965404,2.3788515741

C,0,5.934434366,0.8675951195,1.7150114415

H,0,6.5354829415,2.0633159568,0.0316095855

H,0,5.0559155424,-0.3036125779,3.2892173764

H,0,6.9390569345,0.7830153606,2.1094517407

C,0,-1.4559275148,-0.6451466618,3.8651089536

H,0,-1.8581915732,-1.6012444271,3.5318890437

H,0,-0.5098347288,-0.8422256011,4.371770869

H,0,-2.148629717,-0.1595118472,4.5475541802

C,0,-1.2082268844,0.2245745188,2.6570404567

O,0,-1.7305261274,1.3478209217,2.5729631647

O,0,-0.4280683786,-0.2989764686,1.7770931889

H,0,-1.5661935171,1.8621273185,1.1377287313

Four Carbon

1a

C,0,4.2129898277,-0.7825947995,-1.1683595739

C,0,5.5215177898,-1.2435554229,-1.1700927274

C,0,6.2290228226,-1.3413885599,0.0245455986

C,0,5.6238432955,-0.9728072304,1.220763101

C,0,4.3099392964,-0.5200074782,1.2265510108

C,0,3.5930143116,-0.4291975144,0.0310093136

H,0,3.6528193202,-0.6857443682,-2.0885502758

H,0,5.9925131152,-1.5232803514,-2.1038057853

H,0,7.2521490262,-1.695528115,0.0219105649

H,0,6.1774677751,-1.0284545832,2.1493916354

H,0,3.8603037602,-0.2033080137,2.158898214

C,0,2.176691105,0.0601229556,-0.0450974909

O,0,1.7262911991,0.6056170561,-1.0318819089

N,0,1.4546731764,-0.1286024071,1.1159261257

H,0,1.7105582895,-0.9108598423,1.7028119555

O,0,0.0727363028,0.016121906,1.0628310841

C,0,-1.1713469097,2.8707470712,-0.0164252936

H,0,-0.8483282774,3.8060424436,-0.4812912617

H,0,-2.1261886928,3.0811744944,0.4740981912

C,0,-1.4072562263,1.8411969954,-1.145039827

H,0,-1.8826007455,2.3504380741,-1.9886837025

H,0,-0.4446875418,1.4593856899,-1.494263882

C,0,-2.2446329491,0.7196244012,-0.7427207029

C,0,-2.9193995563,-0.2010568227,-0.3580263655

C,0,-3.6302328543,-1.3237046628,0.1547869517

C,0,-2.9820791125,-2.2197293519,1.0198560461

C,0,-4.9715592935,-1.5590798863,-0.1784257886

C,0,-3.6602344208,-3.3152759976,1.5339995145

H,0,-1.9455817875,-2.0384344409,1.2739701618

C,0,-5.6425849018,-2.6583810932,0.3387970621

H,0,-5.4769226469,-0.8728081328,-0.8452304268

C,0,-4.9918348881,-3.5399431401,1.1964091987

H,0,-3.1478905261,-3.9988370189,2.1998243961

H,0,-6.6782273831,-2.8280141861,0.0715558514

H,0,-5.5183161259,-4.3964373019,1.5981614538

C,0,-0.1250121273,2.4932639262,1.0394915911

H,0,-0.0905888399,3.2982250201,1.780951089

H,0,0.8656237148,2.4529038033,0.5817302559

C,0,-0.3584772328,1.1878513341,1.7913037585

H,0,-1.4201002681,1.0061964885,1.9601233142

H,0,0.1562242999,1.1987950618,2.7562258529

^{1}TS2

C,0,-0.8522447341,-2.1717763286,-1.4704576887
C,0,-1.9015195001,-1.2596471441,-1.763382855
C,0,-2.8099242213,-0.882157755,-0.7652607257
C,0,-2.7185513714,-1.5552569284,0.5012793751
C,0,-1.7386080697,-2.5254589556,0.754657187
C,0,-0.7504653188,-2.8337610002,-0.2238669249
H,0,-0.0997016561,-2.3621868095,-2.2245160528
H,0,-1.9019643799,-0.7550418909,-2.7178346503
H,0,-3.402656072,-1.2690759888,1.2882850986
H,0,-1.6860956745,-2.9898429448,1.731486446
C,0,0.3386469429,-3.8260685581,0.0576221362
H,0,1.1969021373,-3.6587353906,-0.5929162423
H,0,0.6765932279,-3.7468113467,1.0919997725
H,0,-0.0141839388,-4.8483589683,-0.1034146374
C,0,-3.8624837232,0.1896605935,-0.9472685589
H,0,-3.9482321251,0.6860302719,0.0233726081
C,0,-3.4743312827,1.256387705,-1.9713655286
H,0,-4.2041889671,2.0667809256,-1.9538566845
H,0,-2.4948468358,1.6779618315,-1.7456138747
H,0,-3.4575676485,0.8560976935,-2.9882671189
C,0,-5.2151929747,-0.4538772209,-1.2875454955
H,0,-5.5110119056,-1.1887468923,-0.5359707084
H,0,-5.9953806249,0.3076550645,-1.3405775311
H,0,-5.1703405376,-0.960828536,-2.2547463653
Ru,0,-0.7464433977,-0.6003049066,0.1144814974
C,0,0.5883557994,3.1532294552,-1.4349981236
C,0,1.2217577594,2.8794471871,-2.6409282374
C,0,1.5158823359,1.5583245765,-2.9818218612
C,0,1.2206541003,0.5282254787,-2.1037724893
C,0,0.5861161106,0.7861043629,-0.8782684957
C,0,0.2447329717,2.1175283625,-0.5742545385
H,0,0.3166047715,4.1613628332,-1.1473208319
H,0,1.477275395,3.6850422743,-3.3175741946
H,0,1.999731529,1.3362122089,-3.9252807434
H,0,1.5219625358,-0.4830733023,-2.3467080317
C,0,-0.611684327,2.3898796601,0.6223022249
O,0,-0.7466783037,3.5000028529,1.1297870378
N,0,-1.2262634483,1.235789606,0.9638996135
O,0,-2.2599255921,1.3756076199,1.9091264039
C,0,0.4904671648,0.9493832097,3.6433513243
H,0,1.1087507472,1.1017761118,4.5321183142
H,0,0.7824493744,1.718907007,2.9298944115
C,0,0.8396918757,-0.4392904673,3.0439680352
H,0,1.8817848169,-0.6753624814,3.2848668509
H,0,0.2218918648,-1.217921379,3.4986328367
C,0,0.7003166162,-0.4230093136,1.5686721108
C,0,1.4393247755,-0.1235342151,0.55735108
C,0,2.8644677931,-0.2451973037,0.2435506436
C,0,3.5118943458,-1.465999862,0.460332227
C,0,3.6177411601,0.8518168151,-0.1894510866
C,0,4.8806287213,-1.5892079503,0.2503080042
H,0,2.9300102839,-2.315336466,0.7934129128
C,0,4.9847384725,0.7291543,-0.3877528478
H,0,3.1231561251,1.7979636063,-0.3620307948

C,0,5.620351757,-0.4916446347,-0.1736580698

H,0,5.3676237855,-2.5417313071,0.4185506091

H,0,5.5580066027,1.5890453864,-0.7105812517

H,0,6.686764302,-0.5846781776,-0.3362540396

C,0,-0.9742092662,1.1488788759,4.0554725108

H,0,-1.1426899989,0.621652771,5.0027503015

H,0,-1.1476460586,2.2100266163,4.2471012091

C,0,-2.0563825196,0.641874404,3.1110128394

H,0,-1.8869394938,-0.415067509,2.8761758094

H,0,-3.025094023,0.7176685575,3.6102869193

^{1}TS5

C,0,3.1563869269,-1.4246917349,-1.6242496726

C,0,3.6351442521,-0.82983103,-0.4132209838

C,0,3.6004468939,0.5696802381,-0.2207392168

C,0,3.0147123475,1.3585376247,-1.2553482688

C,0,2.4428446714,0.7671155387,-2.3822062982

C,0,2.5250989994,-0.6516702321,-2.5954937849

H,0,3.2127053872,-2.4977192281,-1.7469231904

H,0,4.0444974047,-1.4716557121,0.3523316747

H,0,2.9109589126,2.4252973522,-1.1059996307

H,0,1.9102908616,1.3787773065,-3.0976432605

C,0,1.8771849933,-1.2571226768,-3.8034518817

H,0,1.9842772734,-2.3406959462,-3.8130953275

H,0,0.8114219324,-1.0207073225,-3.8074109855

H,0,2.3170527362,-0.8539520362,-4.7184795648

C,0,4.1209363354,1.2565489316,1.022910351

H,0,3.3878058358,2.0340000549,1.2580244006

C,0,4.2168767077,0.3388737073,2.2408629507

H,0,4.4760414329,0.9253284713,3.1233976909

H,0,3.2681036212,-0.1617715304,2.4325976241

H,0,4.9941248174,-0.4193089543,2.116466122

C,0,5.4682684444,1.9308981298,0.7225689903

H,0,5.3942251541,2.6238778948,-0.1177602584

H,0,5.8141465142,2.4919602725,1.5926211327

H,0,6.2283256276,1.1849238743,0.477356554

Ru,0,1.5236572648,-0.2344671779,-0.5086019062

C,0,-0.2294374282,-2.1417277573,2.8788024707

C,0,-0.0452866145,-3.5071806837,2.7227472048

C,0,0.6018578014,-3.9887695415,1.5822165457

C,0,1.0802707161,-3.1205520382,0.6041808015

C,0,0.2522708212,-1.2859643983,1.8922337946

H,0,-0.7596511337,-1.7291122856,3.7280542679

H,0,-0.4160313504,-4.1982813423,3.4689725879

H,0,0.7272025652,-5.057779777,1.4525970465

H,0,1.5579515254,-3.5337161185,-0.2758837354

C,0,-0.0217066578,0.1796740888,1.8963954499

O,0,-0.8846860892,0.7298822543,2.5586607358

N,0,0.9080162206,0.7436052426,1.0453934528

O,0,0.2500907202,2.4846956288,0.5138785493

C,0,-0.4115240146,3.4271435858,1.3836014912

H,0,-0.0540830902,4.4181392314,1.0769719965

H,0,-0.0303537608,3.2190265306,2.3811394125

C,0,-1.92875366,3.3620934741,1.3774618535

H,0,-2.2805757834,3.9169802304,2.2546435018

H,0,-2.2185578723,2.3257676918,1.5377078116

C,0,-4.3540811505,2.1648174603,0.0603622673

C,0,-4.4135273219,0.9615949685,0.0519578355

C,0,-4.3505329839,-0.4616454308,0.0163517133

C,0,-3.3019268565,-1.1199337161,0.6762704272

C,0,-5.2675835059,-1.2175972686,-0.7265240385

C,0,-3.1591914078,-2.4950652231,0.5676698065

H,0,-2.5980856718,-0.5414952406,1.2581493915

C,0,-5.1247030457,-2.5947165763,-0.8211874454

H,0,-6.0776644688,-0.7136656046,-1.2374682254

C,0,-4.0668355365,-3.2364424489,-0.1826846619

H,0,-2.3271229235,-2.9815154621,1.0594459452

H,0,-5.8362468789,-3.1685210341,-1.4021137158

H,0,-3.9507025154,-4.3095390144,-0.2702027759

C,0,-1.1088171704,0.4194942104,-1.7779547762

C,0,-2.2790903443,-0.0318959168,-2.6218868567

H,0,-2.5795814708,-1.0433393504,-2.3606527656

H,0,-3.1103329916,0.657551639,-2.496976588

H,0,-1.9698541702,-0.014954847,-3.6705507509

O,0,-0.3627316259,-0.5238934411,-1.3422275766

O,0,-0.9205569169,1.6386118845,-1.597343709

C,0,0.9277215665,-1.7401896399,0.7516792929

H,0,-0.2748415156,2.1906947573,-0.3068584989

C,0,-2.6026961473,3.9189454625,0.1232488901

H,0,-2.1493764513,3.4937866876,-0.7728129183

H,0,-2.4714112367,5.0046777263,0.0747154883

C,0,-4.1136175811,3.6025951067,0.0926368153

H,0,-4.6014828475,4.0367933867,0.9729487039

H,0,-4.5726960928,4.0756060938,-0.7803717732

^{1}TS5b

C,0,-0.5905260106,-0.4796909391,-2.6692679656

C,0,0.2262354255,-1.4557497247,-2.0547609886

C,0,1.5299280652,-1.1525425763,-1.6134459269

C,0,1.9801943193,0.18279516,-1.7682290835

C,0,1.157515765,1.145058951,-2.3479487084

C,0,-0.1327622581,0.8340422681,-2.8338643615

H,0,-1.5738201728,-0.7582182615,-3.0243207694

H,0,-0.1655445411,-2.455271,-1.9371590202

H,0,2.967997397,0.4732107425,-1.3854817277

H,0,1.5251729006,2.1602592187,-2.4353929666

C,0,-0.9873620431,1.8987731294,-3.4547381617

H,0,-1.7925181983,1.4704403648,-4.0508603989

H,0,-1.4354799604,2.5233966364,-2.6775562662

H,0,-0.3903739735,2.5471163905,-4.096791049

C,0,2.4428961089,-2.1547486228,-0.9507921601

H,0,2.8352557748,-1.6506603989,-0.0610094899

C,0,1.7465723734,-3.4421124138,-0.5159526566

H,0,2.4469242968,-4.0571313866,0.0493557087

H,0,0.8884512844,-3.2428582566,0.1287642673

H,0,1.4068925098,-4.0360875353,-1.3698246639

C,0,3.6462821248,-2.442511019,-1.8659358485

H,0,4.1818494907,-1.5263915844,-2.11527926

H,0,4.3429521683,-3.1039936085,-1.3494590819

H,0,3.3313794631,-2.9322788943,-2.7917890998

Ru,0,-0.2108723035,0.1278811545,-0.3035967934

C,0,-1.6229733471,-2.5744640941,2.6584288296

C,0,-2.6899679342,-3.2702131096,2.1062347017

C,0,-3.105422393,-2.9813143545,0.8067377095

C,0,-2.4789797504,-1.9898058335,0.0525921569

C,0,-1.4069687722,-1.2940547628,0.599056414

C,0,-0.9894767027,-1.6055499365,1.8885577387

H,0,-1.2676047684,-2.7708283958,3.6624274687

H,0,-3.1957568303,-4.0376214772,2.6778612691

H,0,-3.9352307322,-3.5279368793,0.3749663309

H,0,-2.8517572949,-1.7646135343,-0.9379845977

C,0,0.1728116809,-0.7922640811,2.3265515254

O,0,0.5464470924,-0.6070248442,3.458192403

N,0,0.7795438651,-0.2686253675,1.1573543838

O,0,2.4601506585,1.2384292447,2.0289572302

C,0,2.5204569052,2.4082111525,1.2564629633

H,0,2.1126331006,2.230822789,0.2464306483

H,0,3.5614502698,2.7099134403,1.0958615471

C,0,1.7374176722,3.5032656155,1.9623026908

H,0,1.8899892497,4.456565959,1.4438834193

H,0,2.1448838705,3.6135330882,2.9699251342

C,0,-1.0634828685,1.9803852132,0.2310357465

C,0,-2.0394028728,1.2540518399,-0.0810121407

C,0,-3.4432391612,0.9516814597,-0.2018066794

C,0,-4.0493179155,0.8192405233,-1.4549742805

C,0,-4.2114842329,0.7602005913,0.9523279755

C,0,-5.3989930285,0.5130074172,-1.5524958808

H,0,-3.4584971592,0.9607425195,-2.3490570608

C,0,-5.5591862767,0.4485183963,0.8491003457

H,0,-3.7371461446,0.8367506449,1.9213159134

C,0,-6.1566875771,0.3230322382,-0.4009368197

H,0,-5.8603467026,0.4202654945,-2.527465247

H,0,-6.1427538711,0.2956989457,1.7477319952

H,0,-7.2079123045,0.0770267636,-0.4779747162

C,0,6.4709706435,-0.4046591501,0.1264603771

H,0,7.0595041725,0.050510102,-0.6681686432

H,0,6.9237544468,-0.1937975298,1.0966131937

H,0,6.4678328295,-1.4903728071,0.0050712708

C,0,5.0300988387,0.1034462216,0.113222623

O,0,4.6817109397,0.8861051449,-0.8012838739

O,0,4.2816956955,-0.3377141625,1.0351218493

H,0,3.1175521226,0.5753104934,1.6408608678

C,0,-0.4754867383,3.2552320546,0.6791102087

H,0,0.2232476222,3.6065222771,-0.0843337003

H,0,-1.2958815115,3.9794819741,0.7053471603

C,0,0.2413549018,3.1971928478,2.0567429333

H,0,-0.2403144626,3.9148852413,2.7228902062

H,0,0.1136147691,2.2138608324,2.509888882

^{1}TS10

C,0,-0.4613713196,-2.4358829038,0.0446172663

C,0,0.8735772572,-2.1664906933,0.4031882843

C,0,1.8088970464,-1.768681996,-0.5586221553

C,0,1.3801056726,-1.7133018039,-1.9038504585

C,0,0.0770908077,-2.0107541397,-2.2586680248

C,0,-0.8809367808,-2.3587206254,-1.2908814478

H,0,-1.1530133773,-2.7569257899,0.8122155203

H,0,1.1575894708,-2.2558484436,1.4413720445

H,0,2.0693769486,-1.3679432811,-2.6596231031

H,0,-0.2232727732,-1.9296047095,-3.2955019568

C,0,-2.3044786826,-2.6237929596,-1.6924635565

H,0,-2.8203889169,-3.2481611191,-0.9633492454

H,0,-2.8586712847,-1.685689177,-1.7783226358

H,0,-2.3476482614,-3.1226355455,-2.6612363585

C,0,3.229683198,-1.3639152633,-0.2280083841

H,0,3.3568113248,-0.3858829804,-0.7047686437

C,0,3.4961906701,-1.1904257742,1.2662141116

H,0,4.5027146997,-0.7981479463,1.4161336969

H,0,2.7955169054,-0.4902062484,1.720772047

H,0,3.4335243378,-2.1421119724,1.8014467116

C,0,4.2350509715,-2.3457576693,-0.851632209

H,0,4.0942567244,-2.4448497827,-1.9286881785

H,0,5.2551504887,-1.9984072036,-0.6786770866

H,0,4.1351807101,-3.3387060181,-0.4058514896

Ru,0,-0.1032533651,0.1049340408,-0.1114547405

C,0,0.8521847466,2.0887589864,3.499783815

C,0,0.148047383,1.4708032095,4.5255839967

C,0,-0.6936141735,0.3990066146,4.2341068817

C,0,-0.8532964704,-0.0584049435,2.9252969542

C,0,-0.1443089688,0.5419209009,1.890587892

C,0,0.7021004996,1.612887014,2.2028382753

H,0,1.5135887499,2.926697147,3.6832167886

H,0,0.2515042194,1.8179956821,5.5456863157

H,0,-1.2406898205,-0.0855656298,5.0344513459

H,0,-1.5377483084,-0.8736338755,2.7332330123

C,0,1.4160919463,2.1845996402,1.0208224749

O,0,2.0007975428,3.245669832,0.9598673451

N,0,1.3191918584,1.2184337431,0.0162673986

C,0,0.8640942871,3.5546201404,-2.3461765755

H,0,0.8569451792,4.3232006644,-3.1261739203

H,0,1.7037648818,3.7728977378,-1.6835319839

C,0,-0.4419450272,3.6478151299,-1.5208373508

H,0,-0.9057798884,4.6155693124,-1.7236395249

H,0,-0.204450641,3.657445302,-0.4586495133

C,0,-1.5154070639,2.5634524269,-1.7755863062

H,0,-2.5160748973,3.0054862876,-1.7218216889

H,0,-1.4103284644,2.1652327265,-2.7878112366

C,0,-1.4958265389,1.4439526349,-0.8158626466

C,0,-2.1120364082,0.6848268234,-0.0013149016

C,0,-3.3124067149,0.4437098754,0.7644334923

C,0,-3.7224897262,-0.8405782905,1.1374106993

C,0,-4.1032626752,1.5361295268,1.151374579

C,0,-4.8888589644,-1.0324518281,1.8629882173

H,0,-3.1183405052,-1.6886874017,0.8533374151

C,0,-5.2682967045,1.3427252381,1.878790922

H,0,-3.7831122247,2.5354810591,0.8876404878

C,0,-5.6667813304,0.0584553108,2.2377929062

H,0,-5.1910825502,-2.0346785665,2.1401214084

H,0,-5.8637413908,2.1976243935,2.1736489099

H,0,-6.5740169603,-0.0902825885,2.8091892537

C,0,1.1697901579,2.2143799764,-3.0395793515

H,0,0.3705176771,2.0229769472,-3.7876839948

H,0,2.0949981915,2.3657891289,-3.6261153278

O,0,1.2715862251,1.1497591072,-2.1804659523

^{1}TS18

C,0,-1.3423037685,-1.1977309543,3.0799674416

C,0,-2.192485578,-1.6489397056,2.0224436857

C,0,-2.9813115643,-0.7557673776,1.2946683027

C,0,-2.8888162869,0.6351249733,1.6444119456

C,0,-2.1080892205,1.0751786714,2.716014491

C,0,-1.2973716258,0.1522043652,3.4553292785

H,0,-0.7159037005,-1.9147376925,3.5945645679

H,0,-2.1651290755,-2.6940445633,1.7497241909

H,0,-3.4232969921,1.3596451599,1.0446646643

H,0,-2.0632349328,2.1284097541,2.9533850486

C,0,-0.4516317887,0.626090322,4.5998567911

H,0,0.363671925,-0.0686681189,4.800072117

H,0,-0.0219430271,1.6054249212,4.3936029668

H,0,-1.0596467451,0.7077909001,5.5051033044

C,0,-3.8611067169,-1.1516267717,0.1278489258

H,0,-3.6289007426,-0.4453035133,-0.6755774044

C,0,-3.5950634281,-2.5587285077,-0.404074261

H,0,-4.1907851682,-2.7304434187,-1.3009525093

H,0,-2.5484707115,-2.6970940239,-0.6713285181

H,0,-3.8721448349,-3.3220463948,0.327974217

C,0,-5.3409061662,-0.9801372625,0.5079448576

H,0,-5.5576494543,0.0325439875,0.8524800035

H,0,-5.9779396068,-1.1848551654,-0.3542497415

H,0,-5.6168193279,-1.6738200485,1.3061434893

Ru,0,-0.7821311277,-0.0235631718,1.230707532

C,0,0.3794041952,-3.1406184014,-1.3044607605

C,0,1.1202301609,-4.0342298035,-0.5396245431

C,0,1.5875945714,-3.6569253762,0.7220864852

C,0,1.3172634962,-2.3901190674,1.2205634986

C,0,0.5656164452,-1.4818728964,0.4627250346

C,0,0.0984313269,-1.8751142366,-0.807130664

H,0,0.0037263163,-3.4018990182,-2.2860470219

H,0,1.3402093263,-5.0231253162,-0.9219230739

H,0,2.1709944621,-4.3537623578,1.3118799392

H,0,1.7031025037,-2.0879997878,2.1867601663

C,0,-0.6633493223,-0.8625833396,-1.6051233759

O,0,-0.909909756,-0.9975051897,-2.8007264514

N,0,-0.8971525741,0.2172013749,-0.8187709258

O,0,-1.2512871226,1.389091535,-1.5018396903

C,0,1.902336049,0.7170618098,-1.9397184765

H,0,2.7959200353,0.796517253,-2.5685910205

H,0,1.3379945554,-0.1065362928,-2.364860669

C,0,2.4294915251,0.3297980146,-0.5409027941

H,0,2.9803782144,-0.6089783665,-0.6371629842

H,0,3.1416449828,1.0949929021,-0.2076252205

C,0,1.4522433153,0.2473413025,0.5832061702

C,0,0.9714094236,1.0704176581,1.4423177111

C,0,1.407948045,2.2743315728,2.1075601479

C,0,0.569969958,3.3903538327,2.2441388717

C,0,2.7075265181,2.3512571602,2.6353501209

C,0,1.0214225332,4.5463321942,2.8646524729

H,0,-0.4322066175,3.3439449316,1.8411051264

C,0,3.1513521193,3.5058361767,3.263554382

H,0,3.356572572,1.4886666385,2.5551037127

C,0,2.312317376,4.610239753,3.3812390331

H,0,0.3622656026,5.4016759652,2.9475799435

H,0,4.1562308369,3.5437119098,3.6657956734

H,0,2.6593446065,5.5094205062,3.8737701841

C,0,1.1243355363,2.03359868,-2.1380169524

H,0,1.7873994614,2.8743993931,-1.897459585

H,0,0.9195492861,2.1006482038,-3.209927545

C,0,-0.1858463038,2.340355549,-1.3939889176

H,0,0.0077639545,2.5369124712,-0.33930867

H,0,-0.6113344088,3.2491489082,-1.8251877688

^{1}O

C,0,0.105948484,-3.2679448938,-0.3304991406

C,0,1.0979108672,-2.7513261286,0.4823094843

C,0,1.985006875,-1.7513181462,-0.0233001342

C,0,1.8709439349,-1.3935537946,-1.3932423406

C,0,0.8701344806,-1.9567855525,-2.2277936437

C,0,-0.0534176204,-2.8509088824,-1.6889413759

H,0,-0.6279937856,-3.941132763,0.086048092

H,0,1.1834567466,-3.0871352009,1.5051679404

H,0,2.5892132168,-0.706165365,-1.8153814717

H,0,0.8031120515,-1.6629767554,-3.2659165409

C,0,-1.2369603747,-3.3380137096,-2.4689574965

H,0,-1.2871840285,-4.4292498325,-2.4525775377

H,0,-2.1552334981,-2.956429618,-2.0168555463

H,0,-1.1965175055,-3.0053542734,-3.505398644

C,0,3.1635684983,-1.2358412929,0.7797912375

H,0,3.3894315812,-0.2367464472,0.3990402495

C,0,2.8874762227,-1.111965044,2.2778647897

H,0,3.7168499314,-0.6009559451,2.7690278055

H,0,1.9766933511,-0.5460954019,2.4650081705

H,0,2.7824463323,-2.0900364671,2.7524377256

C,0,4.3878401154,-2.1280423453,0.5193360863

H,0,4.6260437604,-2.1755734756,-0.54451951

H,0,5.261597407,-1.7412925601,1.0476097513

H,0,4.2050205928,-3.1472321803,0.8690182737

Ru,0,0.0120383309,-0.7208808265,-0.3790921493

C,0,-3.6222112083,2.230686518,-1.209157166

C,0,-3.4434305559,3.6019445716,-1.1221134927

C,0,-2.3838315771,4.1081002674,-0.3739517467

C,0,-1.5025002091,3.239147391,0.2540105441

C,0,-1.6523028662,1.8520903127,0.1479891512

C,0,-2.7342004653,1.3529720458,-0.587415362

H,0,-4.4699169288,1.8075378015,-1.7318047138

H,0,-4.132407023,4.2742847036,-1.6176684323

H,0,-2.2399767257,5.1779379913,-0.2847742911

H,0,-0.6696720772,3.6379470987,0.8207458539

C,0,-3.0943909103,-0.0968639005,-0.5176028873

O,0,-4.2763307654,-0.447732698,-0.5417442226

N,0,-2.0511595816,-0.9147924653,-0.2622967082

O,0,-2.3909979784,-2.1004264039,0.4306766785

C,0,-3.1010292621,-1.8816570594,1.6710897901

H,0,-2.8692937018,-2.7828269541,2.2455318067

H,0,-4.1713831107,-1.8567582632,1.457119

C,0,-2.7273028109,-0.6304473637,2.4668315049

H,0,-3.3197005237,-0.6916963621,3.3845333208

H,0,-3.1025093636,0.2508104252,1.9484508924

C,0,-0.5682156228,1.0005123494,0.7831074328

C,0,0.5858455389,1.0108873934,-0.0317667609

C,0,1.7287107996,1.8754332325,-0.2061025862

C,0,2.3782515935,1.9776241828,-1.4455027379

C,0,2.202638961,2.6564276673,0.8616364202

C,0,3.4749831281,2.810694363,-1.6057955753

H,0,1.9819463001,1.4217506192,-2.2840883034

C,0,3.3134841224,3.4711191466,0.7043162636

H,0,1.6975553129,2.6088740089,1.8168015454

C,0,3.955471912,3.5503208968,-0.528629341

H,0,3.9539105478,2.8899539078,-2.5736590717

H,0,3.6744793476,4.0553462894,1.5414995897

H,0,4.8156262796,4.1957348338,-0.6527477483

C,0,-0.5841493418,0.8447954963,2.3027640623

H,0,-1.1087918242,1.7029353362,2.7365398866

H,0,0.4407635056,0.878460926,2.680322262

C,0,-1.2342725163,-0.4555601306,2.8188526177

H,0,-0.6645501733,-1.296911731,2.419568944

H,0,-1.104827554,-0.4813610841,3.9047790477