Supporting Information

[3,3]-Sigmatropic Rearrangement vs. Carbene Formation in Gold-Catalyzed Transformations of Alkynyl Aryl Sulfoxides: Mechanistic Studies and Expanded Reaction Scope

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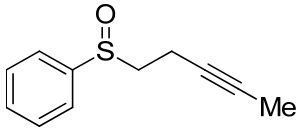
General Ethyl acetate (ACS grade), hexanes (ACS grade), diethyl ether (ACS grade) and anhydrous 1,2-dichloroethane (HPLC grade) were purchased from Fisher Scientific and used without further purification. Methylene chloride and tetrahydrofuran were purified using MBraun Solvent Purifier. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using Sorbent Technologies' pre-coated silica gel plates. Flash column chromatography was performed over Sorbent Technologies' silica gel (230-400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on a Varian 500 MHz Unity plus spectrometer and a Varian 400 MHz spectrometer using residue solvent peaks as internal standards. Infrared spectra were recorded with a Perkin Elmer FT-IR spectrum 2000 spectrometer and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Micromass QTOF2 Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization or Waters GCT Premier time-of-flight mass spectrometer with a field ionization (FI) ion source.

General procedure A: preparation of sulfoxide

To a solution of thiophenol (10 mmol) and pent-4-yn-1-yl *p*-tosylate (10 mmol) in dry acetone (40 mL) was added potassium carbonate (12 mmol). After the reaction mixture was refluxed under N_2 for 2 h, it was then cooled and filtered through a plug of celite. The filtrate was concentrated to give crude sulfide without further purification.

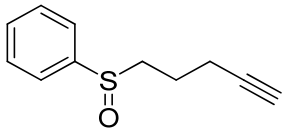
The crude sulfide was dissolved in acetonitrile (20 mL) and water (20 mL) at 0 ºC. Oxone (about 8-9 mmol) was added in portions. The reaction mixture was stirred for 0.5 h and was then quenched with brine. After extracted with ethyl acetate 3 times, the filtrate was dried and concentrated. The residue was purified through silica gel flash chromatography to give sulfoxide typically in good yields.

(Pent-3-yne-1-sulfinyl)-benzene (23)



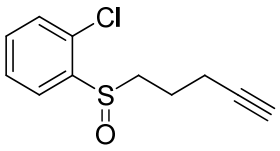
This compound was prepared in 79 % yield according to the general procedure A but using pent-3-yn-1-yl tosylate as the alkylating reagent (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 – 7.65 (m, 2H), 7.50 – 7.54 (m, 3H), 2.91 – 2.96 (m, 2H), 2.65 – 2.68 (m, 1H), 2.36 – 2.41 (m, 1H), 1.76 (t, 3H, *J* = 1.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.3, 131.3, 129.4, 124.2, 78.3, 75.6, 56.2, 12.8, 3.8; IR (neat): 3055, 2918, 1477, 1442, 1085, 1043, 692; MS (ES^+) Calculated for $[C_{11}H_{12}NaOS]^+$: 215.1; Found: 215.0.

(Pent-4-yne-1-sulfinyl)benzene ((29a)



This compound was prepared in 75 % yield according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.62 (m, 2H), 7.51 – 7.53 (m, 3H), 2.94 – 3.00 (m, 1H), 2.84 –2.90 (m, 1H), 2.31 – 2.38 (m, 2H), 1.97 –2.03 (m, 2H), 1.81 – 1.86 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.7, 131.1, 129.4, 124.1, 82.6, 70.0, 55.9, 21.2, 17.8; IR (neat): 3294, 3227, 2934, 2116, 1443, 1086, 1043, 1019, 997; MS (ES^+) Calculated for $[C_{11}H_{12}NaOS]^+$: 215.1; Found: 215.1.

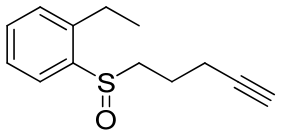
1-Chloro-2-(pent-4-yne-1-sulfinyl)benzene (29b)



This compound was prepared in 71 % yield according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.50 – 7.55 (m, 1H), 7.39 – 7.47 (m, 2H), 3.22 – 2.29 (m, 1H), 2.86 – 2.93 (m, 1H), 2.33 – 2.40 (m, 2H), 2.09 – 2.18 (m, 1H), 1.98 (t, *J* = 2.4 Hz, 1H), 1.80 – 1.89 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.6, 132.1, 130.2, 130.0, 128.1, 126.4, 82.6, 70.0, 53.0,

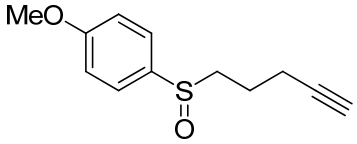
21.3, 17.9; IR (neat): 3301, 3234, 2933, 2116, 1449, 1433, 1062, 1027; MS (ES^+) Calculated for $[C_{11}H_{11}ClNaOS]^+$: 249.0; Found: 249.0.

1-Ethyl-2-(pent-4-yne-1-sulfinyl)benzene (29c)



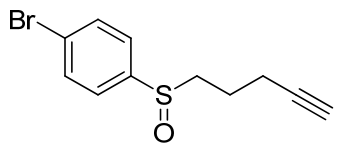
This compound was prepared in 77% yield according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^1H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.92 (m, 1H), 7.41 – 7.44 (m, 2H), 7.25 – 7.28 (m, 1H), 2.95 – 3.00 (m, 1H), 2.74 – 2.84 (m, 2H), 2.62 – 2.68 (m, 1H), 2.31 – 2.44 (m, 2H), 2.04 –2.09 (m, 1H), 1.97 (t, J = 2.4 Hz, 1H), 1.88 – 1.93 (m, 1H), 1.27 –1.29 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.4, 140.9, 131.2, 128.9, 127.4, 124.0, 82.6, 70.0, 55.1, 24.8, 21.7, 17.7, 15.5; IR (neat): 3293, 3229, 2968, 2934, 2116, 1719, 1436, 1068, 1035; MS (ES^+) Calculated for $[C_{13}H_{16}NaOS]^+$: 243.1; Found: 243.1.

1-Methoxy-4-(pent-4-yne-1-sulfinyl)benzene (29d)



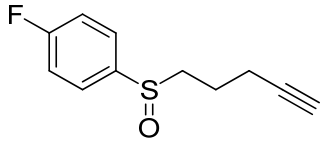
This compound was prepared in 83 % yield according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^1H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, J = 8.5 Hz, 2H), 7.03 (d, J = 8.5 Hz, 2H), 3.85 (s, 3H), 3.05 – 3.11 (m, 1H), 2.87 – 2.93 (m, 2H), 2.31 – 2.36 (m, 2H), 1.97 (t, J = 2.5 Hz, 1H), 1.92 – 1.95 (m, 1H), 1.82 – 1.86 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.1, 134.6, 126.1, 115.0, 82.6, 70.0, 56.1, 55.7, 21.4, 17.9; IR (neat): 3291, 3225, 2942, 2839, 2116, 1595, 1496, 1304, 1251, 1089, 1041; MS (ES^+) Calculated for $[C_{11}H_{11}NNaO_3S]^+$: 245.1; Found: 245.1.

1-Bromo-4-(pent-4-yne-1-sulfinyl)benzene (29e)



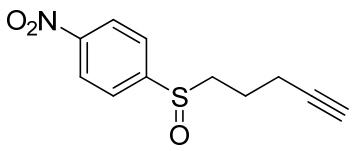
This compound was prepared in 74 % yield according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.69 (m, 2H), 7.48 – 7.51 (m, 2H), 2.94 – 3.01 (m, 1H), 2.81 – 2.88 (m, 1H), 2.32 – 2.39 (m, 2H), 2.33 – 2.40 (m, 2H), 1.99 – 2.05 (m, 1H), 1.97 (t, *J* = 2.4 Hz, 1H), 1.79 – 1.87 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.9, 132.7, 125.8, 125.6, 82.4, 70.2, 55.9, 21.1, 17.8; IR (neat): 2927, 2116, 1471, 1386, 1084, 1047, 1007; MS (ES^+) Calculated for $[C_{11}H_{11}BrNaOS]^+$: 293.0; Found: 293.0.

1-Fluoro-4-(pent-4-yne-1-sulfinyl)benzene (29f)



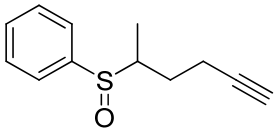
This compound was prepared in 76 % yield according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.66 (m, 2H), 7.21 – 7.26 (m, 2H), 2.93 – 3.00 (m, 1H), 2.83 – 2.89 (m, 1H), 2.33 – 2.39 (m, 2H), 2.33 – 2.40 (m, 2H), 1.99 – 2.05 (m, 1H), 1.98 (t, *J* = 2.4 Hz, 1H), 1.81 – 1.89 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.5 (*J* = 249.6 Hz), 139.2 (*J* = 3.0 Hz), 126.4 (*J* = 9.0 Hz), 116.8 (*J* = 22.3 Hz), 82.5, 70.1, 56.1, 21.2, 17.8; IR (neat): 3297, 3226, 2934, 2858, 2116, 1443, 1085, 1038; MS (ES^+) Calculated for $[C_{11}H_{11}FNaOS]^+$: 233.0; Found: 233.0.

1-Nitro-4-(pent-4-yne-1-sulfinyl)benzene (29g)



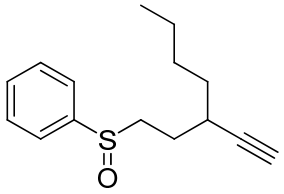
This compound was prepared in 70 % yield according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 – 8.40 (m, 2H), 7.81 – 7.83 (m, 2H), 3.05 – 3.11 (m, 1H), 2.87 – 2.93 (m, 1H), 2.35 – 2.41 (m, 2H), 2.33 – 2.40 (m, 2H), 2.04 – 2.09 (m, 1H), 2.00 (t, *J* = 2.5 Hz, 1H), 1.81 – 1.84 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.5, 149.7, 82.2, 70.5, 55.8, 21.0, 17.7; IR (neat): 3290, 2933, 2116, 1523, 1344, 1084, 1047, 1010, 852; MS (ES^+) Calculated for $[C_{11}H_{11}NNaO_3S]^+$: 260.0; Found: 260.0.

(Hex-5-yne-2-sulfinyl)benzene (29h)



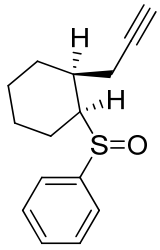
This compound was prepared in 71 % yield (dr: 2:3) according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.60 (m, 5H), 2.90 – 2.97 (m, 0.4H), 2.82 –2.89 (m, 0.6H), 2.49 – 2.57 (m, 0.6H), 2.33 – 2.42 (m, 0.6H), 2.27 – 2.32 (m, 0.4H), 2.18 – 2.25 (m, 0.4H), 2.09 – 2.20 (m, 0.6H), 2.02 (t, *J* = 2.8 Hz, 0.4H), 1.87 – 1.97 (m, 1H), 1.65 – 1.72 (m, 0.6H), 1.53 – 1.63 (m, 0.4H), 1.19 (d, *J* = 7.2 Hz, 1.2H), 1.02 (d, *J* = 7.2 Hz, 1.8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.8, 141.4, 131.3, 130.9, 129.4, 129.1, 125.3, 124.7, 82.7, 82.6, 70.0, 69.7, 57.9, 29.4, 27.3, 16.3, 16.0, 12.7, 10.0; IR (neat): 3229, 2929, 2116, 1443, 1084, 1044; MS (ES^+) Calculated for $[C_{12}H_{14}NaOS]^+$: 229.1; Found: 229.1.

(3-Ethynyl-heptane-1-sulfinyl)benzene (29i)



This compound was prepared in 75 % yield (dr: 1:1) according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 – 7.63 (m, 2H), 7.48 – 7.54 (m, 3H), 3.04 –3.10 (m, 0.5H), 2.93 – 3.02 (m, 1H), 2.81 – 2.87 (m, 0.5H), 2.51 – 2.53 (m, 0.5H), 2.33 – 2.35 (m, 0.5H), 2.06 – 2.07 (m, 1H), 1.96 – 2.04 (m, 0.5H), 1.77 – 1.89 (m, 1.5H), 1.60 – 1.68 (m, 0.5H), 1.37 – 1.45 (m, 2H), 1.25 – 1.35 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.9, 131.2, 131.1, 129.42, 129.40, 124.20, 124.15, 86.2, 70.88, 70.83, 55.18, 55.15, 34.8, 31.3, 30.8, 29.6, 29.5, 27.7, 27.2, 22.7, 22.6, 14.2; IR (neat): 3303, 3226, 2956, 2931, 2859, 2111, 1443, 1087, 1043; MS (ES^+) Calculated for $[C_{15}H_{20}NaOS]^+$: 271.1; Found: 271.1.

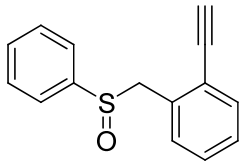
(2-Prop-2-ynyl-cyclohexanesulfinyl)benzene (29i)



This compound was prepared in 72 % yield (dr 1:1) according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.66 (m, 2H), 7.52 – 7.53 (m, 3H), 2.77 – 2.88 (m, 1H), 2.67 – 2.73 (m, 0.5H), 2.48 – 2.61 (m, 1.5H), 1.94 – 2.24 (m, 2H), 2.03 (t, J = 2.8 Hz, 0.5H), 2.00 (t, J = 2.4 Hz, 0.5H), 1.72 – 1.80 (m, 1H), 1.38 – 1.55 (m, 4H), 1.17 – 1.33 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 142.8, 131.8, 131.1, 129.40, 129.35, 125.7, 124.9, 82.8, 70.3, 69.9, 67.8, 66.4, 36.9, 34.0, 29.2, 28.6, 25.4, 24.9, 22.4, 21.6, 21.0, 20.6, 19.2, 17.3; IR (neat): 3297, 3225,

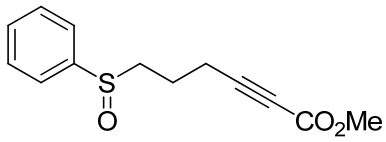
2934, 2858, 2117, 1443, 1085, 1038; MS (ES^+) Calculated for $[C_{15}H_{18}NaOS]^+$: 269.1; Found: 269.1.

1-Benzenesulfinylmethyl-2-ethynylbenzene (29k)



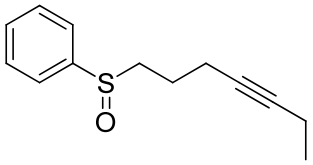
This compound was prepared in 85 % yield according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^1H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.50 (m, 6H), 7.26 – 7.29 (m, 2H), 7.05 – 2.08 (m, 1H), 4.33 (d, *J* = 12.4 Hz, 1H), 4.24 (d, *J* = 12.4 Hz, 1H), 3.27 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 133.1, 132.4, 131.4, 131.2, 129.14, 129.11, 128.5, 124.6, 123.1, 82.6, 81.5, 62.9; IR (neat): 3288, 3211, 3060, 2099, 1483, 1443, 1045; MS (ES^+) Calculated for $[C_{15}H_{12}NaOS]^+$: 263.0; Found: 263.0.

6-Benzenesulfinylhex-2-ynoic acid methyl ester (29m)



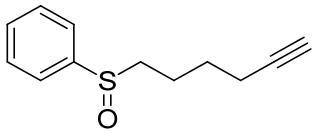
This compound was prepared in 74 % yield according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^1H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.64 (m, 2H), 7.51 – 7.56 (m, 3H), 3.75 (s, 3H), 2.93 – 3.00 (m, 1H), 2.83–2.89 (m, 1H), 2.48 – 2.56 (m, 2H), 2.05 –2.11 (m, 1H), 1.84 – 1.93 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.0, 143.4, 131.3, 129.5, 124.1, 87.3, 74.2, 55.5, 52.9, 20.5, 18.1; IR (neat): 2236, 1713, 1435, 1249, 1078, 1044, 913; MS (ES^+) Calculated for $[C_{13}H_{15}O_3S]^+$: 251.1; Found: 251.1.

(Hept-4-yne-1-sulfinyl)benzene (31)



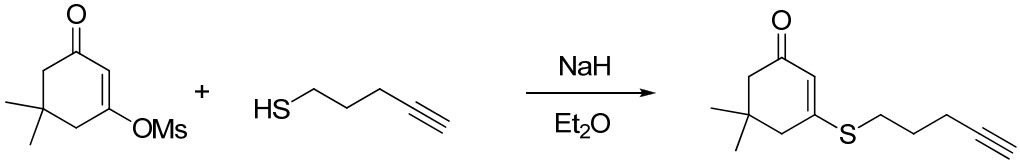
This compound was prepared in 81 % yield according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 – 7.63 (m, 2H), 7.49 – 7.54 (m, 3H), 2.93 – 2.98 (m, 1H), 2.85 – 2.90 (m, 1H), 2.26 – 2.31 (m, 2H), 2.10 –2.14 (m, 2H), 1.90 – 1.94 (m, 1H), 1.75 – 1.80 (m, 1H), 1.08 (t, 3H, J = 8.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.9, 131.1, 129.4, 124.2, 83.5, 77.5, 56.3, 21.8, 18.2, 14.5, 12.6; IR (neat): 2974, 2936, 2914, 1443, 1086, 1045, 748; MS (ES^+) Calculated for $[C_{13}H_{16}NaOS]^+$: 243.1; Found: 243.1.

(Hex-5-yne-1-sulfinyl)benzene (36)



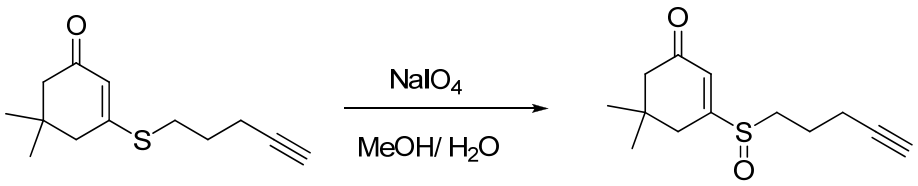
This compound was prepared in 77 % yield according to the general procedure A (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 – 7.62 (m, 2H), 7.48 – 7.53 (m, 3H), 2.82 (t, J = 7.0Hz, 2H), 2.19 –2.22 (m, 2H), 1.93 (t, J = 2.5Hz, 1H), 1.84 – 1.90 (m, 1H), 1.74 – 1.77 (m, 1H), 1.61 – 1.67 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.0, 131.1, 129.4, 124.1, 83.5, 69.3, 56.9, 27.6, 21.6, 18.3; IR (neat): 3295, 3229, 2934, 2360, 2115, 1443, 1087, 1045; MS (ES^+) Calculated for $[C_{12}H_{14}NaOS]^+$: 229.1; Found: 229.1.

5,5-dimethyl-3-(pent-4-ynylthio)cyclohex-2-enone



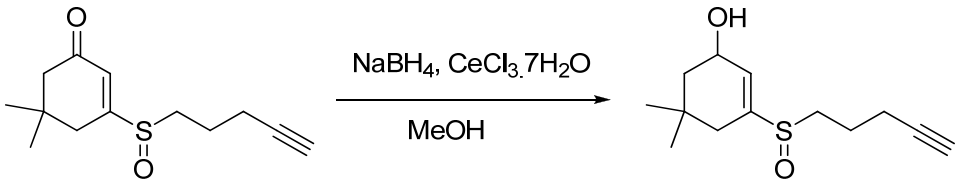
To a solution of pent-4-yne-1-thiol (0.916 g, 9.16 mmol) in dry ether (30 mL) was added NaH (440 mg, 60%, 1.2 eq) at 0 ºC. The mixture was stirred for 0.5 h. Methanesulfonic acid 5, 5-dimethyl-3-oxo-cyclohex-1-enyl ester (1.02 g, 10 mmol) in ether (5 mL) was added dropwise. The mixture was stirred for 24 h at room temperature. Saturated ammonium chloride was added carefully to quench reaction at 0 ºC. After extracted with ethyl acetate for 3 times, the filtrate was dried and concentrated. The residue was purified through silica gel flash chromatography to give sulfide in 34% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.89 (s, 1H), 2.95 (t, *J* = 7.5 Hz, 2H), 2.35 (t, *J* = 7.5 Hz, 2H), 2.33 (s, 2H), 2.26 (s, 2H), 2.02 (t, *J* = 2.5 Hz, 1H), 1.88 – 1.92 (m, 2H), 1.06 (s, 6 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ195.9, 163.3, 118.6, 82.7, 70.0, 51.3, 44.8, 34.4, 29.8, 28.2, 26.8, 18.0; IR (neat): 3290, 2957, 2109, 1652, 1578, 1303, 1245, 1025; MS (ES^+) Calculated for $[C_{13}H_{18}NaOS]^+$: 245.1; Found: 245.1.

5, 5-Dimethyl-3-(pent-4-yne-1-sulfinyl)-cyclohex-2-enone[2] (38)

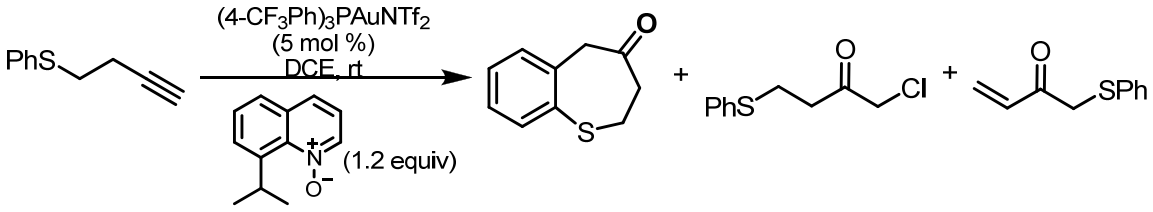


To a solution of sulfide (518 mg, 2.33 mmol) in methanol (4 mL) was added the aqueous sodium periodate (498 mg in 4 mL water) at 0 ºC. The mixture was stirred for 24 h while warming to room temperature slowly. Brine was added carefully to quench reaction at 0 ºC. After extracted with ethyl acetate 3 times, the filtrate was dried and concentrated. The residue was purified through silica gel flash chromatography to give sulfoxide in 73% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.58 (s, 1H), 2.99 – 3.05 (m, 1H), 2.78 – 2.84 (m, 1H), 2.39 – 2.42 (m, 2H), 2.37 (s, 2H), 2.03 (q, *J* = 15.0 Hz, 2H), 2.03 (t, *J* = 2.5 Hz, 1H), 1.87 – 1.92 (m, 1H), 1.13 (s, 3H), 1.10 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.4, 164.3, 127.0, 82.4, 70.5, 52.1, 50.0, 37.2, 35.1, 28.9, 27.7, 20.9, 17.8; IR (neat): 3285, 2959, 2871, 2116, 1676, 1614, 1411, 1347,1066, 911; MS (ES^+) Calculated for $[C_{13}H_{18}NaO_2S]^+$: 261.1; Found: 261.1.

5, 5-Dimethyl-3-(pent-4-yne-1-sulfinyl)cyclohex-2-enol[3] (40)

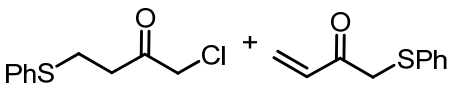


$CeCl_3$•$7H_2O$ (227 mg, 0.61 mmol) and $NaBH_4$ (23.2 mg, 0.61 mmol) were added to a solution of 5, 5-Dimethyl-3-(pent-4-yne-1-sulfinyl)-cyclohex-2-enol (145 mg, 0.61 mmol) in methanol (5 mL) at 0 ºC. The reaction mixture was stirred for 20 min. Brine was added carefully to quench reaction at 0 ºC. After extracted with ethyl acetate for 3 times, the filtrate was dried and concentrated. The residue was purified through silica gel flash chromatography to give alcohol 120 mg in 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.40 (d, *J* = 10.0 Hz, 1H), 4.36 – 4.39 (m, 1H), 2.84 – 2.88 (m, 1H), 2.71 – 2.76 (m, 1H), 2.33 – 2.38 (m, 2H), 1.76 –2.00 (m, 6H), 1.06 – 1.44 (m, 1H), 1.07 (d, *J* = 1.6Hz, 3H), 0.93 (d, *J* = 4.4Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.6, 141.2, 132.9, 132.7, 82.6, 70.1, 65.92, 65.87, 49.5, 49.4, 44.8, 44.6, 35.6, 34.9, 32.5, 31.8, 31.3, 30.9, 26.2, 25.7, 21.1, 20.9, 17.7; IR (neat): 3301, 2953, 2917, 2849, 2116, 1338, 1100, 1048; MS (ES^+) Calculated for $[C_{15}H_{14}NaOS]^+$: 263.1; Found: 263.1.



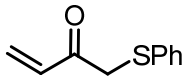
An oven-dried vial was charged with but-3-ynyl(phenyl)sulfane (32.4 mg, 0.2 mmol), 8-methylquinoline 1-oxide (38.2 mg, 0.24 mmol) and dry DCE (2 ml). The mixture was treated with (4-CF_3Ph)$_3$PAuNTf_2 (9.4 mg, 5 mol %). The reaction mixture was stirred at the room temperature until the sulfane was completely consumed. The reaction mixture was concentrated under *vacuum*. The residue was purified through silica gel flash chromatography.

1-Chloro-4-(phenylthio)butan-2-one (19) and 1-(phenylthio)but-3-en-2-one (20)



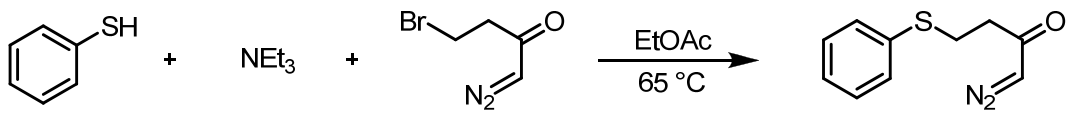
Compound **3** and compound **4** were isolated as a mixture by silica gel flash chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.18 (m, 5H, **3** + **4**), 6.60 (dd, *J* = 17.5, 10.6 Hz, 1H, **4**), 6.30 (dd, *J* = 17.4, 1.1 Hz, 1H, **4**), 5.85 (dd, *J* = 10.6, 1.1 Hz, 1H, **4**), 4.06 (s, 2H, **3**), 3.82 (s, 2H, **4**), 3.19 (t, *J* = 7.1 Hz, 2H, **3**), 2.92 (t, *J* = 7.1 Hz, 2H, **3**); MS (GCMS) Calculated for 3 $[C_{10}ClH_{11}OS]^{+}$: 214; Found:214; MS (GCMS) Calculated for $[C_{10}H_{10}OS]^{+}$: 178; Found:178.

1-(phenylthio)but-3-en-2-one (20)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.33 (m, 3H), 7.33 – 7.19 (m, 14H), 6.60 (dd, *J* = 17.5, 10.5 Hz, 1H), 6.30 (dd, *J* = 17.5, 1.1 Hz, 1H), 5.85 (dd, *J* = 10.7, 1.1 Hz, 1H), 3.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.51, 145.48, 134.10, 130.40, 129.99, 129.33, 127.34, 42.59; IR (neat): 1694, 1482, 1439, 1401; MS (ES^{+}) Calculated for $[C_{10}H_{11}OS]^{+}$: 179.05; Found:179.04.

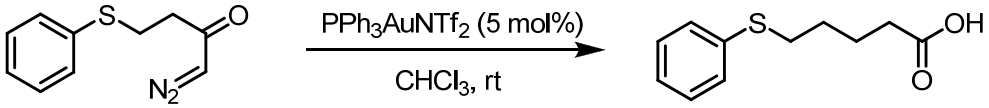
1-diazo-4-(phenylthio)butan-2-one (21)



4-Bromo-1-diazobutan-2-one (177 mg, 1.0 mmol), benzenethiol (132 mg, 1.2 mmol) and triethylamine (202 mg, 2.0 mmol) were mixed in a 10 ml of ethyl acetate. The vial was stirred at 65 °C overnight. The solvent was removed under vacuum. Flash

chromatography afforded 196 mg of compound 5 as yellow oil in 95% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 – 7.36 (m, 5H), 5.24 (br, 1H), 3.20 (t, 2H, *J* = 7.2 Hz), 2.62 (br, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) 192.46, 135.38, 129.72, 129.05, 126.46, 54.98, 40.18, 28.73; IR (neat): 2929, 2841, 2103, 1635, 1494, 1052; MS (ES^+) Calculated for $[C_{10}H_{10}KN_2OS]^+$: 245.02; Found: 245.03.

5-(phenylthio)pentanoic acid (22)



1-diazo-4-(phenylthio)butan-2-one (41.2 mg, 0.2 mmol) and PPh_3AuNTf_2 (7.4 mg, 0.01 mmol) was dissolved in 1 ml of $CHCl_3$. The reaction was stirred at room temperature for 4 h. The organic layer was treated with 1 ml of 10% NaOH solution. The aqueous layer was washed with another 1 ml of $CHCl_3$ followed by 0.5 ml of 6 M HCl solution. Theaqueous layer was extracted by 1 ml of ether twice and the organic layer was concentrated to afford 27.5 mg 4-(phenylthio)butanoic acid as light yellow solid in 71% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.45 (br, 1H), 7.18 – 7.36 (m, 5H), 2.99 (t, 2H, *J* = 6.9 Hz), 2.53 (t, 2H, *J* = 7.2 Hz), 1.96 (quint, 2H, *J* = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) 178.93, 135.73, 129.50, 128.95, 126.20, 32.91, 32.45, 23.95; IR (neat): 2957, 1702, 1481, 1437, 1317, 1245, 1200, 1136, 1093,1025, 914, 734; MS (ES^+) Calculated for $[C_{10}H_{12}KO_2S]^+$: 235.02; Found: 235.04.

General procedure B: gold-catalyzed synthesis of benzothiocine

An oven-dried vial was charged with sulfoxide (0.2 mmol) and dry DCM (4 ml). The mixture was treated with $Ph_3PAuNTf_2$ (7.6 mg, 5 mol %). The reaction mixture was stirred at the room temperature until the sulfoxide was completely consumed. The reaction mixture was concentrated under *vacuum*. The residue was purified to give the desired benzothiocine through silica gel flash chromatography.

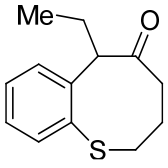
General procedure C: gold-catalyzed synthesis of benzothiocine

An oven-dried vial was charged with sulfoxide (0.2 mmol) and dry DCE (4 ml). The mixture was treated with $IPrAuNTf_2$ (8.6 mg, 5 mol % or 17.2 mg, 10 mol %). The reaction mixture was stirred at 60 ºC for indicated time. The reaction mixture was concentrated under *vacuum*. The residue was purified to give the desired benzothiocine through silica gel flash chromatography.

General procedure D: Mercury-catalyzed synthesis of benzothiocine

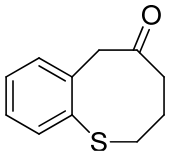
An oven-dried vial was charged with sulfoxide (0.2 mmol) and dry DCM (4 ml). The mixture was treated with $Hg(OTf)_2$ (2.0 mg, 2 mol %). The reaction mixture was stirred at the room temperature until the sulfoxide was completely consumed. The reaction mixture was concentrated under *vacuum*. The residue was purified to give the desired benzothiocine through silica gel flash chromatography.

6-Ethyl-3, 4-dihydro-2*H*, 6*H*-benzo[*b*]thiocin-5-one (32)



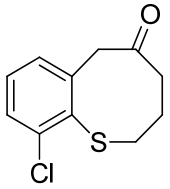
This compound was prepared in 95 % yield according to the general procedure D (eluents: ethyl acetate: hexanes = 1: 6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 7.2Hz, 1H), 7.34 – 7.38 (m, 1H), 7.22 (d, J = 7.6Hz, 1H), 3.35 – 3.38 (m, 1H), 3.03 – 3.08 (m, 1H), 2.41 – 2.54 (m, 2H), 2.34 – 2.40 (m, 2H), 2.14 – 2.18 (m, 1H), 2.05 – 2.17 (m, 1H), 1.51– 1.58 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 212.0, 146.2, 138.3, 135.0, 131.2, 129.4, 128.8, 62.0, 39.5, 38.9, 31.9, 26.3, 12.2; IR (neat): 3056, 2960, 2921, 1696, 1436, 1328, 1176, 1066; MS (ES^+) Calculated for $[C_{13}H_{16}NaOS]^+$: 243.1; Found: 243.1.

3, 4-Dihydro-2*H*, 6*H*-benzo[*b*]thiocin-5-one (30a)



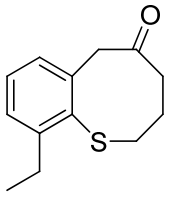
This compound was prepared in 93 % yield according to the general procedure B (eluents: ethyl acetate: hexanes = 1: 6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.2Hz, 1H), 7.29 – 7.38 (m, 2H), 7.25 – 7.31 (m, 1H), 3.89 (s, 3H), 2.82 (t, *J* = 6.0 Hz, 2H), 2.27 – 2.30 (m, 2H), 2.12 – 2.17 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 211.5, 142.1, 137.8, 135.4, 130.3, 129.9, 129.0, 51.8, 39.5, 39.1, 30.8; IR (neat): 2919, 1698, 1469, 1437, 1329, 1177, 1103; MS (ES^+) Calculated for $[C_{11}H_{12}NaOS]^+$: 215.1; Found: 215.1.

10-Chloro-3, 4-dihydro-2*H*, 6*H*-benzo[*b*]thiocin-5-one (30b)



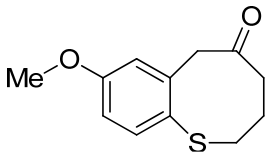
This compound was prepared in 96 % yield according to the general procedure D (eluents: ethyl acetate: hexanes = 1: 3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.0 Hz, 1H), 7.27 – 7.31 (m, 1H), 7.19 (d, *J* = 7.2 Hz), 3.92 (s, 3H), 2.18 – 2.27 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 210.7, 144.7, 141.3, 134.2, 130.6, 129.7, 128.7, 52.6, 38.8, 37.1, 31.3; IR (neat): 2964, 2916, 2848, 1692, 1437, 1421, 1334, 1175; MS (ES^+) Calculated for $[C_{11}H_{11}ClNaOS]^+$: 249.0; Found: 249.0.

10-Ethyl-3, 4-dihydro-2*H*, 6*H*-benzo[*b*]thiocin-5-one (30c)



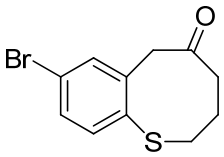
This compound was prepared in 97 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 6). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 – 7.29 (m, 2H), 7.10–7.11 (m, 1H), 3.90 (s, 3H), 2.94 (t, *J* = 7.5Hz, 3H), 2.72 (t, *J* = 6.0Hz, 2H), 2.28 – 2.30 (m, 2H), 2.12 – 2.16 (m, 2H), 1.26 (t, *J* = 7.5Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 211.7, 149.6, 142.8, 134.2, 129.7, 128.8, 127.9, 52.6, 39.2, 38.2, 30.9, 28.1, 15.9; IR (neat): 2963, 2923, 1697, 1432, 1329, 1177, 1103; MS (ES^+) Calculated for $[C_{13}H_{16}NaOS]^+$: 243.1; Found: 243.1.

8-Methoxy-3,4-dihydro-2*H*, 6*H*-benzo[*b*]thiocin-5-one (30d)



This compound was prepared in 72 % yield according to the general procedure D (eluents: ethyl acetate: hexanes = 1: 6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.4 Hz, 1H), 6.83 (dd, *J* = 8.4, 2.8Hz, 1H), 6.78 (d, *J* = 2.8 Hz, 1H), 3.84(s, 2H), 3.81 (s, 3H), 2.76 (t, *J* = 6.0 Hz, 2H), 2.28 – 2.31 (m, 2H), 2.11 – 2.15 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 211.4, 160.8, 143.4, 139.0, 126.2, 115.8, 114.3, 114.2, 55.6, 52.0, 39.6, 39.2, 30.6; IR (neat): 2916, 1696, 1593, 1478, 1238, 1069, 1028; MS (ES^+) Calculated for $[C_{12}H_{14}NaO_2S]^+$: 245.1; Found: 245.1.

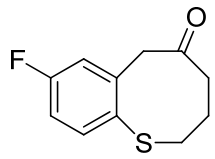
8-Bromo-3, 4-dihydro-2*H*, 6*H*-benzo[*b*]thiocin-5-one (30e)



This compound was prepared in 90 % yield according to the general procedure D (eluents: ethyl acetate: hexanes = 1: 8). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.4Hz, 1H), 7.43 – 7.45 (m, 2H), 3.85 (s, 3H), 2.81 (t, *J* = 6.0 Hz, 2H), 2.28 – 2.30 (m, 2H), 2.13 – 2.16 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 210.4, 144.0, 139.2, 134.5, 133.1, 132.1,

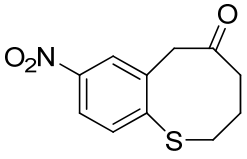
124.2, 51.4, 39.5, 39.2, 30.6; IR (neat): 2955, 2919, 1701, 1574, 1548, 1461, 1329, 1087, 811; MS (ES^+) Calculated for $[C_{11}H_{11}BrNaOS]^+$: 293.0; Found: 293.0.

8-Fluoro-3, 4-dihydro-2*H*, 6*H*-benzo[*b*]thiocin-5-one (30f)



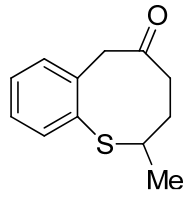
This compound was prepared in 76 % yield according to the general procedure D (eluents: ethyl acetate: hexanes = 1: 6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.67 (m, 1H), 6.97 – 7.03 (m, 2H), 3.86 (s, 3H), 2.79 (t, *J* = 6.0 Hz, 2H), 2.27 – 2.30 (m, 2H), 2.11 – 2.17 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 210.5, 163.5 (*J* = 248.8 Hz), 144.3 (*J* = 8.3 Hz), 139.6 (*J* = 8.1 Hz), 130.8, 117.2 (*J* = 21.9 Hz), 116.0 (*J* = 21.0 Hz), 51.7, 39.5, 39.2, 30.5; IR (neat): 2912, 2853, 2360, 2341, 1697, 1683, 1472, 1234, 965; MS (ES^+) Calculated for $[C_{11}H_{11}FNaOS]^+$: 233.0; Found: 233.1.

8-Nitro-3,4 -dihydro-2*H*, 6*H*-benzo[*b*]thiocin-5-one (30g)



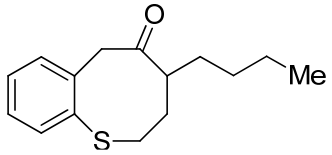
This compound was prepared in 78 % yield according to the general procedure D (eluents: ethyl acetate: hexanes = 1: 3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 – 8.15 (m, 2H), 7.88 (dd, *J* = 5.6, 3.6Hz, 1H), 3.99 (s, 3H), 2.90 (t, *J* = 6.0 Hz, 2H), 2.28 – 2.31 (m, 2H), 2.16 – 2.23 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 209.3, 148.6, 143.9, 143.7, 138.9, 124.8, 123.5, 51.5, 39.8, 39.3, 30.6; IR (neat): 2922, 2852, 1697, 1519, 1349, 1177, 820; MS (ES^+) Calculated for $[C_{11}H_{11}NNaO_3S]^+$: 260.0; Found: 260.0.

2-Methyl-3,4-dihydro-2*H*, 6*H*-benzo[*b*]thiocin-5-one (30h)



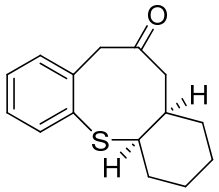
This compound was prepared in 82 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.2 Hz, 1H), 7.35 (dd, *J* = 7.6, 1.2Hz, 1H), 7.25 – 7.31 (m, 1H), 4.00 (d, *J* = 17.6 Hz, 1H), 3.75 (d, *J* = 17.6 Hz, 1H), 2.93 – 2.95 (m, 1H), 2.38 – 2.41 (m, 1H), 2.26 – 2.28 (m, 1H), 2.04 – 2.10 (m, 1H), 1.88 – 1.98 (m, 1H), 1.32 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.6, 142.3, 138.6, 133.6, 130.3, 130.0, 128.6, 51.9, 48.3, 39.0, 37.9, 22.2; IR (neat): 3056, 2955, 2922, 1698, 1470, 1437, 1332, 1185, 1011; MS (ES^+) Calculated for $[C_{12}H_{14}NaOS]^+$: 229.1; Found: 229.1.

4-Butyl-3,4-dihydro-2*H*, 6*H*-benzo[*b*]thiocin-5-one (30i)



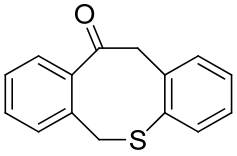
This compound was prepared in 77 % yield according to the general procedure D (eluents: ethyl acetate: hexanes = 1: 6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.29 – 7.37 (m, 1H), 7.24 – 7.26 (d, *J* = 17.6 Hz, 1H), 3.54 (d, *J* = 17.6 Hz, 1H), 3.03 – 3.08 (m, 1H), 2.48 – 3.08 (m, 1H), 2.48 – 2.56 (m, 2H), 2.11 – 2.15 (m, 1H), 1.83 – 1.87 (m, 1H), 1.65 – 1.68 (m, 1H), 1.11 – 1.26 (m, 4H), 0.83 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 214.6, 142.1, 137.8, 135.8, 130.4, 130.0, 129.0, 52.8, 48.1, 38.5, 38.3, 33.9, 29.7, 22.9, 14.1; IR (neat): 2954, 2927, 2856, 1700, 1469, 1441, 1111; MS (ES^+) Calculated for $[C_{15}H_{20}NaOS]^+$: 271.1; Found: 271.1.

1, 3, 4, 4a, 5, 12a-Hexahydro-2*H*, 7*H*-12-thia-dibenzo[*a,d*]cycloocten-6-one (30j)



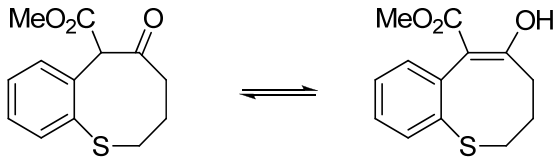
This compound was prepared in 87 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 6). ^{1}H NMR (400 MHz, CD_3SOCD_3, 60 ^{o}C) δ 7.60 (d, *J* = 7.6Hz, 1H), 7.35 – 7.40 (m, 1H), 7.29 – 7.35 (m, 2H), 3.89 (d, *J* = 16.8 Hz, 1H), 3.73 (d, *J* = 16.8 Hz, 1H), 2.98 – 3.00 (m, 1H), 2.52 – 2.55 (m, 1H), 2.20 – 2.22 (m, 1H), 2.02 (d, *J* = 12.0 Hz, 1H), 1.71 – 1.74 (m, 1H), 1.36 – 1.57 (m, 5H), 1.27 – 1.29 (m, 2H); ^{13}C NMR (100 MHz, CD_3SOCD_3, 60 ^{o}C) δ 207.9, 142.0, 137.9, 131.6, 130.2, 129.6, 127.7, 51.7, 50.9, 42.5, 40.7, 30.4, 29.4, 24.2, 21.6; IR (neat): 2929, 2852, 1693, 1469, 1440, 1335, 1118, 1002; MS (ES^{+}) Calculated for $[C_{15}H_{18}NaOS]^{+}$: 269.1; Found: 269.1.

6*H*, 12*H*-5-Thiadibenzo[*a,e*]cycloocten-11-one (30k)



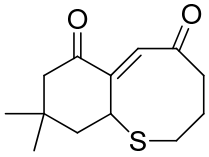
This compound was prepared in 53 % yield according to the general procedure D (eluents: ethyl acetate: hexanes = 1: 6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.33 (m, 3H), 7.20 – 7.22 (m, 1H), 7.14 – 7.16 (m, 1H), 7.09 – 7.13 (m, 2H), 6.99 – 7.03(m, 1H), 4.22 (s, 2H), 4.23 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.8, 140.2, 136.7, 134.0, 133.3, 133.1, 132.1, 130.8, 130.0, 128.1, 127.84, 127.8, 51.8, 37.8; IR (neat): 3072, 2918, 2849, 1676, 1594, 1435, 1252, 913; MS (ES^{+}) Calculated for $[C_{15}H_{12}NaOS]^{+}$: 263.1; Found: 263.1.

5-Oxo-3,4,5,6-tetrahydro-2*H*-benzo[*b*]thiocine-6-carboxylic acid methyl ester (30m)



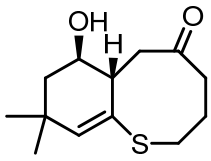
This compound was prepared in 75 % yield according to the general procedure B (eluents: ethyl acetate: hexanes = 1: 6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.1 (s, 0.8H), 7.80 – 7.82 (m, 1H), 7.27 – 7.36 (m, 3H), 4.79 (s, 0.2H), 3.78 (s, 0.6H), 3.70 (s, 2.4H), 3.03 – 3.09 (m, 1H), 2.48 – 2.56 (m, 1H), 2.36 (dd, J = 12.4, 8.4 Hz) , 1.78 – 1.84 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.8, 172.5, 140.5, 138.4, 137.0, 136.5, 131.7, 130.3, 130.1, 129.9, 128.7, 128.6, 103.9, 66.9, 52.8, 52.1, 39.3, 38.8, 37.4, 32,4, 31.6, 26.9; IR (neat): 2951, 2917, 2851, 1745, 1644, 1608, 1442, 1362, 1320, 123az5, 1054; MS (ES^+) Calculated for $[C_{13}H_{14}NaO_3S]^+$: 273.1; Found: 273.1.

9, 9-Dimethyl-3, 4, 6, 8, 9, 10-hexahydro-2*H*-benzo[b]thiocine-5, 7-dione (39)



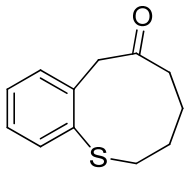
This compound was prepared in 75 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.61 (s, 2H), 2.90 (t, J = 6.4 Hz, 2H), 2.57 (s, 2H), 2.40 – 2.43 (m, 2H), 2.35 (s, 2H), 2.18 – 2.24 (m, 2H), 1.08 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 210.6, 196.2, 154.5, 137.2, 50.7, 48.7, 42.8, 39.3, 33.8, 33.4, 30.2, 28.2; IR (neat): 2955, 1700, 1673, 1347, 1322, 1250, 979; MS (ES^+) Calculated for $[C_{13}H_{18}NaO_2S]^+$: 261.1; Found: 261.1.

7-hydroxy-9,9-dimethyl-3,4,6a,7,8,9-hexahydro-2*H*-benzo[b]thiocin-5(6H)-one (41)

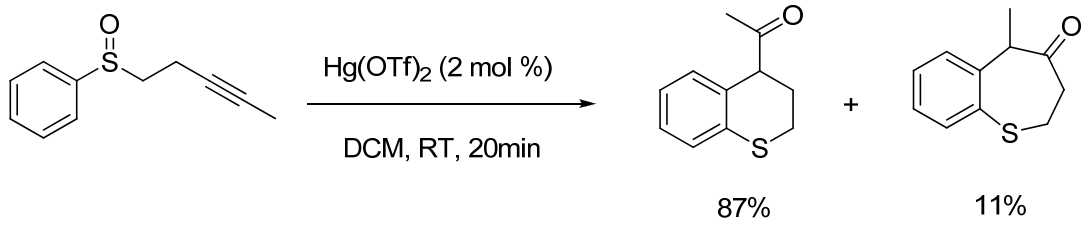


This compound was prepared in 57 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.96 (s, 1H), 3.73 – 3.77 (m, 1H), 3.02 (td, *J* = 15.0 , 3.0 Hz, 1H), 2.93 (dd, *J* = 15.0, 3.0 Hz, 1H), 2.83 – 2.88 (m, 1H), 2.45 – 2.52 (m, 1H), 2.40 (dd, *J* = 15.0, 3.0 Hz, 1H), 2.32 – 2.36 (m, 1H), 2.12 – 2.19 (m, 2H), 1.76 (dd, *J* = 12.5 , 3.5 Hz, 1 H), 1.59 – 1.61 (m, 1H), 1.06 (s, 3H), 1.02 (s, 3H) ; ^{13}C NMR (125 MHz, $CDCl_3$) δ 215.1, 145.2, 131.4, 70.7, 48.8, 47.3, 44.6, 40.3, 35.5, 34.8, 31.0, 30.9, 29.2; IR (neat): 3417, 2956, 2925, 1683, 1447, 1333, 1186, 1056, 913; MS (ES^+) Calculated for $[C_{13}H_{20}NaO_2S]^+$: 263.1; Found: 263.1.

6, 7, 8, 9-Tetrahydro-11*H*-5-thiabenzocyclononen-10-one (37)

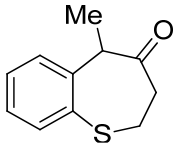


This compound was prepared in 56 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 6). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.0Hz, 1H), 7.31 – 7.34 (m, 2H), 7.26 – 7.31 (m, 1H), 3.91 (s, 2H), 2.82 (t, *J* = 6.0 Hz, 2H), 2.49 (t, *J* = 6.0 Hz, 2H), 1.95 – 1.98 (m, 2H), 1.45 – 1.47 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 212.1, 141.1, 136.3, 133.6, 131.5, 129.4, 128.3, 49.8, 42.5, 36.8, 26.7, 23.2; IR (neat): 3056, 2925, 1703, 1468, 1441, 1177, 1108; MS (ES^+) Calculated for $[C_{12}H_{14}NaOS]^+$: 229.1; Found: 229.1.



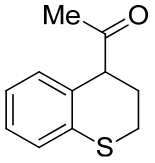
These two compounds below were prepared in according to the general procedure D (eluents: ethyl acetate: hexanes = 1: 8).

5-Methyl-2, 3-dihydro-5*H*-benzo[*b*]thiepin-4-one (24)



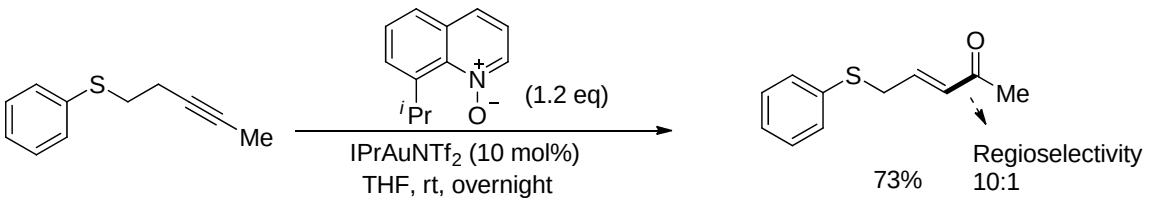
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.0 Hz, 1H), 7.27 – 7.35 (m, 2H), 7.18 – 7.22 (m, 1H), 4.50 (q, *J* = 6.8 Hz, 1H), 3.11 – 3.16 (m, 1H), 2.90 – 3.01 (m, 1H), 2.68 – 2.73 (m, 1H), 1.50 (d, J =7.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 208.9, 143.3, 134.6, 134.2, 129.2, 127.6, 127.3, 51.1, 43.6, 32.0, 14.3; IR (neat): 3058, 2932, 1712, 1459, 1333, 1164, 982; MS (ES^+) Calculated for $[C_{11}H_{12}NaOS]^+$: 215.1; Found: 215.1.

1-Thiochroman-4-yl-ethanone (25)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 – 7.18 (m, 2H), 7.06 – 7.08 (m, 2H), 3.76 (t, *J* = 4.8 Hz, 1H), 3.04 – 3.11 (m, 1H), 2.91 – 2.95 (m, 1H), 2.61 – 2.67 (m, 1H), 2.09 (s, 3H), 2.00 – 2.07 (m, 1H) ; ^{13}C NMR (125 MHz, $CDCl_3$) δ 209.0, 133.6, 132.1, 130.8, 127.9, 127.6, 124.7, 53.1, 28.9, 25.3, 24.4; IR (neat): 2929, 1707, 1354, 1434, 1355, 1158; MS (ES^+) Calculated for $[C_{11}H_{12}NaOS]^+$: 215.1; Found: 215.1.

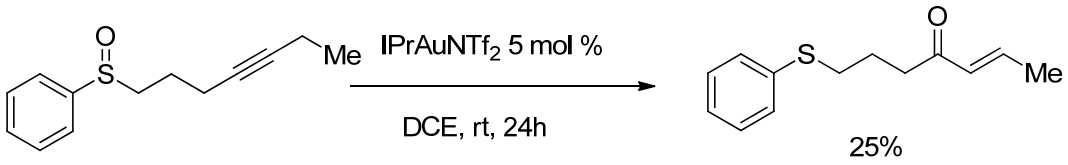
***E*-5-Phenylsulfanylpent-3-en-2-one[4] (26)**



An oven-dried reaction vial was charged with alkyne (35.2 mg, 0.2 mmol), 8-isopropylquinoline N-oxide (0.24 mmol, 1.2 eq), and THF (2 ml). The mixture was treated with $IPrAuNTf_2$ (17.2 mg, 10 mol %). The reaction mixture was stirred at the room temperature until the alkyne was completely consumed. The reaction mixture was

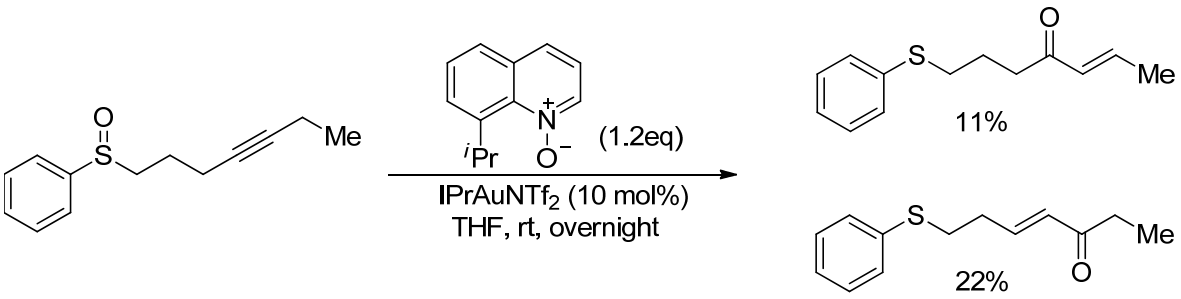
concentrated under *vacuum*. The residue was purified to give *E*-5-Phenylsulfanyl-pent-3-en-2-one in 73% yield through silica gel flash chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 – 7.35 (m, 5H), 6.73 (dt, *J* = 16.0, 6.8 Hz, 1H), 5.98 (d, *J* = 16.0Hz, 1H), 6.73 (dd, *J* = 6.8, 1.2 Hz, 1H), 2.20 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.2, 141.9, 134.4, 132.5, 131.0, 129.2, 127.3, 36.2, 27.3; IR (neat): 2925, 1697, 1674, 1480, 1360, 1251, 975; MS (ES^+) Calculated for $[C_{11}H_{12}NaOS]^+$: 231.0; Found: 231.0.

_E_-7-Phenylsulfanylhept-2-en-4-one (33)



An oven-dried reaction vial was charged with sulfoxide (44 mg, 0.2 mmol) in DCE (4 mL). $IPrAuNTf_2$ (8.6 mg, 5 mol %) was added. The reaction mixture was stirred at the room temperature for 24 h and then concentrated under *vacuum*. The residue was purified to give *E*-5-Phenylsulfanyl-pent-3-en-2-one in 25% yield through silica gel flash chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.35 (m, 2H), 7.26 – 7.30 (m, 2H), 7.15 – 7.19 (m, 1H), 6.85 (dt, *J* = 16.0, 6.8 Hz, 1H), 6.10 (d, *J* = 16.0Hz, 1H), 2.96 (t, *J* = 6.8 Hz, 2H), 2.70 (t, *J* = 7.2 Hz, 2H), 1.94 – 1.99 (m, 2H), 1.89 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.7, 143.1, 136.4, 132.1, 129.4, 129.1, 126.1, 38.4, 33.2, 23.5, 18.5; IR (neat): 2925, 2852, 1696, 1671, 1632, 1439, 1209, 970; MS (ES^+) Calculated for $[C_{13}H_{16}NaOS]^+$: 243.1; Found: 243.1.

(*E*)-7-Phenylsulfanylhept-2-en-4-one (33)and (*E*)-7-Phenylsulfanylhept-4-en-3-one (35)



An oven-dried reaction vial was charged with alkyne (39.2 mg, 0.2 mmol), 8-isopropylquinoline-N-oxide (0.24 mmol, 1.2 eq), and THF (2 ml). The mixture was treated with $IPrAuNTf_2$ (17.2 mg, 10 mol %). The reaction mixture was stirred at the room temperature for 24 h. The reaction mixture was concentrated under *vacuum*. The residue was purified to give the mixture of *E*-7-phenylsulfanyl-hept-2-en-4-one and *E*-7-phenylsulfanyl-hept-4-en-3-one in 33% yield (1:2) through silica gel flash chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.36 (m, 2H), 7.21 – 7.24 (m, 1H), 7.15 – 7.19 (m, 1H), 6.81– 6.87 (m, 1H), 6.09 – 6.15 (m, 1H), 3.04(t, *J* = 7.2 Hz, 1.5H), 2.96 (t, *J* = 6.8 Hz, 0.7H), 2.70 (t, *J* = 7.2 Hz, 0.7H), 2.53 – 2.58 (m, 3H), 1.94 – 1.99 (m, 0.7H), 1.89 (d, *J* = 6.8 Hz, 1.0H), 1.09 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR (105 MHz, $CDCl_3$) δ 201.1, 199.7, 144.0, 143.1, 136.4, 135.7, 132.1, 131.4, 130.0, 129.3, 129.2, 129.1, 126.6, 126.1, 38.4, 33.5, 33.2, 32.5, 32.3, 23.5, 18.5, 8.2; IR (neat): 2925, 2852, 1696, 1671, 1632, 1439, 1209, 970; MS (ES^+) Calculated for $[C_{13}H_{16}NaOS]^+$: 243.1; Found: 243.1.

Reference:

1. Kowalaki, C. J.; Fields, K. W. *J. Org. Chem*. **1981**, *46*, 197.
2. Leonard, N.; Johnson, W. C. *J. Am. Chem. Soc*, **1962**, 74, 831.
3. Trost, B. M.; Seoane, P.; Mignani. S; Acemoglu. M. *J. Am. Chem. Soc*, **1989**, *111*, 7487.
4. Lu, B.; Li, C.; Zhang, L. *J. Am. Chem. Soc*, **2011**, *132*, 14070.

Calculation details. In this paper, density functional theory (DFT) studies have been performed with GAUSSIAN09 program at PBE1PBE/6-31+G**/SDD level in dichloromethane using SMD method. Other methods including B3LYP, B3LYP results with single point energy corrections by MP2/MP4(SDQ) methods, M06 and M062X have also been tested. The results of the PBE1PBE method are shown to be the best compared with the experimental observations. In the Figures, the selected bond lengths are in angstroms, the relative free energies including solvent effect $\Delta G^{o}_{sol}(298K)$ are in kcal/mol.

1. ***All the optimized structures considered on the reaction pathways shown in Scheme 13 in the main text.***

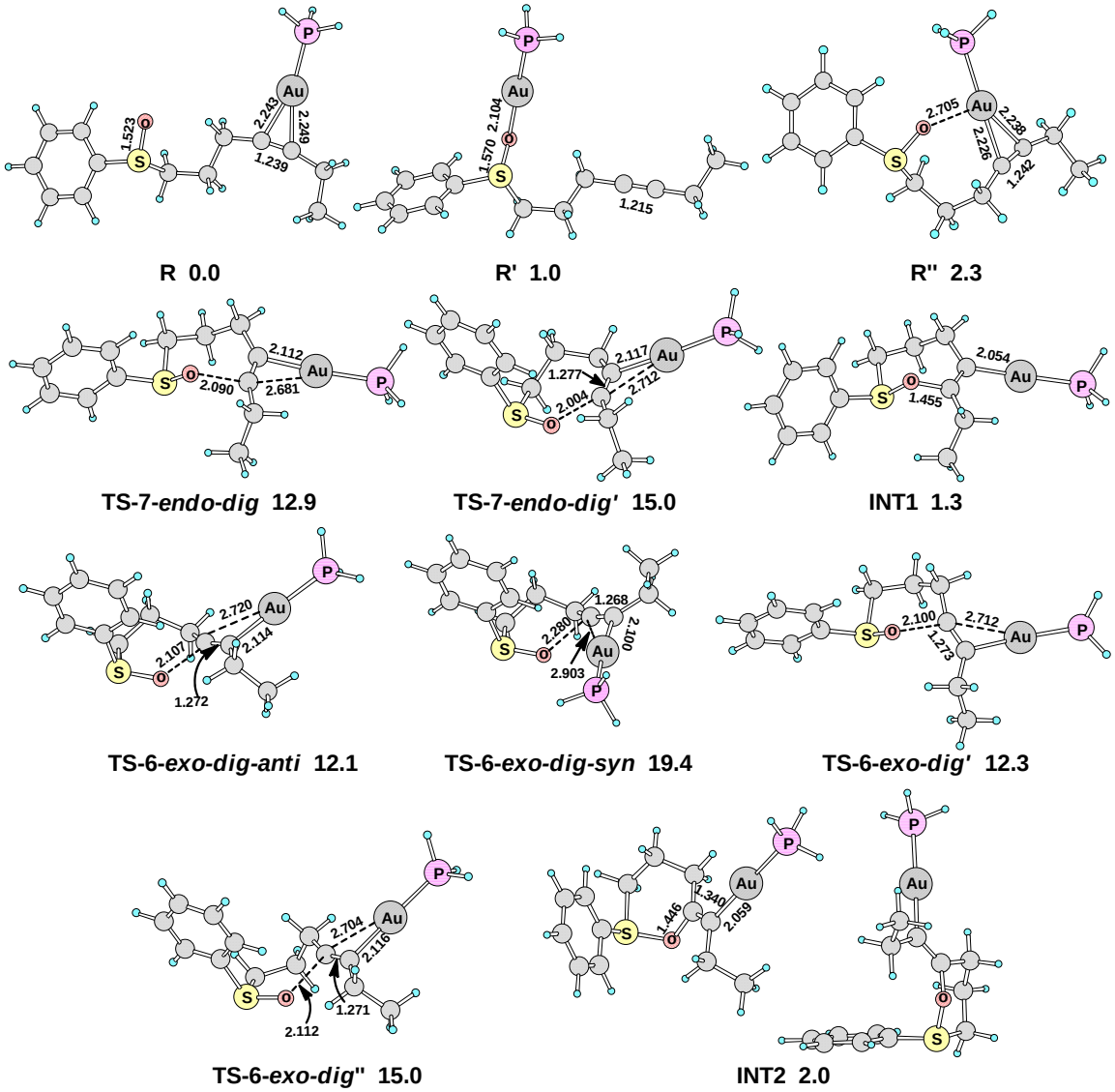


Figure S1. The optimized structures on ***Path-a*** and ***Path-b*** shown in Scheme 13 in the main text. Different conformations were considered for **R**, **TS-7-*endo-dig*** and **TS-6-*exo-dig***. **R'** is a conformer of **R** with higher relative energy, **TS-7-*endo-dig'*** is a conformer of **TS-7-*endo-dig*** with higher relative energy, and so on.

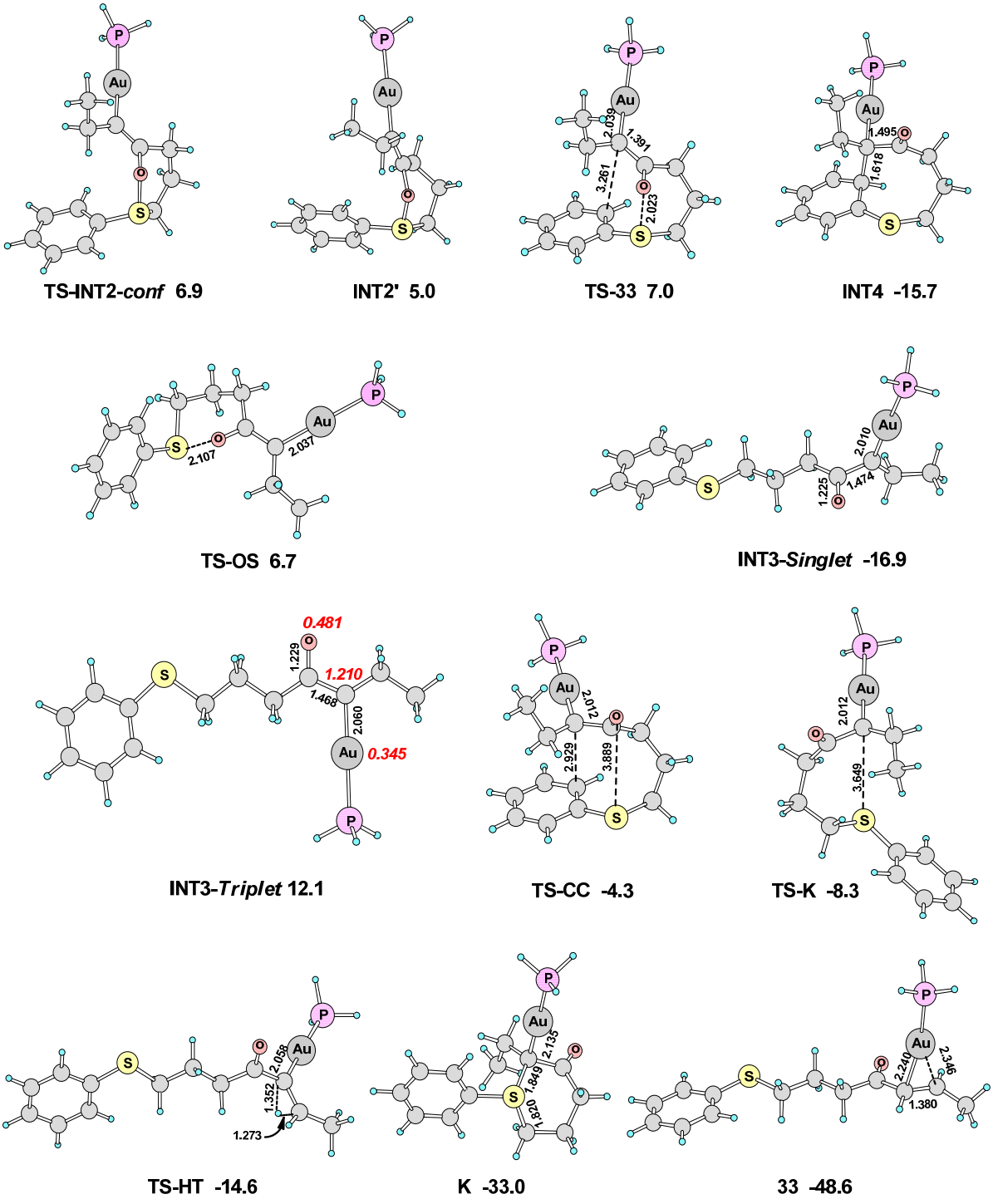
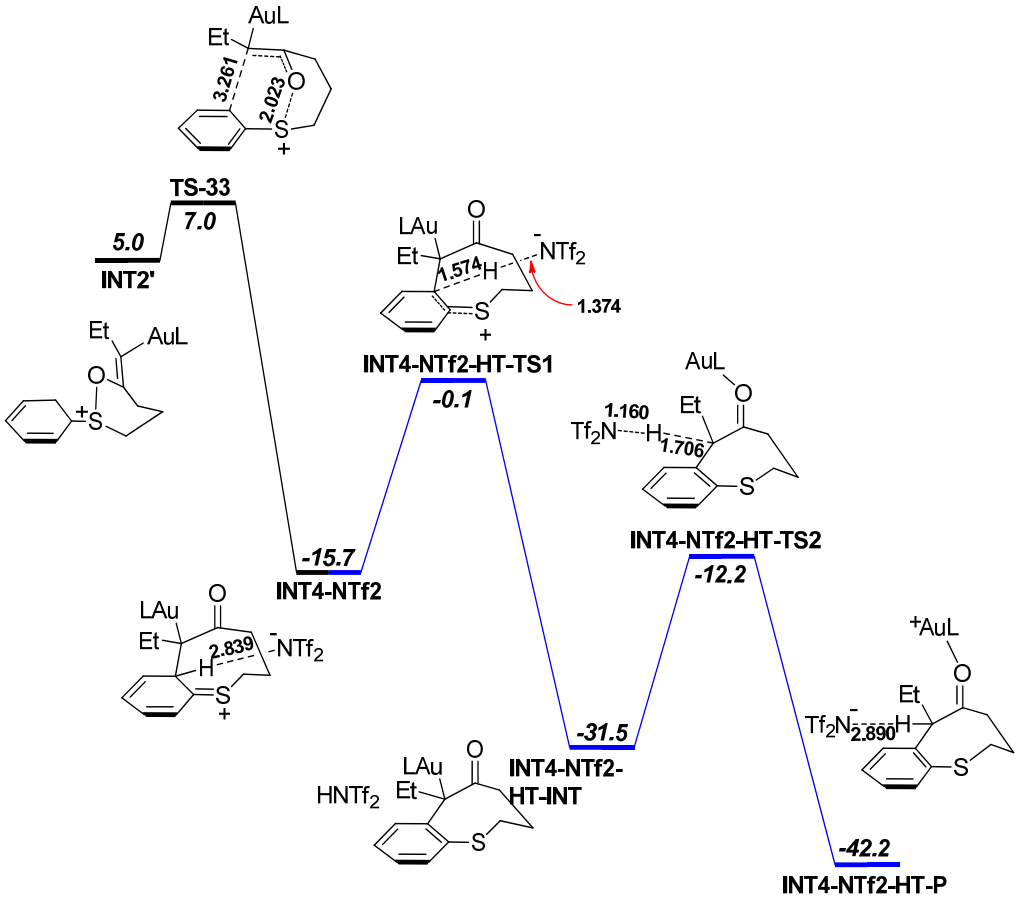


Figure S2. The optimized structures on the reaction pathway ***Path-b1*** and ***Path-b2*** in Scheme 13 in the main text. The α-oxo gold carbene in triplet state **INT3-*Triplet*** was also calculated. The red numbers are Mulliken atomic spin densities with absolute value larger than 0.100.

TS-6-*exo-dig*'' ** can lead to **INT2' directly. However, its energy is much higher (15.0 kcal/mol).

2. *The counterion-assisted 1,2 H transfer of INT4: a deprotonation/protonation process.*

The calculated reaction pathways of the 1,2 H transfer assisted by the NTf_2^- anion of **INT4** are shown in Scheme S1. The barriers of the first and the second steps are 15.6 and 19.3 kcal/mol, respectively.



Scheme S1. The reaction pathway of the counterion-assisted 1,2 H transfer of **INT4**.

Scheme S1 shows that **TS-33** (7.0 kcal/mol) is much higher in energy than **INT4-NTf2-HT-TS1** (-0.1 kcal/mol) and **NT4-NTf2-HT-TS2** (-12.2 kcal/mol). Therefore, the 3,3 rearrangement step is irreversible. In **TS-33**, the H(D) is attached to a carbon center that undergoes rehybridization from sp^2 to sp^3. Therefore an inverse KIE is expected. This is consistent with the experimental results. (Shapiro, N. D.; Toste, F. D. *J. Am. Chem. Soc.* **2007**, *129*, 4160-4161.).

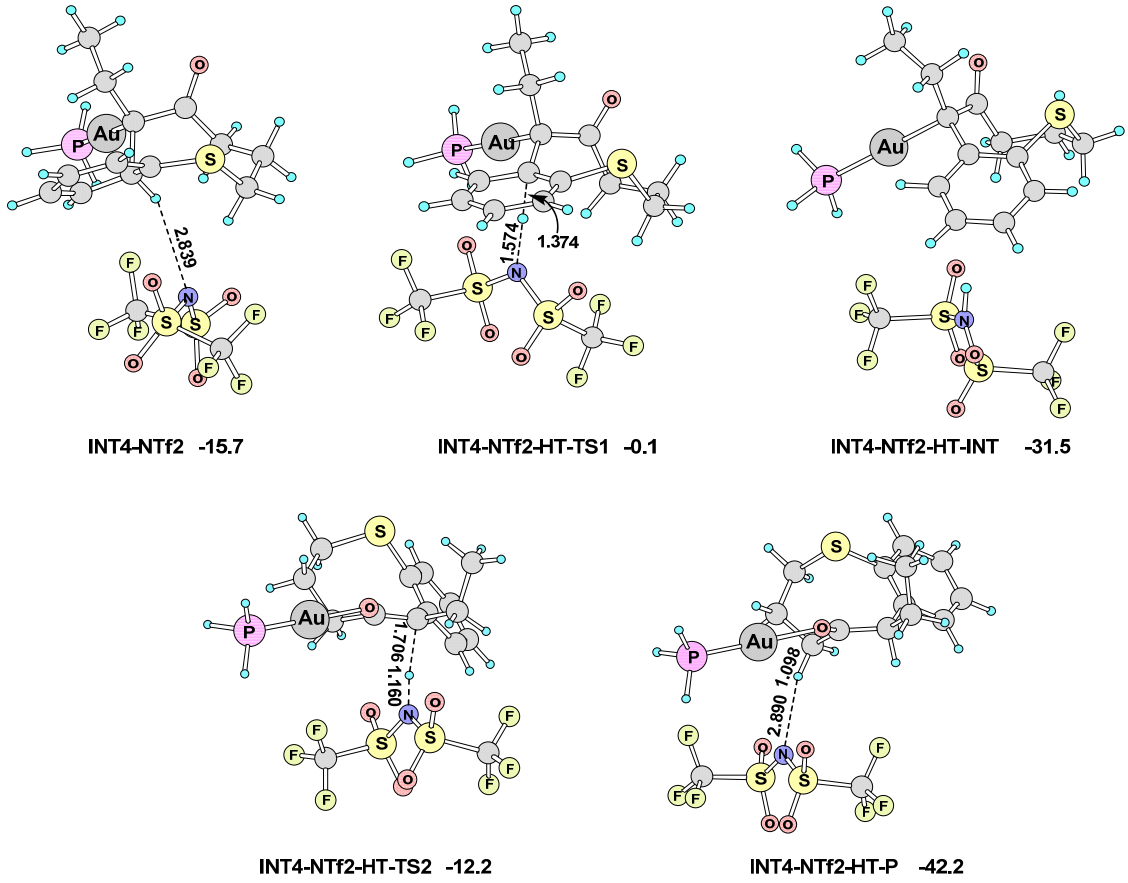


Figure S3. The optimized structures of the counterion-assisted 1,2 H transfer of **INT4**.

3. *The structure of the α-oxo gold carbene.*

As shown in Figure S4, for **INT3**, the singlet state is stable than the triplet state by more than 22 kcal/mol. For the triplet state **INT3-*Triplet***, the spin densities are mainly distributed on Au, C1 and O atoms. However, in **INT3-*Triplet-Syn***, there is nearly one spin distribute on the "PhS" tail, and the spin density on Au atom becomes very small. Obviously, it is no longer a carbene, but a diradical (also see Figure S5).

In **INT3-*Singlet***, the carbonyl group (C2-O) is nearly perpendicular to the C3-C1-Au plane. If we fix the dihedral angle D(O-C2-C1-Au) to 180.0 or 0.0 degree (i.e., confine the carbonyl and the C1-Au bond in the same plane) then do optimization, one of the hydrogen atoms on C3 will shift to C1. This indicates that, to some extent the carbonyl oxygen atom can stabilize the positive charge on C1, i.e., there are some electronic effects between the carbonyl oxygen atom and C1. The angle O-C2-C1 is 109.4 degree, smaller than angle O-C2-C4 (126.7) and C1-C2-C4 (123.8), indicating that the carbonyl oxygen atom becomes closer to C1. The lone pair of the carbonyl oxygen atom may to some extent fill in the empty *p* orbital on C1. The calculated Wiberg bond index of O-C1 is 0.2112. As shown in Figure S6, B3LYP and M06 methods produce similar results with PBE1PBE.

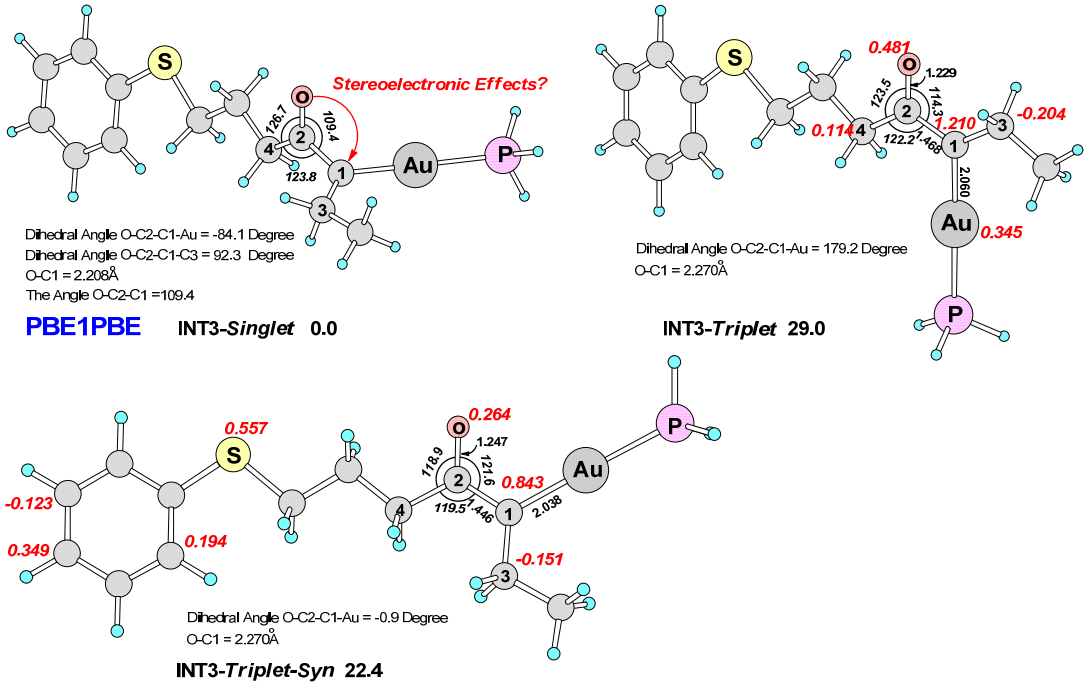


Figure S4. The optimized singlet and triplet states of **INT3**. The red numbers are Mulliken atomic spin densities with absolute value larger than 0.100.

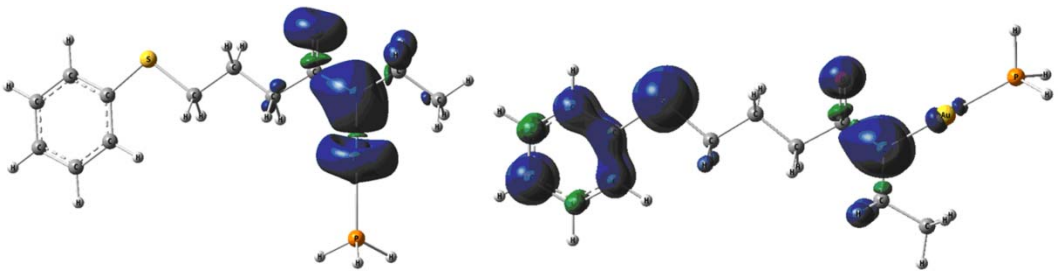
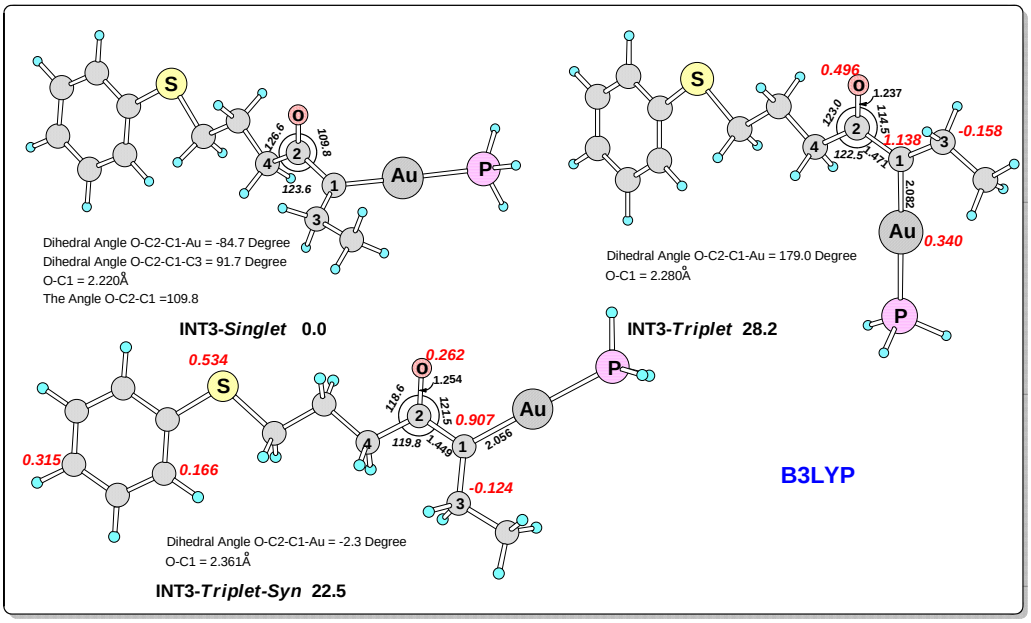


Figure S5. The Mulliken atomic spin densities of **INT3-*Triplet*** and **INT3-*Triplet-Syn***. The distribution of the spin densities is very different.



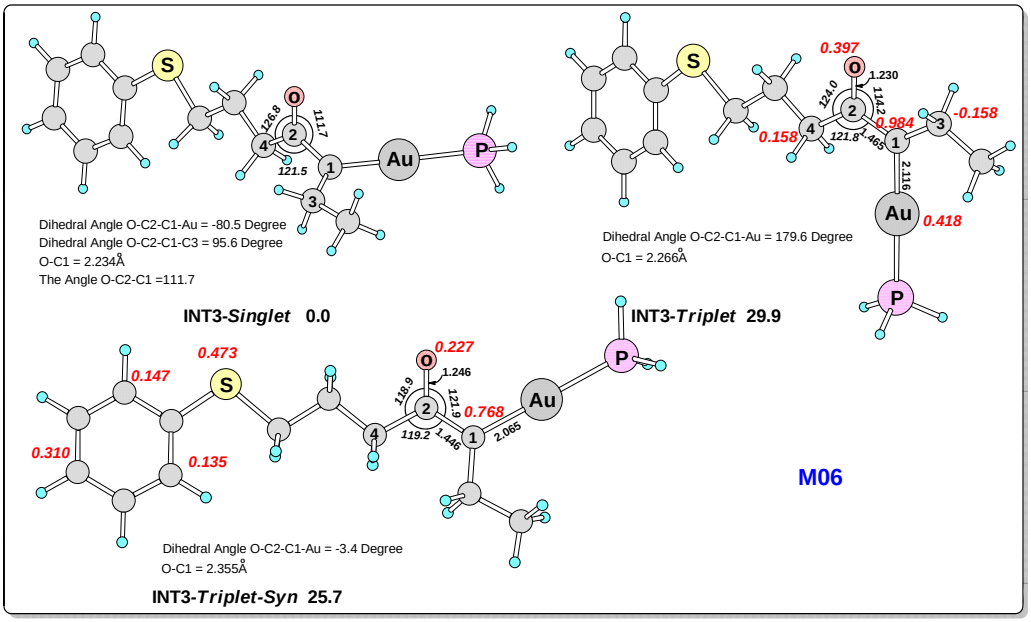


Figure S6. The optimized *singlet* and *triplet* states of **INT3** with B3LYP and M06 functionals. Calculated in DCM using SMD method at 6-31+G**/SDD level. The red numbers are Mulliken atomic spin densities with absolute value larger than 0.100.

Then the *singlet* and *triplet* states of α-oxo gold carbene structure with a terminal H group were studied. As shown in Figure S7, interestingly, for the *singlet* state the angle O-C2-C1 decrease dramatically to 84.8 degree, and the O-C1 distance decrease to 1.803Å, the calculated Wiberg bond index of O-C1 increase to 0.6154.

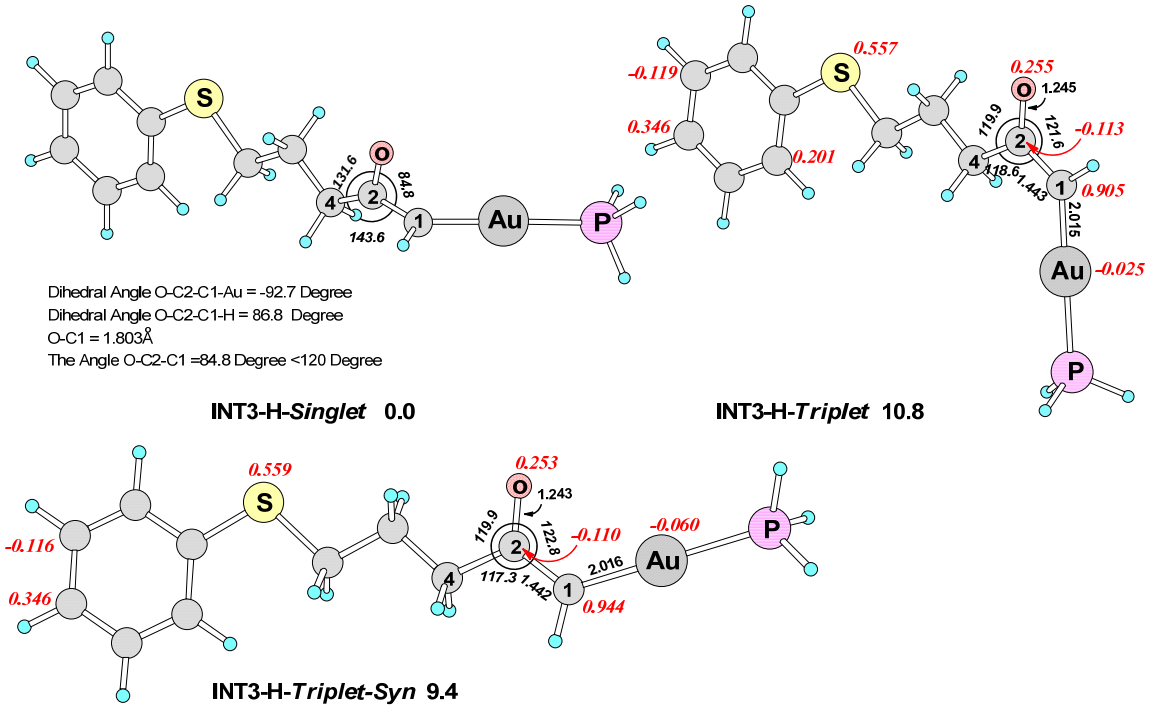


Figure S7. The optimized singlet and triplet states of α-oxo gold carbene structures with terminal H group. The red numbers are Mulliken atomic spin densities with absolute value larger than 0.100.

Without the electronic donating ethyl group, the lone pair of the carbonyl oxygen atom has strong interaction with C1. The energy difference between *singlet* and *triplet* states decrease to 9.4 kcal/mol. However, we failed to locate the *triplet* carbene. The *triplet* states located here are both diradicals with nearly one spin distributing on the "PhS" tail (Figure S7 and S8).

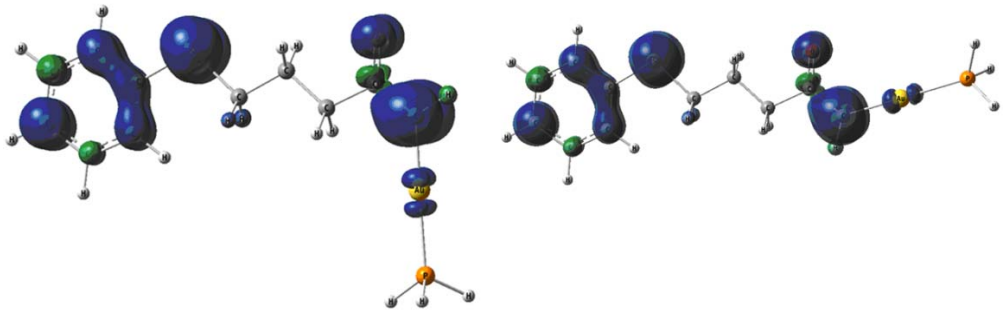
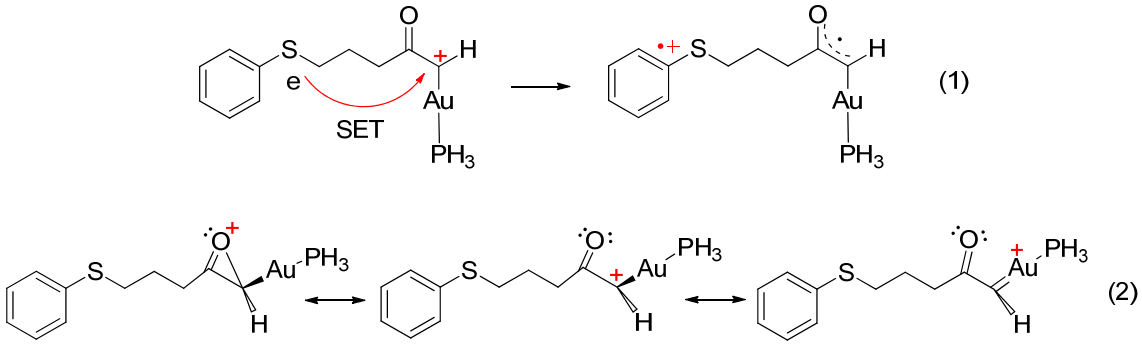


Figure S8. The Mulliken atomic spin densities of **INT3-H-*Triplet*** and **INT3-H-*Triplet-Syn***. They are both diradicals.

It seems that the stability of the *triplet* state has something to do with the "PhS" tail. Thus, as shown in Scheme S2-eq(1), the structure of **INT3-H-*Triplet*** can be understood this way: an intramolecular single electronic transfer (SET) happened between the electron rich PhS tail and the electron deficient carbocation, leading to a diradical structure rather than "a *triplet* state carbene". The total NBO charges on the "PhS" tail in the *triplet* state carbene **INT3-*Triplet*** is only +0.071, whereas in **INT3-H-*Triplet***, it is +0.966, strongly supporting the proposed SET process. It seems that the SET process is easier for unstable oxo carbene with an electronic rich "tail". The structure of the singlet state carbene **INT3-H-*Singlet*** can be rationalized by the resonance structures shown in Scheme S2-eq(2). The strong interaction between the lone pair of the carbonyl oxygen atom and the empty *p* orbital of the carbocation is supported by the molecular orbital analysis (Figure S9).



Scheme S2. The structures of **INT3-H-*Triplet*** and **INT3-H-*Singlet***.

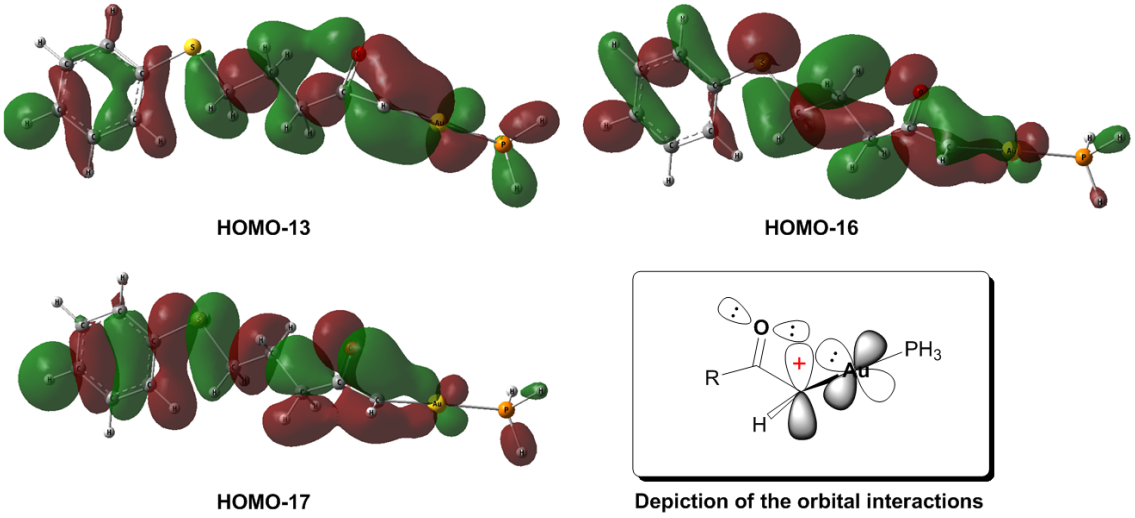


Figure S9. The selected molecular orbitals and the depiction of the orbital interactions in the singlet state α-oxo gold carbene **INT3-H-*Singlet***.

To further clarify the effect of the “PhS” tail, models without the "PhS" tail in which SET cannot happen were also calculated (Figure S10). The spin density distribution and the energy difference of **INT3-NoTail-*Singlet*** and **INT3-NoTail-*Triplet*/ INT3-NoTail-*Triplet-Syn*** are similar with that of **INT3-*Singlet*** and **INT3-*Triplet***. The structure of **INT3-NoTail-H-*Singlet*** is similar with **INT3-H-*Singlet***. However, the relative energy of **INT3-NoTail-H-*Triplet*** increases to 21.2 kcal/mol, and the spin densities are distributed mainly on Au, C1, and O atoms, which is very different from that of the diradical **INT3-H-*Triplet***.

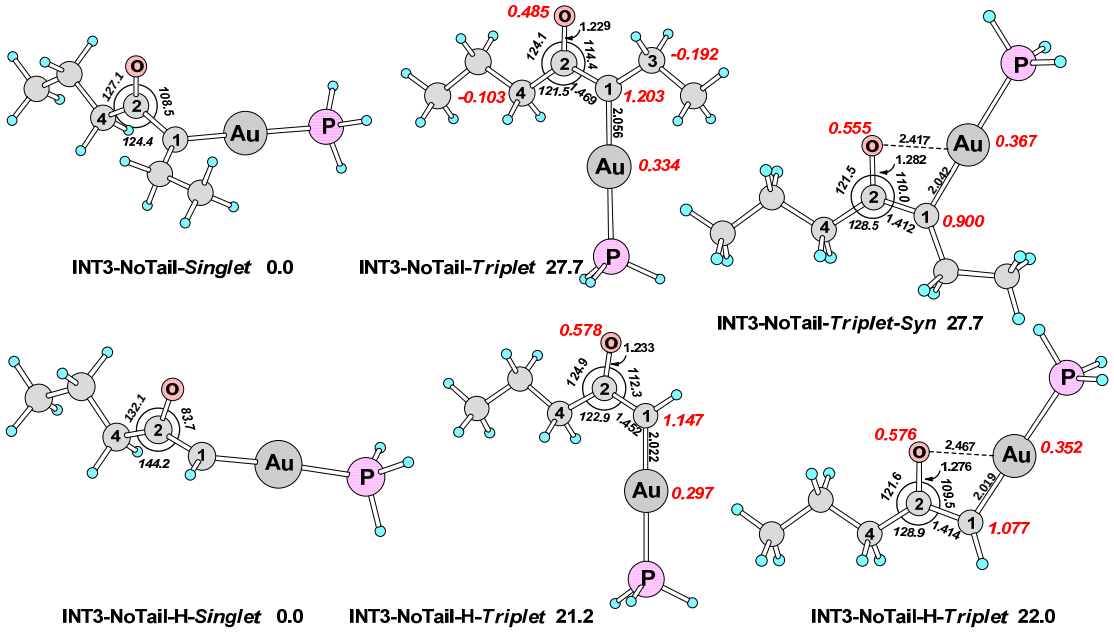


Figure S10. The optimized singlet and triplet states of α-oxo gold carbene structures without the "PhS" tail. The red numbers are Mulliken atomic spin densities with absolute value larger than 0.100.

Based on the calculations above, for the α-oxo gold carbene studied in this paper the singlet state is the ground state.

3. *The relaxed potential energy surface scan for TS-OS-Hg.*

We failed to locate the O-S bond breaking transition state **TS-OS-Hg**. Then a relaxed potential energy surface scan along the O-S bond has been done by a step size of 0.005Å (Figure S11). The energy of the highest point on the PES is used to estimate the energy of the transition state **TS-OS-Hg** approximately. As shown in Figure S11, the O-S bond breaking is accompanied by a hydrogen shift from C3 to C1, indicating that Hg cannot stabilize the newly formed carbocation.

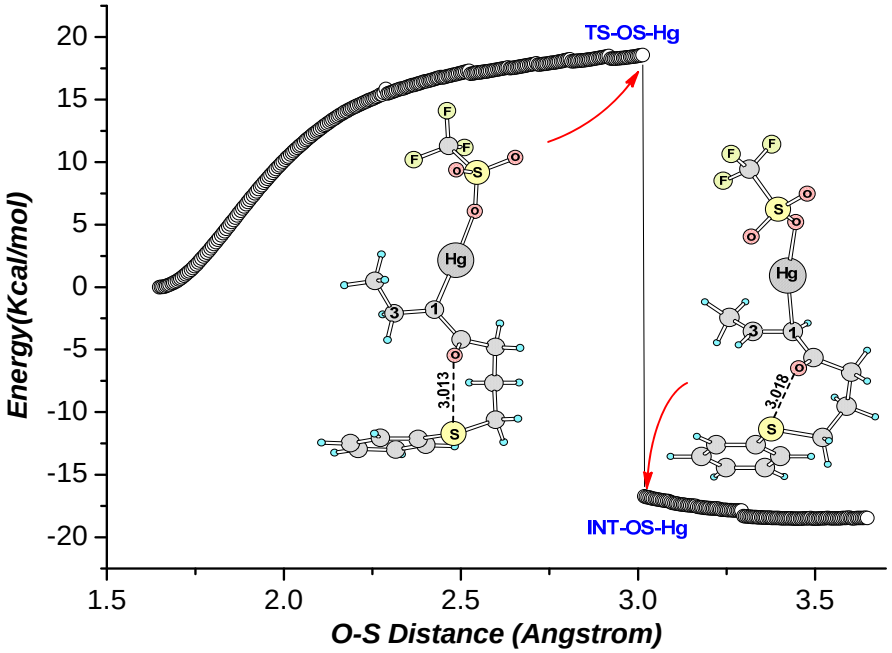


Figure S11. Relaxed potential energy surface scan along the O-S bond. The relative energies including solvent effect ΔE_{sol}(298K) are in kcal/mol. Calculated in DCM using SMD method at PBE1PBE/6-31+G**/SDD level.

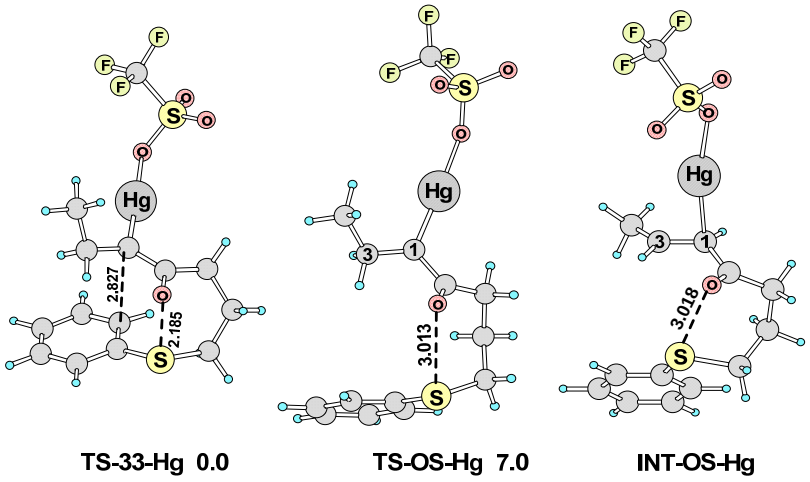
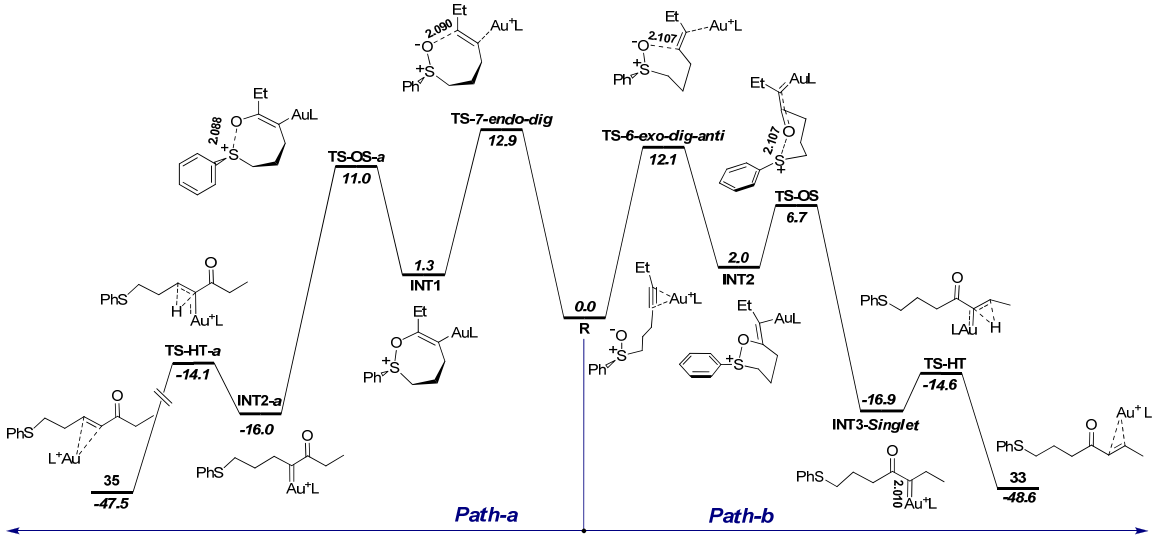


Figure S12. The [3, 3]-sigmatropic rearrangement transition state **TS-33-Hg**, the highest point of the relaxed potential energy surface scan (**TS-OS-Hg**) and the intermediate structure **INT-OS-Hg**. The selected bond lengths are in angstroms, the relative energies including solvent effect ΔE_{sol}(298K) are in kcal/mol. Calculated in DCM using SMD method at PBE1PBE/6-31+G**/SDD level.

The results show that **TS-33-Hg** is much favorable than **TS-OS-Hg** (7.0 kcal/mol, ΔE_{sol}), indicating that the cyclization product **15** is dominant.

4. *Calculations to confirm that the initial cyclization steps are irreversible and determining the selectivity of Path-a and Path-b.*

The S-O bond breaking and the subsequent 1,2 H-shift processes were calculated from **INT1** along ***Path-a***. As shown in Scheme S3, along ***Path-a***, the subsequent transition states are all lower in energy than **TS-7-*endo-dig***. In addition, the overall reaction is irreversible due to the formation of the stable intermediates. A [3,3]-sigmatropic rearrangement transition state cannot be located due to the confine of the 7-memered ring in **INT1**. Along ***Path-b***, the subsequent transition states (along ***Path-b1*** and ***Path-b2***) are all lower in energy than **TS-6-*exo-dig-anti*** (also see Scheme 13 in the main text). Therefore, the cyclization transition states **TS-7-*endo-dig*** and **TS-6-*exo-dig-anti*** are ***irreversible*** and thus determining the selectivity of ***Path-a*** and ***Path-b***. In the experiments, the product ratio of **35**:(**32**+**33**) is 1:32.4. Therefore, the energy difference between **TS-7-*endo-dig*** and **TS-6-*exo-dig-anti*** could be expected to be about 2.0 kcal/mol at room temperature. Thus we think the smaller energy difference of 0.8 kcal/mol between **TS-7-*endo-dig*** and **TS-6-*exo-dig-anti*** may be caused by inaccuracies of the calculation.



Scheme S3. The calculated reaction pathways of the 7-*endo-dig* (***Path-a***) and 6-*exo-dig* cyclization (***Path-b***) of the reactant complex **R**; The selected bond lengths are in angstroms, and the relative free energies in dichloromethane (ΔG^{o}_{sol}) are in kcal/mol. Calculated at the PBE1PBE/6-31+G**/SDD level.

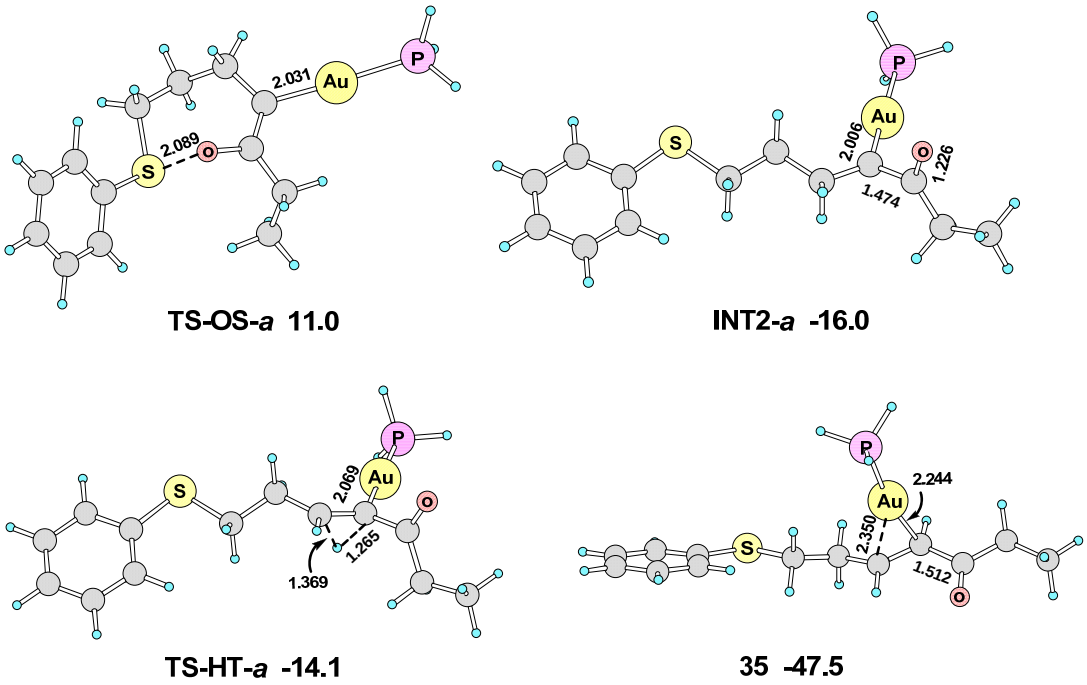
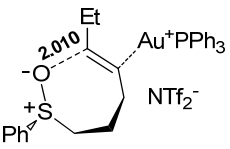
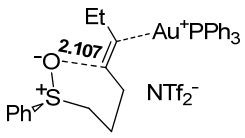


Figure S13. The calculated structures on ***Path-a***. The selected bond lengths are in angstroms, the relative energies including solvent effect ΔE_{sol}(298K) are in kcal/mol. Calculated in DCM using SMD method at PBE1PBE/6-31+G**/SDD level.

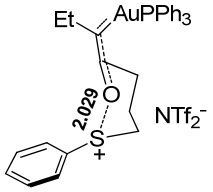
Based on the considerations above, **TS-7-*endo-dig*** and **TS-6-*exo-dig-anti*** were recalculated using full models with the PPh_3 ligand, the counter anion NTf_2^-, and a larger basis set (6-311+G** for C, H, O, N, P, F, and S). As shown in Scheme 4 and Figure S14, the energy difference increased to 1.3 kcal/mol. Under the same calculation conditions, the energy difference between **TS-OS** and **TS-33** remained small (0.2 kcal/mol) [compar with Scheme 13B of the main text].



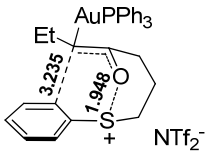
PPh_3-NTf_2-TS-*7-endo-dig*
1.3



PPh_3-NTf_2-TS-*6-exo-dig-anti*
0.0



PPh_3-NTf_2-TS-OS
0.2



PPh_3-NTf_2-TS-33
0.0

Scheme S4. Full model calculation of transition states **TS-7-*endo-dig***, **TS-6-*exo-dig-anti***, **TS-OS** and **TS-33**. The selected bond lengths are in angstroms, and the relative free energies in dichloromethane ($\Delta G^{o}s_{ol}$) are in kcal/mol. Calculated at the PBE1PBE/6-311+G**/SDD level.

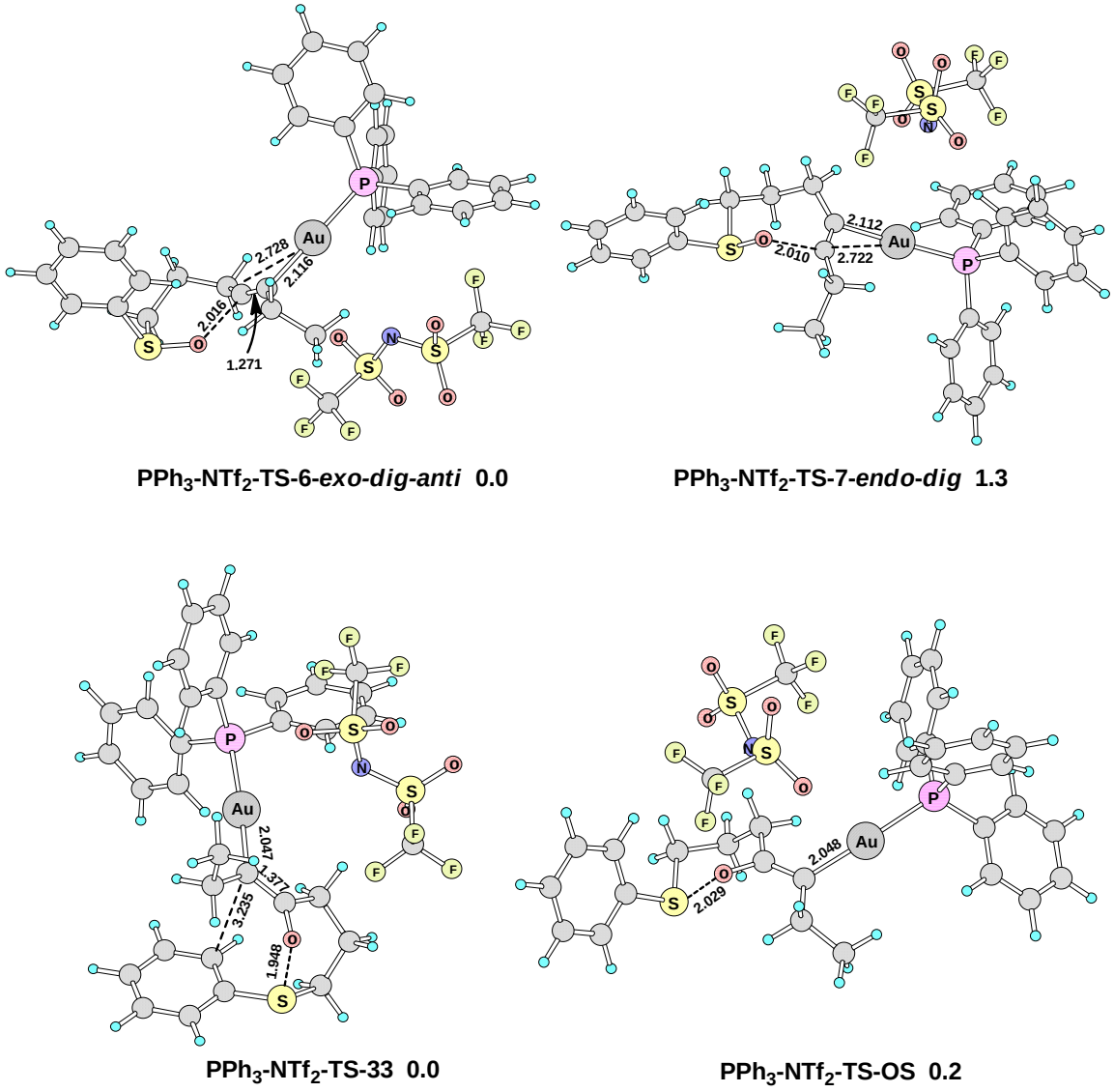
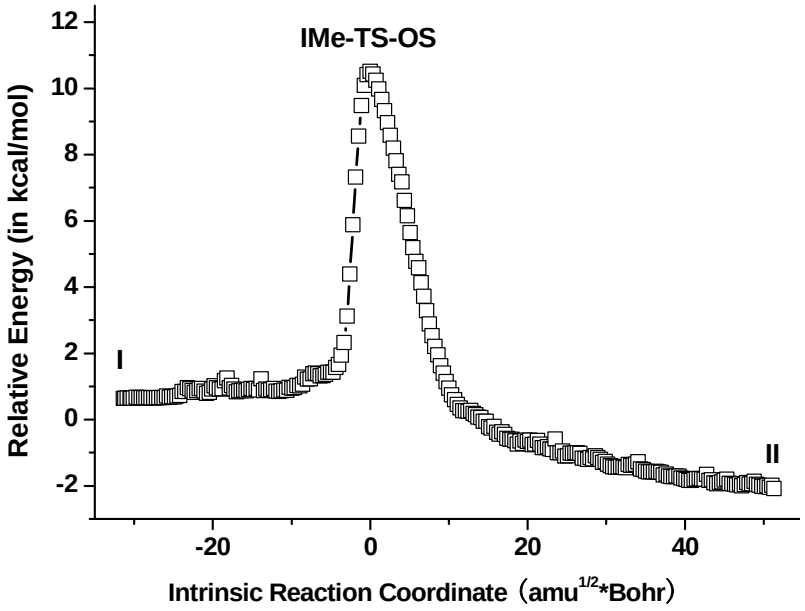


Figure S14. Calculated full models of transition states **TS-7-*endo-dig***, **TS-6-*exo-dig-anti***, **TS-33** and **TS-OS**. The selected bond lengths are in angstroms, and the relative free energies in dichloromethane (ΔG^{o}_{sol}) are in kcal/mol. Calculated at the PBE1PBE/6-311+G**/SDD level.

5. ***The intrinsic reaction coordinate (IRC) calculations of IMe-TS-OS and IMe-TS-33.***

The results show that these transition states connect with the expected reactants and products.



Scheme S5. IRC calculation of transition state **IMe-TS-OS**.

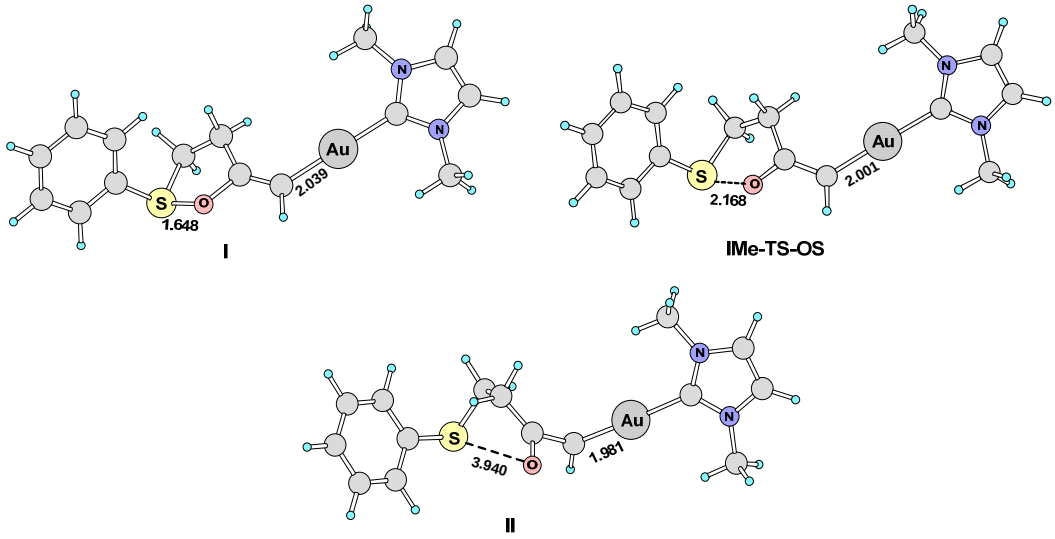
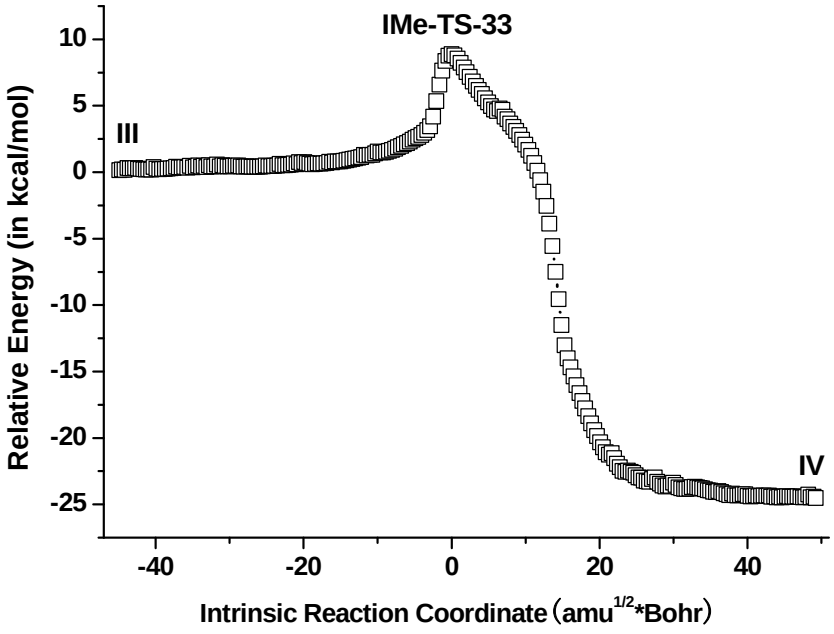


Figure S15. The structures of **I**, **IMe-TS-OS** and **II** shown in Figure S5. The selected bond lengths are in angstroms.



Scheme S6. IRC calculation of transition state **IMe-TS-33**.

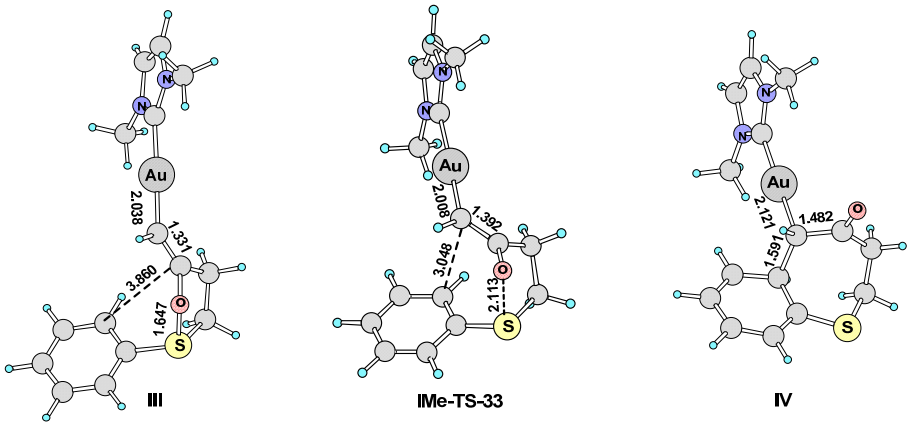


Figure S16. The structures of **III**, **IMe-TS-33** and **IV** shown in Figure S6. The selected bond lengths are in angstroms.

6. ***Calculated total energies and geometry coordinates. Calculated in DCM using SMD method at PBE1PBE/6-31+G**/SDD level. For the calculation of NHC ligand models and the full models using PPh3 ligand, keywords int(ultrafine, acc2e=11) were used to obtain more accurate values.***

6.1 The structures shown in Figure S1, Figure S2 and Figure S4(including all structures shown in Scheme 13 in the main text.

R
SCF Done: E(RPBE1PBE) = -1456.16835747 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.95
Sum of electronic and thermal Free Energies= -1455.937843 A.U.

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C,0,-2.0723296103,1.7342670194,0.1457246844
C,0,5.3343990112,-1.3890948025,-0.1748452312
C,0,5.0523827144,-0.096779185,0.2562682336
H,0,1.0932292762,2.3621394091,-1.0372483819
H,0,3.4187984625,1.9785126694,-0.6595874941
H,0,1.2614920234,2.1596487582,0.7022867923
H,0,2.8099366603,0.4540063911,-1.3516788269
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H,0,0.5077323208,-0.2602428005,0.449914653
H,0,0.3063108148,0.0078443657,-1.2765839736
C,0,-1.0686914041,1.0388680259,-0.066342446
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O,0,2.6918284498,-1.0852199096,1.0511693993
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C,0,7.2767948771,0.6213745974,-0.2971807203
C,0,7.5699845895,-0.6672496673,-0.7482239824
C,0,6.6029806188,-1.6701842879,-0.6830167787
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H,0,8.0344424179,1.3993227373,-0.3358950256
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Au,0,-2.7977614335,-0.3888175287,-0.0075066502
P,0,-4.0516617023,-2.3147044851,-0.0285582337
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H,0,-4.2791848673,-2.9082846349,-1.2810389659
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C,0,-3.038761482,2.810781687,0.4027243052
H,0,-3.7726849321,2.8345859736,-0.4104228954
H,0,-3.5897641113,2.5850465451,1.3221861071
C,0,-2.3335242346,4.1639081774,0.5238621761
H,0,-1.8013932051,4.415779007,-0.3981687348
H,0,-3.0769958716,4.943440401,0.714929688
H,0,-1.6163766505,4.1626328814,1.3499123894

R'
SCF Done: E(RPBE1PBE) = -1456.16737915 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.18
Sum of electronic and thermal Free Energies= -1455.936271 A.U.

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C,0,2.6099233698,-1.6996660596,-0.1979077965
H,0,-1.7580754825,-3.7835009129,-0.202790803
H,0,0.5849773501,-3.5506959151,-0.5531604804
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C,0,-2.2758719705,-1.8148541313,0.5031531707
H,0,-1.9791296271,-0.7712136497,0.3445978075
H,0,-2.0900449969,-2.027172521,1.5642148349
C,0,-3.7015045771,-1.9614578065,0.2190340294
S,0,0.922172289,-1.2386016762,-0.5583575774
O,0,0.5394359728,-0.2000560852,0.5557516998
C,0,3.4138707246,-2.1018493913,-1.2638397516
C,0,4.7280161994,-2.486098687,-1.000922164
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H,0,5.3682296939,-2.8038231625,-1.818718171
H,0,6.2466878611,-2.741161866,0.5020221706
H,0,4.793528835,-1.9906959701,2.3685549179
Au,0,0.210187299,1.8265423514,0.0948055463
P,0,-0.1844392473,3.9941139732,-0.3151550966
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H,0,0.7362023739,4.6321485847,-1.1624462609
C,0,-6.3087051679,-2.2488189285,-0.3148628289
H,0,-6.4549230903,-2.2795655943,-1.4020427521
H,0,-6.650605956,-3.2189577708,0.0674230895
C,0,-7.1608471309,-1.1291787343,0.2876341438
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H,0,-7.0622714779,-1.1031067212,1.3774185005

R''

SCF Done: E(RPBE1PBE) = -1456.16900048 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.99
Sum of electronic and thermal Free Energies= -1455.934117 A.U.

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C,0,5.6660357284,-1.3762720759,-0.3779934915
C,0,5.1336536396,-0.2117403892,0.1645637723
H,0,1.1427115293,2.0613230775,-1.3325638224
H,0,3.4745820971,1.7508175604,-0.7515735834
H,0,1.290411514,1.9398396209,0.4154349425
H,0,2.9216009893,0.30459801,-1.636135251
H,0,5.0226704904,-2.2377287572,-0.5324805002
C,0,0.2848307996,0.2758363386,-0.4782342503
H,0,-0.6942718304,0.757544578,-0.3680216765
H,0,0.4169491367,-0.3745612046,0.392350665
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S,0,3.3922196403,-0.1815309578,0.6316974537
O,0,2.8323289988,-1.5785586882,0.3460804451
C,0,5.9298700505,0.9058333952,0.4191054736
C,0,7.2822301521,0.8583245569,0.0881257386
C,0,7.8280812594,-0.2981798982,-0.4727357453
C,0,7.02294206,-1.4131664833,-0.7015151181
H,0,5.5107479415,1.8017026043,0.8718015199
H,0,7.9117917633,1.7232621441,0.2777848716
H,0,8.885089668,-0.3318127178,-0.7218594453
H,0,7.450672798,-2.3165058717,-1.1279220772
Au,0,1.6020025822,-2.2742066256,-1.9600085151
P,0,2.969998849,-4.1272302223,-2.1715286183
H,0,2.4257564634,-5.2467269854,-2.8231394367
H,0,4.1783717353,-3.9549860428,-2.86834949
H,0,3.4144916154,-4.6875534968,-0.961396346
C,0,-0.7057529728,-1.3940419548,-4.0751216753
H,0,0.0560179619,-1.3448191302,-4.8608907412
H,0,-1.0568413098,-2.4311322752,-4.0409040078
C,0,-1.865342076,-0.4477121516,-4.3934904555
H,0,-1.5239106558,0.5895369638,-4.4596436981
H,0,-2.3060117384,-0.7255856694,-5.3555937453
H,0,-2.6455657498,-0.5081112591,-3.6290328979

TS-7*-endo-dig*
SCF Done: E(RPBE1PBE) = -1456.15164257 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.67
Sum of electronic and thermal Free Energies= -1455.917270 A.U.

C,0,0.8806374775,-2.2433786479,-0.6591655481
C,0,2.3185533862,-1.8198247761,-0.3928701977
C,0,-0.1979117007,0.7393045227,0.4044138599
C,0,4.740800029,0.034921911,1.1627171528
C,0,4.3276223992,0.0363072736,-0.168411802
H,0,4.0063145355,0.0009246505,1.9624429202

C,0,-0.1522713744,-1.8517219574,0.4080410655
C,0,-0.6609437127,-0.4437585787,0.3319085952
S,0,2.5799168998,-0.0318965601,-0.5574157077
O,0,1.8713960593,0.6010630118,0.6657942184
C,0,5.23726766,0.1197562993,-1.2215138161
C,0,6.5997015839,0.1734093945,-0.9285000884
C,0,7.0305935681,0.1616872293,0.3978448604
C,0,6.1042487089,0.0965643873,1.4405096775
H,0,4.8938100891,0.1464802499,-2.2527291664
H,0,7.3217447745,0.2368625195,-1.7376707882
H,0,8.0926891371,0.2120724841,0.6214941492
H,0,6.4428966016,0.09765932,2.4727809058
Au,0,-2.7228229397,-0.0865291761,0.045265308
P,0,-4.9976322193,0.1005996706,-0.245758085
H,0,-5.5737181414,1.348973368,0.0483246184
H,0,-5.4925107189,-0.1397540851,-1.5394669607
H,0,-5.7940231366,-0.7641367225,0.5249811869
C,0,-0.2298960192,2.2028908476,0.4786297375
H,0,-1.259394224,2.4770532343,0.7405387852
H,0,0.3984258955,2.5093565408,1.322076303
C,0,0.198410007,2.9199733931,-0.7992430384
H,0,1.2392665643,2.6973358259,-1.0484244541
H,0,-0.4321659351,2.6302059349,-1.6456721475
H,0,0.1087855512,4.0015207411,-0.6595030127
H,0,-0.9947234104,-2.5419879433,0.3279954816
H,0,0.277006039,-1.997970286,1.4078478614
H,0,2.994436326,-2.2774610131,-1.1249112189
H,0,2.6511934523,-2.0954268555,0.6148683215
H,0,0.5546906219,-1.9010965065,-1.6485003963
H,0,0.9006443474,-3.3385956183,-0.7039860232

TS-7-*endo-dig*'

SCF Done: E(RPBE1PBE) = -1456.15009859 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.54
Sum of electronic and thermal Free Energies= -1455.913867 A.U.

C,0,-1.5939548581,-1.1452835149,1.8495893536
C,0,-2.5011963289,-0.0250481594,2.3336105884
C,0,-0.0638240633,1.0253480183,-0.1003100922
C,0,-3.2692760611,-0.0999044821,-1.3576489637
C,0,-3.835966227,0.0568924997,-0.0967527878
H,0,-2.3489635446,0.4166255814,-1.609704644
C,0,-0.1043034612,-0.8044583131,1.7609103714
C,0,0.3383370506,0.0457756652,0.6139190622
S,0,-3.0790483796,1.1678738253,1.0966915676
O,0,-1.8394240281,1.7931866549,0.4209711824

C,0,-5.0341421997,-0.5703661369,0.2496401791
C,0,-5.6529921615,-1.399858194,-0.6824767392
C,0,-5.0887654749,-1.579718865,-1.9467431578
C,0,-3.903733912,-0.9280327338,-2.2838804408
H,0,-5.4850393222,-0.4194372103,1.2276773662
H,0,-6.5828068632,-1.8977688364,-0.4225210643
H,0,-5.5795736456,-2.2227509637,-2.6719708489
H,0,-3.4681564748,-1.0604397282,-3.2703248949
Au,0,2.3010214304,-0.3026301872,-0.0997704086
P,0,4.4519168213,-0.8264647096,-0.7241680837
H,0,4.8582302419,-0.4228520696,-2.0081608238
H,0,5.48423326,-0.3030604981,0.0737644771
H,0,4.7790873876,-2.1934364363,-0.7432413927
C,0,0.141810189,2.0408373194,-1.1490779148
H,0,0.9218772246,1.6507855692,-1.8129244952
H,0,-0.7687759508,2.1210820222,-1.7508125157
C,0,0.5453046946,3.4121878306,-0.6095225453
H,0,-0.2262173162,3.814971497,0.0514575351
H,0,1.4851350682,3.3517288641,-0.0514701253
H,0,0.6846355826,4.1098455758,-1.4413722829
H,0,0.2177891376,-0.3058496962,2.685568401
H,0,0.4462129179,-1.7490449539,1.7297266329
H,0,-2.0271049633,0.5929007788,3.1052897715
H,0,-3.4312542469,-0.4196691576,2.761862687
H,0,-1.6950225429,-1.957203327,2.5798101849
H,0,-1.9497611217,-1.5503518554,0.8956607546

INT1

SCF Done: E(RPBE1PBE) = -1456.17538388 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.56
Sum of electronic and thermal Free Energies= -1455.935802 A.U.

C,0,-0.6908480437,-2.3637149474,0.7995054643
C,0,-2.161874422,-2.0028074505,0.6486545539
C,0,-0.2279111014,0.5374877234,-0.5293701665
C,0,-4.6379076152,-0.6186809454,-0.9427401901
C,0,-4.0933294228,-0.0111144663,0.1932175922
H,0,-4.034278456,-1.2379926942,-1.5992770486
C,0,0.2037251611,-1.9141445487,-0.3628635648
C,0,0.6485195112,-0.4597671604,-0.3452470981
S,0,-2.399640884,-0.2162288621,0.6423663896
O,0,-1.6311572956,0.2139893984,-0.7375605297
C,0,-4.852145974,0.8056568096,1.0359753631
C,0,-6.1988814507,1.0015878804,0.7391862151
C,0,-6.7577267767,0.403288764,-0.3885609727
C,0,-5.9802180566,-0.3986028733,-1.2283459889

H,0,-4.4041868473,1.2779087229,1.9060691916
H,0,-6.8051883566,1.6280477514,1.386276632
H,0,-7.8068449363,0.5642247251,-0.6200965843
H,0,-6.4215652503,-0.8554033888,-2.1090911095
Au,0,2.6435205252,-0.0529383769,-0.0747182494
P,0,4.9157223821,0.3413609321,0.2403839189
H,0,5.4363660365,1.55740713,-0.2402719117
H,0,5.3916930033,0.3641800999,1.5648628975
H,0,5.8161612536,-0.5715624608,-0.3403041938
C,0,-0.0197593412,2.0126643781,-0.6537365065
H,0,1.0603111477,2.1917303598,-0.6439282628
H,0,-0.3875944517,2.3332014638,-1.6390272247
C,0,-0.6999184045,2.8484523744,0.4301642893
H,0,-1.7909945373,2.7517737865,0.3985748726
H,0,-0.3572750806,2.5596307474,1.4300158915
H,0,-0.4694740929,3.9092371969,0.2870626718
H,0,1.0886941577,-2.5548575735,-0.3583617097
H,0,-0.3183208387,-2.1224853386,-1.3092451016
H,0,-2.7628464864,-2.3575139271,1.4949522935
H,0,-2.5862655935,-2.3935684122,-0.281517183
H,0,-0.2997820834,-1.9917996593,1.7539435585
H,0,-0.6742870437,-3.4583713066,0.858330298

TS-6-*exo-dig-anti*
SCF Done: E(RPBE1PBE) = -1456.15317824 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.54
Sum of electronic and thermal Free Energies= -1455.918607 A.U.

C,0,-1.7054553593,-1.7933516129,-1.5128158153
C,0,-2.9362690724,-2.3146828157,-0.7946595968
C,0,0.527317389,-0.0758682925,0.9532228753
C,0,-3.0365392807,1.2743068255,0.13136648
C,0,-3.8549974591,0.151348573,0.0637910574
H,0,-2.045562781,1.1991625477,0.5669879583
C,0,-0.3999149114,-1.9580306577,-0.7196021279
C,0,-0.1381998348,-0.9416665198,0.3013068916
S,0,-3.3010397377,-1.4187954363,0.7457647429
O,0,-1.9228246487,-1.1798720458,1.394897611
C,0,-5.146177791,0.2173336806,-0.462178113
C,0,-5.608460472,1.432168912,-0.9625338127
C,0,-4.7933168998,2.5647851196,-0.9170156564
C,0,-3.5144007797,2.4864777043,-0.3677994773
H,0,-5.7885491729,-0.6603934709,-0.4814895374
H,0,-6.6104153167,1.4950304562,-1.377488457
H,0,-5.1613124853,3.5118400328,-1.3016473985
H,0,-2.8838679846,3.3701495247,-0.3239055894

Au,0,2.3230260392,0.1265344201,-0.1434225287
P,0,4.3348140445,0.4801201444,-1.2074674411
H,0,5.3383993638,1.0880078317,-0.4335013758
H,0,5.0055676357,-0.6554897208,-1.6939032199
H,0,4.3194169561,1.3066614718,-2.344704038
C,0,0.3369016848,0.7361174046,2.1962051308
H,0,0.374729192,1.7983920391,1.9282568047
H,0,-0.6635131992,0.5266861239,2.5869740595
C,0,1.3929984722,0.4456628026,3.2601559157
H,0,1.375256076,-0.6077970283,3.5575007438
H,0,2.3994594502,0.6791621933,2.8956473392
H,0,1.2026550923,1.0523315902,4.1515210567
H,0,-0.3637105543,-2.9513759736,-0.2544840418
H,0,0.4478693866,-1.9074749361,-1.4130827614
H,0,-2.8116670905,-3.3598774278,-0.4900096092
H,0,-3.8384480687,-2.2441795041,-1.4112661662
H,0,-1.6105499208,-2.3807333773,-2.4324147056
H,0,-1.8418645391,-0.749764346,-1.816174452

TS-6-*exo-dig-syn*

SCF Done: E(RPBE1PBE) = -1456.14177474 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.75
Sum of electronic and thermal Free Energies= -1455.906813 A.U.

C,0,-1.6505531846,-1.681715308,-1.58375283
C,0,-2.9301301562,-2.2915459582,-1.0429881395
C,0,0.4437217967,-0.0984364365,1.0902097732
C,0,-3.2962838366,1.2060508796,0.2713365857
C,0,-4.013794872,0.0696557937,-0.0890112998
H,0,-2.4012552376,1.1087300292,0.8810955043
C,0,-0.4270971218,-1.9044151768,-0.6818078572
C,0,-0.166167179,-0.9334171437,0.3570023951
S,0,-3.4882732676,-1.5418094152,0.5181418071
O,0,-2.1957216941,-1.3120771965,1.3256606718
C,0,-5.1851662637,0.1532798383,-0.8440753927
C,0,-5.6217187428,1.4044966985,-1.2727797937
C,0,-4.9045332968,2.5532855116,-0.9323255606
C,0,-3.7485621113,2.4540076081,-0.1595665807
H,0,-5.7545256439,-0.7383437398,-1.0971512227
H,0,-6.5282438986,1.4818863434,-1.8664512143
H,0,-5.2535779889,3.5270605828,-1.2646874274
H,0,-3.1949519024,3.3486562387,0.1119357613
Au,0,-0.4986134431,0.4604842076,2.8821035006
P,0,-1.3492856436,1.1521547798,4.904738199
H,0,-1.1166470199,2.4913528475,5.2634681965
H,0,-2.7422464725,1.0578595766,5.0739627762

H,0,-0.8848663921,0.4758451815,6.0464141053
C,0,1.8133911361,0.5142677726,0.827418571
H,0,2.4778246548,0.1885736922,1.6349509285
H,0,2.2183791656,0.1159492103,-0.1096407818
C,0,1.7752147781,2.0367801321,0.7756368804
H,0,1.1134232741,2.3923244903,-0.0208256082
H,0,1.420731993,2.4542816677,1.7245462434
H,0,2.7793503978,2.4283648639,0.579984117
H,0,-0.4226950468,-2.9195618234,-0.2663527825
H,0,0.4909056691,-1.8228368568,-1.291077766
H,0,-2.8039548493,-3.3560306659,-0.8160659602
H,0,-3.7624458372,-2.1912304652,-1.7471629555
H,0,-1.4518364797,-2.1730091784,-2.5420852331
H,0,-1.7829486736,-0.6152184518,-1.7942259405

TS-6-*exo-dig'*

SCF Done: E(RPBE1PBE) = -1456.15296986 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.89
Sum of electronic and thermal Free Energies= -1455.918317 A.U.

C,0,1.0726282124,-2.2596487339,-0.7036639297
C,0,2.5437027087,-1.8840795417,-0.6035052014
C,0,-0.801741801,0.7765775199,0.2948365071
C,0,4.7926917771,0.0678643548,1.1846049126
C,0,4.4430748295,0.0685094687,-0.1640365646
H,0,4.0226914343,-0.0062220859,1.9474943263
C,0,0.2032648327,-1.7097981099,0.4369764146
C,0,-0.0873396835,-0.2748669726,0.369119243
S,0,2.7233913893,-0.0780617363,-0.6400459792
O,0,1.8996004423,0.3654313975,0.5977584566
C,0,5.3955323832,0.1992904055,-1.1741056302
C,0,6.7394886455,0.301041912,-0.8173508175
C,0,7.1087597955,0.2928409788,0.5277730146
C,0,6.1386573454,0.1815193139,1.5255160747
H,0,5.1012741872,0.2234189431,-2.220769804
H,0,7.494939235,0.398748748,-1.5918101488
H,0,8.1566763269,0.3820322967,0.8006516879
H,0,6.4291848567,0.1861293878,2.5723374666
Au,0,-2.7690203887,0.0359719353,0.112405514
P,0,-4.9638807182,-0.6297654814,-0.100744915
H,0,-5.921779964,0.3988530731,-0.1174709373
H,0,-5.2985163072,-1.3429703803,-1.2654404078
H,0,-5.4765094517,-1.472787971,0.9008805179
C,0,-0.5475331897,2.2504753548,0.2986428713
H,0,-1.0799585988,2.6904221181,1.1497536476
H,0,0.5242763999,2.4024160298,0.4612411826

C,0,-0.9972507294,2.9361658842,-0.9893364206
H,0,-0.4691939783,2.5314358519,-1.8590852201
H,0,-2.0723607638,2.8063188631,-1.1552821442
H,0,-0.786921454,4.0093883015,-0.9357656431
H,0,2.9881507595,-2.2267230505,0.3372716811
H,0,3.12104346,-2.283788633,-1.4438823531
H,0,0.6571670354,-1.9396372513,1.4083776748
H,0,-0.7701644559,-2.213888042,0.4153394685
H,0,1.0224203498,-3.3529515705,-0.6655740455
H,0,0.6592639988,-1.9545077635,-1.6716394318

TS-6-*exo-dig''*
SCF Done: E(RPBE1PBE) = -1456.14925591 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.64
Sum of electronic and thermal Free Energies= -1455.914670 A.U.

C,0,-1.5170979126,-1.5023833401,-2.2215958928
C,0,-3.0126343138,-1.5054129956,-1.9517316457
C,0,0.5687460742,-0.7486191052,0.7635201768
C,0,-3.1763397274,0.9915670106,1.005653798
C,0,-3.8861434682,0.2025704278,0.1058431
H,0,-1.4037148137,-1.399949509,-3.305949269
H,0,-3.4809533643,-2.4116891215,-2.3451852294
H,0,-1.0746286271,-2.4628090785,-1.9432704622
H,0,-3.5102096519,-0.634371987,-2.3863835598
H,0,-2.2870223634,0.5972938729,1.4885432703
C,0,-0.7562598279,-0.3555092063,-1.5378814151
H,0,-1.3727290023,0.5519149054,-1.5039618825
H,0,0.130515082,-0.1028453194,-2.1301194525
C,0,-0.2605667345,-0.6750543374,-0.1964657446
S,0,-3.364867391,-1.5029119226,-0.1441299892
O,0,-1.9895323001,-1.6414615978,0.5372062445
C,0,-5.0495586808,0.6633578098,-0.5134587765
C,0,-5.4855055099,1.9586696264,-0.2443211316
C,0,-4.7743015495,2.7701989914,0.6418528593
C,0,-3.6248255865,2.2869856619,1.2649643162
H,0,-5.6126371818,0.031027203,-1.196509133
H,0,-6.3861668941,2.3313317969,-0.7240301343
H,0,-5.1222673391,3.7778254971,0.8514123425
H,0,-3.0749260268,2.9148723236,1.9605053462
Au,0,2.3112006249,0.1449232998,-0.0374760073
P,0,4.2834742194,1.1179363462,-0.7148362758
H,0,5.3503797061,1.0345195607,0.1966273559
H,0,4.877379667,0.6220592222,-1.8885990675
H,0,4.2507773493,2.498269354,-0.9798910345
C,0,0.582442782,-1.2635942081,2.1680769214

H,0,0.8066401498,-0.4278992061,2.8412234898
H,0,-0.4225555975,-1.6233886983,2.4092543497
C,0,1.6082766906,-2.3741063001,2.3818134194
H,0,1.4045712433,-3.2309859961,1.7315181619
H,0,2.6244657401,-2.0222669042,2.1721266236
H,0,1.5742215355,-2.7211850762,3.4197163279

INT2

SCF Done: E(RPBE1PBE) = -1456.17447964 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.47
Sum of electronic and thermal Free Energies= -1455.934633 A.U.

C,0,1.5091384052,2.4043152728,-1.1753262549
C,0,2.860814645,2.4937827605,-0.4808544828
C,0,-0.3586482103,0.0228216228,0.8675409611
C,0,3.5393092952,-1.4420002627,0.6888916569
C,0,3.3455776904,-0.3234731281,-0.1313848505
H,0,3.522411466,-1.3496661096,1.7719694641
C,0,0.3502047005,2.267281727,-0.1847261456
C,0,0.4769398598,1.0534561261,0.6798934457
S,0,3.1337260984,1.2013824306,0.7554745296
O,0,1.6709242508,1.120274054,1.492182608
C,0,3.4015770419,-0.4209877767,-1.5238799249
C,0,3.6334288652,-1.6695797574,-2.0956616202
C,0,3.7996914261,-2.7957821143,-1.2910298204
C,0,3.7527616018,-2.6824648953,0.0988810675
H,0,3.2853011542,0.4444824886,-2.1652911842
H,0,3.6819854521,-1.7570855832,-3.1769703743
H,0,3.9765292045,-3.764852485,-1.7490104472
H,0,3.8960135437,-3.5569104234,0.7264792664
Au,0,-2.1612099699,-0.0330180139,-0.1249931893
P,0,-4.2087941862,-0.1482698758,-1.2300746739
H,0,-5.3034618998,-0.6527339761,-0.5032741195
H,0,-4.7546510619,1.0575203498,-1.7088865256
H,0,-4.2860819979,-0.9408596534,-2.3906877392
C,0,-0.0533688446,-1.098883675,1.8298414169
H,0,-0.0930101358,-2.0481503174,1.2795326097
H,0,0.9611361362,-1.0101152404,2.2355373892
C,0,-1.0529176003,-1.1643153465,2.9857611319
H,0,-1.0252073979,-0.2471529881,3.5849835582
H,0,-2.0770141042,-1.288172887,2.6143885173
H,0,-0.8263150145,-2.0070009538,3.6489219311
H,0,0.3093526446,3.1628485913,0.4518997316
H,0,-0.5930201123,2.2052043515,-0.7334155319
H,0,2.9456287869,3.4106235079,0.1133537767

H,0,3.7188331513,2.4592895072,-1.1603746943
H,0,1.4000706541,3.3284613747,-1.7535267389
H,0,1.4852454616,1.5723232984,-1.8844227445

TS-INT2-*conf*
SCF Done: E(RPBE1PBE) = -1456.16443853 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.50
Sum of electronic and thermal Free Energies= -1455.926782 A.U.

C,0,1.1204741167,2.8412671977,-1.0339409661
C,0,2.4807597915,2.1214629403,-1.128455133
C,0,-0.4381088211,0.0755757345,0.7510071123
C,0,4.5182007685,-1.0459792525,0.2430815092
C,0,3.3854210226,-0.4263936436,-0.2951590583
H,0,5.1422270626,-0.5287226907,0.9669123329
C,0,0.2236053996,2.5076288058,0.1721098977
C,0,0.4031049244,1.1152310364,0.6738264021
S,0,3.0385403275,1.1838871082,0.3415130509
O,0,1.7070180903,1.0113511026,1.2810291414
C,0,2.5601898913,-1.0737500512,-1.222565604
C,0,2.8901132114,-2.365129864,-1.6152560825
C,0,4.0253034548,-2.9920463206,-1.0940883138
C,0,4.8376810679,-2.3366636035,-0.1705550749
H,0,1.6773748823,-0.5900153497,-1.6298846528
H,0,2.2606974698,-2.883470268,-2.3324804479
H,0,4.2775144453,-3.9988987461,-1.4147194138
H,0,5.7197660878,-2.8265068889,0.2303415198
Au,0,-2.370917023,0.2774424619,0.0756569751
P,0,-4.5673067481,0.4457341242,-0.6827497277
H,0,-5.5359096895,-0.3310698834,-0.0197023974
H,0,-5.1759915395,1.713486929,-0.6294589545
H,0,-4.828198508,0.0930064036,-2.020255037
C,0,-0.0299662307,-1.2393456358,1.3697182351
H,0,-0.2371519507,-2.0442131268,0.6523056943
H,0,1.0477986693,-1.2656693919,1.5721332594
C,0,-0.7912407061,-1.5340062395,2.6635595887
H,0,-0.5870457664,-0.7713210531,3.4233481854
H,0,-1.8737085443,-1.550457801,2.4901954963
H,0,-0.4973241773,-2.5068343473,3.0736790019
H,0,0.4468522742,3.1944211613,0.9989407914
H,0,-0.8203860488,2.6598235343,-0.1112882254
H,0,2.4953861279,1.4057994169,-1.9502564494
H,0,3.301591738,2.8271983101,-1.2859044671
H,0,1.2963669026,3.9189841537,-1.0597982378
H,0,0.5834448464,2.5767430737,-1.9488892377

INT2'
SCF Done: E(RPBE1PBE) = -1456.16891809 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.44
Sum of electronic and thermal Free Energies= -1455.929853 A.U.

C,0,-1.5897357863,-2.8451002778,-0.6573987275
C,0,-3.0620437121,-2.4966964628,-0.4668733105
C,0,0.4252428913,-0.1758344278,1.052301425
C,0,-2.8789374683,1.4943931798,0.4456553432
C,0,-3.41537662,0.3474742183,-0.1444849069
H,0,-1.5275741309,-3.4396081877,-1.574329726
H,0,-3.6525968485,-3.3313485429,-0.0806080996
H,0,-1.2429402413,-3.4768485705,0.1662586444
H,0,-3.5198261172,-2.1333221169,-1.3893821327
H,0,-2.3156819025,1.4357933904,1.3718669492
C,0,-0.7218637098,-1.593266036,-0.7730557611
H,0,-1.1478305285,-0.9255490567,-1.5362974531
H,0,0.2842173549,-1.8520342948,-1.112980136
C,0,-0.5890491985,-0.8820777887,0.5423543423
S,0,-3.2304204764,-1.1729962334,0.7814302645
O,0,-1.7370005883,-1.0930044014,1.4134679539
C,0,-4.1700935456,0.4074292481,-1.3169908554
C,0,-4.3590023925,1.6483725795,-1.922329898
C,0,-3.8057053981,2.799569412,-1.3644508223
C,0,-3.0682052832,2.7213995277,-0.1838620757
H,0,-4.6233527558,-0.4712979406,-1.7640161281
H,0,-4.9435241463,1.7076158093,-2.835539589
H,0,-3.9553820688,3.7605963652,-1.8479739785
H,0,-2.6401474274,3.6164580068,0.2575051425
Au,0,2.1653213262,0.0004737612,-0.0390048998
P,0,4.1464849642,0.2314245684,-1.2405477693
H,0,4.9610681036,1.3351166871,-0.9247673013
H,0,5.0882060074,-0.8118801748,-1.1632614504
H,0,4.0467293761,0.3799871123,-2.636741398
C,0,0.3527755098,0.4717082525,2.4153082277
H,0,-0.6764471073,0.4781261568,2.7960486783
H,0,0.9300905681,-0.1470921021,3.1172790469
C,0,0.9148546917,1.8913323919,2.4474287141
H,0,1.9679730723,1.9045053785,2.1426669018
H,0,0.3664718693,2.5542901858,1.7682052404
H,0,0.8469737185,2.3127253834,3.4568545452

TS-33
SCF Done: E(RPBE1PBE) = -1456.16426348 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.43
Sum of electronic and thermal Free Energies= -1455.926666 A.U.

C,0,-1.7658727891,-3.0769206992,-0.3934588822
C,0,-2.9880946023,-2.2892306015,-0.8466935963
C,0,0.1715647142,0.0060740902,0.8184436018
C,0,-3.8089208247,1.6685018206,0.0368590884
C,0,-3.103321759,0.5546090724,-0.4615448373
H,0,-1.6160628645,-3.8638852875,-1.1407907674
H,0,-3.8755404061,-2.9286842067,-0.8804581966
H,0,-1.9816710102,-3.5789022865,0.5551599076
H,0,-2.8588716707,-1.8389385932,-1.8345379876
H,0,-4.5853727517,1.5331696108,0.78535453
C,0,-0.4959619276,-2.2358069849,-0.2717209057
H,0,-0.1930294021,-1.860524065,-1.2569872642
H,0,0.3303205383,-2.8624969044,0.0856183367
C,0,-0.6972898966,-1.0701739164,0.6744161642
S,0,-3.4570238483,-0.9561460557,0.3141789951
O,0,-1.7740545705,-1.1294473986,1.4230739387
C,0,-2.0890552915,0.7172670489,-1.4209255378
C,0,-1.8072087587,2.0001262419,-1.8931831487
C,0,-2.5079562548,3.0993219276,-1.4084617127
C,0,-3.5104243225,2.9317966253,-0.4440199033
H,0,-1.5557224688,-0.1296501468,-1.8374530379
H,0,-1.03487581,2.1306449638,-2.6454331189
H,0,-2.2840025315,4.0931392799,-1.7857297278
H,0,-4.0603229498,3.7915715856,-0.0730140845
Au,0,2.0683756379,-0.0918481122,0.0759266022
P,0,4.2528443876,-0.1605245147,-0.7638086752
H,0,5.2952617731,-0.1636878362,0.1813250983
H,0,4.610265124,-1.2679481867,-1.554516838
H,0,4.6554609382,0.9001167679,-1.5962149046
C,0,-0.216889961,1.18783791,1.6502396649
H,0,0.0063566408,2.0932620821,1.0686904471
H,0,-1.2913417108,1.1868076944,1.8655012046
C,0,0.5690222919,1.2595271925,2.9654918093
H,0,1.6490215671,1.2830646835,2.7819410171
H,0,0.2956690967,2.1635193435,3.5204617404
H,0,0.3516619128,0.3926906218,3.5980960431

INT4

SCF Done: E(RPBE1PBE) = -1456.20485935 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.31
Sum of electronic and thermal Free Energies= -1455.962789 A.U.

C,0,-2.1376716996,-2.9524939957,-0.5745121307
C,0,-3.1470864342,-1.9806769107,-1.1651937621
C,0,-0.4193279768,0.0705644639,0.5194821857

C,0,-3.2415064908,1.9687997543,0.032960217
C,0,-2.7101139605,0.7158127946,-0.3043107906
H,0,-2.0848326843,-3.795703658,-1.2733722373
H,0,-4.0808969793,-2.5063480247,-1.3922108168
H,0,-2.505531722,-3.3502123237,0.3772999006
H,0,-2.7928127879,-1.5360093381,-2.1010504175
H,0,-4.2359530372,2.047727299,0.4630833363
C,0,-0.7385831787,-2.372356793,-0.3879551518
H,0,-0.3686612901,-1.9447302659,-1.3259506323
H,0,-0.0565102507,-3.1841218082,-0.112843386
C,0,-0.6963667764,-1.3781061814,0.7634268037
S,0,-3.7528885347,-0.6243784804,-0.1013735953
O,0,-0.8541069749,-1.807257776,1.9048770224
C,0,-1.2903903142,0.6095991831,-0.733330146
C,0,-0.6957975483,1.8830167286,-1.1916786649
C,0,-1.2825355042,3.084196249,-0.9544524882
C,0,-2.5402696464,3.1158195419,-0.290512444
H,0,-1.1719178351,-0.1474437927,-1.5179637696
H,0,0.272034206,1.8119881674,-1.6818013757
H,0,-0.8109884225,4.0133140903,-1.2573178529
H,0,-2.9950803359,4.0785496663,-0.0698295642
Au,0,1.6408261154,-0.0118878664,-0.0748471343
P,0,3.8754646396,-0.1019807893,-0.6899196645
H,0,4.8236279214,-0.0867278874,0.3491430182
H,0,4.2942052731,-1.2300668786,-1.4188733839
H,0,4.3575880403,0.9366446085,-1.5071503589
C,0,-0.6179624255,0.9304570945,1.7714372331
H,0,-0.6833657681,1.9830444331,1.4755187733
H,0,-1.5814236423,0.6722015065,2.234515952
C,0,0.4764023714,0.8102923029,2.8283733589
H,0,1.4429080114,1.1532776792,2.4386750613
H,0,0.2292289015,1.4302700026,3.6985481191
H,0,0.5911687404,-0.2210867955,3.1715807861

TS-OS

SCF Done: E(RPBE1PBE) = -1456.16269212 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.85
Sum of electronic and thermal Free Energies= -1455.927144 A.U.

C,0,1.0777906804,-2.3607249404,-1.1810813201
C,0,2.5557777017,-2.1435494327,-0.8589947946
C,0,-0.7313086883,0.6765157121,-0.0957216627
C,0,4.66886703,-0.6759628787,1.0728154373
C,0,4.393211879,-0.0570117028,-0.1536899614
H,0,4.0077000262,-1.4287980939,1.4876961616
C,0,0.1172851905,-1.7664982326,-0.1463555823

C,0,0.2875872174,-0.2785303053,-0.013040225
S,0,2.9720790198,-0.3995958692,-1.1161346913
O,0,1.4852507676,0.1407145756,0.275753582
C,0,5.239484308,0.9429364854,-0.6598970722
C,0,6.3744356659,1.3035119082,0.0574327117
C,0,6.6623652394,0.6805749022,1.2724556194
C,0,5.8089858771,-0.3026821424,1.7763217185
H,0,5.0162635729,1.4224958198,-1.6093344696
H,0,7.0356549156,2.0699000321,-0.3360772709
H,0,7.5514364847,0.9624426326,1.8294143197
H,0,6.0280382008,-0.7812904159,2.7264686689
Au,0,-2.6597753496,0.1205278505,0.2497586297
P,0,-4.8768072571,-0.5054387769,0.6623721088
H,0,-5.8437131049,0.5161312476,0.6649125684
H,0,-5.4605745378,-1.4222198196,-0.2312578521
H,0,-5.1447574432,-1.1301678383,1.8942319151
C,0,-0.375710759,2.116738217,-0.2705541973
H,0,-0.4148540634,2.5823645167,0.7277755005
H,0,0.6603481714,2.2260335202,-0.6142542367
C,0,-1.3340001353,2.8741541729,-1.1902685747
H,0,-1.3288424494,2.4537042791,-2.2015492851
H,0,-2.3619459423,2.8332273925,-0.8131618377
H,0,-1.0357335533,3.9254647599,-1.2606883381
H,0,2.7752257205,-2.4177770919,0.175777186
H,0,3.2041902938,-2.7210088963,-1.5250415419
H,0,0.3088908889,-2.2381993722,0.8283553461
H,0,-0.9134730774,-1.9971649167,-0.4315994068
H,0,0.92398441,-3.4443295999,-1.2178987361
H,0,0.8475890997,-1.9815286987,-2.1851994173

INT3-*Singlet*

SCF Done: E(RPBE1PBE) = -1456.19377958 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.26
Sum of electronic and thermal Free Energies= -1455.964797 A.U.

C,0,1.806970803,0.3142093191,0.858324871
C,0,3.0993868174,0.1933440045,0.0589052473
C,0,-1.9108583131,1.2369764441,0.0448102586
C,0,5.9075699997,0.0259635987,-1.1722237407
C,0,5.8870720413,-0.292743205,0.1903647172
H,0,4.9919858278,0.2616621857,-1.7042137359
C,0,0.6458371684,0.7026465662,-0.0487028273
C,0,-0.6113105638,0.9902971636,0.6945973727
S,0,4.4217561822,-0.343915685,1.1835767954
O,0,-0.7426777858,1.0672985732,1.9104022904
C,0,7.092631999,-0.5991545745,0.8416018694

C,0,8.2931442038,-0.5836014598,0.1394476638
C,0,8.3154409131,-0.2612031865,-1.2193992658
C,0,7.1194612738,0.0410783635,-1.8660074865
H,0,7.0903369474,-0.8480540027,1.9004847766
H,0,9.216952881,-0.8218376936,0.6604435092
H,0,9.2546661475,-0.2465403431,-1.765165094
H,0,7.1195611989,0.2929479785,-2.9236292872
Au,0,-3.182573004,-0.3088356745,-0.1359210597
P,0,-4.7202499651,-2.0737382757,-0.3006542824
H,0,-6.0082552553,-1.8052857923,0.1923862847
H,0,-4.9974508245,-2.5288329795,-1.6011754927
H,0,-4.3939261872,-3.2682552324,0.3634435959
C,0,-2.1951924694,2.6089150952,-0.3398459033
H,0,-1.5634087192,3.3371476347,0.1864500855
H,0,-1.7208494569,2.5356109949,-1.3545063396
C,0,-3.6405587905,3.0511004133,-0.4776701017
H,0,-4.2138972441,2.3466629078,-1.087571849
H,0,-4.1093988961,3.11854228,0.5084515064
H,0,-3.6880361902,4.0380325663,-0.945897438
H,0,2.9876221852,-0.5359988655,-0.7507814479
H,0,3.3665313179,1.1628589362,-0.3752763132
H,0,0.4272724511,-0.0732869667,-0.7947911561
H,0,0.8769350627,1.6111662246,-0.6271212245
H,0,1.9272907384,1.0667708993,1.6446795706
H,0,1.5764255753,-0.6350357226,1.3553645738

INT3-*Triplet*

SCF Done: E(UPBE1PBE) = -1456.14897461 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.33Sum of electronic and thermal Free Energies= -1455.918559 A.U.

C,0,-1.8934941446,0.730383567,-1.0497617271
C,0,-3.1474501843,0.6000712119,-0.192863037
C,0,1.922808177,1.0419777972,-0.2341620039
C,0,-5.820556657,0.1020985669,1.2245668165
C,0,-5.8927019713,-0.0715685009,-0.162475083
H,0,-4.9202043955,0.4859270627,1.692742466
C,0,-0.6732462254,0.9784249509,-0.172046664
C,0,0.6250818931,1.0530000799,-0.9193879032
S,0,-4.5717315105,0.3028153072,-1.2818485052
O,0,0.6996870149,1.1333848649,-2.1438933368
C,0,-7.0800631434,-0.5577579423,-0.7320940009
C,0,-8.1705294288,-0.8662106055,0.0748390343
C,0,-8.0968351992,-0.7007498895,1.4596175219
C,0,-6.9192576687,-0.2171340415,2.0249614378

H,0,-7.1477779883,-0.7003720139,-1.8082228565
H,0,-9.0812111726,-1.243789998,-0.3830338207
H,0,-8.9481416145,-0.9464352065,2.088317124
H,0,-6.8473104895,-0.0796055137,3.1010525251
Au,0,1.8720655173,0.9336442122,1.8227575539
P,0,1.8157774744,0.8761430455,4.1840642912
H,0,2.7786689307,0.070873884,4.8159327659
H,0,1.993560205,2.1087372005,4.8343922008
H,0,0.6221983864,0.4108399609,4.7609960494
C,0,3.2234362775,1.1269760727,-0.9385877578
H,0,3.2559398726,0.343513056,-1.7101912378
H,0,3.2563867813,2.0806010858,-1.4887324911
C,0,4.4444997975,1.0112202512,-0.0288081022
H,0,4.4636937039,1.8060430734,0.7254004243
H,0,4.4733619379,0.044249462,0.484359215
H,0,5.3571416003,1.0994338673,-0.6264859125
H,0,-3.0508434053,-0.2438315112,0.4992511297
H,0,-3.3107401679,1.5143291191,0.387641522
H,0,-0.5534436109,0.1899709902,0.586770591
H,0,-0.7674291882,1.9259717827,0.379695592
H,0,-2.0080329429,1.5527309122,-1.764692992
H,0,-1.745351811,-0.1858976714,-1.6324208993

INT3-*Triplet-Syn*

SCF Done: E(UPBE1PBE) = -1456.15690828 A.U. after 1 cycles
SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.07
Sum of electronic and thermal Free Energies= -1455.929135 A.U.

C,0,-1.9004541972,0.6245454882,-0.9384617379
C,0,-3.1512734987,0.4225023706,-0.0918177332
C,0,1.8101117205,1.4071905152,-0.0967278136
C,0,-5.8591034055,-0.1397977411,1.2438583895
C,0,-5.9025387547,-0.2024379214,-0.1728150006
H,0,-4.933561986,0.0901805793,1.7600126389
C,0,-0.7098005539,0.9240628023,-0.0387306821
C,0,0.5882507371,1.1165347358,-0.8139014507
S,0,-4.5526613223,0.064437677,-1.1833066042
O,0,0.5676567695,1.0157502146,-2.0570742553
C,0,-7.1203788096,-0.5060216215,-0.8480312354
C,0,-8.2627204916,-0.7407549138,-0.11224103
C,0,-8.2151340668,-0.6788585521,1.2882471813
C,0,-7.0140270547,-0.3783593191,1.9573155753
H,0,-7.141004594,-0.5501514336,-1.9333718274
H,0,-9.1948853704,-0.9727201939,-0.6171277597
H,0,-9.1162888367,-0.8643894336,1.8651374892

H,0,-6.9969634789,-0.3352202629,3.0416448162
Au,0,3.5301978677,1.6255582342,-1.1682266322
P,0,5.5181562553,1.8803743692,-2.37267514
H,0,6.3267197586,2.9897214332,-2.0593002371
H,0,6.4688822811,0.8455876697,-2.2861691414
H,0,5.4247979785,2.021652982,-3.770112971
C,0,1.7577312015,1.5264545604,1.3985155746
H,0,1.0227982803,2.301831912,1.6743747475
H,0,1.3466365774,0.5936312158,1.8209623494
C,0,3.0846680756,1.83622203,2.0796771311
H,0,3.8256858435,1.0558404604,1.8730787883
H,0,3.4963420836,2.7885963762,1.7272274089
H,0,2.9598059455,1.9038477899,3.166679666
H,0,-3.0436886138,-0.4238033119,0.5962389298
H,0,-3.4049950146,1.3214603024,0.4818704893
H,0,-0.5675389631,0.1117206207,0.6877691399
H,0,-0.901053133,1.8251877223,0.5603986326
H,0,-2.0476220486,1.4502524849,-1.6426144037
H,0,-1.6959407518,-0.2721636612,-1.5327061422

TS-CC

SCF Done: E(RPBE1PBE) = -1456.18207956 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.09
Sum of electronic and thermal Free Energies= -1455.944651 A.U.

C,0,-2.3479655817,-2.8788243238,-0.5959899599
C,0,-3.283670185,-1.8735317927,-1.2549889017
C,0,-0.105291282,-0.2078022884,0.9484597467
C,0,-3.0564299151,2.1092495316,-0.0305157555
C,0,-2.7141715635,0.8731658394,-0.6009557935
H,0,-2.2736131196,-3.734469711,-1.2775635548
H,0,-4.2269145101,-2.374830917,-1.4956613523
H,0,-2.7964950825,-3.2568632353,0.3296825504
H,0,-2.884662187,-1.4946767438,-2.2011680763
H,0,-3.952215055,2.1962859527,0.5795572284
C,0,-0.9232369423,-2.3901039171,-0.3129646827
H,0,-0.4863742086,-1.8980899082,-1.1857155824
H,0,-0.3013155422,-3.2690540589,-0.0991363815
C,0,-0.7877361703,-1.5303842631,0.9128257603
S,0,-3.7999465467,-0.4681469282,-0.219549466
O,0,-1.0077465831,-1.9543703232,2.0428016088
C,0,-1.5567636551,0.7888633065,-1.3923096659
C,0,-0.7685047027,1.9279714537,-1.6131546078
C,0,-1.1006131951,3.1432449781,-1.0297541604

C,0,-2.2531616276,3.2249667579,-0.237329722
H,0,-1.2953781794,-0.1291449991,-1.9038903638
H,0,0.1060399986,1.845503703,-2.2529557739
H,0,-0.4868165992,4.023465157,-1.1963737413
H,0,-2.5348082006,4.1718493171,0.2157996435
Au,0,1.7012871688,-0.1280987841,0.0661765901
P,0,3.7937215387,-0.0454058738,-0.9973521291
H,0,4.9125672234,0.0254419331,-0.1495518175
H,0,4.1265074612,-1.1326878175,-1.8228499043
H,0,4.0163417887,1.0455834562,-1.8546793713
C,0,-0.5996281273,0.8263345716,1.8634671486
H,0,-0.631790757,1.7696552409,1.2943439538
H,0,-1.6023179919,0.6006337038,2.238855398
C,0,0.3822850836,1.0582490617,3.032374102
H,0,1.3714479648,1.3478938841,2.6656319439
H,0,-0.0134739324,1.8632874237,3.6588988723
H,0,0.4803055252,0.1568119529,3.6421796172

TS-K
SCF Done: E(RPBE1PBE) = -1456.18641424
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.61
Sum of electronic and thermal Free Energies= -1455.951117 A.U.

C,0,-1.1470153077,2.5994488955,-1.6612892484
C,0,-2.3275580115,1.8952807849,-0.9991227665
C,0,0.7840352824,0.7105779489,0.835763519
C,0,-4.6408039898,0.2579437922,0.1373546364
C,0,-3.6752152926,-0.5375305007,-0.4893729833
H,0,-1.191400099,3.6556870019,-1.3751379972
H,0,-3.2582335487,2.2329168215,-1.4648198177
H,0,-1.2517574805,2.5577279088,-2.75036684
H,0,-2.3690542863,2.1331326228,0.0683675235
H,0,-4.5120019748,1.331850725,0.2210336258
C,0,0.2322503279,2.0272496936,-1.3136889196
H,0,1.0023196667,2.6557715492,-1.7783479744
H,0,0.3485313105,1.0189207906,-1.724700505
C,0,0.5380690971,2.0096226917,0.1604999916
S,0,-2.1793884145,0.0926807258,-1.2018616341
O,0,0.7334389307,3.0154523389,0.8304901205
C,0,-3.8743455485,-1.9238096801,-0.5790559079
C,0,-5.0231248651,-2.5006319834,-0.0470179382
C,0,-5.9887972687,-1.7086450182,0.5777701231
C,0,-5.7903807005,-0.3326761914,0.6651367401
H,0,-3.1327439787,-2.5504208714,-1.0692127114
H,0,-5.1651190408,-3.5753248928,-0.1258177451
H,0,-6.8864944312,-2.1609918425,0.9896528678

H,0,-6.5342198792,0.2969228796,1.1467148769
Au,0,2.3609572039,-0.3210662273,0.1293309496
P,0,4.1818560332,-1.5589593808,-0.6811507581
H,0,4.205042873,-2.9232010152,-0.3457265798
H,0,4.3518626594,-1.5961099316,-2.0753551918
H,0,5.4475102253,-1.1310992525,-0.2449030203
C,0,0.0891266512,0.3415100136,2.0547942102
H,0,0.2018351811,-0.7257823662,2.2697760561
H,0,0.8757645143,0.7941554166,2.7198237015
C,0,-1.2765360428,0.8972627298,2.4123448531
H,0,-1.3333631642,1.9781333662,2.2645396002
H,0,-2.0503793687,0.4118674567,1.8104981705
H,0,-1.4897812628,0.6858609999,3.463743973

TS-HT
SCF Done: E(RPBE1PBE) = -1456.19140840
SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.34
Sum of electronic and thermal Free Energies= -1455.961125 A.U.

C,0,-0.9146825798,-3.0892162338,0.4356696965
C,0,-1.2870313668,-3.8926846243,1.6763456237
C,0,1.0058321939,0.2813482678,-0.1470166366
C,0,-2.2102860237,-5.7435793312,3.9376157737
C,0,-2.5349400287,-6.2316918307,2.6665780636
H,0,-1.6894851926,-4.7991811835,4.0571695944
C,0,-0.1598097204,-1.823922953,0.8158755827
C,0,0.223843428,-0.9810857767,-0.3643848131
S,0,-2.1481762757,-5.403241996,1.1501793755
O,0,-0.0237268631,-1.25877043,-1.5247425555
C,0,-3.2105124642,-7.457431229,2.5546014236
C,0,-3.5517983509,-8.177737512,3.6944413847
C,0,-3.2272882812,-7.6922479904,4.9633200833
C,0,-2.5581473936,-6.4758778866,5.0747736652
H,0,-3.4683780178,-7.8477100624,1.5725803266
H,0,-4.074621104,-9.1248408622,3.5882928383
H,0,-3.4947783965,-8.2564947582,5.8523500217
H,0,-2.2995518764,-6.0837083191,6.0552702879
Au,0,3.0378326115,0.2094956974,-0.4632671354
P,0,5.3199947376,0.1710508499,-0.8929353585
H,0,5.8619803481,1.3461585238,-1.4411485008
H,0,6.1675812258,-0.0460005873,0.2071854054
H,0,5.7748161923,-0.8027372651,-1.7984446197
C,0,0.2818220787,1.438549163,0.1549004997
H,0,-0.8061294136,1.3589035164,0.2420469348
H,0,0.7777660091,0.7469509067,1.1012443685
C,0,0.8570140064,2.812065971,0.208422057

H,0,1.9497030109,2.7879394437,0.2378311973
H,0,0.5415183733,3.328767879,-0.7064698673
H,0,0.4592574283,3.3761966741,1.0563380814
H,0,-0.3889176261,-4.1663637288,2.2404139078
H,0,-1.9466574978,-3.3077363936,2.3264972255
H,0,0.7642959334,-2.0548323991,1.3654094351
H,0,-0.7521833577,-1.1898108608,1.4934383872
H,0,-1.8184206622,-2.8218221869,-0.1229439974
H,0,-0.2936771347,-3.694599592,-0.234024557

K

SCF Done: E(RPBE1PBE) = -1456.23078181
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.12
Sum of electronic and thermal Free Energies= -1455.990438 A.U.

C,0,-1.1480251384,3.2195927459,-1.4286852645
C,0,-2.1580337038,2.127680683,-1.045661689
C,0,-0.1122061339,0.8664242016,0.4900639937
C,0,-3.7030313343,-0.4525587648,-0.1496506863
C,0,-2.3745496946,-0.7163671957,-0.4798872957
H,0,-1.4781168837,4.1462185704,-0.9505316801
H,0,-2.9410413145,2.0060131542,-1.7987239997
H,0,-1.1704072337,3.3800091302,-2.5095250968
H,0,-2.6113521504,2.3110570491,-0.0697590325
H,0,-4.0946580937,0.5585671896,-0.1309814854
C,0,0.309187739,2.9144836524,-1.0138889143
H,0,0.895047251,3.8359735967,-1.0072798678
H,0,0.7633554784,2.2370922583,-1.7495879404
C,0,0.395075587,2.2718773757,0.3529973913
S,0,-1.2276283843,0.5663109572,-0.9534724758
O,0,0.8466078554,2.8693232267,1.3224485133
C,0,-1.8786112229,-2.0221326179,-0.5294591327
C,0,-2.7262262976,-3.0780194377,-0.2080966285
C,0,-4.0562190264,-2.8302127633,0.1328849369
C,0,-4.5418915434,-1.5241610293,0.1543630318
H,0,-0.8456687667,-2.2127786339,-0.8096663814
H,0,-2.3473093373,-4.0953728938,-0.2356566984
H,0,-4.7165727252,-3.658008212,0.3748743122
H,0,-5.5793903923,-1.329693219,0.4100697048
Au,0,1.6012458946,-0.3347117692,0.0651748933
P,0,3.453615204,-1.6623272769,-0.3173761392
H,0,3.4246168835,-2.9551120114,0.2349022038
H,0,3.7737562391,-1.9415541127,-1.6577368649
H,0,4.6821742953,-1.1800745107,0.1676439813
C,0,-0.6739340974,0.5092067477,1.8676614261
H,0,-0.9525349077,-0.5496696269,1.8822551384

H,0,0.1787240274,0.6024359137,2.5492091466
C,0,-1.8240615163,1.3588425441,2.4050596854
H,0,-1.5904237738,2.4272333218,2.368053682
H,0,-2.7602929275,1.1850862342,1.8669773368
H,0,-2.0085118547,1.0984835228,3.4531058954

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SCF Done: E(RPBE1PBE) = -1456.24925507
SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.28
Sum of electronic and thermal Free Energies= -1456.015354 A.U.

C,0,-1.8879242564,3.2182313631,-0.6775878836
C,0,-2.2703345868,4.0446433649,-1.8999692707
C,0,1.5464070875,1.838576579,0.5565589518
C,0,-3.3770117082,5.7003646766,-4.2284921212
C,0,-4.353594248,5.3687139365,-3.2820956571
H,0,-2.4372288017,2.2696169933,-0.6769758724
H,0,-1.9915329356,3.5174477644,-2.818746148
H,0,-2.1710500762,3.7482311968,0.2385022303
H,0,-1.7592762531,5.0136559584,-1.88351156
H,0,-2.3644243158,5.3211318786,-4.1412165222
C,0,-0.3940214488,2.9377884141,-0.6607183635
H,0,0.1866494016,3.8728829157,-0.6651808391
H,0,-0.0731565048,2.3988507845,-1.5644673501
C,0,0.0686221172,2.142690691,0.5282467516
S,0,-4.0667355767,4.3203593659,-1.8835597772
O,0,-0.6717570005,1.7924882654,1.4305148635
C,0,-5.6546702413,5.8741472301,-3.4338970719
C,0,-5.966864355,6.6963509596,-4.511795356
C,0,-4.9917060528,7.0314993319,-5.4539520423
C,0,-3.7009121962,6.530369802,-5.3035936855
H,0,-6.4222397465,5.6275508963,-2.7037046429
H,0,-6.9787781558,7.080440156,-4.612201084
H,0,-5.2366180666,7.6772174959,-6.2926375287
H,0,-2.930480944,6.780876917,-6.0286838892
Au,0,1.7014838393,-0.3273579115,0.0078076104
P,0,1.6071010029,-2.4225342829,-0.9582629588
H,0,2.7358538549,-3.2385203556,-0.7813367584
H,0,0.5572297423,-3.2466750933,-0.5224183664
H,0,1.442028818,-2.4273931767,-2.3526821338
C,0,2.1401420286,1.273017193,1.6660878966
H,0,2.1664226944,2.3347205542,-0.1914166317
H,0,1.4780315536,0.951656669,2.4725228532
C,0,3.6003018909,1.2763260423,1.9474573661
H,0,3.933850199,0.3093126457,2.3366872679
H,0,4.1969743098,1.5519084983,1.074928725

H,0,3.7828008208,2.0103291606,2.7450633282

6.2 The structures shown in Figure S7 and Figure S10.

INT3-H-*Singlet*
SCF Done: E(RPBE1PBE) = -1377.63643878 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.04
Sum of electronic and thermal Free Energies= -1377.455628 A.U.

C,0,-1.8845231893,0.3210279274,-0.8238775547
C,0,-3.1862692586,0.1567159353,-0.0481315008
C,0,1.9356167942,1.0327539742,-0.2963092783
C,0,-5.9831372671,-0.0809896524,1.170961939
C,0,-5.9874140992,-0.1712441189,-0.2255250981
H,0,-5.0543582911,0.0232025947,1.7219588483
C,0,-0.7225761297,0.5554025046,0.1351916355
C,0,0.5566233432,0.7901777476,-0.527883578
S,0,-4.5313265704,-0.1312002697,-1.2335018166
O,0,0.8647236797,0.8517120492,-1.7348552544
C,0,-7.2100719988,-0.306978902,-0.9018301539
C,0,-8.4037569639,-0.354046488,-0.1893724111
C,0,-8.4013682572,-0.2629098795,1.2043368229
C,0,-7.1882930256,-0.1274950909,1.8749958039
H,0,-7.2267664545,-0.3747461735,-1.9873144498
H,0,-9.3413915225,-0.4585795506,-0.7291606898
H,0,-9.3349860269,-0.2986955872,1.7587370629
H,0,-7.1694299692,-0.055817203,2.9596464784
Au,0,3.3694380779,-0.3720824403,-0.0360812928
P,0,5.0477699751,-1.9474720102,0.3164685374
H,0,6.151662613,-1.8861319242,-0.5511333472
H,0,5.6693725346,-1.9126646286,1.5762218984
H,0,4.6747618762,-3.2986693395,0.2167545064
H,0,-3.1168269216,-0.6914618679,0.6414564669
H,0,-3.3995260666,1.0631932888,0.5284165621
H,0,-0.5639483307,-0.2856895335,0.8260437612
H,0,-0.8856064438,1.4283168142,0.7867064682
H,0,-1.9673889202,1.1682642948,-1.5134683999
H,0,-1.6868031602,-0.5731136914,-1.4254710064
H,0,2.1757289535,2.1001490205,-0.2777154796

INT3-H-*Triplet*
SCF Done: E(UPBE1PBE) = -1377.61561120 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.76

Sum of electronic and thermal Free Energies= -1377.438471 A.U.

C,0,1.5491369503,-1.5745046445,-0.0383882173
C,0,2.6624042474,-0.5347413155,-0.094888988
C,0,-2.3065518129,-1.3286698805,0.2434418224
C,0,5.2597484879,1.1750230413,0.0146448158
C,0,5.4853119051,-0.2209729242,-0.1005782529
H,0,4.2531597953,1.5767584446,0.0437470526
C,0,0.1954718526,-0.885126328,0.0520301491
C,0,-0.9676268453,-1.8595739865,0.1543686338
S,0,4.2523030211,-1.3981629526,-0.1890933242
O,0,-0.7507728677,-3.0854387261,0.1607621317
C,0,6.8129252823,-0.7390439708,-0.1431991653
C,0,7.8821844334,0.1281294901,-0.0662388027
C,0,7.654480867,1.5072299169,0.0505148321
C,0,6.3451105468,2.0213821539,0.0885690671
H,0,6.9734571804,-1.8104877993,-0.2326214125
H,0,8.8961518798,-0.2571895771,-0.0959057421
H,0,8.4981567041,2.1887395673,0.1107654017
H,0,6.1882345757,3.0918384835,0.1770123956
Au,0,-2.8985387119,0.5976803595,0.2474553687
P,0,-3.6389230297,2.8189795605,0.2659534067
H,0,-4.8374981409,3.1049145272,-0.413661071
H,0,-3.9114631377,3.3970988158,1.5199830841
H,0,-2.7907421282,3.796287035,-0.2873875347
H,0,2.5796495567,0.106027076,-0.9805070872
H,0,2.6730591965,0.0933288345,0.8025811272
H,0,0.0248514424,-0.2418780841,-0.8216443763
H,0,0.1559326226,-0.2176004616,0.923522889
H,0,1.685689297,-2.2273747567,0.8304332563
H,0,1.5786827684,-2.2133313899,-0.9278452052
H,0,-3.0492781284,-2.1292587987,0.3138982455

INT3-H-*Triplet-Syn*
SCF Done: E(UPBE1PBE) = -1377.61604874 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.74
Sum of electronic and thermal Free Energies= -1377.440654 A.U.

C,0,1.427461193,1.6536427936,-0.0472005878
C,0,2.4751738009,0.5477300113,-0.0376165439
C,0,-2.4372811813,1.6194345605,-0.1449972695
C,0,4.8814729996,-1.3641067805,-0.0183976352
C,0,5.2448192674,0.0070059958,0.0163401509

H,0,3.8390867662,-1.6616050797,-0.0491041856
C,0,0.0314595056,1.0501776037,-0.0881225526
C,0,-1.0774013313,2.0967541442,-0.1019210441
S,0,4.1248323708,1.2953680657,0.0141471708
O,0,-0.7884183647,3.3053933277,-0.0763152554
C,0,6.6163908554,0.3929726191,0.0559023173
C,0,7.5940123094,-0.5794392797,0.0604539682
C,0,7.2306298931,-1.9337787996,0.0261454012
C,0,5.8770951151,-2.3173328593,-0.0130554212
H,0,6.8816375125,1.4464030668,0.0823726343
H,0,8.6410845695,-0.2959549797,0.0905494824
H,0,8.0026983892,-2.6974714485,0.0298590829
H,0,5.6154579205,-3.3703134103,-0.0393985207
Au,0,-4.0789502567,2.7889858994,-0.1748169503
P,0,-5.9875335825,4.1394265888,-0.2154260343
H,0,-7.1399154978,3.6203058626,-0.8349775344
H,0,-6.5232400741,4.5462250972,1.02115974
H,0,-5.8809461819,5.3811869891,-0.8692512438
H,0,2.379867639,-0.0968403554,0.8436988455
H,0,2.4236283771,-0.0703895917,-0.9411835995
H,0,-0.1323235028,0.3920635686,0.7763939951
H,0,-0.0901645783,0.4129617023,-0.9749171239
H,0,1.5708261057,2.3043576788,-0.9164549148
H,0,1.5293454818,2.2808557405,0.8448710467
H,0,-2.5236557403,0.5283710589,-0.1629305782

INT3-NoTail-*Singlet*

SCF Done: E(RPBE1PBE) = -827.362991500 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.00
Sum of electronic and thermal Free Energies= -827.207384 A.U.

C,0,-1.78382782,0.4056787387,-0.8668182329
C,0,-3.0124312551,0.0029007436,-0.0618413733
C,0,1.94773432,1.3295298723,-0.0568439561
C,0,-0.5932801091,0.7061607589,0.0353890017
C,0,0.6387093522,1.1065483887,-0.6936305875
O,0,0.7591925511,1.2820821953,-1.9014048284
Au,0,3.1691529232,-0.2607170178,0.1023571527
P,0,4.5528885303,-2.1392220559,0.326146497
H,0,5.8680161002,-2.0079759326,-0.1505776094
H,0,4.7643038005,-2.5892112846,1.6404869891
H,0,4.1238164207,-3.3121148727,-0.3178663422
C,0,2.2558684056,2.6871724098,0.3620820228
H,0,1.6220795177,3.4339616496,-0.1351419319
H,0,1.8097647662,2.6009330054,1.387196683

C,0,3.7117743377,3.1044893612,0.4665701171
H,0,4.2927239583,2.3705660757,1.0332498567
H,0,4.149516185,3.1982511958,-0.5316190016
H,0,3.7905543327,4.0743078766,0.9654210525
H,0,-2.8214462701,-0.8961434512,0.5359014853
H,0,-3.3196561462,0.8011309103,0.6238767637
H,0,-0.3324893919,-0.1563306693,0.6656984276
H,0,-0.8216976885,1.5202140724,0.7413856753
H,0,-2.0091672634,1.2877077205,-1.4770032714
H,0,-1.5143279293,-0.3955840929,-1.5648813395
H,0,-3.8581259877,-0.2112868978,-0.7233356404

INT3-NoTail-*Triplet*
SCF Done: E(UPBE1PBE) = -827.318726820 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.09
Sum of electronic and thermal Free Energies= -827.163292 A.U.

C,0,1.5027099304,-1.7097522667,0.2353605385
C,0,2.6098021623,-0.6722883645,0.371349949
C,0,-2.4088296359,-1.5065452377,-0.0832629126
C,0,0.1304361114,-1.0578191465,0.1479375751
C,0,-1.028254977,-1.99881235,0.0119768241
O,0,-0.921239404,-3.2221293111,-0.030084848
Au,0,-2.6346009165,0.5365044614,-0.0188192055
P,0,-2.9393324808,2.8787791864,0.0477730978
H,0,-4.0048343589,3.387638675,-0.7141064291
H,0,-3.19154522,3.4388821502,1.3114883919
H,0,-1.8601183333,3.6562835868,-0.404534014
C,0,-3.5945302041,-2.3826558145,-0.2207235586
H,0,-3.4671515933,-3.0066872518,-1.1185967694
H,0,-3.6113824326,-3.0863672763,0.6255513601
C,0,-4.9188694644,-1.6259251144,-0.2957737326
H,0,-5.097641899,-1.0380565849,0.6111969765
H,0,-4.9480517848,-0.9511141427,-1.1583851219
H,0,-5.7452357686,-2.3362575983,-0.4004300307
H,0,2.6275807522,0.0079973916,-0.4882556705
H,0,2.4803681322,-0.0661667843,1.2757162307
H,0,0.0653617028,-0.3723067028,-0.7119400167
H,0,-0.0807263392,-0.4448023873,1.0385213995
H,0,1.5260886292,-2.394138138,1.0913520977
H,0,1.6723727022,-2.3208193412,-0.6587708485
H,0,3.5905120897,-1.1549162386,0.4329136371

INT3-NoTail-*Triplet-Syn*
SCF Done: E(UPBE1PBE) = -827.320813752 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.07

Sum of electronic and thermal Free Energies= -827.163308 A.U.

C,0,-3.7753279338,-0.5057497865,0.0048581427
C,0,-4.3414060307,-1.9197368339,0.0059622701
C,0,-0.2492919929,1.1688752176,0.0014823731
C,0,-2.2508484673,-0.5065298663,0.0004004191
C,0,-1.6222826111,0.8404577478,0.0003568388
O,0,-2.329671258,1.9092342888,-0.0009084781
Au,0,-0.2931467294,3.2103798233,0.0005446915
P,0,-0.3127027669,5.6002680154,0.0049252252
H,0,0.675985224,6.2261787436,0.7833443723
H,0,-0.1356403512,6.2290817585,-1.2395770014
H,0,-1.4832281363,6.219844202,0.474391151
C,0,0.9174393596,0.2600655646,0.0051690519
H,0,0.8309480509,-0.3883730057,0.8928302015
H,0,0.8155461199,-0.4178977787,-0.8582148996
C,0,2.2750595051,0.9474768812,-0.0176084971
H,0,2.3908141341,1.5621148674,-0.9165475031
H,0,2.4054133773,1.5914613303,0.8585153026
H,0,3.0792780435,0.2055916938,-0.0120907607
H,0,-4.0204233299,-2.4785498817,-0.880898688
H,0,-4.0148388399,-2.4793404189,0.890291486
H,0,-1.8604413013,-1.0467807805,-0.8752078725
H,0,-1.8553199509,-1.049205497,0.8721781939
H,0,-4.1366223188,0.0399354056,0.884669312
H,0,-4.1419540429,0.0407819637,-0.8721984893
H,0,-5.4362596333,-1.9018371244,0.009447708

INT3-NoTail-H-*Singlet*
SCF Done: E(RPBE1PBE) = -748.806337421 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -0.77
Sum of electronic and thermal Free Energies= -748.700702 A.U.

C,0,-1.9020680901,0.5141619943,-0.8593215309
C,0,-3.207164488,0.2320171181,-0.1275354502
C,0,1.9433990283,1.0649828083,-0.2428885468
C,0,-0.7312296952,0.6083220079,0.1123270845
C,0,0.5609454824,0.8843979398,-0.5031010946
O,0,0.9042179878,1.0445678893,-1.693642797
Au,0,3.307838039,-0.4184608023,-0.0304440446
P,0,4.9005960768,-2.0832916643,0.3073066375
H,0,6.0909084372,-1.9664445615,-0.4304522957
H,0,5.3869606612,-2.2131853037,1.6190614128
H,0,4.5078684338,-3.4000672502,0.0128001615
H,0,-3.1592249183,-0.7153423482,0.4215282628

H,0,-3.4402554805,1.0259111094,0.5911611235
H,0,-0.590493662,-0.3163148324,0.6937267485
H,0,-0.8768257101,1.390402275,0.8741764453
H,0,-1.9834988271,1.4522062544,-1.4200506775
H,0,-1.7039141134,-0.2778236279,-1.5905084048
H,0,-4.0398128269,0.1662100374,-0.8345775326
H,0,2.2187735753,2.1167285769,-0.1273123716

INT3-NoTail-H-*Triplet*
SCF Done: E(UPBE1PBE) = -748.770695582 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -0.57
Sum of electronic and thermal Free Energies= -748.666858 A.U.

C,0,1.5319928162,-1.770201423,0.2158612903
C,0,2.6917560487,-0.7873273482,0.3159226896
C,0,-2.3656424973,-1.3725465934,0.0033752231
C,0,0.195232033,-1.0462581715,0.1636865405
C,0,-1.0184737644,-1.9105836004,0.0640207347
O,0,-1.0053247808,-3.1430868123,0.0236120512
Au,0,-2.7080511918,0.6194370421,0.0492372734
P,0,-3.1009544194,2.9503806278,0.1020030258
H,0,-4.1236411758,3.4283200704,-0.7346903988
H,0,-3.4686941532,3.4876882401,1.3472510781
H,0,-2.0175426585,3.7669170322,-0.2619939964
H,0,2.7184201908,-0.111949833,-0.5473130941
H,0,2.6169317119,-0.1721847727,1.220367694
H,0,0.1385860231,-0.3599251245,-0.6952845173
H,0,0.0376587745,-0.4201967633,1.0554951689
H,0,1.5456578261,-2.450952974,1.0750116233
H,0,1.646480593,-2.3912299996,-0.6802250157
H,0,3.6492416965,-1.3167652873,0.3528747954
H,0,-3.2032888627,-2.0712401997,-0.0688337458

INT3-NoTail-H-*Triplet-Syn*
SCF Done: E(UPBE1PBE) = -748.770348512 A.U. after 3 cycles
SMD-CDS (non-electrostatic) energy (kcal/mol) = -0.57
Sum of electronic and thermal Free Energies= -748.665577 A.U.

C,0,3.6895365579,0.4713907235,0.004010982
C,0,4.2532119466,1.8861661479,0.0103825549
C,0,0.1683597744,-1.2218125316,-0.0171072077
C,0,2.1655064214,0.4677605007,-0.0055653411
C,0,1.5401121138,-0.8795861379,-0.010382875
O,0,2.2435847705,-1.9437108708,-0.0082335062
Au,0,0.1451478713,-3.2408563753,-0.0137628463

P,0,0.1108418862,-5.6288520322,0.0011241708
H,0,-0.8597627446,-6.2173168079,0.829564793
H,0,-0.1423944947,-6.2541294874,-1.2314019656
H,0,1.2844154194,-6.2765551977,0.4210106256
H,0,3.9343947915,2.4467848178,-0.8760290868
H,0,3.9238711994,2.4430328117,0.8953130943
H,0,1.7703374278,1.0036343782,-0.8815007946
H,0,1.7594242579,1.0024017394,0.8661265709
H,0,4.0487260951,-0.0757835854,0.8838161845
H,0,4.0598386753,-0.0723508375,-0.8733200246
H,0,5.3479767477,1.8685027853,0.0168230636
H,0,-0.6715100169,-0.5298506008,-0.0211939017

6.3 The structures shown in Figure S12.

TS-33-Hg
SCF Done: E(RPBE1PBE) = -2091.66015672 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.82
Sum of electronic and thermal Free Energies= -2091.427045 A.U.

C,0,4.4444727226,5.1467632219,0.0269179704
C,0,5.6971038498,4.456689836,-0.4993635423
C,0,6.8728223294,0.665758618,0.7398671464
C,0,6.094414178,1.6951511446,0.1601539328
H,0,4.1370763382,5.8534065372,-0.7512715852
H,0,6.4913086012,5.1885168258,-0.676139107
H,0,4.6971744072,5.7402937164,0.9106056681
H,0,5.5273727954,3.9187831172,-1.4361076665
H,0,7.7033001643,0.9148633243,1.3950145871
C,0,3.2831433852,4.2049824718,0.3408966828
H,0,2.8878514574,3.7525669562,-0.5768113791
H,0,2.4598483468,4.7745796494,0.7896668631
C,0,3.7241058471,3.1246933488,1.3014624367
S,0,6.4640342594,3.2892681039,0.6835380357
O,0,4.7473483334,3.3832290126,2.0319476417
C,0,5.0022148917,1.3762569503,-0.6805630901
C,0,4.7360698749,0.0320928353,-0.9701557999
C,0,5.5029402451,-0.9700461359,-0.3993830996
C,0,6.5736017367,-0.649879641,0.4575851711
H,0,4.4525495973,2.1481438201,-1.2066673598
H,0,3.9278624916,-0.2140724985,-1.6522843107
H,0,5.2932973315,-2.0107952079,-0.6291977717
H,0,7.1758673514,-1.4428057042,0.8908387243
C,0,3.5934808469,0.798574559,2.3225370517
H,0,3.6846232636,-0.1433372828,1.7617547959

H,0,4.5840115642,1.0547614829,2.7118783748
C,0,2.6157849504,0.5798749411,3.4856746586
H,0,1.6185685341,0.3046890001,3.1247868929
H,0,2.9834657247,-0.2301030695,4.1228990541
H,0,2.5244550983,1.4833071625,4.0962079713
C,0,3.1347733533,1.8525366445,1.3881166623
S,0,-1.8346922983,2.052591995,-0.2852501385
O,0,-0.5819600186,1.2158658404,-0.5294601496
O,0,-1.5511919794,3.3319609234,0.3597726782
O,0,-2.7176317061,2.0236342283,-1.442457362
C,0,-2.6949280212,1.0398884319,1.012934238
F,0,-3.8183915203,1.6479193453,1.3864223583
F,0,-2.9932561647,-0.1699345345,0.544686027
F,0,-1.9067650369,0.9002918593,2.0830032478
Hg,0,1.3126014846,1.5682008912,0.4380469307

The highest point of the relaxed potential energy surface scan (TS-OS-Hg)
E_{sol}=-2091.64896388 A.U.

C	-3.02775700	-1.73279300	-1.45617900
C	-4.36934600	-2.25725700	-0.93882700
C	-0.80734900	-0.09351900	0.93788700
C	-5.64673500	1.29207300	0.73031600
C	-5.44748900	0.27155900	-0.21505100
H	-5.57430400	1.06881400	1.79215300
C	-1.78351100	-1.97609500	-0.57959000
C	-1.74953800	-1.19932400	0.69930100
S	-5.14740100	-1.34395600	0.43065700
O	-2.41478700	-1.48433100	1.69293200
C	-5.54573200	0.56852000	-1.58283300
C	-5.82791400	1.87084900	-1.99024400
C	-6.02302700	2.88343300	-1.05098100
C	-5.93667100	2.58605000	0.31078700
H	-5.42053800	-0.20423200	-2.33425800
H	-5.90343700	2.08994700	-3.05218000
H	-6.24564700	3.89562600	-1.37665300
H	-6.09121900	3.36585900	1.05165600
C	-1.16857300	1.06664900	1.72043300
H	-1.20291200	1.85817000	0.93351500
H	-2.18354400	0.97668300	2.12114500
C	-0.15122500	1.51280800	2.77894300
H	-0.12073500	0.78103900	3.59049200
H	0.85335800	1.61339200	2.35761200
H	-0.45767500	2.47823900	3.18815500
H	-1.73042500	-3.03884800	-0.31020700
H	-0.89043700	-1.73367100	-1.16549000

H	-4.25782900	-3.27123600	-0.53879800
H	-5.09108200	-2.32339800	-1.75863600
H	-2.83702700	-2.25829800	-2.39864500
H	-3.10418000	-0.66926300	-1.70638700
S	4.37477200	-0.44936700	-0.09659800
O	3.02396300	-0.26875800	-0.80091900
O	4.29219900	-0.29690400	1.35392000
O	5.12013400	-1.57228900	-0.64610200
C	5.24558100	1.07418500	-0.70348400
F	6.46871300	1.11838900	-0.18156300
F	5.34059800	1.06317200	-2.03032900
F	4.57741200	2.16515800	-0.32736200
Hg	1.10503600	-0.26600900	0.15441700

INT-OS-Hg

E_{sol}=-2091.70520381 A.U.

C	-3.60792800	-2.39274300	-0.85271600
C	-4.33711400	-2.20745400	0.47479100
C	-1.02693400	-0.34756900	-0.55965400
C	-5.44353200	1.74834400	1.08034600
C	-5.32768800	0.46236600	0.52872100
H	-4.81539900	2.03729600	1.92027500
C	-2.10184300	-2.67465000	-0.68457900
C	-1.43642000	-1.62535300	0.15765200
S	-4.09710100	-0.58537000	1.26614800
O	-1.30873400	-1.73699500	1.36178400
C	-6.15442000	0.10193900	-0.54094200
C	-7.08319000	1.01602800	-1.04275100
C	-7.19596400	2.29241200	-0.49635800
C	-6.36877700	2.65324300	0.56915500
H	-6.08923100	-0.88180600	-0.99369000
H	-7.72101800	0.71908000	-1.87141800
H	-7.92138900	2.99761400	-0.89213200
H	-6.44794500	3.64243000	1.01272900
C	-1.05747400	0.85545200	0.14143600
H	-1.16834600	-0.31317900	-1.64159800
H	-1.11202800	0.78759800	1.22998800
C	-1.12121200	2.19175000	-0.46498900
H	-0.44681300	2.89177900	0.03892200
H	-0.95824800	2.19018000	-1.54388200
H	-2.13642000	2.56670300	-0.25699300
H	-1.96908200	-3.63329200	-0.17390600
H	-1.63143900	-2.72554000	-1.67224500
H	-3.97557700	-2.92754200	1.21673100

H	-5.41168200	-2.38266700	0.37211500
H	-4.03986000	-3.25658000	-1.37118200
H	-3.76683000	-1.52344200	-1.50019600
S	4.35019800	-0.35828100	0.52959400
O	3.34861700	-0.38239700	-0.63589000
O	3.72217600	-0.02034300	1.80344100
O	5.26662900	-1.48530800	0.46036500
C	5.35549600	1.12705000	0.04665600
F	6.31110400	1.32565900	0.94956700
F	5.91588600	0.94069200	-1.14485900
F	4.57801800	2.20911900	-0.00649000
Hg	1.21911500	-0.19467500	-0.43559400

6.4 The structures shown in Scheme 14 and Figure 4 in the main text.

IPr-R

SCF Done: E(RPBE1PBE) = -2193.42453658 A.U. after 1 cycles
SMD-CDS (non-electrostatic) energy (kcal/mol) = -13.33
Sum of electronic and thermal Free Energies= -2192.734365 A.U.

C,0,1.2605737558,1.4887969856,-0.6172055979
C,0,2.6194748438,1.0133019322,-1.1136122537
C,0,-2.0713345069,1.5353377252,0.227378567
C,0,5.2059981335,-1.5518754016,-1.4399206333
C,0,4.9833147181,-0.3097081533,-0.8547954319
H,0,0.9410951024,2.3116052314,-1.2661039348
H,0,3.2860209035,1.8694133591,-1.2664762676
H,0,1.3468332352,1.9001863668,0.3956134782
H,0,2.5468017827,0.4504731454,-2.0515679044
H,0,4.4594006206,-2.3346569224,-1.3339235944
C,0,0.1920759341,0.3834662109,-0.6455374991
H,0,0.4987541841,-0.464317221,-0.024110243
H,0,0.0747401801,0.0029985511,-1.6671565533
C,0,-1.0933811559,0.8984698547,-0.1786105424
S,0,3.4698826943,-0.0596885907,0.0956835792
O,0,2.7302781827,-1.390444312,0.1154614924
C,0,5.9264747151,0.7156305981,-0.9351117368
C,0,7.1043237238,0.4937958497,-1.6454489408
C,0,7.3361929368,-0.743332359,-2.2505706272
C,0,6.391785486,-1.7639048495,-2.1443529258
H,0,5.7520425698,1.6741360812,-0.4510528464
H,0,7.8444688101,1.2858257192,-1.7196401335
H,0,8.2597578097,-0.9136365117,-2.7971682122
H,0,6.5772107873,-2.7291728463,-2.6077849631
Au,0,-2.8746725808,-0.4924454989,0.0472321251
C,0,-4.065539233,-2.1242246583,0.0470846515
N,0,-4.6305225543,-2.7284313345,1.1174899851

N,0,-4.4993091632,-2.8261599786,-1.0255828495
C,0,-5.408710992,-3.7968908209,0.7218931528
C,0,-4.4514079077,-2.3129299647,2.4835271382
C,0,-5.3250295179,-3.8590788093,-0.6322794726
C,0,-4.1330030613,-2.5489828461,-2.3894422226
H,0,-5.9467212441,-4.4074331744,1.43152394
C,0,-5.3629536909,-1.3930416407,3.0298177878
C,0,-3.3817925416,-2.8585063928,3.2143940314
H,0,-5.7723818519,-4.5376996638,-1.3429952737
C,0,-4.8937029728,-1.6144794416,-3.1132635437
C,0,-3.0390472765,-3.238852235,-2.9407940261
C,0,-5.163513832,-1.0059332547,4.3586366398
C,0,-6.5312762129,-0.8224000075,2.2465035061
C,0,-3.2313016261,-2.4386380271,4.5398063047
C,0,-2.4090844917,-3.8627848169,2.6245327146
C,0,-4.5076922222,-1.3589346028,-4.4330031668
C,0,-6.0974823217,-0.9001024553,-2.5269474023
C,0,-2.6994716504,-2.9467920804,-4.265535961
C,0,-2.2393378256,-4.2724072015,-2.1682907078
C,0,-4.1095228235,-1.5205943956,5.1064409485
H,0,-5.8474052016,-0.2929649559,4.8114313188
H,0,-6.5165632508,-1.2554138584,1.2411719585
C,0,-7.8692206391,-1.2029952281,2.8884304652
C,0,-6.4135667009,0.6969284725,2.096041612
H,0,-2.4139057096,-2.8384129457,5.1343657483
H,0,-2.7015417813,-4.0530052111,1.5869400287
C,0,-2.4672651863,-5.2003154071,3.36953051
C,0,-0.9808663963,-3.3093844429,2.6083218877
C,0,-3.4214019181,-2.0144022183,-5.0035222722
H,0,-5.0706428803,-0.6389588055,-5.0213345392
H,0,-6.2289922778,-1.2416731761,-1.4950781141
C,0,-5.8832792414,0.615986747,-2.488095258
C,0,-7.3772183145,-1.251913543,-3.2922249548
H,0,-1.8580813183,-3.4604753587,-4.7231380378
H,0,-2.6552223794,-4.345131483,-1.1584000354
C,0,-0.7706383829,-3.8610199081,-2.029853321
C,0,-2.3586995896,-5.6578041327,-2.8119149614
H,0,-3.9736605776,-1.2070138289,6.1382619022
H,0,-7.9706215501,-0.7676791396,3.8889969712
H,0,-8.6998474191,-0.8318351297,2.277657535
H,0,-7.9762745199,-2.2891892012,2.9813366576
H,0,-6.4540603409,1.1975768797,3.0701844405
H,0,-5.4732022613,0.9804700945,1.6102971084
H,0,-7.2397601376,1.0820148746,1.4878368737
H,0,-1.7995026154,-5.9263638393,2.89222893
H,0,-2.1488408966,-5.0904363976,4.4124024983

H,0,-3.4796075328,-5.6188520882,3.36739415
H,0,-0.9242787114,-2.3595370003,2.0653010085
H,0,-0.608680671,-3.1384571471,3.6247531068
H,0,-0.3034078414,-4.0192290749,2.1204832214
H,0,-3.1383979165,-1.801910038,-6.0312984419
H,0,-4.9828981967,0.8772843836,-1.9202752257
H,0,-5.7786535339,1.0302414931,-3.4972831229
H,0,-6.7398101555,1.1075198796,-2.0130319871
H,0,-8.2422667031,-0.770676368,-2.8221984934
H,0,-7.3276567763,-0.9085457827,-4.3316874695
H,0,-7.5552075132,-2.3328111903,-3.3021653995
H,0,-0.2772728615,-3.8019204384,-3.0066619028
H,0,-0.6708858537,-2.8864579643,-1.540324779
H,0,-0.2279231148,-4.5977622456,-1.4271327682
H,0,-1.9264201965,-5.6685231927,-3.8189528085
H,0,-1.8219774786,-6.4000972956,-2.2104869486
H,0,-3.4034247156,-5.9775418687,-2.890881861
H,0,-2.7424738333,2.3017452089,0.5717035748

IPr-TS-7-*endo-dig*
SCF Done: E(RPBE1PBE) = -2193.40659927 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -13.60
Sum of electronic and thermal Free Energies= -2192.713707 A.U.

C,0,-3.466956487,-2.3227392807,-0.8624371824
C,0,-4.830515795,-1.6443405238,-0.858329304
C,0,-2.2818448361,0.630333976,0.0122879386
C,0,-7.1515744007,1.0467679978,-0.5637123213
C,0,-6.7592896817,-0.0244572844,0.2340249057
H,0,-6.4024699519,1.6564707355,-1.0606453853
C,0,-2.2980958562,-1.5204930599,-1.445989152
C,0,-1.8329515795,-0.3738209546,-0.6150491895
S,0,-5.0154091856,-0.3865809404,0.4428647423
O,0,-4.2854083161,0.8800409786,-0.076953312
C,0,-7.6840073109,-0.8120245917,0.9197505776
C,0,-9.0411216313,-0.5320558657,0.7726414167
C,0,-9.4538928791,0.5306589857,-0.0324898851
C,0,-8.5126734528,1.3189435862,-0.6950109085
H,0,-7.3578497899,-1.6289784625,1.55943475
H,0,-9.7742515665,-1.1379628368,1.2974720555
H,0,-10.5129192613,0.7503785306,-0.1361049878
H,0,-8.8357018886,2.1515318141,-1.3136681993
Au,0,0.2110366052,-0.0210008423,-0.1901046663
H,0,-1.4672136877,-2.2094584138,-1.6161988269
H,0,-2.5767671999,-1.1200891506,-2.4301531563
H,0,-5.6137371551,-2.3805415967,-0.6434975841

H,0,-5.0638910251,-1.1501497691,-1.8090658078
H,0,-3.2143556936,-2.6741377743,0.14519705
H,0,-3.579100605,-3.2207718301,-1.4813355951
H,0,-2.2101395286,1.5313332379,0.5919996395
C,0,2.2072056351,0.1371273388,0.1069793241
N,0,3.0966153735,-0.8725629942,0.2614853047
N,0,2.9471481236,1.2677575081,0.1883161232
C,0,4.3759766493,-0.3805954031,0.4375711444
C,0,2.7610527586,-2.2706133296,0.2348591853
C,0,4.2814723626,0.9719129196,0.3911344882
C,0,2.4228214992,2.6003831401,0.0656245477
H,0,5.2259701995,-1.031633093,0.5764785912
C,0,2.8151407217,-2.9490571959,-0.9956268524
C,0,2.4150920317,-2.9028117106,1.4419678058
H,0,5.031318087,1.743399299,0.4826263374
C,0,2.3414141271,3.1712946721,-1.2162771
C,0,2.0401375279,3.2831925979,1.2330972663
C,0,2.4814160608,-4.3071108392,-0.9953290797
C,0,3.2264088473,-2.2725243806,-2.2905065184
C,0,2.0936071625,-4.2627742928,1.3851751901
C,0,2.3866122499,-2.1744641601,2.7731525193
C,0,1.8355039278,4.4717468924,-1.3090507733
C,0,2.7860673208,2.4421770288,-2.4706722746
C,0,1.5431521225,4.5818205325,1.0832186198
C,0,2.1521924177,2.6707043031,2.6178196453
C,0,2.1227195591,-4.95820876,0.1806326195
H,0,2.5101765252,-4.8618478867,-1.9296526033
H,0,3.4542853657,-1.2245260089,-2.070588396
C,0,4.4964269931,-2.9065394665,-2.8666482221
C,0,2.090738538,-2.2916299997,-3.3176492668
H,0,1.820918886,-4.783396429,2.2995330388
H,0,2.6491072094,-1.1268210017,2.594438986
C,0,3.4239800083,-2.7510601205,3.742202383
C,0,0.9863284482,-2.1973157432,3.3932669591
C,0,1.4392835336,5.1704158793,-0.1731547028
H,0,1.7561115298,4.9432175129,-2.2853320804
H,0,3.1382412938,1.4466253238,-2.181576869
C,0,1.6231708436,2.253128626,-3.4493988626
C,0,3.9579869035,3.1656097873,-3.1421489979
H,0,1.2356889829,5.1387199948,1.9648301425
H,0,2.5693791469,1.6640629534,2.5126444713
C,0,0.7788116912,2.5292220419,3.2811685776
C,0,3.1080348076,3.4742461761,3.5050522427
H,0,1.8699313832,-6.0152449036,0.1591736856
H,0,4.3276901667,-3.9515747868,-3.1500592615
H,0,4.8155631096,-2.3646113174,-3.76397568

H,0,5.3196439327,-2.8823334053,-2.1442734047
H,0,1.8222944375,-3.3170143796,-3.5968489533
H,0,1.192655828,-1.7990321425,-2.9288542147
H,0,2.396506094,-1.7665405174,-4.2296903986
H,0,3.4258923542,-2.179877253,4.6775034091
H,0,3.2008025892,-3.7954200859,3.9887568135
H,0,4.4343574076,-2.7125919976,3.3205546065
H,0,0.2427002951,-1.7632542004,2.715582724
H,0,0.6721062119,-3.2196477281,3.6327764471
H,0,0.9753186608,-1.619440086,4.3243632268
H,0,1.0506433574,6.1812376493,-0.2670859336
H,0,0.7947095744,1.7068767166,-2.984653075
H,0,1.2372977652,3.2163214115,-3.8018557398
H,0,1.9551211418,1.6856873793,-4.3262534902
H,0,4.3033568345,2.5985717441,-4.0139921291
H,0,3.6650827445,4.1635609302,-3.4876006991
H,0,4.8039830495,3.2818988049,-2.4558599941
H,0,0.3050167139,3.5057592972,3.4326286666
H,0,0.1044805597,1.9150292768,2.6742427319
H,0,0.8808388513,2.0511502115,4.262038681
H,0,2.7299929555,4.4871395023,3.6845584846
H,0,3.2228087088,2.9837853325,4.4781787994
H,0,4.1014032287,3.5617594915,3.0513809985

IPr-INT1
SCF Done: E(RPBE1PBE) = -2193.43147577 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -13.56
Sum of electronic and thermal Free Energies= -2192.734142 A.U.

C,0,-0.8021563506,-1.8569256807,1.4352094675
C,0,-2.2333402348,-1.5130484836,1.0430689071
C,0,-0.0988949209,0.3085231016,-0.7908980596
C,0,-4.5553786428,-0.6839383544,-1.0789097978
C,0,-4.0213356495,0.2679658871,-0.2048390115
H,0,-3.9657296674,-1.5262674614,-1.4265210359
C,0,0.1983039725,-1.9200893486,0.273935481
C,0,0.7199714584,-0.5807960227,-0.2219736884
S,0,-2.3662158437,0.1650784951,0.3948557188
O,0,-1.505262497,0.0486641647,-0.9956810568
C,0,-4.7587907807,1.3713973271,0.2334238687
C,0,-6.0739898059,1.5105187235,-0.2033725159
C,0,-6.6220615693,0.5702900384,-1.0739801905
C,0,-5.8648802791,-0.5183459492,-1.5144770163
H,0,-4.3186103646,2.1064493952,0.9017809627
H,0,-6.6638895345,2.3578611347,0.1325366661
H,0,-7.6461275434,0.6865544871,-1.4173829465

H,0,-6.2961380392,-1.2418961718,-2.1996797166
Au,0,2.7061439529,-0.1071798774,-0.0280279934
H,0,1.040970594,-2.5323110531,0.6043587543
H,0,-0.2651199898,-2.4620311969,-0.5645928518
H,0,-2.9060145349,-1.5235040426,1.9093660199
H,0,-2.6223139142,-2.1935816523,0.2785115295
H,0,-0.443297412,-1.1731000701,2.213601652
H,0,-0.8709931288,-2.8489395036,1.8973413755
C,0,4.6871379343,0.3446385457,0.1945592637
N,0,5.5697334265,-0.1951786791,1.0714391311
N,0,5.4138659239,1.2547508931,-0.5000950209
C,0,6.8250669486,0.3651971057,0.9269729338
C,0,5.2479421119,-1.2202867635,2.0255260038
C,0,6.7266131551,1.2819816459,-0.0679025035
C,0,4.892394561,2.0775400267,-1.5569563124
H,0,7.662505192,0.064057765,1.538483288
C,0,5.4124199327,-2.5644535413,1.6481049135
C,0,4.8019745438,-0.8359395734,3.3022467709
H,0,7.4612364847,1.9428877747,-0.5030426366
C,0,4.9477408211,1.5912681937,-2.8747359452
C,0,4.3600837223,3.336830092,-1.2295348319
C,0,5.0947340584,-3.542739524,2.5956212977
C,0,5.9175897891,-2.9771818034,0.2777175359
C,0,4.5027653157,-1.8542908412,4.2128212863
C,0,4.6333253356,0.6162435959,3.7103302788
C,0,4.4399466111,2.4133717325,-3.8857025153
C,0,5.522805077,0.2303550031,-3.2225578372
C,0,3.8610712277,4.1161060971,-2.2781531204
C,0,4.3069633769,3.8605000539,0.1942331814
C,0,4.6443733071,-3.1938102947,3.8647279838
H,0,5.2053586109,-4.5919293546,2.3336676644
H,0,6.11322643,-2.0691162421,-0.30124113
C,0,7.2369393076,-3.7495779863,0.3814511719
C,0,4.8661037951,-3.7907000826,-0.4830989415
H,0,4.1537354461,-1.5920236241,5.2082669573
H,0,4.9363573812,1.2449479608,2.8668593188
C,0,5.5331341707,0.9729851553,4.8975143005
C,0,3.1677091374,0.9373498964,4.0200130128
C,0,3.899874867,3.6614284572,-3.5923959248
H,0,4.4658843841,2.0675360121,-4.9158815776
H,0,5.8558839965,-0.2452070878,-2.2945519401
C,0,4.4603411415,-0.6788220028,-3.8489277485
C,0,6.7429412871,0.3559167264,-4.1399306933
H,0,3.4370081551,5.0926816074,-2.0594344147
H,0,4.7695648681,3.1141943654,0.8479955887
C,0,2.8604070344,4.0494801473,0.6617523563

C,0,5.1035746635,5.1601225615,0.3469099745
H,0,4.4046972682,-3.9696850582,4.5875034773
H,0,7.1056773616,-4.6952672914,0.9199532082
H,0,7.6159744286,-3.9866898962,-0.6190796715
H,0,8.0038292647,-3.1684852033,0.905325539
H,0,4.6427171138,-4.7326510037,0.0309704052
H,0,3.9299422935,-3.2316751781,-0.5902642277
H,0,5.2311358246,-4.0366116453,-1.4868476531
H,0,5.437568892,2.0380232965,5.1371000893
H,0,5.2573618412,0.4050991914,5.7934578093
H,0,6.5870483191,0.7680812577,4.6796490315
H,0,2.5219397632,0.715668063,3.1627821699
H,0,2.8063955039,0.3581053996,4.8777175003
H,0,3.0565700502,2.0002746875,4.2635692359
H,0,3.5076255121,4.2836728562,-4.3928568851
H,0,3.5918082714,-0.7905137855,-3.1904318621
H,0,4.1102436411,-0.2802935901,-4.8081477025
H,0,4.8775603899,-1.675229274,-4.0345018196
H,0,7.1714889236,-0.6335393424,-4.3357486526
H,0,6.4724325901,0.798223815,-5.1055712724
H,0,7.5238300694,0.979169104,-3.6904322057
H,0,2.3465742599,4.8127788073,0.0658144616
H,0,2.2908107822,3.1166139753,0.5837743264
H,0,2.8406955388,4.373075615,1.708738144
H,0,4.6710780714,5.9689611065,-0.2530793956
H,0,5.0987628048,5.4834294406,1.394078252
H,0,6.1467772768,5.0322924706,0.0377033409
H,0,0.1576868864,1.2827802521,-1.1937880551

IPr-TS-6-*exo-dig*

SCF Done: E(RPBE1PBE) = -2193.41366805 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -13.42
Sum of electronic and thermal Free Energies= -2192.722914 A.U.

C,0,3.9252084025,-2.2564308038,0.3882035447
C,0,5.2125852379,-2.491017891,-0.3813653975
C,0,1.7253028159,0.1001379765,-1.4523071521
C,0,5.2302790302,1.2335214775,-0.2056576942
C,0,6.0749540758,0.1405468108,-0.3721611191
H,0,4.2927076315,1.2787929534,-0.7510299688
C,0,2.6592338048,-2.2188074201,-0.4849416056
C,0,2.3508941862,-0.9363905042,-1.0991810543
S,0,5.6326602924,-1.1543418236,-1.5433730442
O,0,4.2925875159,-0.7450315859,-2.1755561914
C,0,7.3035425384,0.0594258012,0.2853440407

C,0,7.6727724652,1.0850024079,1.1525739496
C,0,6.8290355885,2.1815199657,1.3418533692
C,0,5.6143543241,2.2567720043,0.6619995385
H,0,7.9705138677,-0.7845867243,0.1244143617
H,0,8.6248938579,1.031581794,1.6728929485
H,0,7.125391186,2.9826964628,2.0132371889
H,0,4.9616734204,3.1140770182,0.8018026446
Au,0,-0.1590622728,0.0574255454,-0.5376662099
H,0,2.7013783054,-2.9911644475,-1.263038547
H,0,1.7846746322,-2.4527557496,0.1361091681
H,0,5.1504779252,-3.3936572121,-0.9996631181
H,0,6.0740998804,-2.5980483204,0.2862375165
H,0,3.8216393213,-3.0990964557,1.080080375
H,0,3.9936021978,-1.3511062237,1.0004896307
C,0,-2.0147896806,0.1588844845,0.2622275513
N,0,-2.7529719821,1.2706233877,0.4918427712
N,0,-2.8024659048,-0.8700724692,0.6538132464
C,0,-3.9877768269,0.9420439163,1.0184240753
C,0,-2.3116262743,2.6150852451,0.2336188672
C,0,-4.0192392287,-0.4104476085,1.1206491538
C,0,-2.4227902109,-2.2550575524,0.5957729969
H,0,-4.7220686228,1.6926801787,1.2690860046
C,0,-2.5748049663,3.1780122124,-1.0272350608
C,0,-1.6514647045,3.3128385757,1.2603330359
H,0,-4.7851037628,-1.0816681822,1.4793274036
C,0,-2.6644270025,-2.9682550455,-0.591324345
C,0,-1.8431205409,-2.8398025183,1.7354781429
C,0,-2.1358260571,4.4869000514,-1.250260131
C,0,-3.3093779548,2.429119542,-2.1238263727
C,0,-1.2315254837,4.6175627578,0.9823476096
C,0,-1.3900317964,2.710459982,2.6289035856
C,0,-2.2835059176,-4.3137155397,-0.6202671238
C,0,-3.3168779103,-2.3406664109,-1.8095378063
C,0,-1.4850263802,-4.1893193917,1.6529564252
C,0,-1.601813039,-2.0720446133,3.0228129749
C,0,-1.4684869043,5.1991549679,-0.259013856
H,0,-2.3217578601,4.9526704967,-2.2145062278
H,0,-3.553508701,1.4299586987,-1.7488681409
C,0,-4.6291645664,3.1200031443,-2.4817017446
C,0,-2.4320671704,2.2533607615,-3.3672348686
H,0,-0.7145123866,5.1848664288,1.7519443959
H,0,-1.8192563494,1.7036955167,2.6469088741
C,0,-2.0779684159,3.5185587835,3.7337550225
C,0,0.1112136951,2.5767969282,2.9032228012
C,0,-1.6996542899,-4.91901827,0.4879352806
H,0,-2.4525634719,-4.89532053,-1.5228097967

H,0,-3.5418653006,-1.2949214218,-1.5760529515
C,0,-2.3725472276,-2.350688316,-3.0155048494
C,0,-4.6424143991,-3.0320835909,-2.1448222636
H,0,-1.03415464,-4.6737151707,2.5153803558
H,0,-1.9638094971,-1.0481133279,2.8848520744
C,0,-0.1083846742,-1.9886083407,3.3528929437
C,0,-2.3854604247,-2.6834047925,4.1883758722
H,0,-1.1351356983,6.2152679838,-0.453840594
H,0,-4.4559346902,4.1171477837,-2.9023985331
H,0,-5.171611796,2.5319483309,-3.2305970963
H,0,-5.2766686372,3.2320381337,-1.6052033859
H,0,-2.1817673867,3.2203957385,-3.8183851455
H,0,-1.4953428772,1.7377713142,-3.1276373261
H,0,-2.9612035508,1.6609216187,-4.1222973371
H,0,-1.9257659832,3.0348626716,4.7052726829
H,0,-1.671651367,4.5341387792,3.7998374771
H,0,-3.1568812516,3.5976499036,3.5608362642
H,0,0.6065243519,1.9722510448,2.1351288164
H,0,0.5996015338,3.5576341114,2.9297315986
H,0,0.2763166843,2.0954106129,3.8739153525
H,0,-1.4147633835,-5.9671614905,0.4449777394
H,0,-1.4340936725,-1.8303739774,-2.7923750308
H,0,-2.128797384,-3.3741301642,-3.322505158
H,0,-2.8431651773,-1.8494583804,-3.8689040502
H,0,-5.1272728613,-2.5307685618,-2.9900793189
H,0,-4.4869284024,-4.0804980865,-2.4239089856
H,0,-5.3338517447,-3.0083647774,-1.2952677577
H,0,0.3212773868,-2.9838597484,3.5153496894
H,0,0.4522596599,-1.5024281045,2.5467289642
H,0,0.0440658739,-1.406059384,4.2685346651
H,0,-2.0494872403,-3.7040327408,4.4035175507
H,0,-2.2401716609,-2.0866818793,5.0957591912
H,0,-3.4593912769,-2.7202701127,3.9752666256
H,0,1.9656491348,0.9382119432,-2.0939916991

IPr-INT2

SCF Done: E(RPBE1PBE) = -2193.43638100 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -13.18
Sum of electronic and thermal Free Energies= -2192.739380 A.U.

C,0,1.5840816843,2.9041151974,-0.769914548
C,0,2.8902197679,2.8901064251,0.0082522514
C,0,-0.3743090812,0.2657728278,0.839092062
C,0,3.0120341887,-1.2244094364,0.3525218329
C,0,3.2263869362,0.0538939424,-0.1721976255

H,0,2.7252197471,-1.3611793627,1.3915224357
C,0,0.3740301865,2.6266935556,0.1268348445
C,0,0.4581547046,1.3069045064,0.8219037867
S,0,3.1032002959,1.392018664,0.9983581751
O,0,1.6259436195,1.2250573123,1.6817001064
C,0,3.6139275902,0.2478412984,-1.4984694829
C,0,3.768637803,-0.8695526605,-2.3166798848
C,0,3.5349444616,-2.1488221625,-1.8159872861
C,0,3.1566742015,-2.3253687156,-0.4845089275
H,0,3.800130139,1.2370397618,-1.9021653348
H,0,4.0686184922,-0.731846585,-3.3512185275
H,0,3.652552156,-3.0124077266,-2.4643819969
H,0,2.9794874048,-3.3218672873,-0.0911670494
Au,0,-2.1619815575,0.0976725026,-0.125457189
H,0,0.2859592461,3.4273617463,0.8753242854
H,0,-0.5371545904,2.6328238774,-0.4754101283
H,0,2.9246118089,3.6836031129,0.7636378371
H,0,3.7861785453,2.9898851512,-0.6125612929
H,0,1.4975813354,3.9004051281,-1.21715586
H,0,1.6144857084,2.1798465463,-1.5894944708
C,0,-3.953864704,-0.1442422873,-1.0855958642
N,0,-4.1651503618,-0.586545201,-2.350370379
N,0,-5.1977993117,0.0800729881,-0.5943707939
C,0,-5.5151717977,-0.6381018199,-2.6442163712
C,0,-3.1251246146,-0.9682636497,-3.2660624176
C,0,-6.1684057564,-0.216677747,-1.5328851131
C,0,-5.4808592155,0.5497860446,0.7339650232
H,0,-5.8818683816,-0.9680647902,-3.6045956785
C,0,-2.698455817,-2.3079122464,-3.2775324618
C,0,-2.5949806767,0.0082510693,-4.1267429818
H,0,-7.2215279344,-0.1029275611,-1.3238133558
C,0,-5.6288967839,-0.3962104513,1.7634343699
C,0,-5.6203592628,1.9327653642,0.9437956277
C,0,-1.6899046064,-2.6542185035,-4.1822546422
C,0,-3.2841670898,-3.3649468803,-2.3593954701
C,0,-1.5872168969,-0.3912824213,-5.0102174042
C,0,-3.0793012182,1.4466339483,-4.1332500825
C,0,-5.9123903336,0.0865017159,3.0448703273
C,0,-5.4860445445,-1.8896762262,1.533192016
C,0,-5.9093088704,2.3609843974,2.2432351815
C,0,-5.4709158509,2.9533303033,-0.1694878168
C,0,-1.1372676983,-1.7073271468,-5.0384248477
H,0,-1.3347391934,-3.6810012629,-4.2149679218
H,0,-4.0526342099,-2.8917212471,-1.7400139911
C,0,-3.9618064945,-4.4838906834,-3.1565614982
C,0,-2.2206187788,-3.9342199156,-1.4153137051

H,0,-1.1536896864,0.3392185579,-5.6884272851
H,0,-3.8623057243,1.5467531011,-3.3745966062
C,0,-3.6973524429,1.8166380741,-5.4853559494
C,0,-1.9542870374,2.4178022668,-3.7641386615
C,0,-6.0516587027,1.4498118964,3.2845159087
H,0,-6.0268307985,-0.6174443066,3.8650271755
H,0,-5.3216970069,-2.054811962,0.4634588868
C,0,-4.2700443882,-2.4483346463,2.2788895596
C,0,-6.7603573923,-2.644489431,1.923656205
H,0,-6.022430758,3.4240285257,2.4390922412
H,0,-5.2275805948,2.417811536,-1.0928400595
C,0,-4.3193827959,3.9218705408,0.1168271114
C,0,-6.7796194344,3.7134661138,-0.407735416
H,0,-0.3544591031,-1.9977526861,-5.7345883016
H,0,-3.2405178225,-5.0248616393,-3.7797101021
H,0,-4.4213358598,-5.2078294125,-2.4740555822
H,0,-4.7469261233,-4.0925180493,-3.812883218
H,0,-1.4354029458,-4.460696943,-1.9701580896
H,0,-1.7472522176,-3.1422674973,-0.8243595673
H,0,-2.6759878701,-4.6503857082,-0.7216668428
H,0,-4.0965152086,2.8367176985,-5.4522998437
H,0,-2.9529514113,1.7753348778,-6.2888827743
H,0,-4.5172468801,1.1404371919,-5.7512410411
H,0,-1.5262708987,2.1754410151,-2.7852548665
H,0,-1.1463531081,2.3912965557,-4.5044762519
H,0,-2.3374631207,3.4438826217,-3.7245867955
H,0,-6.2733128526,1.803480584,4.2882816793
H,0,-3.3491643021,-1.935979441,1.9782426575
H,0,-4.3834842802,-2.3355421556,3.3633791897
H,0,-4.1510796547,-3.5166674207,2.0641463842
H,0,-6.6546547689,-3.7095116009,1.688168674
H,0,-6.9628816762,-2.5604532285,2.9974816188
H,0,-7.6352091187,-2.2641450146,1.3850004806
H,0,-4.5140313348,4.5205770267,1.0141735123
H,0,-3.3768973861,3.3840442946,0.2668645802
H,0,-4.1877162506,4.6133896432,-0.7233365352
H,0,-7.0664471722,4.298435473,0.4736741727
H,0,-6.6664623399,4.4089082684,-1.2471424622
H,0,-7.604213457,3.0313148671,-0.6418582989
H,0,-0.0298282043,-0.5663646467,1.4604483108

IPr-TS-INT2-*conf*

SCF Done: E(RPBE1PBE) = -2193.42606378 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -13.28
Sum of electronic and thermal Free Energies= -2192.729933 A.U.

C,0,3.3080034077,-1.5780117817,2.83102755
C,0,4.7202653418,-1.3601637255,2.2510087321
C,0,1.75674325,-1.292640422,-0.4454437637
C,0,6.758957206,-1.127440137,-1.178602525
C,0,5.653369812,-0.8363797388,-0.3725191931
H,0,7.2471731453,-2.0967241238,-1.1207782983
C,0,2.2507553939,-2.2268763808,1.9168997909
C,0,2.4721633016,-1.9456960667,0.4714582626
S,0,5.1103614011,-2.1664500539,0.6544949235
O,0,3.6662721216,-2.6353602746,0.0392350715
C,0,4.9982716186,0.3998707718,-0.4346005012
C,0,5.4736063553,1.3556477696,-1.3249460375
C,0,6.5850902891,1.083092123,-2.1268899375
C,0,7.2278605803,-0.1514492086,-2.0539496085
H,0,4.1336960011,0.616740109,0.1854347499
H,0,4.9750219441,2.3180603302,-1.3914816416
H,0,6.9517240607,1.8415866486,-2.812831855
H,0,8.0922156052,-0.3597552709,-2.6771603851
Au,0,-0.0590603955,-0.4019368435,-0.1968734761
H,0,2.2601339729,-3.3154268593,2.0562362681
H,0,1.2626176089,-1.8649918541,2.2073514996
H,0,4.9269271993,-0.3016587058,2.0938432795
H,0,5.4930055017,-1.757178053,2.9153347912
H,0,3.3977039498,-2.1687392119,3.7454021964
H,0,2.9544341345,-0.5844349194,3.1189831655
H,0,2.215935134,-1.2852966269,-1.4387333885
C,0,-1.8842161018,0.5113173065,-0.0293307643
N,0,-2.1359056336,1.820846871,0.2184263836
N,0,-3.1115897771,-0.0431277615,-0.1918274764
C,0,-3.4933400327,2.0813594538,0.208834538
C,0,-1.1268938935,2.8107703018,0.4757868254
C,0,-4.1105678006,0.9018705547,-0.0503331465
C,0,-3.3543494308,-1.4317672847,-0.4741144611
H,0,-3.889081222,3.0704366136,0.3847223942
C,0,-0.5626646243,3.4989739307,-0.6123064889
C,0,-0.7572646407,3.0585085657,1.8095832942
H,0,-5.1560810125,0.6500740474,-0.1464548523
C,0,-3.3973098563,-1.8481055096,-1.816161774
C,0,-3.5557979901,-2.3117419731,0.6036728634
C,0,0.4126612436,4.460737809,-0.3291279439
C,0,-0.9766659534,3.244191777,-2.0501371487
C,0,0.2230997837,4.0299092339,2.0366448606
C,0,-1.3760398564,2.3197695442,2.982568245
C,0,-3.6399506394,-3.2031291202,-2.0618883876
C,0,-3.1805965486,-0.8967972131,-2.9785714169

C,0,-3.7993387096,-3.6551879114,0.3014956588
C,0,-3.5153090133,-1.8603876513,2.0522815988
C,0,0.8042659166,4.7233259475,0.979706711
H,0,0.8689018324,5.0129500438,-1.1468868397
H,0,-1.7230668284,2.4434170203,-2.0540244524
C,0,-1.6284154527,4.4862490551,-2.6668047966
C,0,0.2073733319,2.7701588372,-2.8981826834
H,0,0.5340385023,4.2450044972,3.0559784432
H,0,-2.1059258221,1.6050484793,2.5890514606
C,0,-2.1256281497,3.2774605522,3.9140144168
C,0,-0.3232122103,1.5201026613,3.7555253374
C,0,-3.8386332061,-4.0988294266,-1.016303399
H,0,-3.6716504203,-3.560552039,-3.0877531124
H,0,-3.0619352697,0.1134817222,-2.5738906971
C,0,-1.8957845185,-1.2442307646,-3.7374663065
C,0,-4.3870226303,-0.8741478641,-3.9221093361
H,0,-3.9589282539,-4.3621328794,1.1117939044
H,0,-3.3056056042,-0.7861388527,2.0693046142
C,0,-2.3891113691,-2.5594708203,2.8197272493
C,0,-4.8650874347,-2.0772426709,2.743388013
H,0,1.5633760399,5.4760946705,1.1771348666
H,0,-0.9206253271,5.3213608053,-2.7212022096
H,0,-1.9666234705,4.2685983433,-3.6862073031
H,0,-2.4960989722,4.8169133754,-2.0855695868
H,0,0.9855754385,3.539106566,-2.9645669937
H,0,0.6592870249,1.8633490105,-2.4806090105
H,0,-0.124758522,2.5442986451,-3.9179235137
H,0,-2.6010271921,2.7182064638,4.7277841805
H,0,-1.4460598712,4.0096668278,4.3647275578
H,0,-2.9082855195,3.8285505775,3.3810991694
H,0,0.1989676727,0.8150995552,3.0996711399
H,0,0.4238497708,2.1796841882,4.2116560014
H,0,-0.7993869967,0.9485916656,4.5603280038
H,0,-4.0267156337,-5.1479378871,-1.2299704375
H,0,-1.0253259858,-1.2281966444,-3.0716797592
H,0,-1.9598155447,-2.2412372844,-4.1886397548
H,0,-1.7223643814,-0.5218915659,-4.5434877307
H,0,-4.2298509518,-0.1376377148,-4.7182518737
H,0,-4.5437955964,-1.8484871404,-4.3987297712
H,0,-5.3073951691,-0.606450803,-3.3914446419
H,0,-2.5533546057,-3.641773777,2.8731167214
H,0,-1.4180277957,-2.3887861746,2.3422250282
H,0,-2.3371059464,-2.1789061548,3.8463033771
H,0,-5.125858258,-3.1409758909,2.7834581127
H,0,-4.8272070355,-1.7033795017,3.7729126997
H,0,-5.6732922105,-1.5523148731,2.2223222787

IPr-INT2'
SCF Done: E(RPBE1PBE) = -2193.43128517 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -13.27
Sum of electronic and thermal Free Energies= -2192.736217 A.U.

C,0,-1.5637488515,-3.1837813103,0.1039302167
C,0,-3.0167849152,-2.8074687747,0.3614364444
C,0,0.5182489703,-0.1538818556,0.8410478595
C,0,-2.8951402316,1.2263389768,0.1368347865
C,0,-3.5523802645,-0.0036028264,0.0958328402
H,0,-1.579901182,-3.9940067516,-0.6320085317
H,0,-3.5491213055,-3.5419225515,0.9709326004
H,0,-1.1044853789,-3.5799628652,1.0150525815
H,0,-3.5606245107,-2.6427939762,-0.5718159536
H,0,-2.0709225339,1.4007119337,0.8204256935
C,0,-0.7672276275,-1.9943919855,-0.4284551266
H,0,-1.3076933711,-1.544347486,-1.2744321088
H,0,0.2032447029,-2.3166154901,-0.813368394
C,0,-0.5095516649,-0.9711427924,0.6332819136
S,0,-3.095805334,-1.2402185989,1.3063670355
O,0,-1.54743157,-0.934250577,1.665753231
C,0,-4.6351150378,-0.2377630888,-0.7538663083
C,0,-5.0400714147,0.7842956787,-1.6092277621
C,0,-4.3750305513,2.0100545749,-1.6082569413
C,0,-3.3091182719,2.2292454004,-0.7372504567
H,0,-5.1712057308,-1.1826448037,-0.7562710205
H,0,-5.8795381581,0.6154171662,-2.2771193563
H,0,-4.6938813409,2.7991213936,-2.2831349223
H,0,-2.793076353,3.1846824793,-0.7303573991
Au,0,2.227318863,-0.0260222105,-0.265040517
H,0,0.4007656491,0.5052050444,1.7071670087
C,0,3.9589014026,0.1707164728,-1.3350280143
N,0,5.0976147821,-0.5594278309,-1.2329510481
N,0,4.2379080529,1.0984200411,-2.2846794469
C,0,6.0699640776,-0.095486982,-2.0991203393
C,0,5.2836595873,-1.6667924461,-0.3360752494
C,0,5.5260538809,0.953440283,-2.764653925
C,0,3.3258915595,2.1151419955,-2.7321385763
H,0,7.0477917546,-0.5491310399,-2.1607565549
C,0,5.0232790443,-2.9651016284,-0.8081377281
C,0,5.7403851213,-1.4066726017,0.9676889424
H,0,5.9307801617,1.6021952742,-3.5268848175
C,0,2.5133842303,1.8475366118,-3.8478831007
C,0,3.3069607882,3.3458115635,-2.0527584403

C,0,5.2163550213,-4.0251719192,0.0832195619
C,0,4.5528213676,-3.2446835855,-2.22365437
C,0,5.9171194021,-2.5029925053,1.8176818111
C,0,6.0420260033,-0.0066964362,1.4702357663
C,0,1.6490284791,2.86137382,-4.2729217192
C,0,2.5382916507,0.519920636,-4.5832967539
C,0,2.4230439964,4.3242676758,-2.5186880242
C,0,4.2038324373,3.6415490149,-0.8647132195
C,0,5.6564212151,-3.7985942284,1.3834038843
H,0,5.0205726715,-5.0416393681,-0.2487316453
H,0,4.4654649263,-2.2882692322,-2.7490100267
C,0,5.5677053849,-4.0987895075,-2.9900050917
C,0,3.1686585976,-3.8992919211,-2.231941621
H,0,6.2657703667,-2.3364900475,2.8335655874
H,0,5.85649781,0.6973067652,0.6524660664
C,0,7.5130668573,0.1357039129,1.8726603613
C,0,5.1161806588,0.3795842042,2.6277681179
C,0,1.601672545,4.0866415194,-3.6160377129
H,0,1.0048993658,2.6857750875,-5.1307783059
H,0,3.2942337412,-0.1166911136,-4.1124409066
C,0,1.1920837938,-0.2016104464,-4.4660665785
C,0,2.938342343,0.6950234343,-6.0511789537
H,0,2.3811901344,5.2865497653,-2.0149622904
H,0,4.801088981,2.7476610159,-0.6577670277
C,0,3.3859559612,3.9471612965,0.3937515666
C,0,5.1767605995,4.7840146216,-1.1756394488
H,0,5.8003648205,-4.6364414618,2.0609295562
H,0,5.6828242865,-5.0885344709,-2.5334526205
H,0,5.234293424,-4.2448684329,-4.0236926223
H,0,6.5545600543,-3.6238476506,-3.01583456
H,0,3.1877702712,-4.8814674514,-1.7459713776
H,0,2.4331265576,-3.2771928524,-1.7101642237
H,0,2.8236198638,-4.042791655,-3.2624150123
H,0,7.7225944053,1.1668043023,2.1792609998
H,0,7.7632081789,-0.5191771833,2.7150634474
H,0,8.1825218928,-0.1129444983,1.0417885919
H,0,4.0627586347,0.3077459369,2.3344549807
H,0,5.2716856175,-0.2698008354,3.4971612037
H,0,5.3125314395,1.411322266,2.9415820064
H,0,0.9226272905,4.8616586814,-3.9626164987
H,0,0.918357392,-0.3656239476,-3.4178384829
H,0,0.3892605372,0.3753399599,-4.9396070553
H,0,1.2417041399,-1.177127594,-4.963334596
H,0,3.0003522252,-0.2822378875,-6.543369479
H,0,2.2039208411,1.29675988,-6.5987264074
H,0,3.9137763649,1.1845423238,-6.1470859294

H,0,2.7840567843,4.8547393642,0.2688526829
H,0,2.7092583684,3.1212299731,0.6398876531
H,0,4.0537579241,4.1052106365,1.2483866155
H,0,4.6433701639,5.7240051015,-1.3581442239
H,0,5.8546584816,4.9441550399,-0.329508961
H,0,5.785216021,4.5653465404,-2.0600542293

IPr-TS-33
SCF Done: E(RPBE1PBE) = -2193.42406847 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -13.40
Sum of electronic and thermal Free Energies= -2192.726549 A.U.

C,0,3.4924391323,-3.6537072619,1.1848665378
C,0,4.7702778031,-2.8290370584,1.2787137572
C,0,1.8810833066,-1.0020406624,-1.0186422079
C,0,5.8000693692,0.2990529878,-1.2455607957
C,0,5.0748790855,-0.4464421766,-0.2911955505
H,0,3.3161920157,-4.0598183366,2.1870123494
H,0,5.614095443,-3.4482377092,1.5981072618
H,0,3.6564349866,-4.5095173044,0.5219054761
H,0,4.6824366671,-1.9923320521,1.9771500442
H,0,6.5282680421,-0.1930652463,-1.884774205
C,0,2.2708438691,-2.8543367226,0.7320479039
H,0,1.9821388469,-2.1254126524,1.4982240126
H,0,1.4139237603,-3.5271827293,0.6027513004
C,0,2.5492145546,-2.1298241661,-0.5652370557
S,0,5.3126559104,-2.1586191574,-0.336209968
O,0,3.5423971493,-2.5999988523,-1.2777942414
C,0,4.113477209,0.1786303495,0.5254404724
C,0,3.9202962507,1.5596416042,0.4090041425
C,0,4.6460151413,2.2936337674,-0.5176507501
C,0,5.5849695803,1.6608719267,-1.3473221751
H,0,3.5833434556,-0.3700781719,1.2956443942
H,0,3.1937302321,2.0488129884,1.0506535198
H,0,4.4908216803,3.3657296892,-0.5998008
H,0,6.1509683211,2.2404500832,-2.070579029
Au,0,0.1050237003,-0.2865991318,-0.4008176427
C,0,-1.7187816197,0.4848921317,0.1495849093
C,0,-3.9304760507,0.7086099444,0.5472446755
C,0,-3.3611419462,1.9284100967,0.7149086317
H,0,-4.9553964784,0.3815028267,0.638124379
H,0,-3.7878946119,2.882918662,0.9842208872
N,0,-2.0106349766,1.770028054,0.467771732
N,0,-2.9103054404,-0.1582237688,0.2047722976
C,0,-3.0941346673,-1.5591345138,-0.0587329764

C,0,-3.3001270159,-1.9744626353,-1.3860609807
C,0,-3.0804361245,-2.451025273,1.0275948573
C,0,-3.4753308738,-3.3437693242,-1.6103377455
C,0,-3.2651615049,-3.8084891886,0.7472747338
C,0,-3.4570003004,-4.2523817214,-0.5570998411
H,0,-3.630988209,-3.7004683522,-2.6251709314
H,0,-3.2596525601,-4.5251155626,1.5645078732
H,0,-3.5969551171,-5.3122849512,-0.7539375221
C,0,-1.0494024692,2.8374050384,0.5300271099
C,0,-0.7907887953,3.576920035,-0.6375543949
C,0,-0.4212642537,3.1077168172,1.7586532562
C,0,0.1392088068,4.617491268,-0.5477677631
C,0,0.4989573028,4.1602877019,1.7926258663
C,0,0.779709537,4.9068188551,0.6526775419
H,0,0.3614775086,5.2086768835,-1.4322979361
H,0,1.0030152253,4.3954540685,2.7264809083
H,0,1.4980278541,5.7214720054,0.701326927
C,0,-1.4796588889,3.2941682731,-1.960115103
H,0,-2.1610770046,2.4494818566,-1.8160534351
C,0,-0.7009643888,2.311443026,3.0205053789
H,0,-1.4734679073,1.5699398213,2.7927526127
C,0,-3.3495404593,-1.0042422139,-2.5522913643
H,0,-3.179804185,0.0048283678,-2.1629744962
C,0,-2.8817800689,-1.9974571532,2.4626030201
H,0,-2.7496445318,-0.9107205252,2.4629625004
C,0,-2.244818958,-1.2942661896,-3.5725717686
H,0,-1.2544106313,-1.2726717157,-3.1040846521
H,0,-2.3786333056,-2.2765986221,-4.040071328
H,0,-2.2598402799,-0.5413160894,-4.3688567102
C,0,-4.7283195638,-1.0109827415,-3.2208386604
H,0,-4.7622265497,-0.2652362383,-4.0231581621
H,0,-4.9527265863,-1.9884214155,-3.6630094263
H,0,-5.5235312502,-0.7746555061,-2.5052339859
C,0,-1.6194944588,-2.6126296525,3.0741206521
H,0,-1.6918605856,-3.7049272872,3.1285137045
H,0,-0.7304474793,-2.360492271,2.4860605773
H,0,-1.4707292733,-2.2368590099,4.0928557804
C,0,-4.1134124686,-2.3127065482,3.3176654994
H,0,-4.2820138914,-3.3932740061,3.3899613744
H,0,-3.9789090835,-1.9272452532,4.3346914626
H,0,-5.0192981646,-1.8587521348,2.9013348113
C,0,-2.3200409792,4.4913236374,-2.4155408946
H,0,-1.6921503132,5.3679802586,-2.6121563843
H,0,-2.8535196004,4.2486170462,-3.341556514
H,0,-3.0631505419,4.7712103954,-1.6606992278
C,0,-0.4701219691,2.8904084018,-3.0390349131

H,0,0.2270719003,3.7067319957,-3.259704225
H,0,0.1154958275,2.0175112506,-2.7294968837
H,0,-0.9916204555,2.6365501356,-3.9688812981
C,0,-1.2381385956,3.2050020354,4.1424632491
H,0,-1.4932341538,2.5974240959,5.0180227172
H,0,-0.4941323343,3.9456765717,4.4571401655
H,0,-2.1395492216,3.7437611418,3.8308388162
C,0,0.5460144076,1.5496498921,3.4815365689
H,0,0.9089042357,0.8685982091,2.703332213
H,0,1.3593945911,2.2381583524,3.7389636664
H,0,0.3175286706,0.9544845047,4.3731523394
H,0,2.3649556171,-0.5683595805,-1.8995978281

IPr-INT4
SCF Done: E(RPBE1PBE) = -2193.47749521 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -13.80
Sum of electronic and thermal Free Energies= -2192.781400 A.U.

C,0,-2.2301380905,-3.0207153252,0.4941515087
C,0,-3.2694346302,-2.2022303302,-0.2594639075
C,0,-0.3357596262,0.0451001375,0.3605743808
C,0,-3.0735856087,1.9313896443,0.0098512053
C,0,-2.6779805569,0.5986949967,-0.1821572864
H,0,-2.2846799155,-4.0351155688,0.0816667367
H,0,-4.2314845216,-2.7256260474,-0.2548480045
H,0,-2.5025702153,-3.0949970649,1.5527974669
H,0,-2.9930483123,-2.0457739264,-1.3076238584
H,0,-3.962026773,2.162611831,0.5908469489
C,0,-0.7968697654,-2.5112886142,0.3537951382
H,0,-0.5331616232,-2.4106245833,-0.7045300614
H,0,-0.117541083,-3.2486697518,0.7942653875
C,0,-0.563835144,-1.2136716335,1.1097638347
S,0,-3.7252103244,-0.5890414761,0.4570943835
O,0,-0.5063409069,-1.2372356001,2.3387914126
C,0,-1.3705503623,0.3048347205,-0.8244562537
C,0,-0.8046006724,1.4301439483,-1.5971619341
C,0,-1.2612870995,2.7021975046,-1.4625416809
C,0,-2.3750726825,2.9475645164,-0.6142585046
H,0,-1.4027915959,-0.6076589959,-1.4307398537
H,0,0.0549330425,1.2023699339,-2.2206256503
H,0,-0.7893330346,3.5270199782,-1.9862264448
H,0,-2.7195327169,3.9701313183,-0.4801804554
Au,0,1.684732271,-0.088845069,-0.2631341986
H,0,-0.4016691439,0.8910336645,1.0530161165
C,0,3.666790776,-0.1337013036,-0.7351544085

N,0,4.3307147957,0.646377542,-1.6234932695
N,0,4.6318222106,-0.8889393368,-0.1566432661
C,0,5.6878660269,0.3855403285,-1.5989672298
C,0,3.7088866499,1.6132700057,-2.4853558301
C,0,5.8780831109,-0.5856534431,-0.6713119083
C,0,4.3927215381,-1.8774216284,0.8590794209
H,0,6.3837490544,0.9089644557,-2.2375194346
C,0,3.5267461474,2.9231053412,-2.00809478
C,0,3.324380479,1.2104173985,-3.7766366096
H,0,6.7748482428,-1.0842842931,-0.3353391055
C,0,4.3815640537,-1.4708584294,2.2046858235
C,0,4.1979068175,-3.2118234471,0.4619408767
C,0,2.9093410477,3.8395021586,-2.8657671101
C,0,3.9797738008,3.3666642539,-0.6289383672
C,0,2.7130962372,2.1673854223,-4.5934004732
C,0,3.5492821437,-0.1966819905,-4.30062324
C,0,4.1407347906,-2.4536848016,3.1699158108
C,0,4.63359842,-0.0367733372,2.6333666847
C,0,3.9660006653,-4.1543688234,1.4684579036
C,0,4.2338772708,-3.6514925815,-0.9908953034
C,0,2.5032616853,3.4671817986,-4.1432174555
H,0,2.751205202,4.8600244739,-2.5266051725
H,0,4.4387664271,2.5079891623,-0.1285128949
C,0,5.0440964517,4.4648547183,-0.7218219555
C,0,2.7969546027,3.8231020833,0.2305109806
H,0,2.4005284183,1.8892136767,-5.5965620252
H,0,4.0341024129,-0.7819911721,-3.5127172917
C,0,4.4856667488,-0.1914519427,-5.5132502073
C,0,2.2260118878,-0.8898230625,-4.6374639706
C,0,3.9324479593,-3.7805657043,2.8080776916
H,0,4.118919717,-2.1738193004,4.2198412366
H,0,4.7944493052,0.5659561488,1.7335015588
C,0,3.4271104554,0.55156815,3.3708169619
C,0,5.9002314258,0.0673188341,3.4894516336
H,0,3.8085905877,-5.1947129316,1.1961183723
H,0,4.4298067182,-2.769808183,-1.6100178428
C,0,2.8875978529,-4.2327878287,-1.4331956748
C,0,5.3672927049,-4.6514654316,-1.241305922
H,0,2.0271261729,4.195786287,-4.7946304578
H,0,4.6440603482,5.3721002763,-1.1888025339
H,0,5.3970738206,4.7332298587,0.2802918838
H,0,5.909242786,4.1374876875,-1.3088094122
H,0,2.304714482,4.7025587611,-0.2011575744
H,0,2.0484928549,3.0291620332,0.3326203093
H,0,3.1418544807,4.09399157,1.2348317028
H,0,4.6850443117,-1.2177087098,-5.8416828439

H,0,4.0421751045,0.3485753443,-6.3576358627
H,0,5.4452792275,0.2814779393,-5.2779399651
H,0,1.5675067742,-0.9422641862,-3.7631752765
H,0,1.6911154727,-0.3634299007,-5.436166543
H,0,2.4129202535,-1.9138441476,-4.9802230901
H,0,3.7461880561,-4.5282733548,3.574806206
H,0,2.5224195973,0.5091979957,2.7541895133
H,0,3.2256593797,0.012266765,4.3033160879
H,0,3.6167013062,1.6005865315,3.6258228486
H,0,6.0993583479,1.1144591576,3.7441490493
H,0,5.7941298474,-0.4899471057,4.427229124
H,0,6.7762405617,-0.3255559504,2.9615576915
H,0,2.6405044356,-5.1405553967,-0.8707427894
H,0,2.0753142138,-3.5123045083,-1.2883130369
H,0,2.921313809,-4.4980650879,-2.4961692899
H,0,5.2150077014,-5.577149564,-0.6744338582
H,0,5.4114095352,-4.9150577137,-2.3041032557
H,0,6.340357639,-4.2379811987,-0.9548482704

IPr-TS-OS

SCF Done: E(RPBE1PBE) = -2193.41949803 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -13.50
Sum of electronic and thermal Free Energies= -2192.724870 A.U.

C,0,3.7575017737,-1.6375151271,2.2304937348
C,0,5.1887773894,-1.194127497,1.9245742406
C,0,1.6647413822,-0.5894489491,-0.6876282291
C,0,7.4139178979,0.5251591649,0.4911409241
C,0,6.9072836055,-0.5327920334,-0.2757733245
H,0,6.979818407,0.7878862797,1.4492087011
C,0,2.6804152223,-0.6922039736,1.6898591113
C,0,2.7425643335,-0.5332614634,0.1988347155
S,0,5.539300459,-1.5227579565,0.1803103216
O,0,3.8684071682,-0.1857706948,-0.3286494765
C,0,7.4825107861,-0.8524410884,-1.5182662586
C,0,8.5634485138,-0.1144888481,-1.983609248
C,0,9.0752529797,0.9370450235,-1.220947141
C,0,8.4999946372,1.2506022756,0.0110803735
H,0,7.0879034154,-1.674879077,-2.1097113963
H,0,9.0088055095,-0.3634063267,-2.9423639562
H,0,9.9222264397,1.511040801,-1.5856805579
H,0,8.8966693193,2.0683602127,0.6058075022
Au,0,-0.2544556092,-0.1627762979,-0.3010706128
H,0,5.3082748939,-0.1251167634,2.1201721051
H,0,5.9195696181,-1.7534618467,2.516033576

H,0,2.8134919047,0.2981397028,2.149290469
H,0,1.6908573294,-1.0600497169,1.9750661066
H,0,3.6660769772,-1.6737931906,3.3209021084
H,0,3.5894335543,-2.6616323988,1.8732961862
C,0,-2.2511930929,0.2354668496,0.001751134
C,0,-4.2135010458,1.3099581959,0.2990462619
C,0,-4.4854662265,-0.0154638417,0.1984136177
H,0,-4.8605859049,2.1617981408,0.4451944334
H,0,-5.4180417561,-0.5580011943,0.2384962829
N,0,-3.2731449681,-0.653215708,0.0171740539
N,0,-2.843051679,1.4414936581,0.1777200973
C,0,-2.1418745686,2.6958624967,0.2318144382
C,0,-1.7226173391,3.1767739178,1.4846352543
C,0,-1.9149606378,3.3919381225,-0.9684292244
C,0,-1.0395773178,4.3969319501,1.5092119872
C,0,-1.2254601974,4.6058633324,-0.8866388042
C,0,-0.7888632436,5.1030014209,0.3370345946
H,0,-0.6998906115,4.7977068557,2.4610005073
H,0,-1.0292661268,5.1686335164,-1.7958154016
H,0,-0.2545474595,6.0487678002,0.377826049
C,0,-3.1189094954,-2.0751902476,-0.1278366181
C,0,-2.954044955,-2.8532759833,1.0314006276
C,0,-3.154160598,-2.627751982,-1.4199660251
C,0,-2.8032815947,-4.2333497964,0.8631878039
C,0,-2.9977938638,-4.0130711546,-1.5308785157
C,0,-2.8217974902,-4.8085772188,-0.4033687671
H,0,-2.6704089686,-4.8643565426,1.7381031433
H,0,-3.0161687815,-4.4726945302,-2.5157340076
H,0,-2.7020543314,-5.8835295851,-0.5119794058
C,0,-2.9344073269,-2.2553581067,2.4264350044
H,0,-3.0728546593,-1.1731477673,2.3359529734
C,0,-3.3548611011,-1.7877048805,-2.6676354462
H,0,-3.4792350197,-0.7445922445,-2.3597306857
C,0,-1.9870761981,2.4337125521,2.7813962592
H,0,-2.5391332581,1.5182248299,2.5455026318
C,0,-2.3950687863,2.886784392,-2.316699611
H,0,-2.8950297978,1.9250019426,-2.1639056108
C,0,-0.6789742073,2.0222985088,3.4633374342
H,0,-0.059596049,1.4075093779,2.8012826233
H,0,-0.0918283338,2.8995262346,3.7583171928
H,0,-0.8903604134,1.4418947916,4.3687353604
C,0,-2.8586457045,3.26115175,3.7312950497
H,0,-3.0855857219,2.6837633396,4.6346088989
H,0,-2.3484988739,4.1795554083,4.0426008439
H,0,-3.8077347733,3.5450885958,3.2637852756
C,0,-1.2241963304,2.6502459607,-3.2750268356

H,0,-0.6984283137,3.5848433276,-3.501552663
H,0,-0.4981044435,1.9464143332,-2.8528138819
H,0,-1.5890961618,2.2353346404,-4.2214770376
C,0,-3.4209952112,3.8441495727,-2.9321902547
H,0,-2.9780123467,4.8255584824,-3.1360241493
H,0,-3.791723068,3.4420075583,-3.8818444365
H,0,-4.2803044518,3.994160628,-2.2694031722
C,0,-4.0845594978,-2.7943811377,3.2829607212
H,0,-3.9895972977,-3.8739443643,3.4462932162
H,0,-4.0838483524,-2.3072553442,4.264686575
H,0,-5.0572059489,-2.6090588993,2.8141368344
C,0,-1.5856435658,-2.4910017794,3.1131553326
H,0,-1.4030629027,-3.5593420436,3.2766441395
H,0,-0.7589058382,-2.0938189404,2.5136545758
H,0,-1.5660077019,-1.9950824994,4.0902815613
C,0,-4.6263491729,-2.1985628394,-3.4168846747
H,0,-4.7865519166,-1.5394557376,-4.2775816288
H,0,-4.5555224488,-3.2259075539,-3.7919361399
H,0,-5.5104755812,-2.1349504847,-2.773024191
C,0,-2.130489712,-1.8542257094,-3.5857636582
H,0,-1.2238730496,-1.5276688037,-3.06382079
H,0,-1.9624052491,-2.873331536,-3.9524665979
H,0,-2.2743060602,-1.204804798,-4.4568244963
H,0,1.9884238724,-0.7489379849,-1.7220953639

IPr-INT3-*Singlet*
SCF Done: E(RPBE1PBE) = -2193.44223520 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -14.12
Sum of electronic and thermal Free Energies= -2192.753951 A.U.

C,0,-2.0261921044,0.5576055876,-0.2657758201
C,0,-3.1584859551,0.4668136951,0.7501626723
C,0,1.867052378,1.0332273836,-0.3978612093
C,0,-5.6466533187,0.139411192,2.5047224917
C,0,-5.9125943002,-0.03784212,1.1422731508
H,0,-4.6562662995,0.4186170719,2.8483175335
C,0,-0.6986588082,0.8181187978,0.4362055008
C,0,0.4455358291,0.8935566594,-0.4793885184
S,0,-4.7115776413,0.1677790228,-0.1431683473
O,0,0.4844927543,0.8055067251,-1.715552788
C,0,-7.2085557209,-0.3929005845,0.7358828942
C,0,-8.2162242664,-0.567205526,1.6787625955
C,0,-7.9515666235,-0.3937575106,3.0391488449
C,0,-6.6658871124,-0.0409298783,3.4421069429
H,0,-7.4272695369,-0.535051663,-0.3200906861

H,0,-9.2136520761,-0.8436698279,1.3467112652
H,0,-8.7397296408,-0.5324596086,3.7738777613
H,0,-6.4442043007,0.0996653071,4.4971394664
Au,0,3.1715156186,-0.4582494758,-0.1553007135
H,0,-2.9786322234,-0.3582888098,1.448015644
H,0,-3.2359417287,1.399121119,1.3197927988
H,0,-0.4543747253,0.0411546108,1.1751189455
H,0,-0.7035419508,1.7610774186,1.004122366
H,0,-2.226384899,1.3629924339,-0.9813469699
H,0,-1.9607232446,-0.3750916813,-0.8369630421
C,0,4.5410436542,-1.94693345,0.1732996737
N,0,5.3597863645,-2.5237444386,-0.7360671339
N,0,4.8199012734,-2.5709562593,1.3405405574
C,0,6.1405691816,-3.4992378282,-0.1476244583
C,0,5.3961865449,-2.1817484017,-2.1329322356
C,0,5.8007158001,-3.5274790822,1.1663046872
C,0,4.1792435296,-2.2797615808,2.5943011152
H,0,6.8569687224,-4.0767331491,-0.7124696235
C,0,6.3045625604,-1.1984553811,-2.561433065
C,0,4.5276760876,-2.8563128362,-3.0086205969
H,0,6.1607950458,-4.1335414079,1.9842287765
C,0,4.7514211586,-1.3045047438,3.4296413151
C,0,3.0182574318,-2.9955230357,2.9352834295
C,0,6.3122656929,-0.8831402669,-3.9237578098
C,0,7.2570353461,-0.4872687929,-1.6171432391
C,0,4.5783723466,-2.5023846299,-4.3604569757
C,0,3.5626844779,-3.932358638,-2.5453300541
C,0,4.1048031062,-1.0387918038,4.6410595571
C,0,6.0176069496,-0.5500008418,3.0671293729
C,0,2.4136834409,-2.6910599447,4.1591236367
C,0,2.4180936511,-4.06407296,2.0393627985
C,0,5.4578964528,-1.524906448,-4.8143848019
H,0,6.9991333623,-0.1244874612,-4.2893130031
H,0,7.0975933607,-0.8808450751,-0.6080335706
C,0,8.7168741589,-0.7617476924,-1.9915510564
C,0,6.9809251798,1.0188342915,-1.5724195547
H,0,3.9185809412,-3.0006142998,-5.0657420647
H,0,3.6790465869,-4.056129673,-1.463535916
C,0,3.881870481,-5.2811263474,-3.1989655352
C,0,2.1086512304,-3.5289010257,-2.8093856565
C,0,2.9483553142,-1.7223248045,5.0026255858
H,0,4.5170034345,-0.2890762906,5.3115069061
H,0,6.3648945246,-0.9091277901,2.0929302953
C,0,5.7527609001,0.9530916967,2.93619556
C,0,7.1354454774,-0.8218944283,4.0785207083
H,0,1.5142769152,-3.2242064204,4.4561345771

H,0,3.0360663071,-4.1441457977,1.1389219071
C,0,1.0032997195,-3.6860457342,1.5909788873
C,0,2.4263677244,-5.4338181028,2.7252689895
H,0,5.4799713354,-1.2641007246,-5.8693729429
H,0,8.9534412909,-0.3675382021,-2.9864108834
H,0,9.3891957508,-0.2794060581,-1.2731253897
H,0,8.9377935446,-1.834723809,-1.9934513404
H,0,7.1712328553,1.487717909,-2.5446245964
H,0,5.9425315713,1.2287153589,-1.2928292865
H,0,7.6349967211,1.5008431305,-0.8369464398
H,0,3.2126889006,-6.0577819552,-2.8118056894
H,0,3.7489621734,-5.2385053634,-4.2859101919
H,0,4.9130338758,-5.5913644593,-2.9978316969
H,0,1.862276411,-2.5756889889,-2.3278256994
H,0,1.9126593496,-3.4247056655,-3.8826285518
H,0,1.4269925126,-4.2932130889,-2.4190242652
H,0,2.4633718833,-1.5021554227,5.9502301201
H,0,4.9785431671,1.1590179737,2.188281329
H,0,5.427534001,1.3854771238,3.8893369263
H,0,6.6674024764,1.4726636248,2.6290385929
H,0,8.0542963603,-0.310609589,3.7705461416
H,0,6.8684052387,-0.4573779676,5.0767860124
H,0,7.353962364,-1.892350963,4.1578203031
H,0,0.3206505134,-3.6102196391,2.4449728145
H,0,0.9964387164,-2.7257168574,1.0628499493
H,0,0.6047842065,-4.448279912,0.9120441226
H,0,1.7981510885,-5.4349786891,3.6231304122
H,0,2.0369615197,-6.1988677222,2.0443473324
H,0,3.4388715177,-5.7279319381,3.0224961404
H,0,2.1866111144,2.0667148109,-0.5730810276

6.5 The structures shown in Scheme 15 and Figure 5 in the main text.

IMe-R
SCF Done: E(RPBE1PBE) = -1299.87539275 A.U. after 1 cycles
SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.47
Sum of electronic and thermal Free Energies= -1299.626253 A.U.

C,0,-1.8060067717,0.2709967767,0.8167319373
C,0,0.2095110837,-2.5379371305,-0.1219684543
C,0,-4.9747788879,0.7152308476,-1.080466256
C,0,-4.4499925707,0.7403710246,0.2075735014
H,0,-4.4478961314,1.2241145493,-1.8833801183
C,0,-1.6470947247,-0.6168636318,-0.412742899
C,0,-0.5646913066,-1.5840944299,-0.2545747743

S,0,-2.9337568711,1.6749282977,0.5062880767
O,0,-2.5116257346,2.2689269306,-0.8269328908
C,0,-5.1057242316,0.1288010552,1.2771260773
C,0,-6.2981132727,-0.550124379,1.0354889886
C,0,-6.8303353618,-0.5971270836,-0.2550427312
C,0,-6.1726163862,0.0364942924,-1.3086915002
H,0,-4.7014340089,0.1804498975,2.2858189011
H,0,-6.8169339077,-1.034627925,1.8580004151
H,0,-7.7645443726,-1.1218765637,-0.4357438682
H,0,-6.5920037764,0.0081722826,-2.3107036249
H,0,-1.4568023789,0.005728844,-1.2952571729
H,0,-2.5648482374,-1.1870255678,-0.603025637
H,0,-2.1905269852,-0.2732289658,1.6847103295
H,0,-0.8532131908,0.7369705183,1.0902198409
H,0,0.631026945,-3.5226643776,-0.0238215321
Au,0,1.5774196398,-0.8373456444,-0.0816104128
C,0,3.1901837511,0.3779426693,0.0230521321
N,0,3.8756565228,0.9242788905,-1.0052700111
N,0,3.8225215868,0.8006796333,1.1402646127
C,0,4.9227776197,1.6825121563,-0.5398937563
C,0,3.5548037611,0.7670744652,-2.4133947089
C,0,4.8905933577,1.6027411761,0.8171960386
C,0,3.4564668965,0.4517709789,2.5021398093
H,0,5.5929566817,2.2070024989,-1.2047059385
H,0,2.7462739121,0.0411507967,-2.5063038118
H,0,3.2362168484,1.7248808608,-2.8318336052
H,0,4.4340716102,0.4058645881,-2.9512013156
H,0,5.5293304064,2.0409349509,1.5697217269
H,0,2.5449063272,-0.1463581331,2.4745626007
H,0,4.259012677,-0.1265395051,2.9661483558
H,0,3.2793444848,1.3617034641,3.0799813816

IMe-TS-6-*endo-dig*

SCF Done: E(RPBE1PBE) = -1299.85774058 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.72
Sum of electronic and thermal Free Energies= -1299.607702 A.U.

C,0,2.658561264,-0.0677039452,1.2373834809
C,0,0.6785926184,0.1558075838,-1.0718161057
C,0,5.9841069716,-1.1055707872,0.3930910488
C,0,5.0419459798,-0.2081228246,-0.1083776704
H,0,5.7016917734,-2.1223614237,0.6556593948
C,0,1.1759607012,-0.3897638936,1.379576462
C,0,0.409201971,-0.0829564157,0.1389303804
S,0,3.3545788792,-0.7761431814,-0.2953698532

O,0,2.7404770309,0.0835489637,-1.4295863889
C,0,5.3849169422,1.0890489068,-0.4842834661
C,0,6.7069391124,1.5007925896,-0.3314559778
C,0,7.6602844419,0.622677048,0.1876025038
C,0,7.3011045142,-0.6758028048,0.549409634
H,0,4.6329987909,1.7540940831,-0.8997802867
H,0,6.9931670392,2.5079625929,-0.6211944435
H,0,8.6902872414,0.9492629262,0.3016924211
H,0,8.0470589823,-1.3614700081,0.9410474055
H,0,1.0254127298,-1.4457704768,1.6325672525
H,0,0.7771279096,0.1870024,2.2197989963
H,0,3.2342008562,-0.4913706431,2.0662706122
H,0,2.8384306119,1.0108577173,1.1807646097
H,0,0.5242981008,0.375108399,-2.1115480945
Au,0,-1.6874959462,0.0112614431,-0.0388393272
C,0,-3.7165156199,0.0584259142,0.0152255946
N,0,-4.5672803708,-0.9850676631,-0.1092999433
N,0,-4.5065182811,1.1364625079,0.2196974337
C,0,-5.8723503324,-0.5673699528,0.0148093504
C,0,-4.177330282,-2.3674852962,-0.3240211264
C,0,-5.8340166645,0.7751566644,0.2210213088
C,0,-4.0398799397,2.4998928794,0.3977561609
H,0,-6.7046651202,-1.2521368177,-0.0534500404
H,0,-3.1001216521,-2.4013183837,-0.4926003243
H,0,-4.4287563038,-2.9681954956,0.5539301399
H,0,-4.6954870508,-2.7644575581,-1.199897946
H,0,-6.6257787695,1.4954826855,0.363585353
H,0,-2.9492842226,2.4930802201,0.4136570636
H,0,-4.3884861862,3.1246098969,-0.4285083479
H,0,-4.4163606852,2.8990218332,1.3423954974

IMe-INT1

SCF Done: E(RPBE1PBE) = -1299.88539299 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.68
Sum of electronic and thermal Free Energies= -1299.631160 A.U.

C,0,1.71145605,-1.7790585461,0.1672734812
C,0,0.2407948016,0.7314813 9,0.126688687
C,0,5.0043463375,-0.117221527,-1.2499491778
C,0,4.0576017835,-0.2196081935,-0.2269793551
H,0,4.7027239003,-0.1246529183,-2.2940227459
C,0,0.196792285,-1.7557187101,-0.0390228112
C,0,-0.4671845084,-0.4003928372,0.0657665132
S,0,2.3841236776,-0.3761040711,-0.746464053
O,0,1.6764194663,0.8331422822,0.1027991792

C,0,4.4114625102,-0.1932202929,1.1255608018
C,0,5.7565142892,-0.0659569563,1.449976174
C,0,6.7195612434,0.0235142269,0.4409185568
C,0,6.3481131445,-0.003553325,-0.9020360363
H,0,3.6614503014,-0.2543169552,1.9081850691
H,0,6.0550815449,-0.0360623083,2.493533918
H,0,7.7682973742,0.1194445748,0.7075295484
H,0,7.0996710963,0.0738843221,-1.6816139422
H,0,-0.2249893234,-2.4261012755,0.7191550789
H,0,-0.0555358589,-2.2087121626,-1.0051474582
H,0,1.9980909275,-1.645664684,1.2140571389
H,0,2.1879653883,-2.6789905494,-0.2348126937
H,0,-0.1440464442,1.7421906331,0.2064528569
Au,0,-2.5190125168,-0.2759567915,0.0649714092
C,0,-4.5640877542,-0.1392615094,0.0524134287
N,0,-5.4191242267,-0.4156879358,1.0650625688
N,0,-5.3574560133,0.2663267198,-0.966712682
C,0,-6.7238057884,-0.1874445667,0.6874196421
C,0,-5.0290146836,-0.8912276565,2.3796702154
C,0,-6.6846869912,0.2444157318,-0.5997154738
C,0,-4.8889771804,0.6640472518,-2.2813402663
H,0,-7.5550561397,-0.3495277923,1.3576351075
H,0,-3.9410038181,-0.9644275564,2.4094441201
H,0,-5.3683560922,-0.1898326483,3.1460297633
H,0,-5.4662853599,-1.8752912004,2.5669385717
H,0,-7.4746945284,0.5339395536,-1.27687198
H,0,-3.7990486263,0.6191881082,-2.2860055331
H,0,-5.2853343178,-0.0147378618,-3.0409171743
H,0,-5.2126243398,1.6847176373,-2.4998267473

IMe-TS-5-exo-dig
SCF Done: E(RPBE1PBE) = -1299.86615824 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.58
Sum of electronic and thermal Free Energies= -1299.617593 A.U.

C,0,-2.7062187207,-1.5828355937,-0.968947878
C,0,-0.1434504208,-0.4248598664,1.3954271301
C,0,-5.861702718,-0.311824018,-1.0776859415
C,0,-4.8946750276,-0.1135049232,-0.0916068346
H,0,-5.9856831988,-1.2819311447,-1.5547320168
C,0,-1.7154697874,-0.4430308845,-0.7841434409
C,0,-1.0286707607,-0.4730964276,0.5015903393
S,0,-3.8838502132,-1.5099747971,0.4264247398

O,0,-2.964740499,-0.995476962,1.5416462424
C,0,-4.7444836586,1.1090246201,0.5552085091
C,0,-5.5676514145,2.1717058448,0.181049632
C,0,-6.525533161,1.9983223722,-0.8171841872
C,0,-6.6727932635,0.7594842912,-1.4449593072
H,0,-3.999591619,1.2177202174,1.3387130678
H,0,-5.4612097599,3.1330902261,0.6757843445
H,0,-7.1668525547,2.8277164537,-1.1021698704
H,0,-7.4271753417,0.6234589382,-2.2147096606
H,0,-0.9434440034,-0.5397992923,-1.5580964757
H,0,-2.2010443798,0.5289326364,-0.9301510228
H,0,-2.2204454238,-2.560505051,-0.8992099488
H,0,-3.2460260604,-1.5089203352,-1.916333445
H,0,-0.1536319099,-0.5181838607,2.4739731124
Au,0,1.6892374249,-0.0811445118,0.4378595283
C,0,3.5505715031,0.2434355265,-0.2993225315
N,0,4.3779513505,-0.6595767609,-0.8721551728
N,0,4.2429994878,1.404665132,-0.2940300728
C,0,5.5712297428,-0.071914236,-1.2260991343
C,0,4.0678821172,-2.0600715379,-1.0971982786
C,0,5.486017793,1.2335010846,-0.8600158093
C,0,3.7580454696,2.6725559231,0.2218200538
H,0,6.3676990802,-0.6262884838,-1.6998125984
H,0,3.079403026,-2.2650677448,-0.6837527884
H,0,4.8093706734,-2.6887168749,-0.5986437238
H,0,4.0682027224,-2.2744277827,-2.1689057978
H,0,6.1939238492,2.0440673462,-0.9500690202
H,0,2.7801273974,2.5108355383,0.677320071
H,0,3.6677421154,3.396676518,-0.5919004184
H,0,4.4515051436,3.0545324205,0.9745876054

IMe-INT2

SCF Done: E(RPBE1PBE) = -1299.88893607 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.54
Sum of electronic and thermal Free Energies= -1299.634843 A.U.

C,0,2.8343715277,-0.4590399423,2.073557239
C,0,0.2337084083,-1.2409157027,-0.4461875809
C,0,4.1446311308,0.7471951097,-1.0117908968
C,0,4.7245510943,-0.0385553392,-0.015700371
H,0,3.1190062893,0.58833441,-1.3298141207
C,0,1.6659046253,0.086536224,1.2707761468
C,0,1.344982187,-0.9148963154,0.2009917199
S,0,3.8258764506,-1.3284947415,0.8146985493

O,0,2.5683403376,-1.6485659597,-0.1510143645
C,0,6.0573758434,0.1085081076,0.3740800403
C,0,6.8171844252,1.1083784245,-0.2279301593
C,0,6.2533495689,1.9150274288,-1.2160097146
C,0,4.9277917302,1.7297821928,-1.6116320507
H,0,6.500118835,-0.5394767629,1.1269370635
H,0,7.8540128747,1.2423923284,0.0653261889
H,0,6.8544845414,2.6845806763,-1.6916751653
H,0,4.4989357508,2.3491632217,-2.3937072559
H,0,0.7999995421,0.2285600027,1.9210461141
H,0,1.9284697218,1.0582202956,0.8363776111
H,0,2.5434264402,-1.2303343186,2.7931686145
H,0,3.4638140799,0.2911397628,2.5573608928
Au,0,-1.6048727788,-0.3901947749,-0.2120850504
C,0,-3.4700658449,0.4343066942,-0.0113297064
C,0,-5.7014072274,0.7333857678,-0.0614144064
C,0,-5.1502365172,1.8533355146,0.4737497199
H,0,-6.7308001537,0.4727759122,-0.2583769468
H,0,-5.6028449586,2.7644457118,0.8361106061
N,0,-3.7883319298,1.6492417741,0.4947689728
N,0,-4.6588100275,-0.1188192149,-0.3502775038
C,0,-2.832926317,2.6218006226,0.9912244626
H,0,-1.8310606104,2.2028639838,0.8868970234
H,0,-2.9032911077,3.5451344888,0.4107366477
H,0,-3.0313616679,2.8376672063,2.0442138839
C,0,-4.8321371092,-1.4345352306,-0.9386429616
H,0,-3.849938455,-1.8956319587,-1.049714471
H,0,-5.4540144565,-2.0550786903,-0.2884518112
H,0,-5.3058231519,-1.3454717464,-1.9195827898
H,0,0.3621627282,-2.031425794,-1.1914814926

IMe-TS-INT2-*conf*

SCF Done: E(RPBE1PBE) = -1299.88777416 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.48
Sum of electronic and thermal Free Energies= -1299.633951 A.U.

C,0,2.9097191608,-0.9596631807,2.0893977925
C,0,0.3155968652,-1.1768078923,-0.645201411
C,0,3.7448409798,1.1656036015,-0.471042291
C,0,4.5368323122,0.0996238817,-0.0307464365
H,0,2.6615752805,1.1187355059,-0.4494573181
C,0,1.5592395202,-0.5285736054,1.5346535578
C,0,1.3623197814,-1.1433469316,0.1711439294
S,0,3.8869674394,-1.410768771,0.6230187784
O,0,2.5868418034,-1.8055789826,-0.2610965562

C,0,5.9331158617,0.1343309075,-0.1057183936
C,0,6.5495307286,1.2810406638,-0.6008066124
C,0,5.7751582315,2.3548266514,-1.0350243107
C,0,4.3805491635,2.2934144292,-0.9777734665
H,0,6.5309576623,-0.716039353,0.2123763885
H,0,7.6327877974,1.3244735858,-0.6592709979
H,0,6.2584345905,3.2428200074,-1.4323806572
H,0,3.7822664176,3.1270630963,-1.3331171192
H,0,0.770194817,-0.867929372,2.2109337246
H,0,1.4971527421,0.5623487496,1.4736676592
H,0,2.8573834403,-1.8817967301,2.6753239611
H,0,3.4488492274,-0.1954426252,2.652678547
Au,0,-1.5243084825,-0.3787208116,-0.2714573029
C,0,-3.3809186207,0.4243750822,0.0544655278
C,0,-5.605731278,0.7675005425,0.0229251525
C,0,-5.0454909096,1.7799745092,0.733969657
H,0,-6.635832043,0.5600503367,-0.2264255341
H,0,-5.489969284,2.6303938202,1.2295029899
N,0,-3.6874207109,1.5506111246,0.740818569
N,0,-4.5722953819,-0.0484995644,-0.3806779967
C,0,-2.7243270585,2.4114154632,1.4019541062
H,0,-1.7293887391,1.9881167025,1.2552039563
H,0,-2.7612275038,3.4154444255,0.9714666719
H,0,-2.9434117103,2.4650214228,2.4715095645
C,0,-4.7524650734,-1.2437324231,-1.1841781976
H,0,-3.785181023,-1.7358048974,-1.2939338919
H,0,-5.452618492,-1.9216165729,-0.6900441438
H,0,-5.1383831807,-0.9771875795,-2.1716471178
H,0,0.5007613205,-1.6774453269,-1.5998833883

IMe- INT2'

SCF Done: E(RPBE1PBE) = -1299.88966004 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.54
Sum of electronic and thermal Free Energies= -1299.635298 A.U.

C,0,2.7757294085,-1.8163966711,1.512274442
C,0,0.479420122,-0.49687351,-1.0360399299
C,0,5.7333392582,0.3445581776,-0.2298483283
C,0,4.4231044277,0.1257903561,0.2113815542
H,0,6.3431904824,-0.4798560172,-0.5903257073
C,0,1.378689277,-1.9760984351,0.9041642579
C,0,1.3755352182,-1.252124665,-0.4058251341
S,0,3.8653219504,-1.5407580106,0.0651222841
O,0,2.6424791248,-1.529879904,-1.0369772413
C,0,3.6124660516,1.1715023492,0.6704135783

C,0,4.1392350588,2.4573001299,0.6852841264
C,0,5.4498026198,2.6889729302,0.2588959884
C,0,6.2460036673,1.6382301909,-0.1935909441
H,0,2.5951341761,0.9963436732,1.0051071826
H,0,3.5250938602,3.2821335672,1.0339262957
H,0,5.8513237617,3.6980371154,0.2819746155
H,0,7.2642705942,1.8219041477,-0.5222812308
Au,0,-1.4247149395,-0.0985959906,-0.428191909
H,0,0.6225304172,-1.5679555721,1.5772180824
H,0,1.1739209805,-3.0409850959,0.7448088155
H,0,2.8730866284,-0.9550636952,2.1748264928
H,0,3.1445293708,-2.7104847648,2.0182717664
C,0,-3.3459620685,0.3391375042,0.1402451552
C,0,-5.2337602981,1.4636737662,0.6323887388
C,0,-5.4917019396,0.1399099702,0.7927741685
H,0,-5.8629407844,2.331291578,0.7655180472
H,0,-6.390722043,-0.3780531121,1.0924842174
N,0,-4.3262224267,-0.5275019175,0.4879332242
N,0,-3.9189491227,1.562247156,0.2339909263
C,0,-4.1862152095,-1.9713531277,0.534730431
H,0,-3.1600187694,-2.226203687,0.2666709558
H,0,-4.4017742711,-2.3342484728,1.5428279376
H,0,-4.8738171976,-2.4374144354,-0.1756415667
C,0,-3.2509569462,2.8200029703,-0.0456225922
H,0,-2.2222246621,2.6062338905,-0.33893212
H,0,-3.7603393399,3.3415040076,-0.8599610791
H,0,-3.2517788239,3.4502809167,0.847489065
H,0,0.8304739562,-0.1024923543,-1.9942629446

IMe-TS-33

SCF Done: E(RPBE1PBE) = -1299.87551398 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.75
Sum of electronic and thermal Free Energies= -1299.621215 A.U.

C,0,3.0422170475,-1.5568010194,1.9141892821
C,0,0.7939565038,-0.7608069753,-0.8342571605
C,0,4.7302674028,1.0888567063,-0.760346186
C,0,3.840202496,0.4848423404,0.1532847773
H,0,5.6134343159,0.5527900232,-1.0977526172
C,0,1.6217637739,-1.8627493275,1.354262074
C,0,1.6698605555,-1.564061043,-0.1092953943
S,0,4.198730416,-1.1537771069,0.5847373234
O,0,2.7435241682,-2.0302388031,-0.6709897935
C,0,2.6848170884,1.1648931168,0.583190425
C,0,2.4441140651,2.4583168545,0.1076227453

C,0,3.3248490684,3.054359428,-0.7836485533
C,0,4.4696131314,2.3671981342,-1.216658791
H,0,2.0266573837,0.7476603074,1.3366250913
H,0,1.5636700352,2.9934862351,0.4504534193
H,0,3.1347387284,4.0622605888,-1.1413124245
H,0,5.157611028,2.8389390002,-1.9118402236
H,0,0.8531632329,-1.2808578018,1.8668346578
H,0,1.4263219871,-2.9273023933,1.5160263771
H,0,3.0459138299,-0.7281405801,2.6264845402
H,0,3.4863068443,-2.4264749694,2.4028449592
Au,0,-1.0918201197,-0.2688823565,-0.3500322305
C,0,-3.0286276424,0.2514515758,0.1247729815
C,0,-4.8179153568,1.2703524191,1.0295270913
C,0,-5.2751638343,0.2770440806,0.2237069816
H,0,-5.3436585304,1.9892722135,1.6401895601
H,0,-6.2797358969,-0.0461436875,-0.0058770238
N,0,-4.1654722512,-0.3317007419,-0.318616715
N,0,-3.4432346029,1.235121434,0.9551286773
C,0,-4.2261085777,-1.4560275756,-1.2354089832
H,0,-3.2076426784,-1.7319372106,-1.5122696315
H,0,-4.7152576452,-2.3054649064,-0.752182573
H,0,-4.783661581,-1.1755806272,-2.1324716075
C,0,-2.5705455141,2.1547610627,1.6615794787
H,0,-1.5392224785,1.8270421077,1.5228862946
H,0,-2.6874436008,3.1663642632,1.2639823409
H,0,-2.8137995467,2.1511674479,2.7266156447
H,0,1.1937489342,-0.5311062865,-1.8276576068

IMe-INT4

SCF Done: E(RPBE1PBE) = -1299.92868209 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -7.26
Sum of electronic and thermal Free Energies= -1299.672516 A.U.

C,0,-3.0983899643,-2.1009895417,-1.1650393993
C,0,-1.2765890065,-0.0580338182,0.5537352212
C,0,-4.3209286285,1.5472146885,0.2069762214
C,0,-3.5716549913,0.4594294226,-0.2608140536
H,0,-5.3432545464,1.4089866986,0.5470718526
C,0,-1.8879324078,-2.4623617498,-0.2942356823
C,0,-1.5515784964,-1.4868408441,0.828341761
S,0,-4.3447635731,-1.0616146817,-0.3534891885
O,0,-1.4468477317,-1.9297137538,1.9708330813
C,0,-2.1345816599,0.6189725578,-0.599789075
C,0,-1.681840332,2.0212677913,-0.7017969134

C,0,-2.4515565146,3.0651430766,-0.30251601
C,0,-3.7635121106,2.8113035082,0.1868710063
H,0,-1.8869172006,0.0983240331,-1.5341048952
H,0,-0.6645248081,2.1687652768,-1.0553605665
H,0,-2.0838934809,4.0850597088,-0.3439322429
H,0,-4.3633190973,3.6477948416,0.5372670759
H,0,-1.013937258,-2.55767083,-0.9501521135
H,0,-2.0558226266,-3.4285086986,0.1864515153
H,0,-2.8216193525,-1.6084265112,-2.1016083497
H,0,-3.652249075,-3.0043709646,-1.4359258734
Au,0,0.8102386722,-0.0018329201,0.1751427016
C,0,2.8320102425,0.0477259181,-0.1029049472
C,0,4.9577726947,0.7643861114,-0.2655364516
C,0,4.9644536716,-0.5822585574,-0.4405367075
H,0,5.7619039721,1.4854328372,-0.2674036529
H,0,5.7756696336,-1.2708876473,-0.6245854527
N,0,3.6560928918,-0.9994776789,-0.3371334319
N,0,3.645519663,1.1281958435,-0.0596840619
C,0,3.238210115,-2.3846629183,-0.4570400946
H,0,2.1577722236,-2.4316214152,-0.3148736554
H,0,3.4954880102,-2.7681847967,-1.4475533345
H,0,3.7309676514,-2.9892540818,0.3083599769
C,0,3.2150857288,2.4955034243,0.1692818674
H,0,2.1391416272,2.494872121,0.348348365
H,0,3.727043784,2.9044602352,1.0437757992
H,0,3.4403498536,3.1103056885,-0.7060632742
H,0,-1.449148573,0.5054836262,1.4767319826

IMe-TS-OS

SCF Done: E(RPBE1PBE) = -1299.87218754 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -6.65
Sum of electronic and thermal Free Energies= -1299.618998 A.U.

C,0,-1.9640526842,-0.887684605,1.8643471502
C,0,0.8471372447,0.7678446215,0.3359329527
C,0,-5.1529869538,0.9810414989,-0.0387208543
C,0,-4.220855347,-0.0035019118,0.3296029841
H,0,-5.0810435136,1.9863804036,0.3686025694
C,0,-0.8691924808,-1.1344472236,0.7960735747
C,0,-0.4351362406,0.2252533143,0.3716270699
S,0,-2.9785287445,0.5430080874,1.4340804167
O,0,-1.4202246949,0.9736759391,-0.0105941577
C,0,-4.3103973926,-1.3029557143,-0.1873271742
C,0,-5.3367170487,-1.6064917351,-1.0761886823
C,0,-6.2619742984,-0.6312008827,-1.4513027883

C,0,-6.1686201277,0.660641121,-0.9308574348
H,0,-3.606399365,-2.0767133764,0.0992742885
H,0,-5.4128188071,-2.6132598808,-1.4765338573
H,0,-7.0593633356,-0.8797111354,-2.1457897533
H,0,-6.8894219805,1.4208689449,-1.217003697
H,0,-0.056168283,-1.7231157391,1.2251744948
H,0,-1.309323596,-1.6781191393,-0.046497885
H,0,-1.5165186059,-0.6170792073,2.824946502
H,0,-2.6067985398,-1.7557979204,2.0254458369
Au,0,2.5769656433,-0.2158968633,0.1266553579
C,0,4.3886665166,-1.1689043587,-0.044260309
C,0,5.9832860088,-2.7498134673,-0.1522088197
C,0,6.5936057467,-1.5409939487,-0.2759017974
H,0,6.3860005182,-3.7519413403,-0.1546776496
H,0,7.6340084631,-1.2815749584,-0.4053033388
N,0,5.6018240398,-0.5910822129,-0.2076727643
N,0,4.6387612668,-2.4986406499,-0.0109882992
C,0,5.8401411302,0.8387431754,-0.2971309731
H,0,4.8764437663,1.3498729383,-0.2947963272
H,0,6.4332098045,1.1739454961,0.5575671796
H,0,6.3718321625,1.067699442,-1.2235970044
C,0,3.6326316981,-3.5340848927,0.1387703305
H,0,2.6598973805,-3.0545928597,0.2548835132
H,0,3.6196787302,-4.1735366455,-0.7475750275
H,0,3.8498888866,-4.1387734143,1.0226107399
H,0,0.8196987028,1.8595723705,0.249388873

IMe-INT3

SCF Done: E(RPBE1PBE) = -1299.89284177 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -7.22
Sum of electronic and thermal Free Energies= -1299.643631 A.U.

C,0,3.1241271546,-0.5247896433,-0.1522199875
C,0,0.7896652089,-1.4009855519,-0.1662610644
C,0,6.9261689854,0.9357770256,-0.8445507602
C,0,5.7866532537,0.3914682986,-0.2326056561
H,0,6.8832582515,1.2660263412,-1.8799513546
C,0,1.8332683978,-0.6988887556,-0.9397628566
C,0,-0.5876534382,-1.7110270484,-0.4714828161
S,0,4.3264476364,0.2990215192,-1.2330118633
O,0,0.8622455927,-1.8687533142,0.9718770072
C,0,5.8567587343,-0.0315487019,1.0989594277
C,0,7.0565190734,0.0885475048,1.8033019231
C,0,8.1880039932,0.6293267853,1.1976620638

C,0,8.1147207885,1.0524698576,-0.131271778
H,0,4.9921018899,-0.4541967663,1.5993073479
H,0,7.0972041511,-0.2452182709,2.8370696489
H,0,9.1178494381,0.7203452128,1.751988251
H,0,8.9886867246,1.4758341956,-0.6194683439
H,0,1.4049760536,0.2603054925,-1.2611639024
H,0,1.9850829437,-1.280520676,-1.8614047363
H,0,3.5159625913,-1.498322404,0.1567759063
H,0,2.9456096716,0.0835090277,0.7396641
Au,0,-2.1373669802,-0.5429713685,-0.1227664096
C,0,-3.7781039549,0.6600677101,0.1427232255
C,0,-5.8804962475,1.3533464936,0.500850677
C,0,-5.1037399184,2.4585050626,0.3350172456
H,0,-6.9377665501,1.2522170874,0.6970072986
H,0,-5.3521764387,3.5093879244,0.3515146994
N,0,-3.8234317623,2.0112842105,0.1194761607
N,0,-5.0504938926,0.266486866,0.3763706166
C,0,-2.6872110865,2.8845267198,-0.1192286238
H,0,-1.7889127223,2.2701266925,-0.1908229606
H,0,-2.8291647623,3.4346938159,-1.0526824932
H,0,-2.5832984349,3.5888863446,0.7092043325
C,0,-5.4902284564,-1.1116729968,0.5127194107
H,0,-4.6501427109,-1.7680823771,0.2828236802
H,0,-5.8267744458,-1.2955444172,1.5359253895
H,0,-6.3088140834,-1.3074464409,-0.1832486092
H,0,-0.70803555,-2.7511334448,-0.7988873536

6.6 The structures shown in Figure S13.

TS-OS-*a*
SCF Done: E(RPBE1PBE) = -1456.15716092 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.66
Sum of electronic and thermal Free Energies= -1455.920337 A.U.

C,0,-0.8219258686,-2.1465816143,1.1831671332
C,0,-2.2708285767,-1.94849581,0.7316588004
C,0,-0.1957102076,0.6027154931,-0.1926257436
C,0,-4.8632527725,-1.0000597795,-0.7188548701
C,0,-4.3242530975,-0.0601500391,0.1712414343
H,0,-4.3394179556,-1.9188434888,-0.957972607
C,0,0.2818308595,-1.8279585793,0.1617146625
C,0,0.7513249878,-0.413143291,-0.0216538044
S,0,-2.7733657836,-0.2317944524,0.9583684833
O,0,-1.3992152944,0.2389360712,-0.5422507974

C,0,-5.0195518698,1.1250598135,0.4698450906
C,0,-6.2531916624,1.3611658267,-0.122956217
C,0,-6.7956259307,0.4277112473,-1.0084803261
C,0,-6.1013040848,-0.7471069325,-1.3004495953
H,0,-4.6003604103,1.8484972531,1.1645102614
H,0,-6.7931518988,2.2744879208,0.1090351891
H,0,-7.760649018,0.6152813583,-1.4707126377
H,0,-6.5238901872,-1.4738561722,-1.9881782095
Au,0,2.7450846205,-0.0597183072,-0.1827158789
P,0,5.0567791703,0.2521515313,-0.3556644402
H,0,5.518564781,1.5255506011,-0.7348088863
H,0,5.8148656743,0.0273474766,0.8077216349
H,0,5.7353894072,-0.5654391712,-1.2775265118
C,0,0.08655847,2.0761496962,-0.0706943671
H,0,1.1706240632,2.2269023757,-0.049508469
H,0,-0.3046087174,2.5815405113,-0.9625327482
C,0,-0.542150047,2.6971948679,1.178438777
H,0,-1.6344368379,2.6239412246,1.1628075595
H,0,-0.1796489099,2.2136620792,2.0924578005
H,0,-0.2881043094,3.7604582809,1.2358827936
H,0,1.1451303622,-2.4525104667,0.4072973498
H,0,-0.0459906391,-2.176162778,-0.8356351887
H,0,-2.9584027851,-2.5645003513,1.3196889916
H,0,-2.373436894,-2.1999993723,-0.328737937
H,0,-0.630879759,-1.6306259413,2.1326383245
H,0,-0.7377338788,-3.215864082,1.4065369491

INT2-*a*

SCF Done: E(RPBE1PBE) = -1456.19421405 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.27
Sum of electronic and thermal Free Energies= -1455.963294 A.U.

C,0,0.6385201929,-0.9372499614,-1.2237989754
C,0,1.8998354569,-0.9187577799,-2.079266992
C,0,-1.3232108355,1.9431745001,0.4213097276
C,0,4.4698409425,-1.2280200349,-3.7066363503
C,0,3.9044503064,-2.4555647575,-3.3434938185
H,0,4.0036058303,-0.2911413639,-3.4208672258
C,0,0.164150337,0.4821488663,-0.9416137498
C,0,-1.1175794706,0.6626545293,-0.2797741943
S,0,2.4094521668,-2.6287707971,-2.4084002285
O,0,-0.938546377,1.8359557739,1.5801194183
C,0,4.5379087396,-3.6461428071,-3.7330657751
C,0,5.7152205267,-3.604312629,-4.4726167878
C,0,6.2809992532,-2.3800324996,-4.8354623441
C,0,5.6531558015,-1.1989340411,-4.4476333438

H,0,4.1087212339,-4.6062766345,-3.4557939985
H,0,6.1924050942,-4.5357588848,-4.7661700548
H,0,7.2010173053,-2.3496811441,-5.4124737114
H,0,6.081898538,-0.2380067318,-4.7208687149
Au,0,-2.5941168071,-0.691366746,-0.1761443222
P,0,-4.3421358747,-2.252462512,-0.0329884689
H,0,-5.4382379184,-1.8976767996,0.7708945016
H,0,-4.9653559195,-2.5911167756,-1.2461387234
H,0,-3.9980702527,-3.5155115027,0.4779003609
C,0,-1.9301440575,3.1457505468,-0.2105094332
H,0,-1.2649507845,3.4336152386,-1.0387704757
H,0,-2.8646172764,2.8240862503,-0.6900701013
C,0,-2.1516887821,4.2962506491,0.7567572791
H,0,-2.8317425504,4.0106517046,1.5647175709
H,0,-1.2113234205,4.6270052713,1.2065225624
H,0,-2.591740599,5.1445682329,0.2254360007
H,0,0.9475489652,1.1242838216,-0.5136009275
H,0,-0.0999809009,0.9954632027,-1.9020174274
H,0,2.7041882526,-0.3948367764,-1.5515069305
H,0,1.7089471601,-0.4047197765,-3.0279726894
H,0,-0.1640446821,-1.4907721848,-1.725075407
H,0,0.8376482856,-1.436891087,-0.2691994998

TS-HT-*a*

SCF Done: E(RPBE1PBE) = -1456.18900133 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.41
Sum of electronic and thermal Free Energies= -1455.960261 A.U.

C,0,0.9185226661,0.1524270134,0.8341582319
C,0,2.3160071893,0.5414226898,0.3615110999
C,0,-2.3074386362,2.2822253724,0.413940666
C,0,5.2382306695,0.9889217433,-0.4062638044
C,0,5.0021510063,-0.2874153968,0.1155299795
H,0,4.4338194375,1.7095724944,-0.5110207865
C,0,-0.068250332,1.259308687,0.7065268315
C,0,-1.3950427058,1.0896086997,0.3174647174
S,0,3.4177921063,-0.8697236155,0.6545642056
O,0,-2.8792882575,2.4529684953,1.4764770395
C,0,6.068360877,-1.1922224853,0.2342698319
C,0,7.3483201663,-0.8209640549,-0.1640596848
C,0,7.586964984,0.452948774,-0.6842557703
C,0,6.5281033689,1.3498256621,-0.8016314569
H,0,5.8964317285,-2.1869679993,0.6393258728
H,0,8.1633206945,-1.5333552028,-0.0655765514
H,0,8.587773113,0.7410172212,-0.9933640848

H,0,6.6977292731,2.3451139888,-1.2045512563
Au,0,-2.2923488317,-0.7326647131,-0.0770774664
P,0,-3.3299031866,-2.7715409371,-0.4559854844
H,0,-4.7248175398,-2.7480814806,-0.6266255615
H,0,-2.916799969,-3.4829919052,-1.5956851647
H,0,-3.1825276244,-3.7402828049,0.5515740854
C,0,-2.4952289688,3.1468510633,-0.7984395675
H,0,-1.5045887112,3.5450191037,-1.0653575677
H,0,-2.7710296212,2.4846817563,-1.631174614
C,0,-3.5067675417,4.2625905801,-0.6107910379
H,0,-4.4971528782,3.8636421828,-0.3720996323
H,0,-3.2127891606,4.9355421452,0.1998178787
H,0,-3.589668602,4.8511025604,-1.5291714421
H,0,0.2773670893,2.2636693506,0.9746736171
H,0,-0.5244155986,1.2594567507,-0.5848052278
H,0,2.6739823543,1.4122792402,0.9201104044
H,0,2.3034414475,0.7838402588,-0.7062644286
H,0,0.5354294417,-0.7422819055,0.3292116849
H,0,0.9364653643,-0.0735271366,1.9120278106

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SCF Done: E(RPBE1PBE) = -1456.24725937 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.33
Sum of electronic and thermal Free Energies= -1456.013600 A.U.

C,0,0.8365115276,0.2748015109,-0.2469736058
C,0,2.195782684,0.5728445601,0.3814106823
C,0,-2.4706531755,2.3429637652,0.0187445176
C,0,5.0709836424,0.957652985,1.3227714342
C,0,4.8679138161,-0.272437655,0.6871867939
H,0,4.2560869514,1.6622616106,1.4528626291
C,0,-0.1459322979,1.3745919944,-0.0034934618
C,0,-1.5007168055,1.1941040027,0.1760356331
S,0,3.3105519105,-0.8163903416,0.0392033049
O,0,-2.0775924695,3.4696771621,-0.2283760945
C,0,5.9485098533,-1.155417139,0.5359639482
C,0,7.2081643898,-0.8092972518,1.0138223865
C,0,7.4131674892,0.4184586018,1.6470350717
C,0,6.3407382575,1.2942018176,1.7968089395
H,0,5.8042639321,-2.1139020555,0.0424779714
H,0,8.0341240886,-1.5044972891,0.8876698691
H,0,8.3982903874,0.687460683,2.0175909174
H,0,6.4845374912,2.2547033316,2.2852261272
Au,0,-0.7252740142,1.3693751682,2.2740159689

P,0,-0.3392906149,1.4706371374,4.5506998456
H,0,-1.354915473,0.9279809952,5.3544770657
H,0,0.8038962573,0.7920259288,5.0029196639
H,0,-0.1724685661,2.7559301118,5.0909777041
C,0,-3.9218157001,1.9816613162,0.159934398
H,0,-4.1354246215,1.2119436362,-0.596669149
H,0,-4.0333799687,1.4641563217,1.124166238
C,0,-4.8744517032,3.1551607906,0.0386293413
H,0,-4.6703589045,3.9144595188,0.7998084681
H,0,-4.7907493624,3.6352412431,-0.9409642101
H,0,-5.9077204392,2.8176557325,0.1633520984
H,0,0.2049321306,2.3973188744,-0.1592328799
H,0,-1.9197422485,0.1867642302,0.161374696
H,0,2.0920829583,0.704686813,1.4644769023
H,0,2.6096102361,1.490366406,-0.0489037492
H,0,0.9500000745,0.2101793678,-1.3401539068
H,0,0.432838247,-0.6844424048,0.0932697605

6.7 The structures shown in Figure S14.

PPh_3-NTf_2-TS-6-*exo-dig-anti*
SCF Done: E(RPBE1PBE) = -3975.22055033 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.19
Sum of electronic and thermal Free Energies= -3974.731824 A.U.

C,0,4.0134563493,-0.6708088586,2.0562757767
C,0,4.9748249419,-1.826256324,1.8703101662
C,0,2.0977839133,-0.1670738593,-1.1218105995
C,0,5.9574521398,0.3758728361,-0.9676947041
C,0,6.4327445797,-0.6553028165,-0.1707175916
H,0,4.9557834832,0.3261972312,-1.3786661203
C,0,2.652851468,-0.8856918251,1.3832209345
C,0,2.6062490856,-0.6492049819,-0.0617357957
S,0,5.409559384,-2.1033504688,0.1281947635
O,0,4.0882830907,-1.8875458515,-0.6408015342
C,0,7.7226365272,-0.6434806359,0.3527739086
C,0,8.5405566624,0.4489222188,0.0923991854
C,0,8.0751300064,1.4993139923,-0.6951726794
C,0,6.7904842096,1.460626427,-1.2260230631
H,0,8.0904172997,-1.4712002963,0.9526794217
H,0,9.5468280142,0.473609041,0.4973246472
H,0,8.7207830812,2.3466389278,-0.9020576212
H,0,6.431159504,2.2751800045,-1.8464927952
Au,0,0.5040272777,1.0469700212,-0.4424503582
P,0,-1.2246934505,2.4498367233,0.1933368466
C,0,2.3553957617,-0.2998109182,-2.5882277406

H,0,2.5041947379,0.699222234,-3.0113522278
H,0,3.2827691201,-0.8619374467,-2.728633264
C,0,1.2091331408,-0.9900730127,-3.3217395606
H,0,1.046982318,-2.0010185984,-2.9377916187
H,0,0.2730893453,-0.4350236335,-3.2092955295
H,0,1.4375386708,-1.0640712665,-4.3892987031
H,0,2.2887763908,-1.8981483098,1.5919002654
H,0,1.9229927659,-0.1970528367,1.8207004299
H,0,4.5380585732,-2.7730519476,2.2024972973
H,0,5.920880715,-1.6782034501,2.3980566083
H,0,3.8423249782,-0.5779047986,3.1328885092
H,0,4.4645820549,0.2688620682,1.7231393447
C,0,-0.6862291379,4.1852628077,0.3670860992
C,0,0.5754815366,4.4332215669,0.9156032252
C,0,-1.4985638081,5.2555080082,-0.0102627652
C,0,1.0115258551,5.7393012027,1.0991164184
H,0,1.216401162,3.6013718211,1.1950942666
C,0,-1.0532154194,6.561878796,0.1671564556
H,0,-2.4761343822,5.0739402572,-0.4452348628
C,0,0.1978751563,6.8050401772,0.7235996622
H,0,1.9911894203,5.9252241143,1.5278154845
H,0,-1.6876586264,7.3903681278,-0.1314561624
H,0,0.5422643649,7.8254040197,0.8598724552
C,0,-2.6171177585,2.4716314459,-0.9813396259
C,0,-3.9442813733,2.5161022807,-0.5530043933
C,0,-2.3282592481,2.4576817331,-2.3484476725
C,0,-4.9734347285,2.5562016011,-1.4882997963
H,0,-4.1787913167,2.5120078046,0.5065613095
C,0,-3.3592462373,2.5059823162,-3.2775292315
H,0,-1.2966998092,2.4024648662,-2.6844359812
C,0,-4.6826342331,2.5540757059,-2.8481233826
H,0,-6.0047619182,2.5834593348,-1.1510864669
H,0,-3.1296034547,2.492001586,-4.3381982417
H,0,-5.4878508684,2.5801997694,-3.5757021044
C,0,-1.9246248606,1.9815920099,1.8110469982
C,0,-2.3204955155,2.934803024,2.7511413788
C,0,-2.068519466,0.6203889557,2.0953245465
C,0,-2.8603978107,2.5265026906,3.9666563357
H,0,-2.2061889246,3.9933325748,2.5407876775
C,0,-2.6137251774,0.2203813914,3.3091434408
H,0,-1.759811737,-0.1284482822,1.3704603348
C,0,-3.0081428453,1.171672987,4.2458105723
H,0,-3.1652258529,3.2704067287,4.6960035261
H,0,-2.721893777,-0.8379711987,3.5235594649
H,0,-3.426720942,0.8557507645,5.1963352521
F,0,0.4043486162,-5.366718914,0.945957541

C,0,-0.1286368298,-4.4009395475,0.1987647284
S,0,-1.5997675351,-3.6807353143,1.0945092476
F,0,0.7944855705,-3.4694037229,-0.0100788054
F,0,-0.4881550805,-4.9158245558,-0.9694322605
O,0,-2.5287118515,-4.7917393193,1.222570682
O,0,-1.0201644337,-3.11082742,2.3010978547
N,0,-2.0481472089,-2.4680303483,0.1531775021
S,0,-3.0901021947,-2.5721539121,-1.059225028
C,0,-4.7122329589,-2.1200437719,-0.2528228528
O,0,-3.3143092697,-3.8984630047,-1.6111251562
O,0,-2.8317731975,-1.4667561669,-1.9661424275
F,0,-5.0227162092,-2.9898035182,0.7011824433
F,0,-5.6744505141,-2.1342498949,-1.172590827
F,0,-4.6522741924,-0.9055492888,0.2806950248

PPh_3-NTf_2-TS-7-*endo-dig*

SCF Done: E(RPBE1PBE) = -3975.21956452 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.19
Sum of electronic and thermal Free Energies= -3974.729743 A.U.

C,0,3.1676934414,-0.3273237824,2.42335768
C,0,4.6316923057,-0.2798048893,2.0183427377
C,0,2.3895567716,-1.0552666584,-0.7359424412
C,0,7.1831093599,0.0318222857,-0.3646646615
C,0,6.7593078634,-1.011178121,0.4487203406
H,0,6.4565772466,0.6258933641,-0.9088334186
C,0,2.180347332,0.3081284582,1.4380293471
C,0,1.7959027217,-0.5427984203,0.2655833551
S,0,5.0085175089,-1.356788559,0.609953582
O,0,4.3585527785,-0.6684012204,-0.6185084095
C,0,7.6554065567,-1.8211199516,1.1382420172
C,0,9.0158248494,-1.5556274804,1.0268547712
C,0,9.4591635283,-0.5084574276,0.2242852381
C,0,8.546887187,0.2791361185,-0.4724341726
H,0,7.3039084064,-2.6465306295,1.7503963271
H,0,9.7290849425,-2.1757784085,1.5596561713
H,0,10.5223598126,-0.3100674706,0.1347017327
H,0,8.8960987628,1.0889593555,-1.1046361555
Au,0,-0.2203524136,-1.1274739355,0.0337992071
P,0,-2.4475199283,-1.7493465906,-0.0747963598
C,0,2.4426242024,-1.7396865961,-2.0306645535
H,0,1.4240280155,-1.7112197842,-2.4333608595
H,0,3.0584646267,-1.1348743252,-2.7038030845
C,0,2.9519061563,-3.1758041996,-1.9833568209

H,0,3.9855132755,-3.2204806508,-1.6330462645
H,0,2.3346091075,-3.7912743561,-1.322650928
H,0,2.9183814611,-3.6117375381,-2.9855978162
H,0,1.282072353,0.5910237964,1.9872117219
H,0,2.6042232436,1.2412829877,1.0473633811
H,0,5.273099021,-0.6417787872,2.8286744544
H,0,4.9515769364,0.7271465451,1.7317747955
H,0,2.8666883607,-1.3540851991,2.6580444926
H,0,3.103469373,0.2344884144,3.3613904757
C,0,-3.3964965389,-1.2606104577,1.4027526074
C,0,-2.7531153392,-1.2898857824,2.6427128318
C,0,-4.7371423269,-0.8795216741,1.3265111268
C,0,-3.4501484911,-0.9560772434,3.7971344194
H,0,-1.7035472667,-1.5648098219,2.7007102781
C,0,-5.4287438796,-0.5408849841,2.4849300781
H,0,-5.242154807,-0.8380102827,0.3667890442
C,0,-4.7883764269,-0.5814038324,3.7190752821
H,0,-2.9439603086,-0.9766046929,4.7569678347
H,0,-6.4695872885,-0.2399443891,2.4199417942
H,0,-5.3300383597,-0.3123887241,4.6205175498
C,0,-3.3178351194,-1.028317267,-1.5051066714
C,0,-4.3017417657,-1.7304605095,-2.204279578
C,0,-2.9857222464,0.2740014058,-1.8885498773
C,0,-4.9548883543,-1.1270544769,-3.2740327506
H,0,-4.5578226998,-2.7463457496,-1.9205849892
C,0,-3.645212158,0.8719300697,-2.955488017
H,0,-2.2115547662,0.8223478717,-1.358608812
C,0,-4.6294841804,0.1729497586,-3.6483763226
H,0,-5.7178793085,-1.6766027551,-3.8164526851
H,0,-3.3732224475,1.8807661209,-3.247696713
H,0,-5.1380668101,0.6397007557,-4.486267217
C,0,-2.6555647125,-3.5572586922,-0.2291089981
C,0,-3.6374595634,-4.2559952436,0.473947256
C,0,-1.802269949,-4.2465549161,-1.0960612319
C,0,-3.7671205242,-5.6315132337,0.3052390825
H,0,-4.3000951749,-3.7327506745,1.1556177699
C,0,-1.9418113163,-5.6176449327,-1.2678817539
H,0,-1.0272146472,-3.7083478143,-1.6347614628
C,0,-2.9239740197,-6.3120351875,-0.5660527533
H,0,-4.5309224486,-6.1699023654,0.8573939916
H,0,-1.2778512833,-6.1461615677,-1.9446073708
H,0,-3.0274221232,-7.3847992021,-0.6954743094
F,0,1.8099906776,4.2835840892,-2.6291952886
C,0,1.3771391882,3.5339995662,-1.6179678429
S,0,-0.4776900209,3.6944668434,-1.484302422
F,0,1.7272016469,2.2734596633,-1.8450316406

F,0,1.9667027711,3.9462490735,-0.500969672
O,0,-0.7099244564,5.1206703727,-1.3280390734
O,0,-0.9701815763,3.032251254,-2.6815577072
N,0,-0.8199424674,2.7622725633,-0.2290012735
S,0,-0.9892804055,3.2673810733,1.280343292
C,0,-2.8250854747,3.5811965608,1.40120444
O,0,-0.374889287,4.5410411314,1.6176156223
O,0,-0.7719483163,2.1315937119,2.161976872
F,0,-3.1995370892,4.5151142999,0.5342534321
F,0,-3.1181309173,3.9993391071,2.6305051463
F,0,-3.509544433,2.4707708102,1.1552994363

PPh_3-NTf_2-TS-33
SCF Done: E(RPBE1PBE) = -3975.22928347 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -9.98
Sum of electronic and thermal Free Energies= -3974.739002 A.U.

C,0,3.0873620748,-2.4938640836,2.3601971211
C,0,4.5825591757,-2.3157153386,2.1517738994
C,0,2.1279055245,-0.5904571071,-0.8153270228
C,0,6.4446224351,-1.0080653898,-1.2919792923
C,0,5.581501152,-0.9848696812,-0.1833786167
H,0,2.9104332981,-2.3823668874,3.4345504765
H,0,5.155186334,-3.0818172767,2.6796843834
H,0,2.7993539541,-3.5161131852,2.0997668943
H,0,4.9442940537,-1.3368569347,2.4715563809
H,0,6.8331495543,-1.9515878777,-1.6620462814
C,0,2.2325989689,-1.4890469645,1.5912098333
H,0,2.3927450932,-0.4770986836,1.9801957948
H,0,1.172623961,-1.716486448,1.7469244569
C,0,2.5431962286,-1.5198568235,0.1113581246
S,0,5.0722739643,-2.5375142985,0.402490002
O,0,3.2510280257,-2.5678689541,-0.288776013
C,0,5.0556631575,0.2218965201,0.2964440903
C,0,5.4216770466,1.4091190412,-0.3320022981
C,0,6.2812398813,1.3908562047,-1.420978149
C,0,6.7946834882,0.1821715402,-1.8989973255
H,0,4.4107129204,0.2555203426,1.1654193121
H,0,5.0267203566,2.3492354442,0.0378242373
H,0,6.5616631449,2.3220405678,-1.9024900067
H,0,7.4704903923,0.1736746187,-2.7473629523
Au,0,0.7436635737,0.830122779,-0.3107421973
C,0,2.5981859779,-0.671269782,-2.2346362274
H,0,2.8937564606,0.3363522463,-2.5534036753
H,0,3.4761666326,-1.3189697494,-2.3266356816
C,0,1.4995654575,-1.1716569356,-3.1771692241

H,0,0.607439889,-0.540839644,-3.1185985907
H,0,1.8557632323,-1.1691714613,-4.2123037224
H,0,1.1998673458,-2.1921338947,-2.9214407871
P,0,-0.7263350367,2.5740220331,0.2529756253
C,0,0.1414984066,4.1795783181,0.3625633334
C,0,1.3659451218,4.2149930685,1.0376670294
C,0,-0.3715978048,5.3510498597,-0.1944457605
C,0,2.057424379,5.4123683376,1.1679678669
H,0,1.7772332198,3.3022679962,1.4601156066
C,0,0.3293595017,6.5473243852,-0.0688119616
H,0,-1.3157264641,5.335531459,-0.7290164386
C,0,1.5398442885,6.5807312316,0.613982965
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H,0,-0.0754654866,7.4544148458,-0.5064609071
H,0,2.0836787494,7.5151011289,0.7113786556
C,0,-2.0754712934,2.8219888079,-0.9497447411
C,0,-3.3445021726,3.2601279318,-0.5666997931
C,0,-1.809035528,2.5664195492,-2.297363251
C,0,-4.3329629708,3.4489479771,-1.5268355168
H,0,-3.5682298531,3.4446314366,0.4791183237
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H,0,-2.5864878787,2.5546346327,-4.2975108266
H,0,-4.8368667157,3.344125348,-3.6147890596
C,0,-1.5353178119,2.3561645277,1.8745495865
C,0,-1.8298018857,3.43466529,2.7116062268
C,0,-1.8844555763,1.0601308057,2.2644242709
C,0,-2.4796054083,3.2168296265,3.9220624716
H,0,-1.5525644792,4.4438629202,2.4233030575
C,0,-2.5386921101,0.8491581038,3.4723883353
H,0,-1.6434137511,0.2163894691,1.6243081274
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H,0,-2.7066226168,4.0583922361,4.5690777102
H,0,-2.8090394714,-0.1597478018,3.7674091817
H,0,-3.3457561016,1.7599522444,5.2458283864
F,0,-0.5003581741,-5.5811259631,1.3511205294
C,0,-0.7684051596,-4.6971508096,0.3908946086
S,0,-1.9281225759,-3.3974491377,1.0619753414
F,0,0.3725107354,-4.1482213173,-0.0082591159
F,0,-1.3171328789,-5.3366321154,-0.634338026
O,0,-3.1197442726,-4.1346028305,1.4497737001
O,0,-1.1469561146,-2.7398309572,2.0992174462
N,0,-2.0712184639,-2.3768541371,-0.1582227222
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C,0,-4.5071929113,-1.3090129367,-0.6623856343
O,0,-3.8466712088,-3.7262419604,-1.4975694126
O,0,-2.6626106554,-1.750668804,-2.4764441412
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F,0,-5.4979530478,-1.2421028865,-1.5493616411
F,0,-4.0244627746,-0.0876266898,-0.4714070969

PPh_3-NTf_2-TS-OS
SCF Done: E(RPBE1PBE) = -3975.22995919 A.U.
SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.30
Sum of electronic and thermal Free Energies= -3974.738624 A.U.

C,0,2.1420798751,-2.2661898559,2.8398244204
C,0,3.6536103147,-2.1757834107,2.6553313767
C,0,0.6394143858,-2.1650169944,-0.5354480769
C,0,5.8473897045,-0.9342098113,0.6422227971
C,0,5.6016181416,-2.3068281763,0.5597092978
H,0,5.1303375181,-0.2600460596,1.0947043752
C,0,1.3491514597,-1.4336914781,1.831861743
C,0,1.5980197428,-1.8758845738,0.4208182713
S,0,4.1189615561,-3.0404619703,1.1337768817
O,0,2.8532348216,-1.8924482286,0.0397155975
C,0,6.509964872,-3.1690458379,-0.0635938957
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C,0,7.9471629424,-1.2855459125,-0.4934843634
C,0,7.0286121898,-0.4333842294,0.1148674457
H,0,6.301437702,-4.2320110733,-0.1313356215
H,0,8.3990887672,-3.3132137988,-1.0619684442
H,0,8.8678667014,-0.8826050725,-0.9025394277
H,0,7.2279101447,0.6313855275,0.173816684
Au,0,-1.2365289812,-1.3743732322,-0.314996203
C,0,1.0425411462,-2.848714313,-1.8022263569
H,0,1.2142835235,-2.0633775622,-2.5540960737
H,0,2.0045475467,-3.3600256659,-1.6791020069
C,0,-0.0106327637,-3.8119363085,-2.3409583047
H,0,-0.2276550302,-4.6073141449,-1.6208870798
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H,0,0.2821331826,-1.5060883264,2.0542484857
H,0,1.9306223751,-1.8961993204,3.8472802977
H,0,1.820447652,-3.3146491708,2.8199454053
P,0,-3.3596029342,-0.3977423713,-0.0757684959

C,0,-4.7382300399,-1.5967476952,-0.0733866817
C,0,-4.6795333075,-2.6660320558,-0.9720632104
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C,0,-5.7214326665,-3.5828243387,-1.0351481938
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H,0,-7.7329019342,-2.284318846,1.3716061164
H,0,-7.6307455893,-4.169631782,-0.2360790333
C,0,-3.5265243256,0.5336331225,1.4865240826
C,0,-3.959161568,1.8588332993,1.5251129441
C,0,-3.1809980158,-0.1161921754,2.6761708299
C,0,-4.0530751717,2.5245578143,2.7443524364
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H,0,-2.0939253598,2.9109539173,-3.4857748287
H,0,-4.421628019,3.3694545369,-4.2129374223
F,0,3.4589688516,2.4507295969,-3.4553054603
C,0,3.3711821885,2.0725483148,-2.1820633161
S,0,1.6503253069,2.4168837256,-1.5508019507
F,0,3.6513531494,0.7780053107,-2.1023789687
F,0,4.2718418315,2.7489752076,-1.4757592707
O,0,1.461711718,3.8444001474,-1.749982538
O,0,0.8117771621,1.4919039786,-2.2960118542
N,0,1.7430078331,1.9030894574,-0.0397987552
S,0,2.0279181065,2.8180990849,1.2381902776
C,0,0.3020460226,3.1623766123,1.8560448605
O,0,2.610644555,4.128165686,1.0005257773
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F,0,-0.4016700517,3.8170803667,0.9394456261

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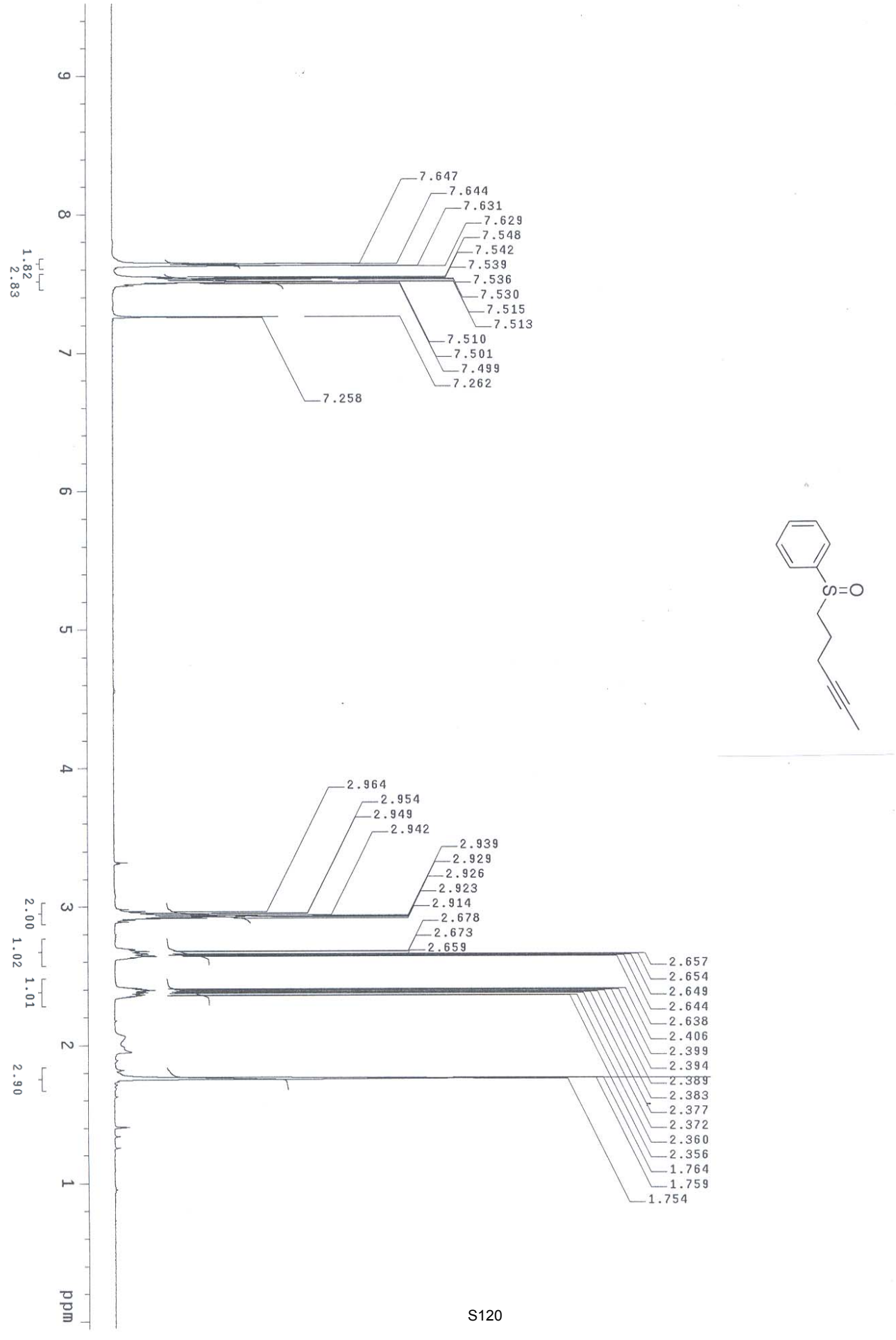
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7.631
7.629
7.548
7.542
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7.536
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7.515
7.513
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7.501
7.499
7.262
7.258
1.82
2.83
2.964
2.954
2.949
2.942
2.939
2.929
2.926
2.923
2.914
2.678
2.673
2.659
2.657
2.654
2.649
2.644
2.638
2.406
2.399
2.394
2.389
2.383
2.377
2.372
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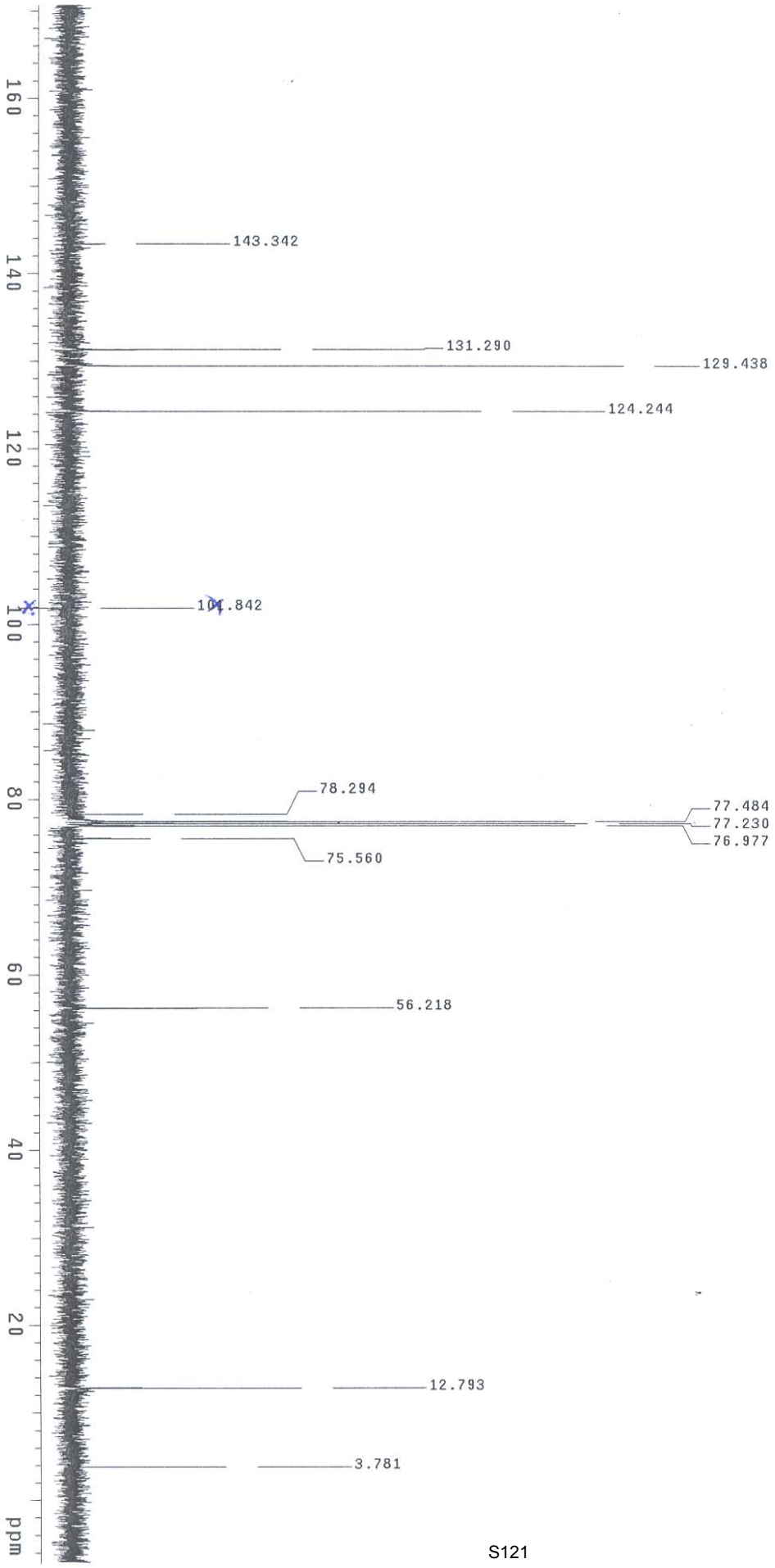
2.356
1.764
1.759
1.754
2.00
1.02
1.01
2.90
S=O
ppm


160
140
120
100
80
60
40
20
ppm
143.342
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129.438
124.244
101.842
78.294
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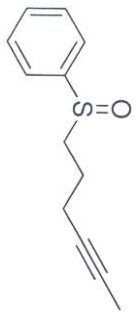
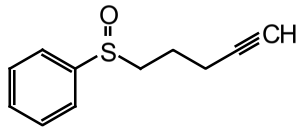
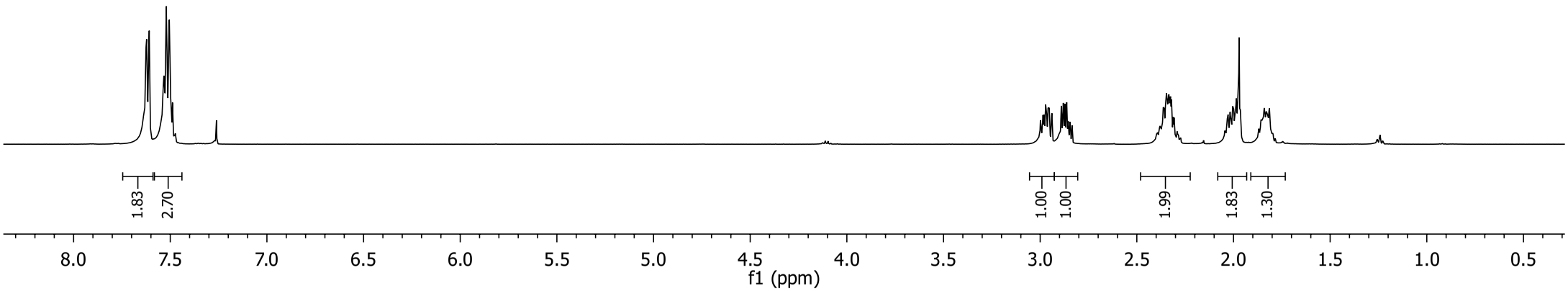
77.230
76.977
75.560
56.218
12.793
3.781

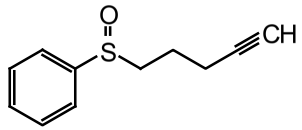

S=O

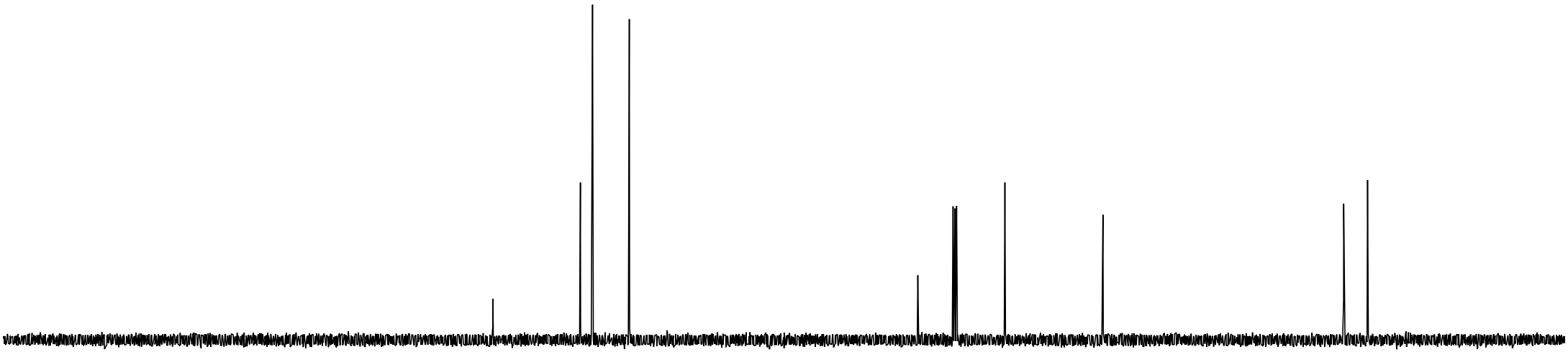
Title lb-III-17
Solvent CDCl3
Spectrometer Frequency 499.86

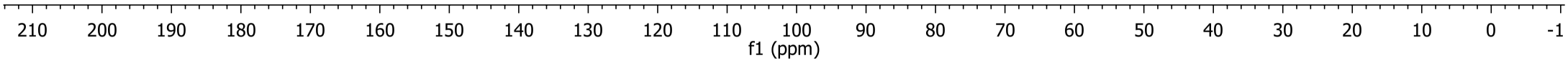




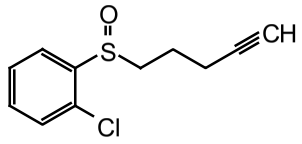
Title lb-III-17-C13
Solvent cdcl3
Spectrometer Frequency 125.70

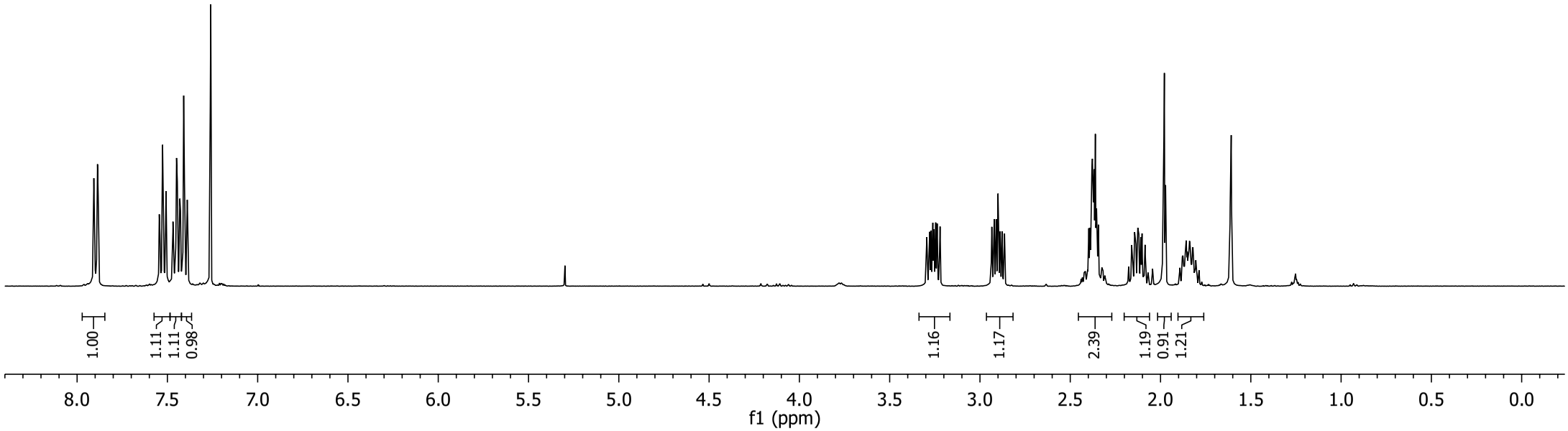




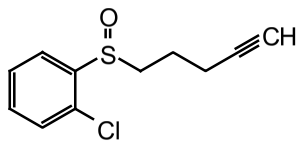


Title lb-III-31-2
Solvent cdcl3
Spectrometer Frequency 399.95

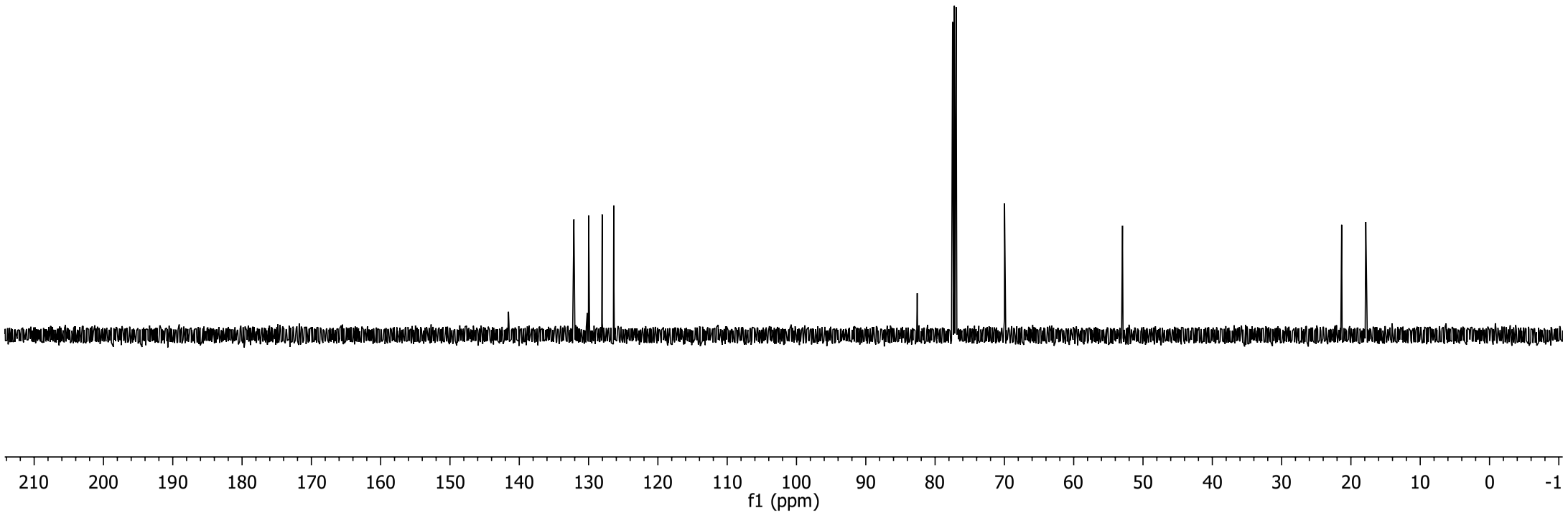




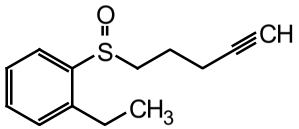
Title lb-III-30-C13
Solvent cdcl3
Spectrometer Frequency 125.70

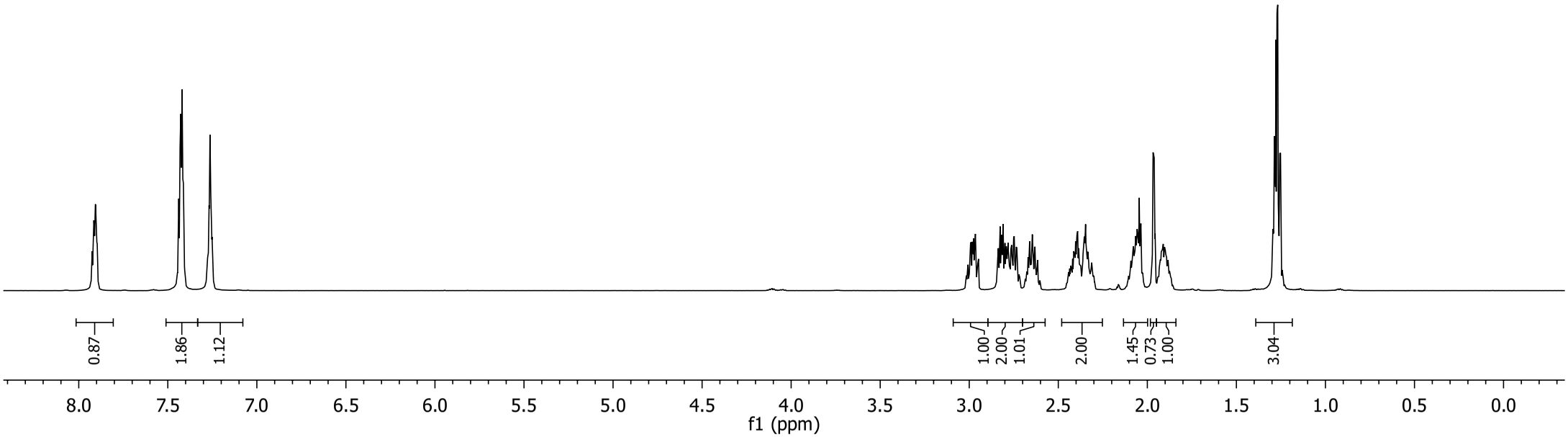


12b

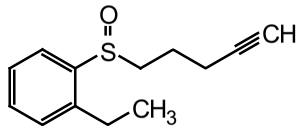


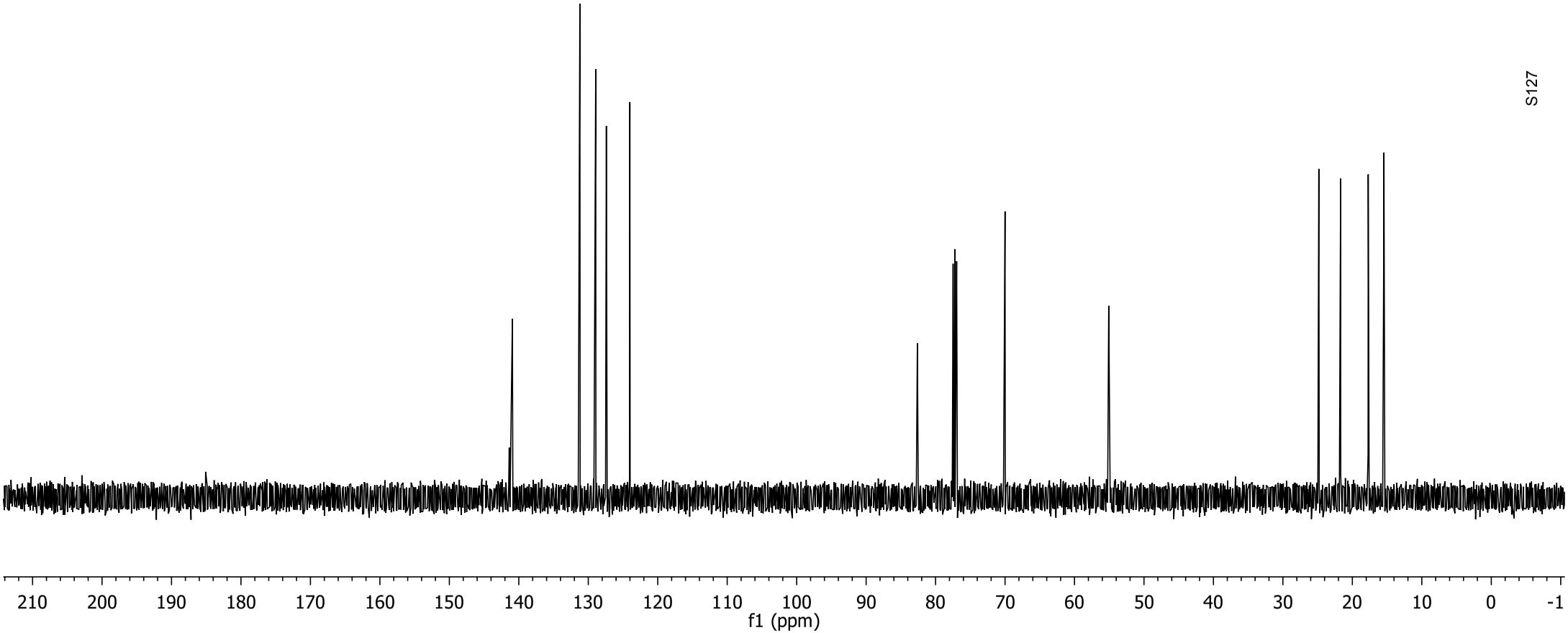
Title lb-III-47-2
Solvent CDCl3
Spectrometer Frequency 499.86



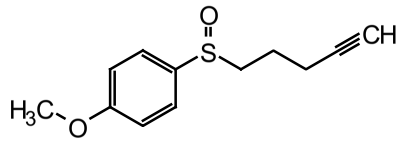


Title lb-III-47-2-C13
Solvent cdcl3
Spectrometer Frequency 125.70





Title Ib-III-53
Solvent CDCl3
Spectrometer Frequency 499.86

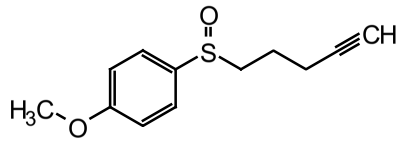


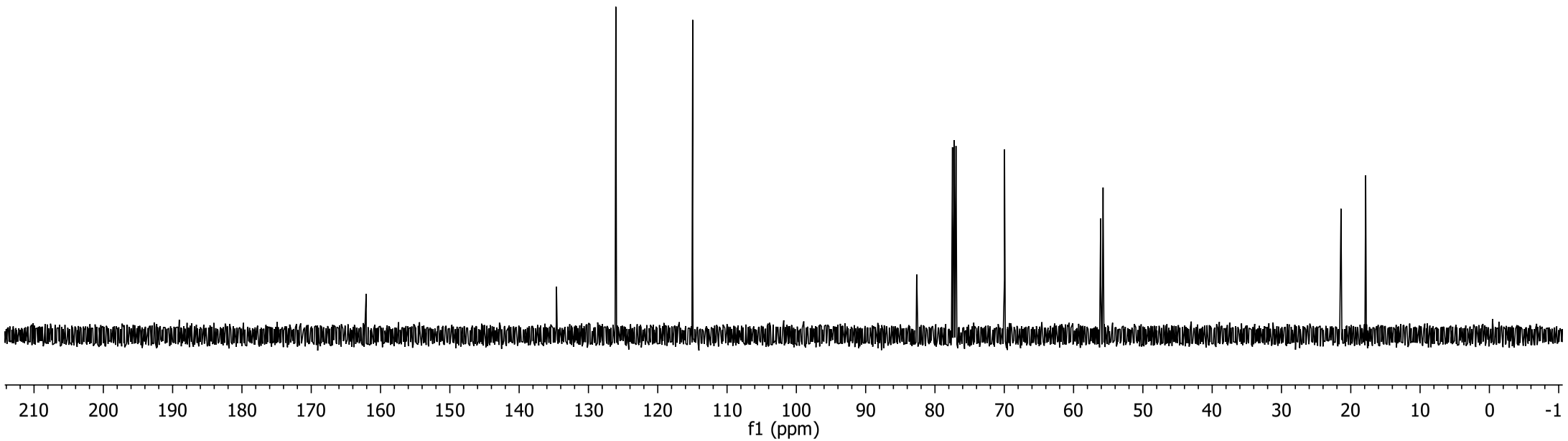
S128

1.79 1.85 2.99 1.94 1.93 1.72 1.00

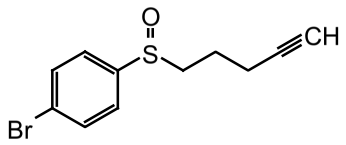
7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4
f1 (ppm)

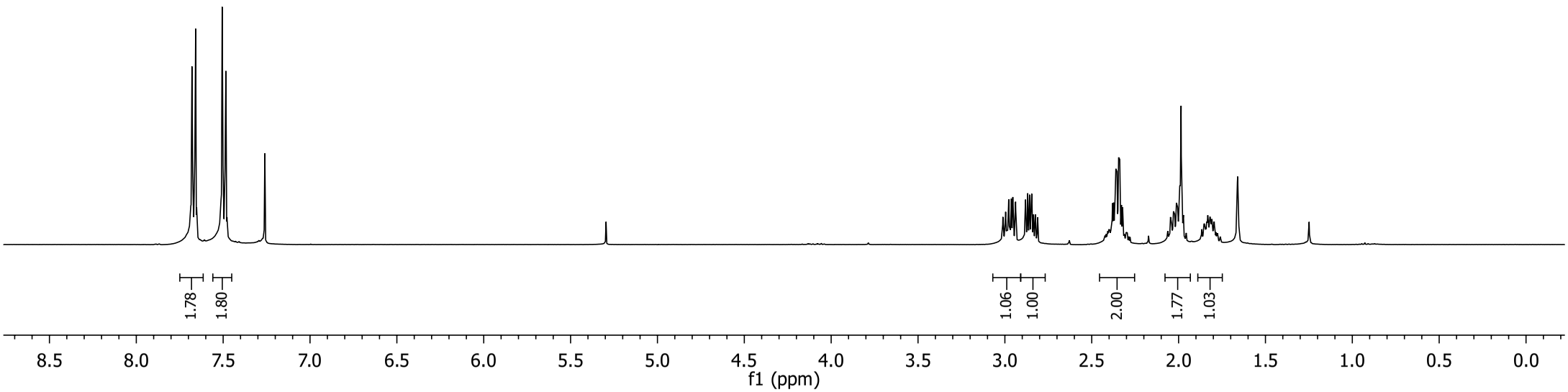
Title lb-III-53-C13
Solvent cdcl3
Spectrometer Frequency 125.70



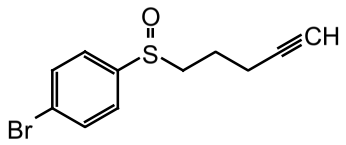


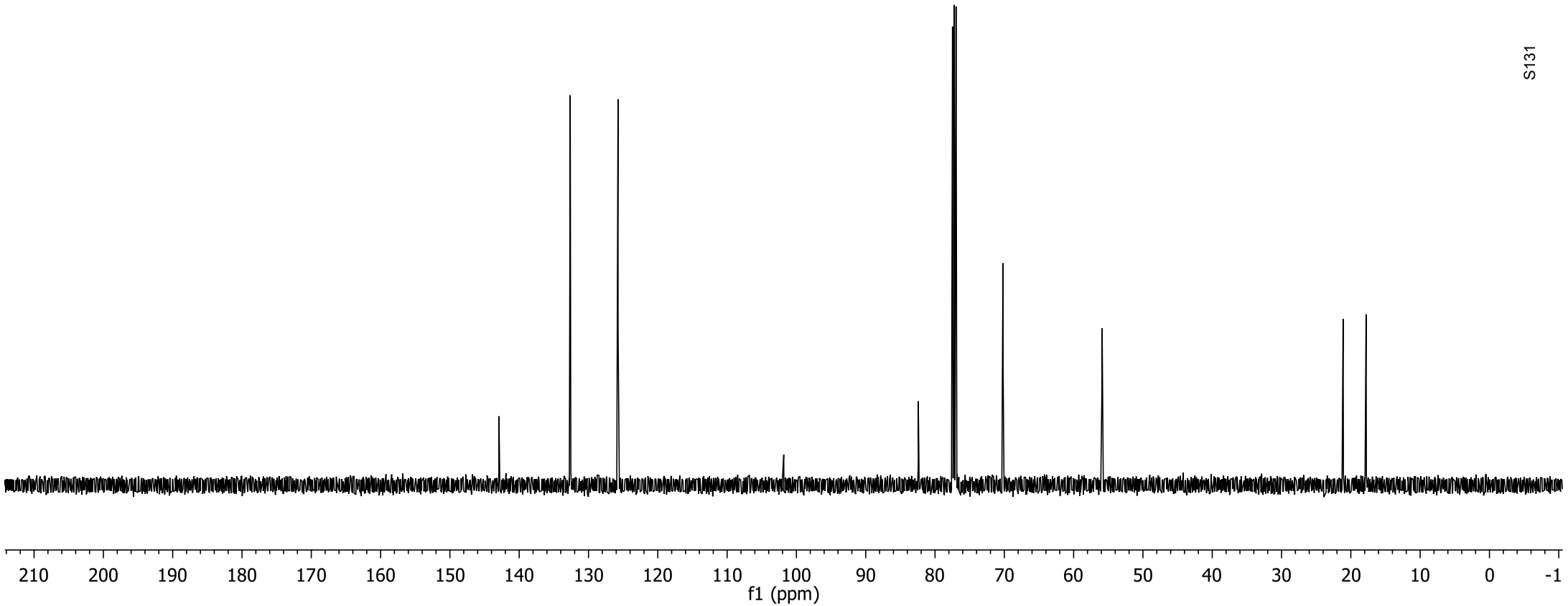
Title lb-III-46
Solvent cdcl3
Spectrometer Frequency 399.95



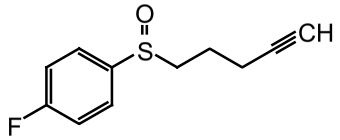


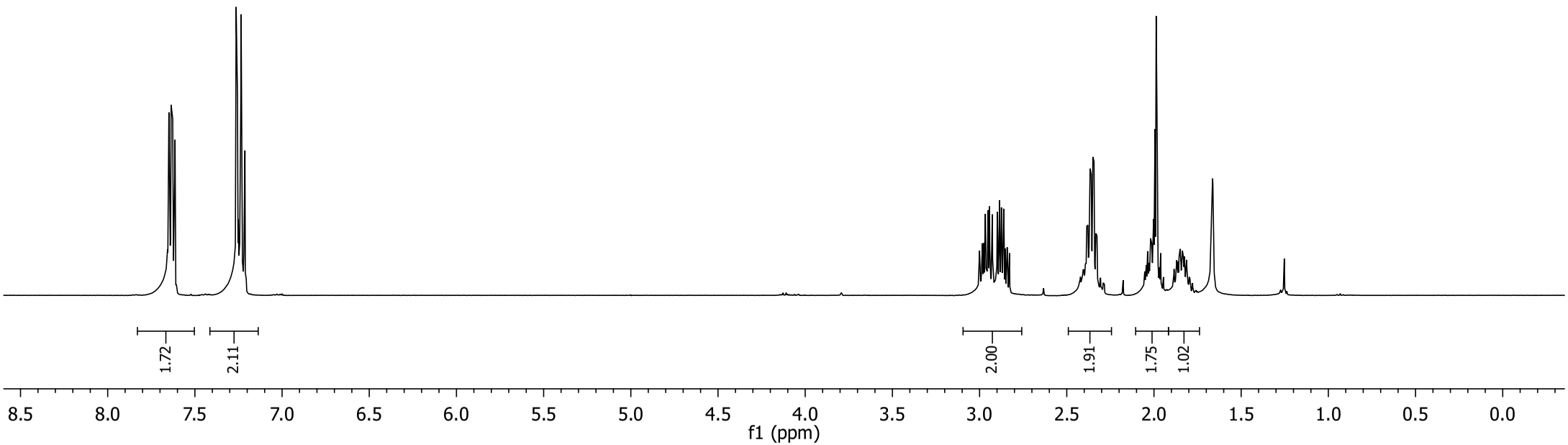
Title lb-III-46-1-C13
Solvent cdcl3
Spectrometer Frequency 125.70



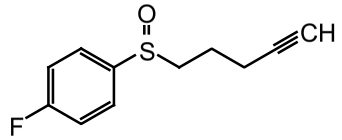


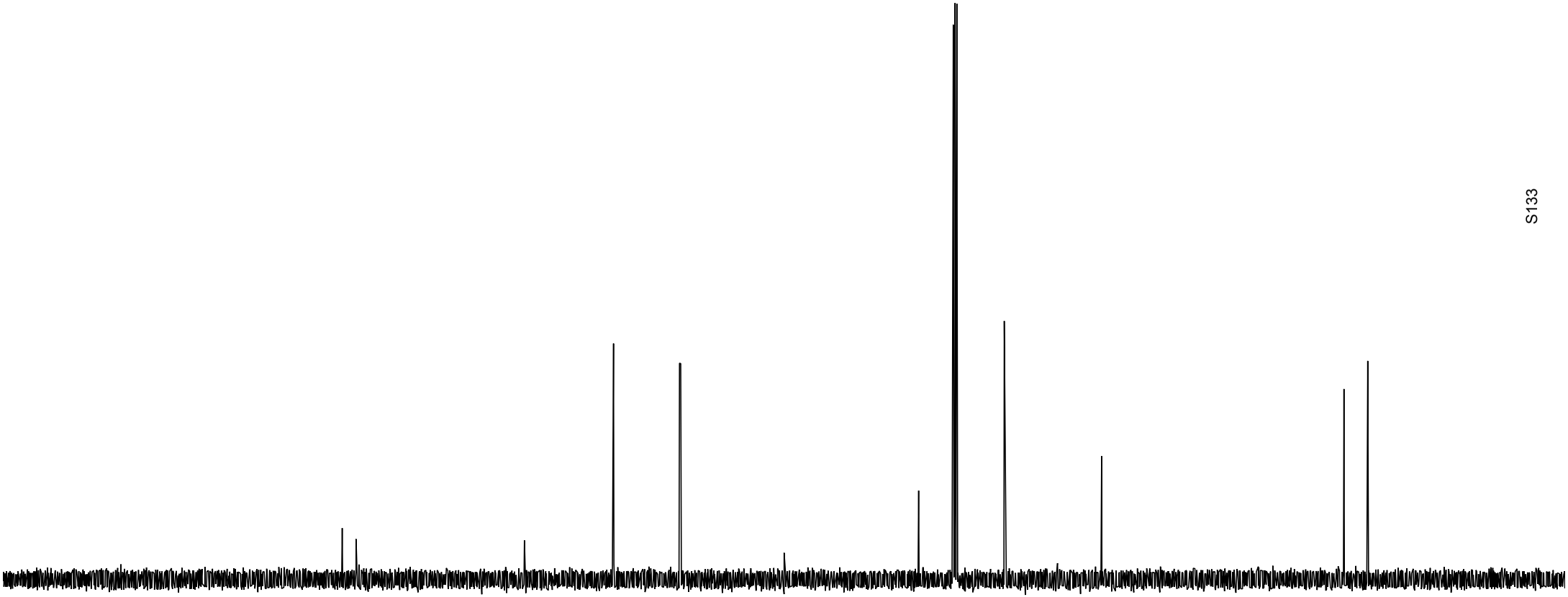
Title lb-III-51-2
Solvent cdcl3
Spectrometer Frequency 399.95

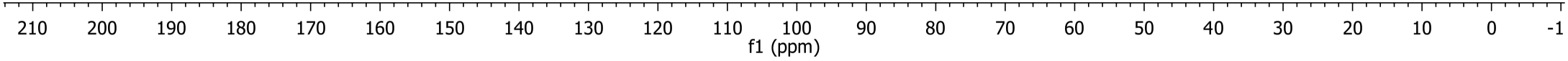




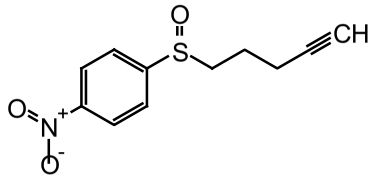
Title lb-III-51-2-C13
Solvent cdcl3
Spectrometer Frequency 125.70

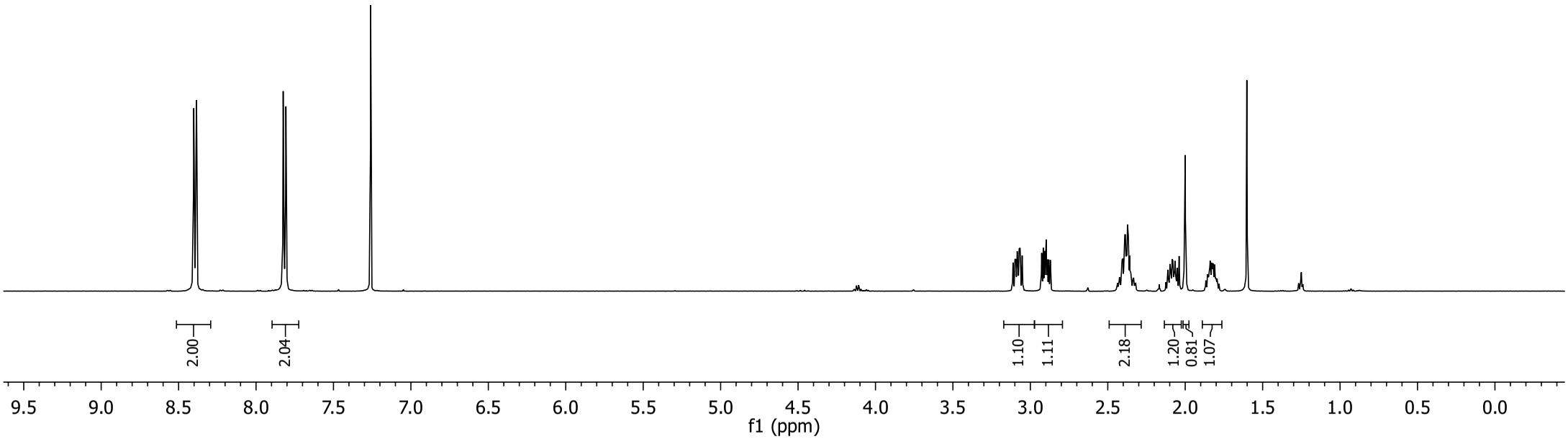




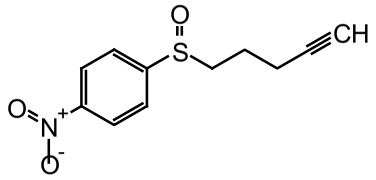


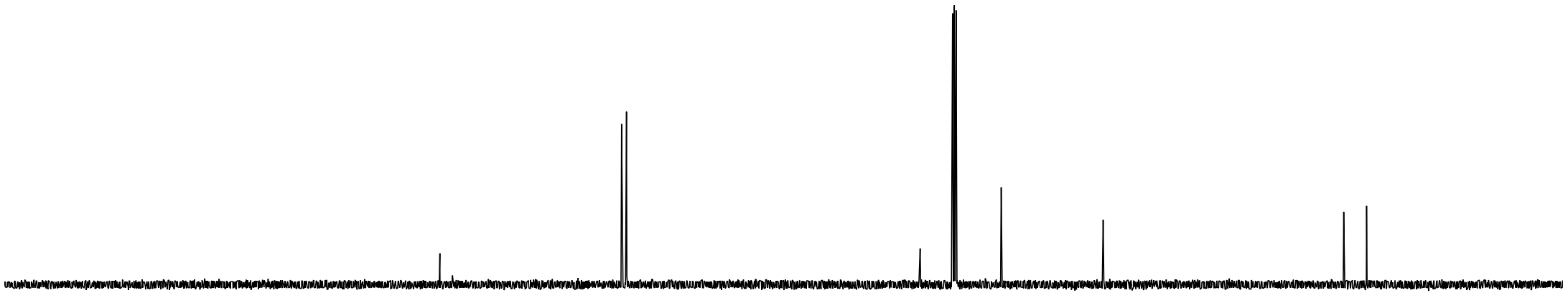
Title lb-III-46-2
Solvent CDCl3
Spectrometer Frequency 499.86

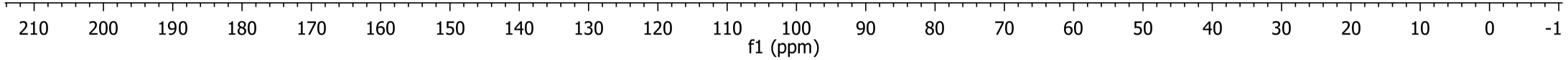


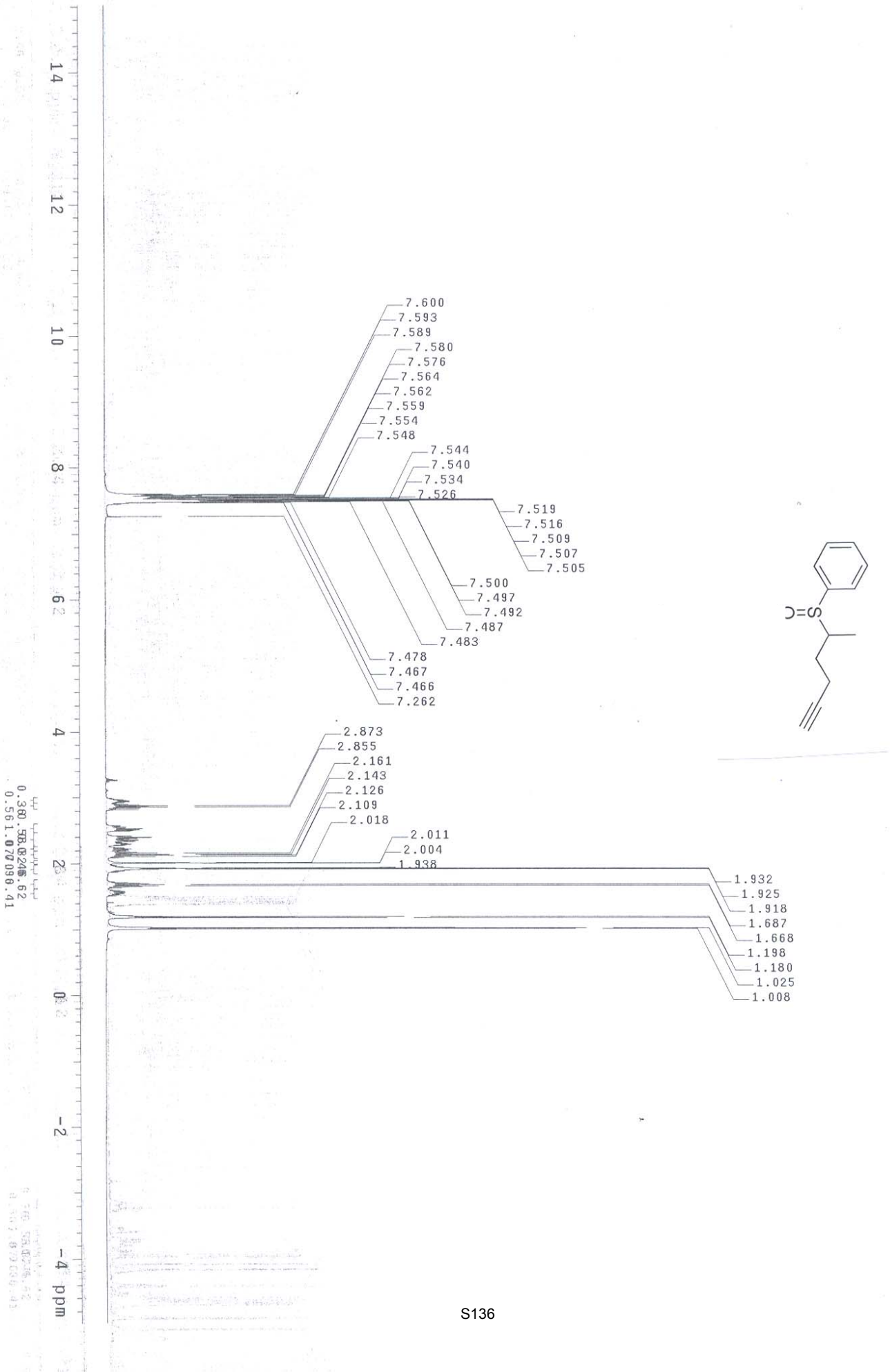


Title lb-III-46-2-C13
Solvent cdcl3
Spectrometer Frequency 125.70

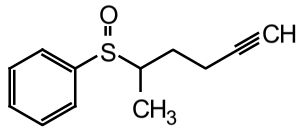


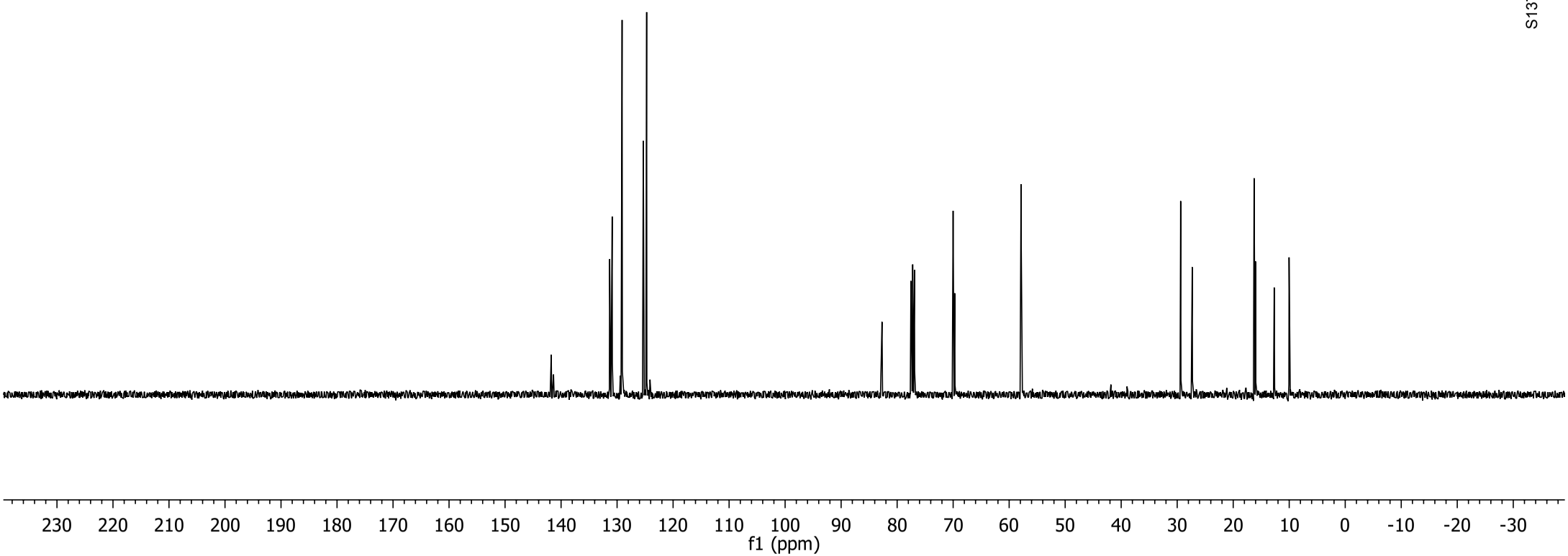




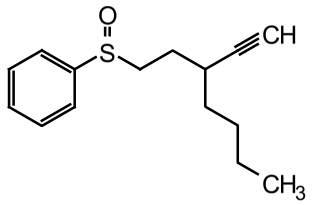

7.600
7.593
7.589
7.580
7.576
7.564
7.562
7.559
7.554
7.548
7.544
7.540
7.534
7.526
7.519
7.516
7.509
7.507
7.505
7.500
7.497
7.492
7.487
7.483
7.478
7.467
7.466
7.262
2.873
2.855
2.161
2.143
2.126
2.109
2.018
2.011
2.004
1.938
1.932
1.925
1.918
1.687
1.668
1.198
1.180
1.025
1.008
14
12
10
8
6
4
2
0
-2
-4 ppm

Title lb-III-70-2-C13
Solvent cdcl3
Spectrometer Frequency 100.58

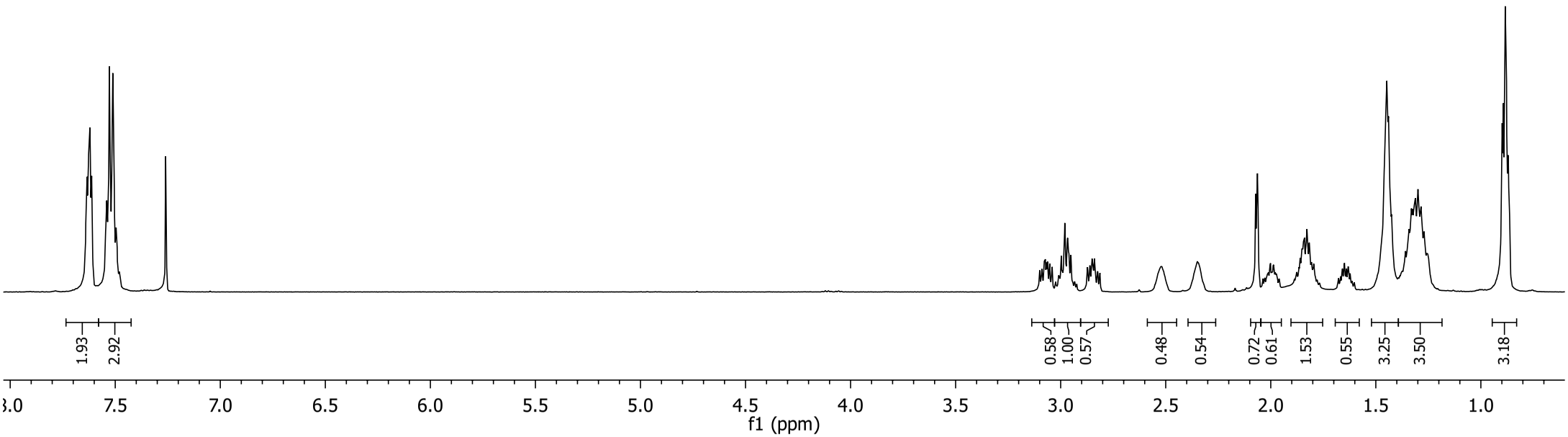




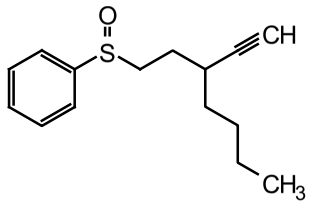
Title
Solvent CDCl3
Spectrometer Frequency 499.86

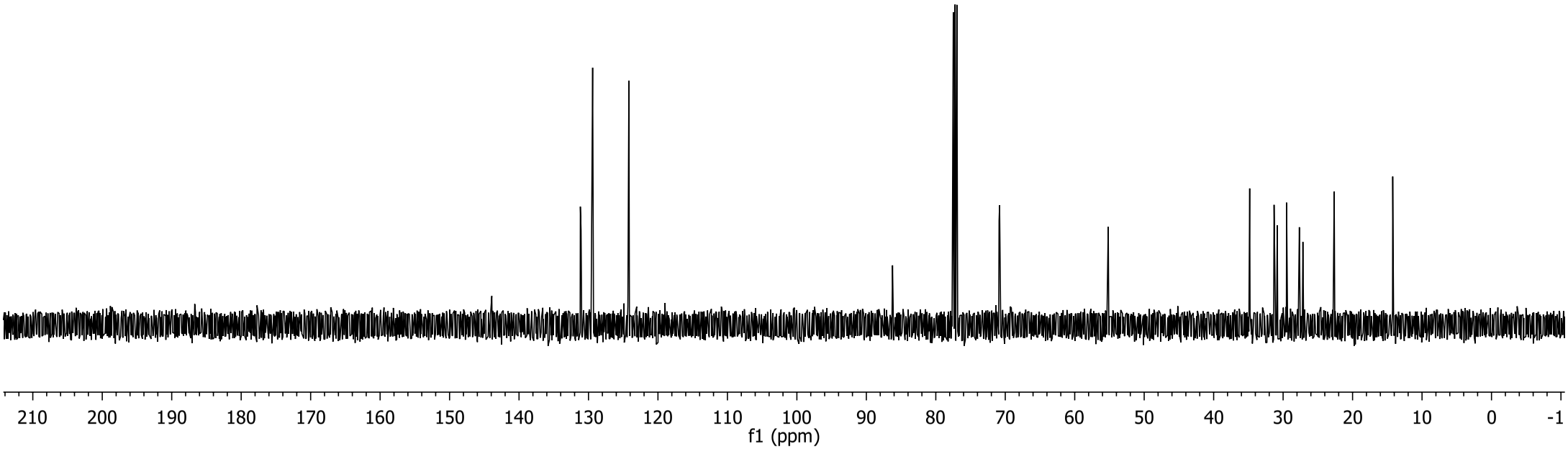


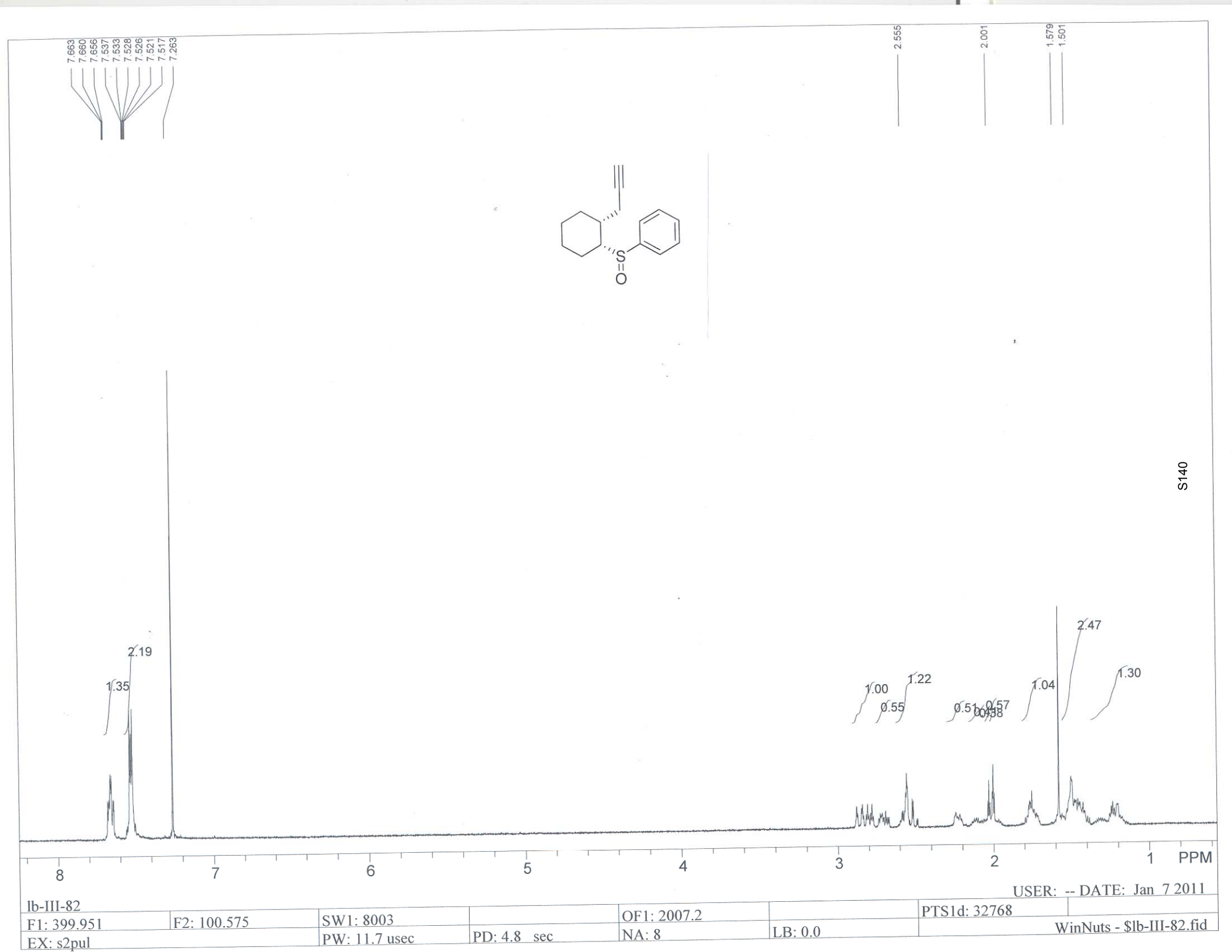
S138



Title lb-III-89-2-C13
Solvent cdcl3
Spectrometer Frequency 125.70







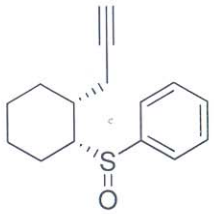
USER: -- DATE: Jan 7 2011

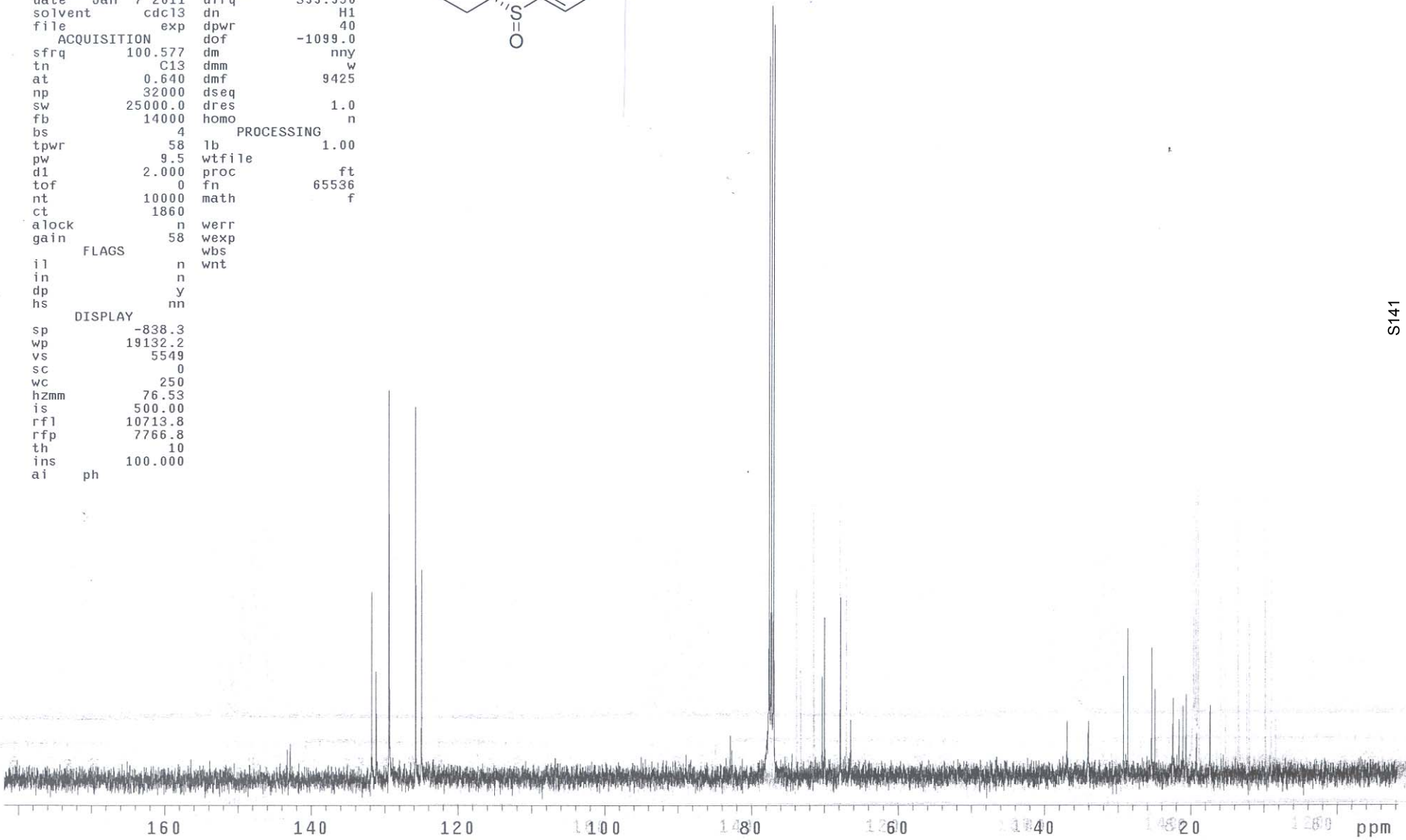
lb-III-82							
F1: 399.951	F2: 100.575	SW1: 8003		OF1: 2007.2		PTS1d: 32768	
EX: s2pul		PW: 11.7 usec	PD: 4.8 sec	NA: 8	LB: 0.0	WinNuts - $lb-III-82.fid	

Standard c13 run using qnp probe

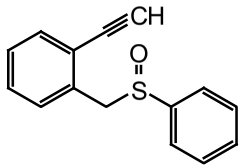
exp1 std13c

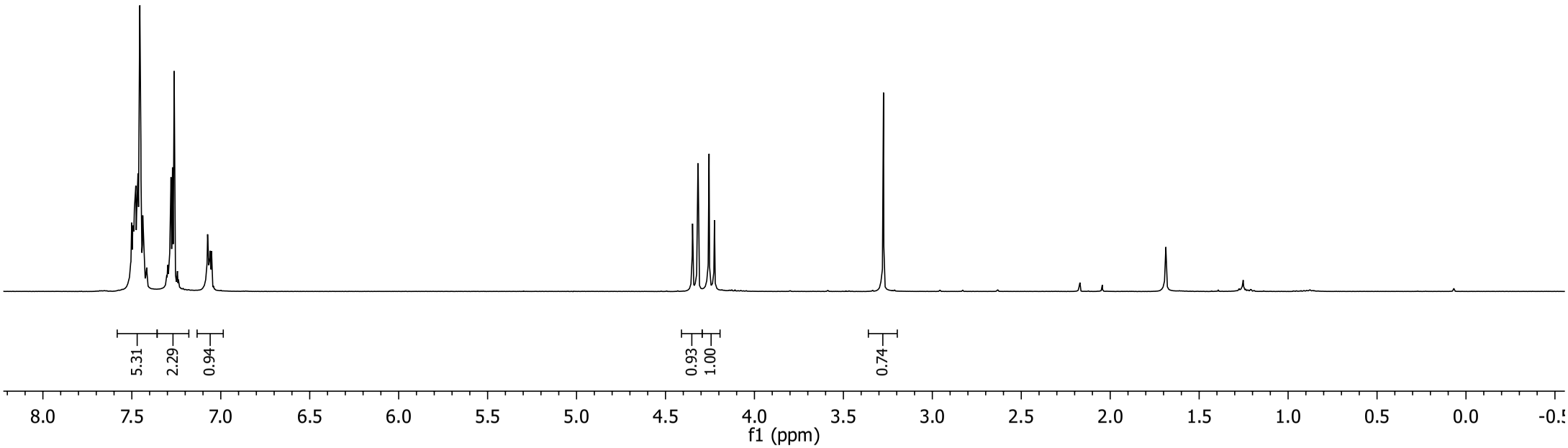
SAMPLE		DEC. & VT	
date	Jan 7 2011	dfrq	399.950
solvent	cdcl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	-1099.0
sfrq	100.577	dm	nny
tn	C13	dmm	w
at	0.640	dmf	9425
np	32000	dseq	
sw	25000.0	dres	1.0
fb	14000	homo	n
bs	4	PROCESSING	
tpwr	58	lb	1.00
pw	9.5	wtfile	
d1	2.000	proc	ft
tof	0	fn	65536
nt	10000	math	f
ct	1860		
alock	n	werr	
gain	58	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-838.3		
wp	19132.2		
vs	5549		
sc	0		
wc	250		
hzmm	76.53		
is	500.00		
rfl	10713.8		
rfp	7766.8		
th	10		
ins	100.000		
ai	ph		



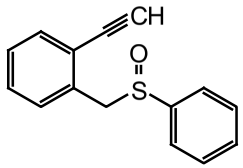


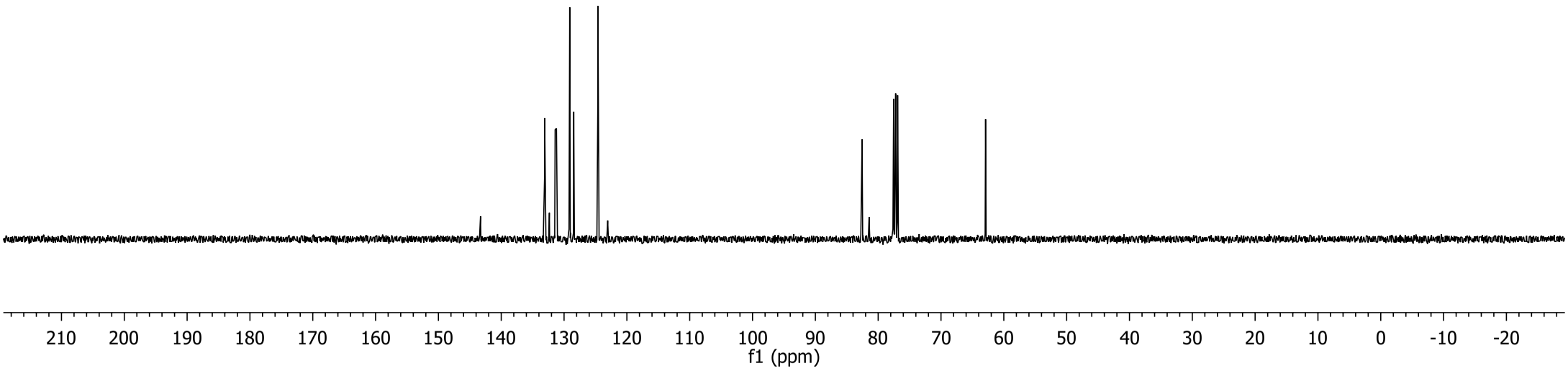
Title lb-III-109
Solvent cdcl3
Spectrometer Frequency 399.95



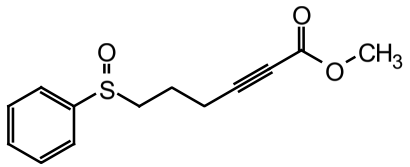


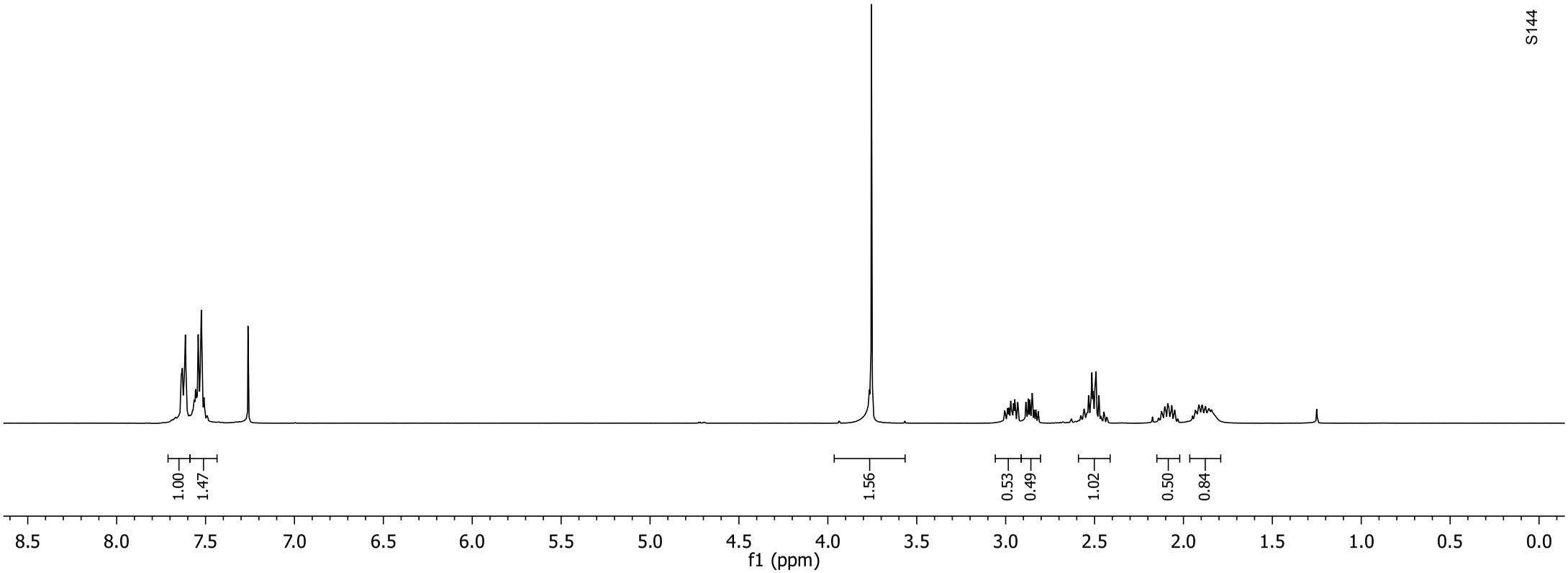
Title lb-III-109-C13
Solvent cdcl3
Spectrometer Frequency 100.58



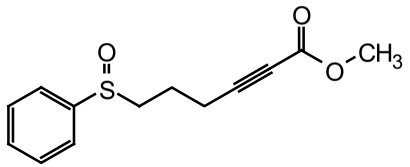


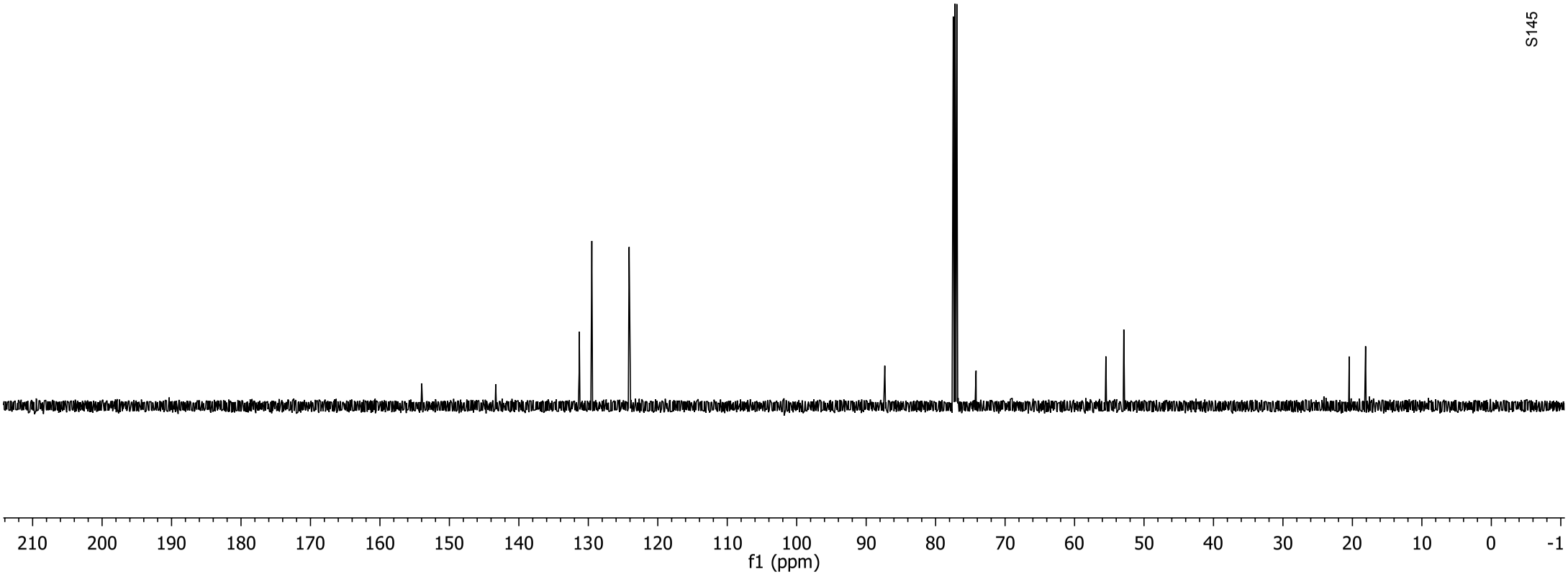
Title lb-III-58-B
Solvent cdcl3
Spectrometer Frequency 399.95

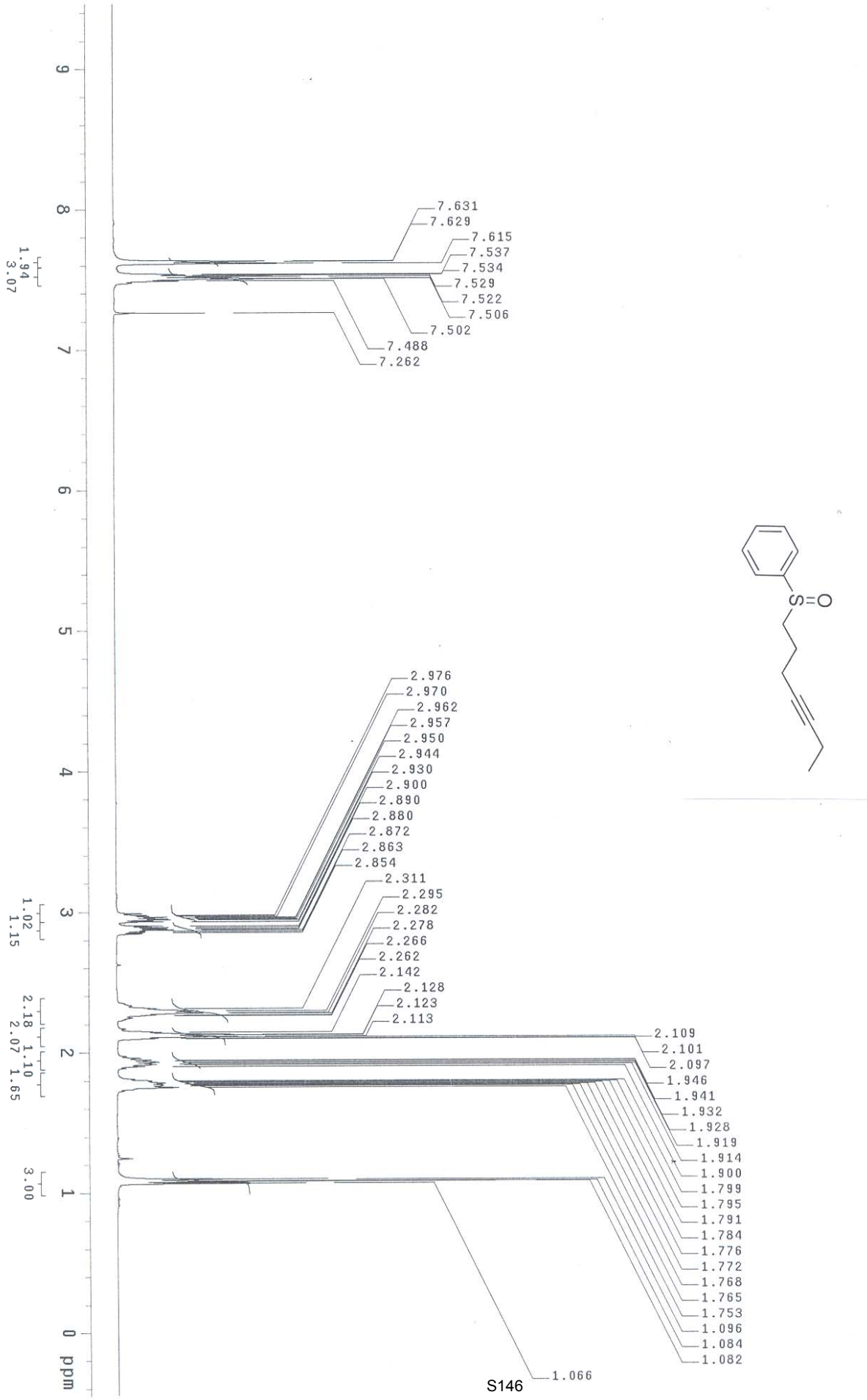


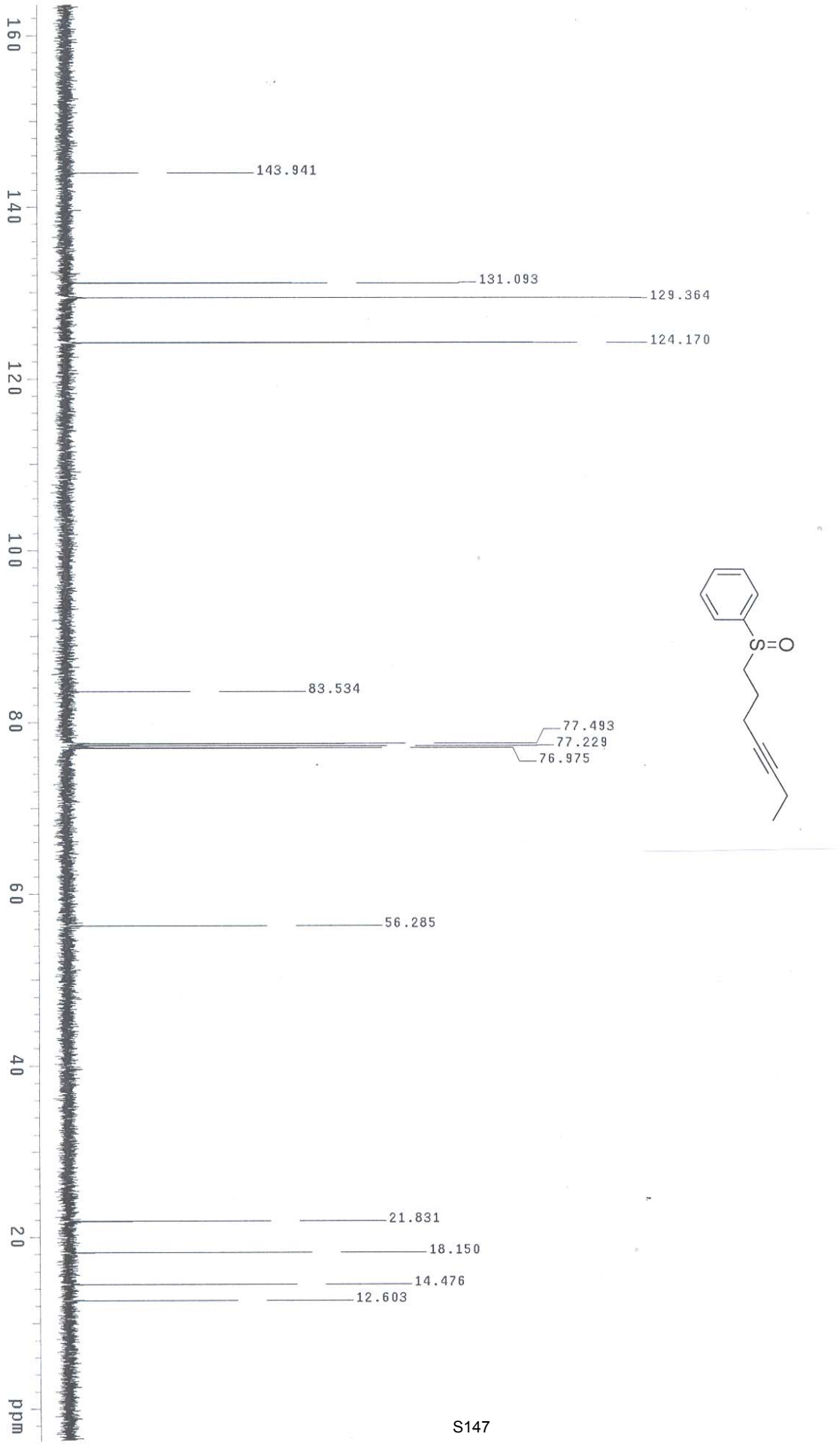


Title lb-III-58-B-C13
Solvent cdcl3
Spectrometer Frequency 125.70






7.631
7.629
7.615
7.537
7.534
7.529
7.522
7.506
7.502
7.488
7.262
2.976
2.970
2.962
2.957
2.950
2.944
2.930
2.900
2.890
2.880
2.872
2.863
2.854
2.311
2.295
2.282
2.278
2.266
2.262
2.142
2.128
2.123
2.113
2.109
2.101
2.097
1.946
1.941
1.932
1.928
1.919
1.914
1.900
1.799
1.795
1.791
1.784
1.776
1.772
1.768
1.765
1.753
1.096
1.084
1.082
1.066
1.94
3.07
1.02
1.15
2.18
1.10
2.07
1.65
3.00
S=O
9
8
7
6
5
4
3
2
1
0
ppm


160
140
120
100
80
60
40
20
ppm
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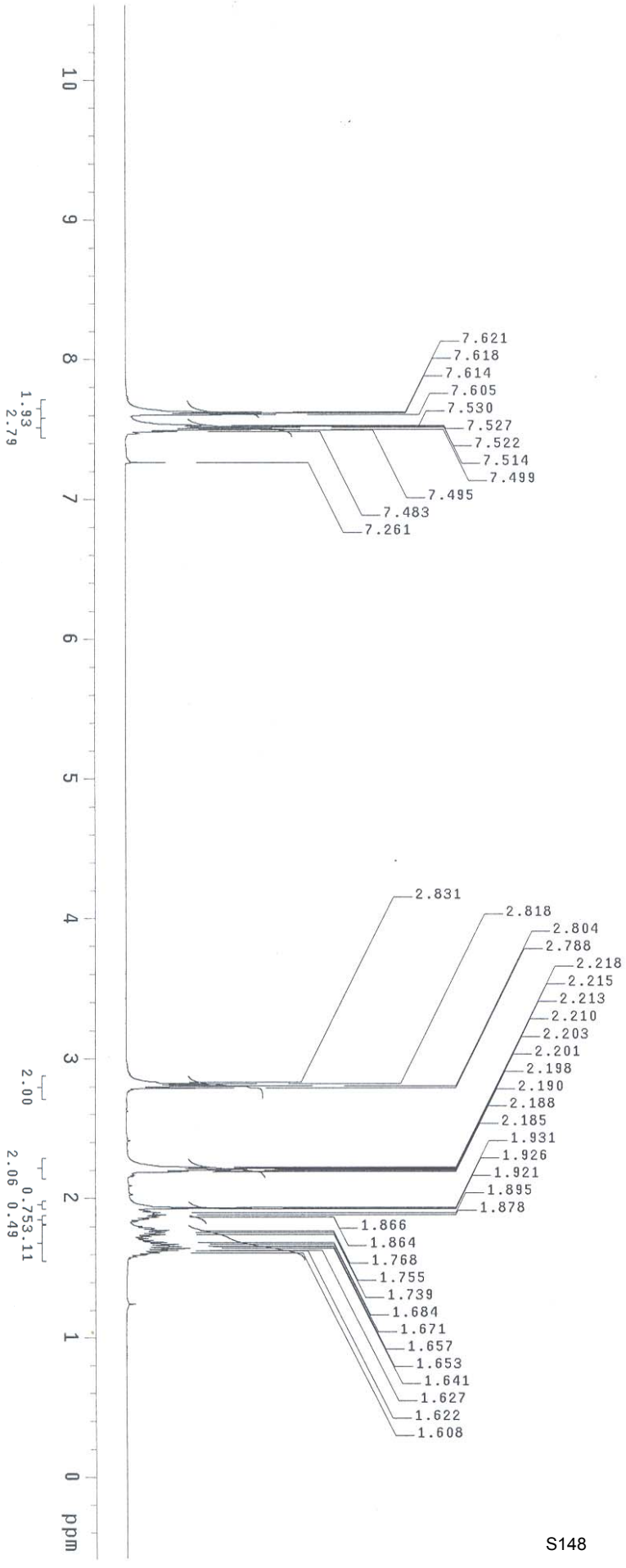
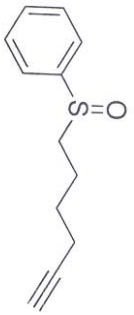
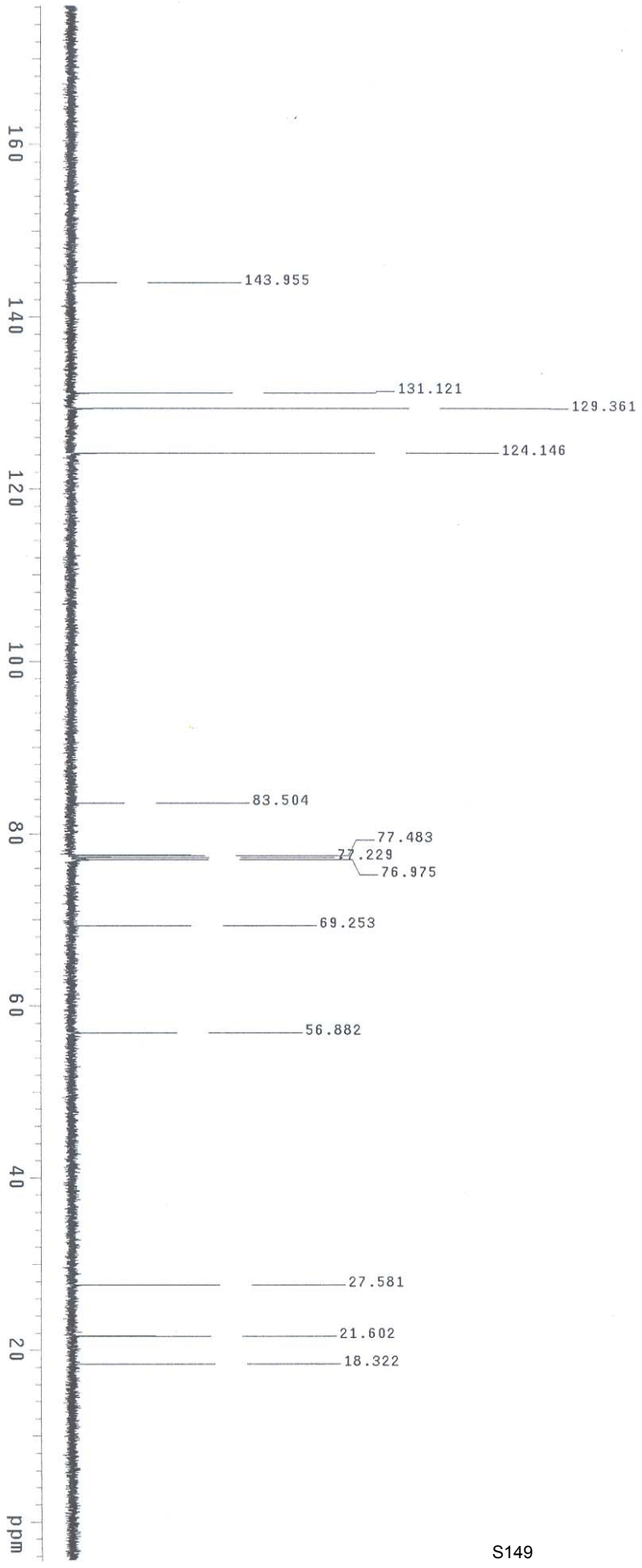
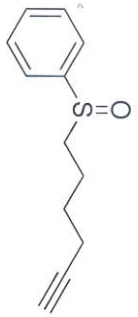
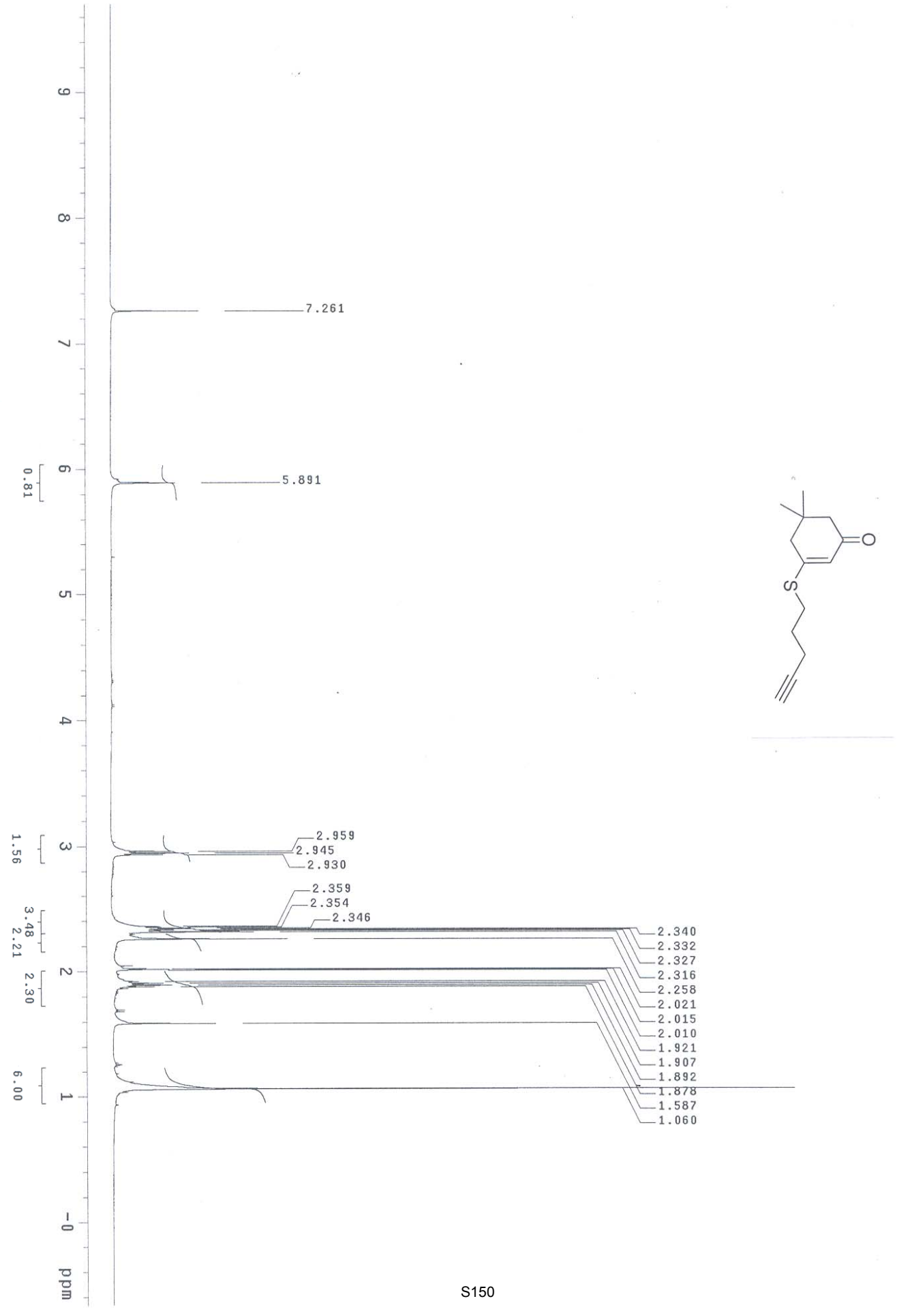
131.093
129.364
124.170
83.534
77.493
77.229
76.975
56.285
21.831
18.150
14.476
12.603
S=O


7.621
7.618
7.614
7.605
7.530
7.527
7.522
7.514
7.499
7.495
7.483
7.261
2.831
2.818
2.804
2.788
2.218
2.215
2.213
2.210
2.203
2.201
2.198
2.190
2.188
2.185
1.931
1.926
1.921
1.895
1.878
1.866
1.864
1.768
1.755
1.739
1.684
1.671
1.657
1.653
1.641
1.627
1.622
1.608
1.93
2.79
2.00
2.06
0.75
3.11
0.49
10
9
8
7
6
5
4
3
2
1
0
ppm


S=O


160
140
120
100
80
60
40
20
ppm
143.955
131.121
129.361
124.146
83.504
77.483
77.229
76.975
69.253
56.882
27.581
21.602
18.322


S=O


7.261
5.891
2.959
2.945
2.930
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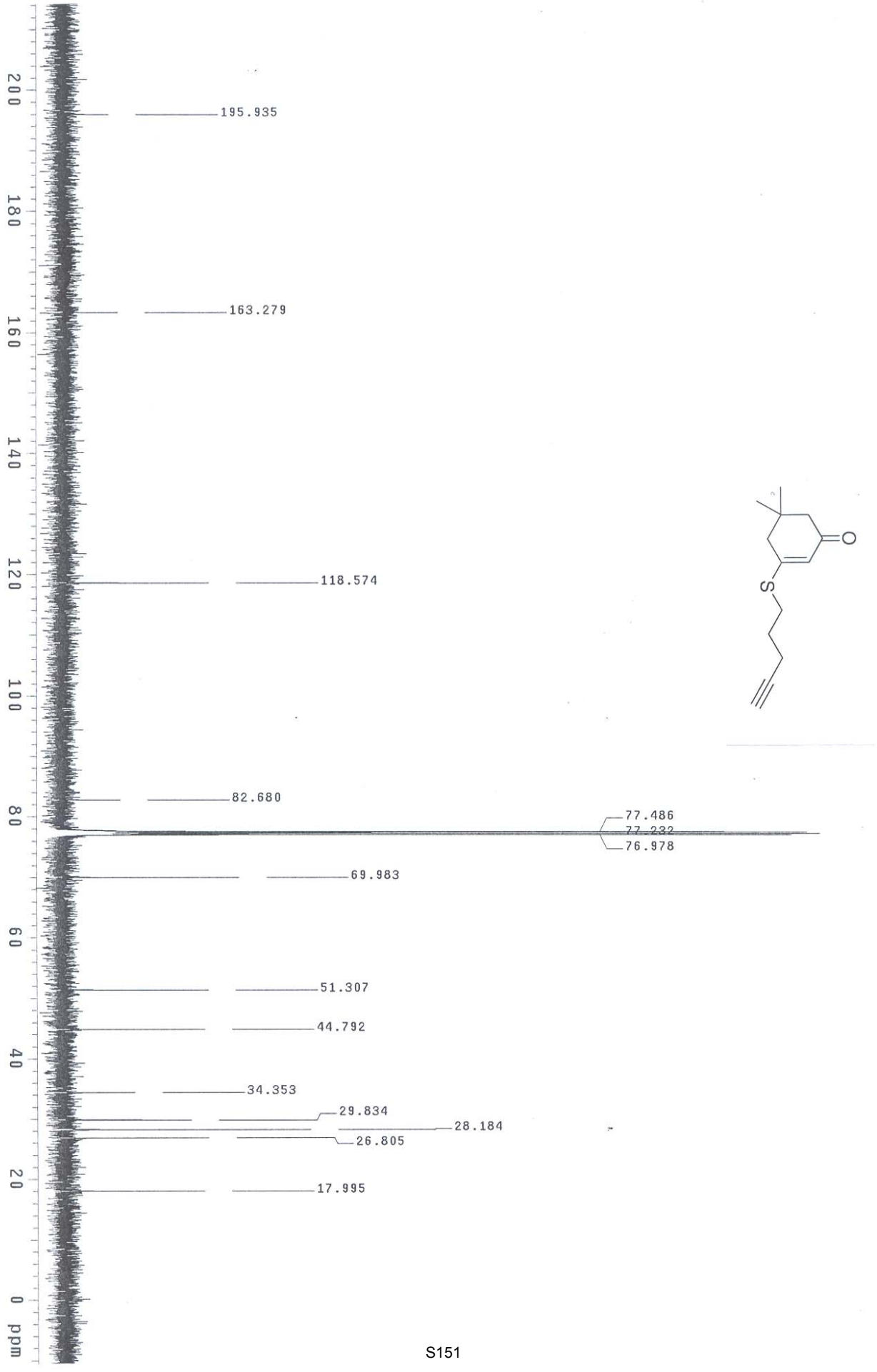
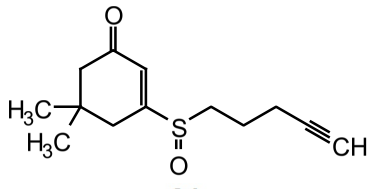
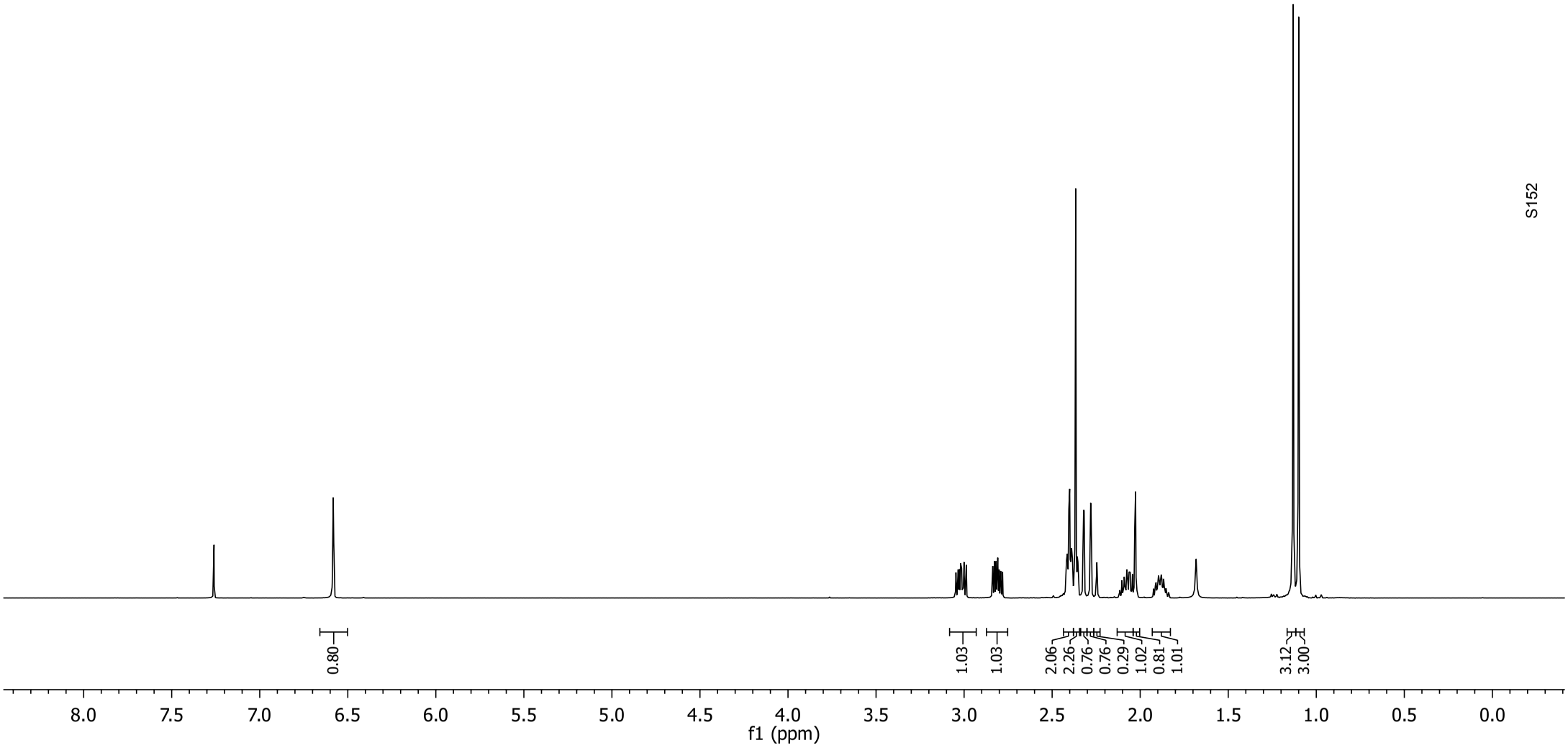
2.354
2.346
2.340
2.332
2.327
2.316
2.258
2.021
2.015
2.010
1.921
1.907
1.892
1.878
1.587
1.060
0.81
1.56
3.48
2.21
2.30
6.00
ppm
O
S

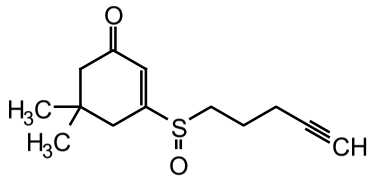

195.935
163.279
118.574
82.680
77.486
77.232
76.978
69.983
51.307
44.792
34.353
29.834
28.184
26.805
17.995
200
180
160
140
120
100
80
60
40
20
0
ppm
O
S

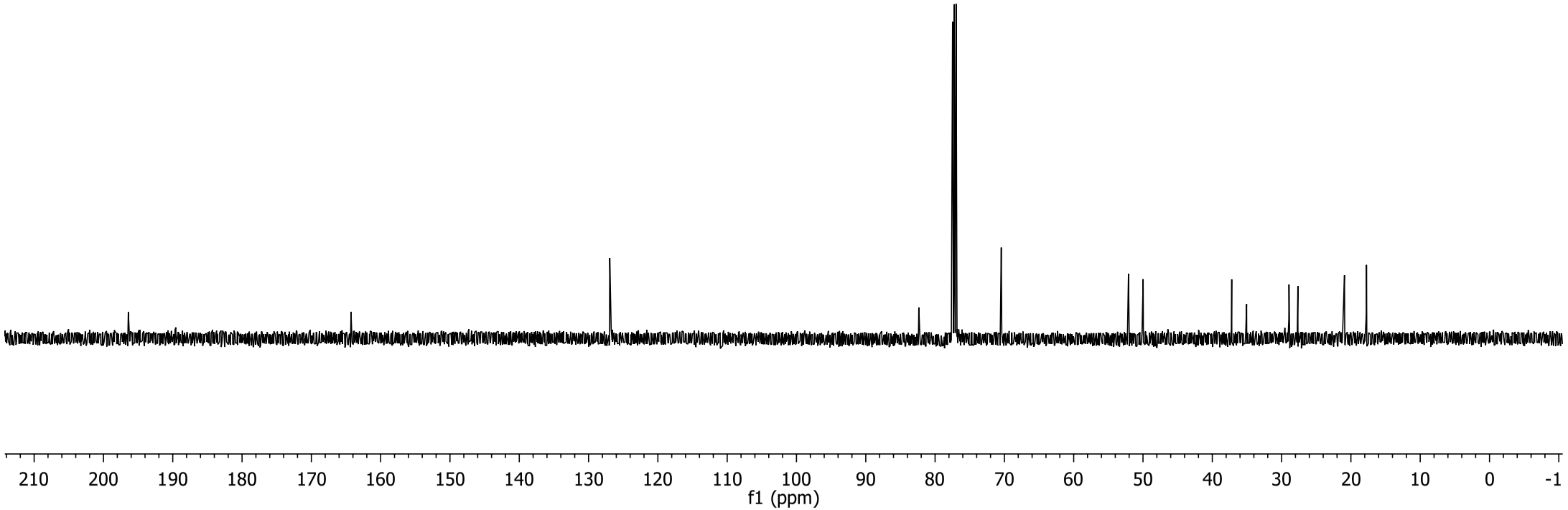
Title lb-III-50
Solvent cdcl3
Spectrometer Frequency 499.86



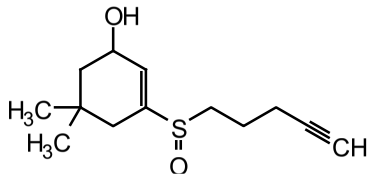


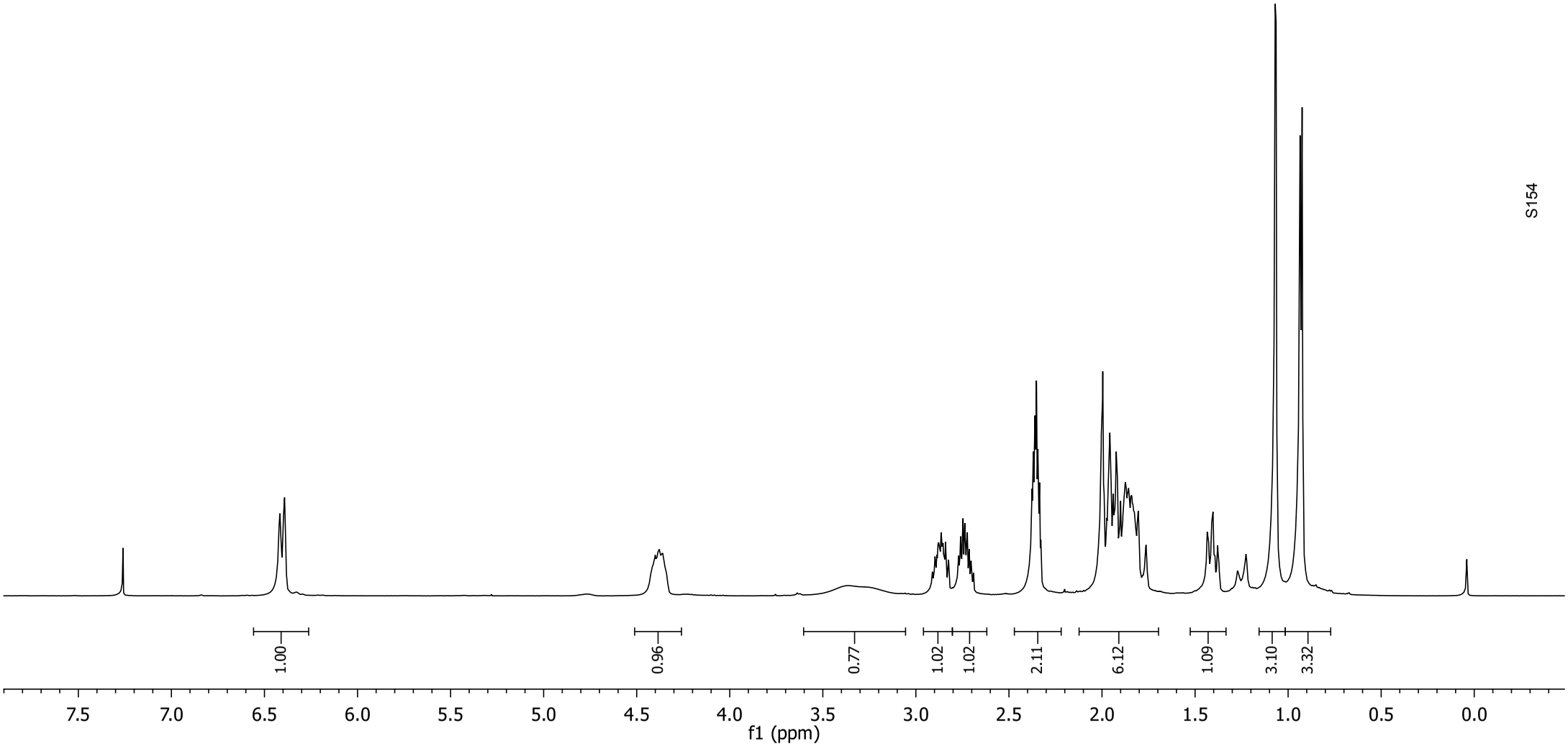
Title lb-III-50-C13
Solvent cdcl3
Spectrometer Frequency 125.70



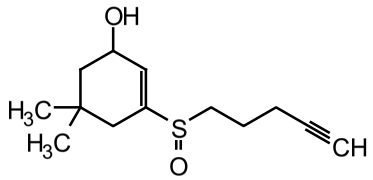


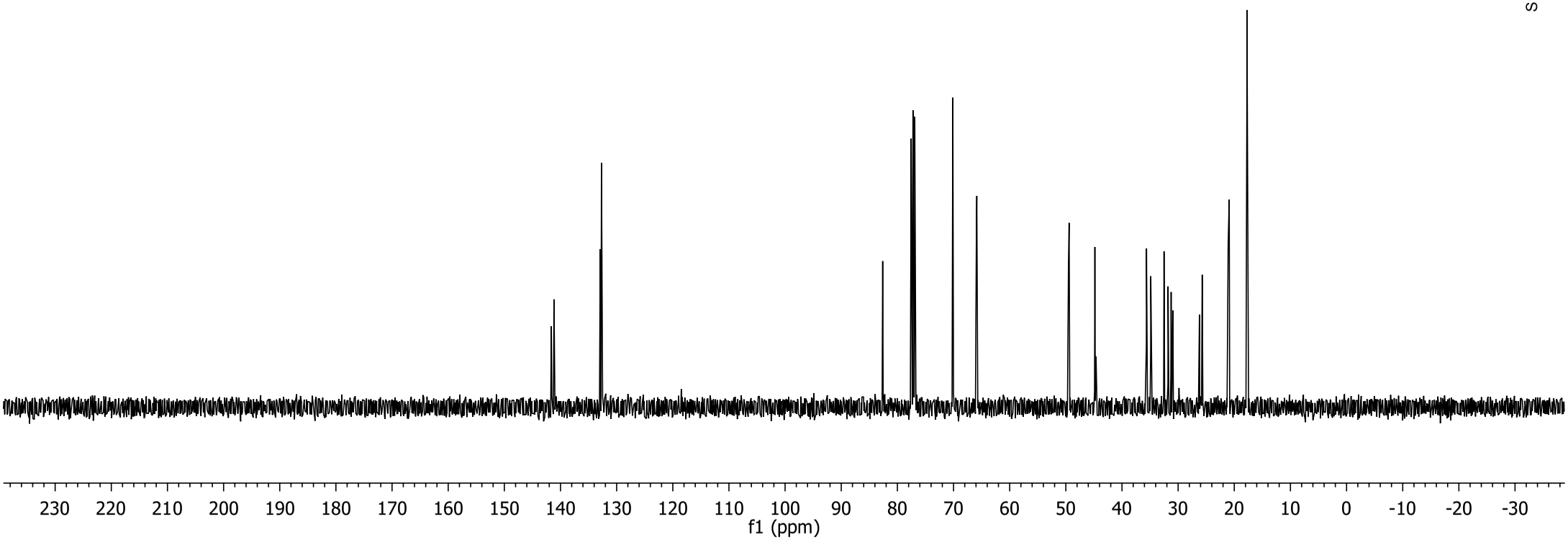
Title lb-III-128
Solvent cdcl3
Spectrometer Frequency 399.95



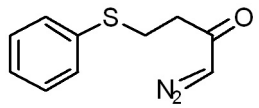


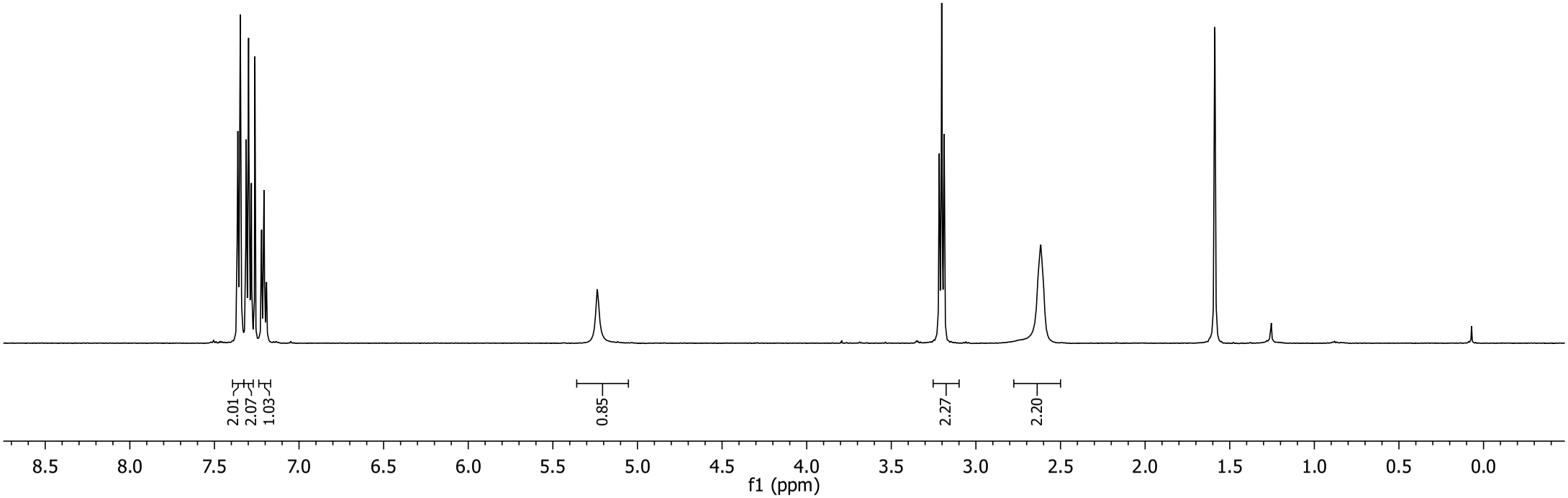
Title lb-III-128-C13
Solvent cdcl3
Spectrometer Frequency 100.58



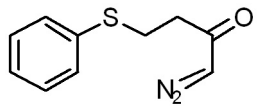


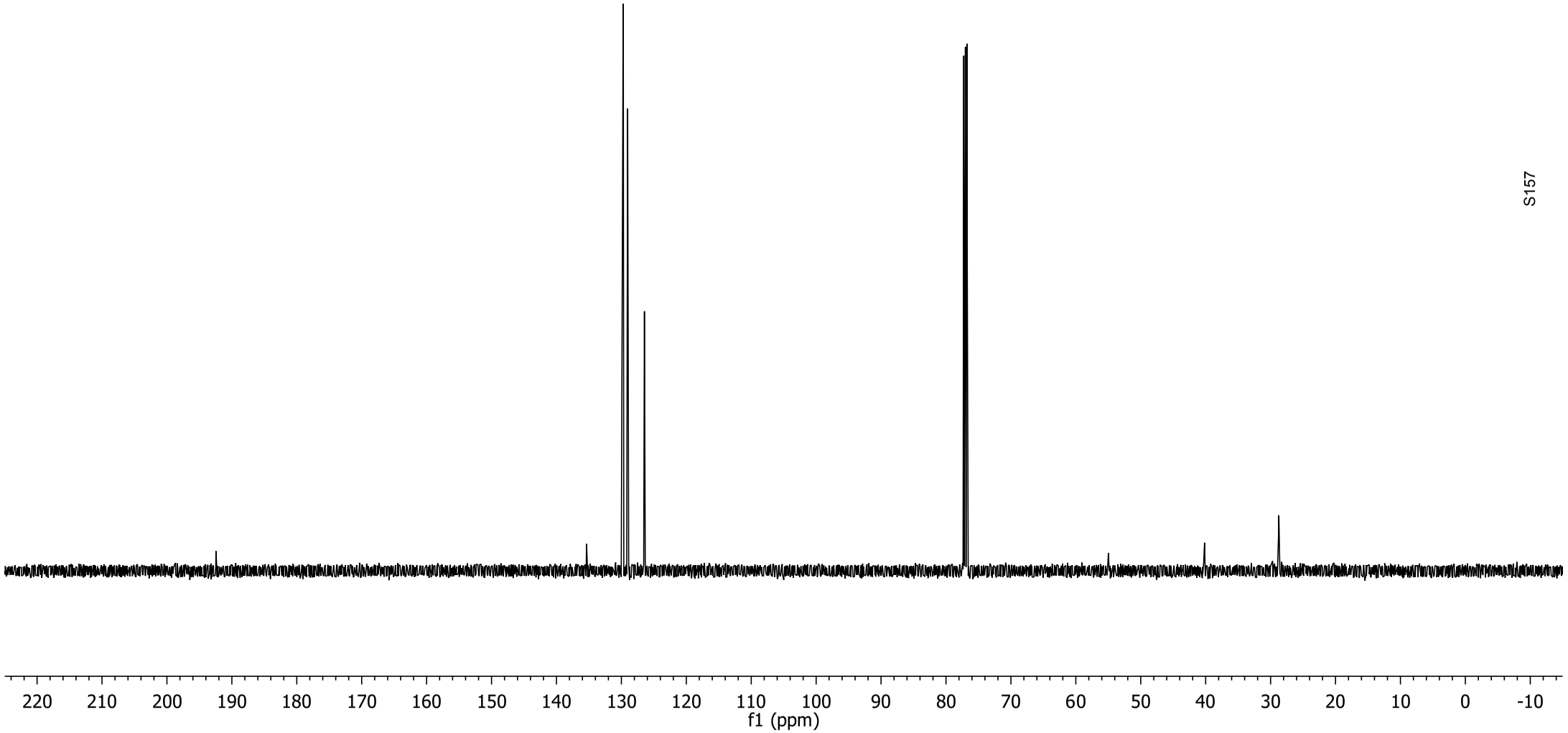
Title lyd-2-145-3
Solvent CDCl3
Spectrometer Frequency 499.86



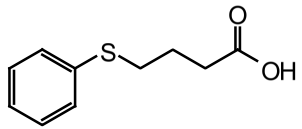


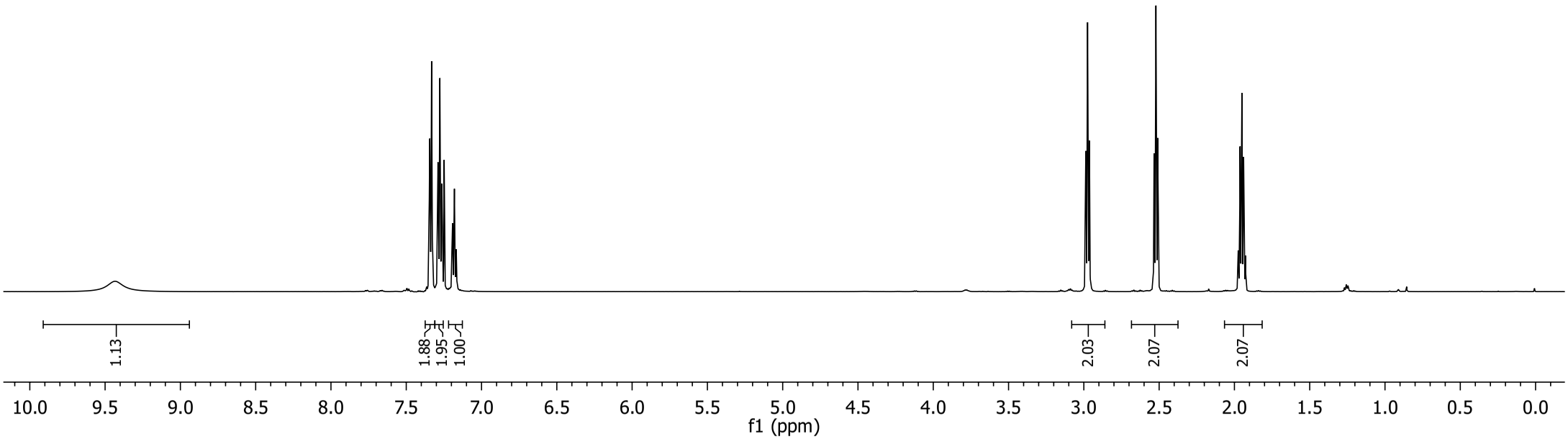
Title lyd-2-145-3-C
Solvent CDCl3
Spectrometer Frequency 125.70



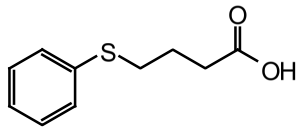


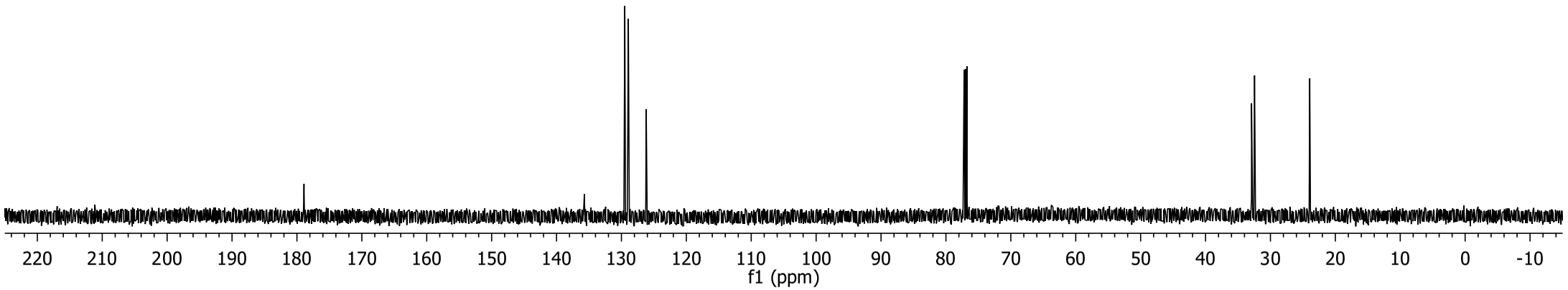
Title lyd-3-31-1-acid
Solvent cdcl3
Spectrometer Frequency 599.63



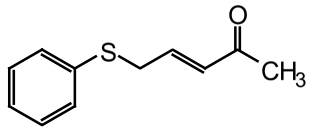


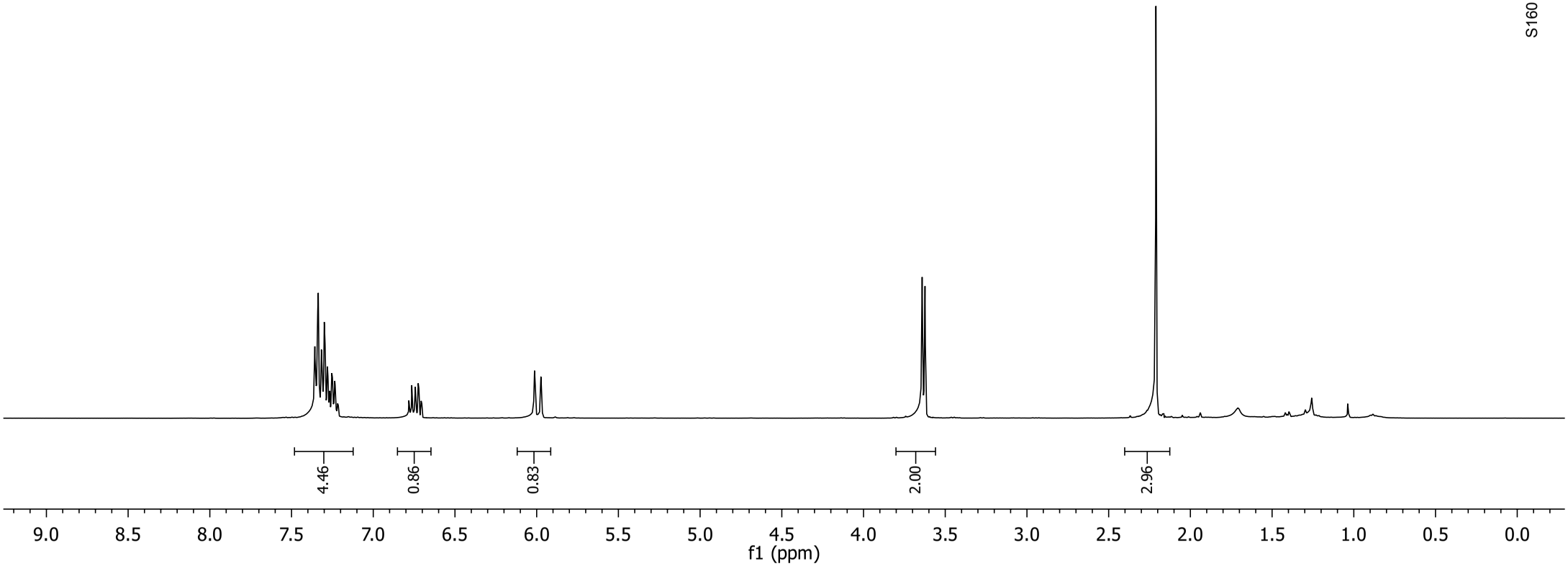
Title lyd-3-31-1acid-c
Solvent cdcl3
Spectrometer Frequency 150.79



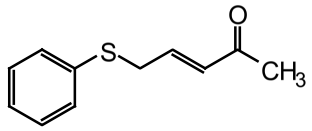


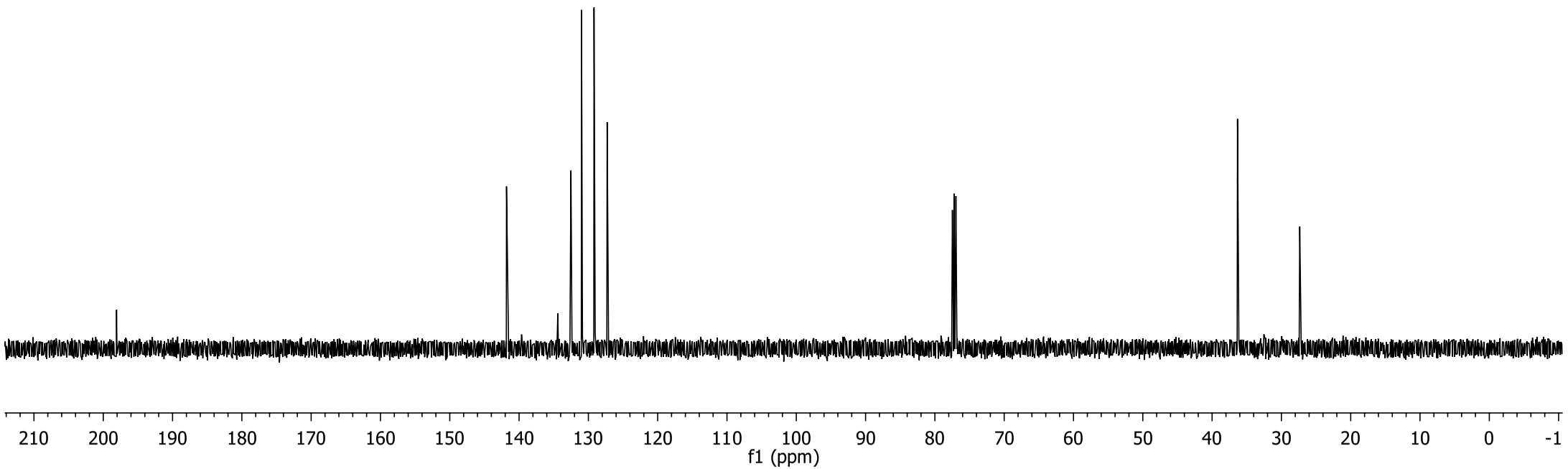
Title lb-III-66
Solvent cdcl3
Spectrometer Frequency 399.95



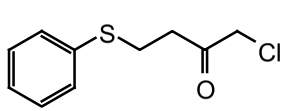


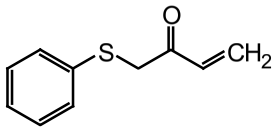
Title lb-III-66-C13
Solvent cdcl3
Spectrometer Frequency 125.70

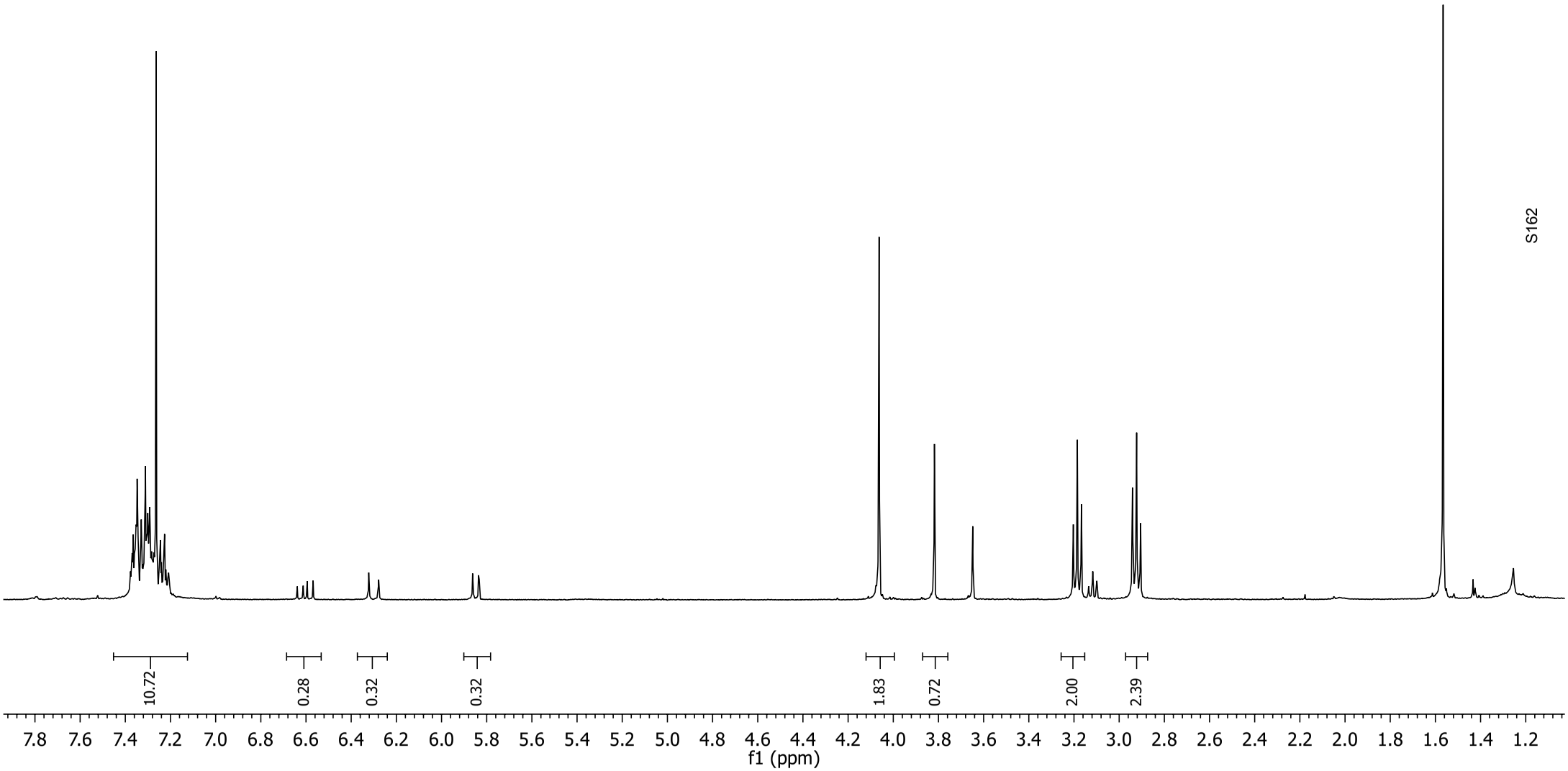




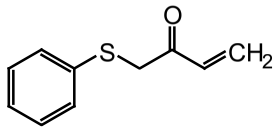
Title lb-III-98
Solvent cdcl3
Spectrometer Frequency 399.95

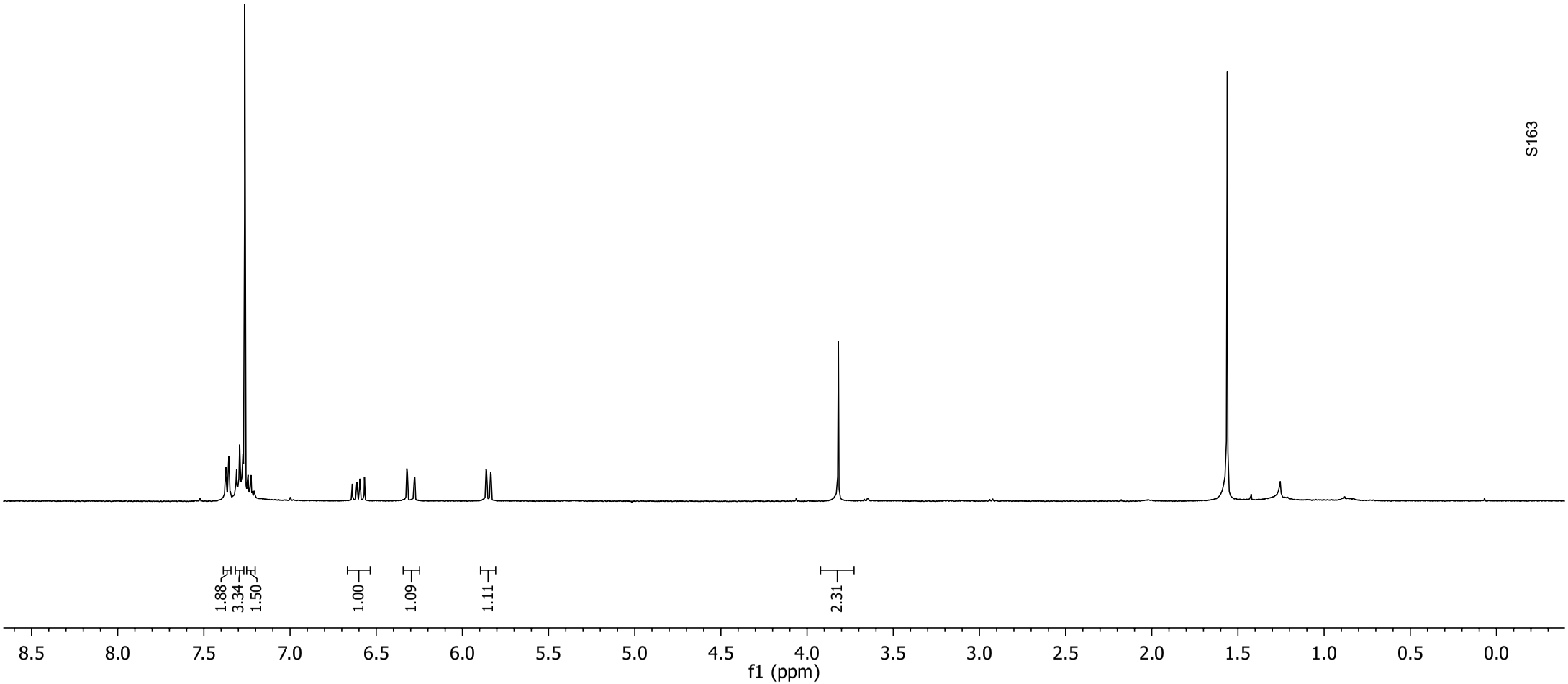




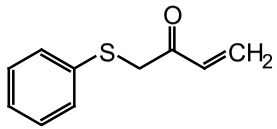


Title lb-III-94-B-2
Solvent cdcl3
Spectrometer Frequency 399.95

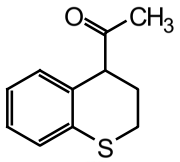




Title lb-III-94-B-1-C13
Solvent cdcl3
Spectrometer Frequency 100.58



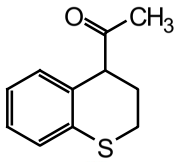
Title lb-III-63-major
Solvent cdcl3
Spectrometer Frequency 399.95

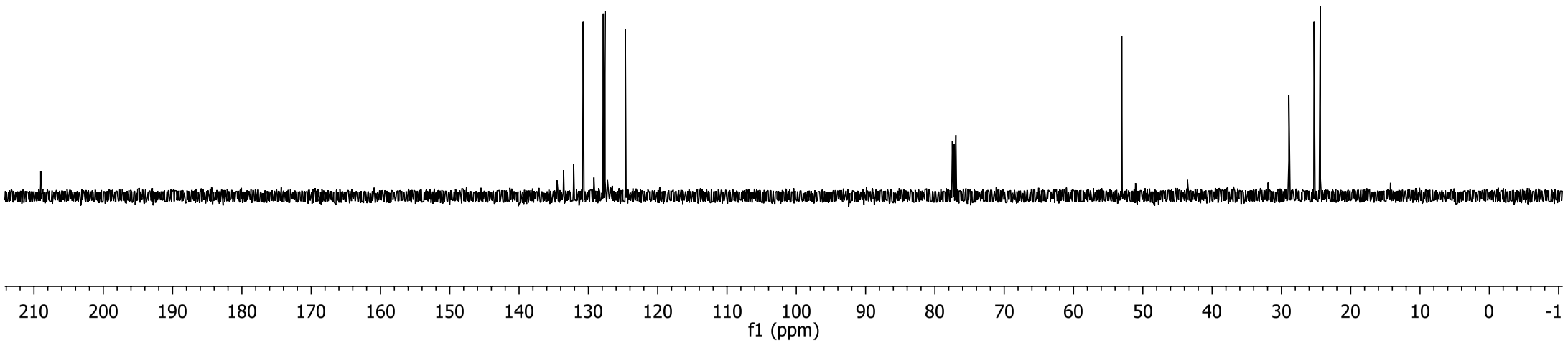


1.91 1.88 1.00 1.07 1.10 1.13 2.86 1.17

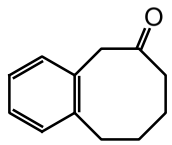
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

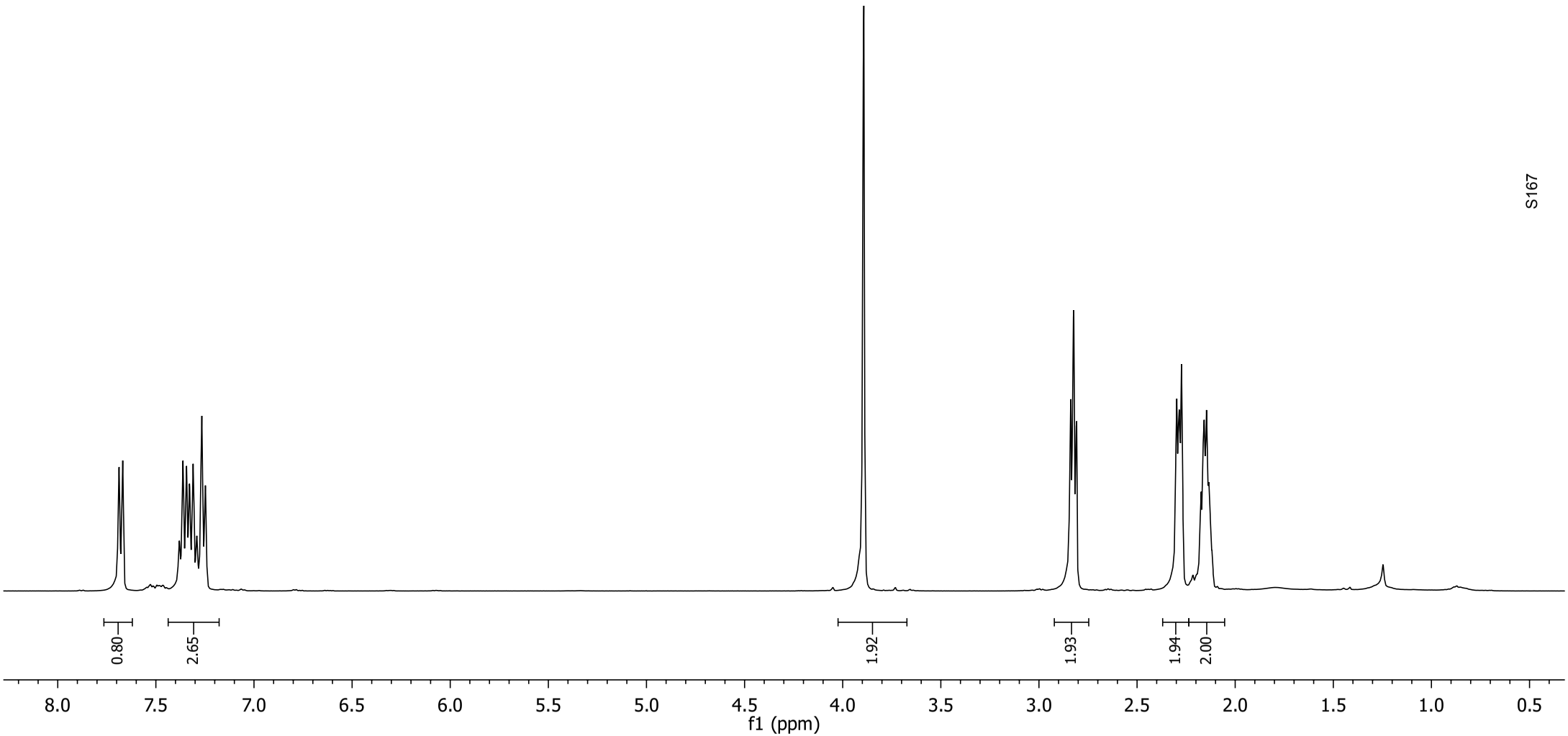
Title lb-III-63-C13
Solvent cdcl3
Spectrometer Frequency 125.70



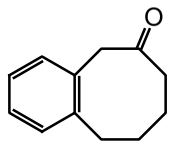


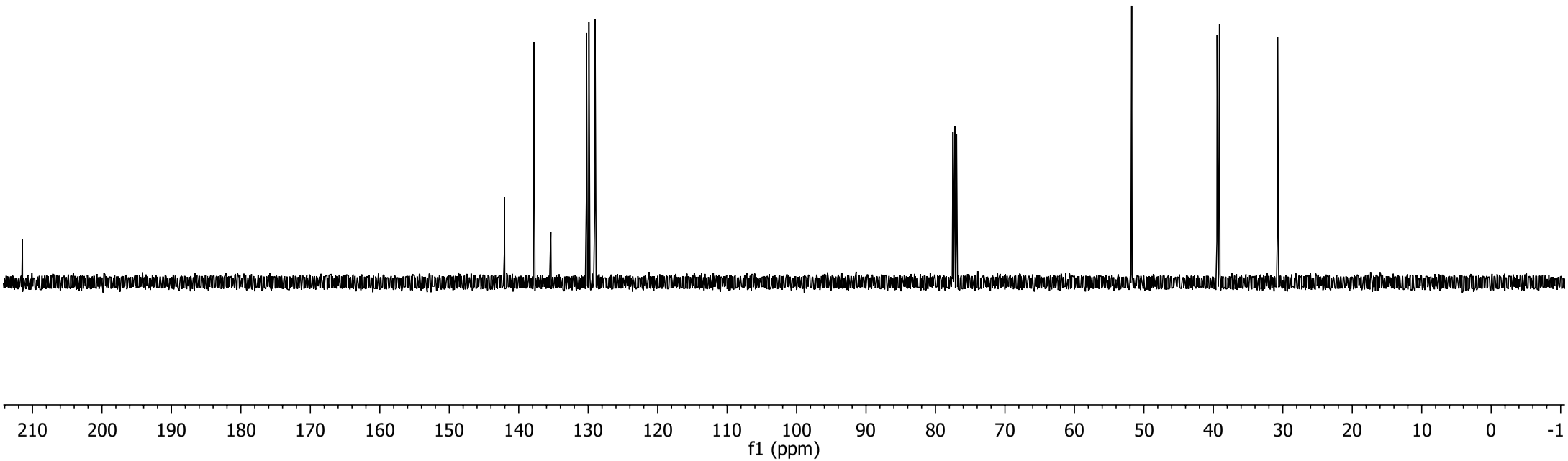
Title lb-III-38-1
Solvent cdcl3
Spectrometer Frequency 399.95



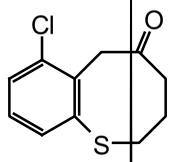


Title lb-III-38-1-C13
Solvent cdcl3
Spectrometer Frequency 125.70





Title lb-III-32-1
Solvent cdcl3
Spectrometer Frequency 399.95

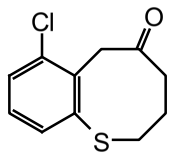


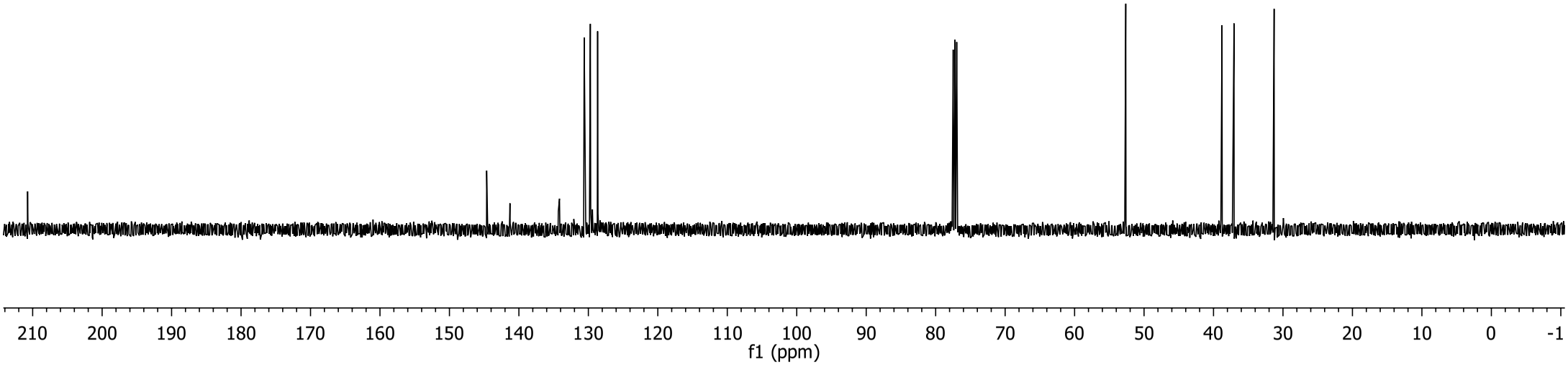
S169

1.23
1.10
0.93
2.00
1.99
4.13

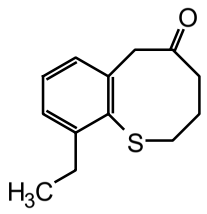
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

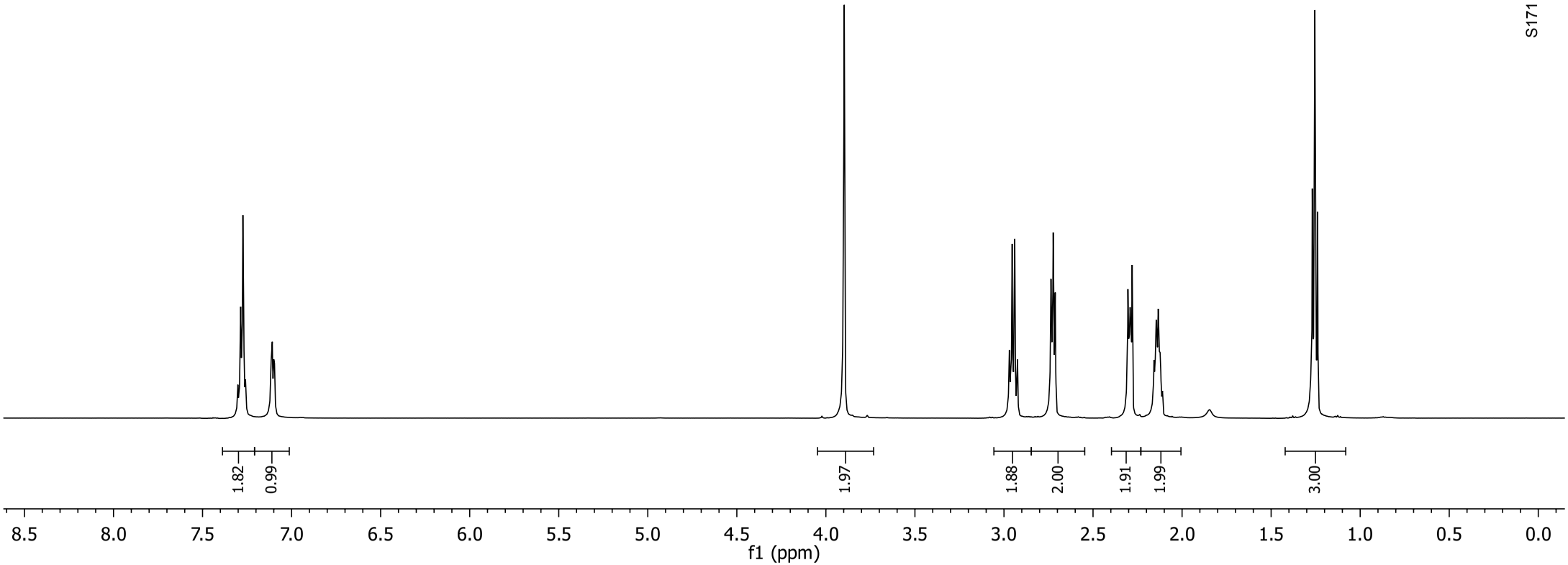
Title lb-III-32-1-C13
Solvent cdcl3
Spectrometer Frequency 125.70



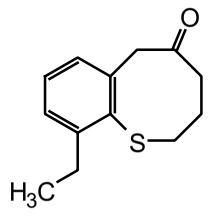


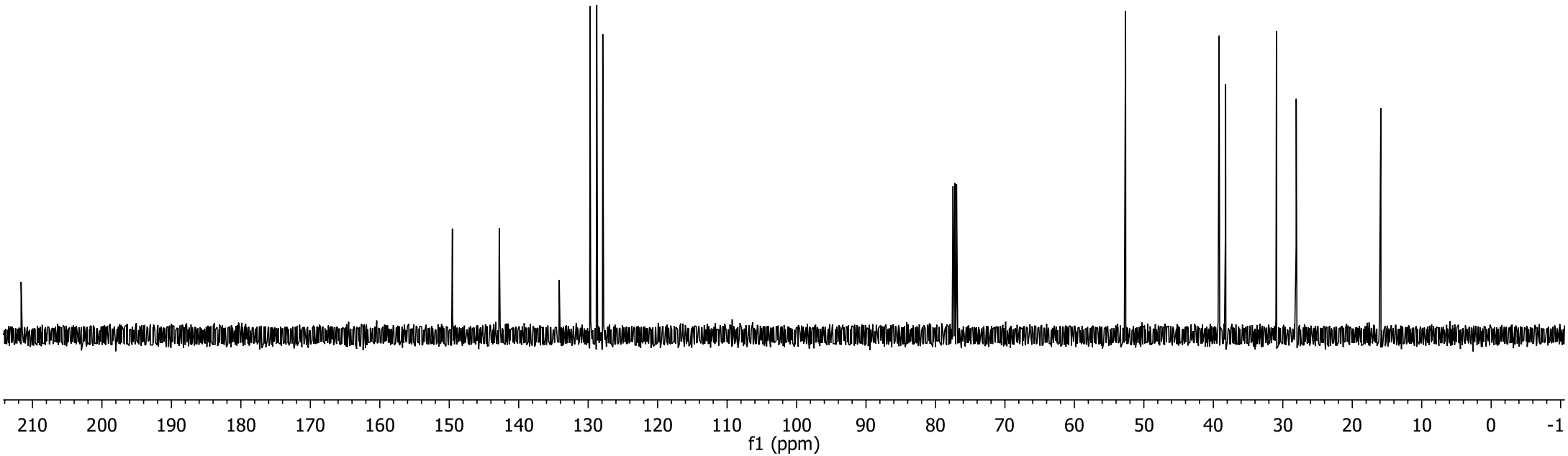
Title lb-III-57-A
Solvent CDCl3
Spectrometer Frequency 499.86



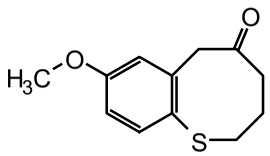


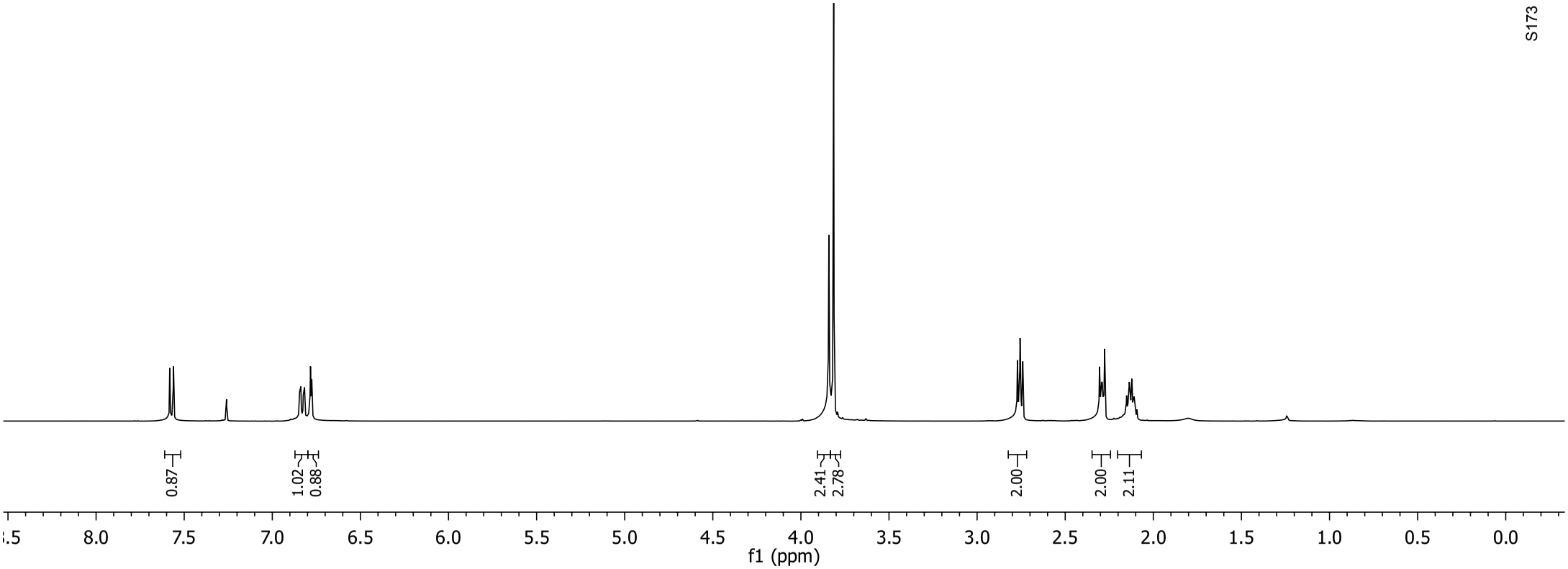
Title lb-III-57-A-C13
Solvent cdcl3
Spectrometer Frequency 125.70



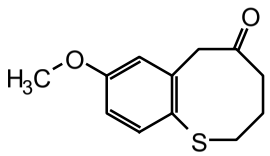


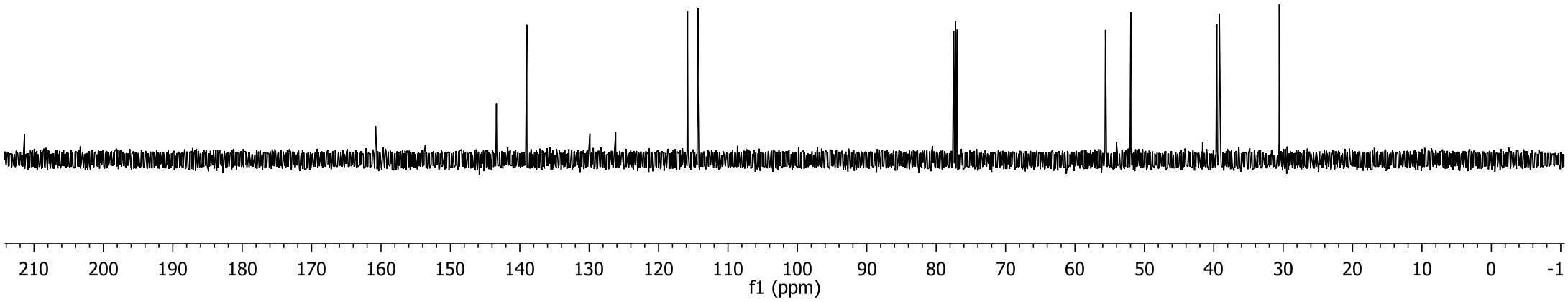
Title lb-III-59
Solvent cdcl3
Spectrometer Frequency 399.95



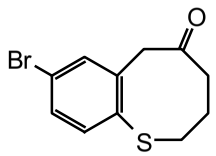


Title lb-III-55-B-C13
Solvent cdcl3
Spectrometer Frequency 125.70





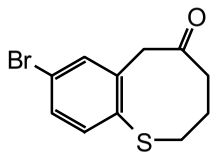
Title lb-III-57-B
Solvent CDCl3
Spectrometer Frequency 499.86

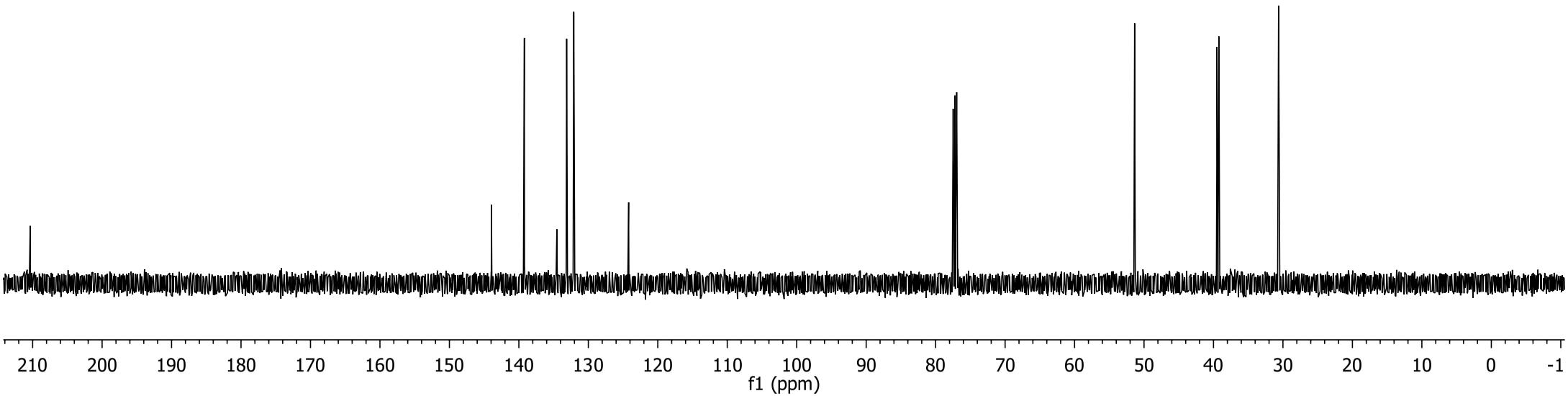


1.00 2.03 2.31 2.28 2.23 2.42

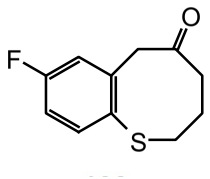
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

Title lb-III-57-B-C13
Solvent cdcl3
Spectrometer Frequency 125.70





Title lb-III-56-B
Solvent cdcl3
Spectrometer Frequency 399.95

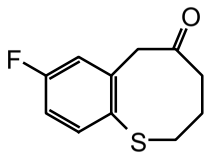


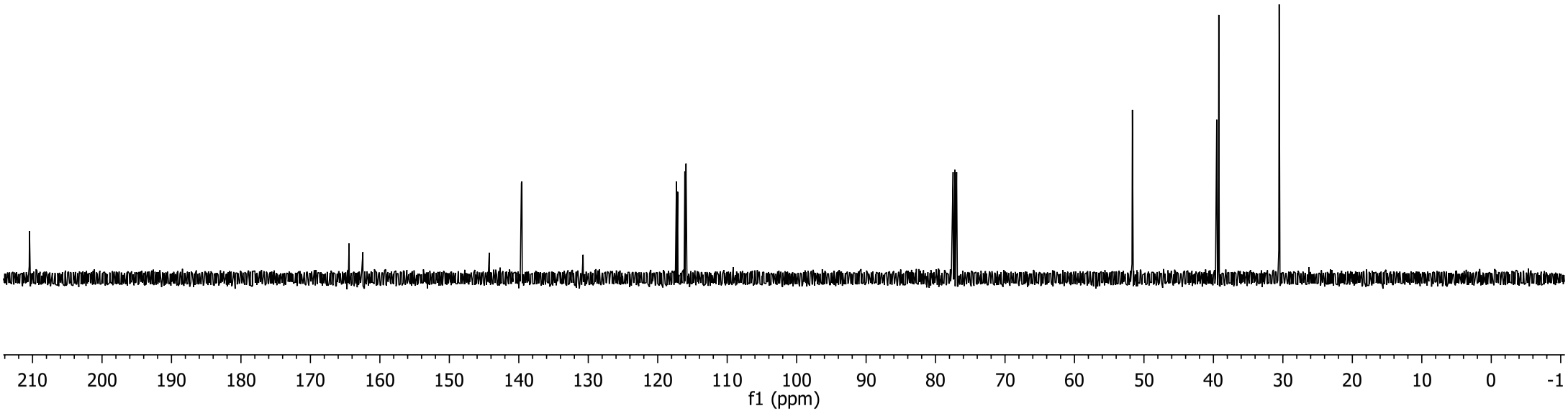
S177

1.00 2.10 2.34 2.32 2.35 2.46

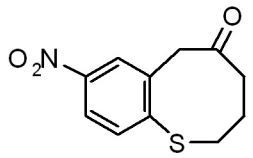
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

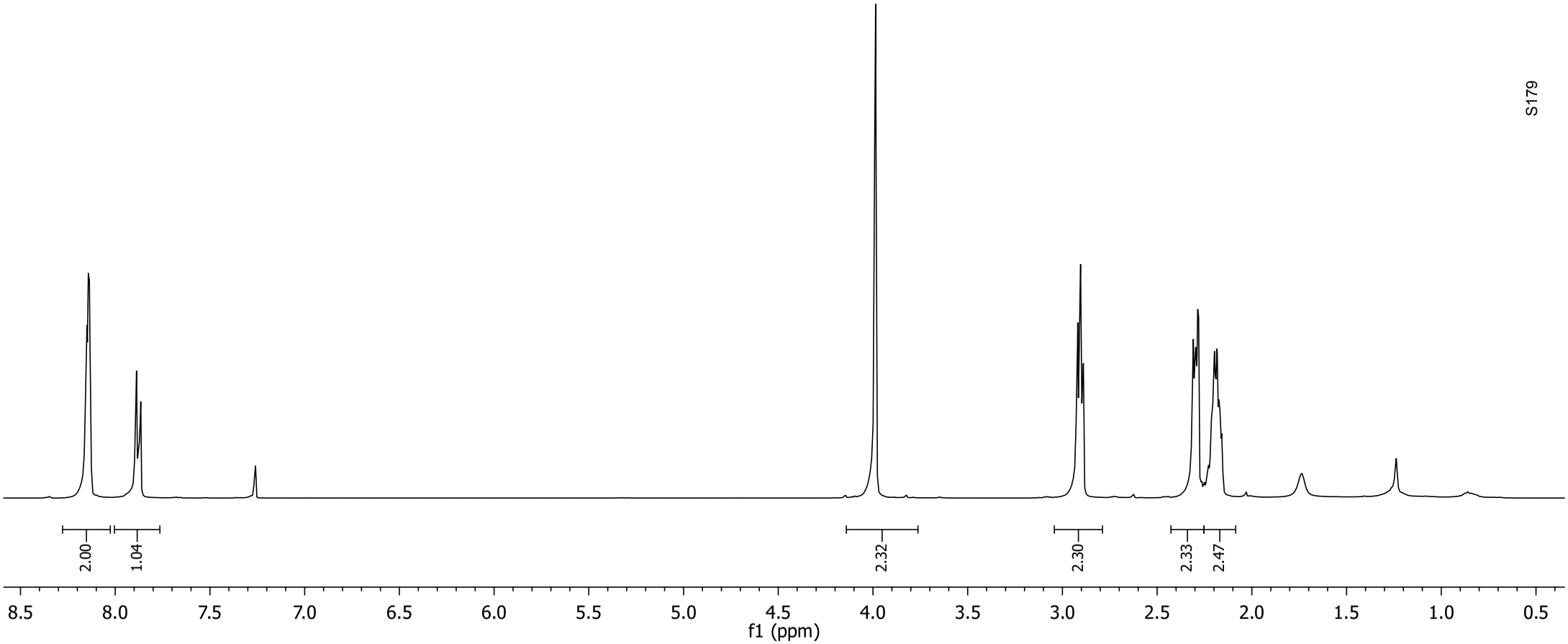
Title lb-III-56-B-C13
Solvent cdcl3
Spectrometer Frequency 125.70



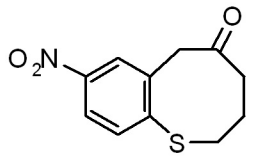


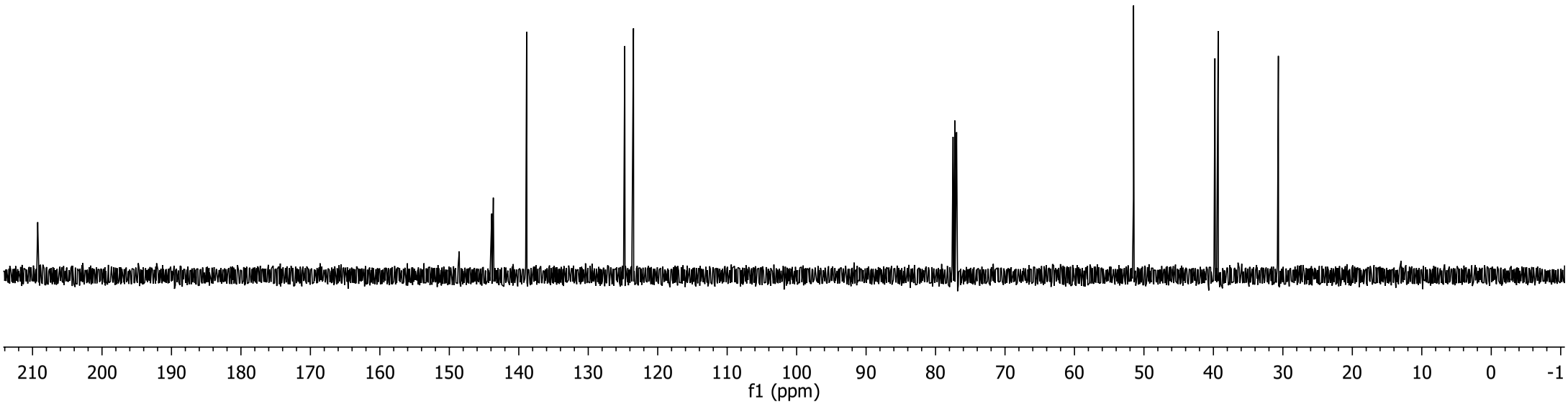
Title lb-III-56-A
Solvent cdcl3
Spectrometer Frequency 399.95



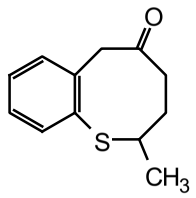


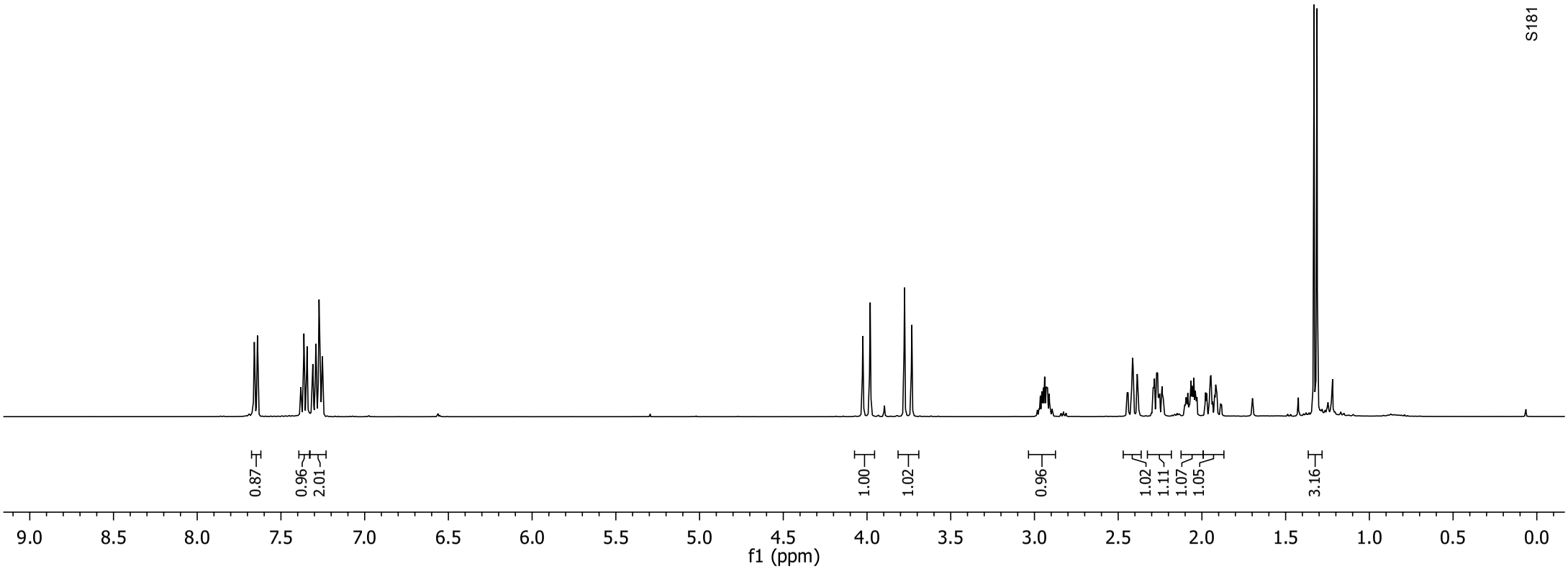
Title lb-III-56-A-C13
Solvent cdcl3
Spectrometer Frequency 125.70



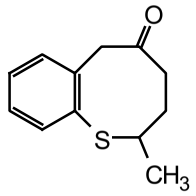


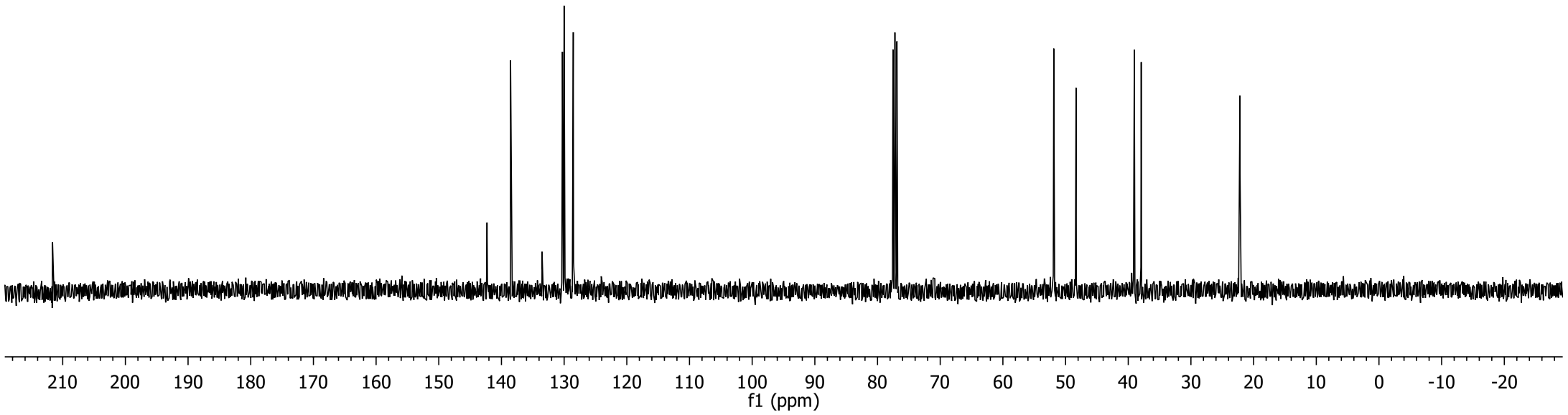
Title lb-III-103
Solvent cdcl3
Spectrometer Frequency 399.95



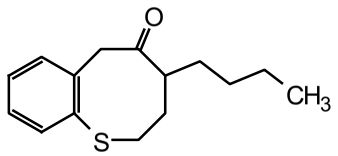


Title lb-III-103-C13
Solvent cdcl3
Spectrometer Frequency 100.58





Title	lb-III-100
Solvent	cdcl3
Spectrometer Frequency	399.95

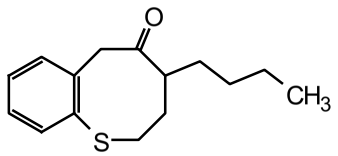


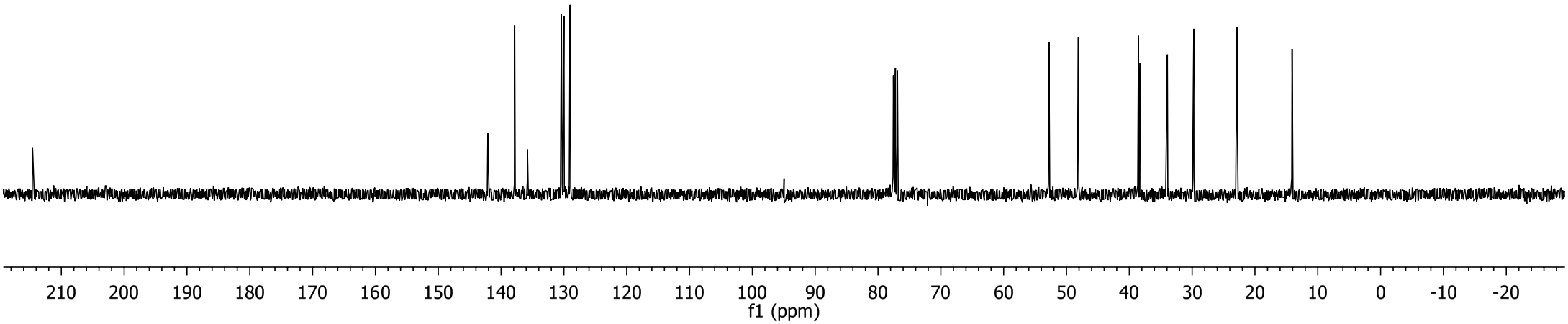
S183

1.00 2.15 1.17 1.10 1.12 1.10 2.19 1.15 1.12 1.30 6.05 3.50

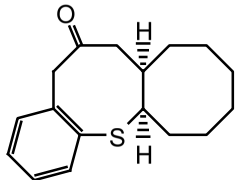
f1 (ppm)

Title lb-III-100-C13
Solvent cdcl3
Spectrometer Frequency 100.58





Title lb-III-111-DMSO
Solvent cdcl3
Spectrometer Frequency 399.95

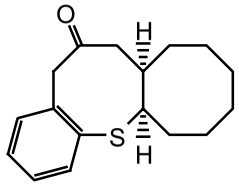


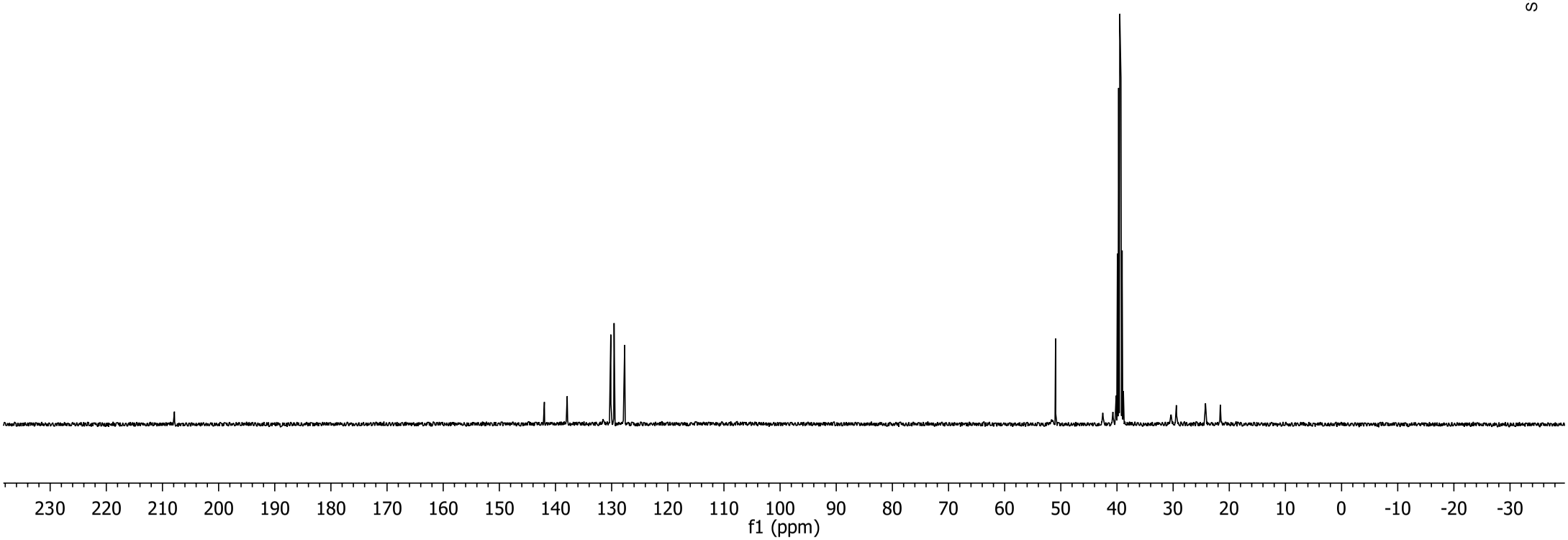
1.00 3.02 2.04 6.00 1.04 1.70 2.06 1.31 7.50

9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

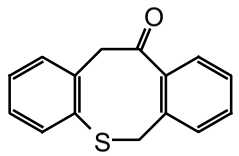
f1 (ppm)

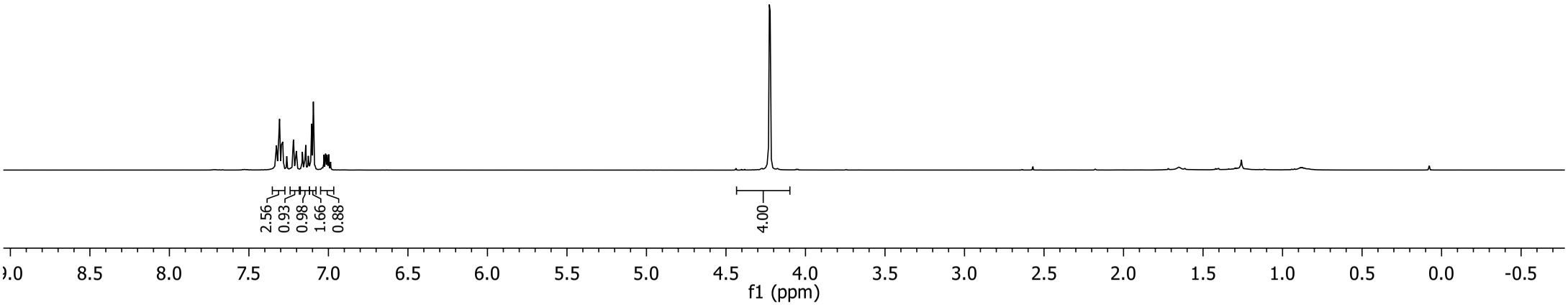
Title lb-III-111-C13
Solvent dmso
Spectrometer Frequency 100.58



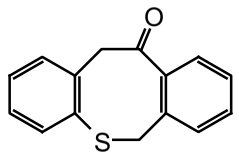


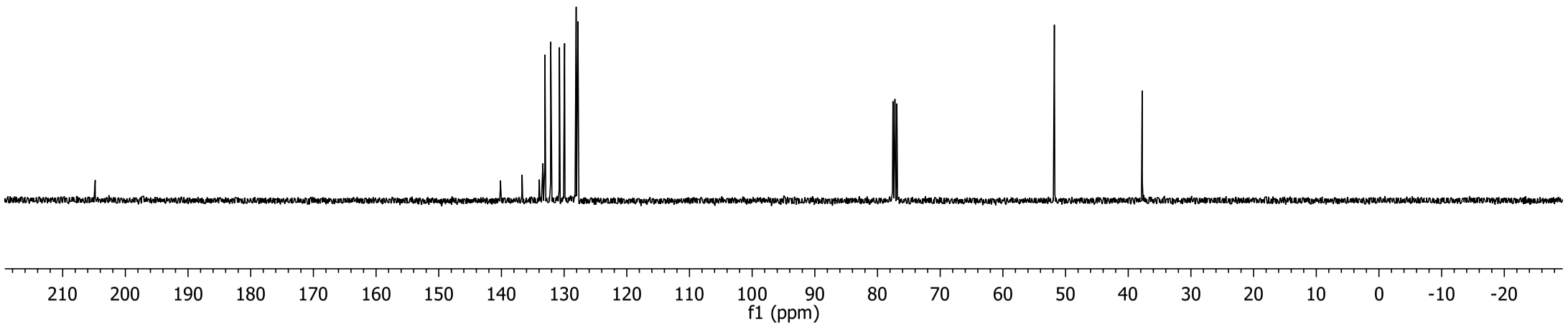
Title lb-III-112
Solvent cdcl3
Spectrometer Frequency 399.95





Title lb-III-112-C13
Solvent cdcl3
Spectrometer Frequency 100.58

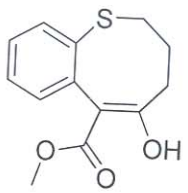




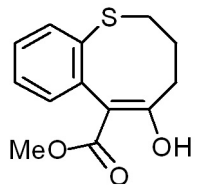
STANDARD 1H OBSERVE - profile

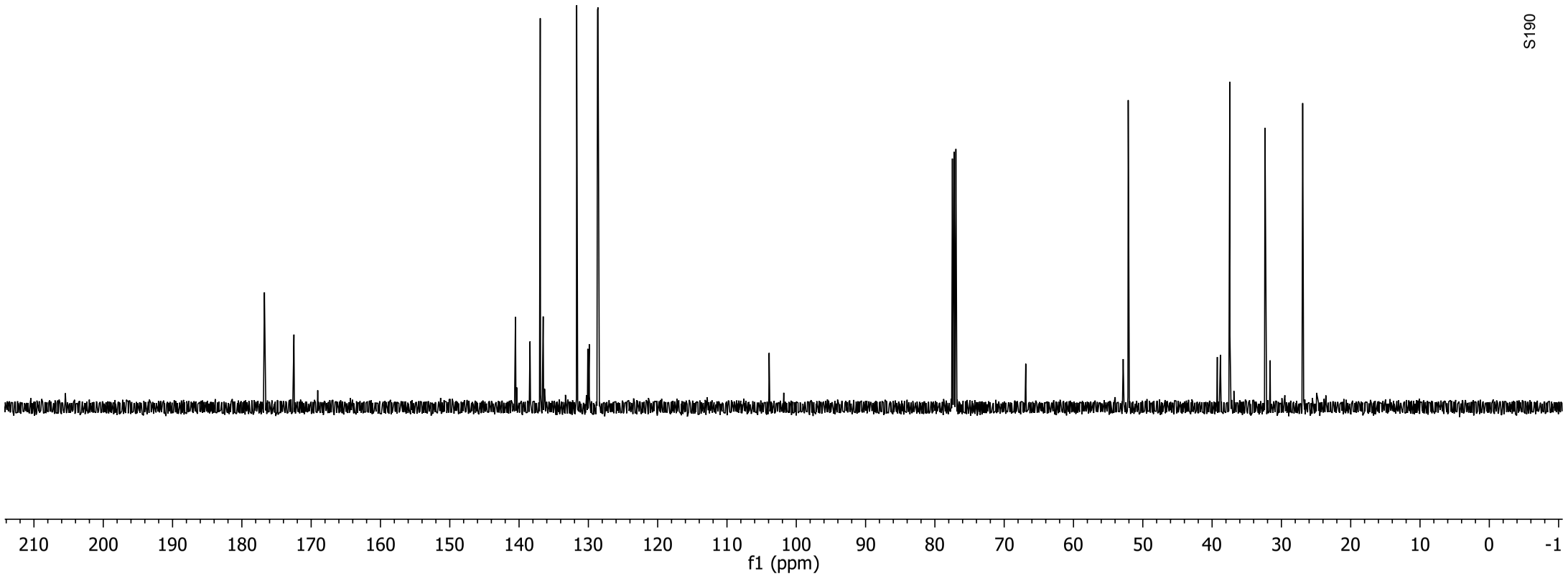
exp1 Proton

SAMPLE		SPECIAL	
date	Jan 16 2007	temp	25.0
solvent	cdcl3	gain	20
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	6410.3	pw90	13.900
at	2.049	alfa	6.600
np	26264	**FLAGS**	
fb	4000	il	n
bs	32	in	n
d1	1.000	dp	y
nt	8	hs	nn
ct	8	**PROCESSING**	
TRANSMITTER		lb	0.20
tn	H1	fn	65536
sfrq	399.782	**DISPLAY**	
tof	399.5	sp	-171.2
tpwr	59	wp	5774.9
pw	6.950	rfl	806.4
DECOUPLER		rfp	0
dn	C13	rp	116.2
dof	0	lp	-28.2
dm	nnn	**PLOT**	
dmm	c	wc	250
dpwr	34	sc	0
dmf	29412	vs	11320
		th	12
		ai	cdc ph

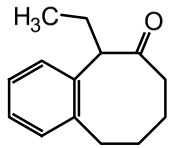


Title lb-III-61-A-C13
Solvent cdcl3
Spectrometer Frequency 125.70





Title lb-III-38-2
Solvent cdcl3
Spectrometer Frequency 399.95

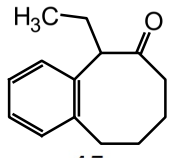


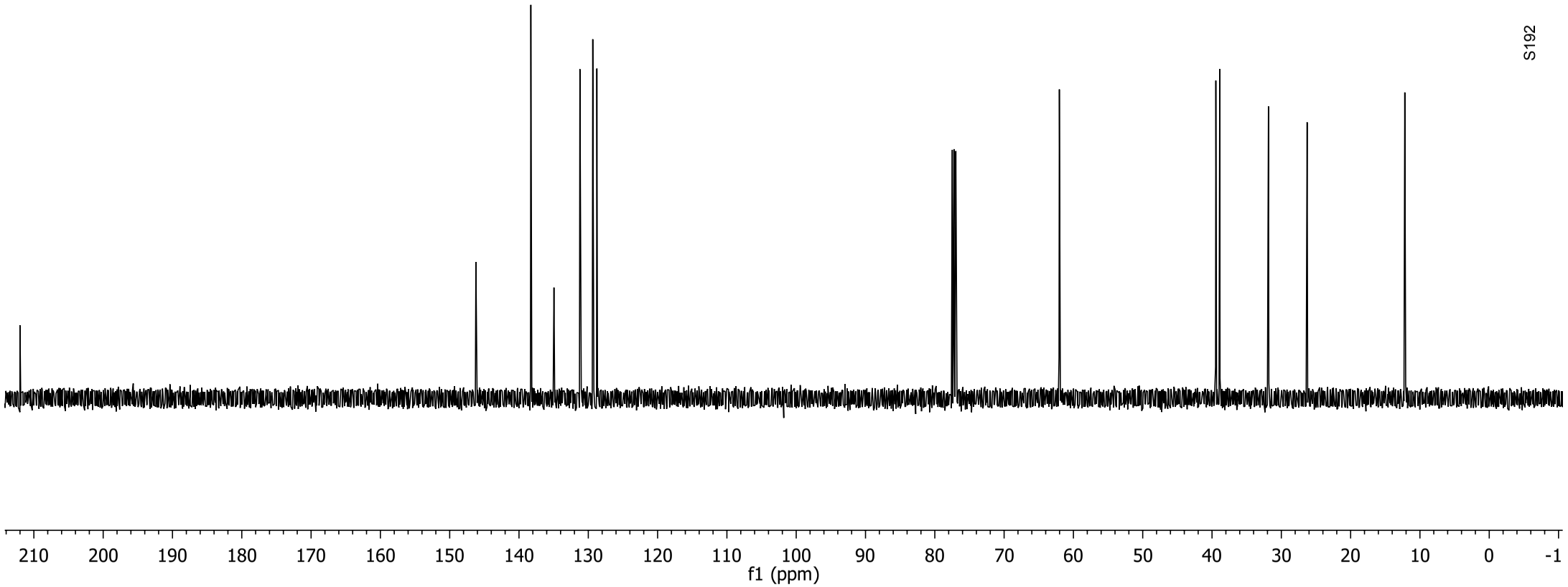
S191

1.69 3.71 1.83 1.84 1.94 3.94 3.96 2.10 2.05 2.02 6.00

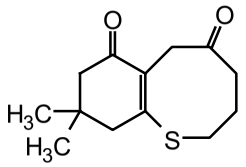
f1 (ppm)

Title lb-III-38-2-C13
Solvent cdcl3
Spectrometer Frequency 125.70





Title lb-III-60
Solvent cdcl3
Spectrometer Frequency 399.95

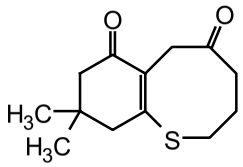


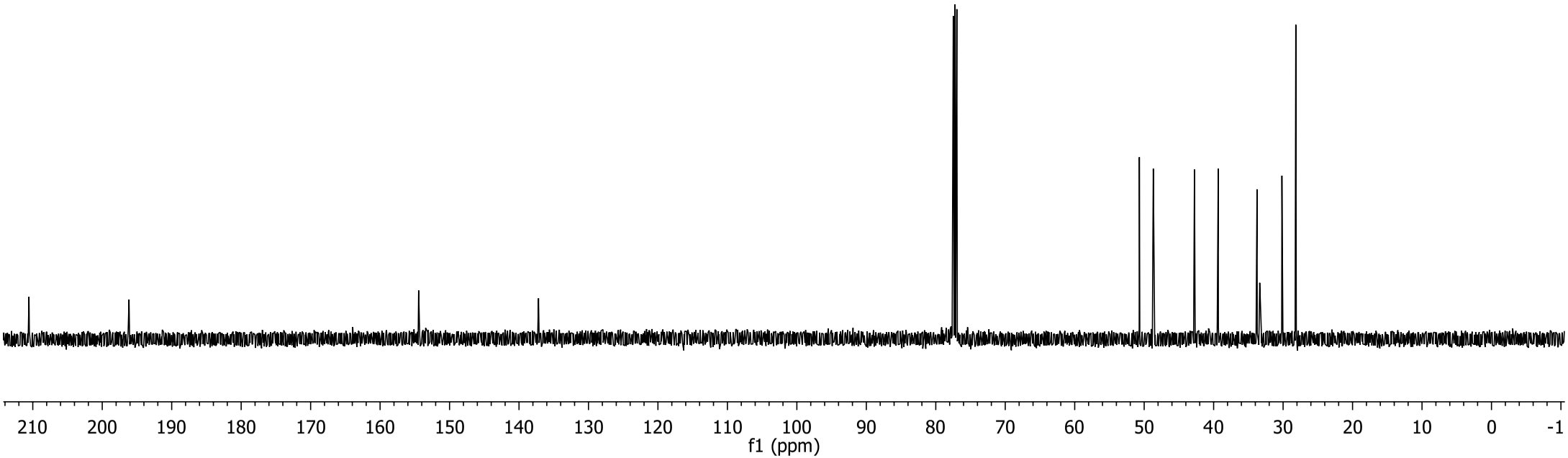
S193

1.00 1.00 1.03 1.04 1.02 1.07 3.16

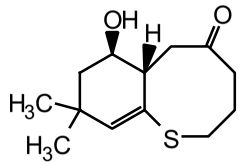
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

Title lb-III-60-C13
Solvent cdcl3
Spectrometer Frequency 125.70





Title lb-III-132-1
Solvent cdcl3
Spectrometer Frequency 499.86

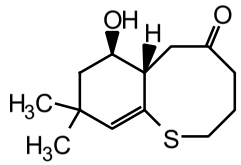


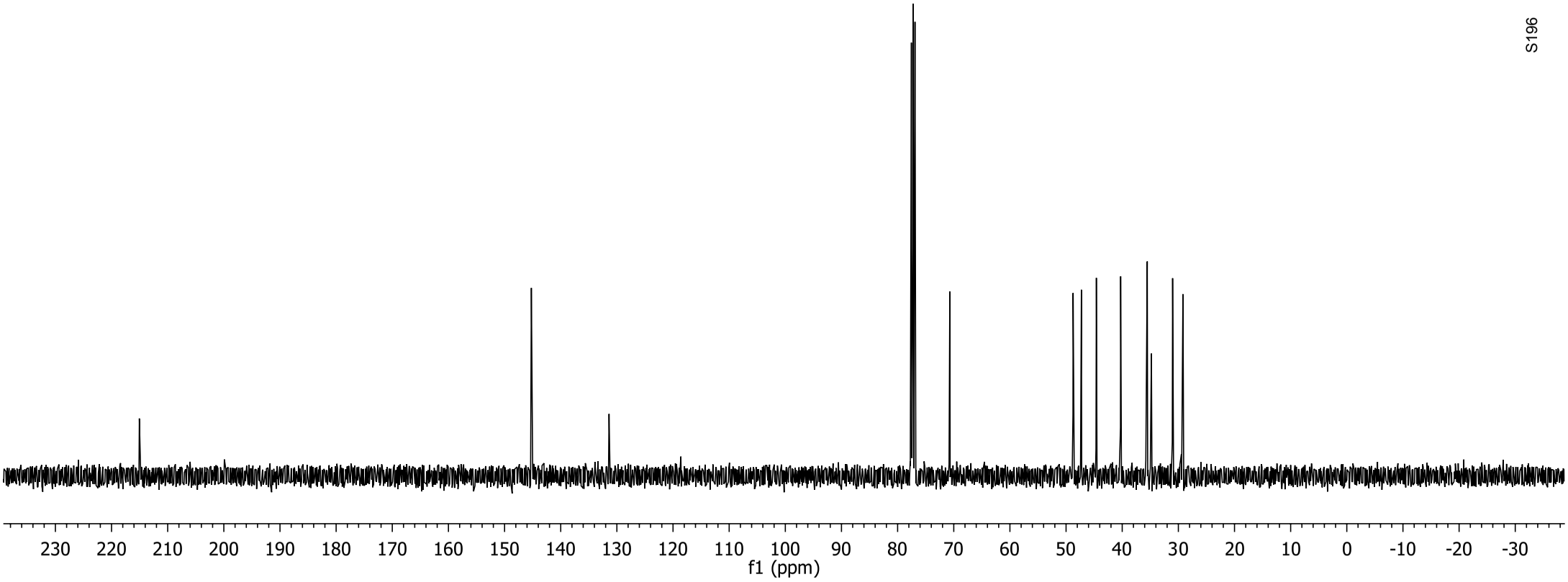
S195

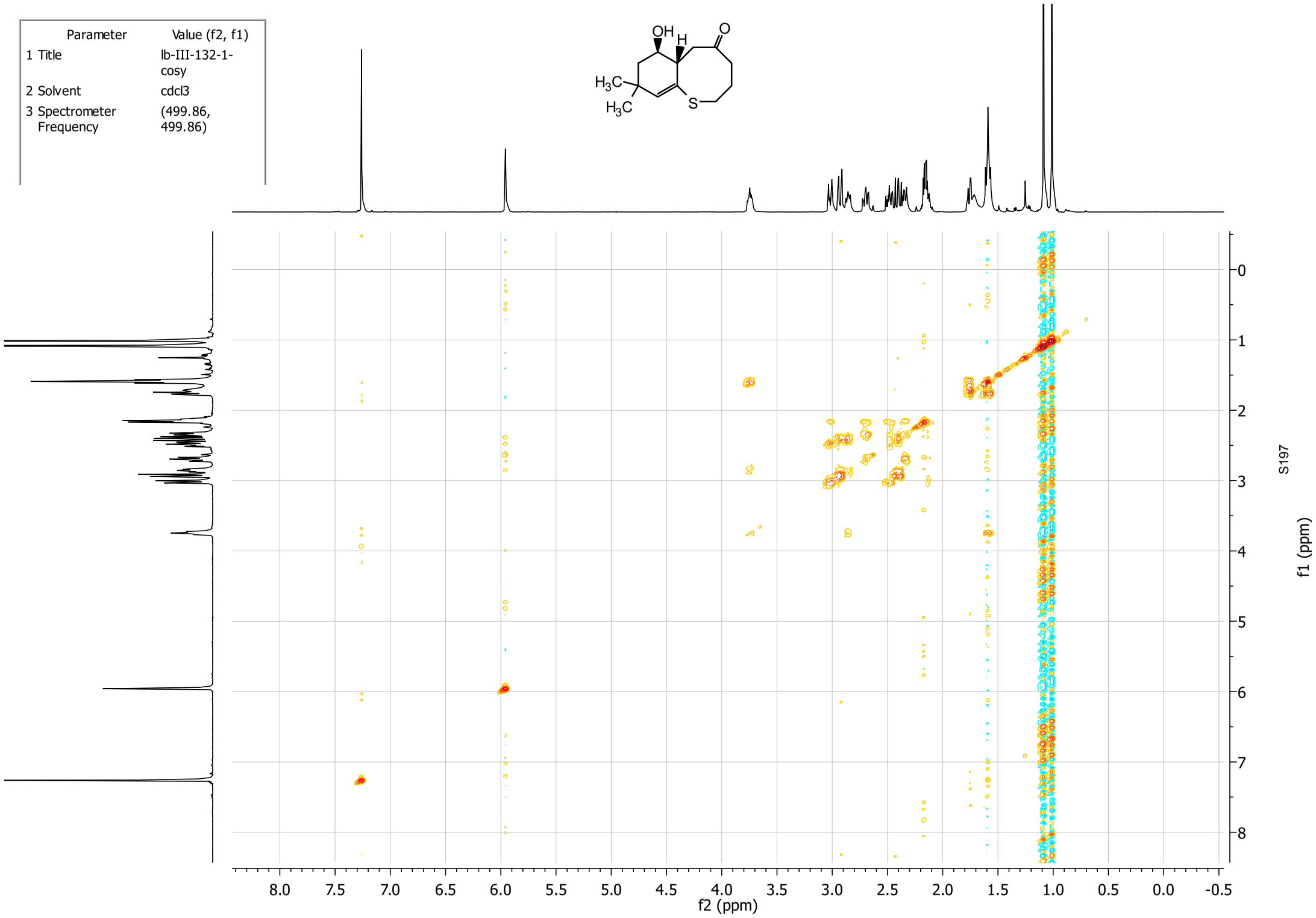
1.00 1.12 1.10 1.09 1.15 1.06 1.07 1.07 1.16 2.37 1.11 3.76 3.38 3.19

8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

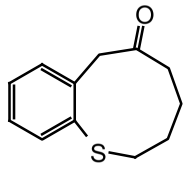
Title lb-III-132-1-C13
Solvent cdcl3
Spectrometer Frequency 100.58

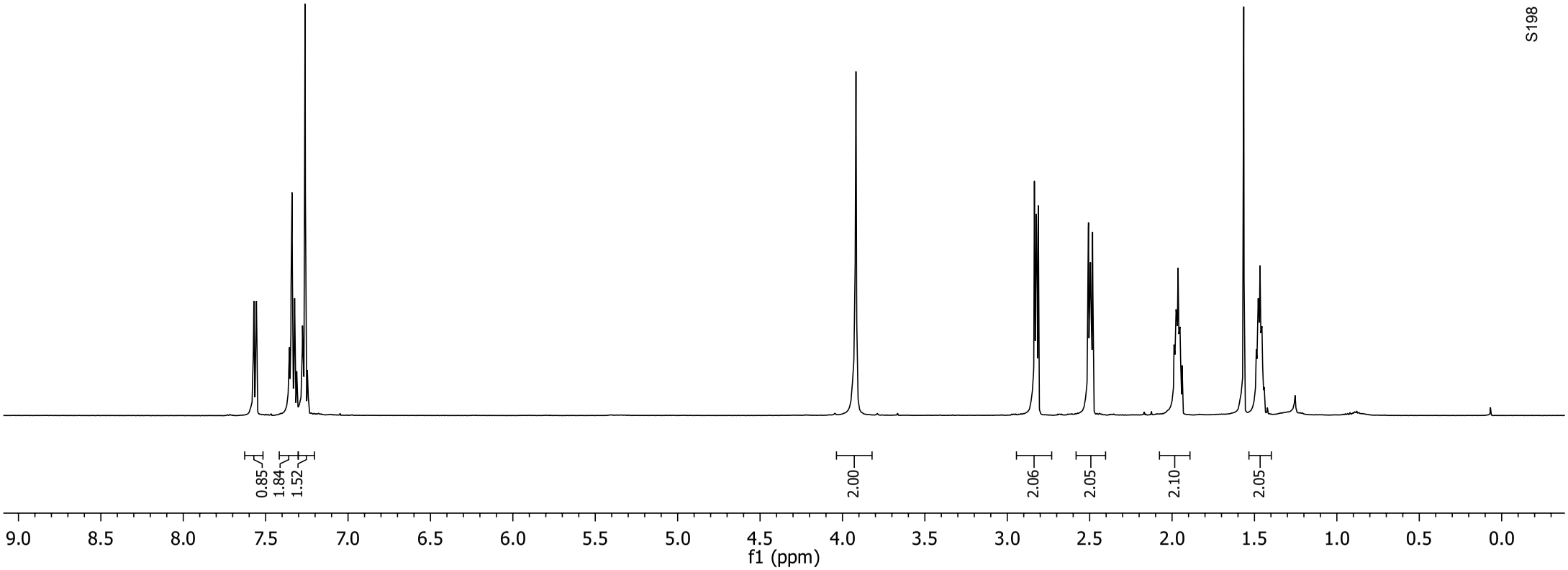




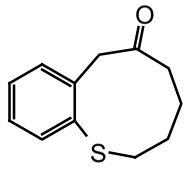

Parameter
Value (f2, f1)
1 Title
lb-III-132-1-cosy
2 Solvent
cdcl3
3 Spectrometer Frequency
(499.86, 499.86)
OH
H
O
H3C
H3C
S
f2 (ppm)
f1 (ppm)
S197

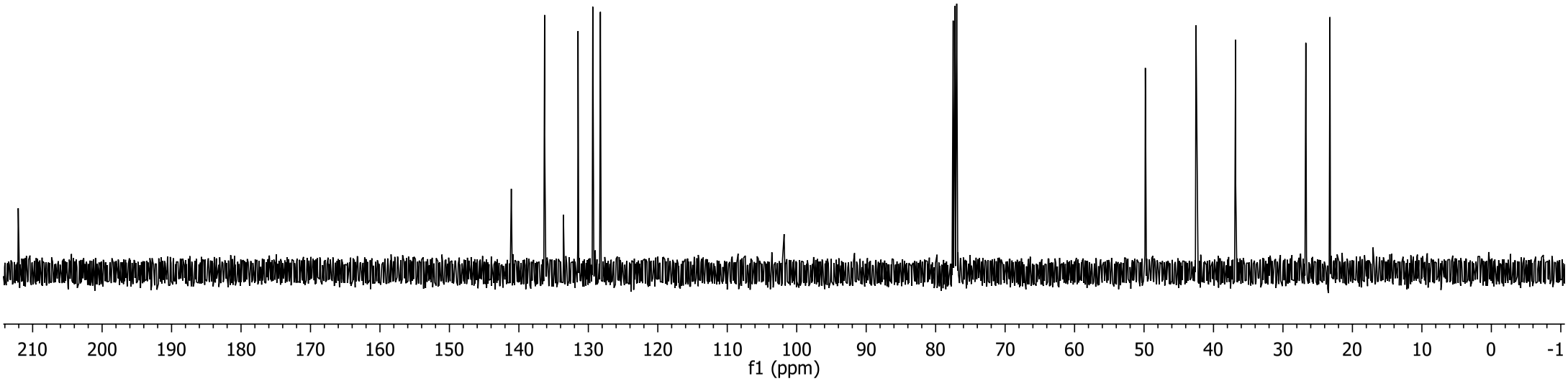
Title lb-III-39
Solvent cdcl3
Spectrometer Frequency 499.86



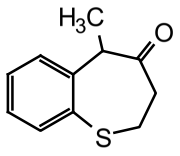


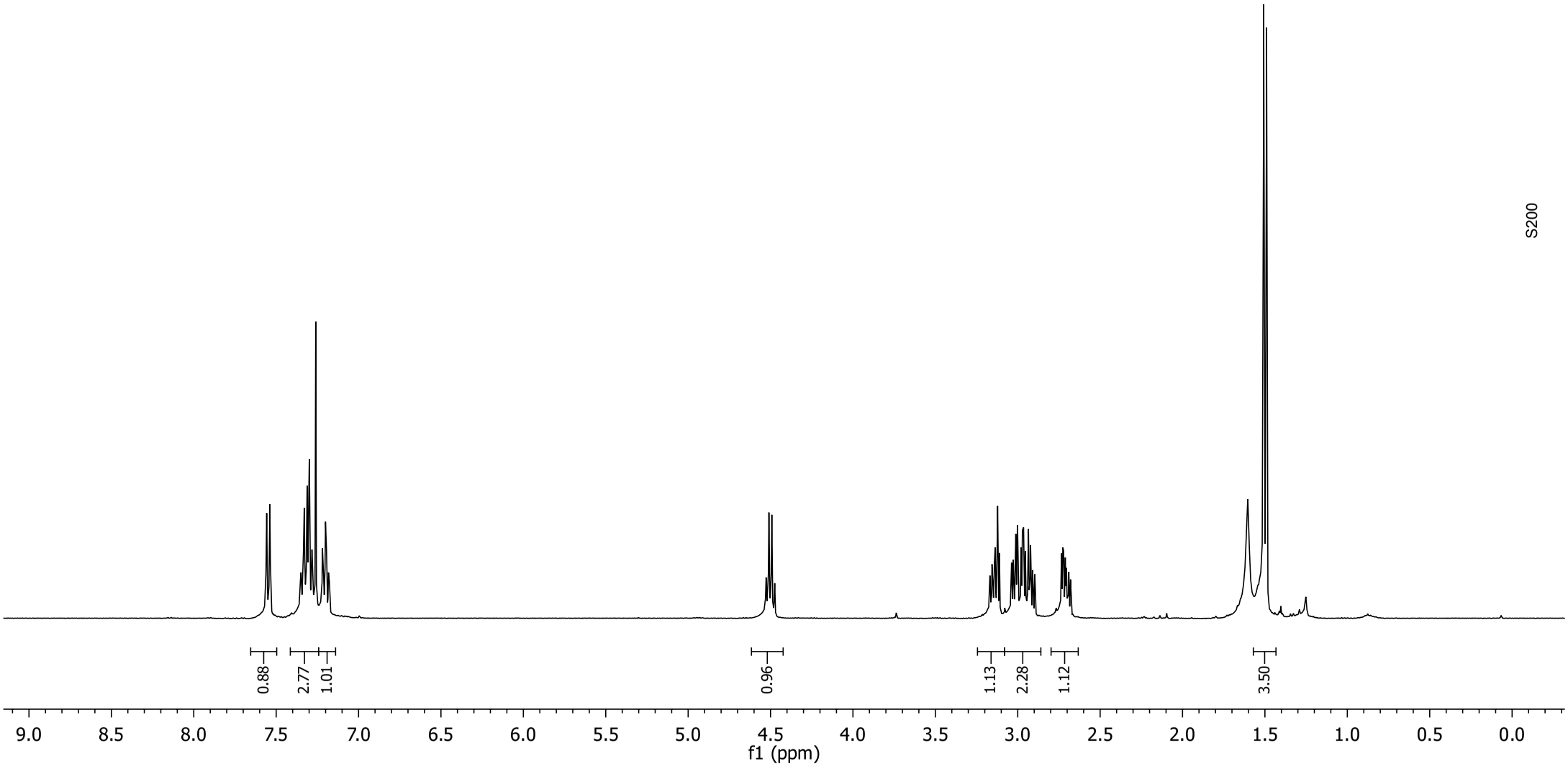
Title lb-III-39-C13
Solvent cdcl3
Spectrometer Frequency 125.70



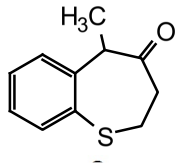


Title lb-III-63-minor
Solvent cdcl3
Spectrometer Frequency 399.95



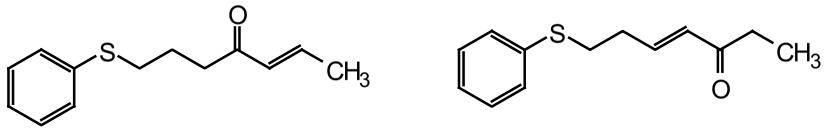


Title lb-III-63-minor-C13
Solvent cdcl3
Spectrometer Frequency 125.70

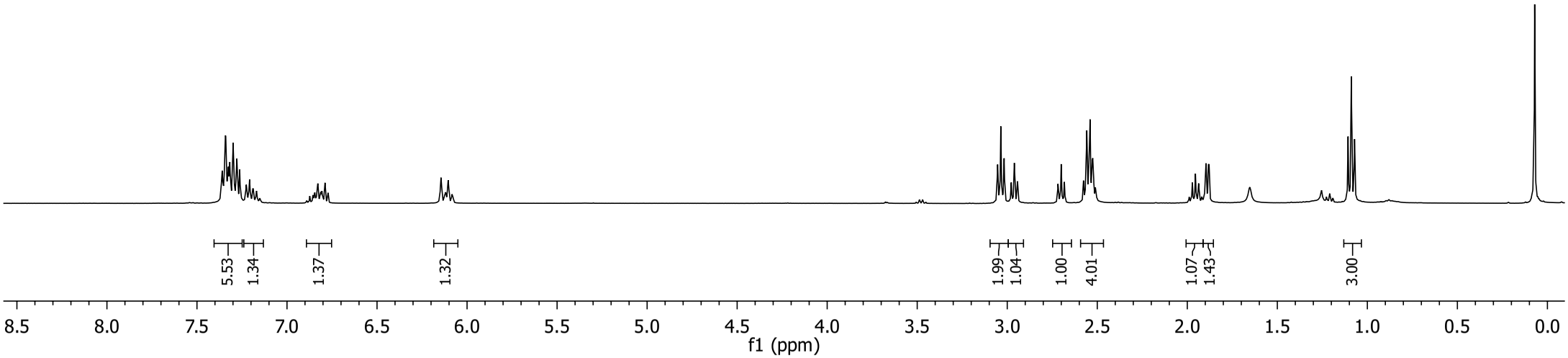


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

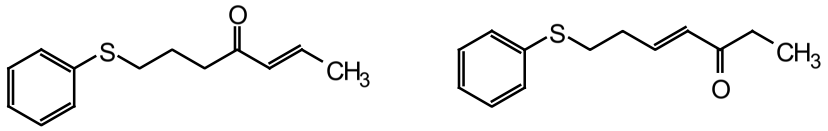
Title lb-III-123
Solvent cdcl3
Spectrometer Frequency 399.95

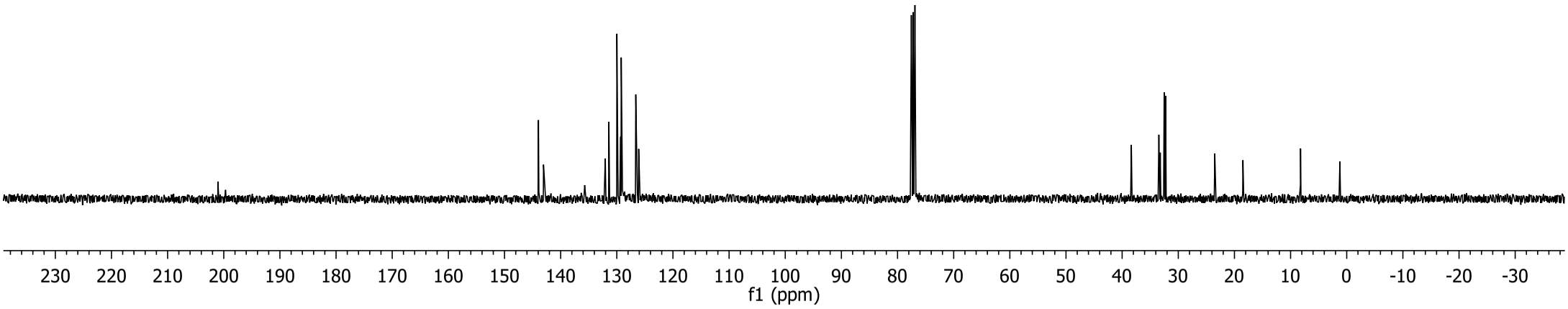


S202

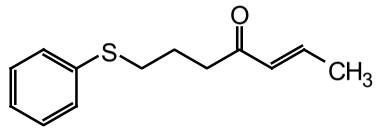


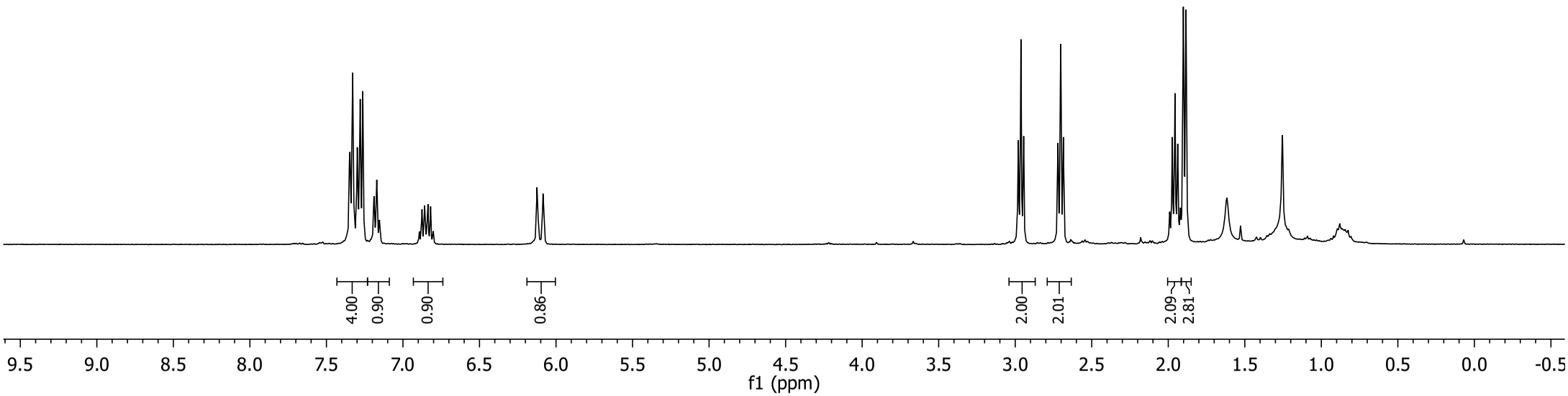
Title lb-III-123-C13
Solvent cdcl3
Spectrometer Frequency 100.58





Title lb-III-120
Solvent cdcl3
Spectrometer Frequency 399.95





Title lb-III-120-C13
Solvent cdcl3
Spectrometer Frequency 100.58