

Supporting Information
for
A Predictive Model for the [Rh₂(esp)₂]-catalyzed Intermolecular C(sp³)-H Bond Insertion
of β -carbonyl Ester Carbenes: Interplay Between Theory and Experiment

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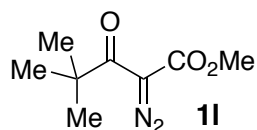
1. General Methods

All solvents used in the reported reactions were purchased anhydrous from commercial sources or freshly distilled. Chromatographic purification was performed as flash chromatography with Dynamic Adsorbents silica gel (32-65 μ m) and solvents indicated as eluent with 0.1-0.5 bar pressure. For quantitative flash chromatography, technical grades solvents were utilized. Analytical thin-layer chromatography (TLC) was performed on EMD silica gel 60 F254 TLC glass plates. Visualization was accomplished with UV light. Infrared (IR) spectra were obtained using an IRAffinity-1S from Shimadzu. The IR bands are characterized as weak (w), medium (m), and strong (s). Proton and carbon nuclear magnetic resonance spectra (^1H NMR and ^{13}C NMR) were recorded on a Varian Mercury Vx 300 MHz spectrometer or a Bruker 500 MHz spectrometer with solvent resonances as the internal standard (^1H NMR: CDCl_3 at 7.26 ppm; ^{13}C NMR: CDCl_3 at 77.0 ppm). ^1H NMR data are reported as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, dd = doublet of doublets, dt = doublet of triplets, ddd = doublet of doublet of doublets, t = triplet, m = multiplet, br = broad), coupling constants (Hz), and integration. Mass spectra were obtained through EI on a Micromass AutoSpec machine or through ESI on a Thermo Orbitrap XL. The accurate mass analyses run in EI mode were at a mass resolution of 10,000 and were calibrated using PFK (perfluorokerosene) as an internal standard. The accurate mass analyses run in EI mode were at a mass resolution of 30,000 using the calibration mixture supplied by Thermo.

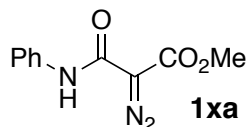
2. Experimental Procedures

A. Diazo Compounds

Diazo compounds **1a**,¹ **1b**,² **1d**,³ **1e**,² **1g**,⁴ **1h**,⁵ **1j**,⁶ **1o**,⁷ and **1s**² were prepared via reported protocols and matched literature characterization.

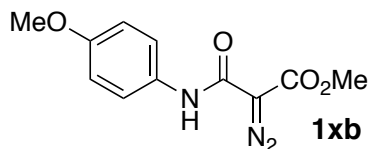


Methyl 2-diazo-4,4-dimethyl-3-oxopentanoate (11): To a dry round bottom flask containing methyl 4,4-dimethyl-3-oxopentanoate (1 mL, 6 mmol), triethylamine (1 mL, 7.4 mmol), in acetonitrile (20 mL) at 0 °C was added 4-acetamidobenzenesulfonyl azide (1.7 g, 7.1 mmol). The ice bath was removed allowing the reaction to warm to room temperature. The reaction mixture was stirred for 18 h. Upon completion of the reaction, solvents were removed via rotary evaporation. Cold dichloromethane (100 mL, 0 °C) was added to the crude material causing a white byproduct to precipitate. This precipitate was removed via vacuum filtration. The filtrate was purified via flash silica gel chromatography. **11** was afforded as a yellow liquid (993 mg, 90% yield). ^1H NMR (300 MHz, CDCl_3) δ = 3.79 (s, 3H), 1.27 (s, 9H). ^{13}C NMR (75 MHz, CDCl_3) δ = 197.12, 161.26, 52.07, 44.28, 25.71. IR: 2957 (m), 2137 (s), 1724 (s), 1638 (s) cm^{-1} . HRMS-EI (m/z): $[\text{M}+\text{H}]^+$ Calcd. for $\text{C}_8\text{H}_{13}\text{O}_3\text{N}_2$ 185.0921; Found 185.0916.

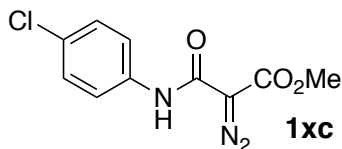


Methyl 2-diazo-3-oxo-3-(phenylamino)propanoate (1xa): *To a dry round bottom flask containing methyl 3-oxo-3-(phenylamino)propanoate (1.3 g, 6.7 mmol), triethylamine (1 mL, 7.4 mmol), in acetonitrile (30 mL) at 0 °C was added 4-acetamidobenzenesulfonyl azide (1.7 g, 7.1 mmol). The ice bath was removed allowing the reaction to warm to room temperature. The reaction mixture was stirred for 18 h. Upon completion of the reaction, solvents were removed via rotary evaporation. Cold dichloromethane (100 mL, 0 °C) was added to the crude material causing a white byproduct to precipitate. This precipitate was removed via vacuum filtration. The filtrate was then washed treated with 1 M HCl and extracted into dichloromethane. The filtrate was purified via flash silica gel chromatography **1xa** was afforded as a yellow solid (1.1 g, 75% yield). [m.p. = 83-84 °C]. ¹H NMR (300 MHz, CDCl₃) δ = 9.57 (s, 1H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.32 (dd, *J* = 8.4, 7.6 Hz, 2H), 7.10 (t, *J* = 7.4 Hz, 1H), 3.88 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ = 164.90, 158.30, 137.83, 129.00, 124.28, 119.81, 52.63. IR: 3279 (m), 2957 (w), 2137 (s), 1699 (s) 1651 (s) cm⁻¹. HRMS-EI (*m/z*): [M]⁺ Calcd. for C₁₀H₉O₃N₃ 219.0644; Found 219.0641.

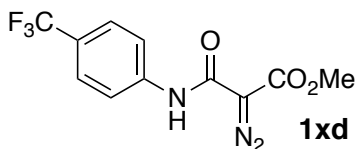
*Note: compounds **1xb-1xg** were all prepared via the procedure used to synthesize **1xa**.



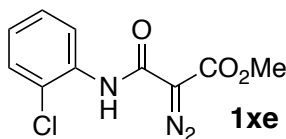
Methyl 2-diazo-3-((4-methoxyphenyl)amino)-3-oxopropanoate (1xb): **1xb** was afforded as a yellow solid (2.83 g, 52% yield). [m.p. = 115-116 °C]. ¹H NMR (300 MHz, CDCl₃) δ = 9.41 (s, 1H), 7.46 (d, *J* = 9.0 Hz, 2H), 6.85 (d, *J* = 9.1 Hz, 2H), 3.86 (s, 3H), 3.77 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ = ¹³C NMR (75 MHz, Chloroform-*d*) δ 164.96, 158.02, 156.36, 130.99, 121.54, 114.10, 55.43, 52.57. IR: 3280 (m), 2957 (w), 2135 (s), 1684 (s), 1651 (s) cm⁻¹. HRMS-EI (*m/z*): [M]⁺ Calcd. for C₁₀H₉O₃N₃ 219.0644; Found 219.0641.



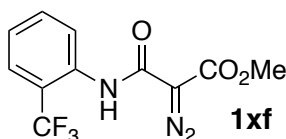
Methyl 3-((4-chlorophenyl)amino)-2-diazo-3-oxopropanoate (1xc): **1xc** was afforded as a yellow solid (4.38 g, 78% yield). [m.p. = 141-142 °C] ¹H NMR (300 MHz, CDCl₃) δ = 9.60 (s, 1H), 7.52 (d, *J* = 9.0 Hz, 2H), 7.28 (d, *J* = 11.8 Hz, 2H), 3.90 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ = 164.82, 158.41, 136.38, 128.98, 128.95, 121.01, 52.72. IR: 3267 (w), 2143 (s), 1686 (s), 1658 (s) cm⁻¹. HRMS-EI (*m/z*): [M]⁺ Calcd. for C₁₀H₈O₃N₃Cl 253.0254; Found 253.0250.



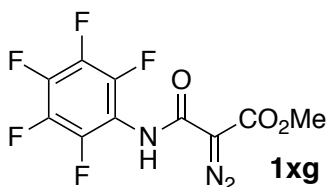
Methyl 2-diazo-3-oxo-3-((4-(trifluoromethyl)phenyl)amino)propanoate (1xd): 1xd was afforded as a white solid (1.62 g, 80% yield). [m.p. = 117-118 °C] $^1\text{H NMR}$ (300 MHz, CDCl_3) δ = 9.59 (s, 1H), 7.50 (d, J = 8.7 Hz, 2H), 7.39 (d, J = 8.7 Hz, 2H), 3.72 (s, 3H). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ = 164.79, 158.73, 140.81, 126.25 (q, J = 3.8 Hz), 125.92 (q, J = 32.8 Hz), 124.06 (q, J = 271.6 Hz), 119.35, 52.77. **IR:** 3279 (m), 2963 (w), 2148 (s), 1687 (s), 1661 (s) cm^{-1} . **HRMS-EI** (m/z): $[\text{M}]^+$ Calcd. for $\text{C}_{11}\text{H}_8\text{O}_3\text{N}_3\text{F}_3$ 287.0518; Found 287.0507.



Methyl 3-((2-chlorophenyl)amino)-2-diazo-3-oxopropanoate (1xe): 1xe was afforded as a white solid (2.48 g, 76% yield). [m.p. = 116-117 °C]. $^1\text{H NMR}$ (300 MHz, CDCl_3) δ = 10.12 (s, 1H), 8.41 (d, J = 8.3 Hz, 1H), 7.37 (d, J = 8.0 Hz, 1H), 7.25 (t, J = 7.9 Hz, 1H), 7.02 (t, J = 7.7 Hz, 1H), 3.90 (s, 3H). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ = 164.60, 158.60, 135.08, 129.15, 127.54, 124.54, 123.12, 121.33, 52.77. **IR:** 3211 (m), 2962 (w), 2143 (s), 1695 (s), 1651 (s) cm^{-1} . **HRMS-EI** (m/z): $[\text{M}]^+$ Calcd. for $\text{C}_{10}\text{H}_8\text{O}_3\text{N}_3\text{Cl}$ 253.0254; Found 253.0249.



Methyl 2-diazo-3-oxo-3-((2-(trifluoromethyl)phenyl)amino)propanoate (1xf): 1xf was afforded as a white solid (1.35 g, 67% yield). [m.p. = 103-105 °C]. $^1\text{H NMR}$ (300 MHz, CDCl_3) δ = 9.99 (s, 1H), 8.26 (d, J = 8.3 Hz, 1H), 7.62 (d, J = 7.9 Hz, 1H), 7.55 (t, J = 7.9 Hz, 1H), 7.22 (t, J = 7.7 Hz, 1H), 3.92 (s, 3H). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ = 164.41, 159.13, 135.08, 132.71, 126.04 (q, J = 5.4 Hz), 124.31, 124.12, 123.80 (q, J = 272.9 Hz), 120.49 (q, J = 30.7 Hz), 52.80. **IR:** 3277 (w), 3051 (w), 2148 (s), 1716 (s), 1664 (s) cm^{-1} . **HRMS-EI** (m/z): $[\text{M}]^+$ Calcd. for $\text{C}_{11}\text{H}_8\text{O}_3\text{N}_3\text{F}_3$ 287.0518; Found 287.0511.

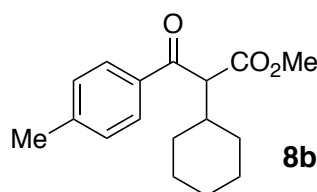


Methyl 2-diazo-3-oxo-3-((perfluorophenyl)amino)propanoate (1xg): 1xg was afforded as a white solid (1.10 g, 64% yield). [m.p. = 91-93 °C]. $^1\text{H NMR}$ (300 MHz, CDCl_3) δ = 9.15 (s, 1H), 3.91 (s, 3H). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ = 164.52, 159.23, 143.16 (d, J = 239.6 Hz), 140.16 (d, J = 254.0 Hz), 137.76 (d, J = 253.8 Hz), 111.32, 52.90. **IR:** 3246 (m), 2970 (w), 2158 (s), 1691 (s), 1651 (m) cm^{-1} . **HRMS-EI** (m/z): $[\text{M}]^+$ Calcd. for $\text{C}_{10}\text{H}_4\text{O}_3\text{N}_3\text{F}_5$ 309.0173; Found 309.0167.

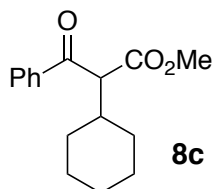
B. C-H Insertion Products

For compounds **8b-8e**, **8g**, **8h**, **8o**, and **8xa**, Procedure A was used: To a dry round bottom flask containing Rh₂esp₂ (1 mol %) and refluxing cyclohexane (7 mL, 81 °C) was added a solution of diazo compound **1** (0.5-0.7 mmol, 1 equiv.) in cyclohexane (3 mL) via syringe pump over 15 minutes. When the TLC showed complete consumption of the diazo compound, methanol (1 mL, 20 mmol) was added, and the temperature was reduced to 65 °C. The mixture continued to stir for 30 minutes. The crude material was purified via flash silica gel chromatography

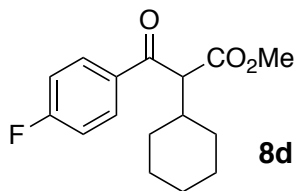
For compounds **8xf-8xg**, Procedure B was used: To a dry round bottom flask containing Rh₂esp₂ (1 mol %) and cyclohexane (5 equiv.) in refluxing dichloromethane (3 mL, 40 °C) was added a solution of diazo compound **1** (0.28 mmol, 1 equiv.) in dichloromethane (2 mL) via syringe pump over 15 minutes.



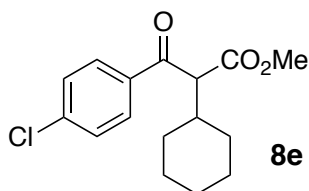
Methyl 2-cyclohexyl-3-oxo-3-(p-tolyl)propanoate (8b): 127 mg (0.580 mmol) of methyl 2-diazo-3-oxo-3-(p-tolyl)propanoate **1b** was used. The crude material was purified via flash silica gel chromatography (25% EtOAc/Hexane, R_f = 0.78). **8b** was afforded as a clear oil (33 mg, 21% yield). ¹H NMR (300 MHz, CDCl₃) δ = 7.91 (d, J = 8.3 Hz, 2H), 7.26 (d, J = 8.5 Hz, 2H), 4.17 (d, J = 9.7 Hz, 1H), 3.65 (s, 3H), 2.41 (s, 3H), 2.42 – 2.30 (m, 1H), 1.80 – 1.57 (m, 5H), 1.42 – 1.20 (m, 2H), 1.19 – 1.04 (m, 2H), 0.97 – 0.85 (m, 1H). ¹³C NMR (75 MHz, CDCl₃) δ = 194.25, 169.60, 144.48, 134.61, 129.44, 128.71, 60.25, 52.28, 38.36, 31.36, 30.95, 26.14, 26.00, 25.95, 21.65. IR: 3030 (w), 2927 (w), 2854 (w), 1734 (s), 1681 (s) cm⁻¹. HRMS-ESI (m/z): [M+H]⁺ Calcd. for C₁₇H₂₃O₃ 275.1642; Found 275.1638.



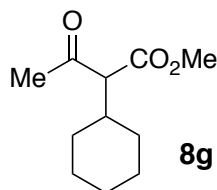
Methyl 2-cyclohexyl-3-oxo-3-phenylpropanoate (8c): 118 mg (0.580 mmol) methyl 2-diazo-3-oxo-3-phenylpropanoate **1c** was used. The mixture continued to stir for 30 minutes. The crude material was purified via flash silica gel chromatography (25% EtOAc/Hexane, R_f = 0.56). **8c** was afforded as a clear oil (51 mg, 34% yield). ¹H NMR (300 MHz, CDCl₃) δ = 8.04 (ddt, J = 8.01 (d, J = 7.1 Hz, 2H), 7.58 (t, J = 7.3 Hz, 1H), 7.47 (t, J = 7.4 Hz, 2H), 4.19 (d, J = 9.7 Hz, 1H), 3.66 (s, 3H), 2.44 – 2.29 (m, 1H), 1.79 – 1.59 (m, 5H), 1.43 – 1.02 (m, 4H), 1.00 – 0.84 (m, 1H). ¹³C NMR (75 MHz, CDCl₃) δ = 193.03, 169.34, 165.99 (d, J = 255.8 Hz), 133.44 (d, J = 3.1 Hz), 131.28 (d, J = 9.4 Hz), 115.91 (d, J = 21.9 Hz), 60.49, 52.41, 38.31, 31.37, 30.88, 26.09, 25.96, 25. IR: 3030 (w), 2928 (w), 2855 (w), 1734 (s), 1684 (s) cm⁻¹. HRMS-ESI (m/z): [M+H]⁺ Calcd. for C₁₆H₂₁O₃ 216.1485; Found 216.1481.



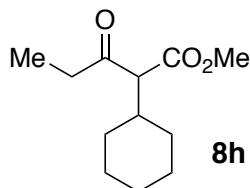
Methyl 2-cyclohexyl-3-(4-fluorophenyl)-3-oxopropanoate (8d): 129 mg (0.58 mmol) of methyl 2-diazo-3-(4-fluorophenyl)-3-oxopropanoate **1d** was used. The crude material was purified via flash silica gel chromatography (25% EtOAc/Hexane, R_f = 0.59). **8d** was afforded as a clear oil (79 g, 49% yield). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ = 8.04 (ddt, J = 8.2, 5.0, 2.5 Hz, 2H), 7.21 – 7.07 (m, 2H), 4.13 (d, J = 9.8 Hz, 1H), 3.66 (s, 3H), 2.36 (qt, J = 9.6, 2.7 Hz, 1H), 1.80 – 1.58 (m, 5H) 1.33 (pt, J = 13.5, 3.4 Hz, 2H), 1.09 (pt, J = 11.7, 2.6 Hz, 5H), 0.90 (qd, J = 11.5, 2.3 Hz, 1H) $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ = 193.03, 169.34, 165.99 (d, J = 255.8 Hz), 133.44 (d, J = 3.1 Hz), 131.28 (d, J = 9.4 Hz), 115.91 (d, J = 21.9 Hz), 60.49, 52.41, 38.31, 31.37, 30.88, 26.09, 25.96, 25.91. **IR:** 3059 (w), 2929 (w), 2853 (w), 1734 (s), 1684 (s) cm^{-1} . **HRMS-ESI** (m/z): $[\text{M}+\text{H}]^+$ Calcd. for $\text{C}_{16}\text{H}_{20}\text{O}_3\text{F}$ 279.1391; Found 279.1386.



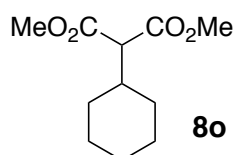
Methyl 3-(4-chlorophenyl)-2-cyclohexyl-3-oxopropanoate (8e): 138 mg, (0.58 mmol) of methyl 3-(4-chlorophenyl)-2-cyclohexyl-3-oxopropanoate **1e** was used. The mixture continued to stir for 30 minutes. The crude material was purified via flash silica gel chromatography (25% EtOAc/Hexane, R_f = 0.66). **8e** was afforded as a clear oil (110 mg, 62% yield). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ = 7.94 (d, J = 8.8 Hz, 2H), 7.43 (d, J = 8.8 Hz, 2H), 4.11 (d, J = 9.7 Hz, 1H), 3.65 (s, 3H), 2.35 (qt, J = 11.5, 3.0 Hz, 1H), 1.79 – 1.55 (m, 5H), 1.30 (pt, J = 12.1, 3.0 Hz, 2H), 1.11 (pt, J = 11.8, 3.0 Hz, 2H), 0.90 (td, J = 11.8, 8.2 Hz, 1H) $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ = 193.45, 169.23, 140.10, 135.30, 129.95, 129.08, 60.48, 52.42, 38.30, 31.35, 30.86, 26.07, 25.95, 25.91. **IR:** 3059 (w), 2927 (m), 2853 (m), 1734 (s), 1684 (s) cm^{-1} . **HRMS-EI** (m/z): $[\text{M}+\text{H}]^+$ Calcd. for $\text{C}_{16}\text{H}_{20}\text{O}_3\text{Cl}$ 295.1101; Found 295.1086.



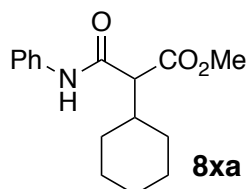
Methyl 2-cyclohexyl-3-oxobutanoate (8g): 94 mg, (0.66 mmol) methyl 2-diazo-3-oxobutanoate **1g** was used. **8g** was afforded as a clear oil (99 mg, 75% yield). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ = 3.66 (s, 3H), 3.21 (d, J = 9.8 Hz, 1H), 2.17 (s, 3H), 2.14 – 2.00 (m, 1H), 1.73 – 1.49 (m, 5H), 1.33 – 1.05 (m, 3H), 1.04 – 0.84 (m, 2H). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ = 203.16, 169.54, 66.61, 52.11, 37.97, 30.77, 30.71, 29.31, 25.93, 25.83. **IR:** 2924 (m), 2851 (m), 1734 (s), 1707 (s) cm^{-1} . **HRMS-EI** (m/z): $[\text{M}+\text{H}]^+$ Calcd. for $\text{C}_{11}\text{H}_{19}\text{O}_3$ 199.1334; Found 199.1338.



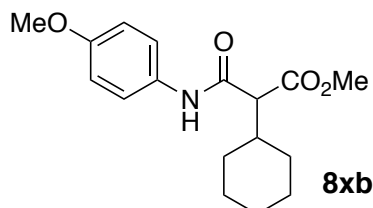
Methyl 2-cyclohexyl-3-oxopentanoate (8h): 90 mg, (0.58 mmol) of methyl 2-diazo-3-oxopentanoate **1h** was used. **8h** was afforded as a clear oil (48 mg, 39% yield). ¹H NMR (300 MHz, CDCl₃) δ = 3.67 (s, 3 H), 3.28 (d, *J* = 9.9 Hz, 1 H), 2.50 (m, 2 H), 2.13 (m, 1 H), 1.65 (m, 4 H), 1.53 (m, 1 H), 1.21 (m, 3 H), 1.02 (t, *J* = 7.2 Hz, 3 H), 0.92 (m, 2 H). ¹³C NMR (75 MHz, CDCl₃) δ = 205.72, 169.54, 65.60, 52.13, 38.11, 36.12, 30.87, 30.85, 26.00, 25.87, 7.46. IR: 2928 (m), 2852 (m), 1740 (s), 1713 (s) cm⁻¹. HRMS-ESI (*m/z*): [M+H]⁺ Calcd. for C₁₂H₂₁O₃ 213.1485; Found 213.1481.



Dimethyl 2-cyclohexylmalonate (8o): 104 mg, (0.66 mmol) of dimethyl diazomalonate **1o** was used. **8o** was afforded as a clear oil (103 mg, 73% yield). Characterization matches that previously reported.⁸ ¹H NMR (300 MHz, CDCl₃) δ = 3.67 (s, 6H), 3.15 (d, *J* = 8.8 Hz, 1H), 2.05 (qt, *J* = 8.5, 2.9 Hz, 1H), 1.75 – 1.56 (m, 5H), 1.26 (pt, *J* = 12.3, 2.5 Hz, 2H), 1.16 – 0.94 (m, 3H). ¹³C NMR (75 MHz, CDCl₃) δ = 168.93, 57.98, 51.88, 37.94, 30.66, 25.94, 25.86.

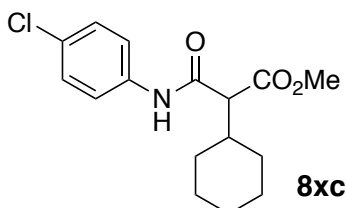


Methyl 2-cyclohexyl-3-oxo-3-(phenylamino)propanoate (8xa): 134 mg (0.62 mmol) of **1xa** was used. **8xa** was afforded as white solid (149 mg, 89% yield). [m.p. = 158-160 °C]. ¹H NMR (300 MHz, CDCl₃, 40 °C) δ = 8.66 (s, 1H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.32 (t, *J* = 7.0 Hz, 2H), 7.10 (t, *J* = 7.4 Hz, 1H), 3.77 (s, 3H), 3.18 (d, *J* = 9.1 Hz, 1H), 2.14 – 1.95 (m, 1H), 1.87 – 1.60 (m, 5H), 1.39 – 1.01 (m, 5H). ¹³C NMR (75 MHz, CDCl₃, 40 °C) δ = 173.22, 165.53, 137.61, 128.91, 124.35, 119.87, 60.56, 52.27, 41.28, 31.00, 30.76, 25.90, 25.84. IR: 3280 (m), 3064 (w), 2920 (m), 2847 (m), 1742 (s), 1655 (s) cm⁻¹. HRMS-ESI (*m/z*): [M+H]⁺ Calcd. for C₁₆H₂₂O₃N 276.1594; Found 276.1588.

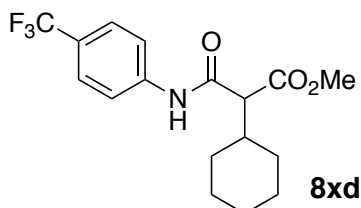


Methyl 2-cyclohexyl-3-((4-methoxyphenyl)amino)-3-oxopropanoate (8xb): 70 mg (0.28 mmol) of **1xb** was used. **8xb** was afforded as a white solid (21 mg, 24% yield). [m.p. = 161-163

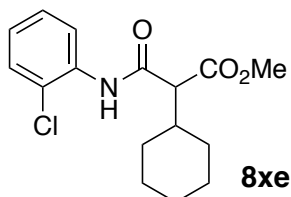
°C]. **¹H NMR** (300 MHz, CDCl₃, 40 °C) δ = 8.58 (s, 1H), 7.44 (d, J = 9.1 Hz, 2H), 6.84 (d, J = 9.1 Hz, 2H), 3.77 (s, 1H), 3.76 (s, 3H), 3.15 (d, J = 9.2 Hz, 1H), 2.12 – 1.92 (m, 1H), 1.90 – 1.55 (m, 5H), 1.16 (m, 5H). **¹³C NMR** (75 MHz, CDCl₃, 40 °C) δ = 173.27, 165.41, 156.41, 130.73, 121.58, 114.07, 60.39, 55.46, 52.35, 41.23, 30.99, 30.75, 25.92, 25.90, 25.84. **IR**: 3283 (m), 3004 (w), 2920 (m), 2849 (m), 1738 (s), 1653 (s) cm⁻¹. **HRMS-EI** (m/z): [M]⁺ Calcd. for C₁₇H₂₃O₄N 305.1627; Found 305.1627.



Methyl 3-((4-chlorophenyl)amino)-2-cyclohexyl-3-oxopropanoate (8xc): 110 mg (0.43 mmol) of **1xc** was used. **8xc** was afforded as a white solid (65 mg, 66% yield). [m.p. = 164-165 °C]. **¹H NMR** (300 MHz, CDCl₃, 40 °C) δ = 8.80 (s, 1H), 7.51 (d, J = 8.7 Hz, 2H), 7.27 (d, J = 8.8 Hz, 2H), 3.77 (s, 3H), 3.17 (d, J = 8.7 Hz, 1H), 2.10 – 1.95 (m, 1H), 1.84 – 1.60 (m, 5H), 1.36 – 1.03 (m, 5H). **¹³C NMR** (75 MHz, CDCl₃, 40 °C) δ = 173.40, 165.76, 136.12, 129.32, 128.94, 121.10, 60.37, 52.47, 41.47, 30.96, 30.78, 25.89, 25.88, 25.78. **IR**: 3277 (m), 3117 (w), 2920 (m), 2848 (m), 1742 (s), 1654 (s) cm⁻¹. **HRMS-ESI** (m/z): [M+Na]⁺ Calcd. for C₁₆H₂₀O₃NCINa 332.1024; Found 332.1022.

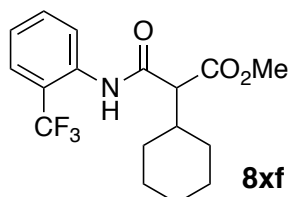


Methyl 2-cyclohexyl-3-oxo-3-((4-(trifluoromethyl)phenyl)amino)propanoate (8xd): 81 mg (0.28 mmol) of **1xd** was used. **8xd** was afforded as a white solid (61 mg, 63% yield). [m.p. = 156-158 °C]. **¹H NMR** (300 MHz, CDCl₃) δ = 9.00 (s, 1H), 7.68 (d, J = 8.5 Hz, 2H), 7.57 (d, J = 8.6 Hz, 2H), 3.78 (s, 3H), 3.19 (d, J = 9.0 Hz, 1H), 2.03 (m, 1H), 1.82 – 1.63 (m, 5H), 1.38 – 1.06 (m, 5H). **¹³C NMR** (75 MHz, CDCl₃, 40 °C) δ = 173.39, 166.03, 140.56 (d, J = 1.3 Hz), 126.21 (q, J = 3.8 Hz), 125.87 (d, J = 6.0 Hz), 129.58 – 119.46 (m), 119.47, 60.40, 52.54, 41.55, 30.96, 30.77, 25.86, 25.74. **IR**: 3300 (m), 2918 (m), 2848 (m), 1738 (s), 1668 (m) cm⁻¹. **HRMS-ESI** (m/z): [M+Na]⁺ Calcd. for C₁₇H₂₀O₃NF₃Na 366.1283; Found 366.1287.

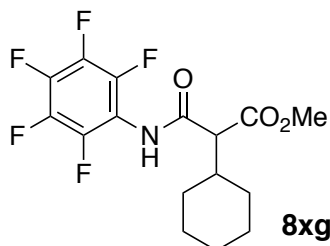


Methyl 2-cyclohexyl-3-oxo-3-(phenylamino)propanoate (8xe): 71 mg (0.28 mmol) of **1xe** was used. **8xe** was afforded as a white solid (60 mg, 69% yield). [m.p. = 123-125 °C]. **¹H NMR** (300 MHz, CDCl₃, 40 °C) δ = 9.24 (s, 1H), 8.36 (d, J = 8.3 Hz, 1H), 7.37 (d, J = 8.0 Hz, 1H), 7.25 (t, J

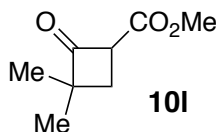
= 7.2 Hz, 1H), 7.11 – 6.98 (m, 1H), 3.79 (s, 3H), 3.21 (d, J = 9.1 Hz, 1H), 2.10 – 1.95 (m, 1H), 1.85 – 1.60 (m, 5H), 1.34 – 1.04 (m, 5H). ^{13}C NMR (75 MHz, CDCl_3 , 40 °C) δ = 172.83, 165.83, 134.51, 129.09, 127.56, 124.76, 123.29, 121.60, 60.86, 52.51, 41.50, 31.00, 30.75, 25.89, 25.87, 25.80. **IR**: 3238 (m), 3043 (w), 2927 (m), 2852 (m), 1740 (s), 1653 (s) cm^{-1} . **HRMS-EI** (m/z): $[\text{M}]^+$ Calcd. for $\text{C}_{16}\text{H}_{20}\text{O}_3\text{NCl}$ 309.1132; Found 309.1140.



Methyl 2-cyclohexyl-3-oxo-3-((2-(trifluoromethyl)phenyl)amino)propanoate (8xf): 81 mg (0.28 mmol) of **1xf** was used. **8xf** was afforded as a white solid (72 mg, 75% yield). [m.p. = 129–131 °C]. ^1H NMR (300 MHz, CDCl_3 , 40 °C) δ = 9.05 (s, 1H), 8.19 (d, J = 8.3 Hz, 1H), 7.61 (d, J = 9.3 Hz, 1H), 7.58 – 7.48 (m, 1H), 7.25 – 7.17 (m, 1H), 3.79 (s, 3H), 3.20 (d, J = 9.3 Hz, 1H), 2.08 – 1.96 (m, 1H), 1.83 – 1.61 (m, 5H), 1.37 – 1.01 (m, 5H). ^{13}C NMR (75 MHz, CDCl_3) δ = 172.64, 166.03, 134.92 (q, J = 1.8 Hz), 132.93 – 132.17 (m), 126.01 (q, J = 5.4 Hz), 124.48, 124.32, 123.86 (q, J = 273.0 Hz), 120.49 (q, J = 29.8 Hz), 60.72, 52.50, 41.41, 30.98, 30.64, 25.84, 25.77. **IR**: 3252 (m), 3003 (w), 2924 (m), 2855 (m), 1741 (s), 1657 (m) cm^{-1} . **HRMS-ESI** (m/z): $[\text{M}+\text{Na}]^+$ Calcd. for $\text{C}_{17}\text{H}_{20}\text{O}_3\text{NF}_3\text{Na}$ 366.1282; Found 366.1287.

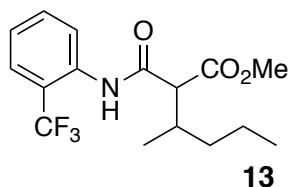


Methyl 2-cyclohexyl-3-oxo-3-((perfluorophenyl)amino)propanoate (8xg): 87 mg (0.28 mmol) of **1xg** was used. **8xg** was afforded as a white solid (84 mg, 82% yield). [m.p. = 152–153 °C]. ^1H NMR (300 MHz, CDCl_3 , 40 °C) δ = 8.60 (s, 1H), 3.80 (s, 3H), 3.27 (d, J = 8.7 Hz, 1H), 2.12 – 1.94 (m, 1H), 1.86 – 1.58 (m, 5H), 1.36 – 1.02 (m, 5H). ^{13}C NMR (75 MHz, CDCl_3 , 40 °C) δ = 173.11, 166.33, 144.42, 141.97 – 138.96 (m), 136.09, 111.57, 59.31, 52.66, 41.72, 30.88, 30.55, 25.92, 25.90, 25.73. **IR**: 3215 (m), 2926 (m), 2854 (w), 1742 (s), 1656 (m) cm^{-1} . **HRMS-EI** (m/z): $[\text{M}]^+$ Calcd. for $\text{C}_{16}\text{H}_{16}\text{O}_3\text{NF}_5$ 365.1050; Found 365.1047.



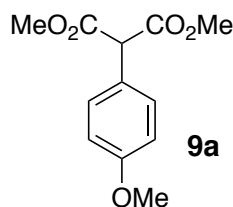
Methyl 3,3-dimethyl-2-oxocyclobutane-1-carboxylate (10l): To a dry round bottom flask containing Rh_2esp_2 (4.1 mg, 5.4 μmol) and refluxing cyclohexane (7 mL, 81 °C) was added a solution of methyl 2-diazo-4,4-dimethyl-3-oxopentanoate (100 mg, 0.54 mmol) in cyclohexane (3 mL) via syringe pump over 15 minutes. When the TLC showed complete consumption of the diazo compound, methanol (1 mL, 20 mmol) was added, and the temperature was reduced to 65 °C. The mixture continued to stir for 30 minutes. The crude material was purified via flash silica gel

chromatography (25% EtOAc/Hexane, R_f = 0.36). **101** was afforded as a clear oil (61 mg, 72% yield). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ = 4.20 (dd, J = 10.2, 7.7 Hz, 1H), 3.72 (s, 3H), 2.27 (dd, J = 11.6, 7.7 Hz, 1H), 2.04 (dd, J = 11.6, 10.3 Hz, 1H), 1.23 (d, J = 5.5 Hz, 6H). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ = 206.62, 167.73, 60.24, 59.54, 52.44, 29.08, 23.22, 21.98. **IR** 2957 (m), 1786 (s), 1730 (s) cm^{-1} . **HRMS-ESI** (m/z): $[\text{M}+\text{H}]^+$ Calcd. for $\text{C}_8\text{H}_{13}\text{O}$ 157.0865; Found 157.0869.

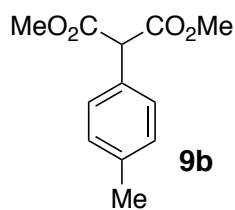


Methyl 3-methyl-2-((2-(trifluoromethyl)phenyl)carbamoyl)hexanoate (13): To a dry round bottom flask containing Rh_2esp_2 (2.64 mg, 3.5 μmol) and refluxing n-pentane (5 mL, 38 $^\circ\text{C}$) was added a solution of **1xf** (101 mg, 0.35 mmol) in DCM (0.5 mL) dropwise. The mixture continued to stir for 30 minutes. The crude material was purified via flash silica gel chromatography. **13** was afforded as a clear oil (101 mg, 87% yield). [m.p. = 50-51 $^\circ\text{C}$]. $^1\text{H NMR}$ (300 MHz, CDCl_3 , 40 $^\circ\text{C}$) δ = 9.15 (s, 1H), 8.26 (d, J = 8.3 Hz, 1H), 7.61 (d, J = 8.3 Hz, 1H), 7.53 (t, J = 7.9 Hz, 1H), 7.21 (t, J = 7.6 Hz, 1H), 3.78 (s, 3H), 3.27 (t, J = 8.3 Hz, 1H), 2.35 – 2.14 (m, 1H), 1.49 – 1.17 (m, 4H), 1.02 (dd, J = 12.8, 6.7 Hz, 3H), 0.93 – 0.77 (m, 3H). $^{13}\text{C NMR}$ (75 MHz, CDCl_3 , 40 $^\circ\text{C}$) δ = 172.81, 172.64, 166.49, 166.21, 134.92 (q, J = 1.7 Hz), 132.77 – 132.63 (m), 126.01 (q, J = 5.4 Hz), 124.50, 124.35 (d, J = 1.8 Hz), 123.85 (q, J = 273.0 Hz), 120.54 (q, J = 29.7 Hz), 60.01, 59.84, 52.52, 52.45, 36.73, 36.68, 36.66, 36.32, 19.76, 19.75, 16.95, 16.78, 13.97, 13.92. **IR**: 3250 (m), 2956 (m), 2860 (w), 1741 (s), 1654 (s) cm^{-1} . **HRMS-ESI** (m/z): $[\text{M}]^+$ Calcd. for $\text{C}_{16}\text{H}_{20}\text{O}_3\text{NF}_3$ 331.1395; Found 331.1386.

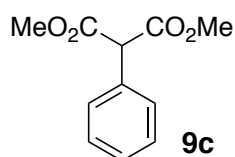
C. Wolff Rearrangement Products



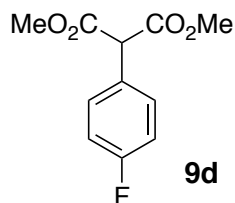
Dimethyl 2-(4-methoxyphenyl)malonate (9a): To a dry round bottom flask containing Rh_2esp_2 (4.4 mg, 5.8 μmol) and refluxing cyclohexane (7 mL, 81 $^\circ\text{C}$) was added a solution of methyl 2-diazo-3-(4-methylphenyl)-3-oxopropanoate **1a** (136 mg, 0.580 mmol) in cyclohexane (3 mL) via syringe pump over 15 minutes. The reaction was monitored by TLC. When the TLC showed complete consumption of the diazo compound, methanol (1 mL, 20 mmol) was added, and the temperature was reduced to 65 $^\circ\text{C}$. The mixture continued to stir for 30 minutes. The crude material was purified via flash silica gel chromatography (25% EtOAc/Hexane, R_f = 0.39). **9a** was afforded as a clear liquid (134 mg, 97% yield). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ = 7.32 (d, J = 8.9 Hz, 2H), 6.89 (d, J = 8.9 Hz, 2H), 4.60 (s, 1H), 3.79 (s, 3H), 3.74 (s, 6H). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ = 168.82, 159.56, 130.34, 124.64, 114.07, 56.71, 55.23, 52.78. **IR**: 3003 (w), 2954 (w), 1732 (s) cm^{-1} . **HRMS-ESI** (m/z): $[\text{M}+\text{H}]^+$ Calcd. for $\text{C}_{12}\text{H}_{15}\text{O}_5$ 239.0914; Found 239.0911.



Dimethyl 2-(*p*-tolyl)malonate (9b): (See procedure for **8b**) To a dry round bottom flask containing Rh₂esp₂ (4.4 mg, 5.8 μmol) and refluxing cyclohexane (7 mL, 81 °C) was added a solution of methyl 2-diazo-3-(4-methylphenyl)-3-oxopropanoate **1b** (127 mg, 0.58 mmol) in cyclohexane (3 mL) via syringe pump over 15 minutes. The reaction was monitored by TLC. When the TLC showed complete consumption of the diazo compound, methanol (1 mL, 20 mmol) was added, and the temperature was reduced to 65 °C. The mixture continued to stir for 30 minutes. The crude material was purified via flash silica gel chromatography (25% EtOAc/Hexane, *R_f* = 0.63). **9b** was afforded as a white solid (100 mg, 78% yield). [m.p. = 68-70 °C]. ¹H NMR (300 MHz, CDCl₃) δ = 7.29 (d, *J* = 8.3 Hz, 2H), 7.18 (d, *J* = 7.9 Hz, 2H), 4.63 (s, 1H), 3.75 (s, 6H), 2.35 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ = 168.73, 138.16, 129.60, 129.39, 129.06, 57.20, 52.81, 21.13. IR: 3041 (w), 2959 (w), 1744 (s), 1724 (s) cm⁻¹. HRMS-EI (*m/z*): [M]⁺ Calcd. for C₁₂H₁₄O₄ 222.0892; Found 222.0892.

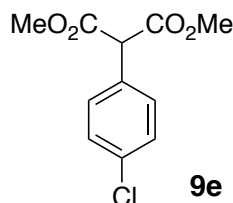


Dimethyl 2-phenylmalonate (9c): (See procedure for **8c**) To a dry round bottom flask containing Rh₂esp₂ (4.4 mg, 5.8 μmol) and refluxing cyclohexane (7 mL, 81 °C) was added a solution of methyl 2-diazo-3-oxo-3-phenylpropanoate **1c** (118 mg, 0.580 mmol) in cyclohexane (3 mL) via syringe pump over 15 minutes. The reaction was monitored by TLC. When the TLC showed complete consumption of the diazo compound, methanol (1 mL, 20 mmol) was added, and the temperature was reduced to 65 °C. The mixture continued to stir for 30 minutes. The crude material was purified via flash silica gel chromatography (25% EtOAc/Hexane, *R_f* = 0.41). **9c** was afforded as a white solid (73 mg, 60% yield). [m.p. = 50-51 °C]. ¹H NMR (300 MHz, CDCl₃) δ = 7.43 – 7.33 (m, 5H), 4.66 (s, 1H), 3.75 (s, 6H). ¹³C NMR (75 MHz, CDCl₃) δ = 168.55, 132.55, 129.22, 128.67, 128.33, 57.56, 52.86. IR: 3040 (w), 2959 (w), 1732 (s) cm⁻¹. HRMS-ESI (*m/z*): [M+H]⁺ Calcd. for C₁₁H₁₃O₄ 209.0808; Found 209.0805.



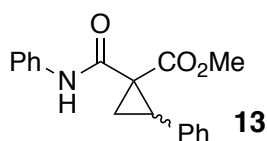
Dimethyl 2-(4-fluorophenyl)malonate (9d): (See procedure for **8b**) To a dry round bottom flask containing Rh₂esp₂ (4.4 mg, 5.8 μmol) and refluxing cyclohexane (7 mL, 81 °C) was added a solution of methyl 2-diazo-3-(4-fluorophenyl)-3-oxopropanoate **1d** (129 mg, 0.580 mmol) in cyclohexane (3 mL) via syringe pump over 15 minutes. When the TLC showed complete consumption of the diazo compound, methanol (1 mL, 20 mmol) was added, and the temperature was reduced to 65 °C. The mixture continued to stir for 30 minutes. The crude material was

purified via flash silica gel chromatography (25% EtOAc/Hexane, R_f = 0.41). **9d** was afforded as a white solide (64 mg, 49% yield). [m.p. = 49-50 °C]. $^1\text{H NMR}$ (300 MHz, CDCl_3) δ = 7.38 (dd, J = 8.8, 5.1 Hz, 2H), 7.05 (t, J = 8.7 Hz, 2H), 4.63 (s, 1H), 3.76 (s, 6H). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ = 168.42, 162.70 (d, J = 247.5 Hz), 130.99 (d, J = 8.3 Hz), 128.31 (d, J = 3.3 Hz), 115.62 (d, J = 21.7 Hz), 56.68, 52.95. **IR**: 3059 (w), 2954 (w), 1736 (s) cm^{-1} . **HRMS-EI** (m/z): $[\text{M}]^+$ Calcd. for $\text{C}_{11}\text{H}_{11}\text{O}_4\text{F}$ 226.0641; Found 226.0644.



Dimethyl 2-(4-chlorophenyl)malonate (9e): (See procedure for **8e**) To a dry round bottom flask containing Rh_2esp_2 (4.4 mg, 5.8 μmol) and refluxing cyclohexane (7 mL, 81 °C) was added a solution of methyl 3-(4-chlorophenyl)-2-cyclohexyl-3-oxopropanoate **1e** (138 mg, 0.58 mmol) in cyclohexane (3 mL) via syringe pump over 15 minutes. When the TLC showed complete consumption of the diazo compound, methanol (1 mL, 20 mmol) was added, and the temperature was reduced to 65 °C. The mixture continued to stir for 30 minutes. The crude material was purified via flash silica gel chromatography (25% EtOAc/Hexane, R_f = 0.41). **9e** was afforded as a clear oil (44 mg, 31% yield). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ = 7.34 (s, 4H), 4.62 (s, 1H), 3.76 (s, 6H). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ = 168.18, 134.46, 130.96, 130.63, 128.85, 56.83, 52.99. **IR**: 3007 (w), 2954 (w), 1730 (s) cm^{-1} . **HRMS-ESI** (m/z): $[\text{M}+\text{H}]^+$ Calcd. for $\text{C}_{11}\text{H}_{12}\text{O}_4\text{Cl}$ 243.0419; Found 243.0416.

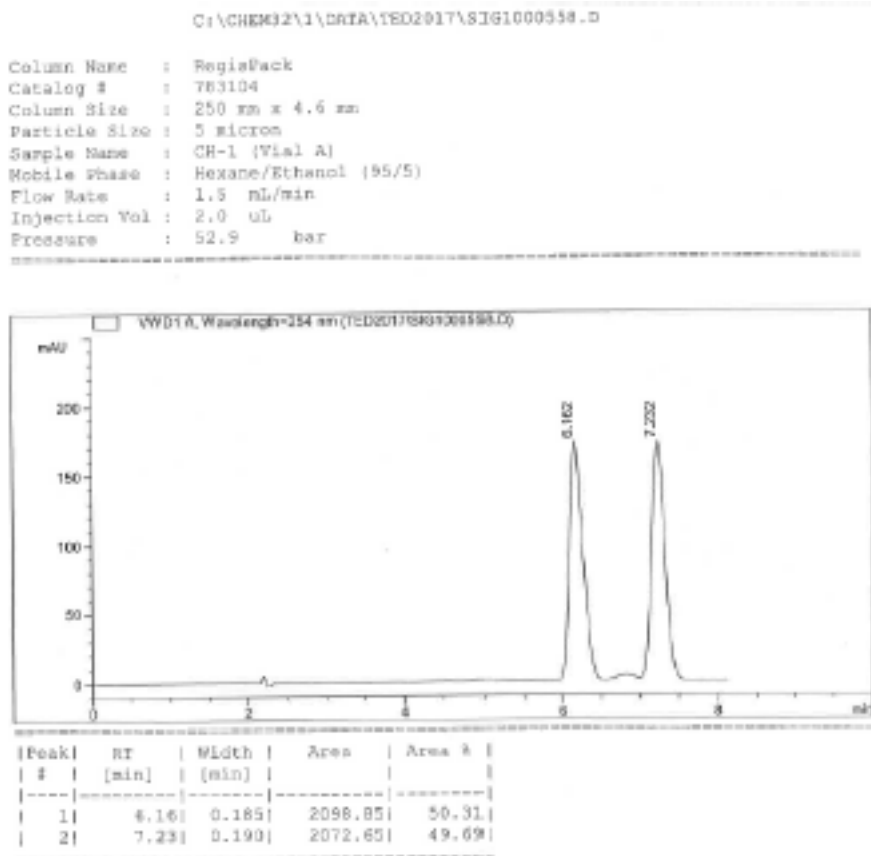
D. Cyclopropane Products



Methyl 2-phenyl-1-(phenylcarbamoyl)cyclopropane-1-carboxylate (13): To a dry round bottom flask containing Rh_2esp_2 (2.7 mg, 3.5 μmol), dichloromethane (4 mL), and styrene (0.160 mL, 1.41 mmol) was added a solution of methyl 2-diazo-3-oxo-3-(phenylamino)propanoate **1a** (155 mg, 0.707 mmol) in dichloromethane (3 mL) via syringe pump over 15 minutes. The reaction was monitored by TLC and stopped when the TLC showed complete consumption of the diazo compound. Two diastereomers were isolated via flash silica gel chromatography (25% EtOAc/Hexane, R_f = 0.71 and 0.36); **13-d1** (white solid; 131 mg, 63% yield, [m.p. = 181-182 °C]) and **13-d2** (yellow oil; 32 mg, 15% yield). $^1\text{H NMR}$ (**13-d1**, 300 MHz, CDCl_3) δ = 9.81 (s, 1H), 7.34 – 7.16 (m, 9H), 7.09 – 6.97 (m, 1H), 3.83 (s, 3H), 3.17 (t, J = 9.0, 1H), 2.60 (dd, J = 8.4, 4.8 Hz, 1H), 2.14 (dd, J = 9.4, 4.8 Hz, 1H). $^{13}\text{C NMR}$ (**13-d1**, 75 MHz, CDCl_3) δ = 172.91, 162.72, 137.83, 134.28, 129.12, 128.71, 128.14, 127.52, 124.05, 52.85, 37.91, 36.37, 18.72. $^1\text{H NMR}$ (**13-d2**, 300 MHz, CDCl_3) δ = 10.63 (s, 1H), 7.63 (d, J = 7.5 Hz, 2H), 7.39 – 7.24 (m, 7H), 7.12 (t, J = 7.4 Hz, 1H), 3.30 (t, J = 8.8 Hz, 1H), 3.20 (s, 3H), 2.41 – 2.32 (m, 2H). $^{13}\text{C NMR}$ (**13-d2**, 75 MHz, CDCl_3) δ = 171.75, 166.17, 138.07, 135.14, 129.21, 128.96, 128.11, 127.45, 124.18, 120.03,

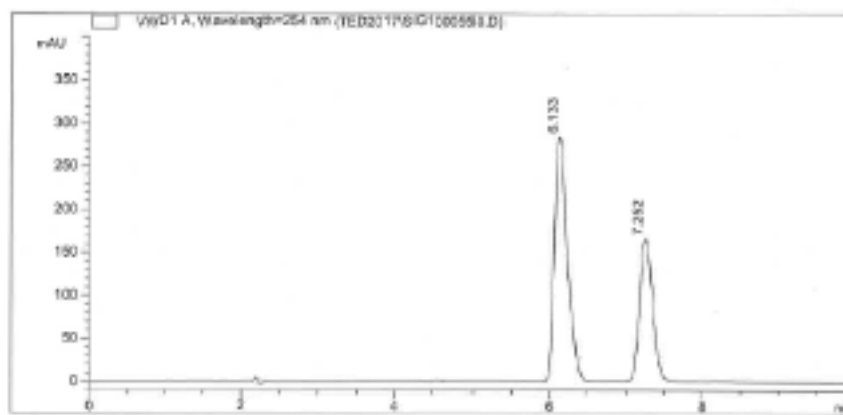
51.63, 38.77, 35.59, 19.39. IR: 3231 (m), 3055 (w), 2949 (m), 1720 (s), 1653 (s) cm^{-1} . HRMS-EI (m/z): $[\text{M}]^+$ Calcd. for $\text{C}_{18}\text{H}_{17}\text{O}_3\text{N}$ 295.1208; Found 295.1206.

Asymmetric Cyclopropanation: To a dry round bottom flask containing $\text{Rh}_2(\text{S-PTAD})_4$ (5.5 mg, 3.5 μmol), dichloromethane (4 mL), and styrene (0.160 mL, 1.41 mmol) was added a solution of methyl 2-diazo-3-oxo-3-(phenylamino)propanoate **1a** (155 mg, 0.707 mmol) in dichloromethane (3 mL) via syringe pump over 15 minutes. The reaction was monitored by TLC and stopped when the TLC showed complete consumption of the diazo compound. HPLC analysis was performed by Regis Technologies with a RegisPack analytical column: RegisPack (95% hexanes/5% EtOH, 1.5 mL/min) enantiomer 1 = 6.1 min, enantiomer 2 = 7.2 min. Racemate were made by the standard reaction conditions with Rh_2esp_2 .



C:\CHEM32\1\DATA\TED2017\SIG1000559.D

Column Name : RegisPacK
 Catalog # : 783104
 Column Size : 250 mm x 4.6 mm
 Particle Size : 5 micron
 Sample Name : (Vial B7)
 Mobile Phase : Hexane/Ethanol (95/5)
 Flow Rate : 1.5 mL/min
 Injection Vol : 2.0 uL
 Pressure : 53.1 bar



Peak #	RT (min)	Width (min)	Area	Area %
1	6.13	0.180	3402.87	62.68
2	7.25	0.192	2026.06	37.32

3. Listed and Calculated Electronic and Steric Parameters and Correlations

A. Tabulated Values and General Correlations

Table S1. Listed and Calculated Values for Steric and Electronic Parameters

Label	PA	r	r'	A-value	σ_p	$\Delta H^\ddagger_{C-H}$	$\Delta G^\ddagger_{C-H}$
a	237.8	3.08	3.16	3	-0.268	3.1	18.3
b	236.8	3.13	3.16		-0.17	2.4	15.5
c	234.9	3.11	3.11		0	1.9	15.6
d	234.6	3.1	3.14		0.062	1.4	13.5
e	232.6	3.09	3.13		0.227	0.7	13.5
f	234	2.62	2.58	0		-6.4	7.2
g	239.1	2.89	2.88	1.7		-2.7	10.7
h	238	2.9	2.91	1.75		-2.6	12.5
i	237.9	2.98	2.89	2		-2.1	13.9
j	238.1	2.96	2.97	2.15		2.1	16.4
k	238.1	2.95	2.97	2.15		1.8	16.9
l	237.9	3.25	3.3	4.5		2.6	18.5
m	233.6	2.96	3			-2.7	11.1
n	241.6	2.67	2.64			-6.1	9
o	242.9	2.79	2.85			-2.4	13.7
p	242.6	2.79	2.86			-1.9	12.7
q	234.3	2.79	2.83			-2.9	9.9
r	248.5	3.05	3.08			6.5	20.3
s	250.6	3.09	3.14			5.9	18.6
t	246.8	2.96	3			1.9	17
u	242.8	2.97	3.04			2	16.2
v	248.6	2.78	2.79			-2.8	12.3
w	250.3	2.77	2.77			-2.9	12.6
xa	242.1	2.75	2.74			-4.1	8.5
xb	244	2.75	2.75				
xc	241.1	2.75	2.74				
xd	238.3	2.75	2.74			-4.9	9.7
xe	239.2	2.75	2.75				
xf	238.1	2.75	2.75				
xg	238	2.72	2.72				

B. Calculated Proton Affinities

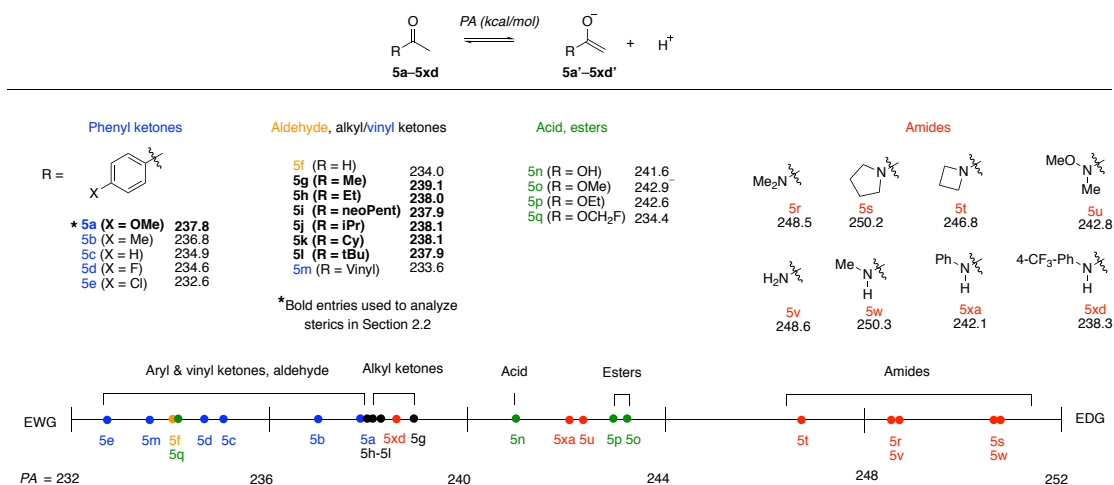


Figure S1. Calculated proton affinities

C. Calculated r Values

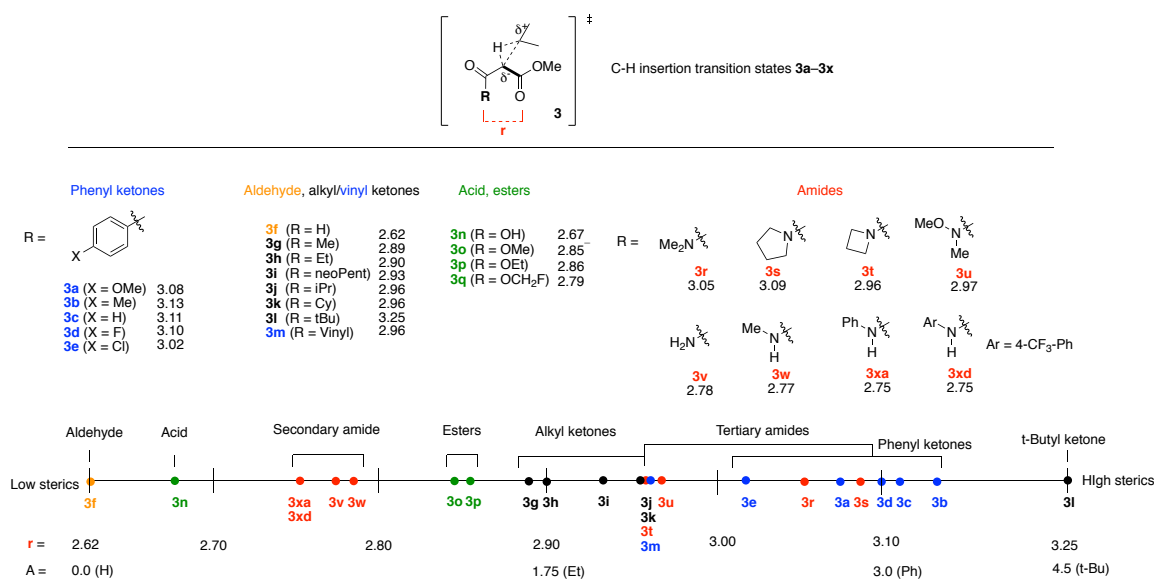


Figure S2. Calculated r values

D. Correlations

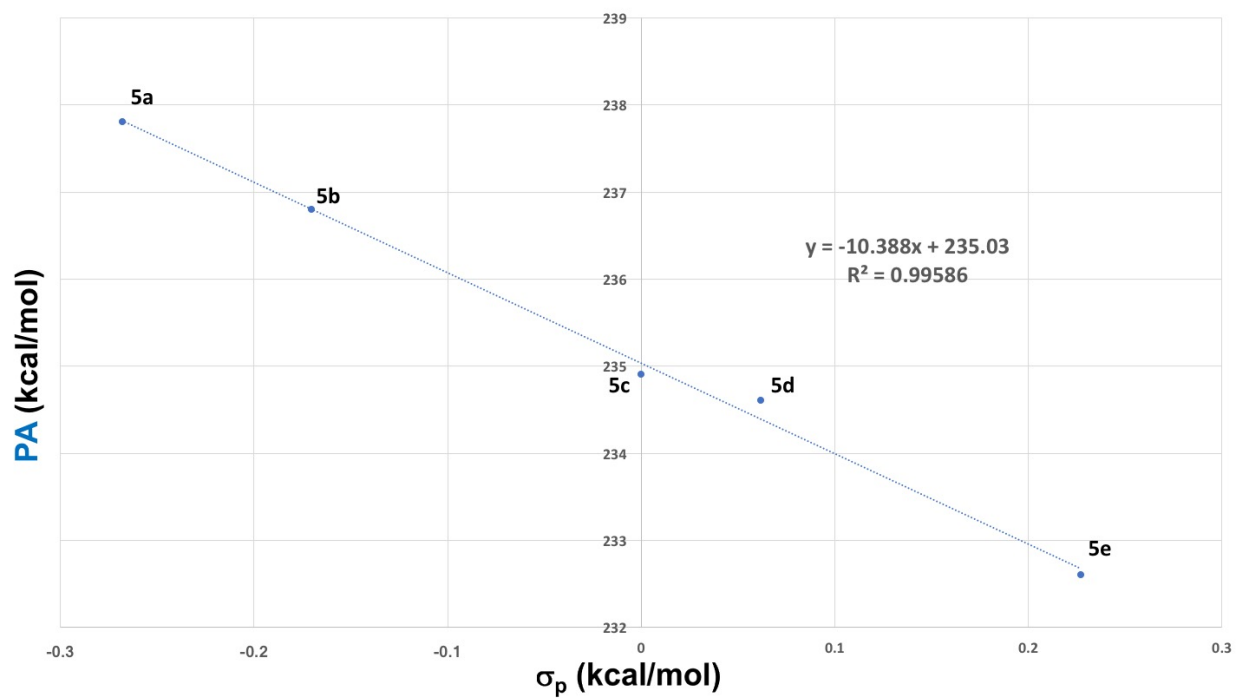
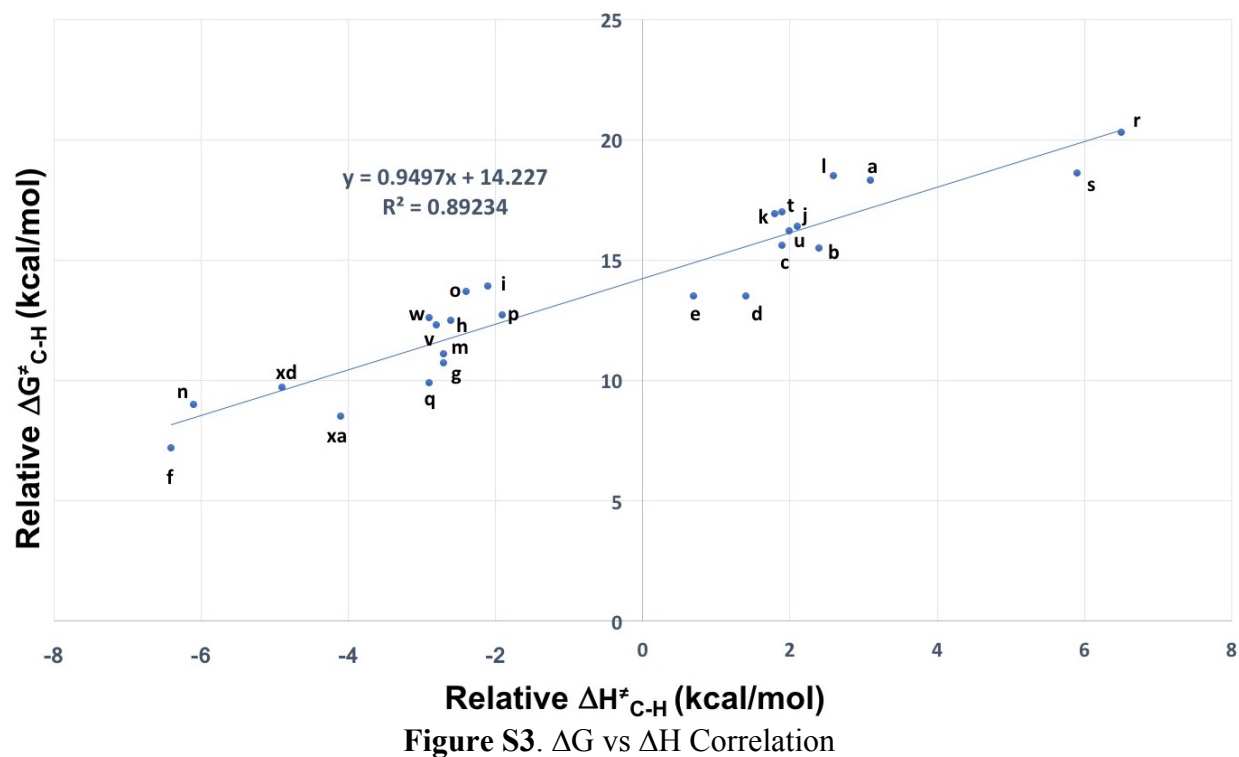


Figure S4. PA vs Hammett Coefficients Correlation

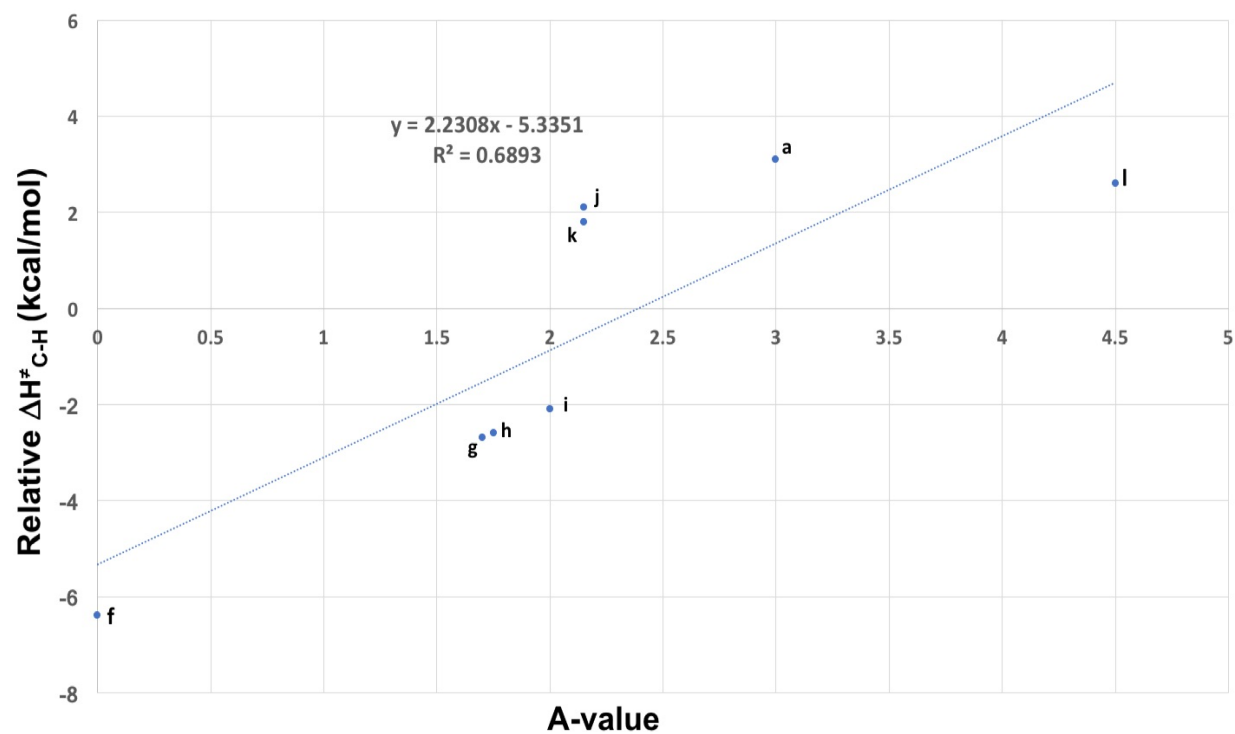


Figure S5. ΔH vs A-value Correlation

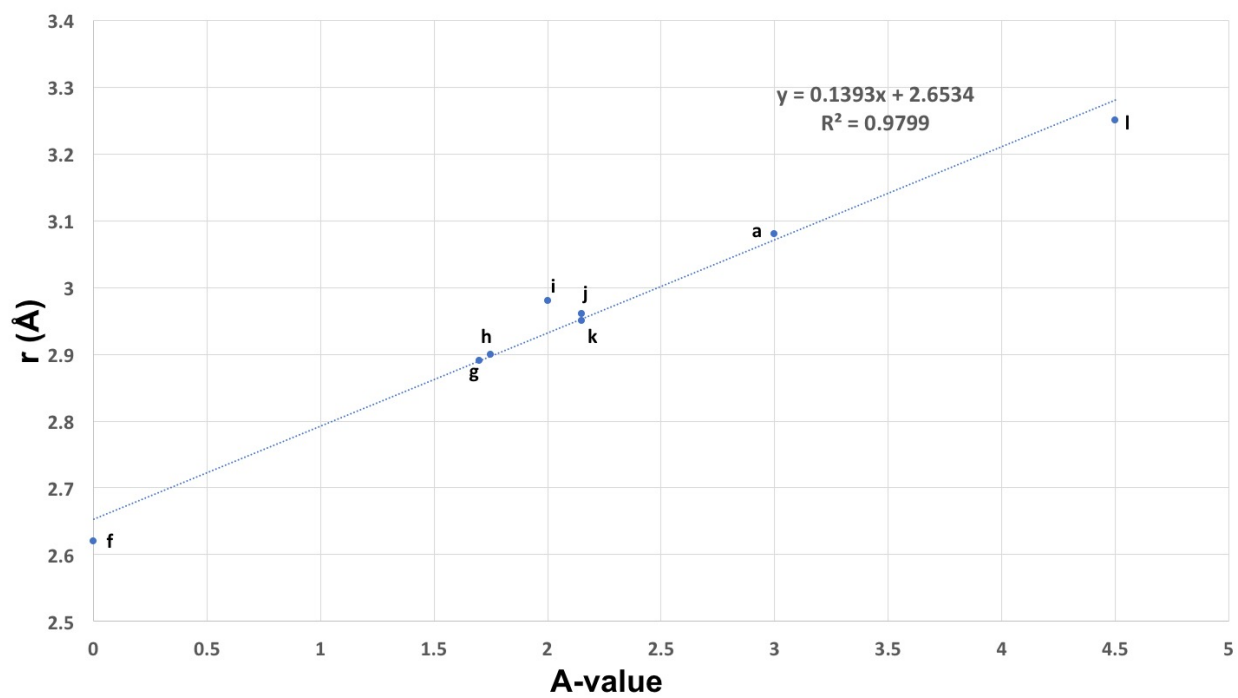


Figure S6. r vs A-value Correlation

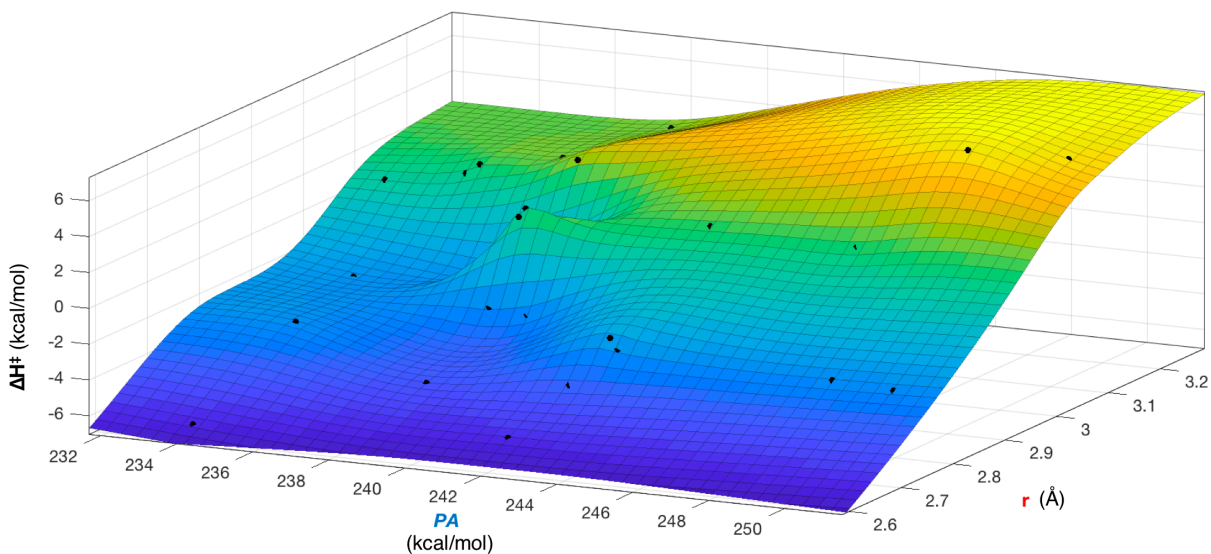


Figure S7. 3D-Chemical Space map (ΔH , PA, r)

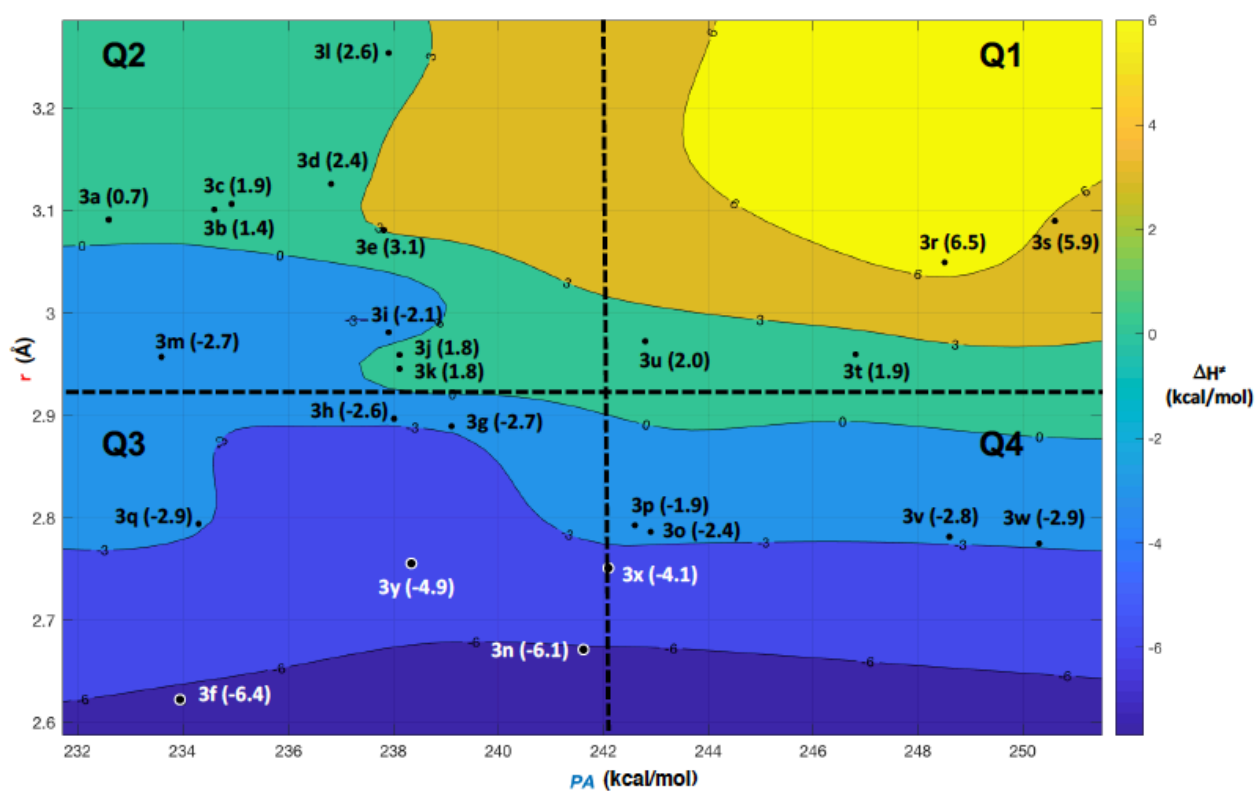


Figure S8. Contour plot of chemical space map (ΔH , PA, r)

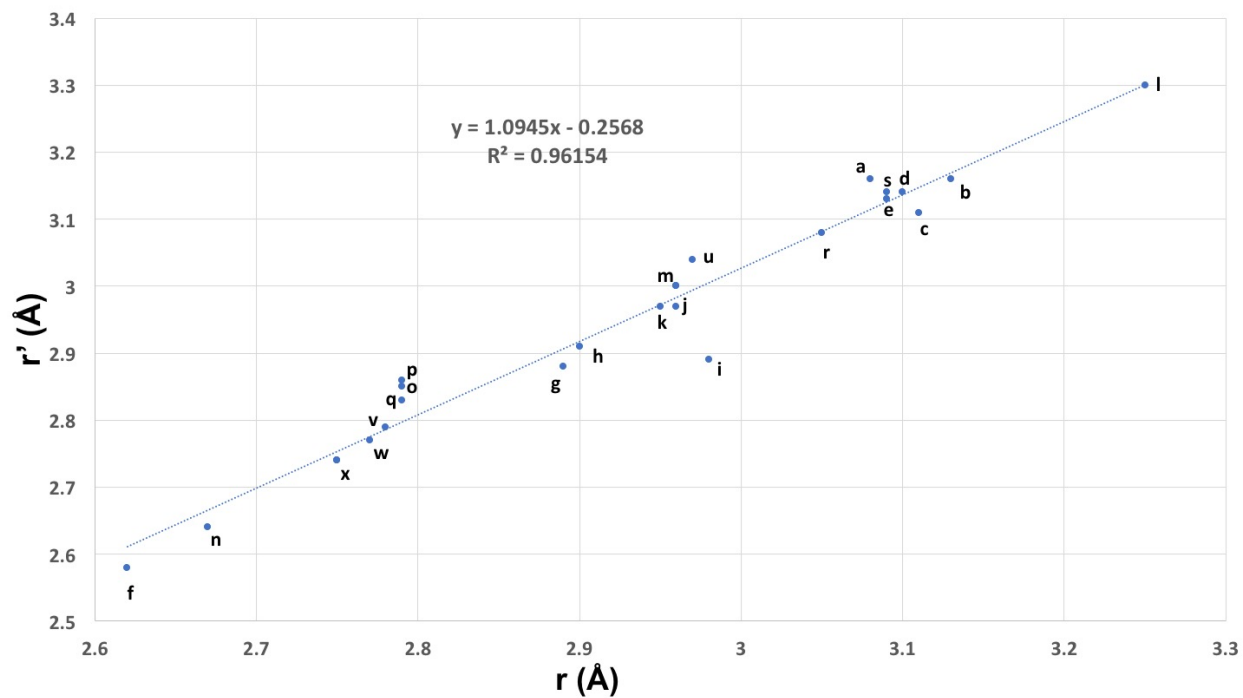


Figure S9. r - vs. r' -Value Correlation

r' vs. PA

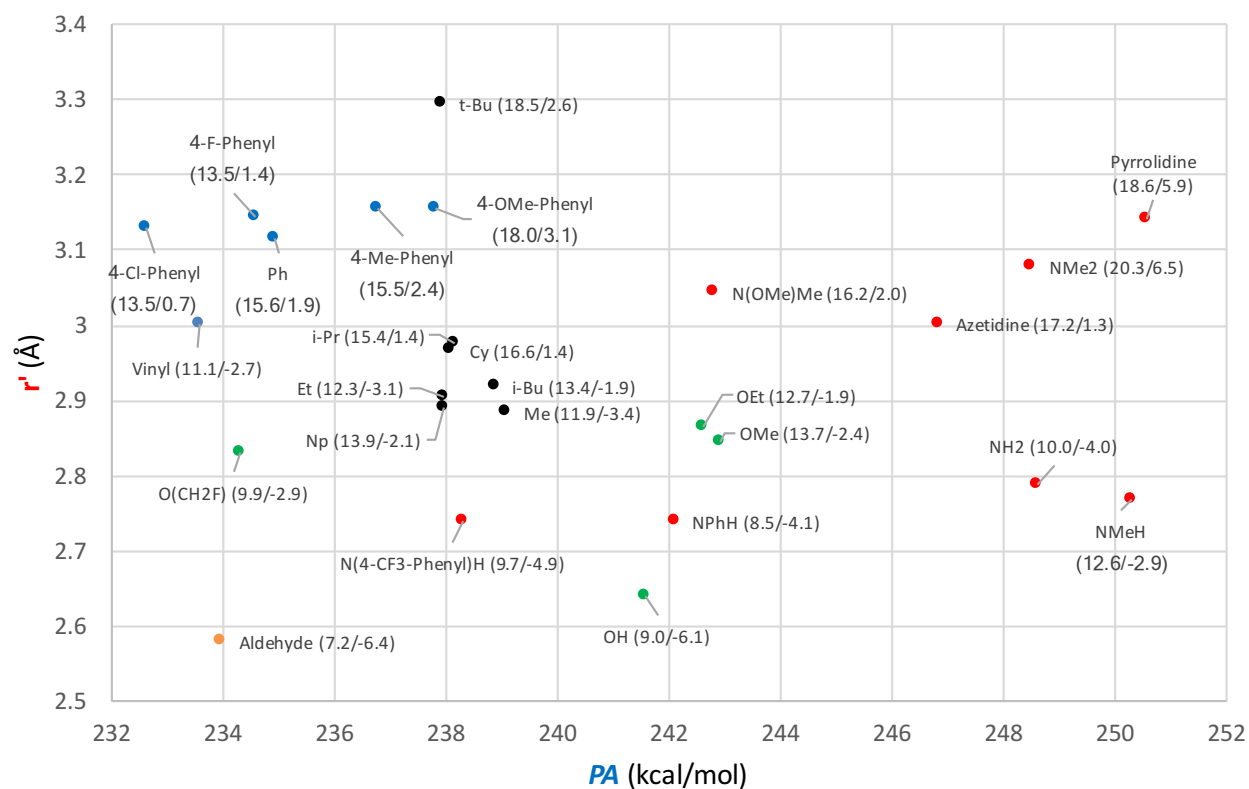


Figure S10. r' vs PA Correlation

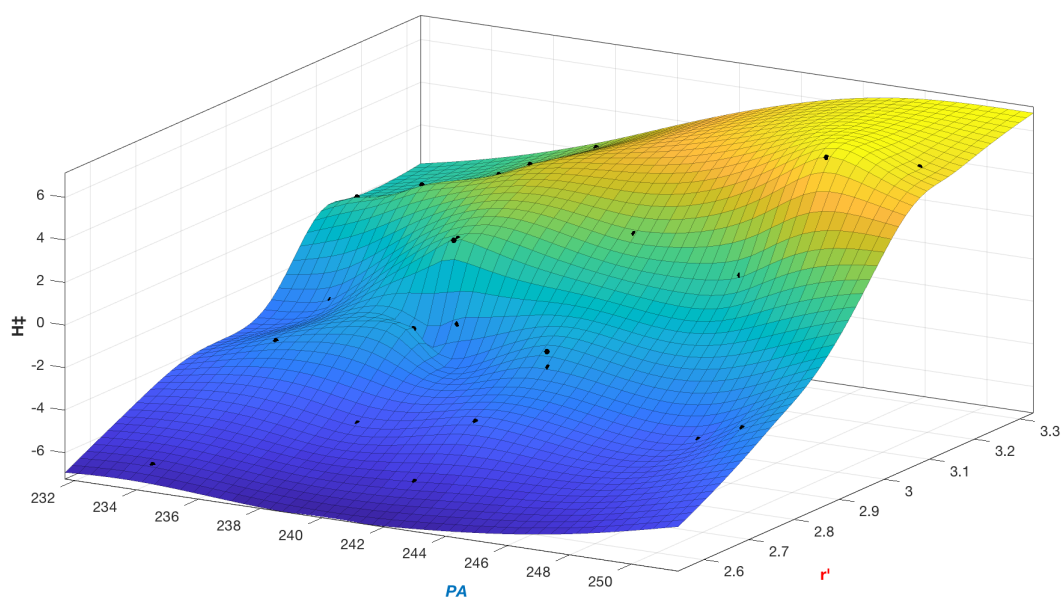


Figure S11. 3D-Chemical Space map (ΔH , PA , r')

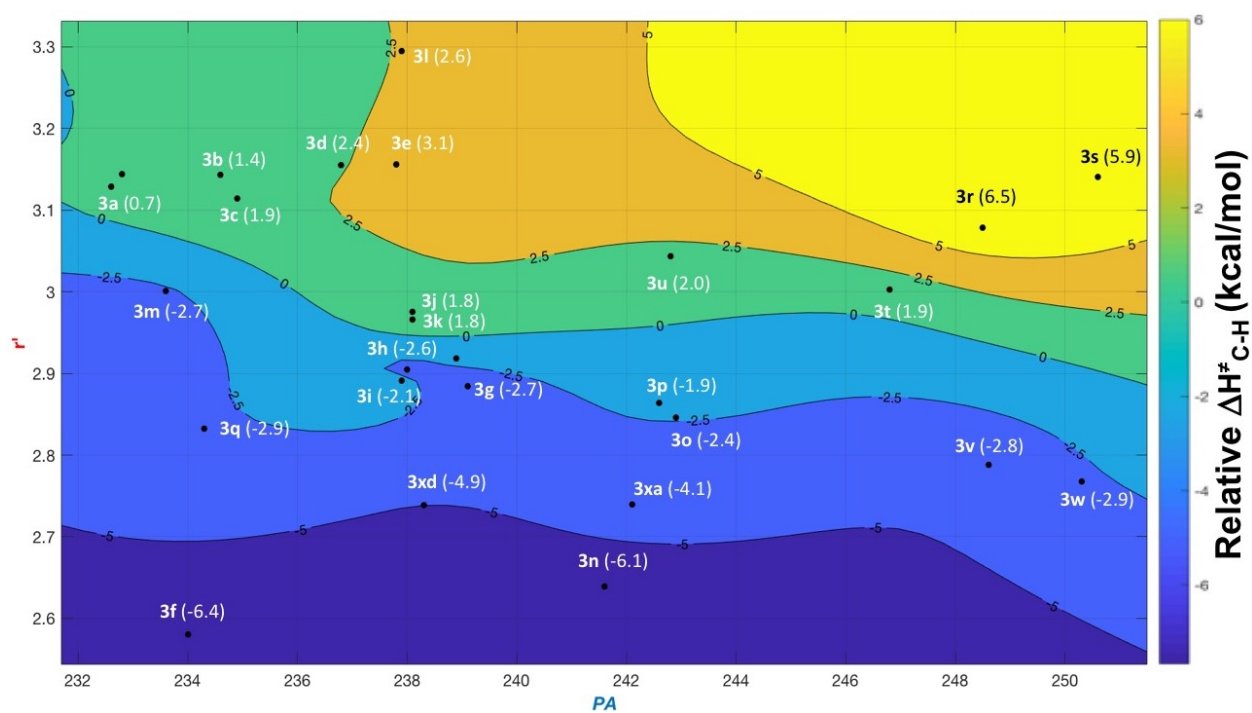


Figure S12. Contour plot of chemical space map (ΔH , PA , r')

4. Computational Detail

A. Computational Method

All calculations were performed using the Gaussian-09 package and the M06L level of density functional theory in conjunction with the 6-31G(d,p) basis sets for all atoms except Rh, for which we used Hay-Wadt pseudopotential and related LanL2DZ basis sets LanL2dz.^{9,10} Gaussian's default solvation model, the Polarizable Continuum Model implemented via integral equation formalism (IEF-PCM), was employed to simulate a dichloromethane solvent.^{11,12} Transition state calculations were verified to have a single imaginary vibrational frequency. Forward and reverse intrinsic reaction coordinate (IRC) calculations were performed for transitions state **6g** to confirm continuity between the metal carbene **2g**, C-H insertion transition state **6g**, and the product **4g**.

B. Structure Energies (a.u.) and Imaginary Frequencies (cm⁻¹)

Label	E	ZPE+E	H	G	Im. Freq.
Rh2(esp)2	-2066.698649	-2066.023256	-2065.981125	-2066.092778	none
2a	-2792.68590	-2791.81904	-2791.76149	-2791.90563	none
2b	-2717.48565	-2716.62388	-2716.56699	-2716.70991	none
2c	-2678.16901	-2677.33567	-2677.28039	-2677.41956	none
2d	-2777.39524	-2776.56862	-2776.51284	-2776.65277	none
2e	-3137.745755	-3136.921692	-3136.865238	-3137.008133	none
2f	-2447.11354	-2446.36125	-2446.31061	-2446.43953	none
2g	-2486.44148	-2485.66128	-2485.60975	-2485.74054	none
2h	-2525.75339	-2524.94518	-2524.89128	-2525.02786	none
2i	-2643.68500	-2642.79096	-2642.73357	-2642.87671	none
2j	-2565.06668	-2564.22996	-2564.17499	-2564.31292	none
2k	-2681.79534	-2680.89082	-2680.83457	-2680.97477	none
2l	-2604.37421	-2603.50906	-2603.45280	-2603.59331	none
2m	-2524.51816	-2523.73113	-2523.67859	-2523.81143	none
2n	-2522.36940	-2521.61158	-2521.55993	-2521.69234	none
2o	-2561.66164	-2560.87534	-2560.82215	-2560.95750	none
2p	-2600.97736	-2600.16253	-2600.10820	-2600.24549	none
2q	-2660.88366	-2660.10372	-2660.05038	-2660.18548	none
2r	-2581.11599	-2580.28856	-2580.23417	-2580.36997	none
2s	-2658.53216	-2657.66830	-2657.61299	-2657.75213	none
2t	-2619.19049	-2618.35633	-2618.30179	-2618.43968	none
2u	-2656.25984	-2655.42937	-2655.37372	-2655.51266	none
2v	-2502.50800	-2501.73822	-2501.68611	-2501.81894	none
2w	-2541.81036	-2541.01216	-2540.95835	-2541.09561	none
2xa	-2733.53769	-2732.68439	-2732.62859	-2732.76901	none
2xd	-3070.54246	-3069.68648	-3069.62645	-3069.77785	none
(propane)	-119.127481	-119.023932	-119.018429	-119.049617	none
4g	-538.927368	-538.713801	-538.699908	-538.753165	none

5a	-499.379834	-499.208725	-499.19752	-499.244776	none
5b	-424.17919	-424.01379	-424.00317	-424.04946	none
5c	-384.86375	-384.72556	-384.71684	-384.75814	none
5d	-484.08965	-483.95984	-483.95029	-483.99369	none
5e	-844.44351	-844.31508	-844.30518	-844.34977	none
5f	-153.817908	-153.762352	-153.757505	-153.787308	none
5g	-193.14078	-193.05688	-193.05057	-193.08488	none
5h	-232.44926	-232.33585	-232.32869	-232.36527	none
5i	-350.38170	-350.18395	-350.17291	-350.21835	none
5j	-271.76101	-271.61986	-271.61118	-271.65134	none
5k	-388.48889	-388.28049	-388.27050	-388.31436	none
5l	-311.07157	-310.902154	-310.892365	-310.934773	none
5m	-231.21486	-231.12544	-231.11865	-231.15443	none
5n	-229.07246	-229.010331	-229.004876	-229.037313	none
5o	-268.36633	-268.27660	-268.27033	-268.30497	none
5p	-307.68120	-307.56272	-307.554508	-307.594164	none
5q	-367.58979	-367.50713	-367.49954	-367.53854	none
5r	-287.80799	-287.67731	-287.66872	-287.70894	none
5s	-365.22667	-365.05887	-365.04980	-365.09168	none
5t	-325.88631	-325.74888	-325.74033	-325.78121	none
5u	-362.95599	-362.82227	-362.81246	-362.85618	none
5v	-209.20730	-209.13312	-209.12711	-209.16051	none
5w	-248.50849	-248.40630	-248.39968	-248.43518	none
5xa	-440.23380	-440.07818	-440.06812	-440.11366	none
5xb	-554.74560	-554.55716	-554.54466	-554.59581	none
5xc	-899.81380	-899.66763	-899.65639	-899.70492	none
5xd	-777.24270	-777.08220	-777.06856	-777.12336	none
5xe	-899.81316	-899.66692	-899.65583	-899.70374	none
5xf	-777.23959	-777.07922	-777.06569	-777.11977	none
5xg	-936.31718	-936.20300	-936.18823	-936.24399	none
5a'	-498.84067	-498.68386	-498.67290	-498.71948	none
5b'	-423.64215	-423.49046	-423.48021	-423.52556	none
5c'	-384.32844	-384.20442	-384.19683	-384.23532	none
5d'	-483.55495	-483.43923	-483.43078	-483.47146	none
5e'	-843.91193	-843.79762	-843.78880	-843.83072	none
5f'	-153.28546	-153.24344	-153.23899	-153.26768	none
5g'	-192.60027	-192.52959	-192.52394	-192.55626	none
5h'	-231.91017	-231.81061	-231.80380	-231.83939	none
5i'	-349.84300	-349.65849	-349.64805	-349.69191	none
5j'	-271.22184	-271.09405	-271.08600	-271.12433	none

5k'	-387.94951	-387.75516	-387.74541	-387.78926	none
5l'	-310.53252	-310.37682	-310.36754	-310.40854	none
5m'	-230.68304	-230.60694	-230.60076	-230.63481	none
5n'	-228.52708	-228.47956	-228.47422	-228.50587	none
5o'	-267.81947	-267.74464	-267.73752	-267.77469	none
5p'	-307.13423	-307.03001	-307.02220	-307.06063	none
5q'	-367.05611	-366.987592	-366.980469	-367.017771	none
5r'	-287.25112	-287.13505	-287.12705	-287.16531	none
5s'	-364.66693	-364.51354	-364.50483	-364.54573	none
5t'	-325.33213	-325.20926	-325.20133	-325.24011	none
5u'	-362.40858	-362.28873	-362.27983	-362.32033	none
5v'	-208.650906	-208.590769	-208.585275	-208.617168	none
5w'	-247.950147	-247.861947	-247.855118	-247.890616	none
5xa'	-439.687318	-439.546448	-439.536627	-439.580687	none
5xb'	-554.196073	-554.022485	-554.01011	-554.060294	none
5xc'	-899.270541	-899.139477	-899.128295	-899.176375	none
5xd'	-776.702085	-776.556661	-776.543153	-776.597469	none
5xe'	-899.271266	-899.139966	-899.129007	-899.175912	none
5xf'	-776.699509	-776.554055	-776.540583	-776.594423	none
5xg'	-935.777504	-935.677682	-935.663264	-935.717642	none
proton	-0.148025	-0.148025	-0.145664	-0.158024	none
3a	-2911.80769	-2910.83702	-2910.77500	-2910.92614	-208.9
3b	-2836.60814	-2835.64353	-2835.64353	-2835.64353	-242.02
3c	-2797.29291	-2796.35590	-2796.29584	-2796.44425	-193.34
3d	-2896.51880	-2895.59025	-2895.52912	-2895.68093	-204.97
3e	-3256.87105	-3255.94383	-3255.88251	-3256.03338	-282.58
3f	-2566.25031	-2565.394817	-2565.339239	-2565.47769	-315.39
3g	-2605.57351	-2604.689377	-2604.632495	-2604.773134	-374.74
3g	-2644.88463	-2643.97220	-2643.91382	-2644.057537	-339.87
3i	-2762.81479	-2761.81693	-2761.75533	-2761.90418	-228.49
3j	-2684.19028	-2683.24961	-2683.19002	-2683.33646	-358.8
3k	-2800.92032	-2799.91059	-2799.85012	-2799.99740	-279.63
3l	-2723.49758	-2722.52741	-2722.46702	-2722.61351	-183.48
3m	-2643.64797	-2642.75883	-2642.70132	-2642.84332	-310.18
3n	-2641.50575	-2640.64426	-2640.58800	-2640.72756	-154.44
3o	-2680.79193	-2679.90178	-2679.84439	-2679.98528	-280.99
3p	-2720.10698	-2719.18863	-2719.12967	-2719.27480	-266.5
3q	-2780.01403	-2779.13207	-2779.07346	-2779.21936	-140.46
3r	-2700.23189	-2699.30148	-2699.24230	-2699.38720	-188.36
3s	-2777.64864	-2776.68260	-2776.62202	-2776.77212	-187.45

3t	-2738.31397	-2737.37621	-2737.31724	-2737.46212	-295.63
3u	-2775.38169	-2774.44886	-2774.38890	-2774.53649	-182.41
3v	-2621.63914	-2620.76572	-2620.70903	-2620.84902	-287.38
3w	-2660.941146	-2660.039687	-2659.981345	-2660.125116	-331.11
3xa	-2852.66916	-2851.71514	-2851.65381	-2851.80516	-246.07
3xd	-3189.67653	-3188.71750	-3188.65276	-3188.81197	-207.94
8a	-726.72934	-726.528394	-726.513268	-726.570389	none
8b	-651.53008	-651.33473	-651.32102	-651.37483	none
8c	-612.21631	-612.04805	-612.03534	-612.08698	none
8d	-711.44279	-711.28281	-711.26936	-711.32264	none
8e	-1071.79884	-1071.64007	-1071.62626	-1071.68075	none
8f	-381.183246	-381.09671	-381.088266	-381.129118	none
8g	-420.49767	-420.38236	-420.37282	-420.41570	none
8h	-459.80768	-459.66474	-459.65430	-459.70018	none
8i	-577.73857	-577.51072	-577.49583	-577.55143	none
8j	-499.11822	-498.94592	-498.93372	-498.98285	none
8k	-615.84649	-615.60749	-615.59368	-615.64708	none
8l	-538.42394	-538.224146	-538.210723	-538.262082	none
8m	-458.57558	-458.45516	-458.44489	-458.48979	none
8n	-456.43605	-456.342676	-456.33407	-456.374994	none
8o	-495.71599	-495.59578	-495.58511	-495.63149	none
8p	-535.03037	-534.88138	-534.869637	-534.918308	none
8q	-594.94670	-594.83345	-594.82230	-594.87047	none
8r	-515.146893	-514.986081	-514.974021	-515.022921	none
8s	-592.56321	-592.36552	-592.35271	-592.40421	none
8t	-553.23020	-553.06214	-553.05030	-553.09922	none
8u	-590.30045	-590.13603	-590.12309	-590.17398	none
8v	-436.55934	-436.45420	-436.44504	-436.48711	none
8w	-475.85905	-475.72683	-475.71657	-475.76149	none
8xa	-667.59370	-667.40805	-667.39431	-667.44858	none
8xb	-782.10363	-781.88586	-781.86943	-781.93011	none
8xc	-1127.17614	-1126.99995	-1126.98508	-1127.04196	none
8xd	-1004.60673	-1004.41627	-1004.39909	-1004.46164	none
8xe	-1127.17554	-1126.99939	-1126.98459	-1127.04111	none
8xf	-1004.60319	-1004.41284	-1004.39557	-1004.45875	none
8xg	-1163.67484	-1163.53080	-1163.51222	-1163.57772	none

C. Structure Cartesian Coordinates

Rh₂(esp)₂

Rh -0.04492600 -0.00019500 -1.19008200
O -1.49970400 1.46267100 -1.09994600
O 1.39633700 1.49256100 -1.16159800
O 1.39766900 -1.49132000 -1.16171400
O -1.49809300 -1.46452100 -1.09993700
Rh 0.04471400 -0.00004800 1.19052700
C -1.85502800 -1.89428000 0.04308800
O -1.39778500 -1.49146500 1.16219000
C 1.85501800 -1.89404800 -0.04260900
O 1.49805500 -1.46435100 1.10041200
C -1.85502300 1.89413300 0.04290800
O -1.39643500 1.49274300 1.16200200
O 1.49949700 1.46270400 1.10035200
C 1.85499700 1.89394300 -0.04256500
C -2.91277300 2.99622800 0.09605000
C -2.91292200 -2.99618500 0.09638900
C 2.91307600 -2.99581500 -0.09601200
C 2.91287900 2.99590200 -0.09574400
C -4.09227600 2.50667000 0.98008600
H -4.83421500 3.31481300 0.99620500
H -3.71831000 2.38905000 2.00320900
C -3.39549300 3.35534600 -1.30389000
H -4.15589500 4.14096600 -1.24049500
H -2.57226000 3.72594300 -1.91992200
H -3.83369600 2.49462200 -1.81501300
C -2.28431600 4.22427300 0.76248000
H -3.02948700 5.02148600 0.84824600
H -1.91532200 3.98713300 1.76362000
H -1.44945100 4.61050700 0.16924700
C -4.09235300 -2.50629100 0.98029600
H -4.83439300 -3.31433800 0.99659100
H -3.71834900 -2.38848100 2.00338300
C -2.28457500 -4.22414600 0.76313000
H -3.02980900 -5.02128700 0.84902000
H -1.44970200 -4.61056400 0.17001600
H -1.91563000 -3.98683900 1.76425500
C -3.39557600 -3.35563200 -1.30349100
H -2.57234100 -3.72660900 -1.91928700
H -4.15616800 -4.14105100 -1.23994800
H -3.83349200 -2.49497100 -1.81496300
C 3.39666300 -3.35444800 1.30375400

H 4.15727500 -4.13984900 1.24016200
H 3.83489300 -2.49347100 1.81443600
H 2.57385900 -3.72514200 1.92028400
C 2.28427900 -4.22420000 -0.76159600
H 1.91489500 -3.98759300 -1.76273100
H 3.02940000 -5.02147300 -0.84727300
H 1.44964600 -4.61012400 -0.16782300
C 4.09183700 -2.50633200 -0.98097800
H 4.83382200 -3.31442600 -0.99759800
H 3.71711100 -2.38869900 -2.00380700
C 4.09182700 2.50673600 -0.98069100
H 3.71721600 2.38935600 -2.00359600
H 4.83369500 3.31493500 -0.99703300
C 2.28403200 4.22432900 -0.76116100
H 1.44951900 4.61022500 -0.16720600
H 3.02914300 5.02160100 -0.84693000
H 1.91442200 3.98774800 -1.76221100
C 3.39638800 3.35438300 1.30409500
H 4.15674600 4.14004300 1.24065000
H 2.57348800 3.72469100 1.92074100
H 3.83488700 2.49344700 1.81460300
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C -4.22543800 0.00018400 0.98019400
C -5.77469900 1.20822400 -0.40176300
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H -3.42377800 0.00018100 1.71616100
C -6.30162600 0.00017500 -0.85163200
H -6.18686500 2.15001600 -0.75903400
C -5.77471500 -1.20786400 -0.40174200
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H -6.18691900 -2.14965400 -0.75896300
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C 4.22508800 0.00019900 -0.98121500
C 5.77513900 1.20818100 0.39991600
C 4.72180000 -1.22253100 -0.52046600
H 3.42303600 0.00018000 -1.71674300
C 6.30234000 0.00013200 0.84944400
H 6.18744000 2.14997200 0.75704200
C 5.77512800 -1.20789500 0.39985700
H 7.13072600 0.00011800 1.55302300
H 6.18746000 -2.14970400 0.75689400

2a

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O 1.53238200 -0.70514400 -2.31842300
O -1.06710200 0.58603500 -2.36867100

O 0.14480300 2.95809200 -0.99263100
O 2.69003000 1.56597000 -0.85549000
C 2.91767600 1.24303700 0.34839400
O 2.10366900 0.64888400 1.13423100
C -0.34403700 3.01919800 0.17649600
O -0.44006800 2.04459600 0.99203000
C 1.38724400 -1.69321200 -1.54062500
O 0.87830000 -1.64940300 -0.37049900
O -1.66739000 -0.22411000 -0.33842900
C -1.89137200 0.05668300 -1.56209900
C 1.84467300 -3.07315200 -2.01387300
C 4.28085100 1.57399900 0.95542300
C -0.84791700 4.37930400 0.65725400
C -3.27794400 -0.29468100 -2.10403600
C 2.91173100 -3.60893700 -1.02079900
H 3.24288100 -4.58171000 -1.40510000
H 2.41578300 -3.79150000 -0.06000200
C 2.41023800 -2.99780500 -3.42680700
H 2.72010700 -3.99740900 -3.74912800
H 1.66379700 -2.62770600 -4.13399900
H 3.27940700 -2.33773600 -3.48005000
C 0.63566000 -4.01309500 -1.97904500
H 0.93053600 -5.01041800 -2.31998100
H 0.23632200 -4.10151800 -0.96531300
H -0.16471800 -3.65746700 -2.63602400
C 4.91853400 0.24987400 1.45554500
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H 4.29460600 -0.13224900 2.27217900
C 4.05635500 2.49039600 2.16258500
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H 3.39120200 2.02437500 2.89505000
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H 4.73184000 3.19947500 -0.40977300
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C -1.48749300 4.27155500 2.03665900
H -1.86848900 5.25217300 2.34085700
H -2.31834600 3.56177700 2.04391900
H -0.76263100 3.94066200 2.78452200
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H 0.82797100 5.42332500 -0.27189700
H 0.03097600 6.31964100 1.03521600
H 1.10700700 4.97030400 1.42079900
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H -1.32703500 5.08261000 -1.32464500
C -3.89330900 0.98229300 -2.73579700
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C -3.09159400 -1.35300400 -3.19607100
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C -4.17891500 -0.84379500 -1.00263200
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H -3.76313200 -1.75699900 -0.56724700
H -4.31523800 -0.12455200 -0.19086700
C 4.08431400 -2.69329700 -0.81091400
C 4.02313800 -1.72404400 0.19455700
C 5.23038000 -2.75472100 -1.61069300
C 5.06035800 -0.81042200 0.40144100
H 3.14582300 -1.68508300 0.83791000
C 6.28113600 -1.86325300 -1.40601100
H 5.30407200 -3.51417000 -2.38694100
C 6.19612600 -0.89349400 -0.41038800
H 7.17295400 -1.92779400 -2.02361500
H 7.02046400 -0.20073800 -0.25143000
C -4.04580600 2.12694800 -1.77426900
C -2.98227500 3.00858800 -1.55844700
C -5.22430600 2.31590100 -1.04531100
C -3.05531400 4.04027900 -0.61746100
H -2.07050900 2.88707800 -2.13960700
C -5.32289000 3.34914800 -0.11753000
H -6.06872900 1.64977200 -1.21299100
C -4.24332400 4.20104200 0.10298000
H -6.24685500 3.49272600 0.43652000
H -4.32355200 5.00555700 0.83172400
Rh 0.20479500 0.15573600 0.44867900
C -0.22977400 -0.69482800 2.15846500
C -1.61242700 -0.95720500 2.57593900
O -2.03124400 -0.08069900 3.34730500
C -2.38489900 -2.07657300 2.06696400
C -3.70833900 -2.25181800 2.48862400
C -1.82806100 -2.98402500 1.14788000
C -4.47321800 -3.30370900 2.01453200
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C -2.57885400 -4.03763200 0.66799000
H -0.80635200 -2.83787500 0.79844000
C -3.90688300 -4.20563000 1.09884600
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H -2.17362800 -4.74701700 -0.04679100

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O 1.58853700 -1.97569400 2.85327500
O 1.08546200 -0.08247000 4.00734100
C 2.24461100 -0.30798300 4.83149200
H 3.14832200 -0.30325300 4.21705700
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H 2.16449100 -1.26358300 5.35199900
C -5.91241600 -5.46511100 0.96357700
H -6.24611900 -6.35282900 0.42937800
H -5.99443300 -5.63512000 2.04229000
H -6.53876700 -4.61185600 0.68240400
O -4.55870700 -5.26165400 0.57391000

2b

Rh -0.53036200 -1.09701600 -1.71106900
O -1.51988800 0.62019700 -2.28001100
O 1.25659800 -0.21602800 -2.34258100
O 0.46183100 -2.80050800 -1.07914400
O -2.28177000 -1.88044800 -0.91143700
C -2.57367700 -1.65657300 0.30050500
O -1.88928800 -0.95300100 1.11937300
C 0.94482800 -2.82801300 0.09366100
O 0.86759100 -1.88633500 0.94966000
C -1.55964800 1.57912700 -1.45405100
O -1.07474900 1.56350200 -0.27334800
O 1.68508000 0.61603700 -0.27841500
C 1.96693000 0.42222900 -1.50699900
C -2.23801600 2.88216400 -1.87399700
C -3.85740200 -2.26610400 0.86670700
C 1.66291500 -4.10598100 0.52450500
C 3.27501800 1.03402000 -2.01351400
C -3.41614600 3.15339500 -0.89842000
H -3.91405600 4.06636800 -1.24827600
H -2.99184100 3.37203600 0.08845500
C -2.72444000 2.79136200 -3.31526900
H -3.21273800 3.73003100 -3.59737900
H -1.88946600 2.62158700 -4.00000100
H -3.43877600 1.97668900 -3.45352700
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H -0.35652500 3.87111500 -2.37849000
C -4.78241400 -1.11040300 1.33877700
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H -4.81685700 -2.54291500 -1.07064800
C 2.24471400 -3.96515600 1.92646600
H 2.74248900 -4.89816800 2.21150300
H 2.97589700 -3.15522300 1.98489900
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C 4.12941300 -0.08879000 -2.65866000
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H 3.83068300 2.50263800 -3.50215100
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C -6.12168600 -0.18115700 -0.60698100
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C 4.45933000 -1.21824000 -1.72397100
C 3.57748500 -2.29540900 -1.59587000
C 5.60807200 -1.20055200 -0.92606000
C 3.79406400 -3.32239400 -0.67250000
H 2.69515100 -2.33472400 -2.23145400
C 5.85421100 -2.22830700 -0.01927000
H 6.31384000 -0.37741500 -1.02205000

C 4.94931400 -3.27793900 0.11442800
H 6.75506300 -2.20979600 0.58803900
H 5.14051400 -4.07595900 0.82944100
Rh -0.09467400 -0.11913400 0.47479100
C 0.20748600 0.73273100 2.20998600
C 1.53596500 1.21569200 2.61069200
O 2.15354000 0.39605100 3.30187900
C 2.04684900 2.50811900 2.16336400
C 3.31288300 2.94269500 2.57838700
C 1.28030700 3.31715300 1.31410400
C 3.80171300 4.16305900 2.14407500
H 3.89579200 2.30633200 3.23859500
C 1.78092800 4.53701500 0.88123900
H 0.30087300 2.97473200 0.98091900
C 3.04753200 4.97892300 1.28505800
H 4.78346300 4.50003500 2.46851300
H 1.18816700 5.16388300 0.21868500
C -0.93229900 0.86674100 3.11720600
O -1.72781600 1.78035200 2.95754200
O -1.01846200 -0.08875600 4.04146700
C -2.17327500 0.00633100 4.89788600
H -3.08865100 -0.04014700 4.30421600
H -2.10954100 -0.84735200 5.56795400
H -2.15367800 0.94087500 5.46078300
C 3.59870800 6.27932600 0.79504000
H 4.10428400 6.82868400 1.59398300
H 4.34370400 6.11421500 0.00845300
H 2.81822400 6.91864000 0.37660000

2c

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O -1.52114300 0.48885700 -2.26008300
O 1.35673300 0.06552800 -2.29672700
O 0.91707900 -2.60335000 -1.02404000
O -1.91789000 -2.08190100 -0.88964700
C -2.24552200 -1.90599800 0.32102800
O -1.67720100 -1.10938800 1.14408500
C 1.38891900 -2.56802700 0.15314200
O 1.18435200 -1.64041200 1.00444700
C -1.69774600 1.43842000 -1.44166100
O -1.21606600 1.50212100 -0.26115700
O 1.65950200 0.93792700 -0.22676000
C 1.97100400 0.78881600 -1.45448100
C -2.55642300 2.62764700 -1.87100800
C -3.42835500 -2.69698100 0.87885700
C 2.26366700 -3.74257500 0.58922800

C 3.18873200 1.57027600 -1.95223800
C -3.77469800 2.72058800 -0.91149400
H -4.39460200 3.55497300 -1.26271600
H -3.39833100 2.99207800 0.08260800
C -3.01324300 2.46442300 -3.31574600
H -3.62949000 3.32234200 -3.60351500
H -2.15968500 2.41427600 -3.99660800
H -3.60409900 1.55582300 -3.45357200
C -1.72125400 3.90287700 -1.72120800
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H -1.43499500 4.06490000 -0.67860700
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C -4.51970200 -1.68832100 1.32860100
H -5.37763400 -2.27964300 1.67152300
H -4.13292400 -1.14876200 2.20064400
C -2.95137300 -3.47023600 2.11188200
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H -2.18352400 -4.20404400 1.84757000
H -2.53530100 -2.79317100 2.86315800
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H -4.81499900 -4.22155600 0.25819300
H -4.33952900 -3.12833800 -1.05426000
C 2.81094700 -3.53180500 1.99574200
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H 3.42777300 -2.63231200 2.06164200
H 2.00222300 -3.43561100 2.72420200
C 1.39768500 -5.00641100 0.54816100
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H 2.00175500 -5.87551400 0.82640900
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C 3.41675100 -3.89865200 -0.43856700
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C 2.70030000 2.54241700 -3.03115000
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H 4.17331400 1.69144600 -0.00814200
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H -7.17789700 -0.21874300 -2.24174500
H -6.55260400 -1.88656800 -0.51829200
C 4.65948700 -0.50363200 -1.64215700
C 3.92585100 -1.68602700 -1.51055700
C 5.79923300 -0.33634800 -0.84839200
C 4.28084200 -2.67956100 -0.59325200
H 3.05009400 -1.83570300 -2.13859400
C 6.18241500 -1.32520100 0.05383400
H 6.39075900 0.57202100 -0.94635200
C 5.42553900 -2.48643900 0.18705800
H 7.07606400 -1.19002500 0.65734100
H 5.72612800 -3.25560200 0.89611300
Rh -0.01368300 -0.02702300 0.51440100
C 0.11425000 0.88720700 2.24111100
C 1.35333200 1.52662100 2.70167600
O 2.00903500 0.84346000 3.49470200
C 1.75768500 2.84718000 2.20599800
C 2.96115400 3.40055100 2.65760000
C 0.95273600 3.55377100 1.30244500
C 3.35979100 4.65081900 2.20580300
H 3.56784800 2.83190400 3.35672200
C 1.35554100 4.80610100 0.85261100
H 0.02730200 3.10586700 0.94050200
C 2.55725900 5.35304300 1.30447900
H 4.29459500 5.08182000 2.55116800
H 0.73903100 5.35556200 0.14646300
C -1.00831200 0.73761500 3.17530700
O -0.96865600 -0.01200200 4.13347300
O -2.06297100 1.47659700 2.80780600
C -3.22724800 1.32518900 3.64007100
H -3.05095000 1.76584600 4.62301500
H -4.02718800 1.85170900 3.12257600
H -3.47348700 0.26730300 3.75787600
H 2.87186800 6.33054500 0.94975900

2d

Rh -0.50609800 -1.07924500 -1.70514200
O -1.50693400 0.63127900 -2.27282300
O 1.27675400 -0.18322900 -2.32414600

O 0.49306400 -2.77946700 -1.08117000
O -2.25136400 -1.88281300 -0.91573400
C -2.54748200 -1.67280800 0.29748700
O -1.87321600 -0.96604300 1.12227100
C 0.97703500 -2.81347200 0.09095700
O 0.89674200 -1.87669900 0.95258100
C -1.55751800 1.58527600 -1.44220600
O -1.07854400 1.56521400 -0.25885700
O 1.69459700 0.64187800 -0.25488500
C 1.98218200 0.45316000 -1.48343900
C -2.24389200 2.88568100 -1.85709000
C -3.82519100 -2.30281800 0.85497300
C 1.69840600 -4.09335300 0.51016100
C 3.28940200 1.07125700 -1.98369300
C -3.44620500 3.12657000 -0.90235300
H -3.95479100 4.03230900 -1.25552500
H -3.04557000 3.34653800 0.09409600
C -2.70070100 2.80792700 -3.30869700
H -3.19632000 3.74355500 -3.58784400
H -1.85096600 2.65798900 -3.97983400
H -3.40128000 1.98564000 -3.47027400
C -1.25467200 4.04037800 -1.67762300
H -1.72571300 4.98059600 -1.98052100
H -0.95060600 4.13313700 -0.63171800
H -0.35756600 3.90226300 -2.29007000
C -4.77694900 -1.16063100 1.30618700
H -5.70798200 -1.63603300 1.63917900
H -4.32960500 -0.67813800 2.18365300
C -3.45717500 -3.13936300 2.08343000
H -4.36359700 -3.55926900 2.53089200
H -2.80149500 -3.97264800 1.81266200
H -2.94568100 -2.53341100 2.83635900
C -4.49412800 -3.18096300 -0.19587400
H -3.83884400 -4.00202000 -0.49851200
H -5.41233900 -3.61188300 0.21692000
H -4.75271700 -2.61489700 -1.09372800
C 2.28358400 -3.96472100 1.91160300
H 2.77540700 -4.90294400 2.18962900
H 3.02188100 -3.16152600 1.97239900
H 1.50288600 -3.75615300 2.64704400
C 0.67514300 -5.23417600 0.47490000
H 0.22834600 -5.33678400 -0.51716900
H 1.16720800 -6.17758200 0.73200000
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C 2.81008300 -4.39335500 -0.53101500
H 3.29774600 -5.32320600 -0.21275900

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C 4.14370100 -0.04288100 -2.64376100
H 3.59679800 -0.41652600 -3.51628700
H 5.05929000 0.43526900 -3.01402800
C 2.92698000 2.11638500 -3.04386200
H 2.32733900 2.92217700 -2.60613200
H 3.83927300 2.56467400 -3.45006700
H 2.36265400 1.67207600 -3.86761000
C 4.05114300 1.74165600 -0.84553300
H 4.98506400 2.16564800 -1.22986700
H 3.46184700 2.55064000 -0.40566600
H 4.29643800 1.03899400 -0.04517300
C -4.40568700 1.97582400 -0.81242700
C -4.22993200 1.00444900 0.17712300
C -5.45699900 1.81999100 -1.72182500
C -5.05402800 -0.12156700 0.25829500
H -3.43282300 1.12953600 0.90946200
C -6.29802000 0.71295600 -1.64485700
H -5.62392800 2.57791300 -2.48466900
C -6.09523500 -0.25697900 -0.66604300
H -7.11922000 0.60733300 -2.34879600
H -6.75636900 -1.11957300 -0.60779200
C 4.48001800 -1.18066100 -1.72143600
C 3.60199600 -2.26179500 -1.60034200
C 5.63144500 -1.16686900 -0.92727500
C 3.82466400 -3.29632000 -0.68680600
H 2.71824100 -2.29865000 -2.23396600
C 5.88394700 -2.20219600 -0.03101200
H 6.33435700 -0.34070700 -1.01793200
C 4.98253300 -3.25561000 0.09645700
H 6.78699400 -2.18664000 0.57308400
H 5.17873800 -4.05964700 0.80333200
Rh -0.08231500 -0.11233300 0.48728000
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C 1.47994000 1.29122400 2.65657200
O 2.08959000 0.52584600 3.41320900
C 1.98627900 2.57411500 2.17334600
C 3.22815300 3.03836700 2.62843300
C 1.24514500 3.33581200 1.25836700
C 3.73213200 4.24632300 2.17492900
H 3.78735800 2.43380600 3.33666200
C 1.74046000 4.54510100 0.79267800
H 0.28776800 2.96488100 0.89492900
C 2.97652100 4.97694800 1.26213500
H 4.68914700 4.63107200 2.50897100
H 1.19563200 5.15337600 0.07820700

F 3.46214100 6.14414000 0.81673200
C -0.97938000 0.83487700 3.10720300
O -1.80254900 1.72160700 2.93808700
O -1.05748500 -0.13963000 4.01166900
C -2.26093100 -0.12831700 4.80295700
H -3.13199700 -0.25121100 4.15465800
H -2.17035600 -0.97095100 5.48404200
H -2.34782500 0.80833600 5.35555900

2e

Rh -0.79705100 -1.07577800 -1.71345600
O -1.49470700 0.77778800 -2.29222100
O 1.10936500 -0.50267500 -2.36483500
O -0.10203500 -2.91756800 -1.06475800
O -2.64816900 -1.55613400 -0.90580000
C -2.88473200 -1.28345900 0.30860400
O -2.08554500 -0.69777600 1.11585900
C 0.37207500 -3.01503100 0.10785900
O 0.46168300 -2.06373700 0.95172600
C -1.36414900 1.74162800 -1.48205100
O -0.86743100 1.66229100 -0.30811200
O 1.68825500 0.25243400 -0.30797300
C 1.92449500 0.00833700 -1.53775000
C -1.83251700 3.13198600 -1.91151900
C -4.24139900 -1.66580700 0.89842600
C 0.86625900 -4.39013100 0.55283000
C 3.31344600 0.38260800 -2.05785400
C -2.95955300 3.59212800 -0.94559600
H -3.31285600 4.56405000 -1.31184700
H -2.50658900 3.76200300 0.03842800
C -2.32863000 3.11077300 -3.35207900
H -2.65571300 4.11554900 -3.63904400
H -1.53750800 2.80101400 -4.03988400
H -3.17081300 2.42678500 -3.48096000
C -0.65661300 4.10327500 -1.77086700
H -0.96354500 5.10464100 -2.08809500
H -0.32047900 4.16195800 -0.73236300
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C -4.00464300 -2.58350300 2.10191300
H -4.96120800 -2.82711000 2.57499800
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C -5.10307800 -2.37339100 -0.13958600

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 C 3.95119200 -0.87932300 -2.69786800
 H 3.33741500 -1.17005900 -3.55765300
 H 4.93273200 -0.57909600 -3.08509000
 C 3.13023400 1.45283200 -3.13862500
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 H 4.10275100 1.72034900 -3.56364100
 H 2.48481700 1.09737100 -3.94606800
 C 4.19581700 0.92590200 -0.93875200
 H 5.18359900 1.17527500 -1.34148800
 H 3.76746200 1.83148300 -0.50033400
 H 4.32847600 0.19932800 -0.13293700
 C -4.10411400 2.62993400 -0.80318200
 C -4.05110800 1.65278400 0.19480900
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 C -5.06442400 0.70369600 0.35255100
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 C -6.24759400 1.73484000 -1.49141500
 H -5.28810500 3.42656300 -2.41890200
 C -6.17099200 0.75945600 -0.50063000
 H -7.11708700 1.77791600 -2.14173200
 H -6.97978300 0.04179600 -0.37751800
 C 4.09324400 -2.03878800 -1.75284600
 C 3.03566700 -2.93731000 -1.58350800
 C 5.25354600 -2.22699400 -0.99477400
 C 3.09665800 -3.98713700 -0.66205700
 H 2.13861200 -2.81558600 -2.18752700
 C 5.34003600 -3.27766800 -0.08548200
 H 6.09354700 -1.54720400 -1.12558100
 C 4.26664000 -4.14798200 0.08728100
 H 6.25012900 -3.42078300 0.49110200
 H 4.33794300 -4.96718100 0.80041100
 Rh -0.18741800 -0.16535200 0.45616500

C 0.22239300 0.63586900 2.19423200
 C 1.60043600 0.88602400 2.62726800
 O 2.03994400 0.00584800 3.37629500
 C 2.37461100 2.02946800 2.14155300
 C 3.69455000 2.19203400 2.57711400
 C 1.81302100 2.95010200 1.24750400
 C 4.45434700 3.25927800 2.12695100
 H 4.11311500 1.46583500 3.26749900
 C 2.56241400 4.02454400 0.78876600
 H 0.79271400 2.80859100 0.89251800
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 H 5.47959100 3.39549400 2.45271000
 H 2.14582900 4.74219200 0.09021200
 C -0.91101700 0.90846300 3.08088600
 O -1.61279200 1.89025200 2.89337000
 O -1.09969200 -0.01696600 4.02037200
 C -2.26788300 0.18301800 4.83966300
 H -3.16513300 0.19069900 4.21625800
 H -2.28775700 -0.65893600 5.52729700
 H -2.19563100 1.12558000 5.38443700
 Cl 4.82985700 5.49897400 0.65522400

2f

Rh 0.11045500 0.36738400 -1.67705800
 O -1.29922800 1.85943800 -1.45530100
 O 1.60353500 1.76954100 -1.30561000
 O 1.48750400 -1.18488100 -1.80151000
 O -1.40146800 -1.02419100 -1.90151600
 C -1.78325300 -1.64716100 -0.86696500
 O -1.33346400 -1.47644200 0.31688000
 C 1.88475100 -1.78944100 -0.76055500
 O 1.51604800 -1.52151400 0.43386600
 C -1.64871600 2.13585200 -0.26890900
 O -1.22260000 1.56026000 0.78802600
 O 1.62575500 1.35567800 0.92133500
 C 2.02608900 1.96808700 -0.12621200
 C -2.67213500 3.24527000 -0.03557700
 C -2.87747200 -2.70346500 -1.00058600
 C 2.89532700 -2.91814600 -0.94488800
 C 3.11358400 3.02498900 0.05852500
 C -3.87235900 2.64060300 0.74496100
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 H -3.51434300 2.34952800 1.73913200
 C -3.12712100 3.84952100 -1.35807300
 H -3.85774300 4.64153100 -1.16433700
 H -2.28697600 4.28810600 -1.90228900

H -3.59419000 3.10480700 -2.00666300
 C -2.01694500 4.32101600 0.83695200
 H -2.74425300 5.10797300 1.05868100
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 H -1.16998400 4.78592900 0.32300100
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 H -4.80881500 -3.08551900 -0.14771900
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 H -2.55164600 -3.09433800 -3.11169000
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 H 3.71740300 -2.83283600 1.07371400
 H 2.38139700 -3.97225300 0.88453700
 C 2.27043200 -3.96568800 -1.87132600
 H 1.97448500 -3.52514500 -2.82650300
 H 2.99518400 -4.76203600 -2.06637800
 H 1.38854800 -4.42305000 -1.41237600
 C 4.15250700 -2.32650900 -1.64089600
 H 4.86985900 -3.14958400 -1.74678600
 H 3.86379100 -2.01777700 -2.65174600
 C 4.33640000 2.61358400 -0.80715500
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 C 2.57361600 4.35996000 -0.46287200
 H 1.71881900 4.69932300 0.13001900
 H 3.35314500 5.12451800 -0.39055200
 H 2.26101100 4.28231400 -1.50706900
 C 3.50705600 3.15983200 1.52509900
 H 4.27830900 3.93032000 1.62587600
 H 2.65102700 3.45367000 2.13828600
 H 3.90297400 2.22512000 1.92895800
 C -4.52693100 1.46394900 0.07802600
 C -4.07026600 0.16862200 0.34177400
 C -5.57704400 1.62845300 -0.83166400
 C -4.61334900 -0.94997500 -0.29822100
 H -3.28062500 0.02276300 1.07707600
 C -6.14594100 0.52392500 -1.46019300
 H -5.95814700 2.62766300 -1.03470300
 C -5.66374500 -0.75646800 -1.20186200

H -6.97106000 0.66163300 -2.15394900
 H -6.11088700 -1.61695000 -1.69622100
 C 4.87244400 1.24120300 -0.51421700
 C 4.36202700 0.13480200 -1.19946800
 C 5.85226800 1.02597900 0.46061600
 C 4.78026200 -1.16894000 -0.91757600
 H 3.61872800 0.29369600 -1.97848300
 C 6.29595700 -0.26360100 0.74182700
 H 6.27577400 1.87639800 0.99161200
 C 5.76005800 -1.35524300 0.06354000
 H 7.06672900 -0.41842000 1.49176500
 H 6.11169000 -2.36107600 0.28554300
 Rh 0.12457500 -0.04553100 0.71999100
 C -0.32111200 -0.24652800 2.59144800
 C -0.12186000 0.85945600 3.51602500
 O -0.03793900 0.66093200 4.72629600
 C -1.16531800 -1.37522700 3.03396400
 O -2.36714500 -1.25050200 3.19703700
 O -0.48583700 -2.51608700 3.17257300
 C -1.27264500 -3.63761400 3.61458800
 H -2.10722500 -3.80886100 2.93179500
 H -0.59542900 -4.48822300 3.61789900
 H -1.66274600 -3.45351900 4.61744000
 H 0.04999200 1.85812900 3.06859900

2g

Rh 0.05280300 0.18569000 -1.75849100
 O -1.34663500 1.69364800 -1.61988700
 O 1.56233500 1.61466400 -1.52104500
 O 1.43534000 -1.35276700 -1.84386500
 O -1.46490300 -1.22922800 -1.79559400
 C -1.85025000 -1.75427000 -0.70880200
 O -1.40854800 -1.47546400 0.45782300
 C 1.83041200 -1.89120200 -0.76496900
 O 1.45924100 -1.55794000 0.40906000
 C -1.70184900 2.05153800 -0.45785500
 O -1.28027100 1.54931500 0.63857300
 O 1.59933200 1.35472400 0.72957600
 C 2.00056600 1.88212900 -0.36220500
 C -2.71969900 3.18211900 -0.31579800
 C -2.94377300 -2.82139800 -0.75317800
 C 2.83800200 -3.03366300 -0.88097600
 C 3.10554800 2.93274200 -0.25485000
 C -3.92903100 2.65236300 0.50337500
 H -4.64633200 3.47917400 0.57913800
 H -3.57665100 2.43302500 1.51856700

C -3.16222900 3.68058000 -1.68623000
 H -3.89256500 4.48720600 -1.56391400
 H -2.31472800 4.07039900 -2.25559500
 H -3.62468400 2.88690300 -2.27755200
 C -2.06533500 4.32275100 0.46928900
 H -2.77999900 5.14240800 0.59206300
 H -1.74971200 3.99178600 1.46212400
 H -1.19198300 4.71838500 -0.05896400
 C -4.12362600 -2.34102200 0.13646500
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 H -3.76727700 -2.30310600 1.17243800
 C -2.37540500 -4.11129500 -0.15292400
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 C 3.23169300 -3.56181800 0.49335600
 H 3.95190900 -4.37860100 0.37845000
 H 3.68867900 -2.78623400 1.11240000
 H 2.36160900 -3.94614200 1.03187900
 C 2.19196600 -4.15059100 -1.70614200
 H 1.87822200 -3.78796300 -2.68817100
 H 2.90986900 -4.96407500 -1.85005100
 H 1.31742900 -4.56439300 -1.19428100
 C 4.08149400 -2.50702400 -1.64965400
 H 4.79037500 -3.34213000 -1.71041300
 H 3.76925700 -2.27207600 -2.67322600
 C 4.29583900 2.47761900 -1.14232100
 H 3.95880500 2.48158500 -2.18474000
 H 5.07351000 3.24578400 -1.04942300
 C 2.55462500 4.25051800 -0.80819600
 H 1.71001800 4.60599900 -0.20854200
 H 3.33281100 5.01941200 -0.77668700
 H 2.21971000 4.13846200 -1.84257100
 C 3.54815500 3.12195300 1.19224600
 H 4.35320400 3.86323100 1.23363300
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 H 3.91425500 2.19155500 1.63317500
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 C -4.14879500 0.16140000 0.30641000
 C -5.61834800 1.52797500 -1.01658100
 C -4.68616500 -1.00292900 -0.25016100
 H -3.36954700 0.07499900 1.06132200

C -6.18145400 0.37807200 -1.56402000
 H -5.98681200 2.50877700 -1.31159900
 C -5.71512600 -0.87960300 -1.18979600
 H -6.99058000 0.46280400 -2.28457600
 H -6.15802500 -1.77602700 -1.62012000
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 C 4.31282300 -0.02144000 -1.38528000
 C 5.85943600 0.96982900 0.16248000
 C 4.73713800 -1.30552000 -1.03079100
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 C 6.31121800 -0.29997200 0.51187100
 H 6.29953700 1.85164100 0.62449100
 C 5.74968500 -1.43141000 -0.07395300
 H 7.10643600 -0.40872100 1.24436800
 H 6.10436700 -2.42239300 0.20334300
 Rh 0.07892100 -0.03916300 0.66083900
 C -0.07545600 -0.09717400 2.60734000
 C 0.62639200 0.89502400 3.43240600
 O 1.63478800 0.49124300 4.00549900
 C -1.07065900 -0.97427600 3.22573500
 O -2.22536400 -0.59082700 3.33288800
 O -0.60405100 -2.16780300 3.58397100
 C -1.58276000 -3.04935600 4.17106000
 H -2.38252600 -3.25152100 3.45615200
 H -1.04353600 -3.96180400 4.41236200
 H -2.00518900 -2.60178300 5.07222200
 C 0.12823900 2.29958600 3.44947300
 H 0.67865000 2.89151000 4.18227700
 H 0.26005400 2.72550900 2.44842000
 H -0.94652200 2.32717400 3.65957100

2h

Rh 0.00561300 0.29133500 -1.81134700
 O 1.37112800 -1.24587900 -1.96488900
 O -1.53119900 -1.11318400 -1.94162900
 O -1.33830400 1.85550300 -1.58666600
 O 1.54412400 1.64611900 -1.50383300
 C 1.92301700 1.89869500 -0.32233000
 O 1.46207400 1.36507800 0.74475700
 C -1.74821400 2.14988900 -0.42287300
 O -1.41428700 1.55120400 0.65318400
 C 1.67586000 -1.87190900 -0.90671800
 O 1.23496200 -1.61447200 0.26361000
 O -1.64683300 -1.34713500 0.30982900
 C -2.01054500 -1.62063400 -0.88295300
 C 2.65698800 -3.03962900 -1.00177900

C 3.03835100 2.92386400 -0.12259200
 C -2.72735300 3.31466100 -0.29372200
 C -3.13017000 -2.64884200 -1.04062500
 C 3.87791900 -2.72404400 -0.09532200
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 H 3.53124900 -2.71688500 0.94465900
 C 3.09348700 -3.25970800 -2.44510100
 H 3.79822400 -4.09657700 -2.48956800
 H 2.23958000 -3.49880800 -3.08376400
 H 3.58442900 -2.37583000 -2.85905900
 C 1.96194500 -4.29514900 -0.46554800
 H 2.64917500 -5.14580600 -0.50917500
 H 1.64597000 -4.16030600 0.57224600
 H 1.08128100 -4.54779300 -1.06468800
 C 4.21001000 2.22704400 0.61963600
 H 5.00764100 2.97239400 0.72805500
 H 3.86168200 1.97630000 1.62730300
 C 2.50088700 4.05317200 0.76209500
 H 3.29477600 4.78076200 0.95794000
 H 1.67770100 4.58211500 0.27176000
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 H 2.68828400 3.99141800 -1.98296000
 H 4.30448200 4.21386100 -1.29299800
 H 3.88711900 2.70170700 -2.11852600
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 C -4.30708900 -1.96806100 -1.78887500
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 H -5.10535500 -2.71584700 -1.87294300
 C -2.59992600 -3.80102000 -1.89936700
 H -1.76397200 -4.30806800 -1.40612400
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 H -2.25928000 -3.44560900 -2.87495100
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H -3.92075900 -2.38075800 0.97979700
 C 4.56611000 -1.42504700 -0.40634600
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 C 5.59228900 -1.34175100 -1.35360700
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 C 5.75248300 1.04432500 -1.00796100
 H 6.98990400 -0.06427200 -2.37393800
 H 6.21818500 2.00063100 -1.23893800
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 H -6.01131700 2.54866300 0.61699700
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 O 0.50544100 1.41822000 3.95823300
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 H -1.36565900 -4.75237200 3.48120300
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 H -2.61898400 -3.50388900 3.41087000

2i

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 O 1.47172600 -0.08219400 -2.35849700
 O 1.16505500 -2.67061500 -0.87899200
 O -1.72858900 -2.28756000 -0.87768000

C -2.08697200 -2.03382600 0.30981200
O -1.55141100 -1.17242000 1.08760900
C 1.58534500 -2.51848200 0.30843700
O 1.29558600 -1.54206500 1.07658100
C -1.64878400 1.17886600 -1.69326300
O -1.18286000 1.37051100 -0.52019200
O 1.67472100 0.98251900 -0.36778800
C 2.01010200 0.76126200 -1.57996600
C -2.56000200 2.28360800 -2.22592000
C -3.26114800 -2.80526400 0.91121700
C 2.51480900 -3.59146800 0.87388000
C 3.17178800 1.58179700 -2.14028300
C -3.74907100 2.45396200 -1.24111900
H -4.39746800 3.23392500 -1.65947600
H -3.34885900 2.83693600 -0.29457900
C -3.05548900 1.94619500 -3.62654600
H -3.68772400 2.76023600 -3.99624100
H -2.22017900 1.82012900 -4.31980000
H -3.64252300 1.02468900 -3.63852200
C -1.75935100 3.59013700 -2.25125600
H -2.40160200 4.41128300 -2.58462900
H -1.37193500 3.83596200 -1.25847600
H -0.91585000 3.52461700 -2.94582800
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C -2.74560800 -3.57756700 2.13008500
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H 3.58429600 -4.05282900 2.68418400
H 3.48354600 -2.31381100 2.35338300
H 2.06792900 -3.17607700 2.95911200
C 1.76477400 -4.92683000 0.84738500
H 1.44262900 -5.18021800 -0.16562900
H 2.41967800 -5.72431600 1.21223700
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C 3.75517000 -3.70220700 -0.05407000
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H 2.91725600 3.30790300 -0.85619300
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C -4.53418400 1.19898200 -0.98296100
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C -5.63323400 0.83944300 -1.77039500
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C -6.32336300 -0.34410400 -1.51970000
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C -5.91586400 -1.19055800 -0.49202300
H -7.18548000 -0.60624000 -2.12704000
H -6.45805000 -2.11457400 -0.29922600
C 4.76664000 -0.32470200 -1.49436000
C 4.13159700 -1.55260000 -1.28920700
C 5.82357100 0.02769700 -0.64937800
C 4.50650900 -2.41692600 -0.25635600
H 3.32235500 -1.84600900 -1.95566400
C 6.22313700 -0.82752700 0.37409400
H 6.34099200 0.97276700 -0.80373900
C 5.56682400 -2.03952700 0.57434600
H 7.05451800 -0.55071600 1.01679400
H 5.88528700 -2.70640400 1.37347000
Rh 0.05057800 -0.04000700 0.40987100
C -0.00816500 1.02077400 2.04876700
C 0.83038700 2.20716000 2.26226400
O 1.74185400 2.07549600 3.07718400
C -1.09891200 0.74940700 2.98976900
O -2.17935100 1.29792700 2.83412100
O -0.80513900 -0.14678600 3.92857900
C -1.89579300 -0.46938400 4.81395200
H -2.73368200 -0.87257200 4.24039100
H -1.50398500 -1.21776300 5.49805000
H -2.22120800 0.41869400 5.35774200
C 0.53427000 3.41718900 1.43024100
H 0.94943400 3.19382600 0.43390800
C 1.03458700 4.77899200 1.93940900
C 0.47319700 5.04843200 3.33607400
H 0.75361700 6.05063800 3.67694300

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H 0.85664600 4.32917500 4.06559300
C 0.51453000 5.83945200 0.96736700
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H 0.84811100 6.83785100 1.26982600
H 0.88135900 5.65806600 -0.05022400
H -0.55497400 3.44363000 1.27097300
C 2.56299700 4.83529200 1.96968800
H 2.97770300 4.09803100 2.66008500
H 2.98580700 4.64556500 0.97696000
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2j

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O -1.57431700 -1.02986700 -2.01231000
O -1.43676900 1.91564100 -1.55211300
O 1.47191200 1.76783200 -1.56663100
C 1.85414900 1.99478900 -0.38095100
O 1.40395400 1.43258700 0.67476700
C -1.82664900 2.14777500 -0.36732400
O -1.45132200 1.51445600 0.67384300
C 1.68955500 -1.74999000 -1.09870500
O 1.27385000 -1.54548600 0.09135400
O -1.59310600 -1.38086700 0.22622000
C -2.00102000 -1.59996900 -0.96297900
C 2.70069100 -2.88388500 -1.25461600
C 2.95809900 3.02431700 -0.14489300
C -2.83538000 3.27646100 -0.16402000
C -3.10206000 -2.64572500 -1.12789800
C 3.89714000 -2.60553800 -0.30420100
H 4.61116400 -3.42674300 -0.44364900
H 3.52891300 -2.66875600 0.72630900
C 3.16673300 -2.99697700 -2.70086700
H 3.88919400 -3.81490900 -2.78974500
H 2.32887400 -3.20757600 -3.36983500
H 3.64707900 -2.07793700 -3.04506100
C 2.02116400 -4.18610900 -0.81848900
H 2.73223200 -5.01557700 -0.88336600
H 1.66191300 -4.12006000 0.21271600
H 1.17113600 -4.42435200 -1.46564900
C 4.11028200 2.32590000 0.62779200
H 4.89055400 3.08010200 0.78883500
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C 2.38353500 4.14014000 0.73440400
H 3.16586000 4.86869300 0.96930900

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H 2.64935600 4.11198400 -1.99892300
H 4.24625600 4.33543900 -1.26604700
H 3.86013400 2.83211400 -2.12113700
C -3.21726400 3.41269200 1.30568100
H -3.92498900 4.23991700 1.42416800
H -3.68649300 2.50300400 1.68774800
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H -2.23526500 -3.38431700 -2.98934800
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H -3.87925800 -2.43929200 0.90395400
C 4.57100500 -1.28023200 -0.52310000
C 4.12182400 -0.14421200 0.15841600
C 5.62974800 -1.13957400 -1.42676700
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C 6.21340900 0.10613200 -1.64267100
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C -4.31260100 0.50045000 -1.42022000
C -5.85055000 -0.86252500 -0.17606100
C -4.73643200 1.64809100 -0.74353400
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C -5.74381200 1.51853000 0.21843400

H -7.09145000 0.18475200 1.23395700
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C 0.00518200 -0.38538000 2.44126400
C -0.70902000 -1.55536500 2.97615700
O -1.76410100 -1.33546600 3.56398400
C 0.60126100 0.59845000 3.35058800
O -0.07644000 1.46756700 3.87098700
O 1.92008200 0.44282800 3.49914900
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H 2.15681500 1.39552200 5.34253300
H 3.61436300 1.18068800 4.32305600
H 2.39843500 2.43194000 3.91388500
C -0.14152900 -2.92315900 2.69142200
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C -0.92523800 -4.00953100 3.40330800
H -0.56461900 -4.99728600 3.10345300
H -0.81207100 -3.92531000 4.48862600
H -1.99230200 -3.94717600 3.17784300
C 1.35381700 -2.94958100 3.00922100
H 1.53110300 -2.81147400 4.08128300
H 1.78861500 -3.91041800 2.71892300
H 1.89350200 -2.16388300 2.46874900

2k

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O -1.23877700 -0.03127400 -2.47231800
O 1.64758200 0.27756300 -2.29198000
O 1.79360500 -2.39758700 -0.96188400
O -1.12067000 -2.57815500 -1.07533000
C -1.57051100 -2.46163200 0.10294600
O -1.22585400 -1.57071900 0.95197900
C 2.13673200 -2.22040400 0.24674100
O 1.64330200 -1.35204100 1.03898100
C -1.70598400 0.86014600 -1.70479700
O -1.32445700 1.08620000 -0.50670000
O 1.51307600 1.28394800 -0.26530200
C 1.95423900 1.18355500 -1.45920600
C -2.80982300 1.77863600 -2.22410800
C -2.61217400 -3.46185400 0.60038600
C 3.23929900 -3.11877900 0.80360200
C 2.94435700 2.25263400 -1.91993200
C -3.97082700 1.77785200 -1.19256400
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H -3.59204700 2.19451700 -0.25208300
C -3.29715700 1.32662100 -3.59551900

H -4.08941700 1.99909800 -3.94129500
H -2.48762100 1.35081400 -4.32863700
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H -3.00488300 3.90679900 -2.58607600
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H 4.33715500 -3.43260000 2.62955700
H 3.86779300 -1.74144100 2.37213800
H 2.66021200 -2.91921300 2.88964600
C 2.76832200 -4.57172400 0.68833400
H 2.53746700 -4.83211200 -0.34752000
H 3.55364300 -5.24399500 1.04784900
H 1.87473700 -4.74704900 1.29612000
C 4.50241200 -2.93239700 -0.08120700
H 5.28292200 -3.57581300 0.34359700
H 4.27431000 -3.31781700 -1.08126300
C 4.25740900 1.53921300 -2.34163600
H 4.04063700 0.93705400 -3.23106600
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C 2.34958000 2.95360100 -3.14452800
H 1.42463400 3.47969100 -2.88536400
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H -6.99348000 -1.66018600 -2.14446100
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C 4.86360600 0.66852300 -1.27772700
C 4.49368100 -0.67690000 -1.18647500
C 5.77435200 1.17328700 -0.34368100
C 4.98547900 -1.51334100 -0.18031700
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H 7.00920200 0.74814500 1.36470800
H 6.30476800 -1.62280600 1.51860500
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C 0.51721400 2.13422700 2.31971800
O 1.58252500 2.19820600 2.92629700
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O 0.14752100 -0.60239200 3.99824600
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H -3.55286000 -0.47873500 4.41862500
H -2.25420200 -1.70914200 4.31627900
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C -1.69537000 3.25670900 2.07455800
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H -0.14079600 3.12516000 0.60836800
C -2.45549200 4.42949500 1.46808700
H -1.78490600 3.28854100 3.17052900
H -2.13457400 2.30257200 1.75208400
C -0.33375200 5.77938900 1.39159100
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H 1.48687800 4.63597700 1.74009400
C -1.80140600 5.76395300 1.80635000
H -3.49810000 4.40996100 1.80479200
H -2.48529900 4.31171400 0.37565700
H 0.12904400 6.73884100 1.64673200
H -0.26432400 5.68322900 0.29687900
H -2.34576600 6.58529700 1.32788400
H -1.86944000 5.93658100 2.89027500

2I

Rh -0.02052400 0.49979500 -1.91862600
O 1.38289300 -0.98012100 -2.26485400

O -1.55989600 -0.88160300 -2.16905400
O -1.36152100 2.01684700 -1.49186200
O 1.50879800 1.84126500 -1.49728400
C 1.80395400 2.05292700 -0.28402100
O 1.32256100 1.43323400 0.72445600
C -1.81313400 2.11118800 -0.30897100
O -1.52025000 1.34107900 0.66300300
C 1.81783300 -1.62658900 -1.26727600
O 1.41398500 -1.49410000 -0.06277800
O -1.51332600 -1.50147600 0.01155000
C -1.97219100 -1.55807100 -1.17807400
C 2.91143900 -2.67235400 -1.48108100
C 2.83250000 3.13186900 0.05247400
C -2.79633000 3.24491100 -0.02281500
C -3.10541500 -2.55164900 -1.44117400
C 4.06638400 -2.39940000 -0.47946400
H 4.82828300 -3.16784300 -0.66018900
H 3.67798700 -2.56325700 0.53206100
C 3.41209800 -2.63671600 -2.91973700
H 4.20319500 -3.38211300 -3.05120000
H 2.60779800 -2.86450600 -3.62339300
H 3.81859000 -1.65682700 -3.18260600
C 2.31761800 -4.04895400 -1.16211900
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H 1.46183700 -4.27572600 -1.80667200
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H 4.72886800 3.23799400 1.05435000
H 3.59731400 2.08532200 1.77496000
C 2.16070200 4.15386900 0.97531000
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H 3.80789500 3.11716200 -1.89705200
C -3.18880800 3.26548700 1.44989500
H -3.88378300 4.09163600 1.63335000
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C -2.12078300 4.56607900 -0.40074000
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C -4.26252200 -1.80928700 -2.15889000
H -3.89193300 -1.46006300 -3.12856500
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C -2.55496900 -3.63389700 -2.37677300
H -1.72198100 -4.17035700 -1.90897300
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H -2.80372200 -3.77381300 0.32515600
H -3.93074700 -2.43835600 0.57614900
C 4.67568200 -1.02891200 -0.57277300
C 4.15035000 0.02758100 0.17915800
C 5.75632600 -0.76992500 -1.42272800
C 4.65189100 1.32880300 0.07169400
H 3.32876800 -0.16721700 0.86765400
C 6.28667900 0.51359300 -1.52074700
H 6.18944100 -1.58485100 -1.99991200
C 5.73294600 1.55840800 -0.78589600
H 7.13562400 0.70082100 -2.17285100
H 6.14538100 2.56234900 -0.86846100
C -4.82619100 -0.65416000 -1.38050200
C -4.27759500 0.62176700 -1.53414100
C -5.86699100 -0.82400600 -0.46085700
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C -6.33123100 0.25484800 0.28695100
H -6.31718600 -1.80715900 -0.33807800
C -5.75416800 1.51376500 0.13802000
H -7.14714500 0.11379400 0.99077000
H -6.11663200 2.35360900 0.72793600
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C 0.01360600 -0.55428200 2.35138200
C -0.60704800 -1.75725800 2.92179800
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C 0.67398200 0.39998000 3.25439200
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C 0.47948900 2.30756200 4.59315000
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H -0.25738000 3.09400800 4.73673400
H 0.71647100 1.82788000 5.54473200
C 0.12206700 -3.08981400 3.01033800
C -0.32150100 -3.80111500 4.28748400

H 0.12626600 -4.79870800 4.32886700
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C 1.63492100 -2.88411900 2.99161400
H 1.98365700 -2.34571400 3.87697000
H 2.13752800 -3.85681300 2.96427000
H 1.95033700 -2.32205900 2.10537500
C -0.30525500 -3.91603700 1.78653400
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H -0.05668900 -3.41167400 0.84780000
H 0.21232000 -4.88115100 1.81118600

2m

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O 1.51152600 1.56083200 -1.71149600
O 1.37084400 -1.41923200 -1.95010300
O -1.52961100 -1.28928800 -1.76908600
C -1.88260500 -1.77130000 -0.65226900
O -1.40104000 -1.45504300 0.48921200
C 1.78886400 -1.92505000 -0.86345300
O 1.46774000 -1.53762000 0.30676900
C -1.74203200 2.01275100 -0.53394700
O -1.30325800 1.52959000 0.56446800
O 1.58541300 1.40731900 0.55061600
C 1.95625500 1.89216900 -0.57003200
C -2.75686200 3.14549400 -0.39793300
C -2.97501100 -2.84024000 -0.62266600
C 2.77308300 -3.09083300 -0.95565000
C 3.04656500 2.96441300 -0.52546900
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H -3.51827600 2.48218500 1.51123000
C -3.26756200 3.57597200 -1.76798800
H -3.99264700 4.38812300 -1.65052900
H -2.44918800 3.93706400 -2.39556400
H -3.75723000 2.75471800 -2.29652000
C -2.05787600 4.32383700 0.28863000
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H -1.22422700 4.69441700 -0.31618500
C -4.11910100 -2.34537100 0.30458000
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C -2.37199000 -4.11185900 -0.01604000
H -3.13956900 -4.88841900 0.05926700

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C -3.49197800 -3.12609700 -2.02673600
H -2.69022800 -3.49205300 -2.67303000
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C 3.08131700 -3.65360100 0.42751500
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H 2.17344900 -4.02229600 0.91305300
C 2.15757300 -4.17795300 -1.83977700
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H 2.86837400 -5.00162500 -1.95938600
H 1.24692300 -4.58613000 -1.39027100
C 4.06656400 -2.56842700 -1.63999000
H 4.78080300 -3.40118100 -1.64425200
H 3.82595700 -2.34365400 -2.68515700
C 4.28449600 2.41918600 -1.28930100
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C 3.41114000 3.31724700 0.91227200
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H 2.54618200 3.71501500 1.45023300
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C -4.15563800 0.16138600 0.41659200
C -5.67611300 1.48397300 -0.89317000
C -4.70633000 -1.02004900 -0.08956300
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C 4.77269000 1.08037500 -0.81539000
C 4.28256700 -0.08222400 -1.41577500
C 5.69051500 0.95157800 0.23220000
C 4.66901400 -1.35590600 -0.99048300
H 3.57723200 0.00794100 -2.24082500
C 6.09647800 -0.30911700 0.66251400
H 6.09843500 1.84506600 0.70115200
C 5.58976700 -1.45641400 0.05757500

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C 0.13497500 -0.12370200 2.52893000
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O 2.18870000 -0.13907500 3.49995800
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O -1.98235500 -0.40761800 3.43237300
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C -1.61155100 -2.99279300 3.99303700
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H -1.90244300 -2.60796400 4.97184500
C 1.00391700 1.91739300 3.78918200
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H 1.81953500 2.32586000 4.38168200
H -0.23621200 3.63708500 3.85963900
H -0.89329900 2.19955000 2.88771300

2n

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O -1.57672400 -1.67231000 -1.44531500
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O 1.41442600 1.18085100 -1.86937800
C 1.79556900 1.73918000 -0.79792500
O 1.34931400 1.49236800 0.37372500
C -1.87654900 1.85154800 -0.75248400
O -1.49823500 1.54107100 0.42817100
C 1.68318900 -2.08912400 -0.43019900
O 1.23981500 -1.57205400 0.66080400
O -1.61115900 -1.35990400 0.79824800
C -2.00636900 -1.92302100 -0.27914600
C 2.71636200 -3.19965000 -0.27255700
C 2.88631800 2.80615300 -0.85775900
C -2.89477600 2.98136700 -0.88342100
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H 3.62772300 -2.88545100 -2.22840500
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C -5.77637400 1.36229900 -0.01216100
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H -6.13873700 2.35495000 0.24865200
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O 2.26442400 1.04345800 3.26268400
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C 1.28502700 3.47735500 3.74971200
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H 0.64961500 4.35904500 3.76613300
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O 0.31214500 -2.16740300 3.16275800
H 0.76687400 -2.14333200 2.29167800

2o

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C 1.68270800 -1.93744600 -0.97166400
O 1.40974500 -1.55376200 0.21135400
C -1.81763300 2.00523200 -0.45370300
O -1.31103200 1.54059000 0.62243500
O 1.57349300 1.38713700 0.41764900
C 1.84697400 1.89847500 -0.71866500
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H -3.56113700 2.48256700 1.63083200
C -3.33488300 3.61820800 -1.63260800
H -4.03787800 4.44519800 -1.48759000

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 C 2.39617500 4.19463300 -1.51025300
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 H 2.41896300 3.78375800 1.22874900
 H 3.68427700 2.55454300 1.26184900
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 C -4.76661600 -1.01345500 0.04999300
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 H -6.12008700 2.45886100 -1.07223600

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 C 4.15495400 -0.08407300 -1.57045800
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 C 4.53764100 -1.35361900 -1.13053100
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 O 1.30771100 1.58712900 3.67701100
 C -0.69031400 -0.88779600 3.26870300
 O -0.44300000 -2.03491400 3.60462800
 O -1.84242000 -0.24723600 3.46396800
 C -2.86322000 -1.01960200 4.12352300
 H -2.57214300 -1.23637900 5.15278100
 H -3.75750800 -0.40067600 4.10045500
 H -3.02754900 -1.95738400 3.58784700
 O 2.56664600 -0.18691900 3.01145100
 C 3.72445800 0.43469500 3.60119300
 H 3.99272900 1.33144300 3.03736600
 H 3.52815600 0.70185300 4.64062200
 H 4.51771600 -0.30591100 3.53515100

2p

Rh -0.06068700 -0.43870800 -1.83508300
 O -1.38394400 1.12744100 -2.05135100
 O 1.51547900 0.91975900 -2.02350800
 O 1.24236300 -2.02618900 -1.55176900
 O -1.63657000 -1.74287900 -1.44729200
 C -1.99141000 -1.94308400 -0.24864400
 O -1.49408600 -1.38013800 0.78613300
 C 1.66669800 -2.26830800 -0.38073100
 O 1.37534400 -1.59939900 0.66504700
 C -1.68181300 1.79083400 -1.01371800
 O -1.26219000 1.55441500 0.16739900
 O 1.61439400 1.29945300 0.20961200
 C 2.00108600 1.47850600 -0.99335500
 C -2.62339300 2.98487300 -1.14671600
 C -3.12155500 -2.93409000 0.02933900

C 2.61158900 -3.45533200 -0.20507700
 C 3.15740100 2.45531600 -1.21119900
 C -3.86161600 2.72787700 -0.24384400
 H -4.54669300 3.57133700 -0.39564100
 H -3.52765200 2.76351000 0.79946700
 C -3.03800200 3.18277700 -2.59924800
 H -3.70853000 4.04505100 -2.67499800
 H -2.16896500 3.36830800 -3.23565000
 H -3.55898900 2.30674900 -2.99333100
 C -1.89020000 4.22512200 -0.62611700
 H -2.54813400 5.09790500 -0.68454800
 H -1.58294000 4.08813000 0.41407300
 H -0.99674000 4.43911900 -1.22278000
 C -4.27040600 -2.16621300 0.74006100
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 C -2.59420600 -4.01237400 0.98087300
 H -3.40281300 -4.70087900 1.24586300
 H -1.79748900 -4.59807400 0.51191700
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 C -3.61154000 -3.57446400 -1.26349000
 H -2.80612500 -4.12000500 -1.76154000
 H -4.41562900 -4.28295200 -1.03869200
 H -3.99583100 -2.83122000 -1.96574500
 C 3.01648100 -3.62280700 1.25498100
 H 3.68332900 -4.48578800 1.35336400
 H 3.53777600 -2.74097300 1.63518200
 H 2.14243300 -3.79122400 1.88960700
 C 1.89045400 -4.71340500 -0.69783400
 H 1.58068500 -4.61092300 -1.74079100
 H 2.55889300 -5.57647900 -0.61840100
 H 1.00235100 -4.92340500 -0.09314200
 C 3.85883200 -3.21295300 -1.09899400
 H 4.53141400 -4.06532000 -0.94204400
 H 3.53461800 -3.24504200 -2.14516000
 C 4.28842000 1.70674300 -1.96459100
 H 3.91133900 1.43713400 -2.95716300
 H 5.10323100 2.42659900 -2.11125200
 C 2.64881400 3.59921800 -2.09426700
 H 1.84195900 4.15068600 -1.59960400
 H 3.46201000 4.30475800 -2.29202600
 H 2.27426700 3.22625000 -3.05082000
 C 3.66852500 3.01204700 0.11305100
 H 4.52885700 3.66442100 -0.06990900
 H 2.89714600 3.60538500 0.61051400
 H 3.97583200 2.22017400 0.80114300

C -4.56145500 1.42313100 -0.49913800
 C -4.18456700 0.28596700 0.22186600
 C -5.57092400 1.29846100 -1.45987100
 C -4.76731300 -0.96317200 -0.01039300
 H -3.42208800 0.37807900 0.99342500
 C -6.17812900 0.06596500 -1.68897000
 H -5.89155100 2.17579900 -2.01856600
 C -5.77635400 -1.05991500 -0.97443600
 H -6.97208800 -0.01698700 -2.42638300
 H -6.25510400 -2.02052800 -1.15490400
 C 4.78970700 0.47789800 -1.25980000
 C 4.18854600 -0.75912900 -1.50758600
 C 5.82540800 0.53834000 -0.32148700
 C 4.57544300 -1.92004800 -0.83135300
 H 3.39830400 -0.81987500 -2.25344900
 C 6.23598000 -0.61006000 0.35043200
 H 6.31647200 1.48992100 -0.12666800
 C 5.61191700 -1.83047400 0.10366600
 H 7.04943800 -0.55432100 1.06889000
 H 5.93654700 -2.72548000 0.63126300
 Rh 0.05118400 -0.01421400 0.55437000
 C 0.00798800 0.41494000 2.45106300
 C 0.87751500 1.46676800 2.98221100
 O 1.92191700 1.16575700 3.53884700
 C -1.03959100 -0.16869400 3.29124200
 O -2.12312900 0.38802100 3.37188200
 O -0.71428500 -1.33097100 3.85185700
 C -1.76457700 -1.93975200 4.62910000
 H -2.63540500 -2.13193900 3.99902200
 H -1.34800800 -2.87220100 5.00155800
 H -2.05189500 -1.28810800 5.45583800
 C 1.33539800 3.78368900 3.08914300
 C 0.92483100 4.98290000 2.28318100
 H -0.10474600 5.27581000 2.50247900
 H 1.57785200 5.82777000 2.51365600
 H 0.99892400 4.77445500 1.21098400
 O 0.44272700 2.69488300 2.72188900
 H 2.36233000 3.46771900 2.88558600
 H 1.24031300 3.94816100 4.16673400

2q

Rh -0.08460500 0.39813000 -1.88588800
 O -1.45162400 1.88134800 -1.46887100
 O 1.44625600 1.80983700 -1.65130100
 O 1.26870200 -1.12823800 -2.25295200
 O -1.59262100 -1.02986500 -1.91362000

C -1.92332500 -1.61895500 -0.84210100
O -1.43700700 -1.39147100 0.31841500
C 1.69691000 -1.77958500 -1.25173700
O 1.42447700 -1.53119300 -0.03269000
C -1.71339700 2.15169000 -0.25918300
O -1.22848400 1.54618900 0.75546800
O 1.64225200 1.35539100 0.56104700
C 1.94726800 1.99480800 -0.50082500
C -2.69070600 3.28406500 0.04530200
C -2.99709100 -2.70292000 -0.89930300
C 2.64330500 -2.94955200 -1.51109900
C 3.03699600 3.05707700 -0.35891300
C -3.91066600 2.68043200 0.79538300
H -4.62249200 3.50023600 0.95368800
H -3.56855400 2.35325000 1.78387100
C -3.13019600 3.97562900 -1.23961600
H -3.83151700 4.78107200 -0.99790300
H -2.27744900 4.41394000 -1.76474400
H -3.62490700 3.28403200 -1.92521000
C -1.99490300 4.28633100 0.97105700
H -2.68504100 5.09790300 1.22180800
H -1.66894300 3.80875200 1.89818900
H -1.11906400 4.73009800 0.48677800
C -4.18201500 -2.25589500 0.00042400
H -4.97336300 -3.00622300 -0.12006300
H -3.84875200 -2.29822000 1.04205200
C -2.40596200 -3.99126100 -0.31687900
H -3.16387100 -4.78091200 -0.32267600
H -1.55370000 -4.34048200 -0.90910600
H -2.06706000 -3.83912900 0.71204900
C -3.45655900 -2.93238400 -2.33366500
H -2.62641600 -3.25634300 -2.96697800
H -4.22461300 -3.71255000 -2.35094800
H -3.87846300 -2.02577800 -2.77416200
C 2.86544300 -3.75857500 -0.23715300
H 3.53010000 -4.60203100 -0.45142000
H 3.31482500 -3.15716700 0.55687900
H 1.92065100 -4.15580000 0.14519700
C 2.04081400 -3.83908600 -2.60023700
H 1.86378100 -3.27613700 -3.51949300
H 2.72564600 -4.66292800 -2.82388500
H 1.08976500 -4.27252500 -2.27564400
C 3.98496200 -2.36336600 -2.03557100
H 4.68845900 -3.20180900 -2.11079700
H 3.81425700 -1.99390300 -3.05319000
C 4.29794300 2.53877600 -1.10745500

H 4.09380800 2.58615800 -2.18315800
H 5.10485400 3.25253700 -0.90028300
C 2.56689000 4.34990900 -1.02670300
H 1.68625400 4.75916100 -0.52147300
H 3.36043100 5.10191900 -0.97567700
H 2.31438200 4.18336900 -2.07631700
C 3.35382000 3.31132600 1.11113600
H 4.13665200 4.07243200 1.19225000
H 2.47225200 3.66656500 1.65223000
H 3.70200200 2.40330000 1.60887000
C -4.57128400 1.53089100 0.08881100
C -4.16513800 0.22377900 0.37139600
C -5.56668500 1.72585200 -0.87515600
C -4.70553500 -0.87958500 -0.29683600
H -3.41476900 0.05705400 1.14212000
C -6.12958600 0.63787100 -1.53742800
H -5.91089900 2.73474800 -1.09514500
C -5.69933400 -0.65646600 -1.25572000
H -6.91207300 0.79915000 -2.27403300
H -6.14683600 -1.50384200 -1.77190100
C 4.71105200 1.14196600 -0.74298400
C 4.24746200 0.06953900 -1.50928500
C 5.52708400 0.86643400 0.35954000
C 4.55824700 -1.25673800 -1.19759400
H 3.63000600 0.27551600 -2.38282100
C 5.85985900 -0.44820100 0.67764000
H 5.91925000 1.68719900 0.95754700
C 5.37459300 -1.50483600 -0.08865900
H 6.50936600 -0.65023400 1.52570900
H 5.64663500 -2.52857000 0.16017600
Rh 0.11041000 -0.02168300 0.49545600
C 0.33896600 -0.46312600 2.37299900
C 1.49216100 0.03329400 3.12495500
O 1.37936300 1.00870800 3.84896700
C -0.57343600 -1.43429700 2.97341400
O -0.33941500 -2.62610700 2.91575100
O -1.67515300 -0.86191900 3.50295700
C -2.70433700 -1.72901000 3.95621800
H -2.84643300 -1.54671600 5.02238300
H -2.44851500 -2.76759800 3.73581200
O 2.61255600 -0.64494500 2.88559300
C 3.76901900 -0.18338100 3.61060500
H 4.08459100 0.79118800 3.23202800
H 3.54414500 -0.10775200 4.67543600
H 4.54057500 -0.92738600 3.42927900
F -3.84338000 -1.38247400 3.29148000

2r

Rh 0.11849600 0.23112000 -1.88728000
O 1.46970100 -1.32953600 -1.93951000
O -1.43518900 -1.16604400 -2.00223500
O -1.20844400 1.81804600 -1.76423900
O 1.66522500 1.58365600 -1.56362700
C 2.01128400 1.86170200 -0.37808700
O 1.50672500 1.36774000 0.68797900
C -1.66222100 2.14425200 -0.62496300
O -1.38415400 1.56963500 0.47840700
C 1.73665200 -1.91943400 -0.85147300
O 1.27247600 -1.60785200 0.29641200
O -1.60148800 -1.33840800 0.25431500
C -1.94604500 -1.63253900 -0.93889400
C 2.69567400 -3.10955200 -0.87423900
C 3.13704600 2.87364500 -0.16451400
C -2.62781700 3.32795200 -0.57074800
C -3.08213800 -2.64575800 -1.09321000
C 3.89710100 -2.78182900 0.05283600
H 4.58554200 -3.63440700 -0.00269400
H 3.52303100 -2.73300700 1.08258100
C 3.16605800 -3.39472700 -2.29518800
H 3.85704900 -4.24416500 -2.28740600
H 2.32506400 -3.64545100 -2.94663400
H 3.68280000 -2.53630100 -2.73070000
C 1.96215400 -4.32971100 -0.30897100
H 2.62921900 -5.19737700 -0.31220900
H 1.63464900 -4.15236000 0.71866400
H 1.08436800 -4.58202800 -0.91290400
C 4.27014300 2.17583900 0.63529800
H 5.07378800 2.91222600 0.75997500
H 3.88418300 1.94228000 1.63542700
C 2.58863800 4.03457200 0.67108400
H 3.39013800 4.74828700 0.88675600
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H -3.49699700 2.93999200 -2.50713200
C -4.21783900 -1.98341300 -1.91739700
H -3.83738900 -1.79590100 -2.92757200
H -5.02114200 -2.72538800 -2.00614400
C -2.53931800 -3.84811600 -1.87090800
H -1.73162800 -4.34122100 -1.31896300
H -3.33539700 -4.58373500 -2.02369400
H -2.15345000 -3.54730800 -2.84812600
C -3.60242300 -3.10035100 0.26617000
H -4.43678400 -3.79617500 0.12722100
H -2.82226500 -3.61938300 0.83036400
H -3.95032900 -2.26011500 0.87299800
C 4.60975000 -1.50261500 -0.28281900
C 4.19815700 -0.30737700 0.31320800
C 5.66312900 -1.46011100 -1.20228800
C 4.79370900 0.91804400 0.00175500
H 3.39585400 -0.33080500 1.04807900
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H 6.01003700 -2.38290700 -1.66384500
C 5.84421200 0.93347000 -0.92159900
H 7.10522100 -0.23011600 -2.21900200
H 6.33100400 1.87605100 -1.16562100
C -4.74162600 -0.70515700 -1.32673100
C -4.14898900 0.51247500 -1.67306500
C -5.79106100 -0.69499300 -0.40202500
C -4.55869500 1.72309700 -1.10692600
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C -6.22362800 0.50308700 0.16097300
H -6.27620100 -1.63118700 -0.13145700
C -5.60867500 1.70398600 -0.18320800
H -7.04798900 0.50119800 0.86917100
H -5.95087500 2.63844300 0.25756000
Rh -0.04544300 -0.00586100 0.53117200
C -0.10197100 -0.22025700 2.47452700
C -1.23602500 -0.82459300 3.18262900
O -2.04100000 0.03026600 3.58717500
C 1.02596400 0.31590800 3.24030500
O 2.06125300 -0.32790600 3.32684300
O 0.82749700 1.53468000 3.74194500
C 1.97424500 2.11063800 4.39406100
H 2.80674200 2.18129300 3.68998900

H 1.66037300 3.10110500 4.71495100
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C -2.52483700 -2.72023800 3.95023400
H -2.23314800 -3.30237900 4.82986600
H -3.18480900 -1.90834200 4.25434600
H -3.05790600 -3.37892900 3.25664200
C -0.38628800 -3.07038100 2.74632400
H -0.82586500 -3.63153100 1.91138000
H 0.47703000 -2.51998000 2.36480300
H -0.04556900 -3.77654100 3.50993200

2s

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O -1.50479600 0.56441600 -2.31180900
O 1.40676000 0.28885200 -2.32751700
O 1.06188300 -2.46997900 -1.19306100
O -1.79602900 -2.07214100 -1.05048100
C -2.14597400 -1.94674200 0.16018300
O -1.60954500 -1.16942300 1.02171600
C 1.51495100 -2.46643500 -0.00771800
O 1.26708300 -1.58567800 0.88042900
C -1.72340000 1.47392900 -1.45816200
O -1.24257700 1.51537100 -0.27628600
O 1.63458300 1.08366800 -0.21588900
C 1.97171100 1.00113900 -1.44383300
C -2.63382100 2.64260500 -1.83937800
C -3.31510200 -2.78664200 0.67545900
C 2.43063200 -3.62617800 0.38433700
C 3.16385400 1.85889900 -1.87248300
C -3.81321200 2.69305300 -0.83078500
H -4.45818400 3.52636100 -1.13637900
H -3.40178800 2.94498200 0.15423800
C -3.14285800 2.48540200 -3.26708400
H -3.79853800 3.32636500 -3.51595100
H -2.31630200 2.47540700 -3.98215600
H -3.70912200 1.56018000 -3.39713400
C -1.83100900 3.94110400 -1.71045800
H -2.46323600 4.79387900 -1.97666500
H -1.47403400 4.08666600 -0.68730400
H -0.96690900 3.94458700 -2.38274700
C -4.38857800 -1.82401800 1.25072300
H -5.22022100 -2.44668000 1.60350200
H -3.96025800 -1.32505600 2.12863000
C -2.79835000 -3.67762900 1.80961400
H -3.62740800 -4.24726300 2.24137000

H -2.05678700 -4.39444000 1.44324800
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H -4.27558000 -3.03900200 -1.26491500
C 2.93700500 -3.47365500 1.81320600
H 3.59127300 -4.31612500 2.06119200
H 3.50403900 -2.54942500 1.94740900
H 2.10909000 -3.46351200 2.52652100
C 1.62537800 -4.92261400 0.24904600
H 1.24529000 -5.04944500 -0.76778200
H 2.26242800 -5.77943600 0.48982200
H 0.77597700 -4.93404800 0.93931700
C 3.61184700 -3.67046100 -0.62215500
H 4.24520700 -4.51754800 -0.33095500
H 3.20150000 -3.89760000 -1.61231900
C 4.23328600 0.93384400 -2.51142700
H 3.80557800 0.50130700 -3.42294500
H 5.06814500 1.57618400 -2.81855100
C 2.66962400 2.85436100 -2.92596700
H 1.92189300 3.53343200 -2.50106500
H 3.50618200 3.46290700 -3.28351300
H 2.22379500 2.34087300 -3.78160300
C 3.74650000 2.61472200 -0.68212700
H 4.60272000 3.21409100 -1.00935700
H 3.00496000 3.28851000 -0.24278900
H 4.07923100 1.93733000 0.10860500
C -4.60224800 1.41854100 -0.73402700
C -4.21612600 0.43979000 0.18615800
C -5.69919400 1.15993600 -1.56254400
C -4.87900600 -0.78705100 0.28077700
H -3.37713500 0.64029500 0.84978200
C -6.38077300 -0.05120400 -1.47172500
H -6.02489600 1.91756900 -2.27285400
C -5.97119200 -1.02184500 -0.56084200
H -7.23906900 -0.23815300 -2.11158400
H -6.50899500 -1.96561400 -0.49079900
C 4.72107900 -0.16109300 -1.60544100
C 4.04267300 -1.38238400 -1.55959100
C 5.82628300 0.01762800 -0.76661500
C 4.41912700 -2.40540200 -0.68457300
H 3.19357500 -1.54067600 -2.22176200
C 6.22915300 -0.99784900 0.09657900
H 6.37619700 0.95649300 -0.79859600
C 5.52724000 -2.19945500 0.14343600

H 7.09565600 -0.85215900 0.73610700
 H 5.84276400 -2.99045500 0.82117500
 Rh 0.00884500 0.00547500 0.44860100
 C 0.11394200 0.81338200 2.22502600
 C 1.25753100 1.59984400 2.70857700
 O 2.04032600 0.93664400 3.41160300
 C -1.01240700 0.57256400 3.13018500
 O -2.01710600 1.26323500 3.04290500
 O -0.85239900 -0.46119000 3.95645900
 C -2.00271600 -0.76814400 4.76526700
 H -2.85572700 -1.00910700 4.12616900
 H -1.71805400 -1.63123600 5.36209000
 H -2.25772600 0.07681700 5.40663700
 N 1.40286500 2.88279700 2.36976900
 C 2.49153900 3.71320100 2.88799600
 H 2.68624600 3.46101500 3.93340500
 H 3.41198900 3.52027200 2.32059900
 C 0.47342400 3.63076900 1.51155900
 H 0.34449700 3.11254900 0.55566400
 H -0.51230900 3.70108000 1.99045400
 C 1.96752200 5.12420300 2.66329100
 H 1.32199200 5.41675000 3.49846100
 H 2.77027700 5.86011400 2.58773600
 C 1.14567400 4.99471000 1.38222100
 H 0.41853800 5.79868700 1.25060200
 H 1.80702900 5.00548800 0.50783000

2t

Rh -0.15151400 -0.51078100 -1.89928300
 O -1.46533600 1.06414000 -2.11844800
 O 1.43567200 0.82595000 -2.18545900
 O 1.14419600 -2.10662200 -1.60742000
 O -1.74083800 -1.76844700 -1.41234200
 C -2.07824100 -1.90769100 -0.20013300
 O -1.54184100 -1.32286000 0.80238200
 C 1.58268400 -2.32196400 -0.43620800
 O 1.31508100 -1.62589600 0.59736400
 C -1.73068900 1.76698400 -1.09873700
 O -1.26109700 1.58351300 0.07464900
 O 1.61386400 1.24230800 0.03701300
 C 1.95624500 1.40017500 -1.18189000
 C -2.67886000 2.95463000 -1.25778700
 C -3.22710300 -2.85617900 0.14269900
 C 2.51725700 -3.51407400 -0.23722400
 C 3.10880600 2.36972700 -1.44512000
 C -3.84024800 2.79978600 -0.23902500

H -4.50585800 3.66059500 -0.38065200
 H -3.41545000 2.87857600 0.76873600
 C -3.20829400 3.03206100 -2.68492300
 H -3.88674800 3.88664600 -2.77747700
 H -2.39299800 3.16390000 -3.40031100
 H -3.75538900 2.12902100 -2.96537400
 C -1.90170100 4.23193300 -0.92196300
 H -2.55178700 5.10361000 -1.04637700
 H -1.54200400 4.21806700 0.11014600
 H -1.04107300 4.36044500 -1.58701900
 C -4.30041700 -2.05496900 0.92895500
 H -5.11216900 -2.75420200 1.16546200
 H -3.85280100 -1.73964000 1.87874700
 C -2.67456100 -3.95582900 1.05602700
 H -3.48435800 -4.62548400 1.36280200
 H -1.92118100 -4.55834600 0.53869000
 H -2.21558300 -3.53167900 1.95333500
 C -3.81779100 -3.47472000 -1.11771900
 H -3.06279100 -4.04410300 -1.66529100
 H -4.63009800 -4.15674400 -0.84504400
 H -4.21997300 -2.71631000 -1.79340900
 C 2.92129400 -3.65491500 1.22636400
 H 3.58609600 -4.51757300 1.34136800
 H 3.44229200 -2.76689500 1.59226100
 H 2.04628000 -3.80972300 1.86341300
 C 1.78699400 -4.77661200 -0.70325500
 H 1.47918200 -4.69500000 -1.74858200
 H 2.44806900 -5.64334600 -0.60357600
 H 0.89631300 -4.96544000 -0.09515300
 C 3.76604200 -3.29970800 -1.13629400
 H 4.43426600 -4.15147700 -0.95864000
 H 3.44132700 -3.35563600 -2.18141600
 C 4.24294300 1.58543200 -2.15753100
 H 3.87285500 1.28385900 -3.14367500
 H 5.06598800 2.29210900 -2.32191600
 C 2.60388600 3.46968700 -2.38273500
 H 1.79856600 4.04671600 -1.91530300
 H 3.41862600 4.16257800 -2.61564300
 H 2.22789400 3.05050900 -3.31915800
 C 3.61092100 2.98570300 -0.14343700
 H 4.44384300 3.66502500 -0.35314800
 H 2.81954000 3.56043800 0.34742700
 H 3.95419900 2.22402900 0.56201500
 C -4.60757000 1.51411200 -0.36625100
 C -4.19512800 0.38436000 0.34674900
 C -5.71215000 1.39995300 -1.21710800

C -4.83300400 -0.85169600 0.20350300
H -3.35688300 0.47156800 1.03557300
C -6.37535500 0.18292900 -1.35234900
H -6.05675300 2.27336700 -1.76780000
C -5.93517200 -0.93832000 -0.65353900
H -7.24095200 0.10836700 -2.00524400
H -6.45388400 -1.88886000 -0.76447900
C 4.72570700 0.37716700 -1.40577700
C 4.11604500 -0.86246600 -1.61774600
C 5.75356600 0.46034800 -0.46077800
C 4.48931200 -2.00398700 -0.90215800
H 3.32925500 -0.94174000 -2.36593900
C 6.14915400 -0.66865300 0.25189500
H 6.25120200 1.41374800 -0.29338900
C 5.51906200 -1.89210400 0.03802900
H 6.95649800 -0.59557100 0.97563800
H 5.83328700 -2.77195800 0.59625600
Rh 0.03162700 -0.00913800 0.47627700
C 0.14691600 0.40482200 2.37777600
C 1.28080900 1.13999000 2.95895600
O 2.16158800 0.41583600 3.44964900
C -0.91084000 -0.09353700 3.25723700
O -1.93887400 0.55484200 3.38857200
O -0.66635100 -1.28229800 3.80725500
C -1.74500300 -1.81234000 4.60079900
H -2.63691300 -1.94106700 3.98351700
H -1.39251900 -2.77346200 4.96692600
H -1.97334300 -1.14309200 5.43190500
N 1.30020200 2.47085200 2.89611400
C 2.31499900 3.44361400 3.29379800
C 0.45986900 3.44520700 2.19768200
C 1.43246100 4.54224500 2.67149400
H 3.28103100 3.27373600 2.80505800
H 2.46954300 3.49513500 4.37590000
H 0.43371500 3.26822900 1.11561800
H -0.56825200 3.49769200 2.57393400
H 1.90318700 5.11759100 1.87300500
H 1.00463800 5.23186300 3.39939800

2u

Rh 0.30031900 0.43561600 -1.95926200
O 1.56655000 -1.19774200 -2.04533500
O -1.28621600 -0.85817600 -2.32750100
O -0.95562500 2.07817300 -1.78805800
O 1.88761700 1.66946000 -1.41582400
C 2.16315600 1.81971500 -0.18985500

O 1.55560700 1.26650100 0.79005200
C -1.43436200 2.34940800 -0.64445600
O -1.26229800 1.66351200 0.41494200
C 1.74177400 -1.87992200 -0.99410600
O 1.21652200 -1.63679800 0.14530900
O -1.61637400 -1.25488100 -0.11712000
C -1.87231300 -1.42655500 -1.35658000
C 2.64209900 -3.11209800 -1.05458600
C 3.31855900 2.73971800 0.20156300
C -2.31278400 3.59212200 -0.51294100
C -3.01535300 -2.38088000 -1.70677900
C 3.76558900 -2.95163700 0.00510200
H 4.40979000 -3.83605700 -0.07686000
H 3.30006300 -2.98002100 0.99753700
C 3.22775900 -3.28241700 -2.45116700
H 3.86685500 -4.17112500 -2.47400300
H 2.43896900 -3.40963600 -3.19653900
H 3.83036000 -2.42030700 -2.74588100
C 1.79453000 -4.33574800 -0.69055200
H 2.41176700 -5.23861200 -0.72710900
H 1.37755500 -4.24548600 0.31581300
H 0.96749700 -4.46734500 -1.39557800
C 4.32834400 1.91773000 1.04800100
H 5.15163300 2.59432700 1.30924100
H 3.82863500 1.63478300 1.98193300
C 2.75048800 3.86275800 1.07602200
H 3.56140300 4.51198900 1.42114500
H 2.04223300 4.48137800 0.51558500
H 2.23190400 3.45755500 1.94940800
C 3.99104000 3.32404400 -1.03388500
H 3.28328000 3.90770700 -1.62778000
H 4.80839500 3.98566600 -0.72812200
H 4.40481500 2.54382400 -1.67743000
C -2.64397700 3.86960700 0.95001700
H -3.26504300 4.76869100 1.01981300
H -3.18216900 3.03897200 1.41263000
H -1.73411500 4.03629800 1.53392200
C -1.57160500 4.78506300 -1.11980000
H -1.30816100 4.59817300 -2.16332600
H -2.20623200 5.67574300 -1.07637800
H -0.65252200 5.00309800 -0.56690300
C -3.60891400 3.34089500 -1.33307000
H -4.27354800 4.19332400 -1.14571500
H -3.34390100 3.36587600 -2.39617500
C -4.16178900 -1.52995700 -2.32309000
H -3.83325000 -1.19562000 -3.31362500

H -5.01163200 -2.20681600 -2.47672500
C -2.53277900 -3.37775600 -2.76139400
H -1.74100500 -4.02240000 -2.36707500
H -3.36402600 -4.02077000 -3.06740400
H -2.14940100 -2.86298400 -3.64515000
C -3.49954000 -3.12100400 -0.46811200
H -4.32547700 -3.78965300 -0.73237000
H -2.69539700 -3.72618900 -0.03796000
H -3.84364300 -2.42764300 0.30161700
C 4.57500400 -1.69308200 -0.13637700
C 4.17066400 -0.53046100 0.52674100
C 5.71194400 -1.63592400 -0.94953500
C 4.85003600 0.68164700 0.37187100
H 3.30641000 -0.57087500 1.18727500
C 6.41562400 -0.44301100 -1.09510900
H 6.05075700 -2.53525300 -1.46072200
C 5.98502700 0.71092100 -0.44516900
H 7.30611900 -0.41334500 -1.71713200
H 6.53798000 1.64118200 -0.56189600
C -4.57096000 -0.33707900 -1.50787900
C -3.98538700 0.90458400 -1.76696000
C -5.50873900 -0.42681800 -0.47377700
C -4.30191700 2.04487900 -1.02373100
H -3.25934400 0.98684900 -2.57501200
C -5.83759400 0.69869200 0.27797500
H -5.99290800 -1.37976500 -0.26819900
C -5.23956800 1.92724400 0.00705800
H -6.57473500 0.62049200 1.07260300
H -5.51270100 2.80595400 0.58771500
Rh -0.04321500 -0.00271800 0.41013600
C -0.26259000 -0.32581600 2.32321500
C -1.45183600 -0.89160200 2.97243800
O -2.25066400 -0.05960700 3.41460900
C 0.82715500 0.11584000 3.20205900
O 1.78765500 -0.61735900 3.38521600
O 0.67794700 1.34279700 3.69545000
C 1.78429900 1.81497200 4.48753200
H 2.69896200 1.81776700 3.88966300
H 1.51898200 2.82675800 4.78446600
H 1.92523800 1.18012300 5.36366700
N -1.60870400 -2.23340300 3.00865200
C -0.64222100 -3.21722300 2.58595200
H -1.15290500 -4.02798100 2.05882000
H 0.05791700 -2.74009400 1.89351700
H -0.09214000 -3.62663800 3.43892900
O -2.60477100 -2.70805400 3.85900800

C -3.82511100 -2.90519700 3.13808800
H -3.71436100 -3.68433200 2.37554700
H -4.54573500 -3.22914500 3.88934100
H -4.16204800 -1.97152500 2.67666700

2v

Rh 0.08878500 0.25112600 -1.75627000
O -1.33280900 1.74196000 -1.58742100
O 1.58069200 1.67782700 -1.45377300
O 1.47721300 -1.28648400 -1.84522800
O -1.42703300 -1.16301600 -1.87458400
C -1.82220400 -1.70938300 -0.80257800
O -1.38530100 -1.45930100 0.37158700
C 1.85720100 -1.85333600 -0.77654300
O 1.46867700 -1.55371100 0.40226200
C -1.68019800 2.09487800 -0.42443300
O -1.23444300 1.59309000 0.66706000
O 1.62552100 1.34958700 0.78906700
C 2.01636000 1.91598200 -0.28694800
C -2.71777200 3.20519400 -0.27036900
C -2.91906000 -2.77094900 -0.86424500
C 2.87131100 -2.98836300 -0.90699000
C 3.10965800 2.97665200 -0.15931300
C -3.89643000 2.65854400 0.58208300
H -4.61669400 3.47926800 0.68839100
H -3.51241100 2.43313900 1.58422500
C -3.20242900 3.67693600 -1.63645800
H -3.95204200 4.46441600 -1.50700900
H -2.37816100 4.08409300 -2.22723600
H -3.65536900 2.86456200 -2.20920600
C -2.07340800 4.37526500 0.47917800
H -2.80098700 5.18493300 0.58972500
H -1.74328100 4.08515200 1.48048900
H -1.21299000 4.77250500 -0.06790700
C -4.06568800 -2.33542500 0.08967800
H -4.83728900 -3.11341100 0.03574600
H -3.67164400 -2.33260300 1.11323200
C -2.32806500 -4.08849900 -0.34972100
H -3.10792400 -4.85559400 -0.31265700
H -1.53436200 -4.45119400 -1.01046000
H -1.90904400 -3.97072300 0.65370700
C -3.42683300 -2.94981000 -2.28919400
H -2.62383800 -3.27596500 -2.95477800
H -4.21340300 -3.71162400 -2.30464100
H -3.84059800 -2.02268300 -2.69269900
C 3.25304400 -3.54694600 0.45867000

H 3.97732200 -4.35829500 0.33184400
H 3.70129800 -2.78464900 1.10009300
H 2.37938600 -3.94734800 0.97948600
C 2.23883800 -4.08869400 -1.76449700
H 1.93421400 -3.70527200 -2.74148400
H 2.96142600 -4.89606300 -1.91894700
H 1.36059500 -4.51728200 -1.27151300
C 4.12031400 -2.43724700 -1.64894800
H 4.83466700 -3.26670000 -1.72151400
H 3.81810800 -2.17994100 -2.67008500
C 4.31404300 2.53629300 -1.03629400
H 3.99240300 2.55773500 -2.08337700
H 5.08913700 3.30379800 -0.91940600
C 2.55778400 4.29303300 -0.71493300
H 1.70900000 4.64759600 -0.12124600
H 3.33426000 5.06347300 -0.67915400
H 2.22961700 4.17944600 -1.75119200
C 3.53337200 3.16213600 1.29293800
H 4.31145400 3.93049600 1.35086400
H 2.69071900 3.48278800 1.91117400
H 3.93014900 2.23968300 1.72345000
C -4.56846100 1.44226900 0.00982400
C -4.09991600 0.16553300 0.33495000
C -5.64421100 1.55228000 -0.87770900
C -4.65388100 -0.98899900 -0.22758700
H -3.28807000 0.06377100 1.05292100
C -6.22387900 0.41251400 -1.42840400
H -6.03405800 2.53725700 -1.12825300
C -5.72798800 -0.84972700 -1.11290700
H -7.06785200 0.50829800 -2.10635900
H -6.18144800 -1.73851200 -1.54813800
C 4.86179600 1.17832200 -0.70089100
C 4.33805500 0.04298600 -1.32601500
C 5.86426200 1.00626100 0.25939600
C 4.76257200 -1.24708600 -0.99461800
H 3.57581600 0.16654500 -2.09283100
C 6.31561800 -0.26949900 0.58738900
H 6.29812900 1.87940100 0.74326200
C 5.76453800 -1.38989600 -0.02880100
H 7.10311100 -0.39136400 1.32607400
H 6.11992100 -2.38542700 0.23083600
Rh 0.10017300 -0.03844300 0.66110000
C -0.16800300 -0.18955900 2.58317800
C 0.28044700 0.82163200 3.55331800
O 1.02444500 0.40501900 4.44939700
C -1.07355200 -1.23463400 3.08024000

O -2.25492000 -0.97744400 3.25535200
O -0.51373600 -2.43362100 3.21998900
C -1.41619300 -3.47136000 3.64783800
H -2.24730800 -3.55913800 2.94448400
H -0.82571800 -4.38407600 3.66314300
H -1.80649000 -3.24846300 4.64244700
N -0.11069500 2.09208300 3.36678000
H -0.60537200 2.33667100 2.51832900
H 0.25470700 2.82093500 3.96002500

2w

Rh 0.03500200 -0.11917600 -1.84267700
O -1.37559600 1.38925200 -1.86857100
O 1.53449400 1.33262700 -1.81715400
O 1.41477300 -1.66139000 -1.73377700
O -1.48003600 -1.52757800 -1.69035300
C -1.86754000 -1.87326100 -0.53551600
O -1.41600000 -1.42818800 0.57467600
C 1.79459200 -2.07553500 -0.59686400
O 1.42435500 -1.60264400 0.53049300
C -1.64613000 1.96241500 -0.77480900
O -1.15664900 1.64879600 0.36650900
O 1.66672600 1.33041100 0.44701200
C 2.01164500 1.73665200 -0.71409700
C -2.64316000 3.12008200 -0.77145800
C -2.98027800 -2.91256100 -0.41238900
C 2.78356800 -3.23950900 -0.57273700
C 3.10749700 2.80150600 -0.77236000
C -3.84821000 2.71580100 0.12166900
H -4.55444000 3.55499700 0.09747600
H -3.48614000 2.62678000 1.15265400
C -3.09594300 3.44139000 -2.19031700
H -3.81446300 4.26717700 -2.16563300
H -2.25137600 3.74292300 -2.81509700
H -3.57584700 2.58350900 -2.66661200
C -1.96974300 4.34506100 -0.14548700
H -2.66741200 5.18794500 -0.14280200
H -1.67372000 4.15003500 0.88890500
H -1.08415400 4.64773400 -0.71240700
C -4.13364900 -2.28387300 0.41750400
H -4.92942300 -3.03664200 0.47805000
H -3.76439300 -2.11402500 1.43598300
C -2.42206800 -4.11783500 0.35072700
H -3.21128700 -4.86039600 0.50466900
H -1.61359000 -4.60043300 -0.20795500
H -2.03001000 -3.82036500 1.32711100

C -3.47135700 -3.34630000 -1.78789400
H -2.66700500 -3.80794500 -2.36617400
H -4.27592300 -4.08066800 -1.67565800
H -3.85577800 -2.50182900 -2.36490100
C 3.13562600 -3.63483300 0.85631000
H 3.85222900 -4.46260400 0.84028700
H 3.58092200 -2.80528800 1.41036600
H 2.24862200 -3.96240700 1.40481400
C 2.14102700 -4.42274300 -1.30264800
H 1.86993300 -4.15656900 -2.32714300
H 2.84458700 -5.26040400 -1.33690600
H 1.23953000 -4.76460900 -0.78446100
C 4.05271600 -2.80618700 -1.35691800
H 4.75977700 -3.64298700 -1.29844800
H 3.77409800 -2.69218300 -2.41039800
C 4.32546800 2.19466700 -1.52066700
H 4.03541700 2.04308900 -2.56654700
H 5.11552100 2.95567300 -1.51092300
C 2.58084400 3.99194500 -1.57815700
H 1.72637800 4.45989200 -1.07839700
H 3.36458300 4.74995600 -1.67401500
H 2.26944900 3.68739400 -2.58009600
C 3.49888000 3.25770200 0.62828700
H 4.28448300 4.01751600 0.56230200
H 2.64118800 3.69826400 1.14463700
H 3.86611300 2.43150500 1.24185900
C -4.52943600 1.44051600 -0.28685000
C -4.10124700 0.22213000 0.24885200
C -5.56959600 1.43106700 -1.22192100
C -4.66745400 -0.99556400 -0.14294300
H -3.31408900 0.22025700 1.00136300
C -6.15725900 0.22993200 -1.60986100
H -5.92709000 2.37227400 -1.63526700
C -5.70648700 -0.97626000 -1.07940700
H -6.97521000 0.23402600 -2.32547400
H -6.17120800 -1.91254500 -1.38317700
C 4.82787000 0.90144700 -0.94539300
C 4.29835400 -0.30929100 -1.40114500
C 5.79651900 0.86699600 0.06296200
C 4.69355300 -1.53883800 -0.86622400
H 3.55745500 -0.29329100 -2.19900500
C 6.21536700 -0.34945800 0.59635400
H 6.23135000 1.79834400 0.42059000
C 5.66603900 -1.54479200 0.13943200
H 6.97884400 -0.36653600 1.36953000
H 6.00084400 -2.49322100 0.55504700

Rh 0.11029600 -0.01961500 0.59001100
C -0.12078000 0.17183800 2.51509000
C 0.38258800 1.28351700 3.33912800
O 0.89453900 0.98640700 4.42902200
C -1.09279900 -0.70620000 3.18690700
O -2.25314100 -0.34446400 3.30924900
O -0.61293000 -1.89282800 3.55242000
C -1.58062200 -2.76979700 4.15932000
H -2.41394400 -2.93943300 3.47365300
H -1.05056500 -3.69797800 4.35889300
H -1.95919900 -2.33556600 5.08636100
N 0.28175200 2.53255500 2.85042600
H -0.05683200 2.64247200 1.90206900
C 0.75897600 3.67287400 3.59621400
H 0.20591400 4.56458100 3.30020500
H 0.60788300 3.49003500 4.66160100
H 1.82880000 3.84784500 3.43366900

2xa

Rh 0.58560600 1.11431200 -1.72501300
O 1.36870900 -0.70682000 -2.30942500
O -1.29190400 0.44727400 -2.34442800
O -0.18577700 2.91449300 -1.04301800
O 2.42826900 1.69179300 -0.96950400
C 2.68924100 1.44983200 0.24508200
O 1.92824600 0.83746700 1.06917300
C -0.63111400 2.98789500 0.14223600
O -0.66552300 2.02755000 0.98191000
C 1.27249300 -1.68539200 -1.51604200
O 0.75998400 -1.64241600 -0.34247800
O -1.79864500 -0.37592700 -0.29388500
C -2.05918300 -0.13673200 -1.52211400
C 1.81645500 -3.04394400 -1.95346900
C 4.03269400 1.90146700 0.81297200
C -1.17306800 4.33785200 0.60914900
C -3.42122100 -0.59401900 -2.04408200
C 2.97784700 -3.43299100 -0.99642200
H 3.38498000 -4.38222000 -1.36590500
H 2.54464100 -3.63031000 -0.00908800
C 2.29655300 -2.98667000 -3.39827800
H 2.69020400 -3.96535900 -3.69109000
H 1.47818600 -2.73220400 -4.07702300
H 3.08584600 -2.24366500 -3.53274500
C 0.70503700 -4.08673300 -1.80550700
H 1.07021700 -5.06697000 -2.12605900
H 0.38100000 -4.17073000 -0.76392800

H -0.16412000 -3.83682900 -2.42387700
 C 4.77281100 0.63313900 1.32361800
 H 5.74728900 0.96278100 1.70484300
 H 4.20587100 0.22989200 2.17122400
 C 3.76812400 2.83210800 1.99994700
 H 4.71485400 3.10513700 2.47659100
 H 3.27894600 3.75687800 1.67707200
 H 3.12931400 2.35165300 2.74558500
 C 4.85234400 2.62838400 -0.24574100
 H 4.33622900 3.52746500 -0.59225900
 H 5.81521600 2.93052300 0.17942700
 H 5.04377300 1.99741600 -1.11619400
 C -1.65570000 4.26827000 2.05310900
 H -2.04645900 5.24586900 2.35404400
 H -2.44773200 3.52694800 2.18225000
 H -0.83925300 4.00571200 2.73114700
 C -0.04582100 5.36729800 0.48116300
 H 0.32424300 5.42431600 -0.54555100
 H -0.41460400 6.35568100 0.77257100
 H 0.79399600 5.11751100 1.13741600
 C -2.33152300 4.74980500 -0.34012400
 H -2.72310500 5.70307800 0.03568000
 H -1.90145500 4.94524000 -1.32878900
 C -4.16442500 0.65805600 -2.58695200
 H -3.60813100 1.03293500 -3.45300100
 H -5.14086200 0.31475200 -2.95052600
 C -3.18444300 -1.56819000 -3.20205000
 H -2.66335500 -2.47008700 -2.86155200
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 H -2.59177600 -1.10674800 -3.99571200
 C -4.23527600 -1.27537300 -0.95019900
 H -5.21513100 -1.56014700 -1.34790700
 H -3.74080100 -2.18311000 -0.59325100
 H -4.39036500 -0.62170800 -0.08909700
 C 4.06678800 -2.40624300 -0.86549400
 C 3.97659600 -1.43153600 0.13318600
 C 5.17106300 -2.38299300 -1.72413000
 C 4.94540300 -0.43431900 0.28037000
 H 3.13490900 -1.45447500 0.82391600
 C 6.15550300 -1.40832300 -1.57930100
 H 5.26735800 -3.14426800 -2.49600100
 C 6.04366600 -0.43938400 -0.58596200
 H 7.01847700 -1.40934400 -2.23965800
 H 6.81961800 0.31492700 -0.47163500
 C -4.33374600 1.75384100 -1.57391800
 C -3.35506300 2.74283100 -1.44166000

C -5.43818400 1.79135700 -0.71668200
 C -3.43684000 3.73922700 -0.46395700
 H -2.50412100 2.73624300 -2.12049600
 C -5.54454300 2.78328300 0.25406800
 H -6.22041200 1.04183400 -0.81848900
 C -4.54800700 3.74751200 0.38622100
 H -6.41106700 2.80847800 0.90914200
 H -4.63748900 4.52338200 1.14418700
 Rh 0.05502400 0.17088300 0.45870700
 C -0.14187800 -0.74138100 2.17560500
 C -1.12816100 -1.77766100 2.52117300
 O -1.60441700 -1.77099600 3.66330800
 C 0.92455900 -0.56291900 3.17521900
 O 1.85078800 -1.35851700 3.20865200
 O 0.81501900 0.52357800 3.93569700
 C 1.89100100 0.70684700 4.87520500
 H 2.84902500 0.72641000 4.35077800
 H 1.69768100 1.66029500 5.36091800
 H 1.89694100 -0.10339500 5.60631000
 N -1.46681000 -2.62792400 1.51251600
 H -1.00200500 -2.44595800 0.62831000
 C -2.36401500 -3.70029300 1.52972000
 C -2.52448400 -4.41274200 0.33132400
 C -3.09297100 -4.07930500 2.66570300
 C -3.39522700 -5.49081500 0.26805100
 H -1.96352500 -4.10419000 -0.54893200
 C -3.95808400 -5.16557200 2.58501900
 H -2.97891700 -3.52308500 3.58631000
 C -4.11657500 -5.87612300 1.39754000
 H -3.51083900 -6.02967700 -0.66770700
 H -4.52037500 -5.45434400 3.46832200
 H -4.79844400 -6.71956600 1.35026600

2xd

Rh 1.87893000 0.47741900 -1.65881300
 O 1.08774600 -1.28929900 -2.37961300
 O 0.17727700 1.49422500 -2.32110600
 O 2.66600400 2.20507300 -0.83265000
 O 3.48208400 -0.56643700 -0.86658300
 C 3.39477000 -0.99197900 0.32322500
 O 2.38522500 -0.86030400 1.09546900
 C 2.36490700 2.52736300 0.35660600
 O 1.58236200 1.87318000 1.12531300
 C 0.23965700 -1.89546700 -1.66591400
 O -0.15985000 -1.51754400 -0.50838400
 O -0.88340400 1.24759500 -0.33357200

C -0.80409600 1.66789400 -1.53967000
C -0.38038000 -3.19032700 -2.18433700
C 4.58051100 -1.73680100 0.93338800
C 2.99352700 3.80083100 0.91730500
C -2.00702600 2.43651400 -2.08604900
C -0.03979400 -4.33058200 -1.18425700
H -0.48977000 -5.24603500 -1.58808600
H -0.54870200 -4.11029100 -0.23864900
C 0.13698500 -3.50992400 -3.58132600
H -0.31960700 -4.43937700 -3.93646100
H -0.11552400 -2.71441500 -4.28701600
H 1.22212600 -3.63510300 -3.59275900
C -1.90237300 -3.01955900 -2.21027300
H -2.36987100 -3.92749100 -2.60289900
H -2.29577600 -2.84570000 -1.20444500
H -2.20226000 -2.18506400 -2.85363000
C 4.07810900 -3.12610800 1.41542000
H 4.94533600 -3.65081200 1.83529600
H 3.36509900 -2.96414000 2.23298400
C 5.06668200 -0.93961000 2.14798700
H 5.87092400 -1.48404200 2.65255000
H 5.46197400 0.03589600 1.84798800
H 4.25684400 -0.77481800 2.86368600
C 5.70974900 -1.88150900 -0.07865000
H 6.07551100 -0.90388300 -0.40227800
H 6.54381200 -2.42391100 0.37852000
H 5.39042500 -2.42975300 -0.96773600
C 2.48317000 4.09614900 2.32287100
H 2.94923100 5.01446000 2.69499300
H 1.39900100 4.23045700 2.34309700
H 2.73179400 3.28455400 3.01136400
C 4.51235000 3.59837500 0.94415700
H 4.90063300 3.36784400 -0.05123500
H 4.99819400 4.51142100 1.30223300
H 4.79060600 2.78528500 1.62185300
C 2.66747200 4.97116000 -0.05021400
H 3.13595700 5.86842100 0.37261900
H 3.16339600 4.76685800 -1.00549000
C -1.51820300 3.83030900 -2.56649100
H -0.83506600 3.67702400 -3.40930400
H -2.39860800 4.35716700 -2.95476100
C -2.54438700 1.66262100 -3.29455100
H -2.89805200 0.66744300 -3.00348900
H -3.39156900 2.20031200 -3.73140400
H -1.77660700 1.54270300 -4.06291000
C -3.09714000 2.58230900 -1.03114700

H -3.93819700 3.14404900 -1.45055100
H -3.47161000 1.60782600 -0.70544900
H -2.73754100 3.11234300 -0.14631200
C 1.42741800 -4.53133300 -0.93328400
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C 2.19778800 -5.38230900 -1.73294300
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H 1.46411900 -3.20271200 0.75918200
C 3.56284200 -5.52563100 -1.49916100
H 1.71938800 -5.94490300 -2.53238200
C 4.17872500 -4.81045100 -0.47542400
H 4.14989000 -6.20038600 -2.11635800
H 5.24622700 -4.92445300 -0.29619100
C -0.84099600 4.64875800 -1.50403400
C 0.53524300 4.51592400 -1.29709600
C -1.55674400 5.52352800 -0.68008100
C 1.20038600 5.20226500 -0.27698200
H 1.10589600 3.85957800 -1.95088500
C -0.90717200 6.23468400 0.32562300
H -2.62611900 5.65247200 -0.83604900
C 0.46016500 6.07089900 0.53209800
H -1.47022400 6.92156600 0.95173800
H 0.96288400 6.62763600 1.32061800
Rh 0.68956800 0.15084700 0.44220700
C -0.24067100 -0.41711400 2.06004400
C -1.69392000 -0.49280700 2.29203900
O -2.11695500 -0.35158500 3.44505200
C 0.55643700 -1.09196000 3.10074100
O 0.61208000 -2.31113400 3.13078100
O 1.22692400 -0.26913200 3.90389200
C 2.03435100 -0.92619600 4.89855700
H 2.75740100 -1.58886300 4.41783100
H 2.54042600 -0.12969600 5.43852000
H 1.40441900 -1.50920800 5.57265700
N -2.46727800 -0.66088600 1.17708200
H -1.95601600 -0.71562300 0.30218800
C -3.85217400 -0.78561100 1.08670100
C -4.39678800 -0.92868600 -0.20099300
C -4.70351400 -0.78098400 2.20103600
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H -3.73434300 -0.92623700 -1.06370500
C -6.07118700 -0.93038600 2.01461500
H -4.29016900 -0.66085300 3.19249800
C -6.60755300 -1.07746700 0.73700900
H -6.17267600 -1.18305900 -1.37233000
H -6.72926300 -0.93496700 2.87723400

C -8.08268500 -1.18018900 0.53399700
F -8.72760900 -1.55989400 1.65427100
F -8.62242500 0.00278500 0.15599400
F -8.39971000 -2.06713200 -0.43507900

3

C -1.26394700 -0.25792600 0.00000200
H -1.30508800 -0.90739200 -0.88143100
H -1.30508700 -0.90738300 0.88144300
H -2.16905400 0.35643800 0.00000000
C 0.00000000 0.58562200 -0.00000300
H -0.00000100 1.24902200 -0.87412800
H 0.00000100 1.24903000 0.87411700
C 1.26394700 -0.25792600 0.00000000
H 2.16905400 0.35643800 -0.00000500
H 1.30508900 -0.90738300 0.88144000
H 1.30508600 -0.90739200 -0.88143400

4g

C -1.54330600 -0.98804800 -0.28483700
O -2.69841800 -0.61512700 -0.18473600
C -0.41338400 0.01195800 -0.54445800
C -0.82195600 1.46748300 -0.23201000
H -0.21258800 -0.05683700 -1.62371000
H -1.77696200 1.60339400 -0.75433300
C -1.06132000 1.70744600 1.25311600
H -1.77758700 0.99461700 1.66906600
H -0.13276200 1.62451100 1.82657900
H -1.45925600 2.71409400 1.41149100
C 0.19218100 2.45623500 -0.79081300
H 1.15744400 2.37353300 -0.27732800
H 0.37423000 2.29608000 -1.85828400
H -0.15880700 3.48380700 -0.65839300
C 0.85681100 -0.37171700 0.17403000
O 0.92181600 -0.69851000 1.34380100
O 1.92978500 -0.26769200 -0.63224100
C 3.18774000 -0.53995800 0.00501600
H 3.20981400 -1.56336200 0.38464300
H 3.94572100 -0.39999200 -0.76232600
H 3.34940300 0.15010700 0.83565900
C -1.16165600 -2.43824500 -0.22085700
H -0.70425700 -2.64087900 0.75269000
H -2.04064500 -3.07124600 -0.33909700
H -0.40987900 -2.68812100 -0.97636200

5a

C -2.56503700 0.29224900 0.00010300
O -3.01974700 1.43376200 0.00010700
C -3.48407600 -0.90265000 0.00018000
H -3.31029900 -1.53326500 0.87775000
H -4.52070400 -0.56726700 0.00022900
H -3.31035200 -1.53331400 -0.87736500
C -1.10547300 0.05087800 -0.00003900
C -0.54395300 -1.23790300 -0.00003900
C -0.23916200 1.15084700 -0.00023100
C 0.82659200 -1.41540700 -0.00015800
H -1.18683500 -2.11380100 0.00004100
C 1.13773600 0.99293100 -0.00031300
H -0.67736600 2.14486400 -0.00033200
C 1.67836300 -0.30085800 -0.00018800
H 1.26907000 -2.40653600 -0.00016300
H 1.78153700 1.86513000 -0.00058500
O 3.00203900 -0.57744800 -0.00015100
C 3.90266000 0.52238100 0.00049000
H 4.90248900 0.09108700 0.00120600
H 3.77477900 1.14386700 -0.89254100
H 3.77345000 1.14391400 0.89328200

5b

C -2.17527000 -0.17525200 0.00085700
O -2.72553600 -1.27226600 0.00137800
C -2.98642500 1.09410600 0.00238900
H -2.76106300 1.70723700 -0.87569200
H -4.04752600 0.84828800 0.00462900
H -2.75736900 1.70765600 0.87921100
C -0.69497800 -0.06633900 -0.00086500
C -0.02851800 1.16458400 -0.00225800
C 0.06974100 -1.24229900 -0.00156600
C 1.36045100 1.21499100 -0.00353600
H -0.59248600 2.09337100 -0.00303300
C 1.45268600 -1.18742200 -0.00279700
H -0.45573800 -2.19318100 -0.00164700
C 2.12519200 0.04432100 -0.00275500
H 1.86536800 2.17832000 -0.00529200
H 2.03202300 -2.10818500 -0.00391300
C 3.62038000 0.09474400 0.00480300
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H 4.04341000 -0.47789400 -0.82665400
H 3.99186200 1.11932600 -0.06616300

5c

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O -2.21443200 -1.30973100 -0.00002100
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H -2.31391600 1.66790000 -0.87734600
H -3.58446200 0.78203400 -0.00025400
H -2.31427000 1.66766600 0.87762700
C -0.20974100 -0.05909000 0.00000400
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C 0.57391600 -1.22076400 0.00001200
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H -0.16677900 2.10247800 0.00000600
C 1.95877200 -1.13759400 0.00001000
H 0.06387600 -2.17980400 0.00002900
C 2.58025100 0.11212500 -0.00000300
H 2.29574400 2.24683000 -0.00001500
H 2.55878400 -2.04278100 0.00002000
H 3.66446400 0.17911800 -0.00001300

5d

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H -2.71488400 1.70297300 -0.87780000
H -4.00120200 0.84154200 -0.00038200
H -2.71541200 1.70305500 0.87770700
C -0.64680900 -0.06592800 0.00013100
C 0.01489100 1.16969600 0.00012500
C 0.11435500 -1.24386500 0.00001500
C 1.40200000 1.23399300 0.00004400
H -0.55201000 2.09589800 0.00020100
C 1.49889500 -1.20054200 -0.00007700
H -0.41297700 -2.19308100 0.00001200
C 2.11830300 0.04450400 -0.00004900
H 1.93192100 2.18001500 0.00005200
H 2.10320800 -2.10088100 -0.00016400
F 3.46059200 0.09859500 -0.00014900

5e

C 2.56568300 0.16463100 0.00000900
O 3.11623600 1.25979600 -0.00005300
C 3.36670300 -1.10873400 0.00004800
H 3.13480800 -1.72025400 -0.87748200
H 4.42922300 -0.87004900 -0.00053900
H 3.13552500 -1.71980900 0.87804700
C 1.08066200 0.06655600 0.00001000
C 0.40668400 -1.16068400 0.00000400
C 0.33262400 1.25107900 0.00004500

C -0.98186700 -1.21100900 -0.00005700
H 0.96166400 -2.09410300 0.00008500
C -1.05265900 1.22193400 -0.00001400
H 0.86680700 2.19644600 0.00013400
C -1.69513600 -0.01569600 -0.00008700
H -1.50698400 -2.15991100 -0.00005500
H -1.63434800 2.13738700 0.00005100
Cl -3.43839700 -0.06450200 0.00002500

5f

C 0.22554500 0.39588200 0.00001200
O 1.23826600 -0.27274200 0.00000200
C -1.16204800 -0.15110100 0.00002800
H -1.70579800 0.22195500 -0.87430700
H -1.16021400 -1.24167000 0.00043300
H -1.70632100 0.22279500 0.87364500
H 0.28522200 1.51017100 -0.00003200

5g

C 0.00000000 0.18467200 -0.00001400
O 0.00002700 1.40497300 0.00000300
C -1.27619100 -0.61351400 -0.00233400
H -1.36742700 -1.16887800 0.93727700
H -2.14160100 0.03927000 -0.11686900
C 1.27616600 -0.61355300 0.00233100
H 1.36747300 -1.16885800 -0.93729300
H -1.26735100 -1.36306400 -0.79967900
H 2.14156600 0.03922100 0.11696700
H 1.26728000 -1.36310600 0.79967100

5h

C -0.64014300 -0.17444200 0.03024000
O -1.55015500 -0.94754200 -0.22455900
C -0.85787100 1.31392100 0.08117900
H -0.35165500 1.79377800 -0.76351600
H -1.92164000 1.54591700 0.03273500
C 0.75500400 -0.67518200 0.33502900
C 1.88887500 0.16373300 -0.23602700
H 1.82508600 0.23567700 -1.32599400
H 1.88396300 1.18180300 0.16398500
H 2.85759900 -0.27808800 0.00830900
H 0.83865400 -0.69976100 1.43111500
H -0.41940000 1.74799700 0.98562600
H 0.81343900 -1.71516400 0.00168900

5i

C 1.49005000 -0.19489400 -0.24447100
O 1.76952200 -1.34757700 0.05037900
C 2.42238900 0.94708200 0.05070000
H 3.28376300 0.61320600 0.62964000
H 2.76709400 1.39099700 -0.88995200
C 0.18236800 0.15579900 -0.92012800
C -1.05181000 0.05029400 0.01216700
H 0.23195500 1.17545900 -1.32219400
H 1.89758200 1.74627200 0.58499300
H 0.03777900 -0.52901900 -1.76426300
C -1.31074900 -1.40459500 0.39940000
H -0.46409900 -1.83840000 0.93703300
H -2.19692800 -1.47389500 1.03985900
H -1.49058500 -2.02083700 -0.48852200
C -2.25913700 0.59214600 -0.75249300
H -3.16581200 0.52522300 -0.14124500
H -2.11766600 1.64312400 -1.02785900
H -2.43400800 0.02403900 -1.67276300
C -0.83302200 0.88885600 1.27250200
H 0.00076500 0.50743100 1.87387900
H -0.62098200 1.93575800 1.02574100
H -1.72556300 0.87312800 1.90655900

5j

C -0.74051800 -0.32939800 0.02976000
O -0.93014300 -1.47130600 -0.35858200
C -1.88009100 0.64511700 0.17960300
H -1.90330900 1.31441800 -0.68737200
H -2.82990400 0.11148000 0.22169800
C 0.64983400 0.17736300 0.37983600
C 1.71020100 -0.87790500 0.12465100
H 1.76757700 -1.11794200 -0.94159800
H 2.69390900 -0.52385200 0.44475800
H 1.48728100 -1.80664200 0.65424800
C 0.96322800 1.49038300 -0.34036800
H 0.95301700 1.35254800 -1.42709100
H 0.25070000 2.28206200 -0.09464800
H 1.95959300 1.84497800 -0.06316000
H 0.61089900 0.39922000 1.45873200
H -1.76454300 1.28082400 1.06219700

5k

C -1.81496700 -0.21840400 0.00897900
O -2.25810400 -1.26064900 -0.44828800
C -2.70939700 0.96836400 0.25820200
H -2.60845000 1.67967300 -0.56917400

H -3.75202300 0.65332400 0.30708300
H -2.43387200 1.50805100 1.16888100
C -0.34510100 -0.05163000 0.34185400
C 0.46857000 -1.29791100 0.01324500
C 0.25667500 1.19457400 -0.32859600
H -0.30274700 0.12572700 1.43155300
C 1.93635500 -1.12101000 0.37911100
H 0.37655700 -1.49924300 -1.06334500
H 0.03582300 -2.16760700 0.51846400
C 1.72788100 1.35886100 0.03368600
H 0.15605900 1.09157600 -1.41942900
H -0.30528400 2.09200300 -0.04703300
C 2.53141700 0.10740400 -0.29952100
H 2.50373700 -2.02018100 0.11405700
H 2.02794400 -1.00997600 1.46977800
H 2.14374200 2.23398600 -0.47831200
H 1.80818400 1.56260000 1.11156800
H 3.58031500 0.23851100 -0.01064700
H 2.52625300 -0.04473900 -1.38889500

5l

C 0.90272900 0.32108100 -0.02733600
O 1.25977700 1.48838000 -0.03590000
C -0.58098900 -0.06101400 -0.01043800
C 1.91343800 -0.79683500 -0.01258400
H 2.00293000 -1.21695500 -1.02049400
H 2.88942300 -0.41511700 0.28712600
H 1.61634000 -1.62227300 0.64053300
C -0.92010900 -0.47608100 1.43041900
H -1.97895600 -0.74665000 1.49557400
H -0.33700500 -1.34296500 1.75648200
H -0.73771600 0.34258500 2.13367100
C -1.42832300 1.14220100 -0.40708500
H -1.21140300 1.45924100 -1.43175200
H -2.49192200 0.89151700 -0.34668300
H -1.23435600 1.99424400 0.24842500
C -0.85234900 -1.23567100 -0.95407300
H -1.91728700 -1.48837100 -0.93570000
H -0.58761100 -0.99120000 -1.98819200
H -0.29703300 -2.13317900 -0.66520500

5m

C 0.44239700 0.16327100 -0.00003200
O 0.40001300 1.38736600 0.00025300
C 1.73980600 -0.59455100 -0.00038100
H 1.79290600 -1.25491600 -0.87250600

H 2.59026800 0.08665500 -0.00480300
H 1.79677800 -1.24727900 0.87729900
C -0.79196900 -0.66414100 0.00039300
C -2.00527700 -0.10703700 -0.00031100
H -0.67198700 -1.74632600 0.00117000
H -2.91472500 -0.69817600 -0.00010700
H -2.10308800 0.97585900 -0.00109400

5n

C 0.09153200 0.12309300 0.00030500
O 0.65154000 1.19981300 -0.00004800
C -1.38601700 -0.10100300 0.00012200
H -1.67780500 -0.69068400 0.87194700
H -1.91033900 0.85247400 0.00834500
H -1.67901400 -0.67475900 -0.88206200
O 0.76424200 -1.04895800 0.00004100
H 1.70780800 -0.82640600 -0.00073000

5o

C 0.46050000 0.17577800 -0.00221900
O 0.27711500 1.37601400 -0.00017400
C 1.78967400 -0.51163500 0.00057400
H 1.86547900 -1.19912900 -0.84468700
H 2.59052700 0.22371500 -0.04933300
H 1.90083800 -1.11026200 0.90787400
O -0.54246100 -0.72792400 -0.00268100
C -1.85979500 -0.16354000 0.00175000
H -2.54572000 -1.00836500 0.00116600
H -2.01333000 0.45069300 0.89163400
H -2.01730200 0.45500300 -0.88444600

5p

C 0.88989900 0.16869300 -0.07488700
O 0.68198100 1.35651700 -0.22522400
C 2.19666700 -0.43973500 0.32996600
H 2.42089300 -1.32489900 -0.26754300
H 2.99532500 0.29360600 0.23234900
H 2.14109000 -0.76237300 1.37324000
O -0.04788000 -0.78692300 -0.23939600
C -1.37380700 -0.31855400 -0.58239000
H -1.84558500 -1.17742300 -1.06398500
H -1.28213900 0.49036700 -1.31215700
C -2.13145800 0.12414700 0.64327900
H -1.65031900 0.98866700 1.10612700
H -3.15145700 0.40823700 0.37208900
H -2.18842600 -0.68023400 1.38103500

5q

C -0.85737500 0.17993800 -0.07161700
O -0.65118800 1.36627500 -0.17547900
C -2.15487400 -0.47548000 0.26147600
H -2.11372700 -0.85528000 1.28602400
H -2.96821000 0.24327700 0.18289600
H -2.33787000 -1.33203700 -0.38924700
O 0.12053300 -0.76726400 -0.23938200
C 1.40970800 -0.26657700 -0.49529200
H 1.97300600 -1.09454000 -0.92691200
H 1.36283800 0.59976000 -1.15949500
F 1.99382800 0.11327100 0.68424700

5r

C 0.72992200 -0.29061400 0.00003900
O 1.07566800 -1.47342600 0.00000600
C 1.75304300 0.82087500 -0.00005500
H 1.66266900 1.46276700 0.88084600
H 2.74323200 0.36743300 -0.00016000
H 1.66246200 1.46282100 -0.88088700
N -0.58823800 0.07700200 0.00017300
C -1.07656900 1.43791200 -0.00000200
H -1.69599800 1.62427300 -0.88586700
H -1.69733900 1.62395400 0.88497300
H -0.25966600 2.15577600 0.00071900
C -1.61609100 -0.94125800 -0.00006800
H -2.25301700 -0.84586400 -0.88719900
H -1.13816700 -1.91873500 0.00028800
H -2.25368200 -0.84552200 0.88654000

5s

C 1.44908500 -0.20904500 -0.01266600
O 1.96848100 -1.32658200 -0.07562100
C 2.25554200 1.06180000 0.08588200
H 1.95075700 1.67072500 0.94268000
H 3.31071400 0.80921800 0.18280800
H 2.12273000 1.68223800 -0.80621300
N 0.10086000 -0.05087400 -0.03365400
C -0.62788800 1.21531500 0.05137100
C -0.79411900 -1.20621700 -0.08225500
H -0.23141300 1.94952100 -0.65752600
H -0.53837800 1.64766300 1.05909600
C -2.06533100 0.80766400 -0.25243900
H -0.80157400 -1.63795700 -1.09282500
H -0.43705900 -1.98355900 0.59844100

C -2.14562900 -0.61608200 0.29211200
H -2.22708100 0.80440700 -1.33613800
H -2.79480400 1.48891300 0.19059500
H -2.98222800 -1.18807900 -0.11468400
H -2.25548900 -0.59491900 1.38228400

5t

C -1.16261000 -0.21572200 -0.02918300
O -1.65875400 -1.34086500 0.04827700
C -1.96534800 1.05913600 0.02419500
H -1.58067400 1.82164000 -0.65825100
H -3.00625400 0.84587600 -0.21731700
H -1.92905500 1.48116500 1.03397500
N 0.17350700 -0.04126300 -0.16787000
C 1.05904100 1.11256400 -0.00762000
C 1.23364100 -1.02930000 -0.01371700
C 2.24217600 0.13112000 0.08018900
H 0.86201100 1.69410600 0.90158500
H 1.06054100 1.79663200 -0.86446400
H 1.12107600 -1.63907500 0.89039200
H 1.34256400 -1.70048700 -0.87274600
H 2.80759800 0.17710600 1.01124900
H 2.93627800 0.19201200 -0.75872300

5u

C 0.87958800 -0.50587800 -0.05316100
O 0.65759900 -1.69081100 -0.27527000
C 2.24982200 0.02463100 0.28970400
H 2.25853400 0.56104200 1.24230400
H 2.93314900 -0.82064800 0.35426700
H 2.61425000 0.71421800 -0.47738300
N -0.12640700 0.43017000 -0.04291700
C -0.00463400 1.86818000 -0.07386800
H -0.02288500 2.25386400 -1.09982200
H -0.83349000 2.31135200 0.48382700
H 0.92686700 2.17073900 0.40307300
O -1.35673700 0.00485900 -0.56581900
C -2.16467100 -0.51465600 0.48851100
H -2.33224700 0.23616400 1.26999600
H -3.11674900 -0.77357100 0.02252300
H -1.71010400 -1.41038300 0.92323800

5v

C -0.07755000 0.14236400 -0.00265100
O -0.37028500 1.33525800 0.00042800
C 1.35429700 -0.33295500 -0.00034500

H 1.46354600 -1.41593700 -0.08259900
H 1.88907000 0.14114100 -0.82562400
H 1.83718500 -0.00270400 0.92240700
N -1.01662700 -0.83774000 -0.00222000
H -0.78125700 -1.81494200 0.00380700
H -1.99035500 -0.58189500 0.01209500

5w

C 0.48589500 0.17590200 -0.00020600
O 0.41178000 1.40378700 0.00009700
C 1.80112700 -0.56622000 0.00003800
H 1.89122700 -1.20900600 -0.88031900
H 2.62217700 0.14916500 0.00025600
H 1.89087300 -1.20912700 0.88034800
N -0.61126600 -0.62964100 -0.00015100
C -1.95808500 -0.11455700 0.00009600
H -2.51186600 -0.43451000 0.88821300
H -1.89057000 0.97347200 -0.00031100
H -2.51238300 -0.43516300 -0.88745400
H -0.47846000 -1.62838600 -0.00002400

5xa

C 2.17024100 0.15939900 -0.00699300
O 2.12791100 1.38500300 -0.00879000
C 3.47885500 -0.58889900 0.01100200
H 3.38321900 -1.66757600 -0.12622900
H 4.12669900 -0.18795500 -0.77078300
H 3.97979200 -0.40493300 0.96503800
N 1.05889200 -0.64843700 -0.00756500
H 1.23362800 -1.64241700 -0.00512900
C -0.29876600 -0.28958000 -0.00288900
C -1.23676400 -1.33212600 -0.00363500
C -0.74752100 1.03789800 0.00156000
C -2.59769100 -1.05528300 -0.00001000
H -0.89068200 -2.36337300 -0.00718900
C -2.11537100 1.29673900 0.00510700
H -0.02787300 1.84444600 0.00202500
C -3.04796300 0.26324600 0.00432400
H -3.30712500 -1.87806400 -0.00070100
H -2.45159300 2.32998900 0.00850000
H -4.11171800 0.48055900 0.00695300

5xb

C 3.07360100 -0.13923400 0.01782700
O 3.03255500 -1.36523500 0.07312100
C 4.38325100 0.60774000 -0.00995000

H 4.28337300 1.69484200 -0.01249100
H 4.97877500 0.31182400 0.85637200
H 4.94471200 0.30726500 -0.89794100
N 1.96418000 0.66437500 -0.02967400
H 2.13534800 1.65826800 -0.05892300
C 0.60510300 0.29953700 -0.01986200
C -0.34221400 1.32666500 0.00707000
C 0.15840900 -1.03042300 -0.04188700
C -1.70646900 1.05299800 0.01286800
H -0.01107900 2.36253600 0.02450800
C -1.20088400 -1.30353200 -0.03462800
H 0.87958200 -1.83569200 -0.06253300
C -2.14501100 -0.27243800 -0.00705000
H -2.41036500 1.87748800 0.03428300
H -1.55295500 -2.33065000 -0.05107400
O -3.45385200 -0.65400800 -0.00224700
C -4.41991700 0.38148900 0.02662000
H -4.34327400 1.03139900 -0.85386800
H -5.39287200 -0.10865200 0.02717400
H -4.32534900 0.99787200 0.92916600

5xc

C -3.02891100 -0.24912200 -0.00004300
O -2.90042700 -1.46803200 -0.00032200
C -4.38375200 0.41012400 0.00001000
H -4.35468300 1.50108700 0.00062900
H -4.94063400 0.07514900 -0.87786800
H -4.94100100 0.07415200 0.87725600
N -1.97269800 0.63164700 0.00023700
H -2.21176700 1.61206300 0.00030800
C -0.59742000 0.36133000 0.00009000
C 0.26989500 1.46267400 -0.00007400
C -0.05824000 -0.93231000 0.00020900
C 1.64597600 1.28895700 -0.00013300
C 1.32121400 -1.10767000 0.00014000
H -0.71768200 -1.78823000 0.00035200
C 2.16344500 -0.00219700 -0.00003000
H 2.30786100 2.14760000 -0.00023900
H 1.73813300 -2.10910800 0.00024800
Cl 3.89863000 -0.23830100 -0.00003800
H -0.13788300 2.47042400 -0.00014000

5xd

C 3.67883600 -0.27112400 0.00479700
O 3.53049200 -1.48667100 0.00200800
C 5.04260000 0.36873800 0.00316300

H 5.02910100 1.45990600 0.01582900
H 5.60087800 0.01468200 0.87244800
H 5.58820100 0.03575100 -0.88252400
N 2.63486500 0.62767100 0.00811700
H 2.89112600 1.60386200 0.00984200
C 1.25772600 0.38348000 0.00084800
C 0.41359900 1.50371800 -0.00366100
C 0.69392500 -0.90176000 -0.00636700
C -0.96270200 1.35172200 -0.01680600
H 0.84534700 2.50135100 -0.00082700
C -0.68670200 -1.04123500 -0.02010500
H 1.33834700 -1.76869900 -0.00557800
C -1.52263400 0.07487100 -0.02873500
H -1.60461500 2.22590700 -0.02525200
H -1.11970800 -2.03735500 -0.03232200
C -3.00249800 -0.10722400 -0.00134300
F -3.66031400 0.99968700 -0.40345300
F -3.45893500 -0.39805700 1.24180900
F -3.40625800 -1.12416800 -0.79560600

5xe

C -2.39338700 -0.31841000 -0.00011400
O -2.54713700 -1.53352500 -0.00061700
C -3.56151300 0.63237700 0.00028600
H -3.28455600 1.68783200 0.00003200
H -4.18030200 0.43130400 -0.87677000
H -4.17950100 0.43154600 0.87796600
N -1.16436000 0.30429900 0.00019200
H -1.17440200 1.31459900 0.00045800
C 0.10821300 -0.26939600 0.00011300
C 1.23631300 0.57236600 -0.00002600
C 0.33648300 -1.65386300 0.00022200
C 2.53016800 0.07060400 -0.00007800
C 1.63175800 -2.15637200 0.00016100
H -0.51951100 -2.31341600 0.00033500
C 2.73262300 -1.30541000 0.00000800
H 3.36615200 0.76138100 -0.00018400
H 1.77604200 -3.23251500 0.00025200
H 3.74324400 -1.70054700 -0.00004800
Cl 1.01508900 2.31332600 -0.00011100

5xf

C -2.64489500 -0.03461800 -0.01530300
O -3.13258400 1.07641600 -0.17324300
C -3.49292100 -1.27839700 0.04239800
H -2.94936300 -2.18132100 0.32600500

H -4.30867800 -1.11848900 0.74936400
H -3.94701200 -1.44163000 -0.93815600
N -1.29142600 -0.27675000 0.10743600
H -1.04037500 -1.24680500 0.21879000
C -0.22939600 0.63498800 0.05784300
C 1.09520600 0.14440200 0.00668300
C -0.42820200 2.02201200 0.07053200
C 2.17131600 1.02770900 -0.02689000
C 0.66050200 2.88522400 0.03353700
H -1.43759500 2.40486300 0.10649300
C 1.96348700 2.40093600 -0.01432100
H 3.17702600 0.62467400 -0.06529200
H 0.47864700 3.95601500 0.04634400
H 2.80896700 3.08004200 -0.04068400
C 1.35960200 -1.32637000 -0.01804000
F 2.66420700 -1.62372900 -0.07090500
F 0.76800800 -1.93617100 -1.07760500
F 0.85565700 -1.95196100 1.08322100

5xg

C -2.88709100 -0.03661200 0.28784400
O -2.64666500 -0.87900000 1.13776600
C -4.27517100 0.42928900 -0.05174200
H -4.30078000 1.35376200 -0.63115200
H -4.77862600 -0.34887500 -0.63160500
H -4.84191200 0.56364800 0.87013100
N -1.88887900 0.54578100 -0.47425200
H -2.11333000 1.37109900 -1.01076100
C -0.53066200 0.27161400 -0.28474800
C 0.37837800 1.31860600 -0.12085900
C -0.02491400 -1.03053900 -0.27775700
C 1.73630700 1.09310800 0.05132900
C 1.32819700 -1.27138000 -0.07001600
C 2.21321300 -0.21210000 0.08978700
F -0.82370600 -2.07249300 -0.50598300
F 1.78704300 -2.52476500 -0.06327500
F 3.51338300 -0.44815900 0.26782200
F 2.57342900 2.12143900 0.20245800
F -0.07230500 2.57953300 -0.13680200

5a'

C 3.28162500 1.30072900 -0.16670400
C 2.68621300 0.06645800 0.02216600
H 4.36663300 1.38129700 -0.17499400
O 3.28565400 -1.04772400 0.20507000
H 2.71761400 2.20276900 -0.38172900

C 1.17053100 0.00885400 0.00109700
C 0.56065100 -1.25249800 -0.07629400
C 0.31838500 1.11614900 0.07593400
C -0.81741500 -1.40562400 -0.09909300
H 1.22532500 -2.11203400 -0.11016900
C -1.07072800 0.98933000 0.06237100
H 0.74357800 2.11299800 0.16834000
C -1.64578300 -0.28149200 -0.03023100
H -1.27942300 -2.38805200 -0.16412000
H -1.69089100 1.87770600 0.13109600
O -2.99456400 -0.52505100 -0.05015300
C -3.84370100 0.59941600 0.05291600
H -4.86459600 0.21724000 0.03059600
H -3.68368100 1.14552800 0.99177200
H -3.70194100 1.29681200 -0.78308700

5b'

C -2.99193400 1.10716300 0.04130900
C -2.27601200 -0.07532700 -0.00030000
H -4.07912200 1.07591700 0.04965500
O -2.76747700 -1.25457100 -0.03262500
H -2.52754300 2.08681600 0.08283500
C -0.76033900 0.01949700 -0.00411200
C -0.02897100 -1.17384100 0.01040000
C -0.01908800 1.21226800 -0.02615500
C 1.36304100 -1.18348100 0.01150500
H -0.60559900 -2.09502800 0.01852000
C 1.37067200 1.20614700 -0.02570900
H -0.53514500 2.16925600 -0.05132300
C 2.09468000 0.00606100 -0.00343600
H 1.89997100 -2.13254200 0.02290600
H 1.91275800 2.15173300 -0.04559100
C 3.59373000 0.00645400 0.01532000
H 4.01278000 0.64871700 -0.76714200
H 3.98962600 0.38185800 0.96676400
H 3.99741500 -0.99980700 -0.12856300

5c'

C -2.50951300 1.10281100 -0.00265700
C -1.78997600 -0.07796500 0.00019800
H -3.59651900 1.06809100 -0.00274700
O -2.27771100 -1.25903500 0.00277800
H -2.04930700 2.08529100 -0.00541100
C -0.27353200 0.02148200 0.00014200
C 0.45662200 -1.17497500 -0.00112900
C 0.46097900 1.21830200 0.00151200

C 1.84853300 -1.18577900 -0.00146200
H -0.12355700 -2.09374100 -0.00183600
C 1.85271900 1.21672100 0.00126700
H -0.06045300 2.17235600 0.00307700
C 2.55885000 0.01267400 -0.00030700
H 2.38458800 -2.13345200 -0.00258700
H 2.39262000 2.16179600 0.00239800
H 3.64622600 0.01231200 -0.00050500

5d'

C 2.94791700 1.10427900 0.00223600
C 2.22845100 -0.07588800 -0.00007400
H 4.03472800 1.06961800 0.00223700
O 2.71315400 -1.25808900 -0.00232900
H 2.48784500 2.08675400 0.00456400
C 0.71219900 0.02252900 -0.00008100
C -0.01472300 -1.17543200 0.00094100
C -0.02348100 1.21801800 -0.00127200
C -1.40669400 -1.19951100 0.00112100
H 0.56713900 -2.09260700 0.00157800
C -1.41521400 1.22341900 -0.00116200
H 0.49382300 2.17363300 -0.00257000
C -2.08583000 0.00775700 0.00010400
H -1.96665500 -2.13061200 0.00199200
H -1.98326300 2.14916400 -0.00211800
F -3.44384400 0.00641500 0.00023100

5e'

C 3.38203800 1.10495300 0.00208000
C 2.66453900 -0.07635000 -0.00005200
H 4.46873800 1.07236300 0.00207600
O 3.14738500 -1.25869700 -0.00219100
H 2.92027400 2.08640200 0.00424800
C 1.14986600 0.02407100 -0.00004000
C 0.42377400 -1.17429800 0.00090200
C 0.41323200 1.21864500 -0.00116400
C -0.96701200 -1.20044000 0.00103400
H 1.00548700 -2.09168600 0.00150700
C -0.97758300 1.22372200 -0.00109900
H 0.92757700 2.17574500 -0.00237200
C -1.65448500 0.00676500 0.00006400
H -1.51391600 -2.13926700 0.00184200
H -1.53401100 2.15648600 -0.00200800
Cl -3.41526100 0.00277200 0.00011100

5f'

C -1.17875100 -0.16979000 0.00001500
C 0.09631800 0.35096000 0.00009400
H -1.35845700 -1.24535500 -0.00014200
O 1.22622600 -0.22707600 -0.00002500
H -2.04521100 0.48861400 -0.00005900
H 0.08845500 1.48633000 -0.00025300

5g'

C -1.17064000 -0.80257800 0.00017300
C -0.13412000 0.11071400 -0.00005900
H -2.20816000 -0.47028300 -0.00016200
O -0.21333400 1.38451700 -0.00000700
C 1.28642700 -0.46773900 -0.00001100
H 1.32946700 -1.56352900 -0.00077000
H -0.98795000 -1.87468300 -0.00058800
H 1.84190500 -0.10423100 -0.87479600
H 1.84140900 -0.10579200 0.87575100

5h'

C 1.68437300 -0.73181200 -0.23744200
C 0.63597100 0.10877200 0.07994700
H 2.66082600 -0.33170000 -0.51066300
O 0.63122600 1.38610300 0.08671700
C -0.69205900 -0.56370400 0.47416900
C -1.85284800 -0.03106200 -0.34967600
H -1.82420100 1.06294900 -0.32905700
H -1.76759100 -0.33925500 -1.39886400
H -2.83058800 -0.36481100 0.01540800
H -0.62994000 -1.65806500 0.39648800
H 1.57663400 -1.81363500 -0.20338700
H -0.88756900 -0.33747300 1.53434700

5i'

C -2.42597600 -0.99360000 0.04179300
C -1.58870300 0.07521200 -0.21714500
H -3.39691800 -0.84134500 0.51259500
O -1.82138300 1.31051200 0.02046800
C -0.23820400 -0.26865200 -0.86754300
C 1.01182500 -0.04333500 0.01074800
H -0.22863600 -1.31975500 -1.19490500
H -2.13549700 -2.01613200 -0.18899900
H -0.11795100 0.34460300 -1.77591500
C 1.20649500 1.44127800 0.31719600
H 1.35909700 2.01210100 -0.60757100
H 0.31787700 1.84675200 0.80562500
H 2.08795700 1.59641900 0.95372200

C 0.87646200 -0.81733100 1.32147300
H 0.72660600 -1.88784200 1.13394600
H 1.77691200 -0.70743300 1.93891700
H 0.01685600 -0.46572500 1.90039500
C 2.23952400 -0.55669300 -0.74320200
H 3.15930700 -0.39435500 -0.16624700
H 2.16109000 -1.63101900 -0.95049800
H 2.35582800 -0.04164300 -1.70473500

5j'

C 1.90807800 0.00252400 -0.79301800
C 0.85997900 -0.00059400 0.10396900
H 2.94229900 0.00127500 -0.44971400
O 0.92138800 -0.00469000 1.38039700
C -0.56617600 0.00140400 -0.49570400
C -1.31470300 -1.24808200 -0.04792600
H -1.28809800 -1.30427500 1.04611200
H -2.36396100 -1.24752400 -0.36858200
H -0.84363900 -2.15893600 -0.43523100
C -1.31385200 1.24892800 -0.04106700
H -1.28690700 1.29913300 1.05323100
H -0.84225800 2.16157300 -0.42347500
H -2.36320600 1.25084600 -0.36141400
H -0.50087600 0.00444100 -1.59465600
H 1.73558000 0.00590800 -1.86697600

5k'

C 2.86414300 -0.00049300 -0.89146600
C 1.88670800 0.00013800 0.08253400
H 3.92122500 -0.00056100 -0.62640800
O 2.04528800 0.00065100 1.35106900
H 2.61063900 -0.00089300 -1.94923000
C 0.42366000 0.00001900 -0.40626600
C -0.30427500 -1.24812500 0.09482000
C -0.30447500 1.24827300 0.09424300
H 0.39547000 -0.00025000 -1.50954500
C -1.78938400 -1.25447600 -0.24699300
H -0.16752400 -1.28046000 1.18559400
H 0.18664000 -2.14654000 -0.30354900
C -1.78958900 1.25420000 -0.24758500
H -0.16773200 1.28114700 1.18500000
H 0.18626900 2.14660000 -0.30453700
C -2.48100400 -0.00007300 0.27417400
H -2.27647600 -2.15507100 0.14973600
H -1.91112000 -1.29779400 -1.34071400
H -2.27684200 2.15490000 0.14870600

H -1.91132200 1.29696700 -1.34132900
H -3.54414000 -0.00022700 0.00286500
H -2.44210500 0.00018900 1.37409400

5l'

C 1.79187600 1.06301300 0.00005600
C 1.02477000 -0.08421500 -0.00004500
H 2.87809000 0.98212300 -0.00036000
O 1.45836200 -1.28702500 -0.00006400
C -0.53244500 0.04605800 0.00000200
H 1.37211800 2.06340300 -0.00032100
C -1.05202900 -0.67747100 -1.24310300
H -0.62069500 -1.68178100 -1.28239900
H -2.14742000 -0.75756800 -1.24359700
H -0.75468800 -0.14725700 -2.15665700
C -1.05179200 -0.67761500 1.24312300
H -0.75442100 -0.14739200 2.15665900
H -2.14715700 -0.75777500 1.24362700
H -0.62030800 -1.68186500 1.28229300
C -1.05935100 1.47650100 0.00011400
H -0.72000000 2.02847900 0.88400600
H -0.72064600 2.02838000 -0.88409500
H -2.15794000 1.48982000 0.00048300

5m'

C -1.68333100 -0.68211300 -0.00075900
C -0.54728700 0.11433100 0.00012100
H -2.68010400 -0.24343800 0.00159700
O -0.48681700 1.38850800 -0.00006700
H -1.61237600 -1.76696600 0.00254300
C 0.73663000 -0.65698400 0.00007700
C 1.93790200 -0.06714600 0.00016100
H 0.66788300 -1.74843700 -0.00114600
H 2.87441100 -0.61860300 -0.00052600
H 1.98124200 1.02086000 0.00046400

5n'

C -1.39320000 -0.16458400 0.00107500
C -0.04522600 0.11931800 -0.00017900
H -2.11305800 0.64653000 -0.00248900
O 0.56752900 1.21929300 -0.00002800
H -1.75603700 -1.18665600 -0.00236400
O 0.78671100 -1.03795500 -0.00002200
H 1.66573200 -0.63898700 -0.00012600

5o'

C -1.77854400 -0.56187500 -0.00037300
C -0.58725200 0.13056800 0.00005700
H -2.71415700 -0.01399100 0.00029900
O -0.34684500 1.35984200 0.00008700
H -1.80422500 -1.64554100 0.00041000
O 0.54483100 -0.76574300 0.00029400
C 1.78509500 -0.11192100 -0.00016300
H 2.55391800 -0.89160000 0.00037200
H 1.93242000 0.52821600 -0.88203300
H 1.93237500 0.52948700 0.88077300

5p'

C 2.17219000 -0.46125000 0.37409300
C 1.00306100 0.13510700 -0.04362600
H 3.04780800 0.15004800 0.56141500
O 0.72409100 1.33952100 -0.25158200
H 2.24425600 -1.53563500 0.50067900
O -0.03514700 -0.84612700 -0.26919500
C -1.30259600 -0.30690300 -0.57314700
H -1.85989000 -1.10927900 -1.07535600
H -1.20315300 0.53005900 -1.27682800
C -2.04722200 0.16081400 0.66251100
H -1.49057000 0.97527200 1.13307100
H -3.05008900 0.52622400 0.41379400
H -2.15251600 -0.65044900 1.39046300

5q'

C 2.10357400 -0.61951900 -0.28511900
C 1.01210500 0.14537800 0.02576500
H 3.03786000 -0.13488700 -0.54420800
O 0.81220800 1.37206500 0.08315600
H 2.05215100 -1.70121700 -0.27398000
O -0.14018000 -0.73907200 0.38122100
C -1.32412000 -0.09855400 0.51721200
H -1.97213400 -0.68995100 1.17576000
H -1.19830100 0.93053900 0.87391400
F -2.00501800 -0.00358500 -0.72151700

5r'

C 1.56202600 1.04800900 0.17415900
C 0.84566700 -0.11627400 -0.05651500
H 2.64112200 0.97255100 0.27506900
O 1.30937900 -1.29504100 -0.11866400
H 1.11843800 2.03026500 0.27779200
N -0.59044300 0.00217500 -0.29501100
C -1.22098500 1.27631500 -0.07166500

H -2.27763600 1.22280000 -0.36137500
H -1.18159000 1.61852600 0.98239300
H -0.74394000 2.04962800 -0.68166400
C -1.37689600 -1.09948100 0.20571100
H -2.34568000 -1.14721300 -0.30854700
H -0.82203000 -2.02109500 0.02781200
H -1.58948100 -1.03177000 1.29276800

5s'

C 2.24348200 1.09715600 -0.00344400
C 1.53637700 -0.10199000 0.02521200
H 3.32778000 1.04700300 -0.05724000
O 1.99046800 -1.27364900 -0.15405100
H 1.80593200 2.03232100 0.33416200
N 0.12657500 -0.01976900 0.27556000
C -0.61546900 1.21417200 0.05939300
C -0.69719800 -1.17123500 -0.04140900
H -0.14421500 1.81956300 -0.73209700
H -0.61488500 1.84632500 0.96441700
C -2.03211500 0.76699800 -0.31540900
H -0.58496500 -1.49747500 -1.09431900
H -0.42260400 -2.03330600 0.57573700
C -2.10661500 -0.66262300 0.21282000
H -2.14256700 0.75767800 -1.40697000
H -2.81154300 1.42579800 0.08016600
H -2.87926400 -1.26647300 -0.27340700
H -2.31420800 -0.65872400 1.29006700

5t'

C -1.88123500 1.11667000 0.12290600
C -1.23349300 -0.09367300 -0.06515900
H -2.95267100 1.12908700 0.30050100
O -1.68422600 -1.27252500 0.05032500
H -1.39173300 2.06448300 -0.08412300
N 0.15823900 -0.01251800 -0.44708600
C 1.03705400 1.07266400 -0.00168600
C 1.08999300 -1.02072400 0.06297700
C 2.17728300 0.05993900 0.13047800
H 0.71202700 1.50054900 0.96352900
H 1.16648900 1.90418700 -0.70992700
H 0.80006400 -1.41040400 1.05246200
H 1.26822500 -1.88315500 -0.59405800
H 2.78370200 0.10256600 1.03868800
H 2.84243100 0.05125800 -0.73715900

5u'

C -2.25385900 -0.12495100 -0.01409600
C -0.94408800 -0.56368600 0.03604200
H -3.04339700 -0.87032000 -0.05664300
O -0.50934100 -1.74626000 -0.02782500
H -2.54931000 0.91651300 -0.01618200
N 0.09088000 0.46342800 0.29542600
C -0.24726800 1.84605500 0.03721500
H 0.64083800 2.46584100 0.19006500
H -0.63723400 2.02736300 -0.97948600
H -1.01169400 2.15904800 0.75229200
O 1.23529800 0.19431700 -0.56639400
C 2.22337100 -0.44116000 0.20893300
H 3.07481300 -0.61051400 -0.45980400
H 2.55337600 0.18643300 1.05219400
H 1.85985800 -1.40036700 0.59477700

5v'

C -1.33171800 -0.43671600 0.03011900
C -0.06689900 0.12825200 -0.00986000
H -2.21047800 0.20014200 -0.01385100
O 0.25578600 1.35306500 0.00655200
H -1.47898800 -1.51082800 -0.05848400
N 1.05001300 -0.80069200 -0.11505300
H 0.84511600 -1.68186100 0.34469500
H 1.83966800 -0.37634100 0.35904400

5w'

C -1.74878100 -0.62518800 0.15154600
C -0.59865800 0.12323000 -0.04996600
H -2.71320100 -0.12741700 0.19785600
O -0.47239300 1.38305800 -0.05126000
H -1.74518300 -1.70900400 0.05426200
N 0.60687000 -0.64569500 -0.31963900
C 1.84148700 -0.06913200 0.15909800
H 2.70815700 -0.52926200 -0.33107400
H 1.81952100 0.99511500 -0.08609900
H 1.99980500 -0.14615000 1.25178100
H 0.49767500 -1.60134700 -0.00324300

5xa'

C 3.46328300 -0.62803800 -0.03487500
C 2.30540900 0.12868200 0.01313100
H 4.42565400 -0.12959800 0.00234900
O 2.18029600 1.38066700 0.09820500
H 3.44937300 -1.71114200 -0.11461500
N 1.09535700 -0.67927300 -0.03992000

H 1.25271300 -1.67605800 -0.03373400
C -0.22605900 -0.31198300 -0.01819000
C -0.67962900 1.02729900 -0.05490900
C -1.20884700 -1.33026500 0.02867200
C -2.04076300 1.30606700 -0.04006900
H 0.06334200 1.81338000 -0.08986200
C -2.56319400 -1.02898400 0.03977100
H -0.88463100 -2.36987900 0.05652800
C -3.00226000 0.29520700 0.00770400
H -2.35728100 2.34737500 -0.06846400
H -3.28414100 -1.84354800 0.07651400
H -4.06253200 0.53112100 0.01767400

5xb'

C 4.37371500 0.60513100 0.05321900
C 3.19557200 -0.12102600 0.06858500
H 5.31384600 0.09642400 0.23633700
O 3.02889100 -1.35303200 0.28424200
H 4.39903700 1.66994500 -0.16059500
N 2.01574300 0.68657400 -0.21135700
H 2.17678000 1.68201500 -0.16676800
C 0.68562100 0.33087700 -0.11977500
C 0.22391500 -1.00293000 -0.20331600
C -0.29026100 1.33784300 0.00625400
C -1.13194800 -1.28812100 -0.14874400
H 0.95913200 -1.79189800 -0.29401100
C -1.65331700 1.04949000 0.04667400
H 0.02955800 2.37669900 0.07380500
C -2.08618200 -0.27374700 -0.02589100
H -1.47614400 -2.31788800 -0.21064600
H -2.36134300 1.86659700 0.14420600
O -3.40456000 -0.67206900 0.01072800
C -4.36022400 0.35526100 0.14729800
H -4.32369600 1.06517100 -0.69074400
H -5.33773700 -0.12811700 0.16145900
H -4.22563400 0.91917900 1.08087400

5xc'

C 4.37417600 0.42610100 0.00020300
C 3.16518300 -0.24448000 -0.00010600
H 5.29722700 -0.14221900 0.00010400
O 2.94112200 -1.48504100 -0.00030000
H 4.43908500 1.51012600 0.00032600
N 2.01868200 0.65656100 0.00004200
H 2.25172600 1.63849500 0.00016100
C 0.67697300 0.38917100 0.00002700

C 0.12328600 -0.91359200 -0.00005400
C -0.22797600 1.47789400 0.00009400
C -1.25199000 -1.09983400 -0.00006200
H 0.80412800 -1.75406900 -0.00011800
C -1.60133600 1.28949700 0.00008900
C -2.11174100 -0.00490400 0.00001200
H -1.65915100 -2.10690800 -0.00011900
H -2.27064700 2.14408300 0.00014200
H 0.16591500 2.49273700 0.00015100
Cl -3.85691100 -0.25982100 0.00001400

5xd'

C 5.02891100 0.38362600 -0.01598500
C 3.81277300 -0.27269600 0.00481200
H 5.94522100 -0.19514900 -0.02429100
O 3.56925600 -1.50831100 0.01502800
H 5.10612800 1.46669000 -0.02648300
N 2.67965900 0.64888600 0.01744500
H 2.93218000 1.62641200 0.01554900
C 1.33755400 0.41006300 0.00744000
C 0.75509600 -0.88336500 -0.00444000
C 0.45678800 1.52159100 0.00501300
C -0.61984500 -1.02916400 -0.02221500
H 1.41886700 -1.73687100 -0.00426400
C -0.91454000 1.35832800 -0.01211500
H 0.87818300 2.52506600 0.01182600
C -1.47744800 0.07806200 -0.03272900
H -1.04533300 -2.03033800 -0.03779200
H -1.56125600 2.23085500 -0.01867200
C -2.94395300 -0.11422700 -0.00479200
F -3.35379400 -1.13595000 -0.80068800
F -3.42484000 -0.41662500 1.23580000
F -3.62110800 0.98860900 -0.40268200

5xe'

C 3.53127300 0.72804900 0.06895900
C 2.53471300 -0.22520500 -0.01557000
H 4.56824200 0.41824900 0.01253000
O 2.63345500 -1.47399700 -0.14763900
H 3.31682200 1.78613800 0.18514700
N 1.19511900 0.35927900 0.05982300
H 1.17423600 1.36810300 0.07113000
C -0.02874800 -0.23980800 0.03180200
C -0.22886200 -1.64298800 0.05632500
C -1.21522000 0.53713700 -0.00505500
C -1.50071500 -2.19343800 0.03689600

H 0.66149100 -2.25698900 0.08384800
C -2.48815400 -0.01315800 -0.01901600
C -2.64604200 -1.39591800 -0.00057700
H -1.59839200 -3.27656800 0.05591700
H -3.34784200 0.64963200 -0.04513400
H -3.63996500 -1.83219000 -0.01345900
Cl -1.07750200 2.29956600 -0.03001200

5xf'

C -3.38959200 -1.50921500 0.00051300
C -2.76445400 -0.27711900 -0.00003000
H -4.47275400 -1.55250800 0.00017800
O -3.27383200 0.87386000 -0.00058900
H -2.83824800 -2.44471400 0.00067600
N -1.30280200 -0.39800100 0.00016300
H -0.98461900 -1.35377000 0.00054900
C -0.33315500 0.56243300 0.00006700
C -0.62894600 1.94878100 0.00001300
C 1.04962700 0.20508300 0.00004200
C 0.38040100 2.89471000 0.00008600
H -1.67384400 2.22651500 -0.00005800
C 2.04616700 1.18229500 0.00012700
C 1.73110000 2.53322200 0.00017400
H 0.10508200 3.94737100 0.00006700
H 3.08319100 0.86212500 0.00013400
H 2.51532800 3.28364000 0.00032700
C 1.44483300 -1.22631200 -0.00009400
F 0.96373400 -1.90691300 1.08079300
F 0.96376800 -1.90666900 -1.08113800
F 2.77919200 -1.41495000 -0.00006300

5xg'

C -4.24366800 0.44084500 -0.01961500
C -2.98808700 -0.04071000 -0.31469900
H -5.09436100 0.11886500 -0.60932500
O -2.59476400 -0.86777600 -1.16871300
H -4.40975000 1.14192800 0.79182300
N -1.92720700 0.57415200 0.55259000
H -2.08445800 1.56096900 0.70566100
C -0.60286900 0.29575200 0.31617400
C -0.09226000 -1.01391600 0.29622700
C 0.34235100 1.31748300 0.13961600
C 1.25302300 -1.26792000 0.06676300
C 1.69412600 1.07947900 -0.05307100
C 2.15869900 -0.22842400 -0.11142000
F -0.08486800 2.59873900 0.16465900

F 2.54267900 2.10636800 -0.21665300
F 3.46058400 -0.48794600 -0.31444800
F 1.70004000 -2.53372000 0.06491100
F -0.87296600 -2.06057000 0.59859400

Proton

H 0.00000000 0.00000000 0.00000000

3a

Rh -0.54950400 -1.34488900 -1.87445800
O 0.21684700 -3.06953700 -0.99478500
O -2.44285600 -1.88933600 -1.20160200
O -1.26061200 0.49024300 -2.60004200
O 1.35528300 -0.78699300 -2.44911900
C 2.05340300 -0.09854600 -1.64114700
O 1.68360200 0.29534000 -0.48834900
C -1.35518100 1.46779700 -1.79374900
O -1.04527600 1.44913900 -0.56040200
C 0.57866400 -3.04945200 0.22091000
O 0.53767300 -2.03710900 0.99714200
O -2.09700600 -0.90034300 0.80765700
C -2.79319900 -1.56494800 -0.02357800
C 1.10978500 -4.33910000 0.84860500
C 3.45981200 0.31645200 -2.08125300
C -1.88635600 2.79114600 -2.34773900
C -4.18323800 -2.02211400 0.42548600
C 2.51629300 -4.05268900 1.43946900
H 2.87316100 -4.98926200 1.88632400
H 2.39498900 -3.32797000 2.25311700
C 1.16557200 -5.46486500 -0.17619300
H 1.54309700 -6.37655400 0.29926800
H 0.17343100 -5.67749900 -0.58232100
H 1.82332800 -5.21946400 -1.01352600
C 0.17607200 -4.72547500 1.99992900
H 0.52141800 -5.65563600 2.46225100
H 0.15744700 -3.94739000 2.76807200
H -0.84741900 -4.88757900 1.64633700
C 4.48222700 -0.15018000 -1.01059800
H 5.47258000 0.17420600 -1.35468900
H 4.26798500 0.39146000 -0.08102400
C 3.50486200 1.84549900 -2.14558500
H 4.49177500 2.17333400 -2.48858600
H 2.75982400 2.23933800 -2.84606200
H 3.31421700 2.28363400 -1.16311500
C 3.79784100 -0.27314200 -3.44582800
H 3.11038300 0.09095700 -4.21334500

H 4.81410500 0.02053100 -3.73063300
H 3.74631000 -1.36459700 -3.44169400
C -1.89995900 3.87360100 -1.27268900
H -2.28649200 4.80567200 -1.69908800
H -2.52284700 3.60115900 -0.41686400
H -0.89427800 4.06614600 -0.88953900
C -0.97308000 3.21916200 -3.49981200
H -0.93954100 2.45829800 -4.28352400
H -1.33593000 4.15455500 -3.93751800
H 0.04917400 3.39125300 -3.14280600
C -3.31767500 2.54860800 -2.89639700
H -3.68207100 3.50856100 -3.28316100
H -3.24049900 1.86378300 -3.74831700
C -5.23034000 -1.45751800 -0.57107400
H -5.06378500 -1.93658000 -1.54210600
H -6.21636200 -1.78229600 -0.21556800
C -4.22829300 -3.55135800 0.36431200
H -3.51258200 -3.99503800 1.06430300
H -5.22667300 -3.90646400 0.64004700
H -3.99781500 -3.91531000 -0.64013800
C -4.48600400 -1.55060800 1.84228100
H -5.49595100 -1.86363600 2.12874600
H -3.78057700 -1.97828900 2.55939100
H -4.42235300 -0.46319700 1.92492200
C 3.51227200 -3.52993400 0.44426200
C 3.61073300 -2.15425600 0.21506300
C 4.32896900 -4.39045000 -0.29640000
C 4.47461400 -1.62856100 -0.74992500
H 3.00189500 -1.47019200 0.80376000
C 5.21405100 -3.88205000 -1.24419900
H 4.27648100 -5.46328600 -0.11893000
C 5.28186200 -2.51060500 -1.47614000
H 5.85458400 -4.55813200 -1.80453400
H 5.97278500 -2.11563900 -2.21875500
C -5.19819800 0.03557100 -0.73619700
C -4.37281500 0.60607100 -1.70962200
C -5.95893200 0.88642000 0.07279600
C -4.27447200 1.98973900 -1.88098300
H -3.78784100 -0.04878700 -2.35264200
C -5.88901300 2.26744500 -0.09494700
H -6.61709300 0.46066400 0.82822700
C -5.04944800 2.81741100 -1.06111800
H -6.49380300 2.91936300 0.53002400
H -4.99824600 3.89710900 -1.18859700
Rh -0.20038200 -0.24503000 0.25391600
C 0.15905000 0.83053900 2.23673900

C 1.59544500 1.14460900 2.35471500
 C -0.91838200 1.80944500 2.41089500
 H -0.09920400 -0.19154200 2.61204800
 O 2.36261600 0.33570000 2.90158800
 C 2.13710500 2.39808800 1.78042700
 O -0.85118900 3.01165600 2.21455400
 O -2.07207300 1.19637800 2.78504000
 C -0.05861100 -0.63504500 4.18906000
 C 3.36328700 2.87154500 2.26046300
 C 1.51849500 3.09667200 0.73023500
 C -3.24642100 1.99782100 2.64106600
 H 0.90422000 -1.08209500 3.94225000
 C -0.03217800 0.44899200 5.18587800
 C -1.26097700 -1.47873400 4.04157900
 C 3.94636000 4.02593200 1.75214100
 H 3.85647600 2.31996100 3.05604800
 C 2.09229500 4.23815200 0.20456900
 H 0.59447300 2.72052900 0.30542700
 H -3.48170500 2.11714800 1.57608800
 H -4.04894300 1.45195000 3.13713100
 H -3.11515100 2.98094400 3.09709800
 H 0.86281400 1.06744900 5.10722000
 H -0.93688600 1.06196700 5.15572000
 H -0.01012100 -0.03089600 6.17631300
 H -2.18408300 -0.91640900 4.19075400
 H -1.29302800 -2.00036700 3.08010500
 H -1.19596100 -2.25078100 4.82343400
 C 3.30576900 4.71868300 0.71732600
 H 4.88725500 4.37745800 2.16075900
 H 1.63159500 4.76953600 -0.62396200
 O 3.78281400 5.84937600 0.14235000
 C 5.01846900 6.35408200 0.62477300
 H 5.22620700 7.25121500 0.04325600
 H 4.95787700 6.61591800 1.68728600
 H 5.83040900 5.63188200 0.48064800

3b

Rh -0.26359500 -1.20361500 -1.93859700
 O 0.84922200 -2.77333600 -1.13830600
 O -1.99817200 -2.15302500 -1.30073300
 O -1.33487300 0.47534100 -2.58283200
 O 1.48920000 -0.26304200 -2.48213200
 C 2.04536600 0.50741200 -1.63871200
 O 1.61381800 0.76417900 -0.46911900
 C -1.58655800 1.39765200 -1.74455900
 O -1.25474800 1.40340900 -0.51582600

C 1.19057600 -2.74554100 0.08281700
 O 0.92713800 -1.81055100 0.91067900
 O -1.87588600 -1.17091100 0.73717800
 C -2.41418600 -1.94325400 -0.11777000
 C 1.97884200 -3.92906200 0.64652800
 C 3.34325900 1.20663400 -2.05172600
 C -2.36172300 2.61360200 -2.25510700
 C -3.68484200 -2.68445600 0.30605000
 C 3.28676900 -3.39329200 1.28848100
 H 3.82247800 -4.26087100 1.69438700
 H 3.00768300 -2.75655700 2.13624600
 C 2.28412400 -4.94968900 -0.44304300
 H 2.85548600 -5.78173700 -0.01765000
 H 1.36438000 -5.35275700 -0.87440600
 H 2.87070000 -4.51266200 -1.25503600
 C 1.13437700 -4.57694200 1.74854300
 H 1.66257100 -5.44176700 2.16265300
 H 0.94330500 -3.87109600 2.56165100
 H 0.17203200 -4.92727500 1.36077800
 C 4.41868100 0.94172700 -0.96425700
 H 5.32359900 1.48137100 -1.27175400
 H 4.06810000 1.39537000 -0.02893400
 C 3.07137800 2.71261900 -2.10576000
 H 3.98188600 3.24406300 -2.40276500
 H 2.29286900 2.94875600 -2.83947900
 H 2.75157500 3.08988100 -1.13132000
 C 3.81314200 0.71685400 -3.41642600
 H 3.07415000 0.94060500 -4.18973300
 H 4.74896700 1.21980600 -3.68351700
 H 3.99040900 -0.36133700 -3.42411700
 C -2.55997700 3.64374800 -1.14890200
 H -3.13287600 4.49266900 -1.53755100
 H -3.09819400 3.22517200 -0.29508600
 H -1.60190300 4.01976600 -0.77978600
 C -1.56608300 3.23582500 -3.40524400
 H -1.39657500 2.51366000 -4.20765300
 H -2.11056400 4.09205700 -3.81621100
 H -0.59246800 3.59602400 -3.05386400
 C -3.73380500 2.12522600 -2.79176000
 H -4.28072800 3.01340400 -3.13206900
 H -3.55103400 1.50016400 -3.67300500
 C -4.83783400 -2.26315300 -0.64440700
 H -4.60927200 -2.65284300 -1.64277600
 H -5.74142600 -2.77954100 -0.29645700
 C -3.44218100 -4.18675100 0.13963200
 H -2.63499400 -4.52957700 0.79576300

H -4.34652700 -4.74364100 0.40524200
 H -3.17397800 -4.43125100 -0.89089900
 C -4.04460800 -2.37506800 1.75406200
 H -4.98732000 -2.86914200 2.01297800
 H -3.27312400 -2.73966900 2.43729900
 H -4.15393500 -1.30153400 1.92409800
 C 4.16872400 -2.62558800 0.34622700
 C 3.97775800 -1.25074900 0.17730900
 C 5.15933500 -3.26216500 -0.40806900
 C 4.72339500 -0.51321300 -0.74739400
 H 3.23017300 -0.74226900 0.78376600
 C 5.93139400 -2.53742700 -1.31238800
 H 5.32863700 -4.32952500 -0.27703300
 C 5.70997400 -1.17385700 -1.48741600
 H 6.70878100 -3.03766600 -1.88399900
 H 6.31026900 -0.61101900 -2.20024400
 C -5.07880300 -0.78246800 -0.72944800
 C -4.38997100 -0.02696800 -1.68288600
 C -5.96472200 -0.12233600 0.12845900
 C -4.54629100 1.35777000 -1.78736000
 H -3.71216700 -0.53300200 -2.36770600
 C -6.14782900 1.25506700 0.02824300
 H -6.52233300 -0.69476500 0.86781200
 C -5.44051300 1.99242700 -0.91875600
 H -6.84835300 1.75671800 0.69103200
 H -5.58925700 3.06796400 -0.99437800
 Rh -0.13060300 -0.15592400 0.23569000
 C 0.04728100 0.81033600 2.30639000
 C 1.42462900 1.30476100 2.44036600
 C -1.16462600 1.59515400 2.54380400
 H -0.06169300 -0.26715400 2.56680900
 O 2.30791900 0.56075600 2.89637400
 C 1.79587100 2.66848200 1.97971700
 O -1.29295800 2.80440400 2.44244800
 O -2.20192800 0.77646500 2.86435900
 C 0.08591000 -0.84105900 4.14424100
 C 2.96808900 3.23290400 2.49682600
 C 1.08672000 3.37387300 0.99839900
 C -3.49242000 1.38170700 2.77776500
 H 1.10292500 -1.09017200 3.84207400
 C -0.05512700 0.14973200 5.22267100
 C -0.96343200 -1.85120200 3.91752700
 C 3.40709700 4.47738200 2.06442600
 H 3.52698700 2.67683300 3.24421000
 C 1.53477500 4.61397400 0.56608700
 H 0.20395700 2.92958200 0.55055700

H -3.73974600 1.56885400 1.72606600
 H -4.19355900 0.66030700 3.19787200
 H -3.53121300 2.31990300 3.33488200
 H 0.72397100 0.91234900 5.19501000
 H -1.05001000 0.60291800 5.24157000
 H 0.05872500 -0.39711300 6.17163500
 H -1.96599700 -1.46426700 4.10758500
 H -0.91480200 -2.28893800 2.91609700
 H -0.76821200 -2.66603000 4.63222300
 C 2.70146200 5.18827900 1.08708300
 H 4.31456500 4.90719500 2.48362400
 H 0.98650700 5.14058300 -0.21377800
 C 3.19829600 6.50361000 0.57492800
 H 2.38750000 7.23052800 0.46998300
 H 3.96077400 6.93269200 1.22939400
 H 3.64720100 6.39058400 -0.41916100

3c

Rh -0.05868600 -1.11511100 -1.94576100
 O 1.22484900 -2.54249400 -1.13299200
 O -1.67153200 -2.26787800 -1.30944800
 O -1.32686900 0.41070600 -2.60334400
 O 1.57090100 0.04450700 -2.47017900
 C 2.02920000 0.86891400 -1.61877300
 O 1.56792300 1.06284700 -0.44780600
 C -1.68225900 1.30977900 -1.77757300
 O -1.34470400 1.37280100 -0.55257400
 C 1.53689200 -2.48336000 0.09448200
 O 1.15772600 -1.58389500 0.91748100
 O -1.68494300 -1.25720400 0.71728200
 C -2.11758600 -2.10040800 -0.13064400
 C 2.44443300 -3.57254100 0.67017300
 C 3.23317600 1.72423200 -2.01678600
 C -2.60189700 2.41522100 -2.30165600
 C -3.28652200 -2.99145000 0.29614200
 C 3.70239100 -2.89680500 1.27855700
 H 4.33433100 -3.70015500 1.67795900
 H 3.37550600 -2.28783200 2.12992800
 C 2.83417500 -4.58169800 -0.40299900
 H 3.47550500 -5.35421400 0.03476500
 H 1.95190200 -5.07031900 -0.82438500
 H 3.37945300 -4.11084500 -1.22443100
 C 1.68932300 -4.27719600 1.80134800
 H 2.31238500 -5.07141500 2.22465900
 H 1.43844200 -3.57587700 2.60210900
 H 0.76314800 -4.73636400 1.44051700

C 4.34413000 1.54490400 -0.94756700
 H 5.18584900 2.18016200 -1.25137700
 H 3.96261100 1.93964000 0.00165800
 C 2.79279300 3.19097600 -2.01066400
 H 3.63127900 3.83099800 -2.30424600
 H 1.97540700 3.36443000 -2.71937300
 H 2.45519700 3.49475500 -1.01640400
 C 3.74126200 1.33925000 -3.40120700
 H 2.96813300 1.48864300 -4.15884900
 H 4.60262100 1.96331000 -3.66288800
 H 4.05314100 0.29289700 -3.44401900
 C -2.91234600 3.43630500 -1.21225100
 H -3.59019300 4.19971700 -1.60900300
 H -3.38245700 2.97653000 -0.33915500
 H -2.00277400 3.93684600 -0.86890300
 C -1.89876000 3.10520100 -3.47339600
 H -1.65072600 2.39117400 -4.26250400
 H -2.54862200 3.87857600 -3.89513200
 H -0.97316400 3.59017300 -3.14393500
 C -3.90832000 1.75626400 -2.81934800
 H -4.56084300 2.56794000 -3.16508400
 H -3.65423600 1.14898700 -3.69536700
 C -4.47498000 -2.72769500 -0.66680700
 H -4.18832000 -3.08835800 -1.66103600
 H -5.30905400 -3.35259100 -0.32350800
 C -2.85644700 -4.45334900 0.14956400
 H -2.02133300 -4.68594600 0.81856000
 H -3.68808600 -5.11525500 0.41188200
 H -2.54777100 -4.67448800 -0.87490000
 C -3.69246700 -2.71607300 1.73964700
 H -4.55394400 -3.33838900 2.00475500
 H -2.87729600 -2.95563500 2.42751400
 H -3.95892400 -1.66791600 1.89803900
 C 4.48099100 -2.04264300 0.31967500
 C 4.13760300 -0.69745400 0.15675800
 C 5.53211700 -2.56175900 -0.44309900
 C 4.79808100 0.12572700 -0.75971100
 H 3.33691400 -0.27745300 0.76272200
 C 6.21661500 -1.74988400 -1.34432200
 H 5.82111800 -3.60395500 -0.31799500
 C 5.84993100 -0.41632600 -1.50626400
 H 7.04215700 -2.15830700 -1.92151900
 H 6.38725100 0.21615900 -2.21083800
 C -4.89396100 -1.28835900 -0.75569200
 C -4.30543300 -0.45607700 -1.71158700
 C -5.83864000 -0.73626600 0.11592600

C -4.61704300 0.90297600 -1.80598200
 H -3.57785800 -0.88015000 -2.40129200
 C -6.17516100 0.61245500 0.02740200
 H -6.31868000 -1.37082500 0.85890500
 C -5.56613400 1.42949100 -0.92226000
 H -6.91836200 1.02963200 0.70204500
 H -5.83494900 2.48207700 -0.98842400
 Rh -0.06554300 -0.05240300 0.22456200
 C -0.01671600 0.92294100 2.29971900
 C 1.27828800 1.59894200 2.43783800
 C -1.32204100 1.53592600 2.54803400
 H 0.02480400 -0.15984000 2.55283100
 O 2.26236900 0.97830800 2.86928900
 C 1.44749900 3.02155000 2.03052500
 O -1.61648300 2.71501800 2.44020000
 O -2.23017100 0.58503200 2.89360800
 C 0.25865800 -0.72412600 4.13154700
 C 2.48471200 3.73955900 2.64020300
 C 0.67795600 3.64138900 1.03878700
 C -3.59189700 1.01484000 2.87325400
 H 1.29033300 -0.85589200 3.80585400
 C 0.02794000 0.24380000 5.21456400
 C -0.67504200 -1.84310500 3.91934900
 C 2.72800400 5.06297900 2.29488600
 H 3.08882700 3.23874700 3.39128100
 C 0.93201400 4.96282300 0.68483100
 H -0.09743600 3.07785800 0.53002100
 H -3.92382600 1.14758500 1.83658900
 H -4.16706700 0.21675700 3.34309800
 H -3.72063000 1.95159200 3.41918600
 H 0.71860600 1.08705100 5.17866700
 H -1.01015200 0.58512900 5.24934300
 H 0.21388900 -0.28934700 6.15998000
 H -1.71137800 -1.56277600 4.11460000
 H -0.58394800 -2.28007400 2.92062100
 H -0.38822600 -2.62553200 4.63948300
 C 1.94919800 5.67822100 1.31576300
 H 3.52434400 5.61495500 2.78609600
 H 0.34310900 5.43327000 -0.09861900
 H 2.13936900 6.71178400 1.03902300

3d

Rh -0.21853500 -1.26004600 -1.91119700
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 O -1.34318900 0.36684000 -2.59489200

O 1.50416700 -0.27944300 -2.48465400
C 2.04364100 0.52413300 -1.66174500
O 1.61207200 0.79555100 -0.49498300
C -1.62060900 1.30069000 -1.77851500
O -1.27231500 1.35219300 -0.55575300
C 1.28178200 -2.71269700 0.14530600
O 0.98992500 -1.76805900 0.95263500
O -1.81987700 -1.19917500 0.77446100
C -2.34047800 -2.00822300 -0.05753000
C 2.10425600 -3.86037600 0.73443500
C 3.31885400 1.25004500 -2.09778000
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C -3.58603100 -2.77480700 0.39437700
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H 3.11981200 -2.62440800 2.18280500
C 2.42435600 -4.90306000 -0.32984700
H 3.01213600 -5.71363700 0.11421600
H 1.51023800 -5.33301800 -0.74702600
H 3.00016000 -4.47633300 -1.15487400
C 1.28834400 -4.49869600 1.86294000
H 1.84336100 -5.33737800 2.29515500
H 1.08743200 -3.77574400 2.65823800
H 0.33161700 -4.88488400 1.49615500
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H 5.30217400 1.58129500 -1.34702400
H 4.06401400 1.48741600 -0.08758800
C 3.00868300 2.74792900 -2.16654500
H 3.89699500 3.29621800 -2.49673800
H 2.20380300 2.95520400 -2.88028600
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C 3.78559600 0.75381800 -3.46124200
H 3.03205800 0.94653900 -4.22878600
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H -3.29627600 4.33154700 -1.63088600
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C -1.66126700 3.11694100 -3.45797100
H -1.45063200 2.39433000 -4.25025800
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H -0.70851300 3.52107700 -3.09728000
C -3.78534200 1.91549100 -2.85876600
H -4.36244600 2.77102800 -3.23139500
H -3.55964800 1.27607300 -3.71951600

C -4.74562400 -2.44827700 -0.58447200
H -4.48872500 -2.86844700 -1.56332800
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H -2.46570600 -4.54563800 0.98974900
H -4.16198400 -4.85282300 0.59410900
H -2.98842900 -4.55798000 -0.70520300
C -3.97024800 -2.40500800 1.82172700
H -4.87464300 -2.94952500 2.11347800
H -3.17394700 -2.66621900 2.52361700
H -4.16084700 -1.33424700 1.92391300
C 4.25713200 -2.51065500 0.37591700
C 4.03330000 -1.14546700 0.17392100
C 5.25351300 -3.14379900 -0.37387600
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C -4.37663800 -0.23191200 -1.69866400
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C -6.20294400 1.03417000 -0.04719200
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H -6.93072700 1.52867500 0.59109100
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C 1.39091100 1.45554800 2.35681100
C -1.20386100 1.60576900 2.49447700
H 0.00496900 -0.19028800 2.57594700
O 2.32744500 0.78110300 2.81369200
C 1.66491600 2.83495700 1.87416800
O -1.40358100 2.79692600 2.32068000
O -2.17709500 0.75324100 2.91021400
C 0.22637900 -0.70969800 4.16763200
C 2.77182400 3.49649600 2.42176800
C 0.92293000 3.46633500 0.86698500
C -3.50120000 1.28824900 2.89500000
H 1.24112500 -0.92439700 3.83264800
C 0.08248700 0.31813700 5.20921000

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C 3.11961300 4.77515800 2.00907000
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H -4.12049900 0.57467000 3.43857400
H -3.53868700 2.26903700 3.37278500
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H -0.92867900 0.73249100 5.24525900
H 0.25035900 -0.18426900 6.17471700
H -1.79685800 -1.40936600 4.22859800
H -0.75620200 -2.23669400 3.02615600
H -0.53705000 -2.54747700 4.74750700
C 2.35336200 5.37565700 1.01904800
H 3.96255400 5.30688200 2.43711100
H 0.71626200 5.23948900 -0.35928500
F 2.68239900 6.61335600 0.60350100

3e

Rh -0.43997700 -1.29328000 -1.91000700
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O -2.30120000 -1.96786900 -1.27101500
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O 1.43933000 -0.61396400 -2.44554400
C 2.08898800 0.08308900 -1.60596700
O 1.68269500 0.41912200 -0.44688700
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O -1.10870100 1.42048000 -0.51375200
C 0.75627100 -3.00714300 0.13945200
O 0.64706900 -2.02920000 0.95246100
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C -2.68209300 -1.70486100 -0.08749700
C 1.34389200 -4.29366000 0.72176300
C 3.47929700 0.58436300 -2.00529800
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C -4.04202100 -2.26792200 0.33080900
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C 1.45422700 -5.37571800 -0.34486000
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C 0.42534900 -4.76500000 1.85385400
H 0.80397900 -5.70180400 2.27472400

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H -3.73261900 -0.18679100 -2.37268600
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C -5.21940500 2.53909400 -1.01835400
H -6.70430200 2.48578700 0.53655500
H -5.24180000 3.62336500 -1.10987500
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C 0.11733900 0.76761600 2.27693800
C 1.52882200 1.15453600 2.39227900
C -1.01738600 1.67088200 2.47838900
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C 1.99817300 2.46956800 1.87024400
O -1.03588300 2.87770300 2.29996500
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C -1.13579200 -1.71916500 4.00960400
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H 3.71254100 2.43194300 3.16003800
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3f

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O 1.42819300 1.37528400 0.99396400
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C 1.98286200 -1.58932900 -1.00660700
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H 6.35388900 -1.68024000 -1.52795100
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C 0.17138600 -3.13646400 2.86057400
C -3.76781800 -0.84825000 2.92069200
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C -0.27968400 -3.22717200 4.26437400
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H -4.39626100 -1.71717400 2.72985000
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H -1.35321900 -3.04924600 4.36363000
H -0.09695400 -4.26179000 4.58861200
H -1.64964200 -3.78094400 1.93105000
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H -0.31108900 -4.94313800 1.93942000
H 0.92252500 0.67998000 3.72844100

3g

Rh 0.27578100 0.57595000 -1.89590800
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O -1.20073600 -0.81288400 -2.37142700
O -1.12975100 2.08907100 -1.57731600
O 1.75652900 1.90162300 -1.31965200
C 2.02034200 2.02027000 -0.08353100
O 1.47684500 1.36370100 0.86280100
C -1.63569600 2.20998800 -0.41581600
O -1.38070000 1.47657900 0.59150500
C 1.93817100 -1.66906500 -1.02525800
O 1.39562600 -1.55898300 0.12544900
O -1.47422000 -1.36658900 -0.19091900
C -1.73806600 -1.47779800 -1.43032100
C 2.97499700 -2.78375600 -1.17267800
C 3.07948500 3.03966100 0.33781900
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C -2.80655000 -2.49894700 -1.82919200
C 4.09712600 -2.55273400 -0.12485200
H 4.82686300 -3.36237600 -0.25312800
H 3.65381600 -2.66961800 0.87140400
C 3.54829000 -2.81167600 -2.58425700
H 4.29319900 -3.61074500 -2.66252400
H 2.76671500 -3.00037400 -3.32447900
H 4.03244100 -1.86685400 -2.84299900
C 2.29127600 -4.11830500 -0.85904000
H 3.00055300 -4.94103100 -0.99423800
H 1.93234600 -4.14329100 0.17353800
H 1.43948700 -4.29828800 -1.52410500
C 4.18356500 2.29515300 1.13511600
H 4.93977800 3.04134000 1.40964700
H 3.73355900 1.92766700 2.06451400
C 2.41148300 4.05724500 1.26850100
H 3.15182300 4.78197900 1.62244400
H 1.62374000 4.61220300 0.74892800

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 H 4.14617600 3.04740900 -1.56183500
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 H -3.81557100 4.21168100 1.38322500
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 H -2.24142000 3.58821500 1.91512900
 C -1.99694700 4.66167800 -0.60831000
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 H -1.13822100 4.89164700 0.03031900
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 H -4.59335800 3.87436000 -0.93490900
 H -3.52298100 3.21284400 -2.17190000
 C -3.98710500 -1.73443500 -2.48679400
 H -3.63209100 -1.32358600 -3.43863500
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 C -2.20248300 -3.45178300 -2.86330200
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 C -3.28837000 -3.28484700 -0.61596600
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 C 4.77319100 -1.21467800 -0.21851700
 C 4.25528900 -0.12785800 0.49178300
 C 5.89879900 -1.01215800 -1.02402600
 C 4.81581900 1.14956000 0.39690200
 H 3.39421800 -0.28245700 1.13984400
 C 6.48000100 0.25005300 -1.11755200
 H 6.32587800 -1.85155300 -1.57006600
 C 5.93946100 1.32609800 -0.41765500
 H 7.36147000 0.39544500 -1.73666300
 H 6.39780900 2.31073200 -0.49195200
 C -4.55893600 -0.62666100 -1.64849800
 C -4.03699200 0.66391000 -1.77038600
 C -5.58660900 -0.84285800 -0.72415400
 C -4.49488700 1.72777000 -0.98878900
 H -3.25098500 0.84705900 -2.50101200
 C -6.06866100 0.20859400 0.05222600
 H -6.01759500 -1.83737900 -0.62322100
 C -5.52412100 1.48477000 -0.07302800
 H -6.87536100 0.03259500 0.75937100

H -5.90682300 2.30334500 0.53377400
 Rh 0.00046200 -0.04078600 0.42257000
 C -0.21515200 -0.69692100 2.61710100
 C 0.95341000 -0.11400200 3.27889300
 C -1.59472600 -0.43085500 3.01389400
 H -0.04976800 -1.68145200 2.10616600
 O 2.03546900 -0.70611200 3.32207000
 O -1.99546100 0.59299400 3.54391000
 O -2.41514100 -1.45596400 2.67466000
 C 0.22665700 -2.98134900 2.93008800
 C -3.81027800 -1.15537000 2.77013400
 H 1.28831400 -2.80557800 2.75251400
 C -0.18504300 -3.04555600 4.34836300
 C -0.49463400 -3.80408900 1.92937400
 H -4.07878500 -0.38643600 2.03727600
 H -4.33295100 -2.08388500 2.54116900
 H -4.07067700 -0.80661300 3.77178200
 H 0.36037400 -2.33835800 4.97454100
 H -1.26347400 -2.92021100 4.47053600
 H 0.06139700 -4.05652400 4.70402000
 H -1.57392900 -3.79940100 2.09286300
 H -0.27566000 -3.49926200 0.90227900
 H -0.13230700 -4.83506300 2.05175600
 C 0.79688500 1.26565000 3.85705500
 H 0.29465200 1.93035200 3.14941900
 H 0.16841300 1.22843200 4.75154500
 H 1.78278300 1.65688700 4.11304100

3h

Rh -0.23039800 -0.13007700 -2.01176200
 O -1.59708400 1.43312400 -1.87132500
 O 1.28040600 1.28691800 -2.18092300
 O 1.13692200 -1.70479600 -1.98000900
 O -1.73628000 -1.51321800 -1.74259900
 C -2.03500800 -1.87588800 -0.56385600
 O -1.50664300 -1.43820200 0.51017500
 C 1.63449400 -2.05597100 -0.86302700
 O 1.38383200 -1.52795100 0.26667400
 C -1.84102700 1.95290900 -0.74002700
 O -1.34552800 1.58244400 0.37662100
 O 1.49742200 1.41607900 0.07078400
 C 1.79888800 1.75321800 -1.11786600
 C -2.81987800 3.12535000 -0.67280000
 C -3.13056500 -2.92987500 -0.40236400
 C 2.62984900 -3.21734400 -0.88014000
 C 2.88987500 2.81216800 -1.28896200

C -4.02497700 2.69377700 0.20699500
H -4.73492000 3.53058300 0.21182100
H -3.66081200 2.56990600 1.23416200
C -3.27919800 3.53128100 -2.06734600
H -3.98208400 4.36811100 -1.99497600
H -2.43282900 3.84874200 -2.68229700
H -3.77709900 2.70838600 -2.58520000
C -2.12258400 4.30277700 0.01457400
H -2.79700800 5.16400400 0.05432200
H -1.83511800 4.04588300 1.03769400
H -1.22189300 4.60751000 -0.52920500
C -4.29245200 -2.30128500 0.41338200
H -5.08706400 -3.05567700 0.47308400
H -3.93115200 -2.12999300 1.43417700
C -2.55693600 -4.10830900 0.38897800
H -3.33341500 -4.86281900 0.55166800
H -1.73503100 -4.58705900 -0.15380900
H -2.18111500 -3.78358100 1.36291100
C -3.62837400 -3.40850600 -1.76165600
H -2.82029200 -3.86471600 -2.33960200
H -4.41413900 -4.15878600 -1.62247200
H -4.03879300 -2.58783700 -2.35486500
C 3.08155900 -3.56883800 0.53294100
H 3.80264400 -4.39261400 0.49260200
H 3.54887100 -2.72007000 1.03904200
H 2.23414900 -3.88317600 1.14861300
C 1.94622700 -4.42492200 -1.52749900
H 1.60690800 -4.19066500 -2.53960900
H 2.64587400 -5.26520700 -1.58186700
H 1.07994500 -4.74840000 -0.94134000
C 3.84097400 -2.80746600 -1.75983000
H 4.55646600 -3.63871800 -1.72740000
H 3.49077900 -2.72391500 -2.79486900
C 4.05453200 2.18326800 -2.09976000
H 3.69051700 1.98815600 -3.11474500
H 4.83841600 2.94701800 -2.17859200
C 2.30787700 3.97962900 -2.08972700
H 1.47314200 4.44541600 -1.55489100
H 3.07398000 4.74640800 -2.24380200
H 1.94629800 3.64980600 -3.06661500
C 3.38784200 3.31039000 0.06295600
H 4.20634000 4.02330600 -0.08421400
H 2.59115900 3.81910600 0.61201100
H 3.74787100 2.49034400 0.68916900
C -4.69947700 1.42727000 -0.23755300
C -4.26644900 0.20027800 0.27336400

C -5.73346300 1.43068300 -1.17952900
C -4.82526700 -1.01186000 -0.14289700
H -3.47145300 0.18729800 1.01778000
C -6.30882400 0.23345000 -1.59817200
H -6.09608900 2.37784900 -1.57452400
C -5.85651800 -0.98102400 -1.08757800
H -7.12047700 0.24741900 -2.32097200
H -6.31504700 -1.91337300 -1.41218800
C 4.60958000 0.91518800 -1.51572800
C 4.05693300 -0.31359500 -1.88809500
C 5.65662200 0.91927500 -0.58818200
C 4.50629600 -1.52356900 -1.35188200
H 3.25192500 -0.32823500 -2.62085300
C 6.12944400 -0.27751700 -0.05425500
H 6.10944000 1.86481300 -0.29428200
C 5.55624300 -1.49109200 -0.42768100
H 6.95198400 -0.26451700 0.65654800
H 5.93209100 -2.42354200 -0.01078900
Rh 0.00683200 0.00294500 0.39042600
C 0.22071400 0.13238800 2.66348800
C -0.95648200 -0.53475000 3.22862600
C 1.59850800 -0.25622400 2.95516400
H 0.07367300 1.22275900 2.42467200
O -2.01457500 0.07555600 3.40528300
O 1.96972000 -1.38396400 3.23943400
O 2.45245900 0.78649900 2.80713100
C -0.12177900 2.30739800 3.51729000
C 3.83328800 0.41782100 2.75110900
H -1.19236000 2.22864900 3.32303600
C 0.29845700 2.00717900 4.90226800
C 0.63124400 3.31179300 2.72960500
H 4.02630500 -0.16035000 1.84055900
H 4.39322500 1.35242400 2.72206100
H 4.12167100 -0.17220300 3.62345700
H -0.26493900 1.18203000 5.34027800
H 1.37333200 1.82612000 4.97886300
H 0.08217200 2.90337000 5.50164200
H 1.70888500 3.22909300 2.88076200
H 0.40339000 3.25908500 1.66131300
H 0.30698300 4.29971200 3.08782500
C -0.84335000 -2.01016000 3.53408400
H -0.43036300 -2.50683500 2.64648500
H -0.06088800 -2.13290800 4.29264900
C -2.15224500 -2.62612300 3.97599400
H -2.92862800 -2.49607200 3.21635300
H -2.03469900 -3.69767500 4.15841800

H -2.52304100 -2.16233800 4.89366200

3i

Rh -0.22391100 -1.63255700 -1.56115000

O 0.98325400 -2.82117900 -0.35789600

O -1.86325700 -2.45106200 -0.59024300

O -1.42519200 -0.32761300 -2.65450000

O 1.42811200 -0.75231900 -2.43675200

C 1.93028400 0.28672700 -1.90926000

O 1.54032600 0.83983300 -0.82917200

C -1.69427400 0.81010500 -2.15308500

O -1.31305100 1.23601600 -1.01681900

C 1.33510300 -2.40536300 0.78797600

O 1.05152700 -1.26688800 1.28961800

O -1.77783400 -0.86375300 1.02504000

C -2.26260100 -1.91072200 0.48896300

C 2.19453900 -3.32599700 1.65520200

C 3.12430200 0.93732800 -2.60678500

C -2.56567000 1.75101500 -2.98737700

C -3.44559800 -2.58195600 1.18838000

C 3.57925600 -2.64792700 1.85058400

H 4.20199400 -3.35140000 2.41800500

H 3.43259600 -1.76372400 2.48277600

C 2.34733800 -4.69553700 1.00393000

H 2.96272900 -5.33987500 1.64062900

H 1.37475700 -5.17700900 0.86962900

H 2.82177600 -4.62823400 0.02227100

C 1.53424400 -3.46950300 3.02845600

H 2.12877400 -4.13639200 3.66074200

H 1.45815000 -2.50104500 3.52953400

H 0.52772700 -3.89386700 2.94714400

C 4.33961200 0.85132800 -1.64389300

H 5.20496900 1.26175600 -2.18020700

H 4.13785900 1.51424900 -0.79622800

C 2.79904400 2.41227800 -2.85554400

H 3.66156900 2.91722400 -3.30299600

H 1.95221300 2.52157000 -3.54116200

H 2.54721700 2.92271600 -1.92135900

C 3.42967500 0.24276100 -3.92857200

H 2.57521300 0.29546300 -4.60856300

H 4.28139400 0.73274200 -4.41251800

H 3.67655600 -0.81189800 -3.78596400

C -2.70488600 3.11000200 -2.30968200

H -3.34242000 3.75954700 -2.91907600

H -3.13973200 3.02988900 -1.31025700

H -1.72984100 3.59361600 -2.19901500

C -1.91757900 1.91836700 -4.36411900

H -1.80007000 0.95379500 -4.86384100

H -2.53999500 2.56227700 -4.99365300

H -0.93010500 2.38424800 -4.28207000

C -3.95725600 1.08790900 -3.17801300

H -4.58165900 1.80932000 -3.72012500

H -3.82702100 0.21959200 -3.83390500

C -4.67544700 -2.48876700 0.24503000

H -4.48542500 -3.13955600 -0.61579700

H -5.52946300 -2.91310700 0.78788400

C -3.10538300 -4.05877300 1.40339000

H -2.22608400 -4.17056600 2.04728100

H -3.94331800 -4.56932500 1.88879400

H -2.89713300 -4.55747000 0.45394100

C -3.74263400 -1.91955900 2.52828000

H -4.62043200 -2.38860300 2.98564600

H -2.90100700 -2.03544300 3.21687100

H -3.93535500 -0.84944700 2.42147500

C 4.26385000 -2.23798800 0.57830400

C 4.05867800 -0.95066700 0.07323600

C 5.08664300 -3.11314500 -0.13857700

C 4.63586900 -0.52744800 -1.12785300

H 3.43538400 -0.25611500 0.63588000

C 5.68167500 -2.70361300 -1.32944200

H 5.27412800 -4.11290400 0.24876000

C 5.45607400 -1.42137500 -1.82440700

H 6.33153600 -3.38553600 -1.87165500

H 5.93035500 -1.10356100 -2.75116700

C -4.99198800 -1.10283700 -0.24076400

C -4.40731600 -0.63859300 -1.42245900

C -5.84492900 -0.24353100 0.45943700

C -4.63611400 0.65053200 -1.91078600

H -3.75747500 -1.30520100 -1.98667400

C -6.09571300 1.04154400 -0.01699600

H -6.32131500 -0.58829600 1.37578000

C -5.49258500 1.49041100 -1.19019400

H -6.76726300 1.69845800 0.53025500

H -5.69793900 2.49339300 -1.55979800

Rh -0.11031600 0.04888300 0.17199100

C 0.04906500 1.59827000 1.84981500

C 1.37369900 2.22889500 1.76185800

C -1.23010300 2.30378000 1.82629300

H 0.04519200 0.65992900 2.47148800

O 2.35759000 1.67532700 2.26601600

O -1.48431400 3.31417300 1.18790700

O -2.16689200 1.64755300 2.55648800

C 0.30067300 0.60896300 4.03918700
 C -3.51014200 2.06618600 2.30011700
 H 1.32488400 0.33345200 3.78486700
 C 0.13969500 1.87067200 4.78766000
 C -0.67243100 -0.48709600 4.23077300
 H -3.77078000 1.85875600 1.25685900
 H -4.14078500 1.47578000 2.96486600
 H -3.63701500 3.13227100 2.50087300
 H 0.85985700 2.63300100 4.48563700
 H -0.88108600 2.25716700 4.73419800
 H 0.33612900 1.63790600 5.84487100
 H -1.69504400 -0.11720600 4.32358500
 H -0.61685900 -1.23626600 3.43624900
 H -0.40000800 -0.98894600 5.17150800
 C 1.48362700 3.52846200 0.99995900
 H 1.44071300 3.26166600 -0.06777300
 H 0.56717900 4.10221000 1.17011000
 C 2.70679700 4.41927400 1.27844500
 C 2.81041400 4.72282200 2.77428500
 H 3.03994100 3.82138800 3.34896500
 H 3.60350200 5.45435300 2.96515100
 H 1.87272200 5.14433700 3.15674600
 C 2.48248600 5.73002900 0.52028700
 H 3.33087800 6.40960100 0.65933300
 H 2.37145700 5.55021800 -0.55573400
 H 1.57955300 6.24484100 0.86747800
 C 4.00881500 3.79216800 0.78159000
 H 4.19249600 2.82395200 1.25218800
 H 3.98087000 3.64711000 -0.30498300
 H 4.85756300 4.45123900 0.99912100

3j

Rh -0.05011600 -0.00022700 -2.13397600
 O -1.47982900 1.50492500 -1.99247400
 O 1.44296700 1.44603000 -2.09415600
 O 1.35004100 -1.54776700 -2.10353300
 O -1.57102900 -1.38699100 -2.08412400
 C -1.99765200 -1.77128700 -0.95060300
 O -1.54022400 -1.41354400 0.18232600
 C 1.74346800 -1.99694200 -0.98001700
 O 1.36892000 -1.58642300 0.16439900
 C -1.78919000 1.96469600 -0.85133400
 O -1.30156600 1.58167600 0.26458100
 O 1.57459100 1.35639800 0.16615400
 C 1.92059600 1.80599100 -0.97263000
 C -2.81741400 3.09541100 -0.77731900

C -3.14916000 -2.77912300 -0.93573800
 C 2.75817100 -3.14282600 -1.00560300
 C 3.01547200 2.87661900 -1.00808700
 C -3.95277900 2.68865000 0.19945300
 H -4.63996100 3.54213200 0.25862600
 H -3.50897100 2.55946200 1.19303800
 C -3.37641300 3.41434400 -2.15838300
 H -4.10602900 4.22767300 -2.08097400
 H -2.58417800 3.72985300 -2.84182500
 H -3.87622000 2.54977600 -2.60238100
 C -2.11108000 4.32833500 -0.20267200
 H -2.80744400 5.17199800 -0.16218400
 H -1.74759300 4.13642300 0.81094600
 H -1.26012500 4.62657400 -0.82398800
 C -4.20253200 -2.32552200 0.10809800
 H -4.97142200 -3.10730300 0.15214300
 H -3.71540200 -2.28690600 1.09025900
 C -2.57145100 -4.13592000 -0.51771500
 H -3.37080700 -4.88275400 -0.47317700
 H -1.82862300 -4.48437800 -1.24276700
 H -2.09329200 -4.08480700 0.46361500
 C -3.77626000 -2.90822700 -2.32052100
 H -3.04674900 -3.27179700 -3.04759300
 H -4.60639300 -3.62209000 -2.28141600
 H -4.16532400 -1.95382900 -2.68357500
 C 3.15032800 -3.55674200 0.40853000
 H 3.91094100 -4.34383400 0.36228700
 H 3.54951300 -2.71859000 0.98586500
 H 2.28771100 -3.94704500 0.95524300
 C 2.12149300 -4.32751300 -1.73744100
 H 1.81876400 -4.05169700 -2.75082100
 H 2.83742300 -5.15325700 -1.80269300
 H 1.23947600 -4.69209200 -1.20071000
 C 4.00386700 -2.68109500 -1.80716200
 H 4.71875600 -3.51344300 -1.79224500
 H 3.69867300 -2.53550100 -2.84944600
 C 4.21222600 2.31963300 -1.82638600
 H 3.88271200 2.19579100 -2.86416800
 H 4.99062700 3.09300300 -1.82276900
 C 2.45840300 4.10770100 -1.72688000
 H 1.60836500 4.53006500 -1.17973200
 H 3.22909300 4.88233000 -1.79426100
 H 2.12650700 3.85945100 -2.73782900
 C 3.46511800 3.25545000 0.39701800
 H 4.27464600 3.99107100 0.33795100
 H 2.64541300 3.69837800 0.96836500

H 3.82480500 2.38644000 0.95209000
C -4.70037200 1.44347900 -0.18632400
C -4.20062500 0.19038700 0.18261900
C -5.87891100 1.50081300 -0.93732400
C -4.82851700 -0.99574600 -0.21090200
H -3.30496600 0.13709000 0.79739900
C -6.53600900 0.33005900 -1.30759700
H -6.28615600 2.46936000 -1.22309800
C -6.01095200 -0.91009700 -0.95424800
H -7.45954500 0.38419300 -1.87823900
H -6.52081800 -1.82376600 -1.25544500
C 4.75651900 1.01852300 -1.31060200
C 4.22406400 -0.18502100 -1.78019100
C 5.76174800 0.96669000 -0.33906800
C 4.64884900 -1.42469300 -1.29505300
H 3.45394000 -0.15540000 -2.54901500
C 6.20951300 -0.25980500 0.14655200
H 6.20010800 1.89260300 0.02907000
C 5.65393500 -1.44838600 -0.32193600
H 6.99947600 -0.29024200 0.89275600
H 6.00946700 -2.40411900 0.05831300
Rh 0.02361000 -0.02572300 0.28419000
C 0.06859500 0.05260600 2.56449600
C -1.14590200 -0.56214300 3.12244700
C 1.42866100 -0.29918700 2.96798700
H -0.06721100 1.15287400 2.33661100
O -2.22922100 0.02439700 3.03773700
O 1.81734800 -1.42733400 3.23101500
O 2.25351300 0.77732700 2.94809200
C -0.37196200 2.28633200 3.37945700
C 3.64700400 0.46172100 3.01037700
H -1.41047600 2.18641500 3.06005900
C -0.09421500 1.97772300 4.79655300
C 0.45538100 3.29253400 2.68090100
H 3.95508600 -0.05689900 2.09488500
H 4.16701600 1.41638000 3.08742200
H 3.87280800 -0.16547600 3.87514600
H -0.70864700 1.16226600 5.18194100
H 0.96601100 1.78090200 4.97377400
H -0.35085000 2.87793000 5.37410200
H 1.50650700 3.22997500 2.96762300
H 0.35953100 3.22787000 1.59346700
H 0.07465100 4.27899900 2.98568200
C -1.04335900 -1.91539300 3.80945200
H -0.14378900 -1.88047300 4.43676600
C -2.26437200 -2.17602800 4.67544800

H -3.17334000 -2.21601200 4.06815900
H -2.16059400 -3.13390700 5.19393400
H -2.40719800 -1.39529100 5.42819800
C -0.84425000 -3.03076900 2.78464200
H -0.04778500 -2.79426200 2.07485700
H -0.60080300 -3.97127000 3.28866700
H -1.76882700 -3.17404800 2.21755400

3k

Rh -0.22766300 -1.42457600 -1.81239300
O 1.05079800 -2.77861300 -0.87869300
O -1.85653500 -2.39521700 -0.95272400
O -1.44048900 0.06247000 -2.63380100
O 1.41397400 -0.44622800 -2.57490900
C 1.96698500 0.44361300 -1.85607600
O 1.57919500 0.82045800 -0.70383200
C -1.70415500 1.09050500 -1.93175200
O -1.30915000 1.30679500 -0.74231900
C 1.41744700 -2.57106500 0.31773600
O 1.07534900 -1.57626200 1.04056700
O -1.77089400 -1.08344200 0.89269300
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C 2.33694100 -3.59502800 0.98680500
C 3.19922000 1.14829000 -2.42920700
C -2.57957200 2.16272300 -2.58255200
C -3.47329800 -2.77133900 0.76110500
C 3.59416700 -2.86490800 1.53274500
H 4.20528300 -3.62234600 2.04009600
H 3.26335100 -2.15024900 2.29506500
C 2.73038300 -4.69585400 0.00965400
H 3.39430300 -5.41015800 0.50849000
H 1.85207900 -5.23874700 -0.34820100
H 3.25486800 -4.29474300 -0.86127200
C 1.58105100 -4.19708100 2.17633500
H 2.19608100 -4.96343200 2.65878100
H 1.34567600 -3.43103700 2.92057600
H 0.64502000 -4.66955000 1.85926400
C 4.29985600 1.19618400 -1.33718900
H 5.14274000 1.76255200 -1.75346300
H 3.91036900 1.76614200 -0.48451900
C 2.79465400 2.57825300 -2.80656100
H 3.65743400 3.10950200 -3.22165400
H 2.00751400 2.57274600 -3.56781100
H 2.43019600 3.14140200 -1.94355600
C 3.70234000 0.43100500 -3.67853400
H 2.95207500 0.45427900 -4.47216300

H 4.60562400 0.92914700 -4.04781000
 H 3.94753300 -0.61463700 -3.47936000
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 H -3.45827200 4.07450800 -2.12184900
 H -3.29670100 3.01552200 -0.70671700
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 H -2.48268800 3.40594400 -4.35245600
 H -0.90721600 3.11993800 -3.60009300
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 H -5.51798600 -3.13334500 0.21611000
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 H 6.37400000 -0.29633200 -2.30445500
 C -5.02510000 -1.17200600 -0.51249200
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 C -4.65972600 0.83486000 -1.86315000
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 C -6.23758500 0.86766100 -0.02422900
 H -6.46257800 -0.96983900 1.08029800
 C -5.59158000 1.51732000 -1.07390400
 H -6.97046700 1.40358800 0.57360200
 H -5.82025600 2.55827100 -1.29438200
 Rh -0.09478500 -0.07524600 0.19266900
 C 0.04189200 1.10449400 2.14525300

C 1.35055900 1.76967400 2.23405800
 C -1.23954900 1.78477800 2.32534100
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 O -1.49468700 2.92159000 1.95672300
 O -2.16328200 0.97150800 2.89443600
 C 0.35009700 -0.35230000 4.03590800
 C -3.51317200 1.43112600 2.78570100
 H 1.36690300 -0.56711000 3.70239400
 C 0.21270200 0.71130700 5.05266800
 C -0.61408800 -1.47447800 4.03016700
 H -3.84921300 1.35191000 1.74415600
 H -4.10722600 0.77091100 3.41710400
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 H 0.43524700 0.25191300 6.02667200
 H -1.62967600 -1.14331500 4.25449300
 H -0.59950700 -2.03171700 3.08942900
 H -0.29619600 -2.16543100 4.82522300
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 C 2.76212300 3.83910200 2.48798800
 C 1.19933400 3.61763900 0.53726400
 H 0.61143200 3.72559900 2.58570300
 C 2.81407600 5.34656000 2.26846000
 H 3.57570100 3.35400600 1.93196600
 H 2.92621000 3.59001900 3.54344300
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 C 2.56173600 5.70543400 0.80800000
 H 3.77944300 5.74491600 2.60128100
 H 2.04926500 5.83072500 2.89390800
 H 1.08748500 5.35173900 -0.74327500
 H 0.40527800 5.59037100 0.86133100
 H 2.58417900 6.79237200 0.66856500
 H 3.37777400 5.29516500 0.19267500

3I

Rh -0.17177400 0.62844800 -2.05468900
 O -1.53653900 2.05668800 -1.41759200
 O 1.34820900 2.00613600 -1.72330200
 O 1.17742400 -0.88239200 -2.54566000
 O -1.69700400 -0.72308900 -2.30011100
 C -2.05010500 -1.44284300 -1.31489500
 O -1.54094400 -1.40999600 -0.14799300

C 1.66832400 -1.58758200 -1.60664600
O 1.41274600 -1.46733400 -0.36698500
C -1.78703000 2.18155800 -0.18023500
O -1.29316600 1.46949900 0.75682400
O 1.56192800 1.34691000 0.43420500
C 1.86764400 2.07267300 -0.56507400
C -2.76873000 3.27409300 0.24891600
C -3.18353400 -2.44545400 -1.55865400
C 2.66038900 -2.68004600 -2.01070300
C 2.96055900 3.12575900 -0.36579700
C -3.97125400 2.59935100 0.96146800
H -4.65878800 3.40228300 1.25663600
H -3.59845800 2.13493000 1.88213500
C -3.23585700 4.08552700 -0.95338700
H -3.94654600 4.85202400 -0.62604500
H -2.39536500 4.58550800 -1.44195300
H -3.72894700 3.45630100 -1.69798400
C -2.06982500 4.18823200 1.25804600
H -2.74064800 5.00231500 1.55054500
H -1.79064200 3.63564800 2.15865200
H -1.16479800 4.63606900 0.83453400
C -4.33468700 -2.15492300 -0.56096900
H -5.13475400 -2.87427600 -0.77709700
H -3.97110000 -2.37184400 0.44997100
C -2.65302600 -3.85709800 -1.29493200
H -3.44113200 -4.59095800 -1.49200300
H -1.80636800 -4.09215300 -1.94857800
H -2.32748400 -3.97568600 -0.25810200
C -3.68718100 -2.34911900 -2.99513600
H -2.88921500 -2.56977500 -3.70851500
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H -4.07352500 -1.35293200 -3.22421100
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H 1.10339900 -4.10877900 -2.53572900
C 3.86449600 -2.00493600 -2.71969300
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H 3.50499100 -1.57458900 -3.66105300
C 4.12416000 2.80334800 -1.34176200
H 3.76306500 2.97066200 -2.36269800
H 4.91393100 3.54153800 -1.15360700

C 2.38157800 4.49569300 -0.72831700
H 1.56205100 4.76756800 -0.05436800
H 3.15632100 5.26368300 -0.63657700
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C 4.66610800 1.40679800 -1.22491500
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C 4.54161200 -0.93987700 -1.90444400
H 3.31072600 0.63106400 -2.69823700
C 6.15705800 -0.23101400 -0.24349500
H 6.15959700 1.86492500 0.25943900
C 5.58032300 -1.23657300 -1.01548200
H 6.97145300 -0.47076400 0.43541700
H 5.94416400 -2.25940600 -0.93855200
Rh 0.03886100 -0.05972300 0.25369400
C 0.23055700 -0.66540300 2.49981400
C -0.94911000 -1.50508900 2.76194000
C 1.63604300 -0.94003500 2.79907500
H -0.01456800 0.42303100 2.53924200
O -2.03128000 -0.94427500 2.97060900
O 2.20523000 -2.02128300 2.81004500
O 2.30268300 0.21661200 3.05151800
C -0.37073500 1.22287700 3.96675600
C 3.72224100 0.08289100 3.12781000
H -1.39025400 1.15340500 3.58642500
C -0.08637800 0.50355000 5.21902200
C 0.40582200 2.42172900 3.59971500
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H 1.43962500 2.37768100 3.94327800
H 0.37479100 2.62344200 2.52438400
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C -0.88366400 -3.04527700 2.79557400
C -2.30876700 -3.58980400 2.73055000
H -2.79166800 -3.30393800 1.79147200
H -2.28411100 -4.68335900 2.78309800
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H 0.97104600 -3.34305300 1.67509900
H -0.11699100 -4.74212000 1.71623800
C -0.27691300 -3.44274700 4.15236700
H -0.24534500 -4.53532700 4.22717600
H 0.74170000 -3.07026500 4.27721200
H -0.89407700 -3.07432100 4.97999500

3m

Rh 0.17447800 0.30308500 -1.99851300
O 1.56182000 -1.24996500 -2.00044400
O -1.33488300 -1.10804700 -2.23848000
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O 1.68268200 1.67905300 -1.65194800
C 1.99720300 1.93887400 -0.44994600
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C -1.67319200 2.12478900 -0.66532700
O -1.39408100 1.51536500 0.41587300
C 1.82933800 -1.85834100 -0.92054600
O 1.33972100 -1.59118500 0.22787400
O -1.51821900 -1.40409500 0.00003000
C -1.83486800 -1.65536800 -1.20520500
C 2.83088100 -3.01277500 -0.96328400
C 3.07974800 2.98612200 -0.18974100
C -2.67463100 3.27838700 -0.57567200
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C 4.02153900 -2.65228800 -0.03438500
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H 4.03225300 -4.08870100 -2.39174600
H 2.47601300 -3.54175500 -3.03999800
H 3.78984800 -2.38366200 -2.81479400
C 2.14869600 -4.26597200 -0.40611500
H 2.83852700 -5.11497500 -0.44590800
H 1.84704300 -4.11870400 0.63469500

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C 2.46934800 4.10132200 0.66478600
H 3.23372100 4.84866100 0.90176400
H 1.65951100 4.61094200 0.13230700
H 2.07060300 3.70120100 1.60119200
C 3.60894300 3.56244000 -1.49758000
H 2.81158800 4.05186300 -2.06281000
H 4.38212000 4.30815800 -1.28371400
H 4.04535300 2.79086300 -2.13621100
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H -3.58026500 2.63716600 1.30197500
H -2.25351600 3.78205600 1.49700600
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H -3.57228200 2.92580700 -2.50509100
C -4.09964800 -2.02113200 -2.18880000
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C 5.73875800 -1.24929600 -1.26677300
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C 6.31437700 -0.01430400 -1.55506200
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C 5.83982600 1.14280800 -0.94210300
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H 6.29575600 2.10527500 -1.16763300
C -4.65159200 -0.80601300 -1.49856400
C -4.10780100 0.45050700 -1.77829700

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 H -3.31653400 0.52727100 -2.52196900
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 H -6.12781800 -1.85744500 -0.33314700
 C -5.58112100 1.49957800 -0.19853100
 H -6.95261800 0.18300000 0.80873200
 H -5.95134300 2.39338400 0.30060600
 Rh -0.01225100 -0.02289400 0.38961300
 C -0.08119900 -0.36308100 2.63894300
 C 1.15668700 0.20866500 3.17382400
 C -1.42505300 0.02641100 3.06043200
 H 0.00841500 -1.43149400 2.30831800
 O 2.18750600 -0.46997900 3.28062000
 C 1.15589300 1.65467300 3.51041200
 O -1.75065400 1.11113100 3.51670600
 O -2.31253900 -0.97095600 2.81732400
 C 0.24031800 -2.65146000 3.30027700
 C 2.20928800 2.21164800 4.11462300
 C -3.68588000 -0.57630100 2.85344500
 H 1.29734100 -2.57003200 3.04491700
 C -0.10259000 -2.44119600 4.71944700
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 H -4.26610900 -1.49621000 2.78383800
 H -3.92312400 -0.04531000 3.77745500
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 H -1.16267000 -2.21346700 4.85819800
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 H -0.25823200 -4.57611300 2.69284700
 H 0.27483200 2.23187300 3.24690500
 H 2.23417500 3.26757900 4.36442100

3n

Rh 0.25827000 0.57863200 -1.89596100
 O 1.68301100 -0.92488000 -2.05079100
 O -1.21215300 -0.82682200 -2.35819900
 O -1.15860800 2.07508500 -1.57042800
 O 1.72839300 1.91813300 -1.31691000
 C 1.98815600 2.04037700 -0.07999000
 O 1.45036900 1.37747200 0.86530400
 C -1.67310700 2.17964000 -0.41159500
 O -1.41968800 1.43430900 0.58781600

C 1.95349300 -1.64694900 -1.04416600
 O 1.42082500 -1.54408300 0.11199800
 O -1.44205300 -1.40740900 -0.17935500
 C -1.72757100 -1.50584300 -1.41554300
 C 2.99973200 -2.75065800 -1.20197300
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 C -2.79511100 -2.53272400 -1.80306300
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 H 4.86635800 -3.30780400 -0.29866500
 H 3.69299100 -2.63342400 0.83723000
 C 3.56173000 -2.76935700 -2.61825800
 H 4.31234200 -3.56208400 -2.70527000
 H 2.77558100 -2.96180200 -3.35267100
 H 4.03606300 -1.81975300 -2.87779800
 C 2.33152000 -4.09268600 -0.88672200
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 H 1.97485200 -4.12183700 0.14663200
 H 1.48093300 -4.28190300 -1.55065000
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 H 4.90460100 3.08447700 1.40203800
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 H 1.94328700 3.56610900 2.16468600
 C 3.60607200 3.79726300 -0.86575200
 H 2.82015100 4.32577800 -1.41122000
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 H 4.08903700 3.10784600 -1.56243500
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 H -2.28614900 3.53653300 1.92369900
 C -2.04555600 4.62852700 -0.60169900
 H -1.70316400 4.60234200 -1.63888400
 H -2.77066400 5.44192200 -0.49617000
 H -1.18841100 4.86220100 0.03753900
 C -3.90626100 3.04140700 -1.12951200
 H -4.64056800 3.83058300 -0.92464800
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 C -3.98243100 -1.77898000 -2.45954100
 H -3.63179500 -1.36677700 -3.41233500
 H -4.74683500 -2.53032100 -2.69405600
 C -2.19225600 -3.48757300 -2.83639400
 H -1.33918200 -4.03279100 -2.41779300

H -2.94053500 -4.22398800 -3.14642400
H -1.85068100 -2.94679800 -3.72221500
C -3.26586400 -3.31611600 -0.58321000
H -4.08134800 -3.98952400 -0.86783500
H -2.45420000 -3.92357000 -0.17363600
H -3.61661100 -2.65527900 0.21362300
C 4.78260600 -1.16025800 -0.25607200
C 4.25630300 -0.08581700 0.46691900
C 5.89585500 -0.93585300 -1.07285900
C 4.79647000 1.20025500 0.37424400
H 3.40615000 -0.25786400 1.12502800
C 6.45687400 0.33561700 -1.16460500
H 6.32976800 -1.76530400 -1.62861000
C 5.90802500 1.39891700 -0.45179500
H 7.32916200 0.49831200 -1.79234500
H 6.35085200 2.39073100 -0.52463500
C -4.56581400 -0.67448100 -1.62480600
C -4.05588900 0.62030900 -1.74933200
C -5.59861700 -0.89605000 -0.70740500
C -4.53065800 1.68406900 -0.97773700
H -3.26786600 0.80769500 -2.47659200
C -6.09744700 0.15474000 0.05907200
H -6.02102600 -1.89408000 -0.60511600
C -5.56473900 1.43592600 -0.06867600
H -6.90784900 -0.02550200 0.76091600
H -5.96081200 2.25399900 0.53024000
Rh 0.00685900 -0.05207000 0.42312200
C -0.14302200 -0.66979300 2.55655200
C 1.01852700 -0.15842500 3.30232200
C -1.49180600 -0.34115100 2.98998300
H -0.00523700 -1.70764500 2.16793600
O 2.10250400 -0.72385900 3.33852200
O -1.78736800 0.71424900 3.55498400
O -2.39593400 -1.27479200 2.65216200
C 0.26900200 -3.11538700 2.96076100
C -3.76770400 -0.86681600 2.74061000
H 1.32265200 -2.92813100 2.74578500
C -0.12632500 -3.09864500 4.37658300
C -0.51235400 -3.87632300 1.97045800
H -3.98764700 -0.14752900 1.94446600
H -4.35770500 -1.77068000 2.59413800
H -3.98347000 -0.42079200 3.71278800
H 0.44369300 -2.37669200 4.96268500
H -1.20138100 -2.95194700 4.50778400
H 0.10606800 -4.09542000 4.78245100
H -1.58667500 -3.81423900 2.15757600

H -0.29229800 -3.57537900 0.94241500
H -0.21332700 -4.93143800 2.07035700
O 0.83844300 1.01448100 3.93169600
H -0.11467300 1.25653700 3.85769400

3o

Rh 0.17645900 0.25929100 -2.00877600
O 1.56085900 -1.29422000 -1.97692100
O -1.32921500 -1.16061500 -2.22499200
O -1.20249300 1.81207200 -1.87129400
O 1.67659200 1.64177100 -1.67693700
C 1.99764900 1.92530000 -0.48255200
O 1.49978700 1.40764100 0.57007500
C -1.68095100 2.10240300 -0.72842400
O -1.40702000 1.51893800 0.36813300
C 1.82478300 -1.88153300 -0.88484100
O 1.34023200 -1.58540100 0.25892900
O -1.51723400 -1.40540300 0.01969400
C -1.83091000 -1.68407700 -1.18077700
C 2.81711900 -3.04499200 -0.90612200
C 3.08592800 2.97680200 -0.26500900
C -2.68444500 3.25664000 -0.67579800
C -2.91818900 -2.74020400 -1.39077400
C 4.02603700 -2.66261400 -0.01028700
H 4.74245100 -3.49205500 -0.06664300
H 3.67079000 -2.61057700 1.02607600
C 3.26900600 -3.34812500 -2.32920900
H 3.98327000 -4.17837600 -2.31922300
H 2.42245100 -3.63425700 -2.95886700
H 3.75266600 -2.48498700 -2.79241100
C 2.13801200 -4.27501700 -0.29703700
H 2.82280500 -5.12870800 -0.31919300
H 1.85409400 -4.09102400 0.74263900
H 1.23799600 -4.55357000 -0.85548200
C 4.25493200 2.31071900 0.50869700
H 5.04226500 3.06749500 0.61646600
H 3.89622800 2.06900700 1.51623000
C 2.50345300 4.10128100 0.59639900
H 3.27951500 4.84005400 0.82160300
H 1.69185900 4.61879400 0.07466900
H 2.10742900 3.71272100 1.53835500
C 3.57463600 3.54055600 -1.59439000
H 2.75973100 4.01947200 -2.14324500
H 4.35031700 4.29200400 -1.41185800
H 3.99585200 2.76253100 -2.23545600
C -3.13587800 3.53078400 0.75366900

H -3.85215500 4.35974300 0.75724200
H -3.61728000 2.65816000 1.20185000
H -2.29093600 3.80445300 1.39019200
C -2.01164600 4.50193000 -1.26013400
H -1.67261200 4.32316100 -2.28352900
H -2.71828800 5.33812600 -1.26878800
H -1.14693200 4.80143900 -0.65934900
C -3.89801200 2.88553200 -1.56877700
H -4.61854900 3.70921500 -1.48824100
H -3.55491700 2.85779000 -2.60901400
C -4.09049400 -2.08222800 -2.16552600
H -3.73275600 -1.83517100 -3.17136500
H -4.87017100 -2.84622500 -2.27772600
C -2.33349100 -3.86857600 -2.24426700
H -1.49697300 -4.35628300 -1.73201800
H -3.09762100 -4.62960800 -2.43262800
H -1.97387000 -3.49312800 -3.20526700
C -3.40824000 -3.29968200 -0.05977300
H -4.20939400 -4.02516400 -0.23777400
H -2.60324500 -3.80985900 0.47534200
H -3.79295000 -2.51238200 0.59318100
C 4.68782000 -1.36495300 -0.37719900
C 4.24901200 -0.17618500 0.21257900
C 5.71762400 -1.30085300 -1.32185200
C 4.79827300 1.06345800 -0.12822500
H 3.45986000 -0.21496700 0.96220400
C 6.28403500 -0.07575900 -1.66515400
H 6.08444400 -2.21854800 -1.77833700
C 5.82555600 1.10077400 -1.07697700
H 7.09222800 -0.03792200 -2.39095300
H 6.27600600 2.05540300 -1.34316900
C -4.64838200 -0.84843800 -1.51431500
C -4.10454400 0.40055300 -1.82669200
C -5.68446600 -0.90689000 -0.57600900
C -4.55217900 1.57825800 -1.22172700
H -3.30699100 0.45695400 -2.56548000
C -6.15400400 0.25719000 0.02798900
H -6.13058400 -1.86876100 -0.32880800
C -5.59015000 1.49144400 -0.28737300
H -6.96726200 0.20263100 0.74734500
H -5.96490800 2.39869800 0.18318500
Rh -0.01655800 -0.01553000 0.38818000
C -0.11090700 -0.26829700 2.60449900
C 1.10662200 0.30696700 3.18637400
C -1.46120500 0.09822800 3.03541800
H 0.00880100 -1.35692200 2.35350200

O 2.17858000 -0.28150300 3.25812900
O -1.81737600 1.18665000 3.44818500
O -2.32123100 -0.93454100 2.82987300
C 0.26205000 -2.56317400 3.36155400
C -3.70224400 -0.56793900 2.84893400
H 1.31584000 -2.46535900 3.09553000
C -0.08161000 -2.31598900 4.77371000
C -0.55441700 -3.49331800 2.55464700
H -3.92592300 0.06815700 1.98486200
H -4.26309500 -1.49984900 2.77936500
H -3.95991400 -0.03595100 3.76710100
H 0.52658700 -1.52993500 5.22369700
H -1.14669100 -2.10882900 4.90701100
H 0.13077000 -3.24526200 5.32342500
H -1.61613600 -3.42730900 2.79840400
H -0.40816900 -3.34977500 1.48002400
H -0.20922000 -4.51018700 2.79542000
O 0.93709200 1.57813000 3.59721700
C 2.11946900 2.20352400 4.10168700
H 1.81837900 3.20692100 4.39783000
H 2.51640500 1.65473500 4.95867600
H 2.89043700 2.25490600 3.32788500

3p

Rh 0.11601700 -0.46811900 -2.04168300
O 1.45549200 -1.97961900 -1.54446600
O -1.45082700 -1.82630600 -1.78947500
O -1.20937500 1.10475900 -2.38253500
O 1.66574000 0.88900800 -2.16865500
C 2.01983400 1.52357600 -1.12783600
O 1.52655800 1.38421100 0.03909300
C -1.66307900 1.74444300 -1.38079600
O -1.39380700 1.51142400 -0.15978500
C 1.72628100 -2.20837200 -0.32705400
O 1.27406800 -1.55796500 0.67384000
O -1.57823100 -1.36236100 0.42506400
C -1.93807700 -1.98256300 -0.62564400
C 2.68718500 -3.35111200 0.00127200
C 3.14094600 2.55469300 -1.26806600
C -2.62927300 2.89344200 -1.67697100
C -3.06250700 -3.01071200 -0.47596400
C 3.92619700 -2.74666300 0.71621500
H 4.61679200 -3.57547700 0.91783200
H 3.59437600 -2.35601700 1.68603100
C 3.09938200 -4.09733300 -1.26167300
H 3.79497700 -4.90281000 -1.00262700

H 2.23281400 -4.54279900 -1.75775400
H 3.59141300 -3.43682100 -1.97938300
C 1.99312600 -4.30788900 0.97431800
H 2.65563700 -5.14727200 1.20824900
H 1.73982300 -3.80062800 1.90939100
H 1.07250700 -4.71712300 0.54503400
C 4.31503700 2.12728100 -0.34666300
H 5.12438800 2.85217200 -0.50041600
H 3.98036100 2.23020500 0.69227900
C 2.60939900 3.90684900 -0.78482100
H 3.41331300 4.65023900 -0.79022200
H 1.80912200 4.27334300 -1.43587200
H 2.21125100 3.82956600 0.23043600
C 3.60861200 2.66541900 -2.71430200
H 2.79006900 2.96941600 -3.37179100
H 4.40103800 3.41829400 -2.78565800
H 4.00314400 1.71794400 -3.08887100
C -3.02909800 3.62249500 -0.39976300
H -3.72577200 4.43199100 -0.64412800
H -3.51288000 2.95539600 0.31790200
H -2.15745000 4.05930000 0.09430800
C -1.94042600 3.86508600 -2.63871700
H -1.63863800 3.36093700 -3.56006100
H -2.62347000 4.68112900 -2.89614000
H -1.04959000 4.30730700 -2.18113700
C -3.88115200 2.30697600 -2.38331100
H -4.57200600 3.14201000 -2.55508000
H -3.57040500 1.93728300 -3.36717800
C -4.24171300 -2.58272600 -1.38931900
H -3.91136000 -2.67482300 -2.43008500
H -5.04556500 -3.31432900 -1.23896700
C -2.53857100 -4.36656000 -0.95622700
H -1.70530800 -4.70923400 -0.33331100
H -3.33258600 -5.11761700 -0.89347000
H -2.19281000 -4.31347800 -1.99143500
C -3.52329100 -3.11959200 0.97327200
H -4.34445300 -3.84129100 1.04347200
H -2.71222000 -3.46634100 1.61872200
H -3.87134700 -2.16058000 1.36516500
C 4.61736900 -1.65394600 -0.04778500
C 4.22717300 -0.32645100 0.14739200
C 5.62952900 -1.92331600 -0.97495800
C 4.80840900 0.72585100 -0.56621400
H 3.45284700 -0.10400800 0.88016600
C 6.22775000 -0.88598000 -1.68624000
H 5.95790600 -2.94987300 -1.12794700

C 5.81891600 0.43055800 -1.48706000
H 7.02253200 -1.10382500 -2.39485400
H 6.29524700 1.23935300 -2.03809900
C -4.74509100 -1.18815000 -1.14624900
C -4.16940300 -0.12026700 -1.83986600
C -5.76244400 -0.91244400 -0.22669800
C -4.56606700 1.20264500 -1.62992000
H -3.38942700 -0.32675600 -2.57046200
C -6.18069000 0.39900500 -0.01168400
H -6.23474700 -1.73159300 0.31266200
C -5.58408700 1.45149900 -0.70293000
H -6.97906200 0.60202900 0.69761400
H -5.91845300 2.47365300 -0.53489500
Rh -0.03852300 0.02117900 0.32397200
C -0.10837300 0.47076000 2.52082800
C 1.13028500 1.17892700 2.86105900
C -1.44592300 0.98245600 2.82130400
H -0.01201300 -0.64279000 2.60198200
O 2.19336900 0.61935000 3.10504400
O -1.77860600 2.15275800 2.86771300
O -2.32580200 -0.04475000 2.96583200
C 0.24833600 -1.47005000 3.94730600
C -3.69982900 0.33707000 2.87288000
H 1.29836900 -1.47473200 3.65118600
C -0.07035800 -0.79507000 5.21877700
C -0.59111100 -2.59438800 3.48333400
H -3.92285600 0.65483100 1.84786300
H -4.27929100 -0.55267100 3.11920600
H -3.93388500 1.14908300 3.56430600
H 0.55684000 0.07819200 5.40246900
H -1.12971300 -0.53576000 5.29163000
H 0.13319500 -1.51733500 6.02358300
H -1.64959100 -2.43274600 3.69556000
H -0.45161900 -2.80980100 2.42005300
H -0.26187700 -3.48442300 4.04037900
C 2.20518600 3.26034000 3.04775200
H 2.91343000 3.00534800 2.24987800
C 1.84774100 4.72022100 3.04542600
H 2.74662200 5.32455600 3.19011400
H 1.38944300 5.01362800 2.09707500
H 1.14479200 4.95569000 3.84816800
O 0.99007000 2.51523100 2.82879100
H 2.65291900 2.94039200 3.99402100

3q

Rh -0.14093700 0.29648500 -2.05408200

O -1.47420500 1.84425000 -1.66067600
O 1.42692100 1.66304400 -1.92361100
O 1.19474500 -1.28878400 -2.28315800
O -1.69036800 -1.06733500 -2.06376100
C -2.03477100 -1.62526700 -0.97647400
O -1.53638500 -1.39273500 0.17362900
C 1.65012800 -1.84578900 -1.23347800
O 1.37739500 -1.51726000 -0.03620600
C -1.74971900 2.15852100 -0.46375800
O -1.30335900 1.57918700 0.58252300
O 1.55571100 1.39080400 0.32206000
C 1.92032500 1.91382000 -0.77941100
C -2.70848900 3.32444400 -0.22363300
C -3.15091600 -2.67022500 -1.03283600
C 2.61388100 -3.01900900 -1.42485800
C 3.05313500 2.94142400 -0.72515300
C -3.95369400 2.77473900 0.52581500
H -4.64734600 3.61511200 0.65591100
H -3.62888500 2.46222700 1.52562200
C -3.10893800 3.97953600 -1.53945400
H -3.79584900 4.80972100 -1.34346600
H -2.23521700 4.37642100 -2.06347200
H -3.60526500 3.27392800 -2.20935300
C -2.01422200 4.34688200 0.68004800
H -2.67646000 5.20074100 0.85461500
H -1.76002800 3.90648600 1.64773400
H -1.09368900 4.72475000 0.22186900
C -4.33686100 -2.16976700 -0.16379600
H -5.14647800 -2.90211300 -0.27395300
H -4.02092500 -2.19826600 0.88519200
C -2.62415900 -3.97728800 -0.43395900
H -3.41885000 -4.73044900 -0.43101600
H -1.79222900 -4.37355000 -1.02513300
H -2.27445300 -3.84031300 0.59222100
C -3.60484900 -2.90553000 -2.46894700
H -2.77890400 -3.26411200 -3.08868100
H -4.39577500 -3.66305000 -2.48287200
H -3.99487000 -1.99415500 -2.92829500
C 3.02074200 -3.61686500 -0.08263200
H 3.70328700 -4.45730300 -0.24965100
H 3.52189800 -2.88572500 0.55679500
H 2.14979400 -3.98228800 0.46730900
C 1.91208100 -4.07980900 -2.27715600
H 1.59389100 -3.66759100 -3.23788000
H 2.59349100 -4.91569400 -2.46560700
H 1.03035700 -4.47699500 -1.76385700

C 3.86144200 -2.51249500 -2.19810000
H 4.54639900 -3.36467800 -2.28991900
H 3.54328100 -2.24392200 -3.21191700
C 4.20878600 2.44874700 -1.63635900
H 3.84711700 2.45628800 -2.67060100
H 5.01013600 3.19516000 -1.56768000
C 2.51983700 4.26366600 -1.28438100
H 1.69173900 4.64211000 -0.67484200
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H 2.16277100 4.14473000 -2.31039500
C 3.54406400 3.14797900 0.70368700
H 4.39235400 3.84096400 0.70506900
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C -4.25655900 0.31536500 0.15225200
C -5.62394500 1.82123700 -1.12907100
C -4.82130900 -0.78791500 -0.49479200
H -3.50250500 0.15103200 0.92143200
C -6.20852000 0.73288800 -1.77158000
H -5.94409900 2.83305700 -1.37113800
C -5.80802600 -0.56417100 -1.46069600
H -6.98488700 0.89579100 -2.51429700
H -6.27214200 -1.41267400 -1.96003800
C 4.73161900 1.08201800 -1.29691900
C 4.15018800 -0.04444900 -1.88419900
C 5.77377100 0.89262400 -0.38289500
C 4.55944300 -1.34228000 -1.56612600
H 3.35308600 0.09233300 -2.61255900
C 6.20812700 -0.39226900 -0.06577400
H 6.24986800 1.75810200 0.07489500
C 5.60127800 -1.50414300 -0.64626100
H 7.02420300 -0.52852900 0.63939500
H 5.94443000 -2.50631900 -0.39555200
Rh 0.02369700 -0.00230500 0.34035200
C 0.17087100 -0.26043100 2.54847100
C -1.07474800 -0.88125900 2.98443200
C 1.49681400 -0.80915000 2.84180400
H 0.12359300 0.85576800 2.58737500
O -2.11499200 -0.27625900 3.21872000
O 1.78151400 -1.98565500 2.97046100
O 2.42038300 0.18911900 2.87136100
C -0.09330600 1.85289400 3.88797100
C 3.77658500 -0.25114900 2.77115300
H -1.14966000 1.83271600 3.61611800
C 0.27461400 1.24266500 5.17430100

C 0.74693900 2.90632600 3.29373300
H 3.96640400 -0.62914100 1.75935400
H 4.39510000 0.62652800 2.95911700
H 3.99341400 -1.03519400 3.49949600
H -0.35878100 0.39430600 5.43663200
H 1.33169400 0.96602200 5.20857100
H 0.12671700 2.01014500 5.94963200
H 1.81072700 2.73549500 3.47232900
H 0.56006200 3.03861400 2.22402000
H 0.46736300 3.85086000 3.78651000
O -1.00091400 -2.23187100 3.05177500
C -2.24724500 -2.85681800 3.28380700
H -2.58280300 -2.68363500 4.31149100
H -2.98642200 -2.49324700 2.56031200
F -2.02924200 -4.18500400 3.09524500

3r

Rh -0.16737200 0.02114100 -2.10241900
O -1.51363500 1.60054100 -1.87008200
O 1.37584800 1.41067600 -2.14947300
O 1.17468300 -1.58752400 -2.13719100
O -1.72136700 -1.32761400 -1.95842400
C -2.02765800 -1.79188300 -0.81702700
O -1.47042900 -1.48641100 0.28765500
C 1.68951900 -1.97529000 -1.04138200
O 1.46821000 -1.47395000 0.10735300
C -1.81956300 1.99903000 -0.70591100
O -1.37197300 1.52154000 0.39056300
O 1.47885200 1.46969300 0.11511800
C 1.83945400 1.84075400 -1.04644500
C -2.80063100 3.16388300 -0.56717900
C -3.16356500 -2.81970800 -0.75373600
C 2.67437800 -3.14500300 -1.10439200
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H -1.17774600 4.61957300 -0.41889200
C -4.27519100 -2.27954600 0.18573400

H -5.06372500 -3.04224300 0.22014500
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C -2.61908600 -4.11573100 -0.14824800
H -3.40199100 -4.88079000 -0.14324600
H -1.77263100 -4.50532900 -0.72375100
H -2.29012000 -3.95827500 0.88224300
C -3.71839400 -3.09852900 -2.14621900
H -2.94640900 -3.50991200 -2.80137900
H -4.53263000 -3.82803500 -2.07749600
H -4.10783100 -2.19347700 -2.61781700
C 3.08393100 -3.58784600 0.29623200
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H -6.14130500 2.53981100 -1.34479400
C -5.92068300 -0.84578700 -1.10479200
H -7.23521100 0.47656100 -2.17743500
H -6.39971200 -1.75033800 -1.47545500
C 4.65909500 1.01115000 -1.42155600
C 4.12968200 -0.19533900 -1.88770700
C 5.66927500 0.96297000 -0.45465800
C 4.56584800 -1.43307700 -1.40812100

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 H 6.91981000 -0.28797400 0.76978300
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 C 0.14438700 -0.01306600 2.56064700
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 O -2.03641800 0.01790600 3.49084400
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 C 3.72957300 0.46076000 2.93273000
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 H 4.23874100 1.41984500 2.83316300
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 H 0.31729600 4.21170300 3.15243900
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 H 0.45346600 -2.43416300 1.89262100
 H 0.49458900 -3.45262200 3.34589800
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 H -2.76315700 -1.92102700 4.49341000
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 H -1.90381200 -3.48620200 4.51754900

3s

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 O 1.42443600 -2.35827400 -1.22755700
 O -1.45666200 -2.22386500 -1.51959000
 O -1.20920500 0.56393400 -2.61315400
 O 1.69269200 0.32752800 -2.37767400
 C 2.07181200 1.11852100 -1.45968500
 O 1.55206900 1.22527300 -0.30159100

C -1.66426500 1.36539100 -1.73652100
 O -1.39935900 1.34591700 -0.49342600
 C 1.70770700 -2.35006300 0.00804700
 O 1.27034800 -1.51488200 0.86972000
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 C -1.94350000 -2.17641600 -0.34621400
 C 2.64838500 -3.43323700 0.54174500
 C 3.25118800 2.04899900 -1.76156800
 C -2.62732900 2.45450000 -2.21580200
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 H 3.65087900 -3.79481000 -1.35894900
 C 1.88825500 -4.24469800 1.59517300
 H 2.51370300 -5.06789000 1.95489400
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 H 0.97059300 -4.67694000 1.18244800
 C 4.33521900 1.85278600 -0.66914500
 H 5.15112900 2.55051900 -0.89765500
 H 3.90208400 2.16038800 0.29094500
 C 2.75181400 3.49384400 -1.68267300
 H 3.56727400 4.18420900 -1.92214500
 H 1.93655500 3.67743000 -2.39086400
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 H 4.66900200 2.44202000 -3.33558100
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H -6.18246900 -1.73933900 0.60409100
C -5.55241400 1.21723800 -0.95925400
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C 1.00077800 1.71967200 2.57243000
C -1.53396400 1.22881500 2.67311200
H 0.05153200 -0.22457500 2.57181600
O 1.99316900 1.28782600 3.18878900
O -1.96836900 2.36521500 2.79893600
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C 0.26270100 -0.83982500 4.13772100
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H 1.31752100 -0.81664900 3.86654700
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H -0.35896200 -2.40225100 2.80568100
H -0.10681900 -2.85285600 4.48975400
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C 0.11416700 3.61675000 1.12016500
H -0.91216100 3.27866800 1.22624200
H 0.46046900 3.34460800 0.11285100
C 2.12302600 3.86493100 2.42962900
H 2.22909800 3.95186300 3.51665000
H 3.05467600 3.41724300 2.06003000
C 0.30691000 5.09664900 1.39961300
H -0.30919100 5.38828800 2.25824500
H 0.02144800 5.72649400 0.55249700
C 1.79305500 5.19566300 1.74746300
H 2.02672900 6.05170700 2.38469800
H 2.38646300 5.30908100 0.83386000

3t

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O -1.38941200 -1.98400600 -1.73099300
O -1.18335700 0.93033100 -2.46961100
O 1.70524400 0.71874800 -2.23336700
C 2.05488100 1.41713600 -1.23318100
O 1.53403400 1.37565100 -0.07040400
C -1.66275000 1.60940600 -1.50712500
O -1.40036500 1.44962400 -0.27260500
C 1.76027000 -2.23816000 -0.20393200
O 1.29048500 -1.53185000 0.74916200
O -1.55709900 -1.38668000 0.44950800
C -1.88869900 -2.07766900 -0.56556900
C 2.71948300 -3.35628900 0.20781400
C 3.20022300 2.41218900 -1.43901700
C -2.65262200 2.72060000 -1.86424400
C -2.99506700 -3.11758100 -0.36916400
C 3.92664300 -2.71601100 0.94471300
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H 3.55550900 -2.28087500 1.88011000
C 3.18149200 -4.15065500 -1.00754000
H 3.87950300 -4.93375800 -0.69245500
H 2.33665400 -4.62891400 -1.51025000
H 3.68694600 -3.51402000 -1.73748900
C 1.99394800 -4.27720800 1.19261900
H 2.64587800 -5.11028000 1.47427600
H 1.71679200 -3.73714800 2.10199000

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H 2.93934800 2.60831700 -3.58697900
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H -1.08818600 4.14431900 -2.38426100
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C 4.24553900 -0.32799200 0.25045600
C 5.69932100 -1.98562800 -0.70985300
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H 6.03574900 -3.01836600 -0.78165100
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H 7.14826000 -1.25190200 -2.12076200
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C -4.69805200 -1.36328900 -1.15711400
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C -6.17129500 0.26046600 -0.12722100
H -6.19290700 -1.84899800 0.31653700
C -5.58624400 1.28197800 -0.87205300
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C -0.17297500 0.60711700 2.46943000
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H 0.13468800 -1.13062700 6.08737500
H -1.60154600 -2.29627100 3.80926400
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H -0.16031200 -3.25722300 4.20180400
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C 2.11337600 3.63604500 2.83073300
C 0.21949300 3.73780200 1.85897000
C 1.30579500 4.77081300 2.18937100
H 2.94139100 3.25858100 2.21480200
H 2.48396800 3.78597000 3.85013100
H 0.20868900 3.39371500 0.81549800
H -0.79835900 3.96493500 2.17065800
H 1.77138700 5.28534100 1.34743900
H 0.97053200 5.51597900 2.91327600

3u

Rh -0.03590000 0.92761500 -1.98693300
O -1.37961900 2.30403600 -1.19003000
O 1.50824900 2.19280900 -1.39108000
O 1.31739800 -0.53323400 -2.62149700

O -1.60708300 -0.33681600 -2.45253800
C -2.01350000 -1.16864200 -1.58240800
O -1.51331700 -1.33410300 -0.42186500
C 1.75447200 -1.36959600 -1.77008600
O 1.45319000 -1.40184200 -0.53429900
C -1.68746100 2.25216100 0.03828500
O -1.28319600 1.37379900 0.87301300
O 1.56677700 1.26414700 0.67532100
C 1.95040000 2.10080400 -0.20316200
C -2.61970200 3.32759000 0.59886100
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C -3.72107100 -1.71652100 -3.34599800
H -2.95209100 -1.88736700 -4.10347100
H -4.58242100 -2.35013800 -3.58371800
H -4.03487000 -0.67277900 -3.41860900
C 3.09407000 -3.40916300 -1.14996100
H 3.82612000 -4.13614600 -1.51749300
H 3.51471400 -2.90369400 -0.27685800
H 2.20964100 -3.95883700 -0.81560100
C 2.10391700 -3.17878200 -3.43531600
H 1.83268300 -2.49398700 -4.24231300
H 2.80464900 -3.92134700 -3.83014400
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C 4.01630500 -1.70272900 -2.77487000
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H 3.74159900 -1.13476100 -3.67098200

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H 5.05660700 3.54850400 -0.41117500
C 2.52516400 4.50783100 -0.01391700
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C -6.31966000 1.32446400 -1.38059000
H -6.00666900 3.21707800 -0.39746400
C -5.89802100 0.00375800 -1.50932100
H -7.15926400 1.68431600 -1.96966600
H -6.40630700 -0.66743100 -2.19938600
C 4.77293900 1.44966500 -0.77992600
C 4.24955900 0.55510300 -1.71728100
C 5.74060400 0.98201400 0.11600600
C 4.65160700 -0.78183200 -1.77299600
H 3.50314000 0.91072600 -2.42595200
C 6.16356600 -0.34443400 0.06818900
H 6.17302000 1.66590200 0.84423600
C 5.62066600 -1.22394600 -0.86578200
H 6.92402900 -0.69460300 0.76162500
H 5.95807500 -2.25805500 -0.90199100
Rh 0.05292200 -0.07607800 0.21587500
C 0.08797400 -1.02047500 2.25270000
C -1.13228800 -1.84314600 2.42531300
C 1.43016500 -1.49748100 2.59722000
H -0.08978400 0.03850300 2.54954200
O -2.16581900 -1.37394100 2.91614900
O 1.81878300 -2.65552000 2.59306600
O 2.24783100 -0.45729100 2.89712300
C -0.37135100 0.59628000 4.11902400
C 3.63275000 -0.79120000 2.99783000
H -1.40741300 0.63606100 3.78216600
C -0.07345300 -0.35547100 5.19882800
C 0.47046000 1.78636300 3.90999000
H 4.02833400 -1.04960200 2.00875700
H 4.13007400 0.10335700 3.37296200

H 3.78960900 -1.62938600 3.68021000
H -0.67645600 -1.26230600 5.13042800
H 0.99233000 -0.59197800 5.26198600
H -0.34067300 0.14068300 6.14526300
H 1.52085600 1.59861600 4.13722800
H 0.37423100 2.19298200 2.89862600
H 0.09983400 2.56006800 4.60082700
N -1.05865500 -3.16878000 2.05284600
C -0.24772600 -3.74435900 1.00350400
H -0.88727400 -3.97848600 0.14863000
H 0.50368000 -3.03024700 0.68052000
H 0.24587100 -4.65515500 1.35354000
O -2.28544200 -3.85387700 2.13952500
C -2.45524100 -4.35026500 3.46286400
H -2.53315400 -3.52960000 4.18414100
H -3.39244700 -4.90932800 3.44570400
H -1.63216200 -5.01774300 3.74311000

3v

Rh 0.23503200 0.57157800 -1.89804300
O 1.66196800 -0.93067300 -2.05731700
O -1.23345200 -0.84278400 -2.34022400
O -1.18363600 2.06579200 -1.56964800
O 1.70923600 1.91710500 -1.34015300
C 1.98268900 2.04279000 -0.10660000
O 1.45610000 1.38552200 0.84805000
C -1.68456800 2.18338800 -0.40595200
O -1.41622700 1.45545800 0.60196400
C 1.93138000 -1.65212600 -1.04965400
O 1.40338500 -1.54582300 0.10754500
O -1.46943000 -1.38768800 -0.15234200
C -1.75070800 -1.50630600 -1.38732100
C 2.97417900 -2.75978200 -1.20845000
C 3.03921900 3.07057900 0.30335200
C -2.70796800 3.30337700 -0.20053900
C -2.81716400 -2.53938400 -1.76407000
C 4.10862300 -2.51630600 -0.17675300
H 4.84610600 -3.31704200 -0.31687200
H 3.68103400 -2.63801300 0.82533200
C 3.52808700 -2.78686900 -2.62776200
H 4.27532900 -3.58281900 -2.71564900
H 2.73706400 -2.97941200 -3.35696500
H 4.00451800 -1.84021800 -2.89417900
C 2.30590200 -4.09907900 -0.88276200
H 3.02275100 -4.91556600 -1.01630300
H 1.95198200 -4.12122300 0.15164300

H 1.45314200 -4.29192100 -1.54281000
C 4.15638200 2.33092800 1.08686300
H 4.90947200 3.08160400 1.35836700
H 3.71547300 1.95522300 2.01773600
C 2.37972700 4.08418600 1.24437200
H 3.11980200 4.81936300 1.57698500
H 1.57344100 4.62739000 0.74123500
H 1.96277300 3.59025500 2.12645700
C 3.60684100 3.78524500 -0.91595400
H 2.82123100 4.31402500 -1.46154800
H 4.35660400 4.51795000 -0.59817800
H 4.08169500 3.08712700 -1.60935900
C -3.15612500 3.37795600 1.25485200
H -3.89556600 4.17793400 1.37000900
H -3.60429600 2.44091500 1.59542900
H -2.31198800 3.59578200 1.91462500
C -2.06560800 4.62993500 -0.61436800
H -1.72574900 4.59783800 -1.65226900
H -2.79198200 5.44279300 -0.51231000
H -1.20704700 4.86928200 0.02106700
C -3.91976300 3.03414200 -1.13262800
H -4.65506500 3.82488800 -0.93720600
H -3.58111800 3.15695700 -2.16770200
C -4.00371900 -1.79426000 -2.43147800
H -3.65130600 -1.39044200 -3.38722100
H -4.76729300 -2.54831200 -2.66024800
C -2.21119800 -3.50620200 -2.78428500
H -1.35884200 -4.04569300 -2.35673200
H -2.95789500 -4.24726900 -3.08722000
H -1.86741200 -2.97596300 -3.67562400
C -3.29180700 -3.30898200 -0.53714300
H -4.10561900 -3.98622000 -0.81796200
H -2.48228500 -3.91068800 -0.11556800
H -3.64820800 -2.63857200 0.24897700
C 4.76604100 -1.16953600 -0.27927900
C 4.24516700 -0.09069600 0.44191300
C 5.87567000 -0.95257500 -1.10306300
C 4.78995700 1.19296100 0.33815900
H 3.40047600 -0.25872800 1.10949500
C 6.44057400 0.31644400 -1.20432900
H 6.30397000 -1.78629100 -1.65696200
C 5.89811100 1.38470900 -0.49417400
H 7.31019400 0.47326800 -1.83733700
H 6.34301000 2.37510100 -0.57446900
C -4.58740200 -0.68305000 -1.60616800
C -4.07523500 0.61001300 -1.73901100

C -5.61740700 -0.89789600 -0.68399600
C -4.54477900 1.67832600 -0.97060400
H -3.28796800 0.79208700 -2.46837100
C -6.11045900 0.15737300 0.08008800
H -6.04117600 -1.89465000 -0.57511800
C -5.57532400 1.43664100 -0.05577700
H -6.91848900 -0.01783700 0.78592000
H -5.96682200 2.25836000 0.54118600
Rh 0.00227700 -0.04299500 0.43155000
C -0.08895800 -0.66114300 2.58871000
C 1.13347200 -0.20187300 3.28985600
C -1.43379400 -0.33604600 3.04683400
H 0.02081400 -1.68431600 2.13144900
O 2.21211300 -0.79794200 3.17505000
O -1.74708700 0.71313900 3.59954100
O -2.33030900 -1.29228800 2.71698800
C 0.25835300 -2.99976300 2.91276600
C -3.70244600 -0.89138800 2.78754800
H 1.32170700 -2.86733400 2.70529400
C -0.12431700 -3.03139200 4.33977900
C -0.53290400 -3.77796800 1.93207300
H -3.91629100 -0.16766400 1.99331400
H -4.28806700 -1.79633800 2.62808700
H -3.93602600 -0.45031000 3.75834000
H 0.45737700 -2.33500800 4.94592100
H -1.19497700 -2.86494500 4.48186700
H 0.09366300 -4.04434600 4.70799400
H -1.60658800 -3.66538800 2.09628100
H -0.28954600 -3.51632500 0.89888700
H -0.27304800 -4.83638800 2.07954100
N 0.99122500 0.91417600 4.04575100
H 1.82663000 1.36604900 4.38025400
H 0.10930300 1.40881200 4.04848600

3w

Rh -0.17081600 -0.10741400 -2.03369000
O -1.55864600 1.43781600 -1.91019400
O 1.33684900 1.32549100 -2.14239800
O 1.21020100 -1.66634200 -1.99323300
O -1.67663800 -1.51065800 -1.80333600
C -1.98176700 -1.88405300 -0.62927700
O -1.46949000 -1.45067600 0.45333700
C 1.69151600 -2.02576000 -0.87200100
O 1.41939100 -1.51164400 0.25907400
C -1.83001800 1.94497700 -0.77960400
O -1.34967200 1.57446100 0.34329100

O 1.49209500 1.44564500 0.11594200
C 1.82390100 1.78826400 -1.06282500
C -2.82559300 3.10391200 -0.71979400
C -3.06606900 -2.95044800 -0.47117000
C 2.69337500 -3.18331000 -0.89411300
C 2.91536500 2.85332200 -1.19556500
C -4.02691000 2.66057800 0.15895500
H -4.74675800 3.48904200 0.16017000
H -3.66299700 2.54275900 1.18655100
C -3.28663200 3.49791800 -2.11710400
H -4.00173100 4.32487600 -2.05012400
H -2.44339200 3.82456200 -2.73144200
H -3.77162500 2.66583600 -2.63271800
C -2.14470600 4.29278000 -0.03585800
H -2.83204800 5.14378700 0.00510000
H -1.85037200 4.04069200 0.98657800
H -1.25086600 4.61018900 -0.58343300
C -4.23009500 -2.33813100 0.35514100
H -5.01535500 -3.10233300 0.41733900
H -3.86340700 -2.16352900 1.37390400
C -2.47581300 -4.12468100 0.31460000
H -3.24710900 -4.88087200 0.49384900
H -1.66210600 -4.60309100 -0.24055300
H -2.08154900 -3.79285600 1.27909700
C -3.56311200 -3.42817000 -1.83041100
H -2.75172400 -3.87375200 -2.41213600
H -4.34133300 -4.18677500 -1.69349600
H -3.98253700 -2.60873900 -2.41903800
C 3.12750300 -3.56546500 0.51591100
H 3.83764100 -4.39821600 0.46617600
H 3.60849400 -2.73366200 1.03671200
H 2.27218500 -3.87885300 1.11983300
C 2.02666200 -4.38026200 -1.57746500
H 1.69695300 -4.12425900 -2.58733600
H 2.73365900 -5.21358100 -1.64348600
H 1.15645500 -4.72389100 -1.00898400
C 3.91810800 -2.75159800 -1.74478600
H 4.63767200 -3.57945500 -1.71361900
H 3.58641800 -2.65148700 -2.78445100
C 4.09744600 2.24390300 -1.99557900
H 3.75218700 2.06143200 -3.01938600
H 4.87774700 3.01352500 -2.04945400
C 2.34378600 4.03275400 -1.98635200
H 1.50122200 4.48957500 -1.45602100
H 3.11101300 4.80258000 -2.11848400
H 1.99634600 3.71737500 -2.97324000

C 3.38742600 3.32952100 0.17398600
 H 4.20479800 4.04876200 0.05278400
 H 2.57948900 3.82532800 0.71828200
 H 3.74250100 2.50075500 0.79178000
 C -4.68586100 1.38546000 -0.28433200
 C -4.23547400 0.16363600 0.22499600
 C -5.72221100 1.37818300 -1.22378500
 C -4.78169800 -1.05364900 -0.19405200
 H -3.44224400 0.15849600 0.97237500
 C -6.28515900 0.17522400 -1.64274700
 H -6.09658600 2.32179100 -1.61657200
 C -5.81652300 -1.03426400 -1.13523600
 H -7.09933500 0.18064200 -2.36291800
 H -6.26457800 -1.97178300 -1.45985900
 C 4.65120400 0.97092400 -1.42107300
 C 4.11836000 -0.25594700 -1.82636700
 C 5.67796700 0.96776800 -0.47067900
 C 4.56718300 -1.47118800 -1.30187100
 H 3.32758900 -0.26534400 -2.57462100
 C 6.15054900 -0.23403600 0.05201100
 H 6.11590300 1.91177200 -0.15096800
 C 5.59756100 -1.44625900 -0.35572500
 H 6.95807100 -0.22629200 0.77992000
 H 5.97431700 -2.38266800 0.05139100
 Rh 0.01292400 0.00838900 0.37969300
 C 0.08382700 0.08410600 2.60301000
 C -1.15325200 -0.50864300 3.17140600
 C 1.41550800 -0.36733600 2.99478400
 H -0.00082900 1.19986300 2.45146200
 O -2.22119500 0.11949700 3.21721300
 O 1.69777400 -1.51971900 3.30684200
 O 2.33739100 0.61437100 2.88946200
 C -0.21777100 2.28574800 3.52853600
 C 3.70085000 0.17899500 2.86300700
 H -1.28150000 2.23610100 3.28877600
 C 0.14733100 1.93286600 4.91598600
 C 0.59714100 3.27545800 2.78736600
 H 3.92283900 -0.26710200 1.88648300
 H 4.30664800 1.07381100 3.00331400
 H 3.89859300 -0.54722200 3.65328400
 H -0.44612400 1.10515900 5.30830600
 H 1.21532500 1.72589900 5.02248700
 H -0.07113100 2.81105300 5.54075100
 H 1.66701700 3.13013700 2.95004100
 H 0.38437200 3.26901900 1.71495600
 H 0.32481800 4.26880000 3.17354100

N -1.04802400 -1.78832400 3.59983400
 H -0.14383500 -2.23814900 3.52431600
 C -2.20495400 -2.51558400 4.05515900
 H -1.88880600 -3.48917400 4.42956100
 H -2.71689100 -1.97546100 4.85668700
 H -2.93037300 -2.67172900 3.24707700

3xa

Rh -0.48672300 -1.23609000 -1.87759300
 O 0.48351900 -2.87423800 -1.04003700
 O -2.28950500 -2.00220900 -1.15254000
 O -1.42162300 0.49486400 -2.57917000
 O 1.33166300 -0.44984900 -2.46993500
 C 1.95923200 0.30417100 -1.66347600
 O 1.57931900 0.62479800 -0.49096100
 C -1.55269400 1.47705500 -1.78232400
 O -1.17677000 1.51104300 -0.56795600
 C 0.82841900 -2.84291900 0.18017500
 O 0.66735600 -1.86033500 0.97822600
 O -2.04468400 -0.93424300 0.83089100
 C -2.66293700 -1.69805300 0.02334300
 C 1.50134300 -4.07986400 0.77782900
 C 3.29676900 0.89113000 -2.11636400
 C -2.22674700 2.73645800 -2.33157400
 C -3.98552000 -2.30125300 0.50187700
 C 2.90501200 -3.67186500 1.30152900
 H 3.37128300 -4.57989800 1.70496700
 H 2.76138400 -2.98065800 2.14055600
 C 1.61310100 -5.19305500 -0.25618300
 H 2.10816800 -6.06169700 0.19107500
 H 0.62676000 -5.50607100 -0.60837800
 H 2.19288500 -4.87826400 -1.12693800
 C 0.66511800 -4.55271100 1.97060300
 H 1.11193600 -5.45177900 2.40729700
 H 0.61743700 -3.78336500 2.74618100
 H -0.35737500 -4.80126800 1.66766500
 C 4.37700200 0.47896100 -1.08150700
 H 5.32745200 0.91368100 -1.41826800
 H 4.12115800 0.95669900 -0.12943100
 C 3.17728500 2.41835700 -2.10777500
 H 4.13798200 2.86767500 -2.38255500
 H 2.42921800 2.76058600 -2.83084300
 H 2.89898100 2.78903700 -1.11748800
 C 3.66444700 0.40554900 -3.51289300
 H 2.91173100 0.70701900 -4.24595900
 H 4.62482200 0.84024300 -3.81092100

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 C -2.27130900 3.83820600 -1.27839800
 H -2.77134000 4.72018100 -1.69380300
 H -2.80784000 3.52430500 -0.37914000
 H -1.26361000 4.12880000 -0.96814100
 C -1.43425600 3.21154000 -3.55261600
 H -1.38100700 2.43223700 -4.31700200
 H -1.91473400 4.09301800 -3.98984300
 H -0.41262900 3.49146100 -3.27580400
 C -3.66130700 2.36274200 -2.79052900
 H -4.13290300 3.28576700 -3.15057500
 H -3.57378300 1.68863500 -3.65006500
 C -5.10885300 -1.82352800 -0.45632400
 H -4.92411600 -2.27087400 -1.43934100
 H -6.05079200 -2.24345400 -0.08155000
 C -3.88084500 -3.82588400 0.41246100
 H -3.10440300 -4.20702500 1.08426500
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 C -4.29572300 -1.88912000 1.93596900
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 C 3.79641900 -3.03047200 0.27698200
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 C 4.51418200 -1.00281100 -0.88088000
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 C 5.38488300 -1.77416700 -1.65875600
 H 6.15263900 -3.74016200 -2.07628000
 H 6.01064900 -1.28686700 -2.40451400
 C -5.21899000 -0.33156000 -0.59737400
 C -4.46994800 0.32760000 -1.57557100
 C -6.04379300 0.43336900 0.23462300
 C -4.51155400 1.71543100 -1.73440400
 H -3.83829600 -0.25828200 -2.24059000
 C -6.10644200 1.81712100 0.08621100
 H -6.64894200 -0.06162500 0.99232800
 C -5.34289400 2.45694200 -0.88774800
 H -6.75887900 2.40091100 0.73050800
 H -5.40036000 3.53757100 -1.00439400
 Rh -0.22210000 -0.12333200 0.25852500
 C 0.09048100 0.93591300 2.19178400
 C 1.49441900 1.40216800 2.26273500

C -1.04685200 1.83950700 2.34655100
 H -0.04872400 -0.07072400 2.67687600
 O 2.41088600 0.65696600 2.62522600
 O -1.06051000 3.01922900 2.00558000
 O -2.13573200 1.20943600 2.83194100
 C 0.10575900 -0.47970800 4.19188200
 C -3.36564800 1.92445500 2.66676100
 H 1.08602200 -0.86867100 3.91157900
 C 0.09976600 0.63531100 5.15798300
 C -1.03511900 -1.41861300 4.14112600
 H -3.61074000 1.99095200 1.60105900
 H -4.12378800 1.34079300 3.18779400
 H -3.29721500 2.92897100 3.08867300
 H 0.93499500 1.32226800 5.01231800
 H -0.85093000 1.17568400 5.15641200
 H 0.21234800 0.19666600 6.16049700
 H -1.99133500 -0.91235600 4.28662300
 H -1.05942500 -1.99869400 3.21449800
 H -0.89760300 -2.13377800 4.96609100
 N 1.66631800 2.69470300 1.83910100
 H 0.79766600 3.18218700 1.62471400
 C 2.85120300 3.36812500 1.53542300
 C 2.72467900 4.64634200 0.96628700
 C 4.13244900 2.83848200 1.74778300
 C 3.85042700 5.37155900 0.60158000
 H 1.73114000 5.05790900 0.80158900
 C 5.25062700 3.57530400 1.36647900
 H 4.23493700 1.85814400 2.19263500
 C 5.12472400 4.83810300 0.79289300
 H 3.72896400 6.35622600 0.15894000
 H 6.23735800 3.14771300 1.52447200
 H 6.00599700 5.40163300 0.50190600

3xd

Rh 1.48595800 1.07261000 -1.86639900
 O 1.30334400 2.95266500 -0.99586500
 O 3.43750600 0.97086600 -1.12973500
 O 1.57645300 -0.87767700 -2.60831900
 O -0.48619300 1.15000100 -2.48214700
 C -1.38443400 0.70879800 -1.69998000
 O -1.19226400 0.23715600 -0.53210500
 C 1.27769000 -1.83413100 -1.82518100
 O 0.93530600 -1.72244100 -0.60511100
 C 0.95016700 3.05598500 0.21790500
 O 0.65940500 2.08648300 0.99599000
 O 2.73405300 0.11205800 0.84621400

C 3.63027000 0.53570700 0.04835100
C 0.85007200 4.45401300 0.82973200
C -2.83652900 0.74196200 -2.18197700
C 1.34788500 -3.25274900 -2.39394600
C 5.07750700 0.50972100 0.54654800
C -0.60715500 4.66618800 1.32276300
H -0.65762300 5.67717700 1.74676400
H -0.78700600 3.95945700 2.14213300
C 1.24367700 5.52054300 -0.18452600
H 1.15962600 6.51208300 0.27289800
H 2.27572900 5.38498800 -0.51854400
H 0.60167300 5.49449600 -1.06785400
C 1.78031700 4.51801000 2.04484500
H 1.75253000 5.52106700 2.48224100
H 1.47374600 3.80287200 2.81328100
H 2.81759500 4.30242200 1.76739800
C -3.66099100 1.58353800 -1.17096500
H -4.69616200 1.60101100 -1.53674800
H -3.66284400 1.04304300 -0.21767900
C -3.38207400 -0.68927800 -2.17259800
H -4.43919900 -0.68643200 -2.45957900
H -2.84405500 -1.32336500 -2.88511000
H -3.30035600 -1.13778200 -1.17923100
C -2.93285300 1.32545800 -3.58618200
H -2.37250200 0.71984900 -4.30334500
H -3.98109400 1.34608800 -3.90355100
H -2.54001900 2.34411000 -3.63150500
C 0.86971000 -4.27479900 -1.36808700
H 0.93585100 -5.28132600 -1.79530600
H 1.46368700 -4.24421700 -0.45141700
H -0.17035900 -4.08903100 -1.08472900
C 0.47076400 -3.31899100 -3.64667900
H 0.79150200 -2.58777200 -4.39260900
H 0.53239100 -4.31731000 -4.09162600
H -0.57926800 -3.12530600 -3.40534300
C 2.81671800 -3.53798900 -2.80888300
H 2.84937300 -4.57232700 -3.17371500
H 3.05701700 -2.88895400 -3.65868700
C 5.89535100 -0.42235500 -0.38729700
H 5.94963400 0.05501000 -1.37210800
H 6.91704800 -0.45835200 0.01127600
C 5.64814100 1.92653900 0.44601000
H 5.09809300 2.61871200 1.09261500
H 6.69488000 1.93145600 0.76635700
H 5.59804400 2.30228800 -0.57887300
C 5.15427500 0.02128600 1.98781700

H 6.20027100 -0.00908600 2.31126800
H 4.61010100 0.69044500 2.65989300
H 4.72721200 -0.97820300 2.09902800
C -1.65801600 4.48203000 0.26544200
C -2.20736400 3.21461300 0.05262800
C -2.08713300 5.54077500 -0.54159800
C -3.14943200 2.97832800 -0.95338600
H -1.89523400 2.38774500 0.68853000
C -3.03696700 5.32691100 -1.53777000
H -1.68292800 6.53832600 -0.37881600
C -3.56207300 4.05392400 -1.74706100
H -3.37312300 6.15858400 -2.15153300
H -4.30733200 3.89262900 -2.52383100
C 5.33737600 -1.80982700 -0.53593300
C 4.41018100 -2.07107300 -1.54861800
C 5.70007600 -2.85657300 0.31823300
C 3.83184400 -3.33126500 -1.72101700
H 4.13198500 -1.26595800 -2.22661700
C 5.14305100 -4.12336900 0.15594800
H 6.43167300 -2.67943800 1.10467500
C 4.21194600 -4.36049300 -0.85318200
H 5.43994000 -4.93306600 0.81788200
H 3.78540400 -5.35377500 -0.97946300
Rh 0.74799000 0.14989400 0.24375100
C 0.01458600 -0.66475000 2.19581400
C -1.45058200 -0.49259000 2.23768500
C 0.66665700 -1.95695900 2.37185100
H 0.56714800 0.20172500 2.63806600
O -1.97686400 0.57364300 2.56917200
O 0.19355100 -3.03764800 2.02765700
O 1.90451900 -1.83465300 2.89100400
C 0.58221000 0.71630000 4.16478700
C 2.73231000 -2.99525700 2.74868400
H -0.14692100 1.45641600 3.83096100
C 0.11811800 -0.25623100 5.16888400
C 2.01012500 1.08380500 4.08682500
H 2.94891800 -3.16246800 1.68792200
H 3.65273200 -2.77257600 3.28764500
H 2.24772900 -3.87901900 3.16795500
H -0.92506000 -0.54236300 5.02610400
H 0.76158800 -1.13856900 5.21805100
H 0.18538400 0.23840700 6.14982300
H 2.66662200 0.23161600 4.27446400
H 2.26817100 1.55287700 3.13263700
H 2.18933900 1.83284800 4.87327400
N -2.14795100 -1.60318400 1.82079800

H -1.56091700 -2.41334600 1.62571400
C -3.49248600 -1.70985500 1.48517900
C -3.90957900 -2.92626500 0.91608800
C -4.43222000 -0.68131500 1.66095800
C -5.22117300 -3.10560900 0.51333400
H -3.18461800 -3.72410500 0.77642600
C -5.74329700 -0.87029900 1.24451500
H -4.12137200 0.25594100 2.10159000
C -6.14734400 -2.07258800 0.66604600
H -5.52641800 -4.04531800 0.06385200
H -6.46154300 -0.06456700 1.36464000
C -7.56892300 -2.27768300 0.27029600
F -8.31860600 -2.77149700 1.28709200
F -7.69109900 -3.15481600 -0.74979000
F -8.16491600 -1.12774400 -0.11305500

8a

C 2.30029000 1.04083200 -0.21056100
C 1.01652500 1.63697300 -0.18345800
C 2.69142900 -0.28512600 0.10000500
H 3.11814000 1.74694600 -0.33578700
O 0.86102400 2.88772100 -0.21706900
O 2.03750300 -1.28774900 0.40722900
O 4.09253600 -0.38547800 0.04561400
C 4.59247000 -1.66883600 0.36346200
H 4.25687300 -2.42955000 -0.35136000
H 5.68108700 -1.59303700 0.32732800
H 4.27915500 -1.99562900 1.36135200
C -0.24617000 0.81930600 -0.14516100
C -0.41000000 -0.39739100 -0.82078300
C -1.36368500 1.35931900 0.49435200
C -1.63202400 -1.05200300 -0.83820400
H 0.43804700 -0.83236100 -1.33839200
C -2.59362900 0.70585800 0.51603000
H -1.25356800 2.32554600 0.98027500
C -2.72882900 -0.51126600 -0.15688000
H -1.76396900 -1.98891400 -1.37293200
H -3.43240400 1.14919600 1.04285200
O -3.88352700 -1.23954000 -0.21390900
C -5.00308100 -0.71531300 0.47449200
H -5.81355300 -1.42930200 0.32893500
H -4.80437900 -0.60757300 1.54822300
H -5.30550300 0.26094300 0.07483000

8b

C 1.86258100 1.07183200 -0.25289500

C 0.55671000 1.61139300 -0.19727300
C 2.32210300 -0.22845200 0.07392300
H 2.64322300 1.80754700 -0.43114200
O 0.34115800 2.85148200 -0.27005200
O 1.72401600 -1.24430200 0.44296900
O 3.72126400 -0.27700200 -0.05171200
C 4.28875800 -1.52413300 0.29568200
H 3.89556400 -2.33999500 -0.32107900
H 5.36434800 -1.42900100 0.13396200
H 4.10024500 -1.78435300 1.34380600
C -0.66940500 0.74205600 -0.08812500
C -0.81072900 -0.48657500 -0.73980100
C -1.78321800 1.25295800 0.58837200
C -2.01605700 -1.18114500 -0.70236700
H 0.03405200 -0.89489500 -1.28485500
C -2.97795700 0.54655700 0.65078500
H -1.69090500 2.23078900 1.05450100
C -3.11756300 -0.68728000 0.00419400
H -2.11029200 -2.12708200 -1.23440600
H -3.82548700 0.95960000 1.19665200
C -4.40018100 -1.45944800 0.07757300
H -4.45797100 -2.05743100 0.99512200
H -5.27276500 -0.79919200 0.07863300
H -4.50176900 -2.15399600 -0.76124500

8c

C -1.30529500 1.16140700 0.27469600
C 0.06554400 1.49686700 0.21353100
C -1.94342300 -0.05234800 -0.08616400
H -1.96923500 1.99523500 0.49081100
O 0.47957300 2.68344600 0.30566700
O -1.49139400 -1.11940900 -0.51263300
O -3.33207900 0.07767900 0.07928600
C -4.06852700 -1.07078500 -0.29106500
H -3.77993100 -1.95042700 0.29542600
H -5.11847600 -0.83652400 -0.10463600
H -3.93275800 -1.32255300 -1.34916900
C 1.13621700 0.44248400 0.08284600
C 1.09736600 -0.77224900 0.77511500
C 2.28672800 0.75016900 -0.65216700
C 2.17078700 -1.65718900 0.72424100
H 0.21522500 -1.01773400 1.35824800
C 3.34974800 -0.14381200 -0.73317300
H 2.33089400 1.71402100 -1.15360600
C 3.29703800 -1.35191300 -0.03896400
H 2.13066800 -2.58921900 1.28338900

H 4.22636700 0.10524000 -1.32656200
H 4.13135100 -2.04754900 -0.08584000

8d

C 1.81150200 1.09420600 -0.26346500
C 0.49635800 1.60771700 -0.20274700
C 2.29455700 -0.19599000 0.07163400
H 2.57776600 1.84329500 -0.44715400
O 0.25062200 2.84183200 -0.27330100
O 1.71248500 -1.21777700 0.45069500
O 3.69207300 -0.22306800 -0.05815200
C 4.28142600 -1.45730700 0.30057400
H 3.89678100 -2.28613600 -0.30387600
H 5.35423100 -1.34705800 0.13089400
H 4.10308300 -1.70695000 1.35289100
C -0.71016600 0.71079000 -0.08939400
C -0.81866500 -0.52586700 -0.73437500
C -1.83124900 1.20517700 0.58688800
C -2.00204500 -1.25814100 -0.69577300
H 0.03645200 -0.91825300 -1.27348600
C -3.01524400 0.47982800 0.66466000
H -1.75557100 2.18665300 1.04639100
C -3.07682500 -0.74454100 0.01524700
H -2.10190400 -2.21155900 -1.20520400
H -3.88275600 0.84893500 1.20290000
F -4.22749000 -1.45689600 0.06924700

8e

C -2.29515700 1.01884300 0.23905500
C -1.03658300 1.65711400 0.19864900
C -2.63795700 -0.31864700 -0.08564100
H -3.13496400 1.68819200 0.41095600
O -0.90512400 2.90751800 0.27917400
O -1.94569500 -1.27852100 -0.43990100
O -4.02505500 -0.48677000 0.02356400
C -4.47636500 -1.79161700 -0.28375800
H -4.07905500 -2.53668000 0.41562200
H -5.56499100 -1.76641700 -0.20818500
H -4.18280500 -2.09826600 -1.29340700
C 0.25324500 0.88219600 0.09422800
C 0.48480500 -0.32997800 0.75153500
C 1.31997600 1.48043800 -0.58488200
C 1.73543800 -0.93955400 0.72234400
H -0.32703300 -0.80338100 1.29215200
C 2.57030800 0.87673900 -0.65629900
H 1.15148200 2.44544300 -1.05534900

C 2.76116200 -0.33185600 0.00578800
H 1.91576900 -1.87218700 1.24758800
H 3.38762900 1.33606800 -1.20302600
Cl 4.33927800 -1.10309700 -0.05383400

8f

C -0.83319100 -0.50743200 0.00064400
C -2.04254300 0.20102800 -0.00016800
C 0.42250800 0.14963300 0.00031800
H -0.84689200 -1.59455400 0.00116600
O -3.20488600 -0.26228000 -0.00019800
O 0.67965800 1.35888200 0.00015100
O 1.47128900 -0.77674900 -0.00032400
C 2.76121000 -0.19558500 -0.00025700
H 2.93750600 0.41241200 0.89447100
H 3.47222600 -1.02371700 -0.02180600
H 2.92092800 0.44729200 -0.87307400
H -1.90016000 1.31386900 -0.00101200

8g

C -0.46107900 -0.75350100 -0.00051800
C -1.79047600 -0.27078900 0.00121800
C 0.71072400 0.03362300 -0.00004300
H -0.33402700 -1.83302500 -0.00206600
O -2.79479300 -1.02585200 0.00109000
O 0.85558700 1.26364700 0.00165500
O 1.85449500 -0.78404500 -0.00152300
C 3.07455100 -0.07169700 0.00035600
H 3.17957600 0.56326300 0.88800900
H 3.86936700 -0.82069300 -0.00662000
H 3.17524100 0.57575000 -0.87868700
C -2.02842800 1.23379500 -0.00040400
H -1.53167900 1.72636700 0.84042100
H -1.60822700 1.70592300 -0.89426400
H -3.10430800 1.42382300 0.03977100

8h

C -0.10902800 0.93216700 -0.00129200
C 1.27949800 0.65904700 -0.00149200
C -1.15188000 -0.01835400 -0.00217900
H -0.39714100 1.98049500 0.00054000
O 2.15134800 1.56324500 -0.00050900
O -1.11645200 -1.25689800 -0.00555700
O -2.40378100 0.62329800 0.00081000
C -3.50430800 -0.26191700 0.00448200
H -3.52815400 -0.88647700 0.90555100

H -4.40158900 0.35965100 -0.02871500
H -3.49239400 -0.93566600 -0.85980300
C 1.75236000 -0.79714400 -0.00252700
H 1.30533300 -1.31866900 0.85301600
H 1.31535700 -1.31394300 -0.86620300
C 3.26204200 -0.92581900 0.00543600
H 3.57620500 -1.97465500 0.00184900
H 3.70565200 -0.43312900 -0.86472400
H 3.69571000 -0.44264700 0.88596800

8i

C 1.27479000 -1.07805500 0.00006700
C -0.14084400 -1.03980400 0.00008500
C 2.15268100 0.02762200 0.00009900
H 1.72853900 -2.06660600 -0.00005600
O -0.83494200 -2.08932200 0.00003200
O 1.92172400 1.24457900 0.00026400
O 3.49064500 -0.40636400 -0.00009300
C 4.43650600 0.64290000 -0.00015500
H 4.33940200 1.28511400 0.88302200
H 5.42153500 0.17106100 -0.00038600
H 4.33907200 1.28529700 -0.88316000
C -0.82162100 0.33243200 0.00017900
H -0.43972400 0.90284400 0.85862800
H -0.43945100 0.90310500 -0.85796900
C -2.35572100 0.38722600 -0.00003400
C -2.76933100 1.86114900 0.00001500
H -2.38516800 2.38377100 -0.88441700
H -3.86169300 1.96393700 -0.00013500
H -2.38542300 2.38364100 0.88463400
C -2.92900000 -0.27907500 -1.25202100
H -2.66195900 -1.33727900 -1.27523200
H -4.02227000 -0.18571100 -1.27695600
H -2.53757200 0.19635800 -2.16022200
C -2.92937400 -0.27927400 1.25167600
H -2.53828400 0.19605400 2.16007700
H -4.02265700 -0.18598200 1.27626900
H -2.66228500 -1.33746800 1.27481800

8j

C 0.34018700 1.02973800 0.12669300
C -1.06365200 0.86543000 0.05955200
C 1.33864700 0.04920000 -0.06658900
H 0.68935500 2.03461100 0.35344400
O -1.86406900 1.81180700 0.26688300
O 1.25612500 -1.16290500 -0.31088600

O 2.61531700 0.62364200 0.06169300
C 3.68036400 -0.28648200 -0.12166200
H 3.68268000 -0.71953800 -1.12887900
H 4.60097800 0.28073800 0.03101400
H 3.63945900 -1.11802600 0.59140600
C -1.65299800 -0.52279500 -0.24357400
C -1.66050200 -1.35736700 1.03567800
H -2.24943700 -0.85977200 1.81688600
H -2.10545000 -2.34554300 0.86712400
H -0.64359900 -1.50367000 1.40891400
C -3.05304600 -0.40941300 -0.82459400
H -3.71871400 0.10820200 -0.12742900
H -3.06060000 0.16328500 -1.75758400
H -3.47410600 -1.39977200 -1.03279200
H -0.99354800 -1.03073300 -0.95664900

8k

C -1.50925300 1.18073200 -0.20656400
C -0.12321100 1.46717400 -0.17834000
C -2.14367400 -0.04671900 0.09119500
H -2.16170400 2.00447500 -0.48757400
O 0.34087300 2.59824300 -0.47117600
O -1.67883400 -1.15119900 0.40772300
O -3.53902700 0.08914600 -0.01619500
C -4.26064100 -1.09417100 0.25837700
H -4.10492700 -1.44413800 1.28579500
H -5.31583500 -0.85195200 0.11484000
H -3.97948800 -1.91381200 -0.41300300
C 0.86605800 0.35621300 0.18883200
C 1.11943200 -0.54308100 -1.02770200
C 2.18745100 0.91081400 0.71176100
H 0.41155800 -0.28301500 0.95784500
C 2.10575700 -1.65906600 -0.70948900
H 1.51873100 0.07881600 -1.84551200
H 0.16662600 -0.95821700 -1.37266100
C 3.17392000 -0.20313400 1.03979000
H 2.61232300 1.57869000 -0.04975600
H 2.01012000 1.54134300 1.59245900
C 3.41777400 -1.10328700 -0.16665400
H 2.28867600 -2.28000500 -1.59591100
H 1.65470700 -2.32237500 0.04454800
H 4.12208300 0.21370300 1.40283300
H 2.77237500 -0.81352400 1.86350900
H 4.10847700 -1.91670000 0.08882800
H 3.91050500 -0.51566800 -0.95629500

8l

C 0.50463400 1.04583400 0.00063900
C -0.91630100 0.98712600 -0.00024500
C 1.51473600 0.05802800 0.00141200
H 0.88144900 2.06691000 0.00050300
O -1.58652000 2.04944700 -0.00125500
O 1.48060100 -1.18225500 0.00158100
O 2.77687200 0.68251100 0.00303300
C 3.86610900 -0.21657800 -0.00295000
H 3.89080400 -0.82871700 -0.91253900
H 4.76997600 0.39426100 0.04648700
H 3.83753800 -0.90178500 0.85163400
C -1.70727800 -0.34942400 -0.00016300
C -1.37638500 -1.15699600 1.25824200
H -1.63413000 -0.58920200 2.16048200
H -1.95936800 -2.08734100 1.27876400
H -0.31666000 -1.41524800 1.29341800
C -3.20467400 -0.04778200 -0.00087000
H -3.49511500 0.53350600 -0.88061700
H -3.77370000 -0.98577400 -0.00077700
H -3.49579000 0.53409000 0.87827100
C -1.37527500 -1.15759900 -1.25793300
H -1.63240600 -0.59025000 -2.16063100
H -0.31548300 -1.41571600 -1.29218900
H -1.95813500 -2.08801200 -1.27846300

8m

C 0.00838500 0.87489200 -0.00003500
C 1.40099700 0.62098300 -0.00001600
C -1.06650900 -0.05040300 0.00010700
H -0.27690500 1.92395100 -0.00003900
O 2.25950300 1.54225300 -0.00026800
O -1.08666300 -1.28812400 -0.00015600
O -2.28509300 0.64068200 0.00081600
C -3.42492900 -0.19637600 -0.00047000
H -3.45756600 -0.84396500 0.88273000
H -4.29282800 0.46561000 -0.00066900
H -3.45635100 -0.84286400 -0.88451500
C 1.87451000 -0.79786800 0.00026000
C 3.17668800 -1.09664600 -0.00005100
H 1.11431400 -1.57596500 0.00089400
H 3.54179800 -2.12007300 0.00037100
H 3.91070300 -0.29268300 -0.00068000

8n

C -0.50784400 -0.78306200 -0.00004000

C -1.80584400 -0.18927600 -0.00003900
C 0.67174100 -0.02812900 0.00002600
H -0.44570100 -1.86496100 -0.00003300
O -2.88222200 -0.79879400 -0.00003600
O 0.78585500 1.22239600 0.00003600
O 1.81964000 -0.80334100 0.00020900
C 3.02953200 -0.06531000 -0.00014300
H 3.11713400 0.57416500 0.88478300
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H 3.11562500 0.57576300 -0.88402700
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H -0.91257200 1.48795100 0.00001700

8o

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8p

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8t

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8v

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8w

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8xa

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8xb

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8xc

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8xg

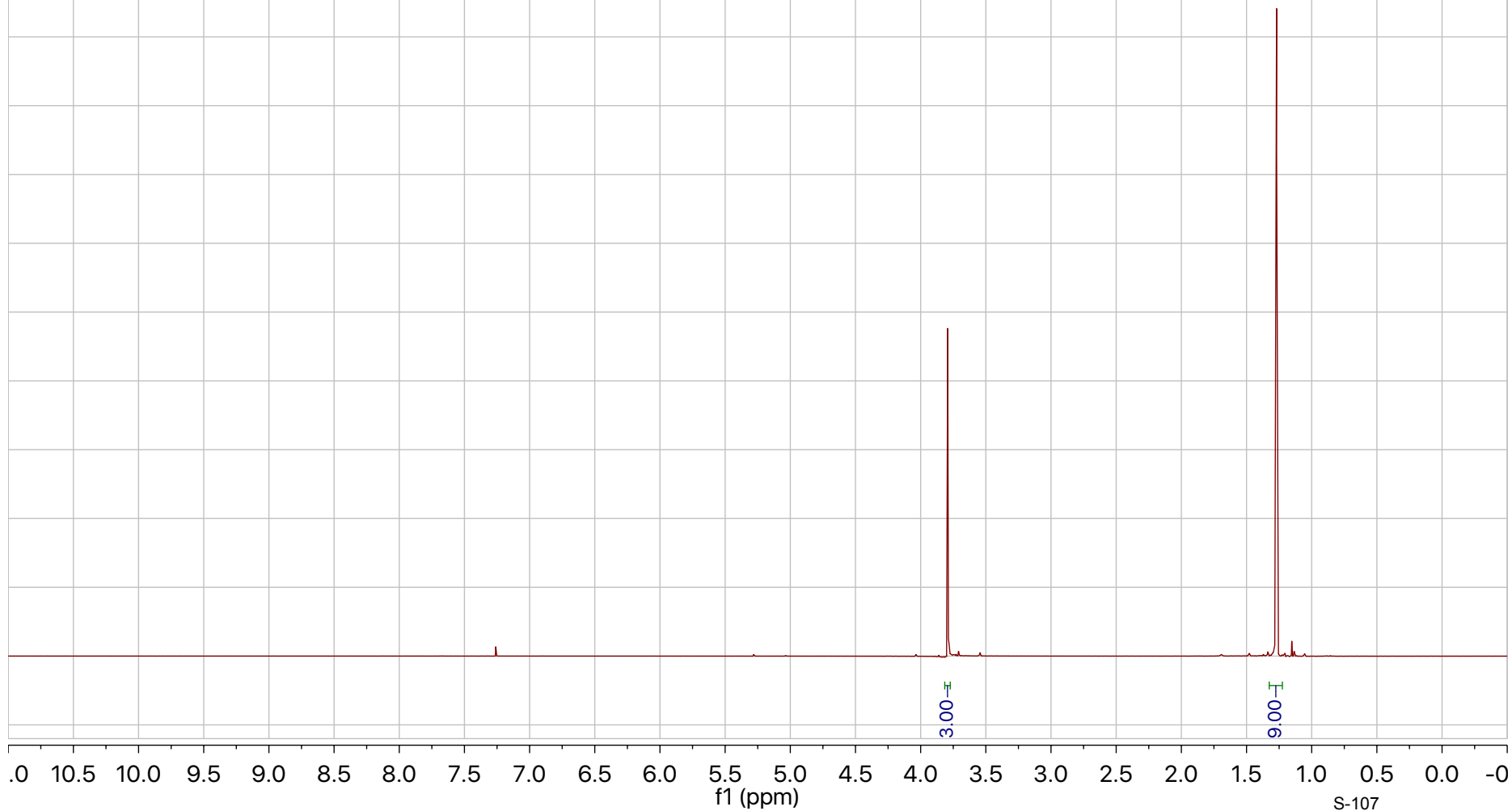
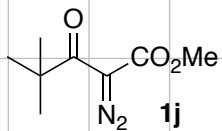
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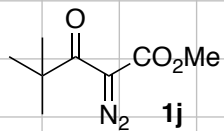
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4. Copies of NMR Spectra



S-107



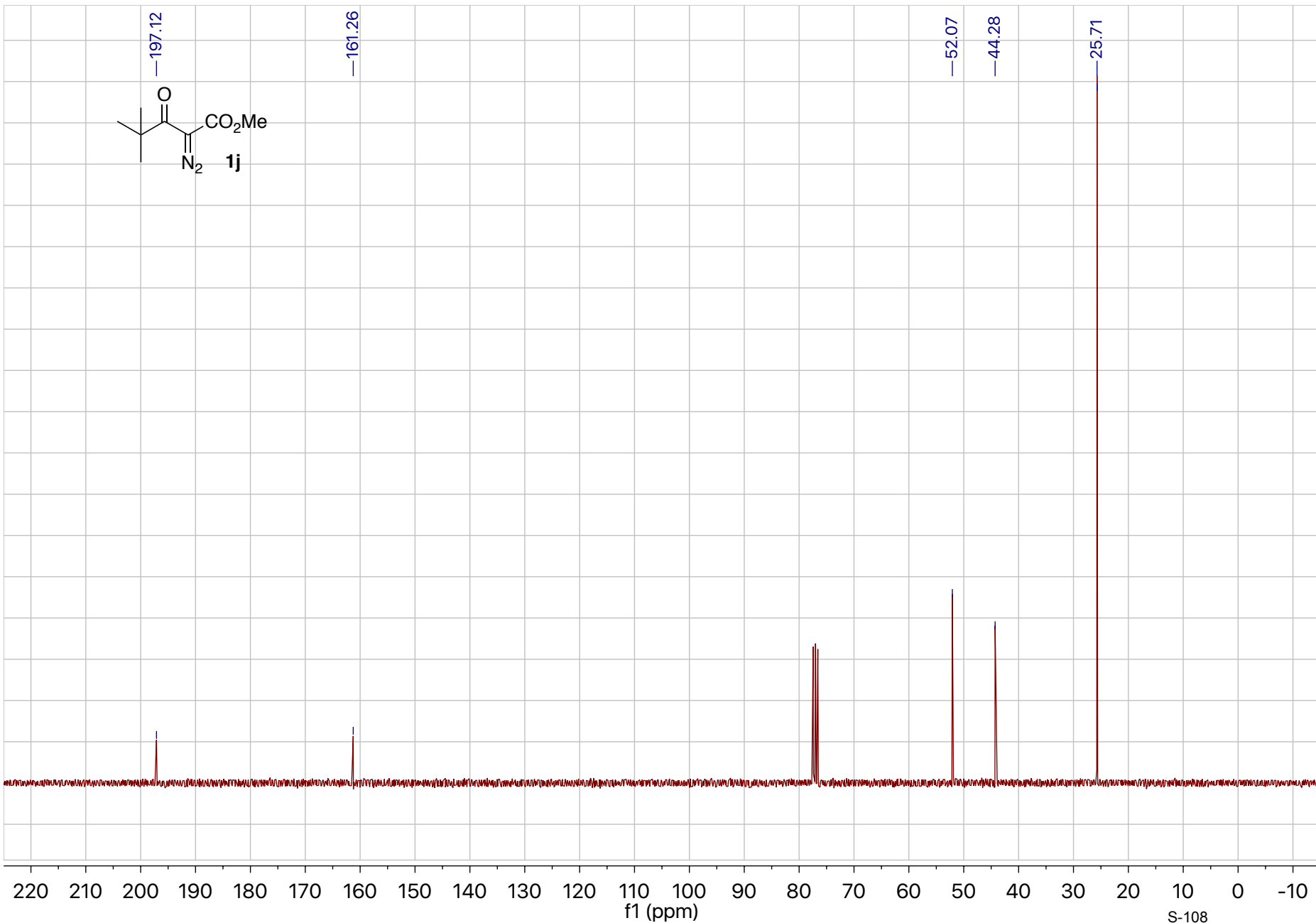
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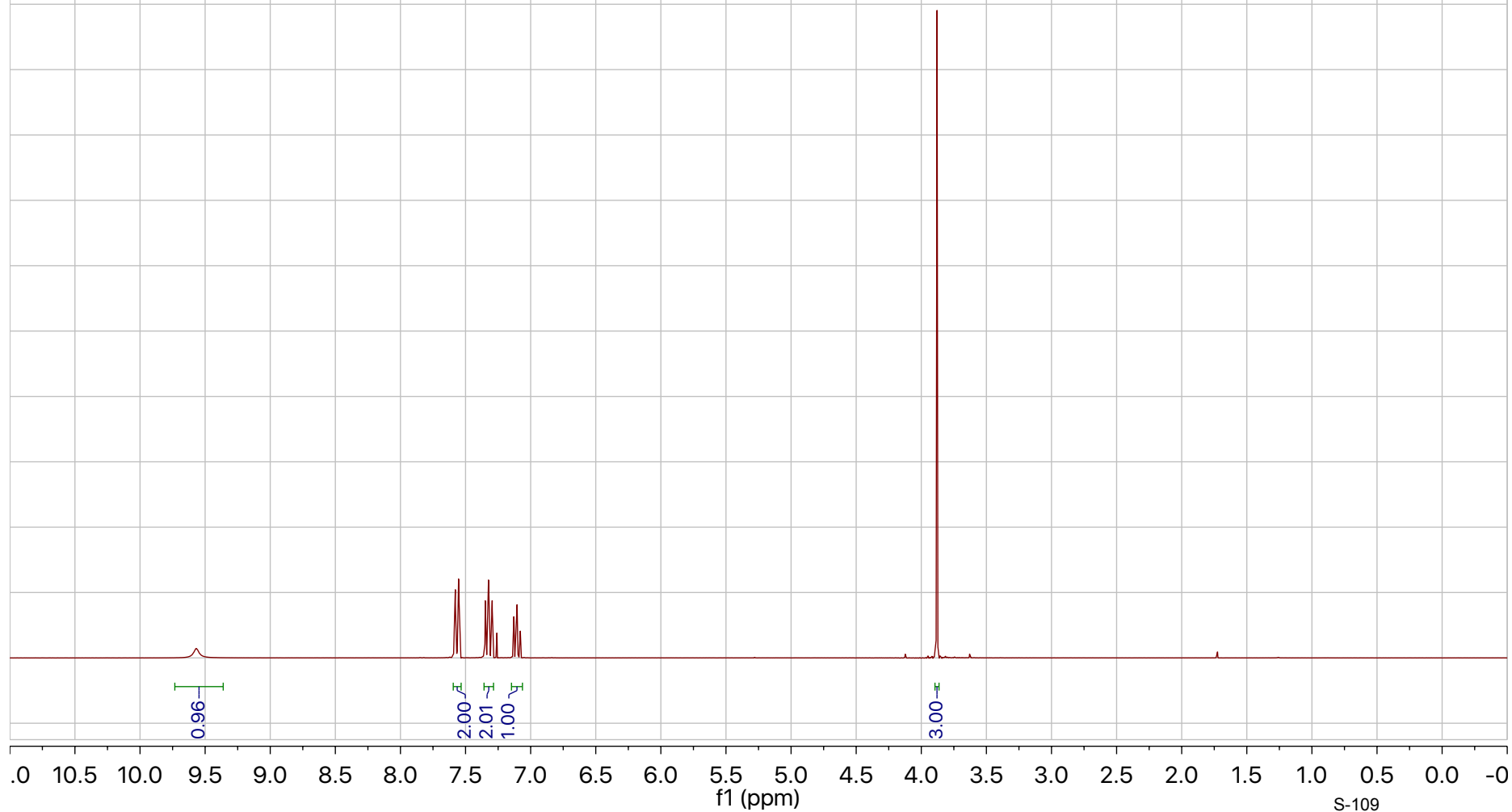
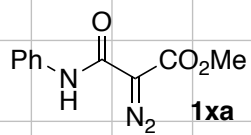
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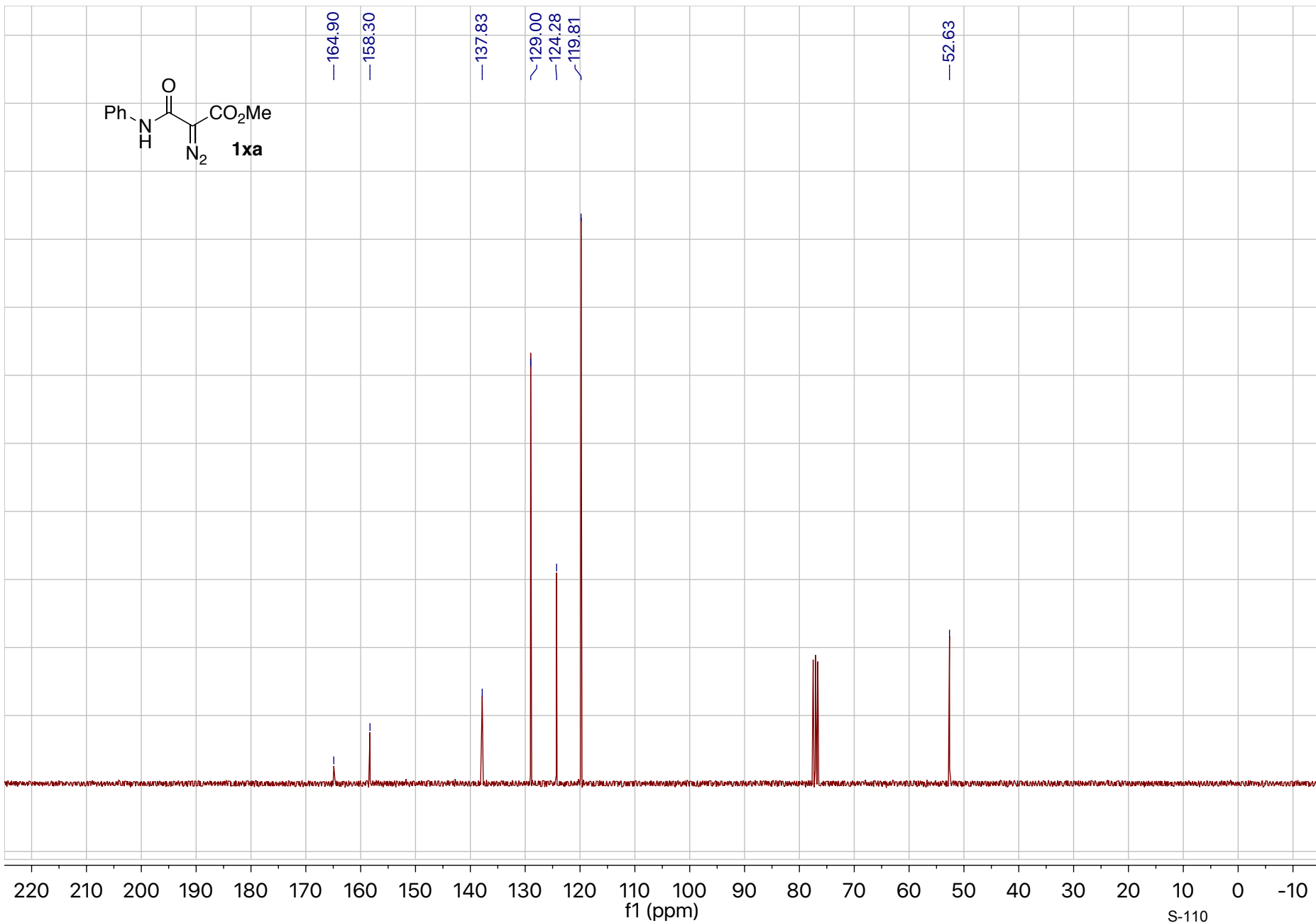
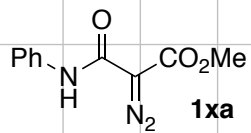
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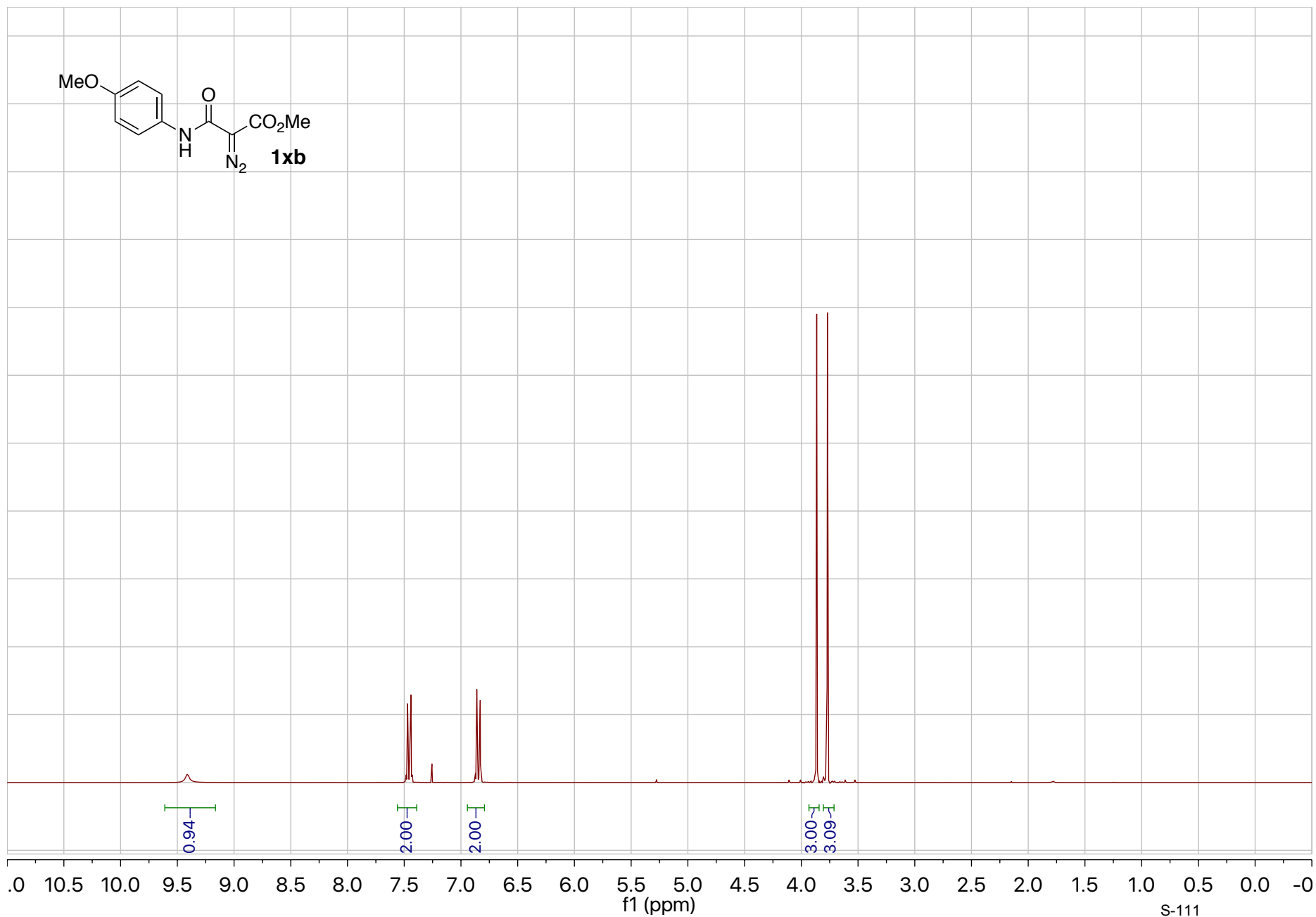
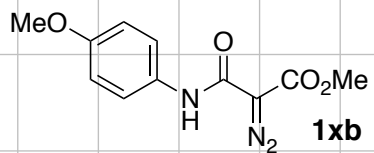
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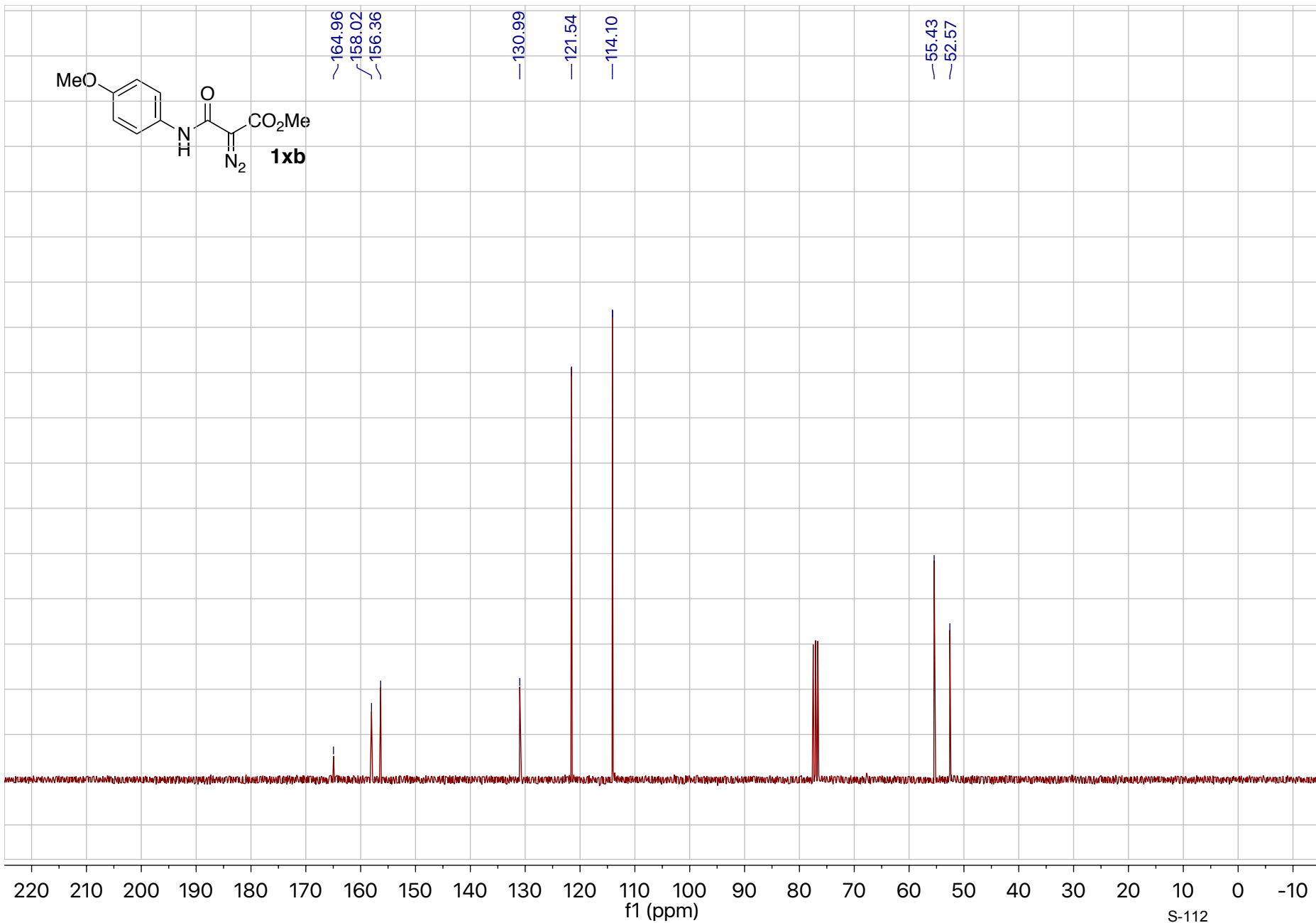
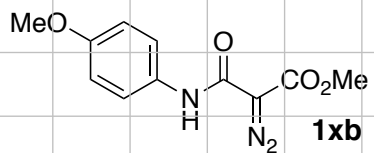
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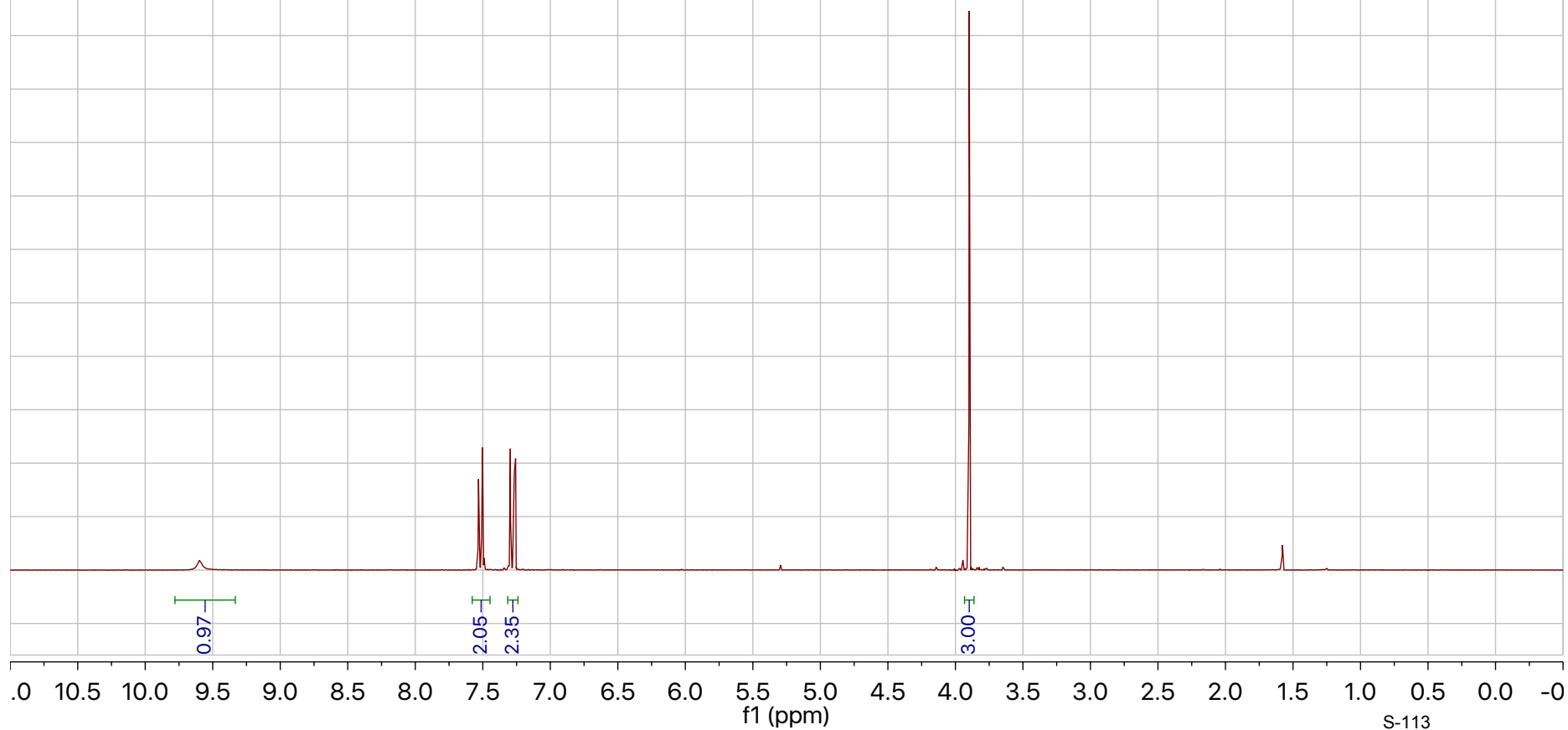
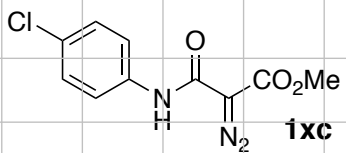


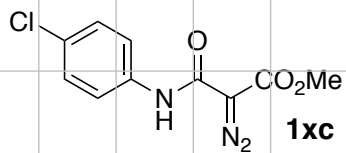












—164.82

—158.41

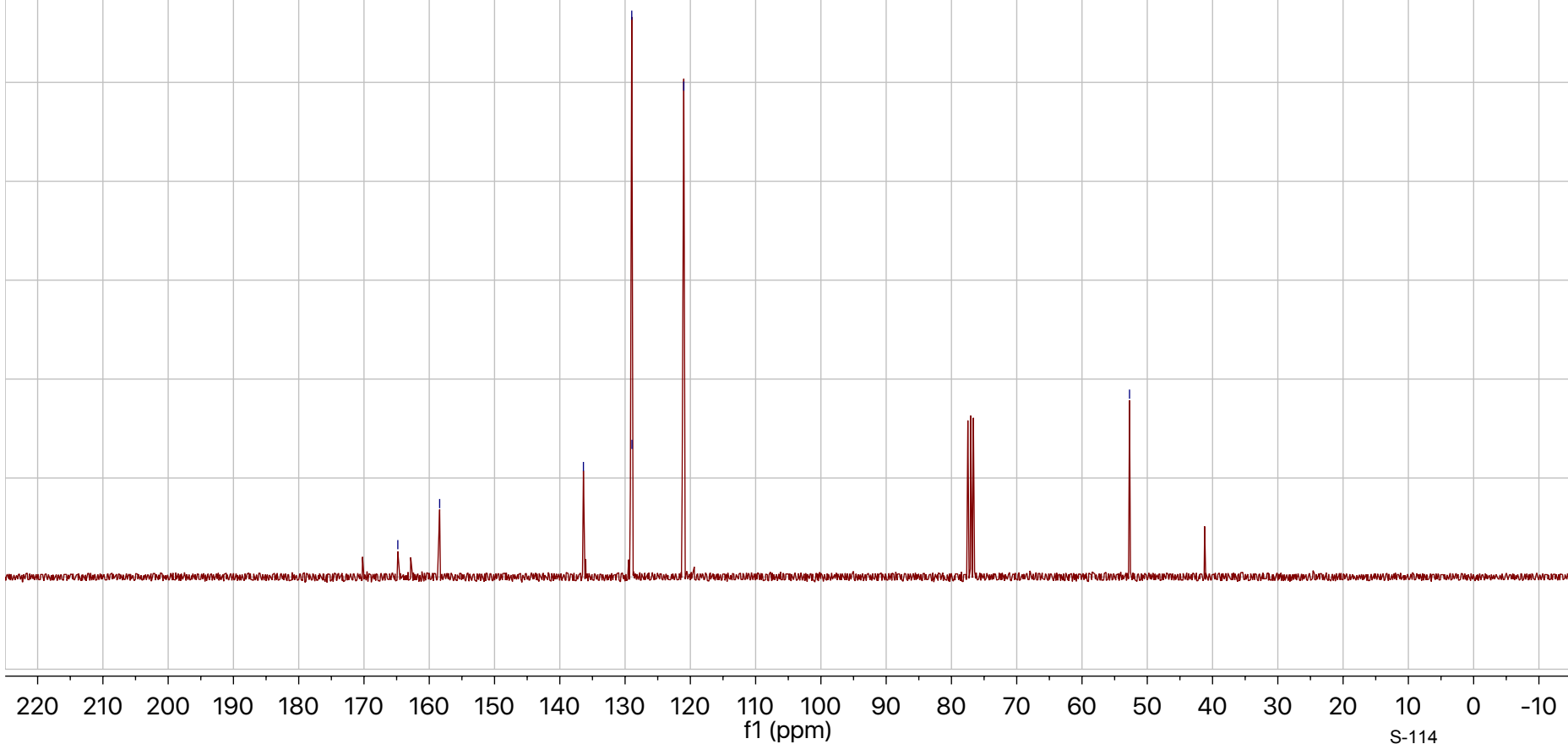
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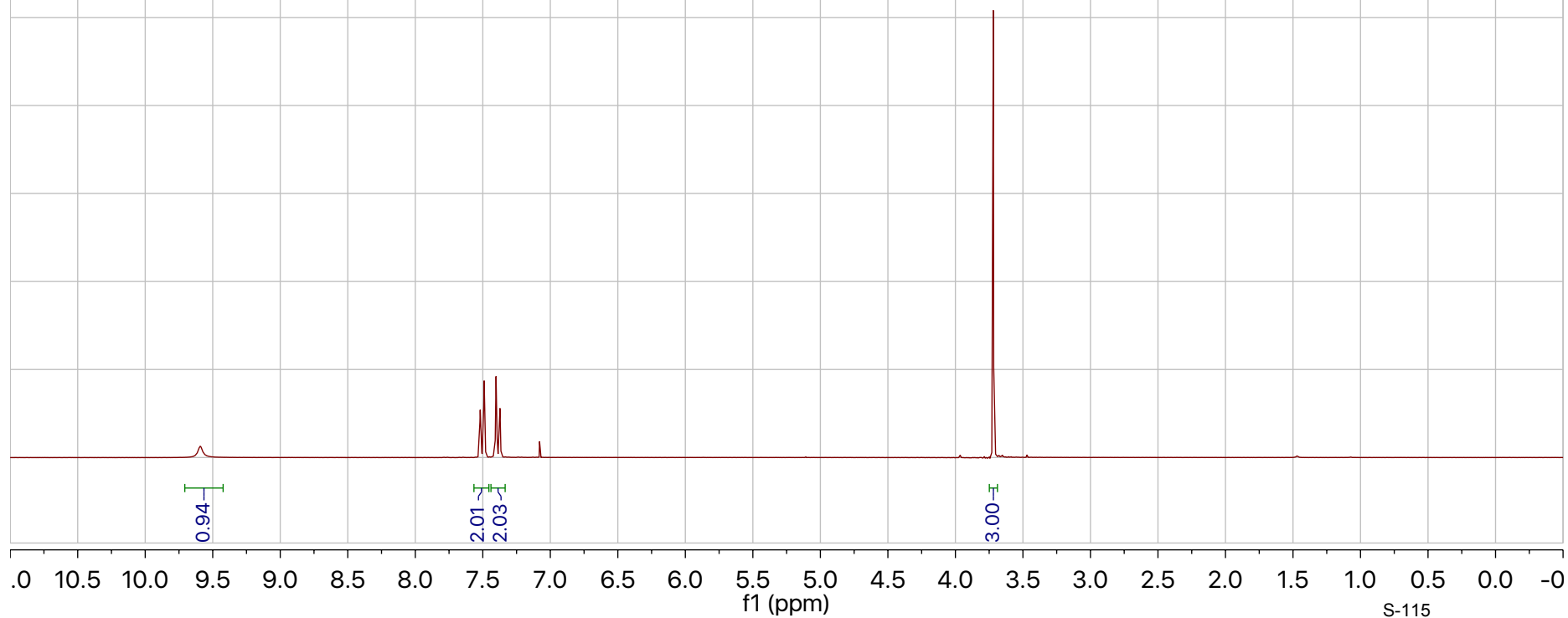
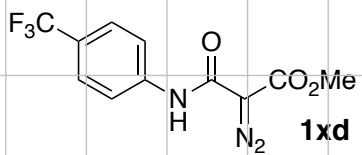
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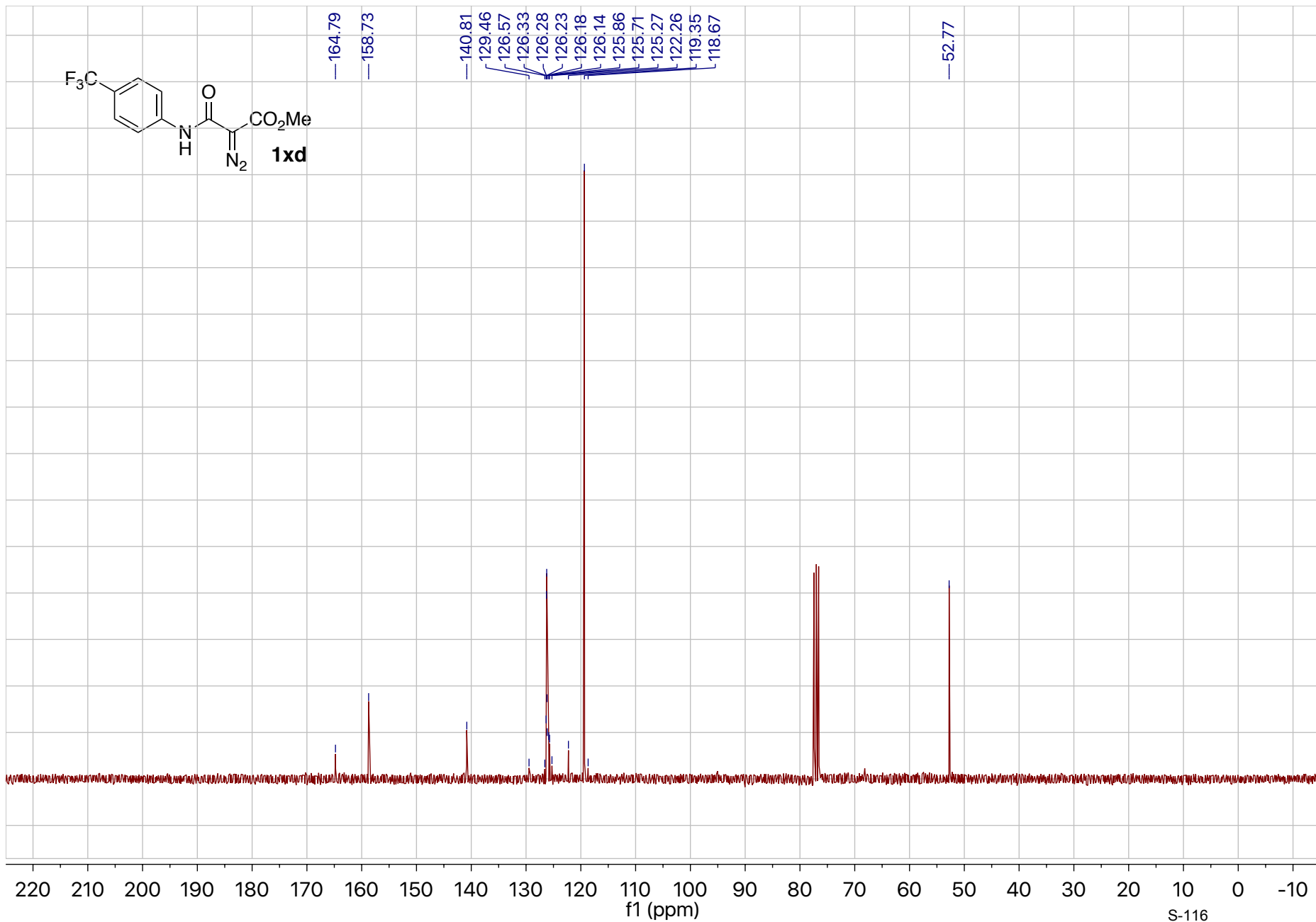
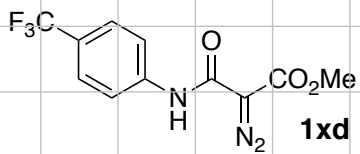
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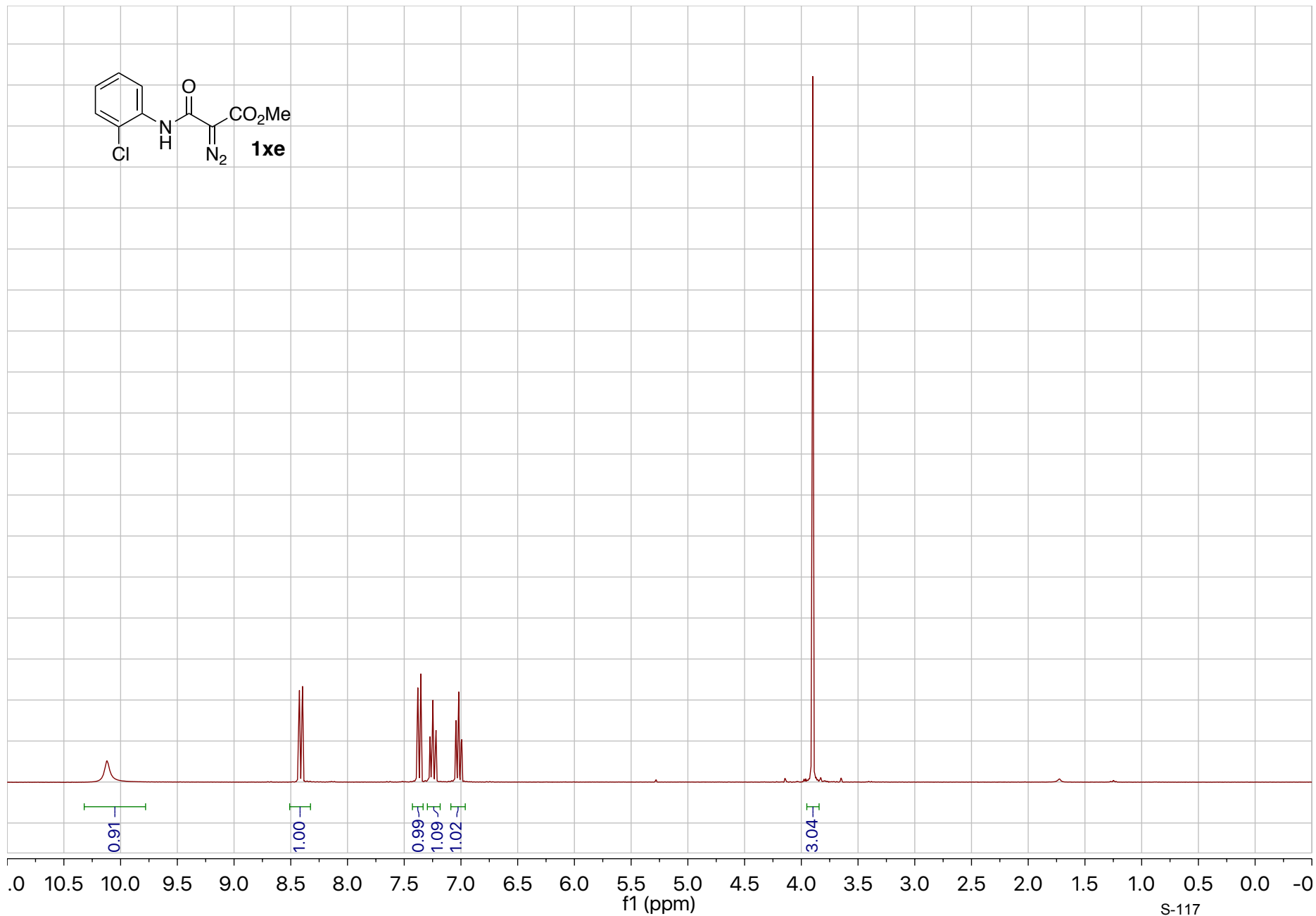
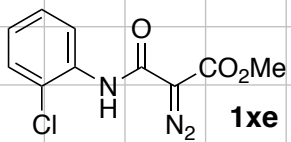
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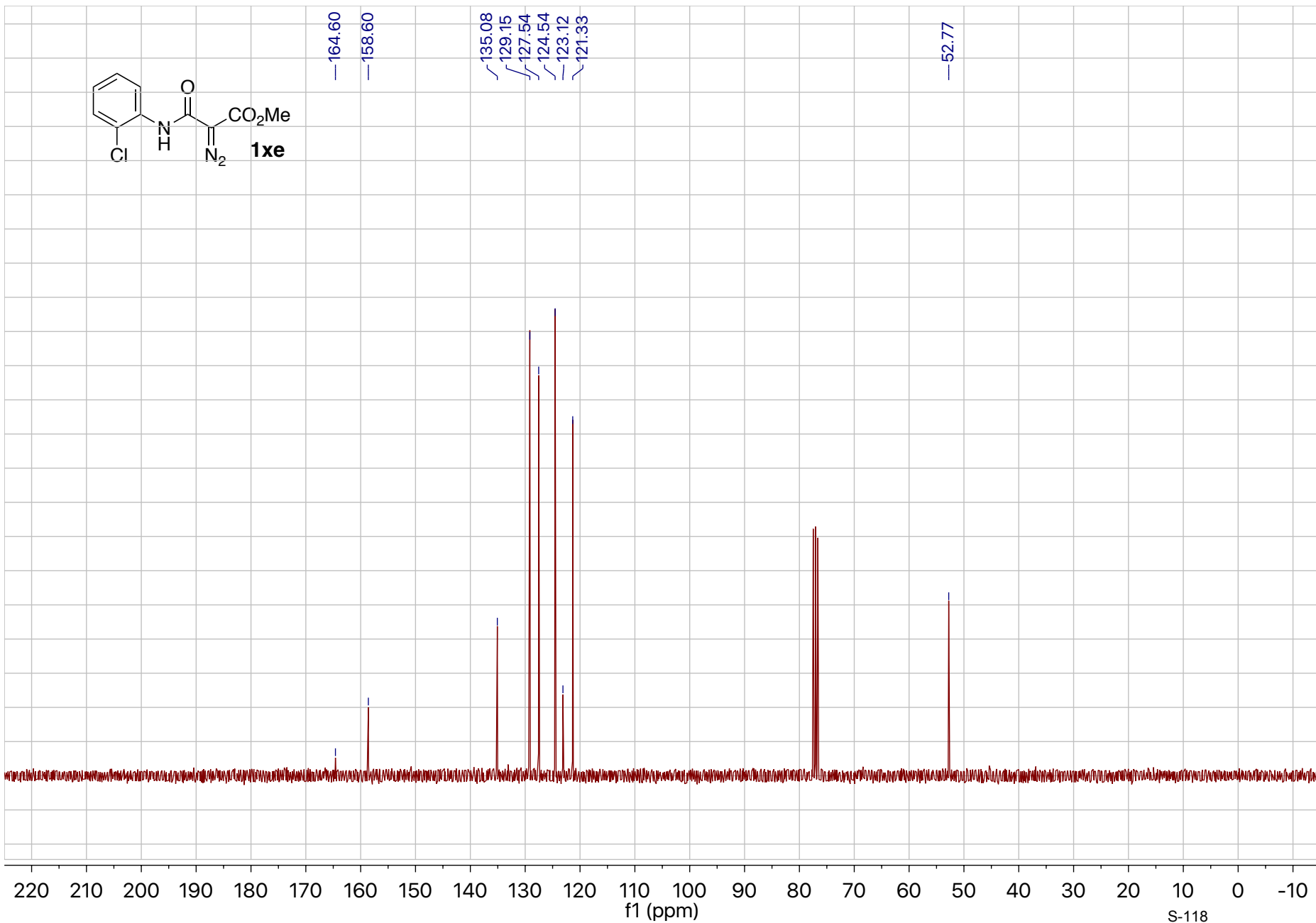
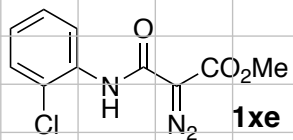
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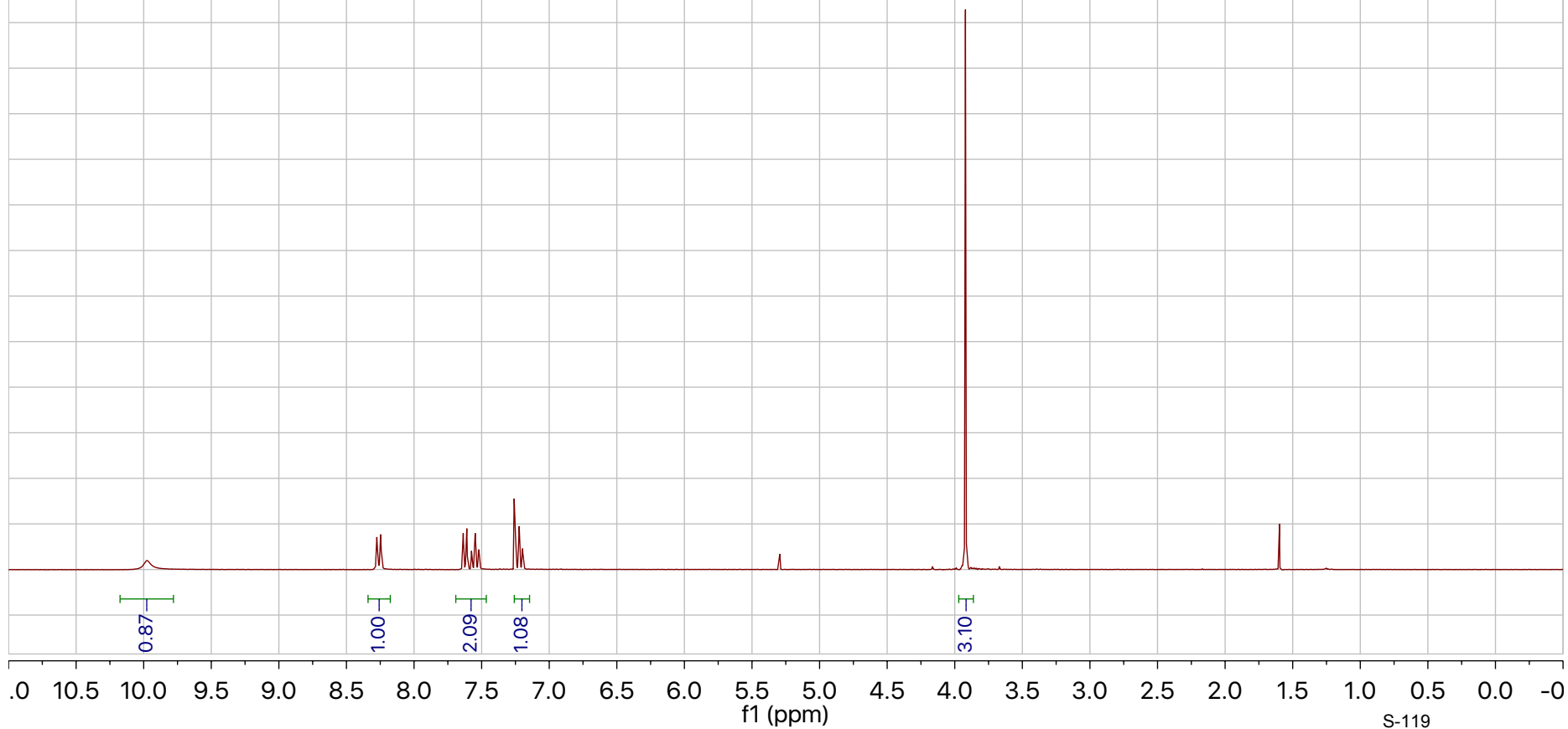
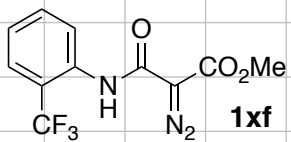


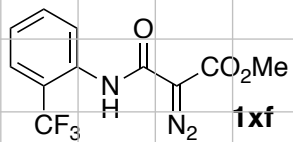




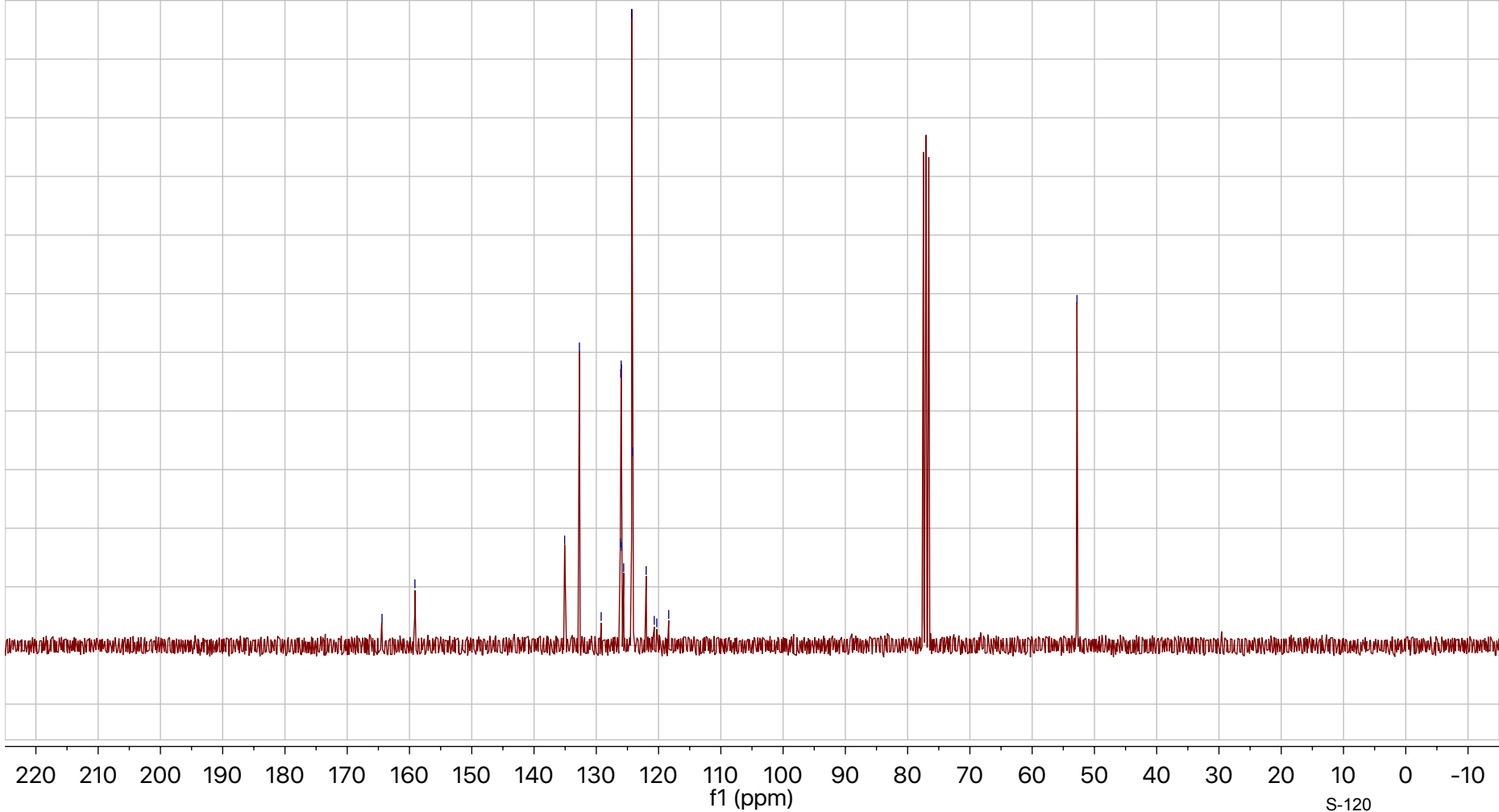




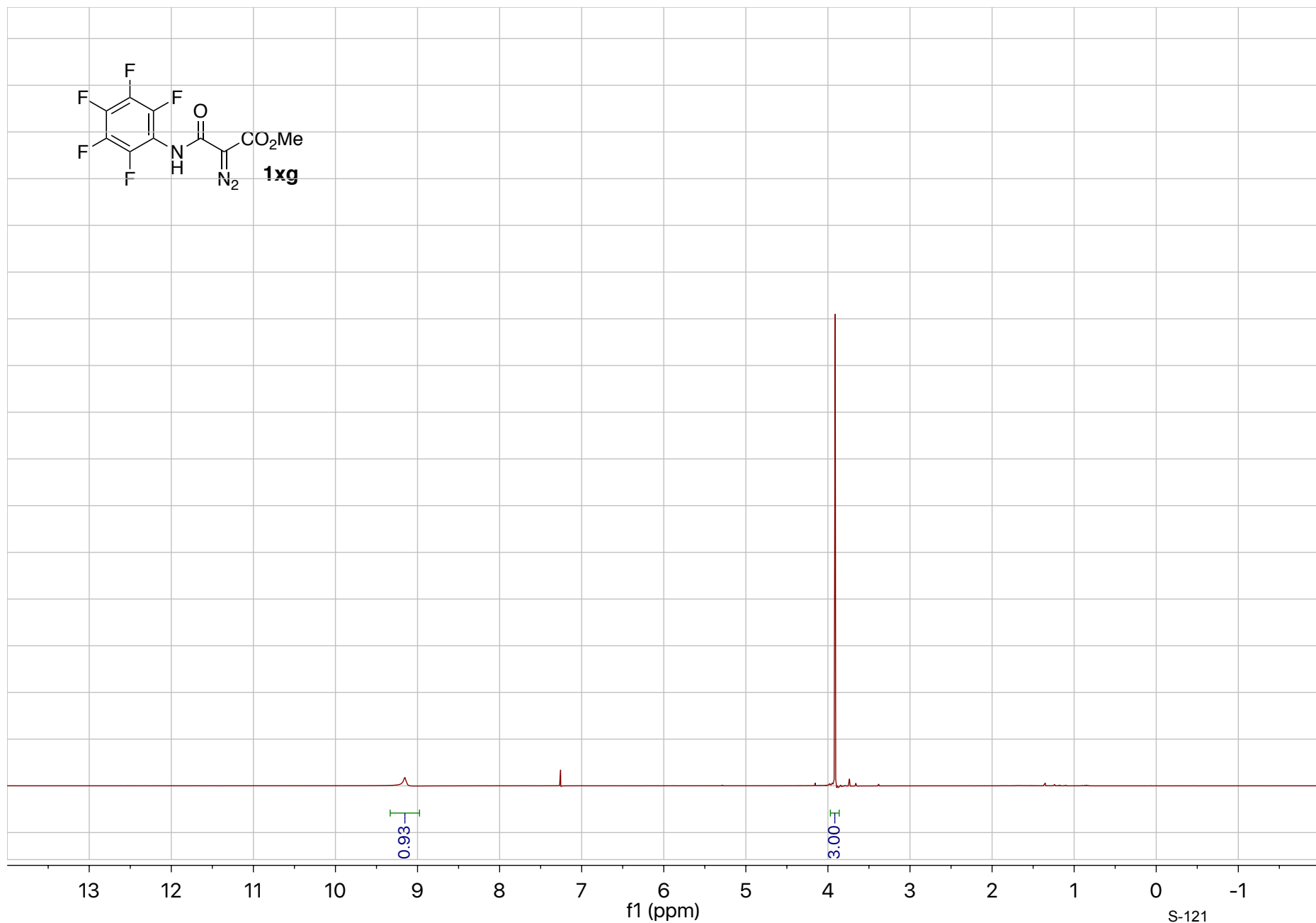
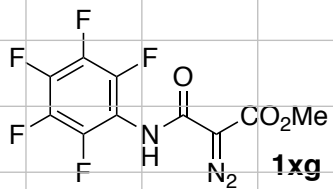


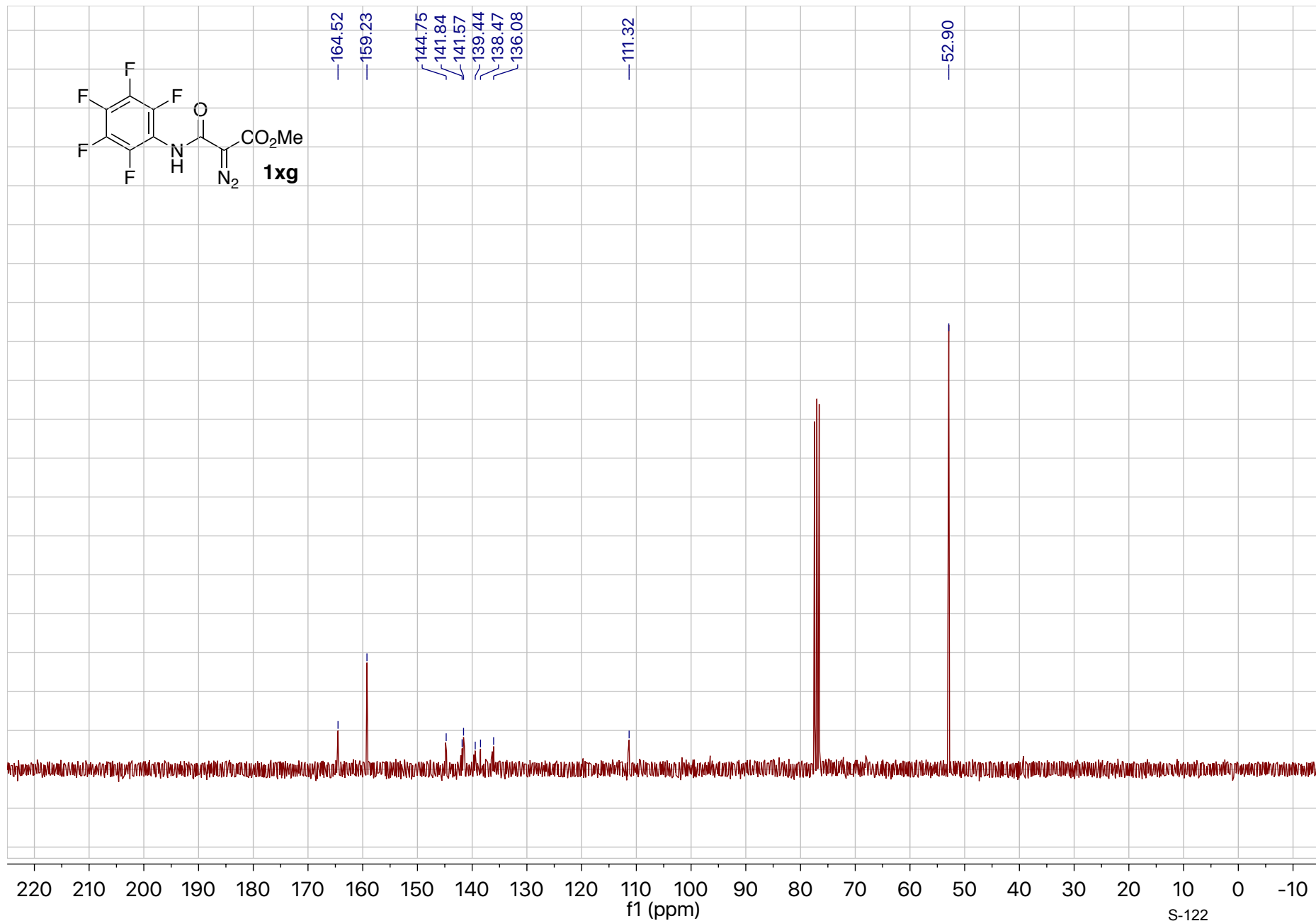
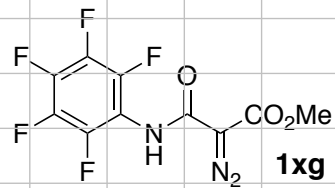


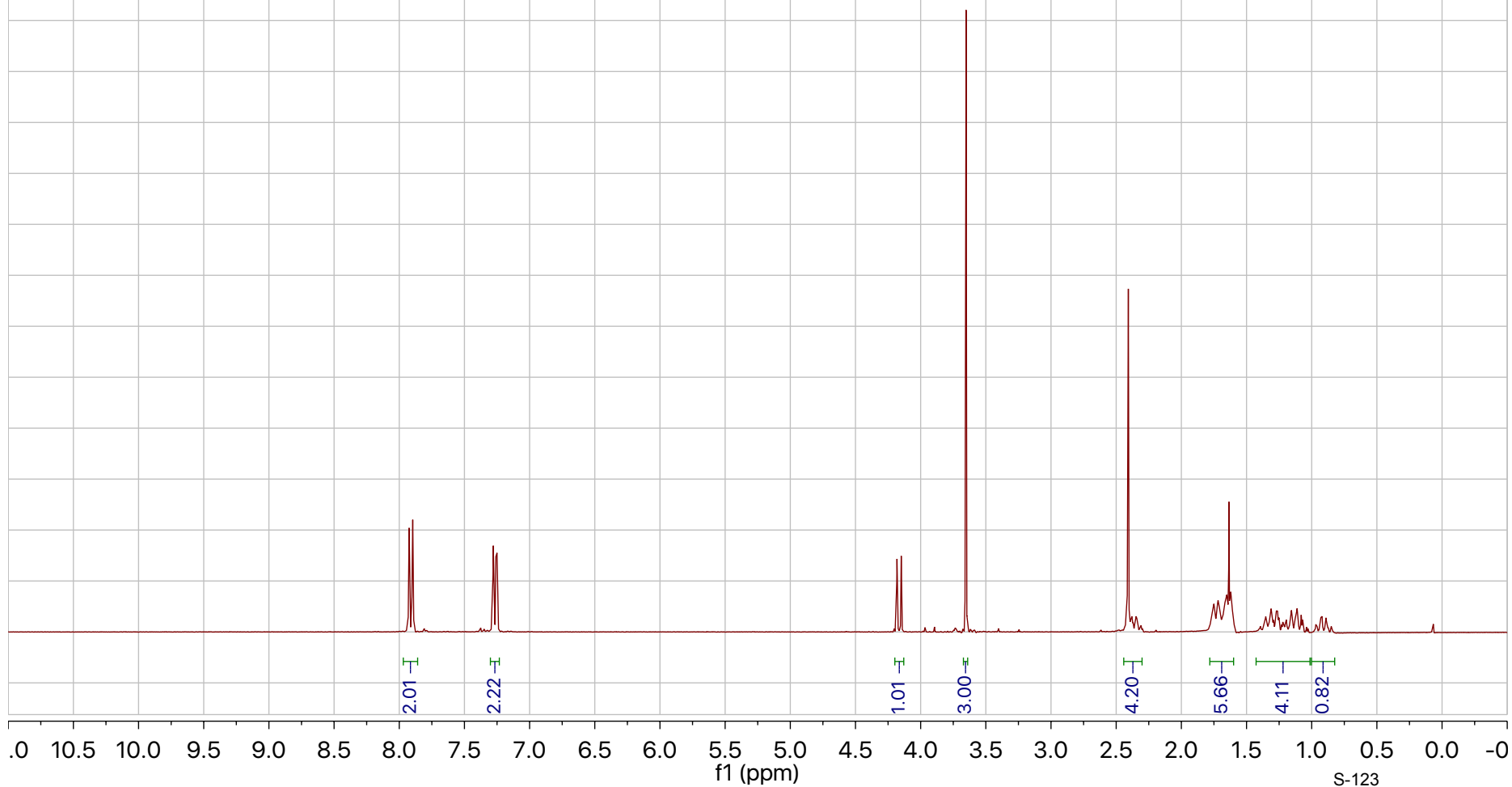
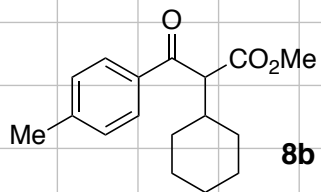
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—159.13
135.08
132.71
129.22
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121.99
120.69
120.29
118.37
—52.80

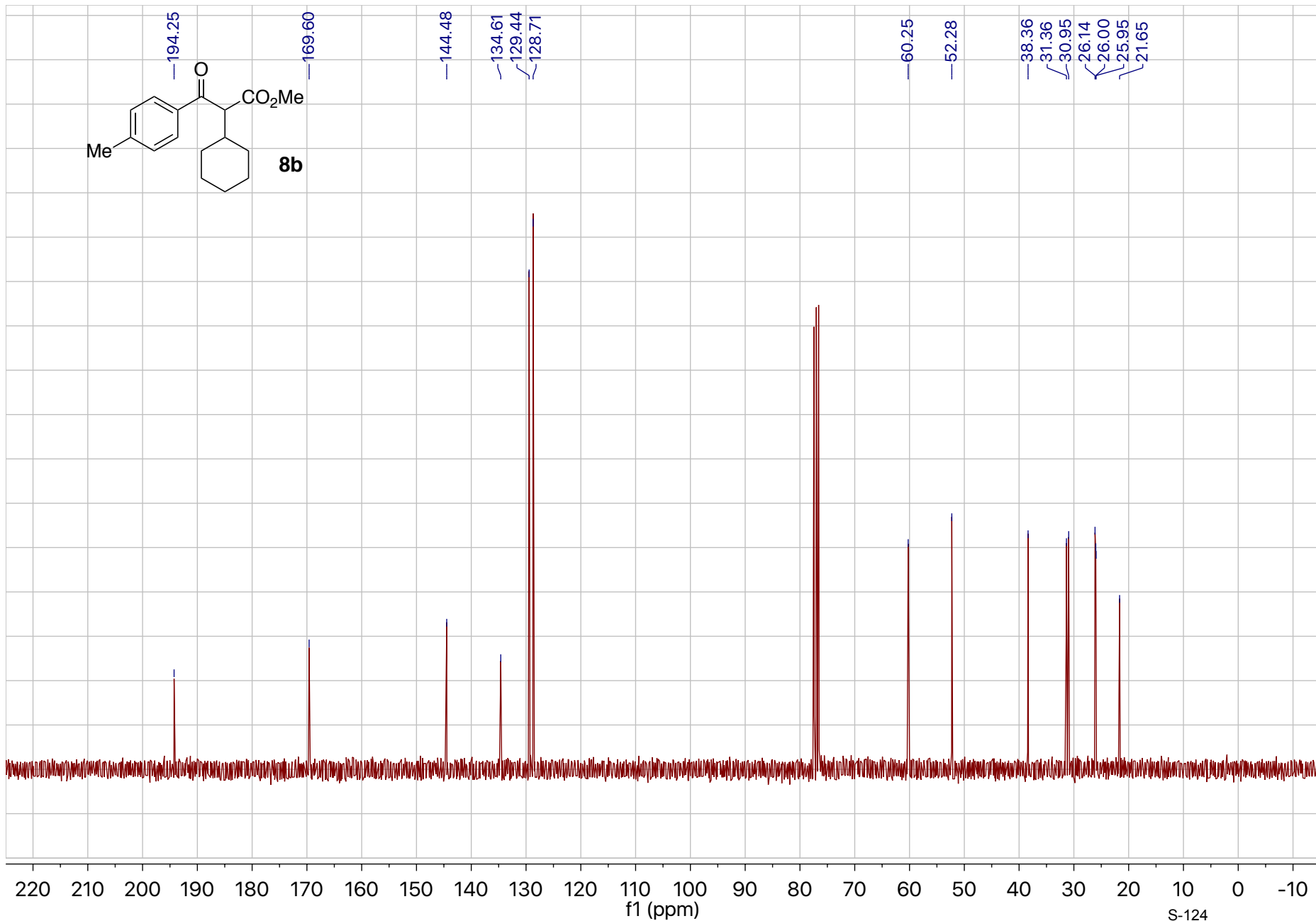
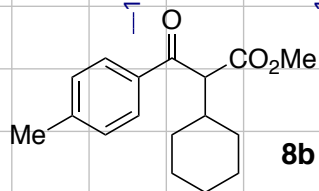


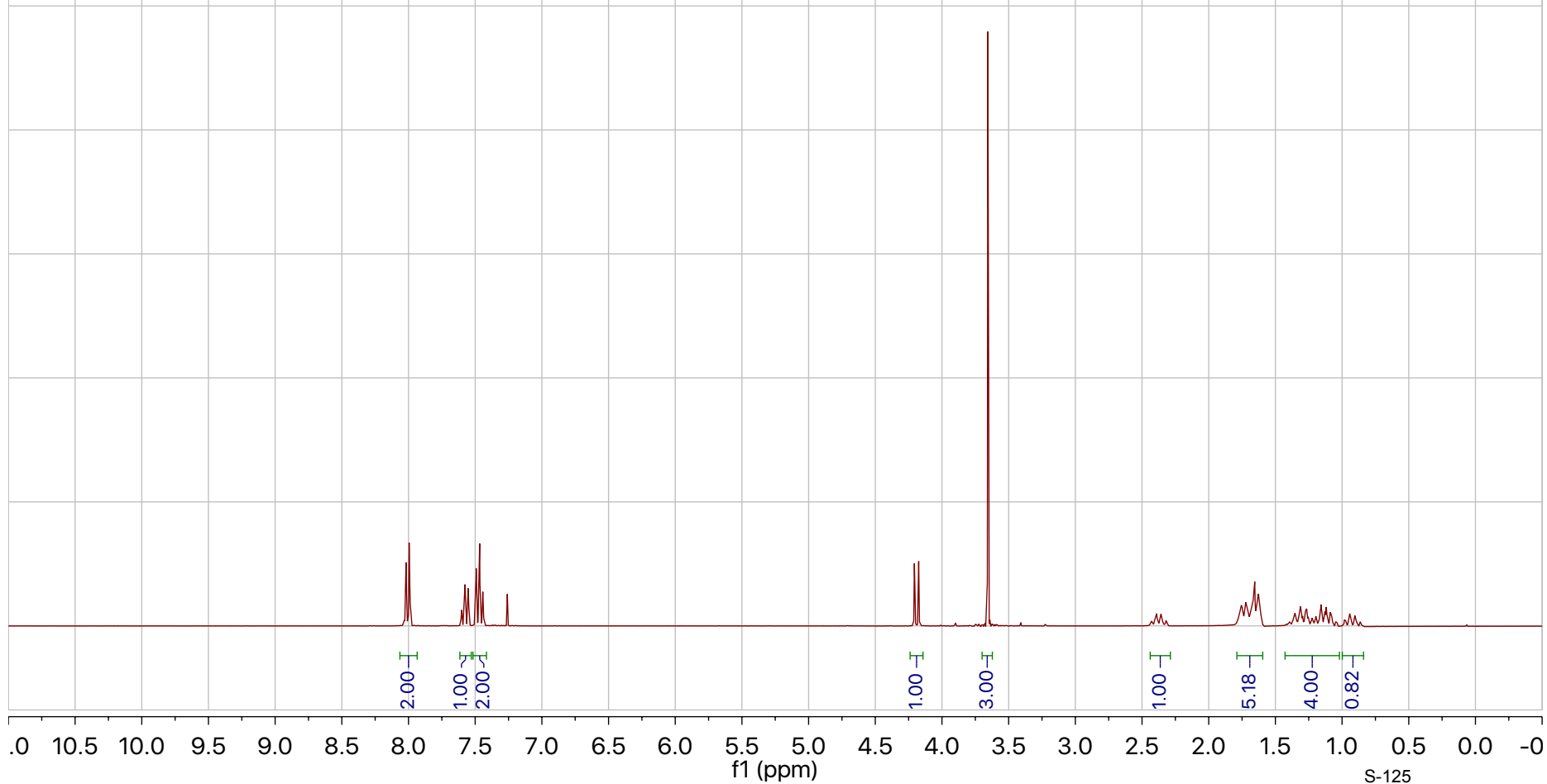
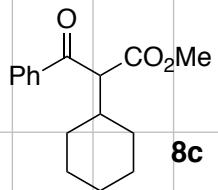
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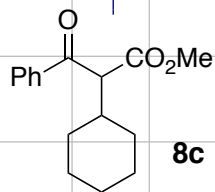








S-125



194.67

169.46

137.07

133.50

128.74

128.54

60.38

52.32

38.39

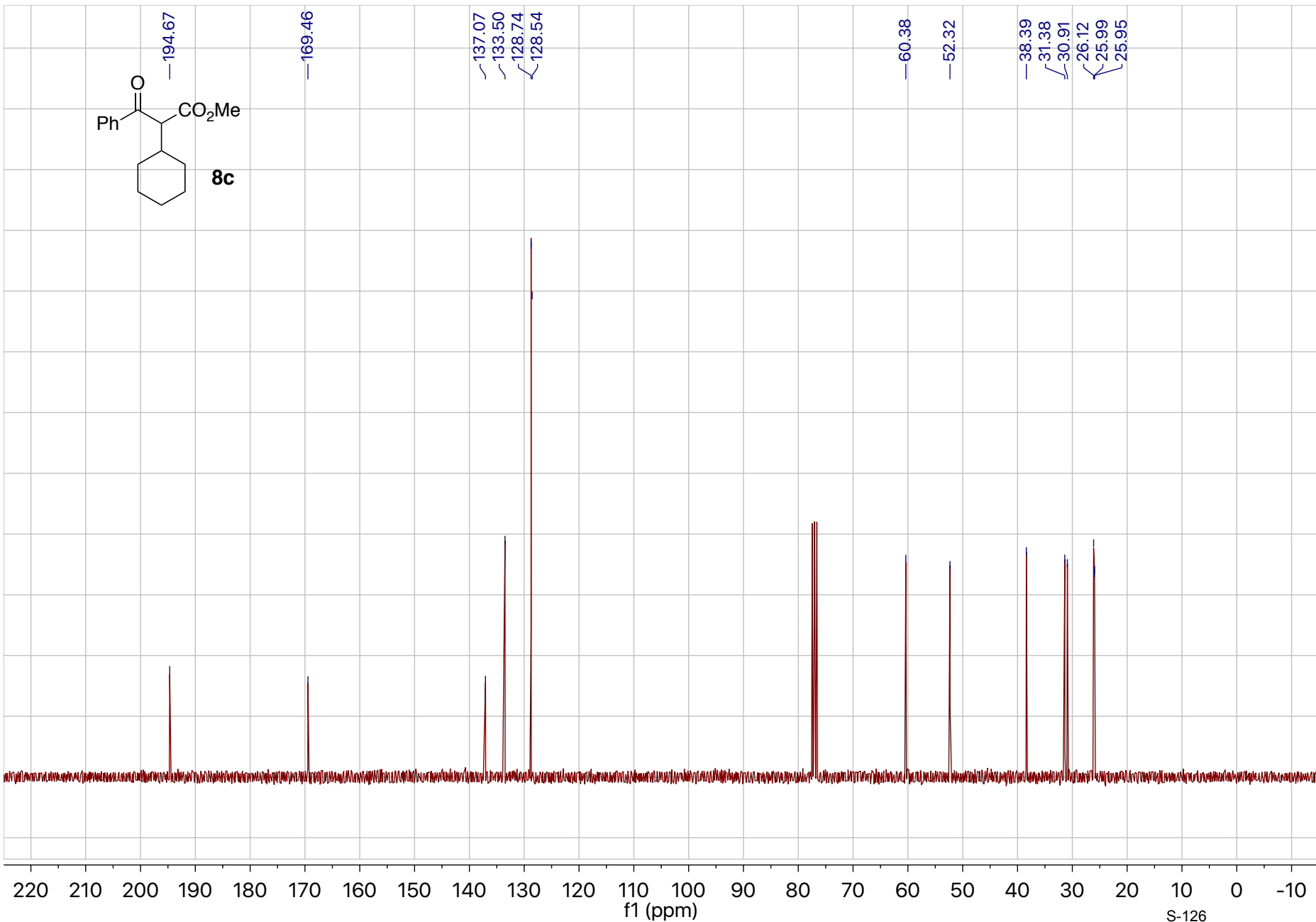
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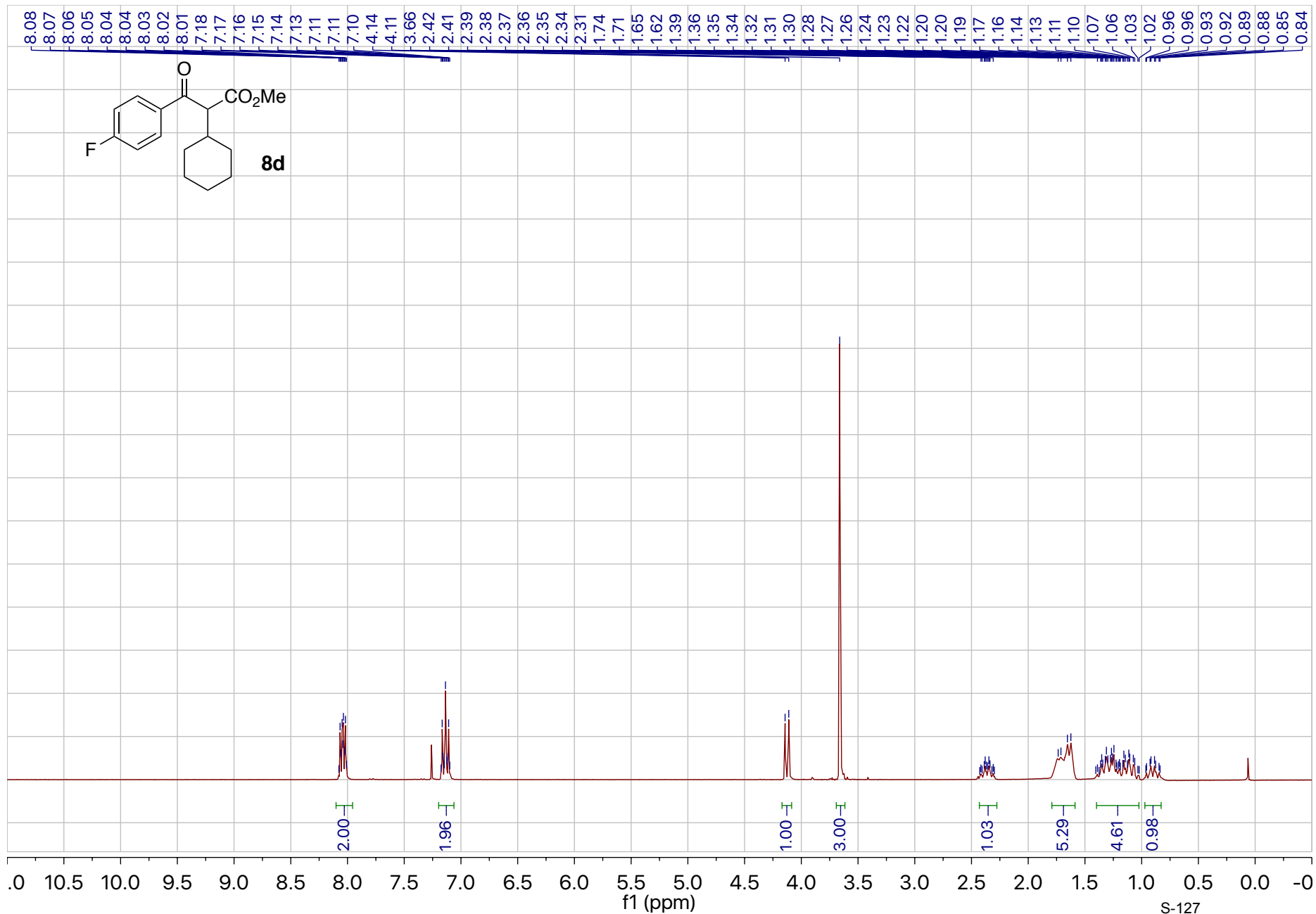
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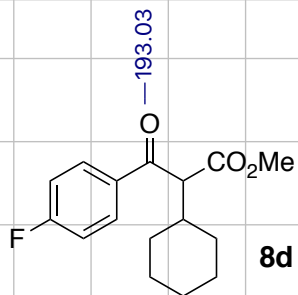
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25.99

25.95







193.03

169.34

167.69

164.30

133.46

133.42

131.34

131.22

116.05

115.76

60.49

52.41

38.31

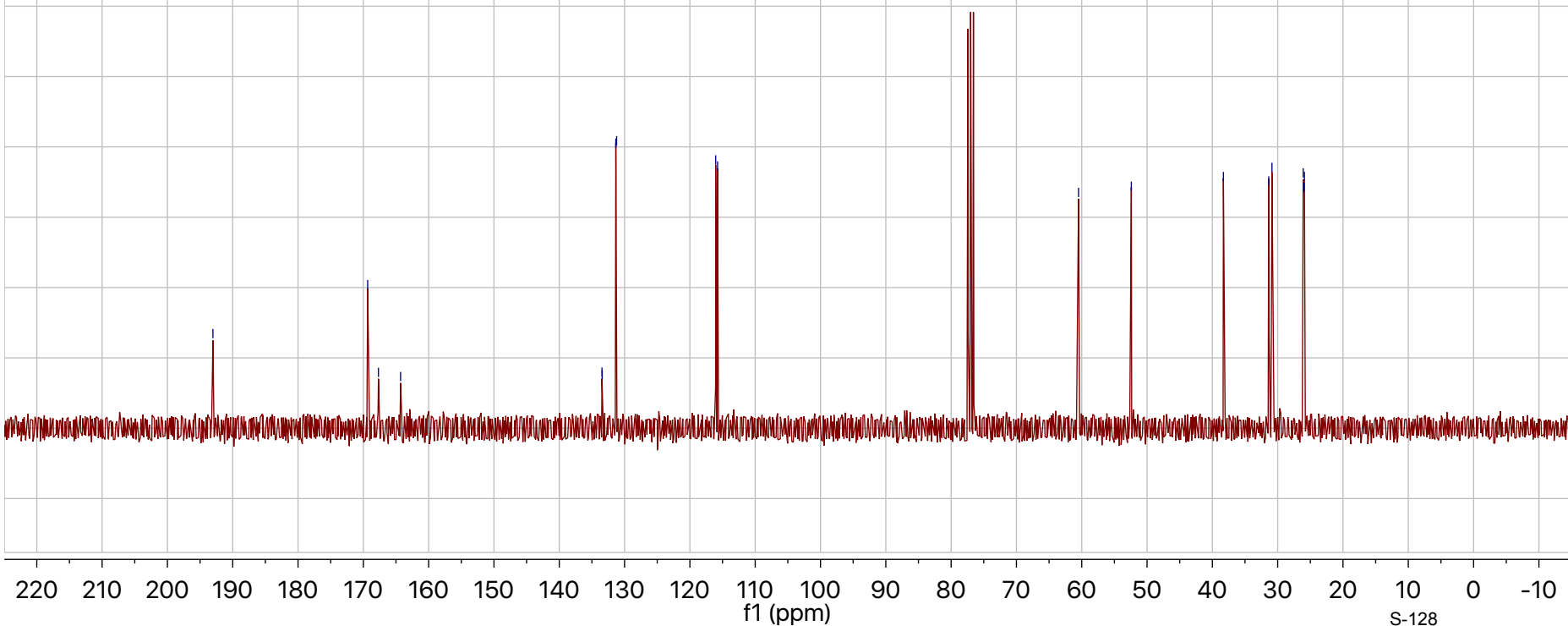
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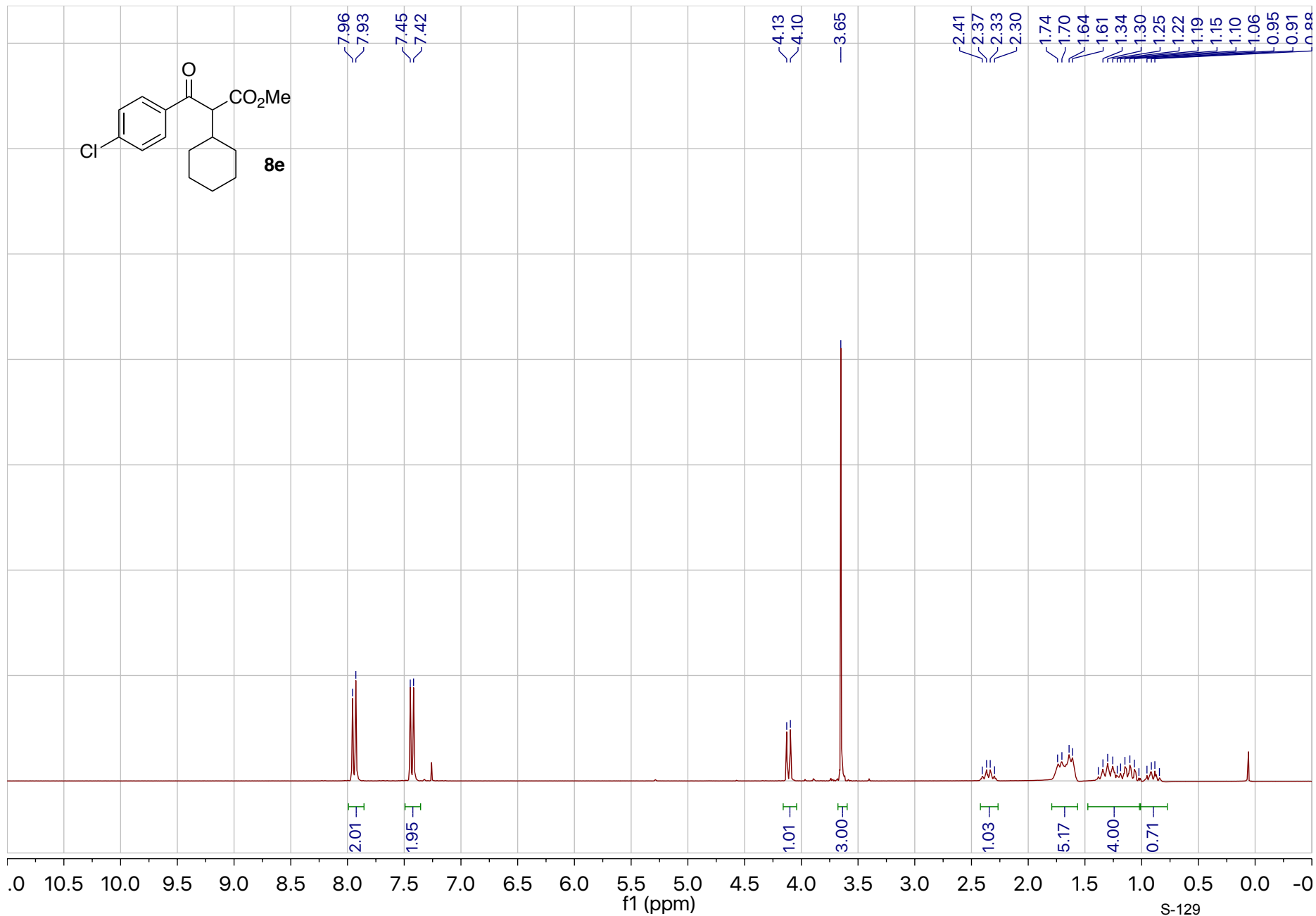
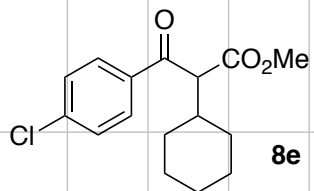
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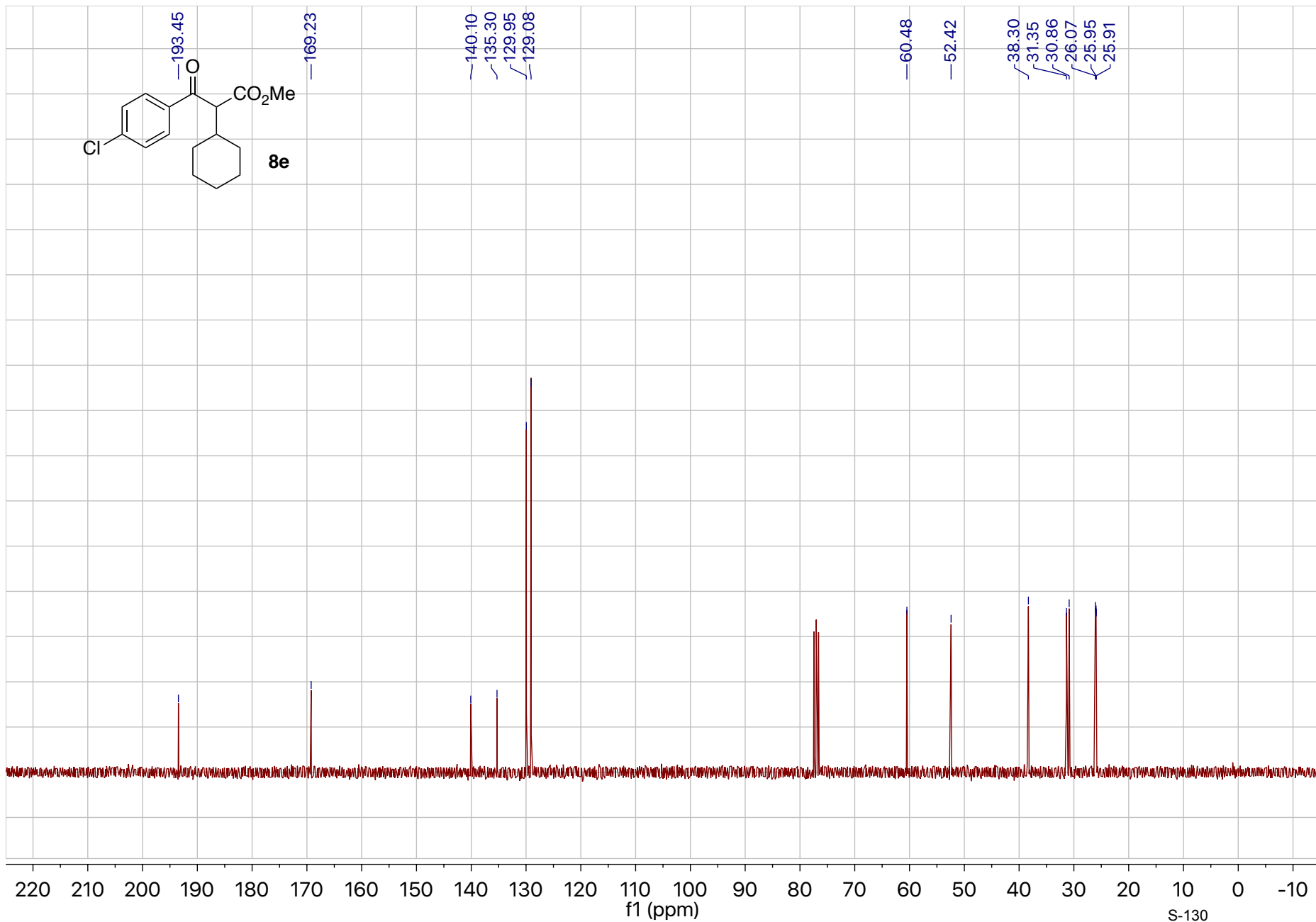
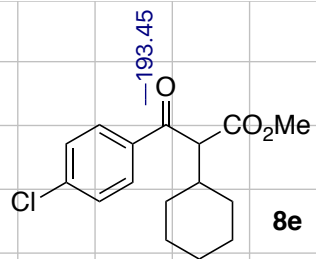
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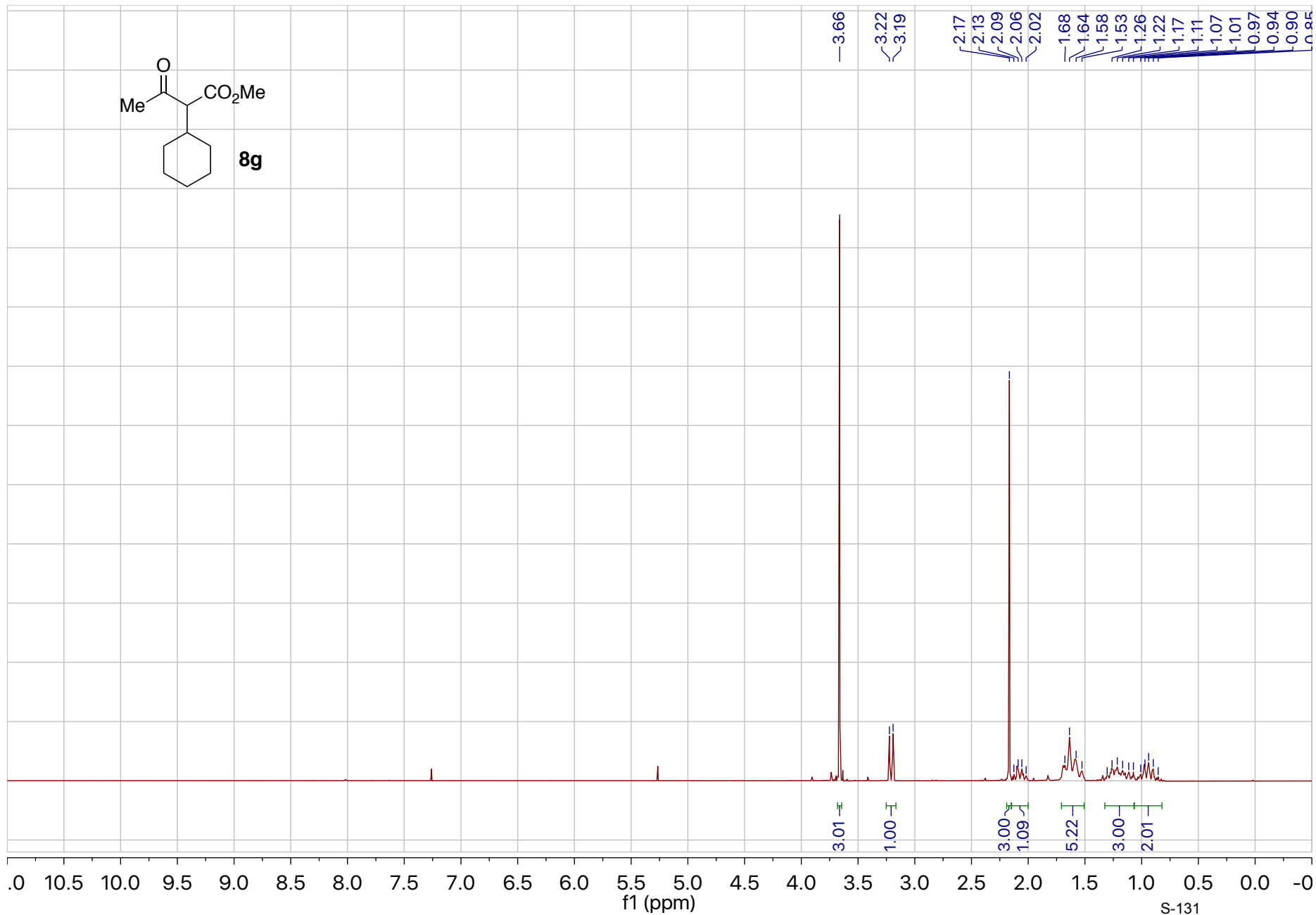
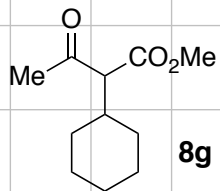
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25.91

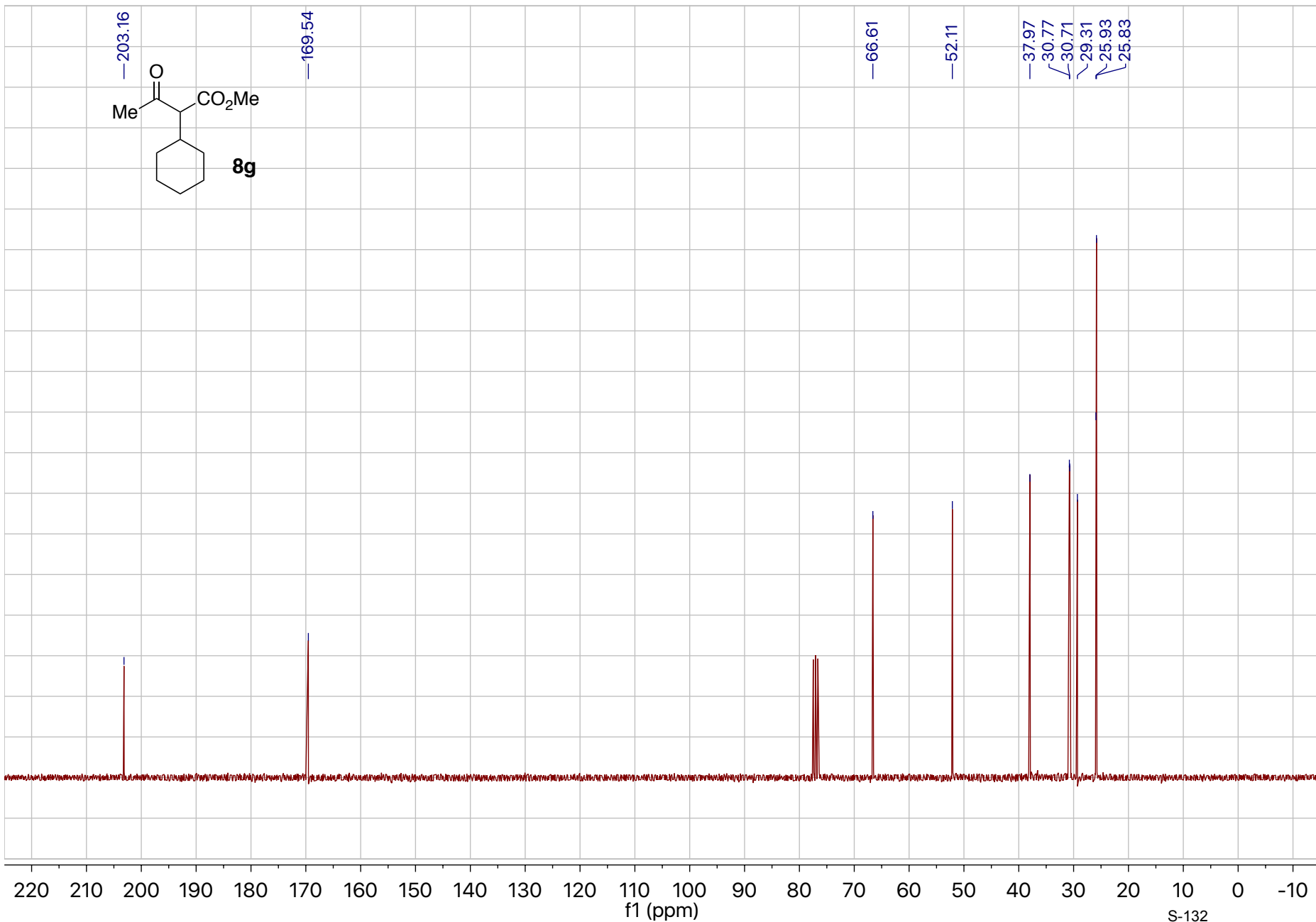
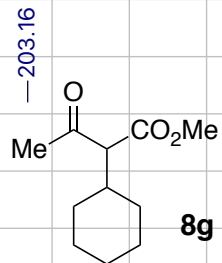


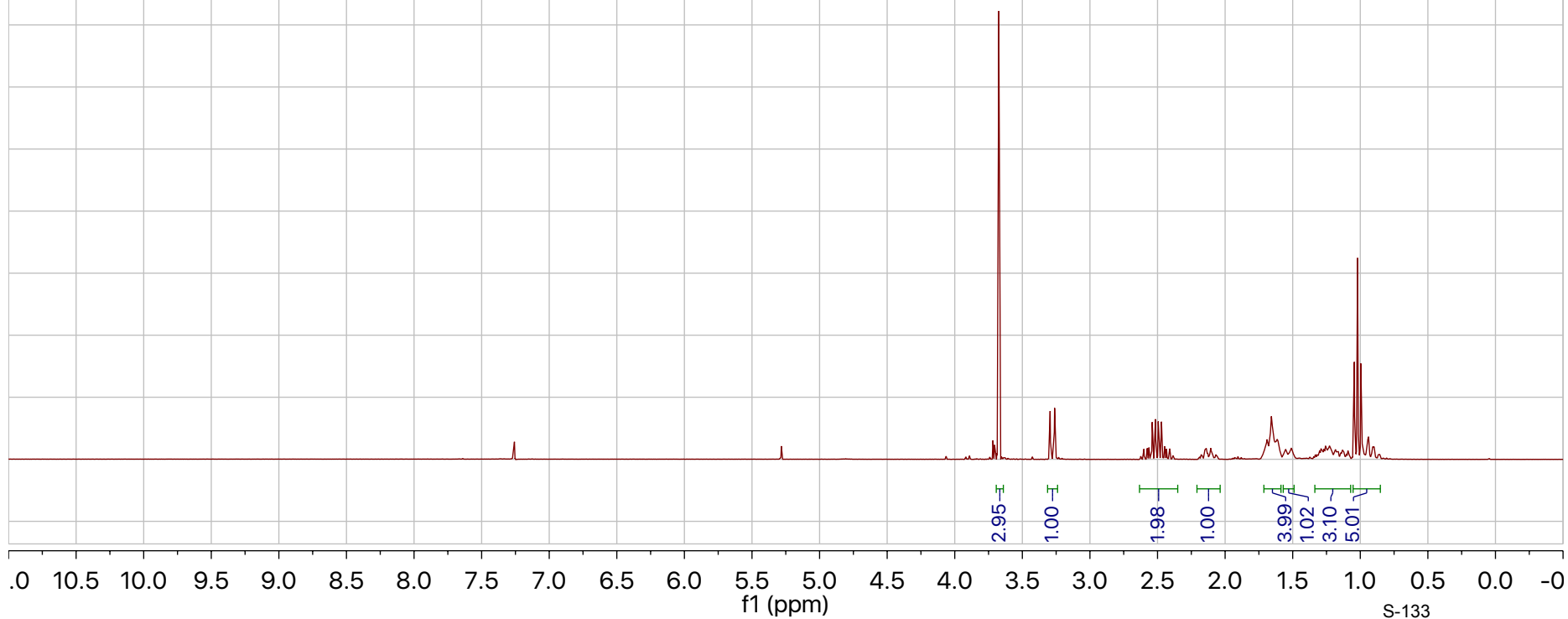
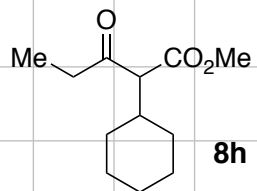




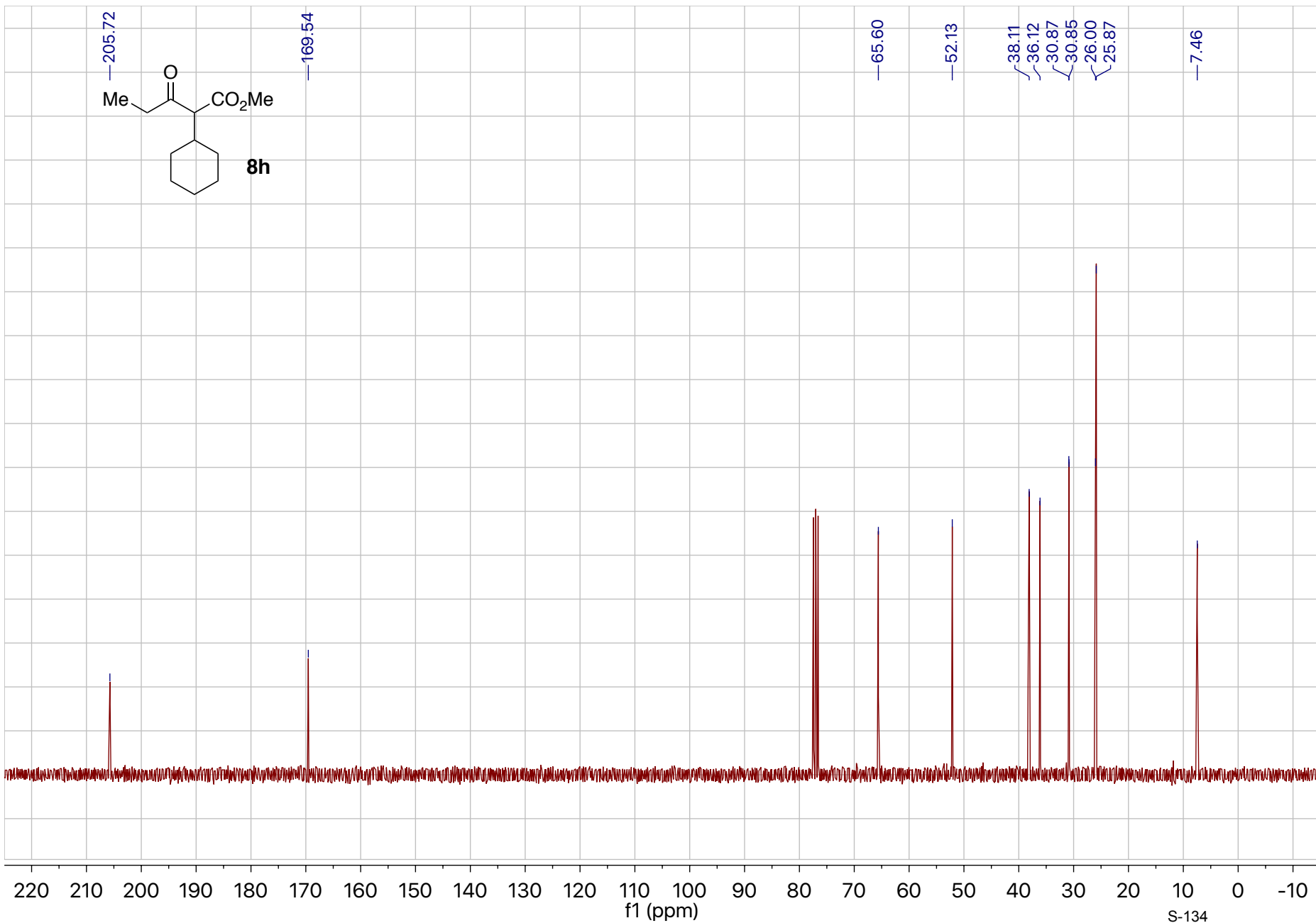
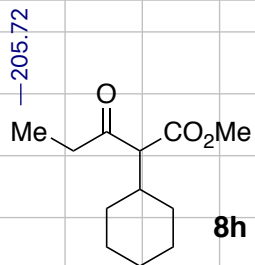


S-131

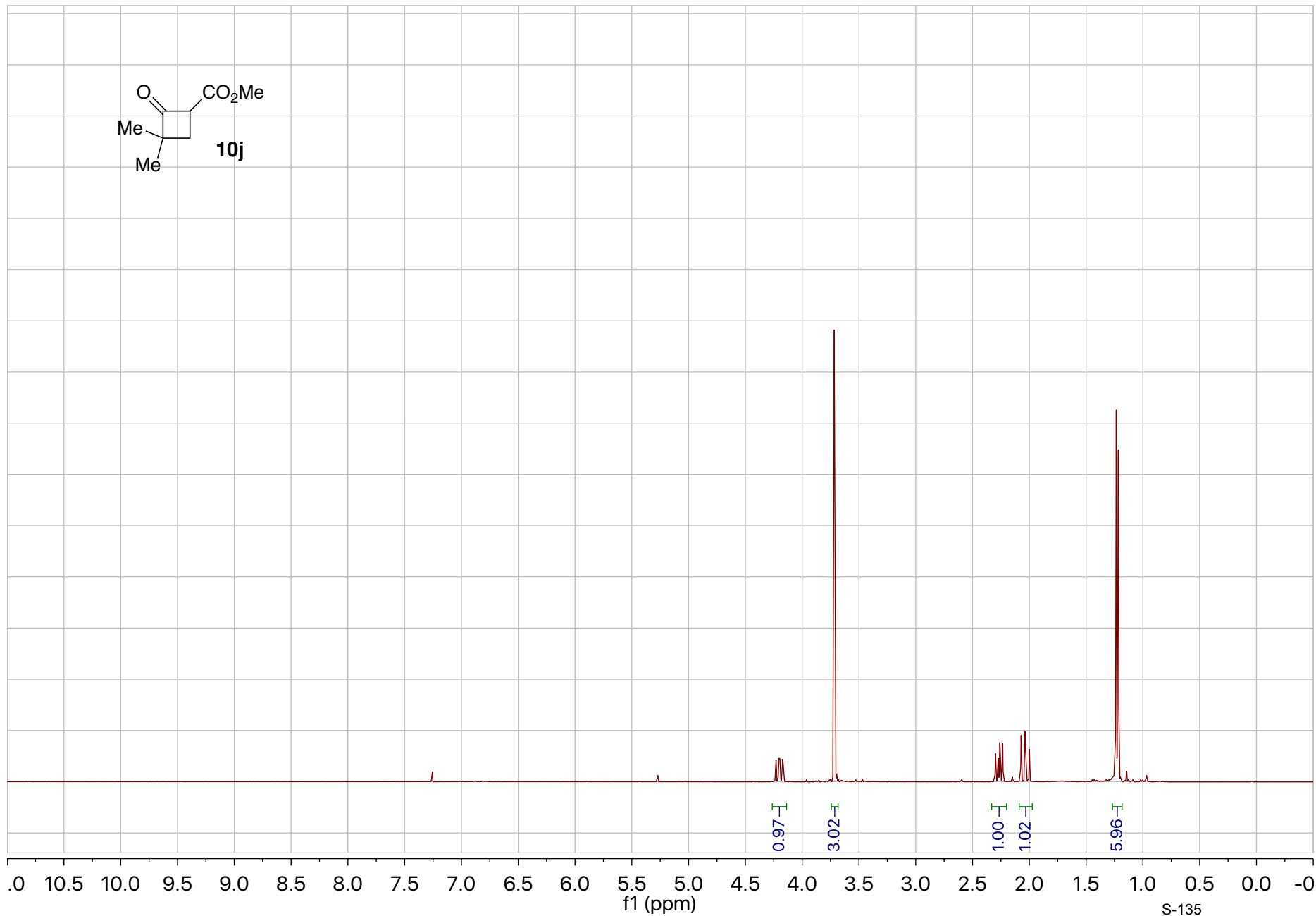
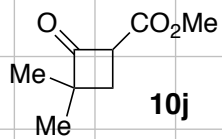




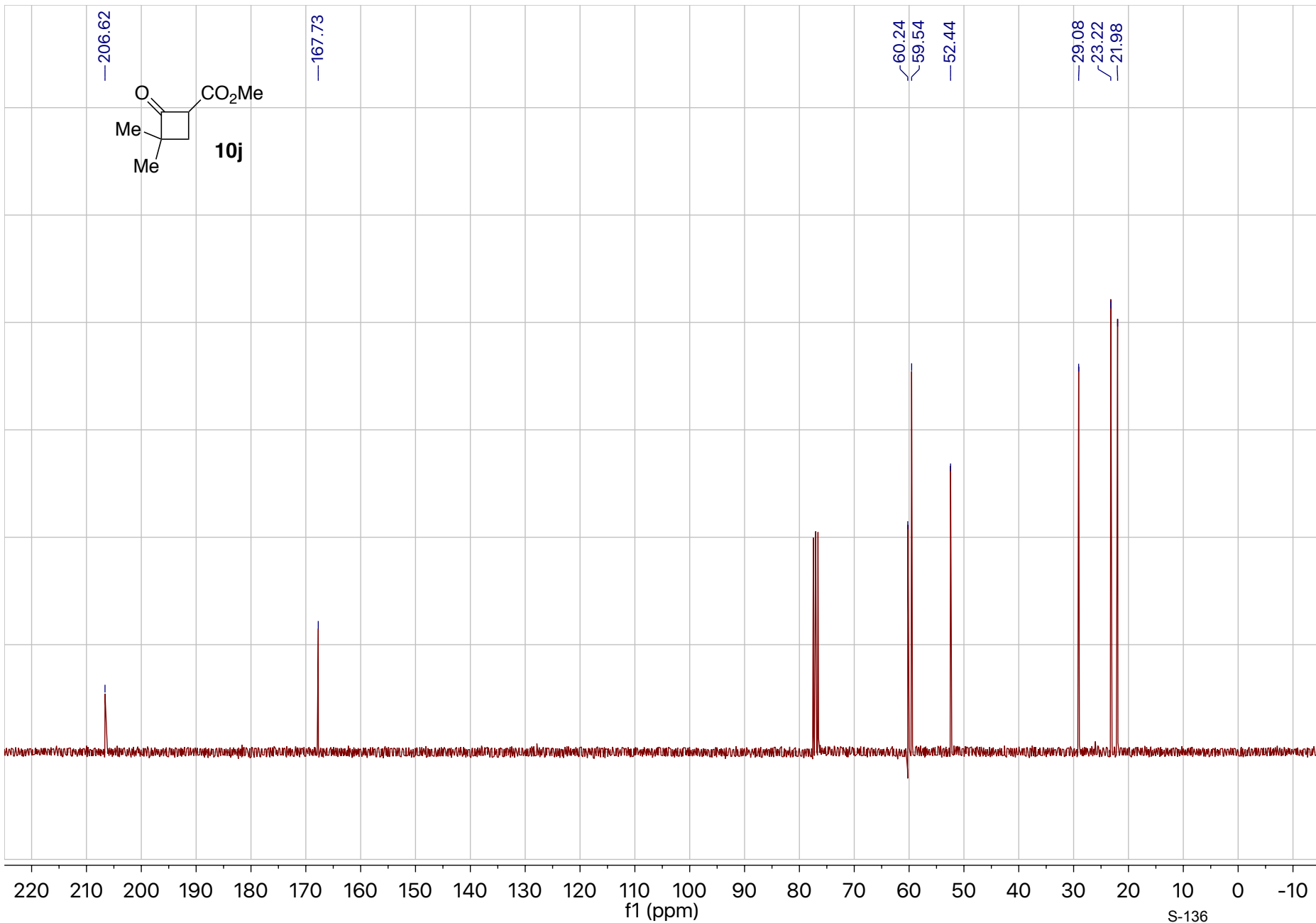
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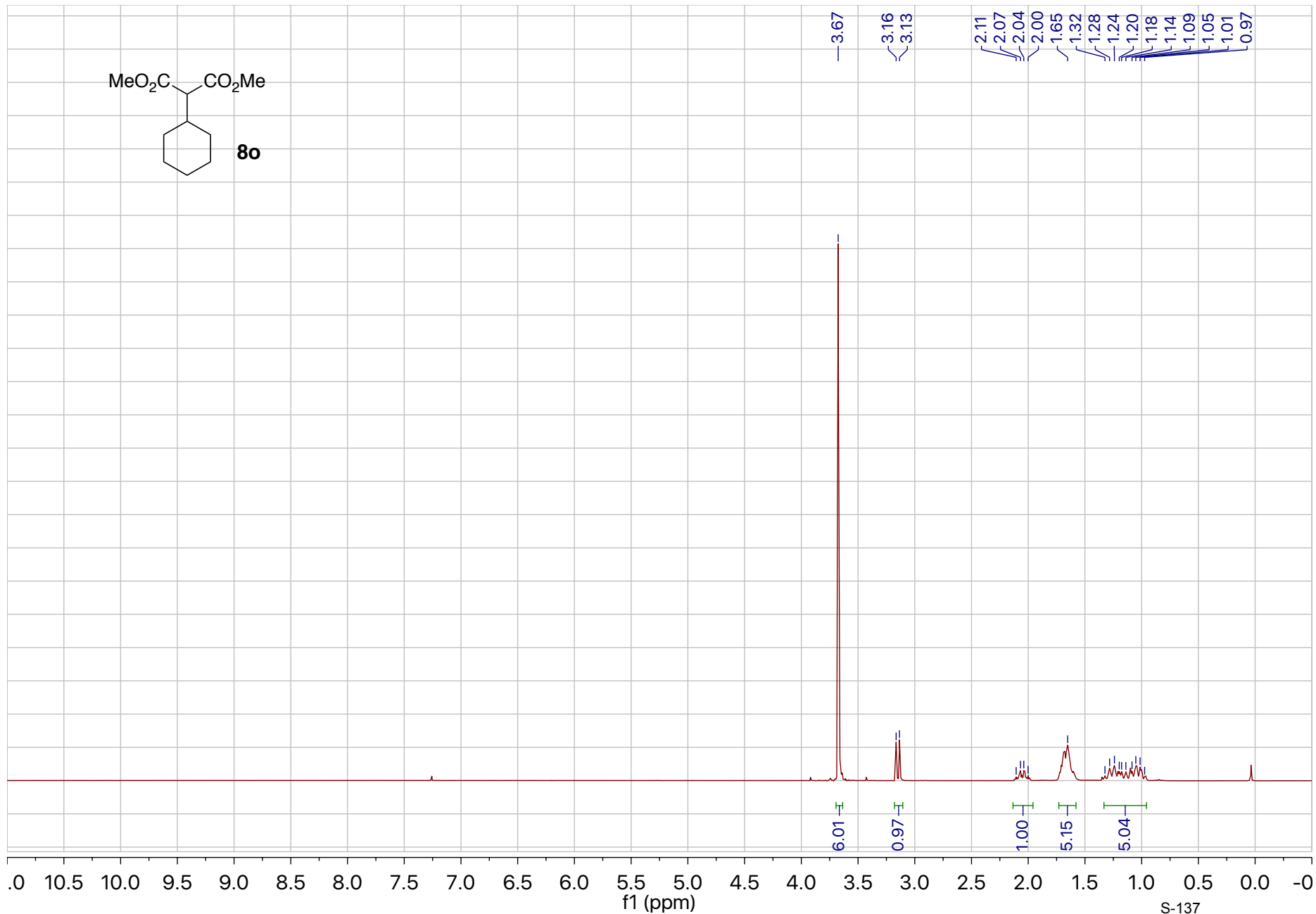
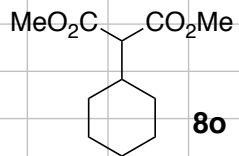


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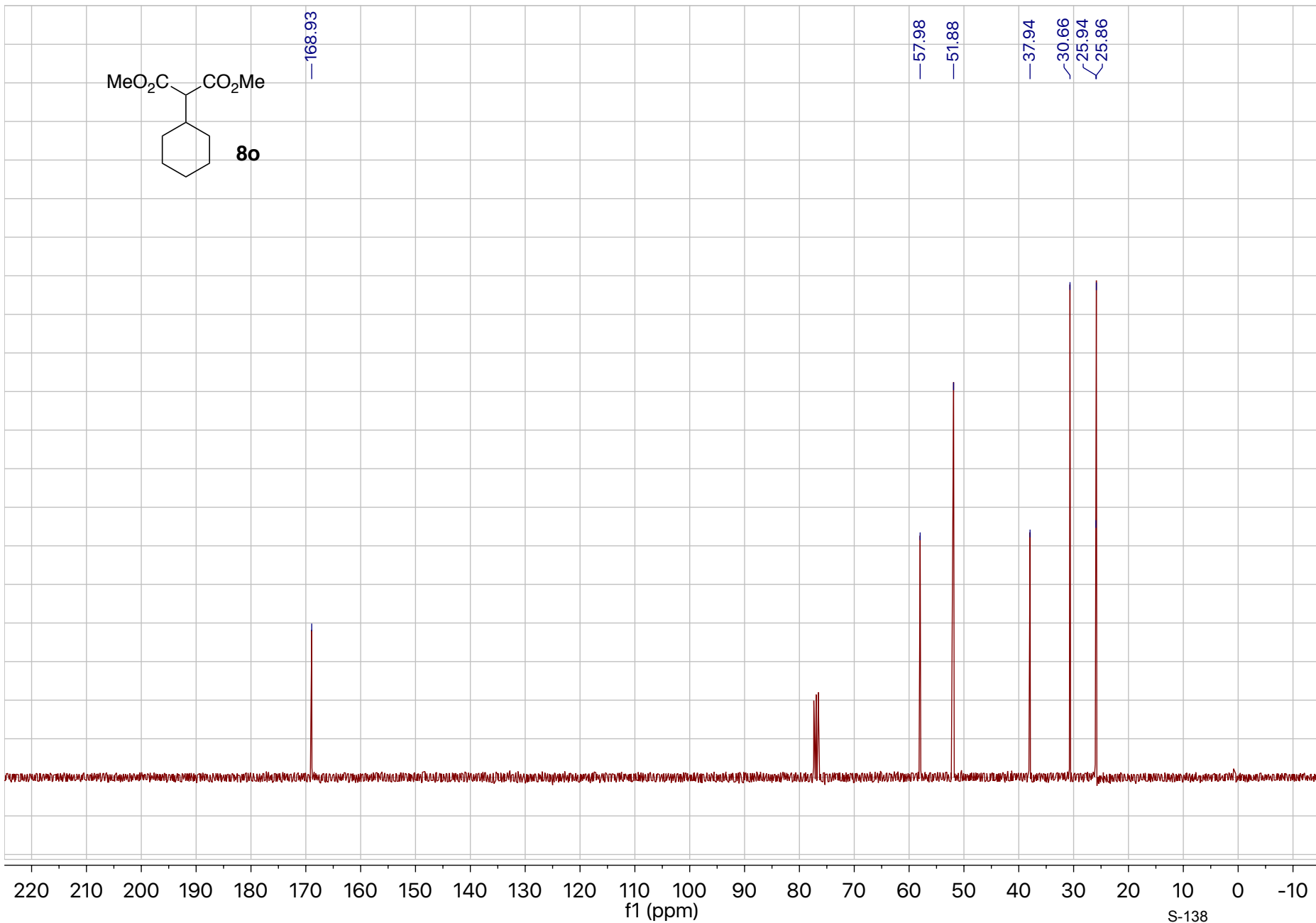
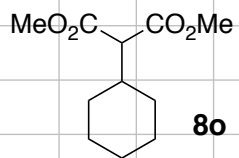


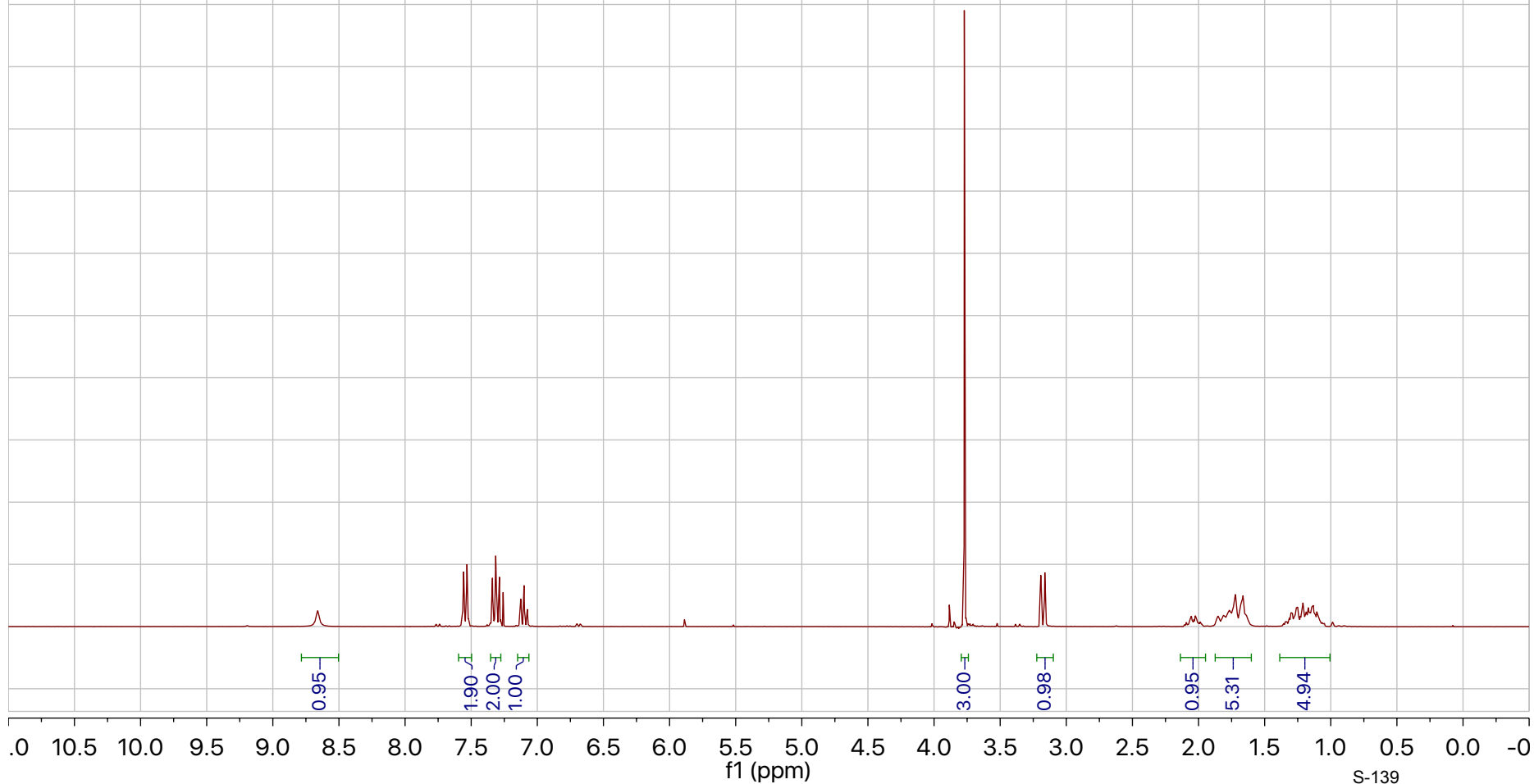
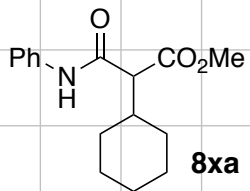
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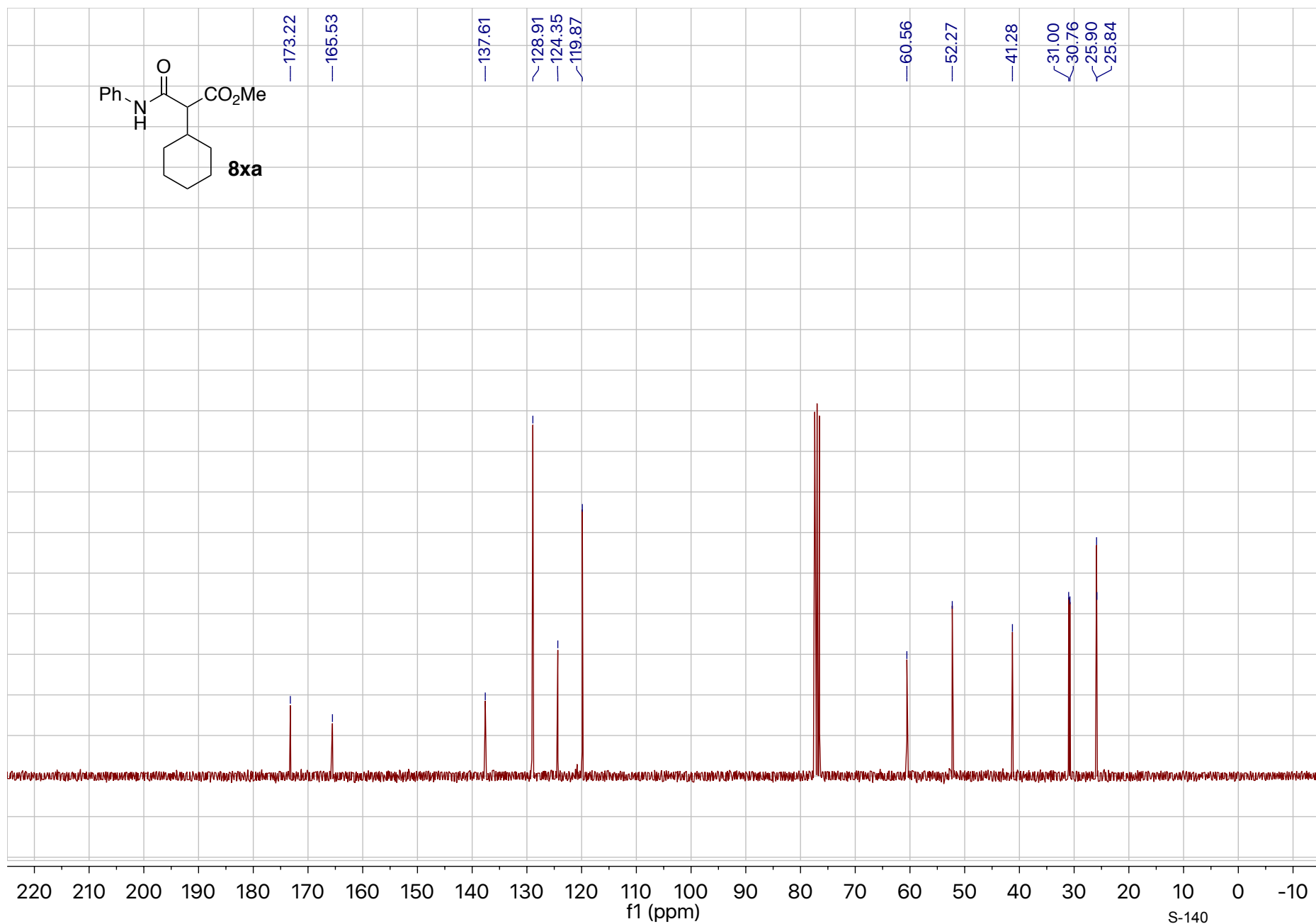
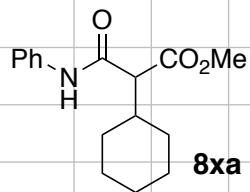


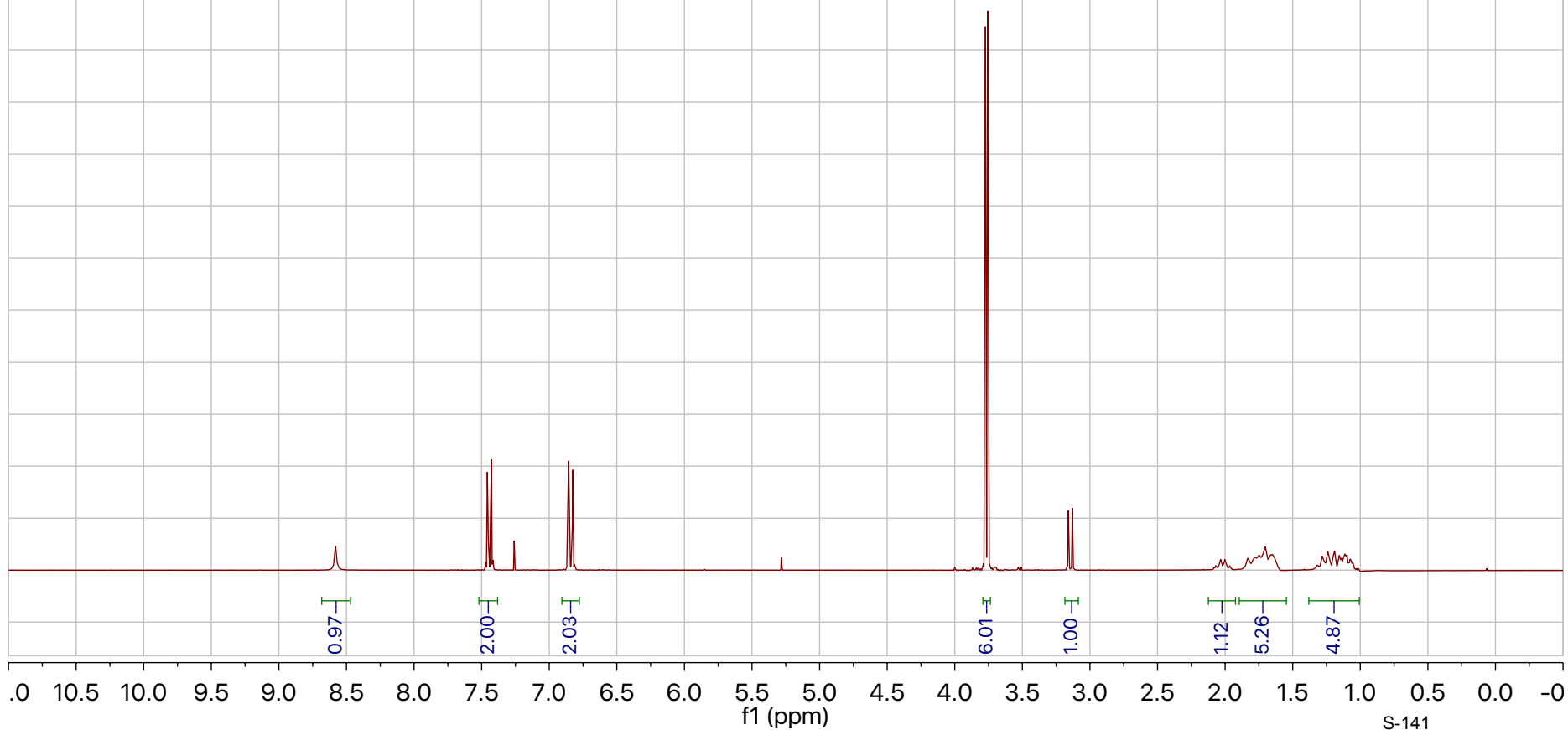
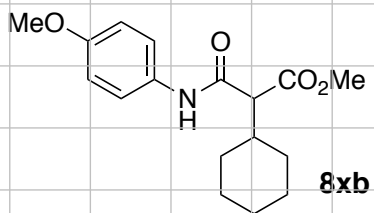


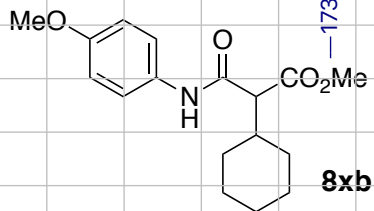
S-137











—173.27

—165.41

—156.41

—130.73

—121.58

—114.07

~60.39

~55.46

~52.35

—41.23

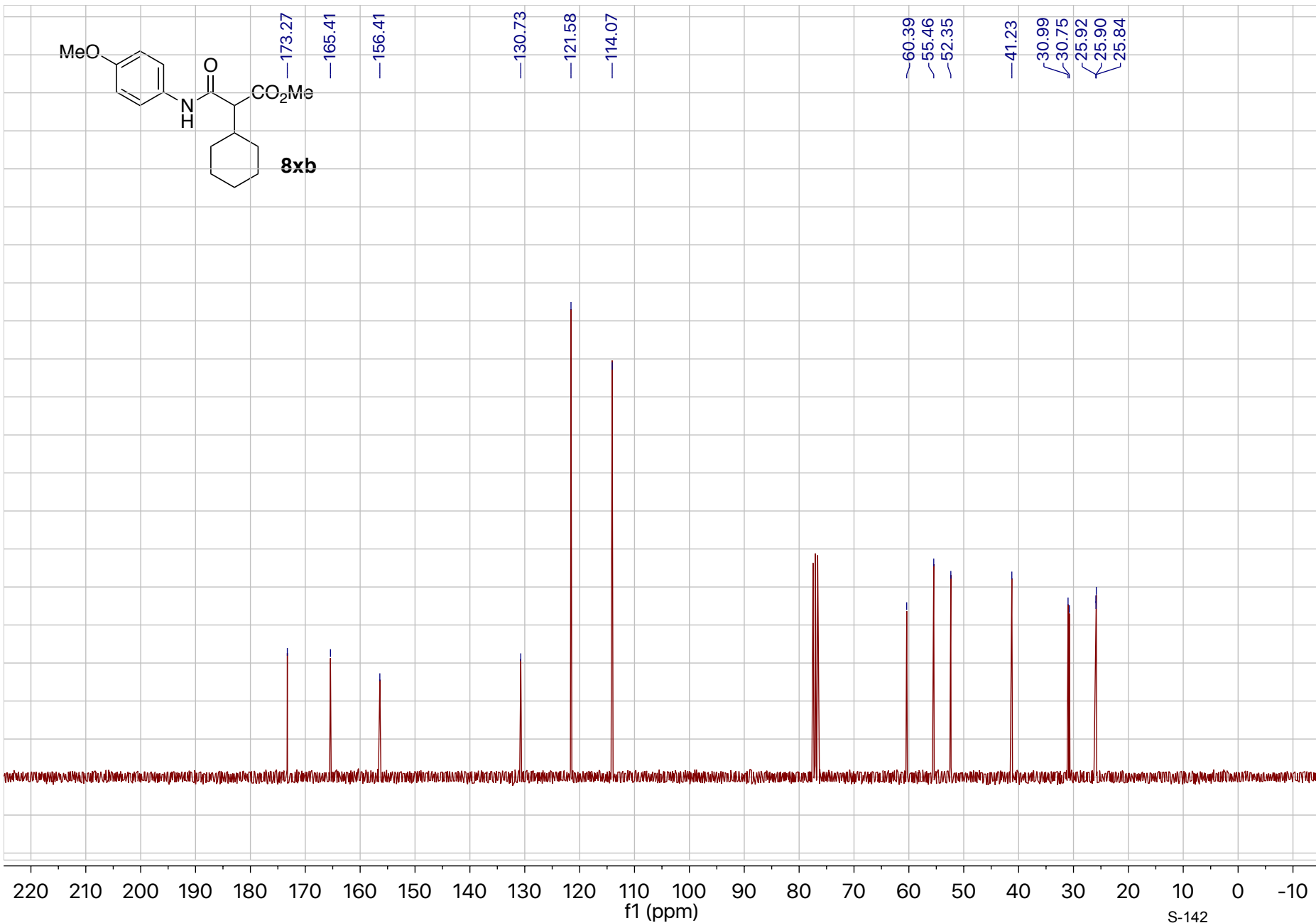
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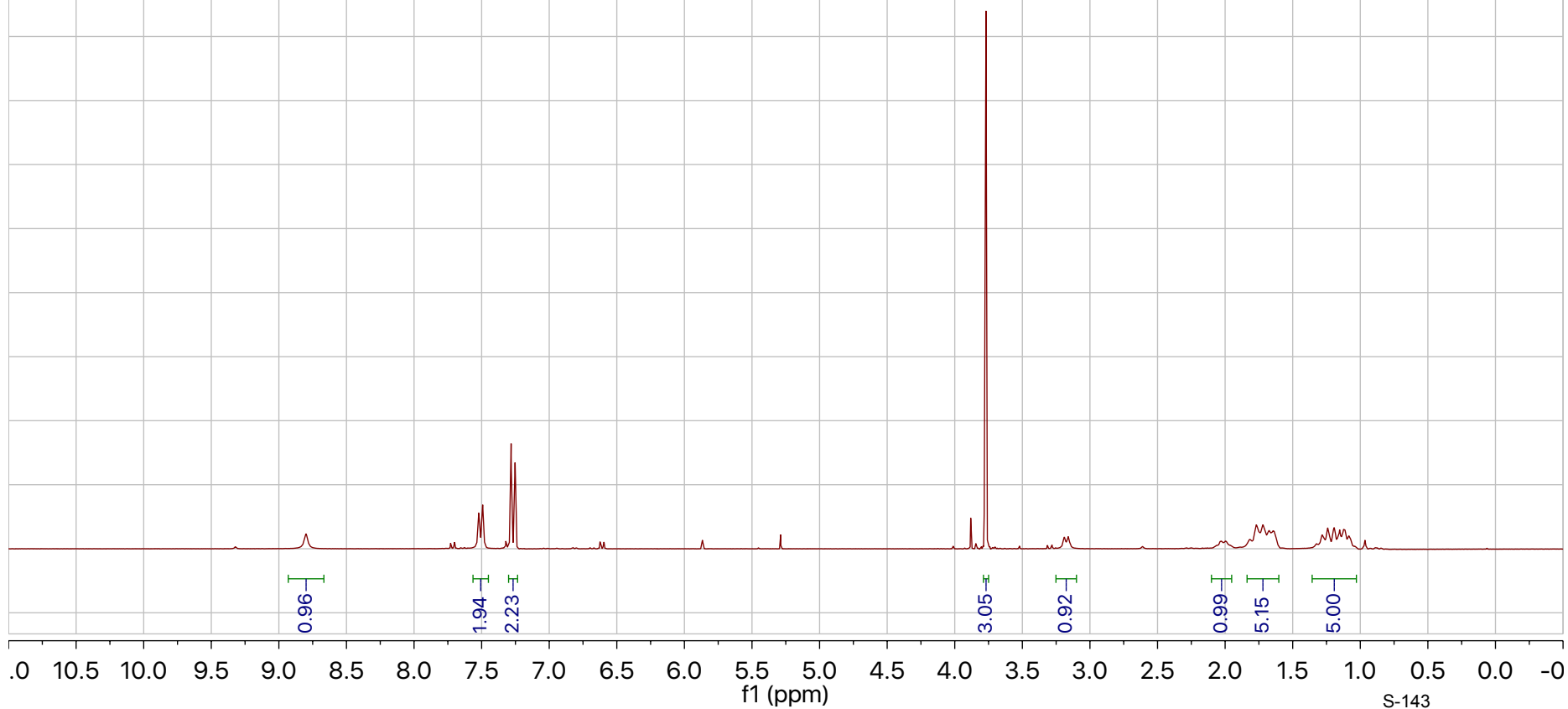
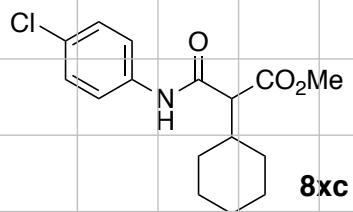
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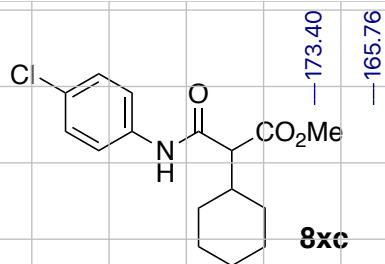
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25.90

25.84







173.40

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136.12

129.32

128.94

121.10

60.37

52.47

41.47

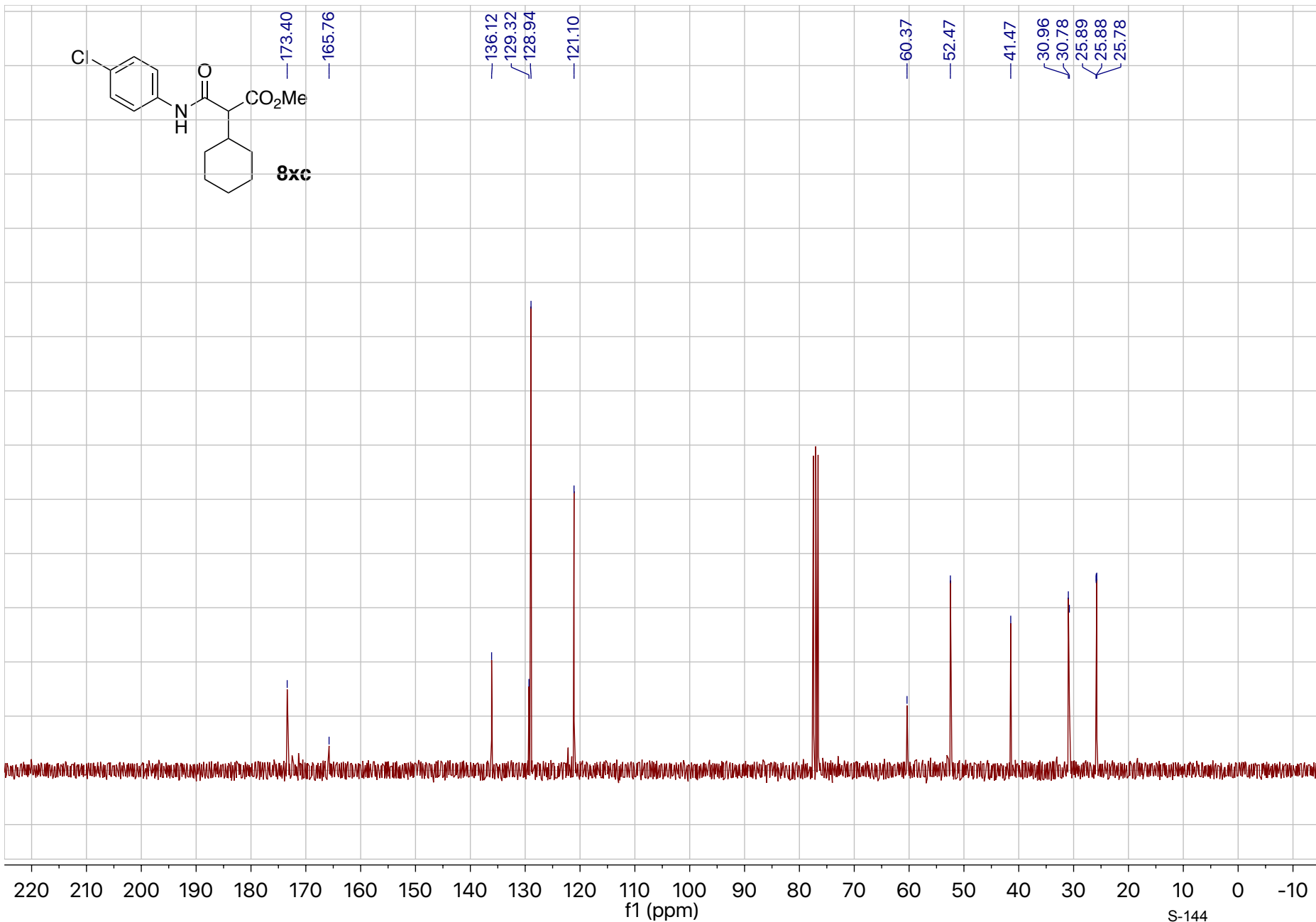
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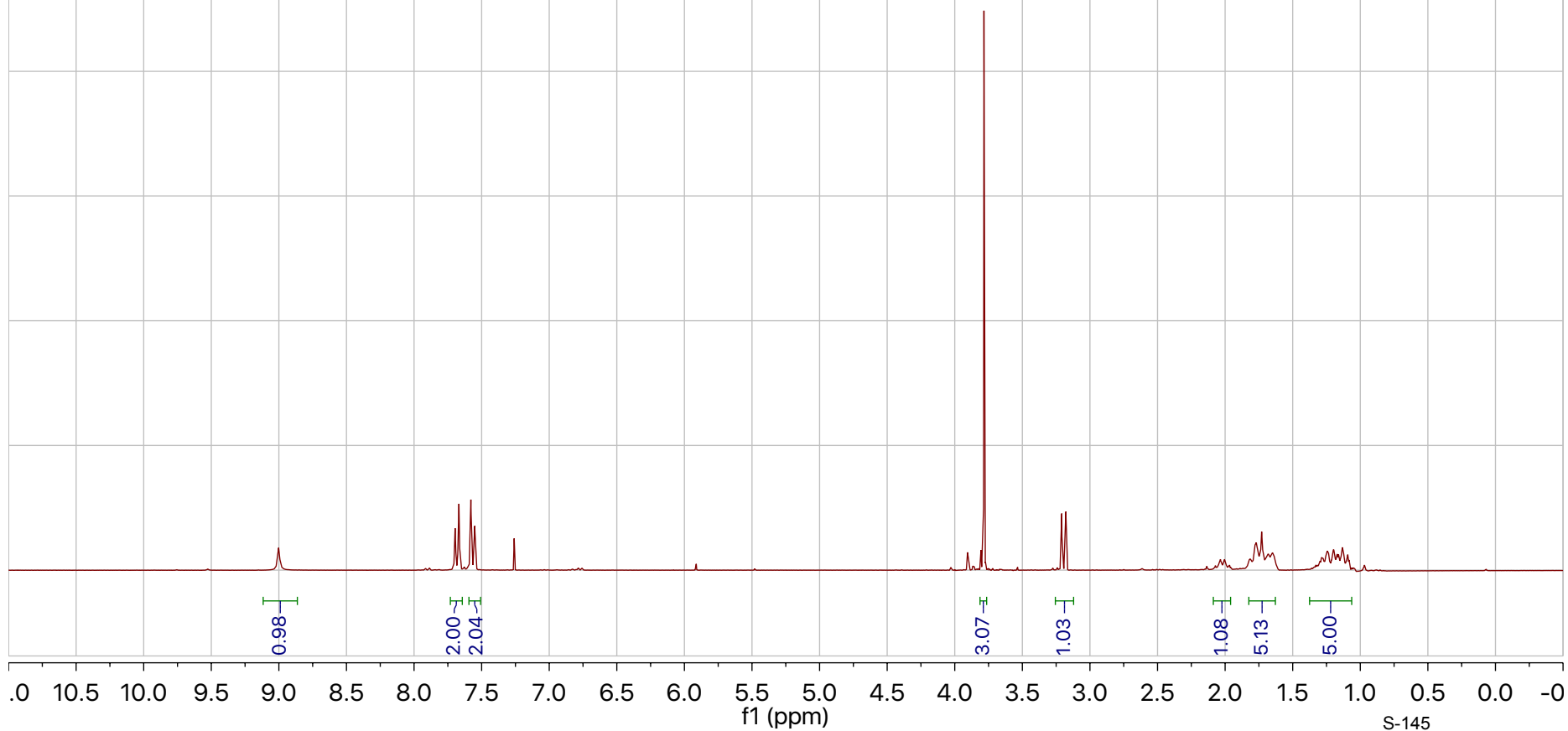
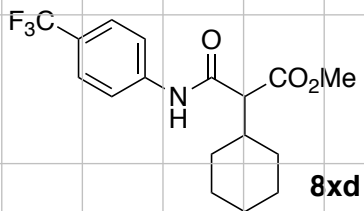
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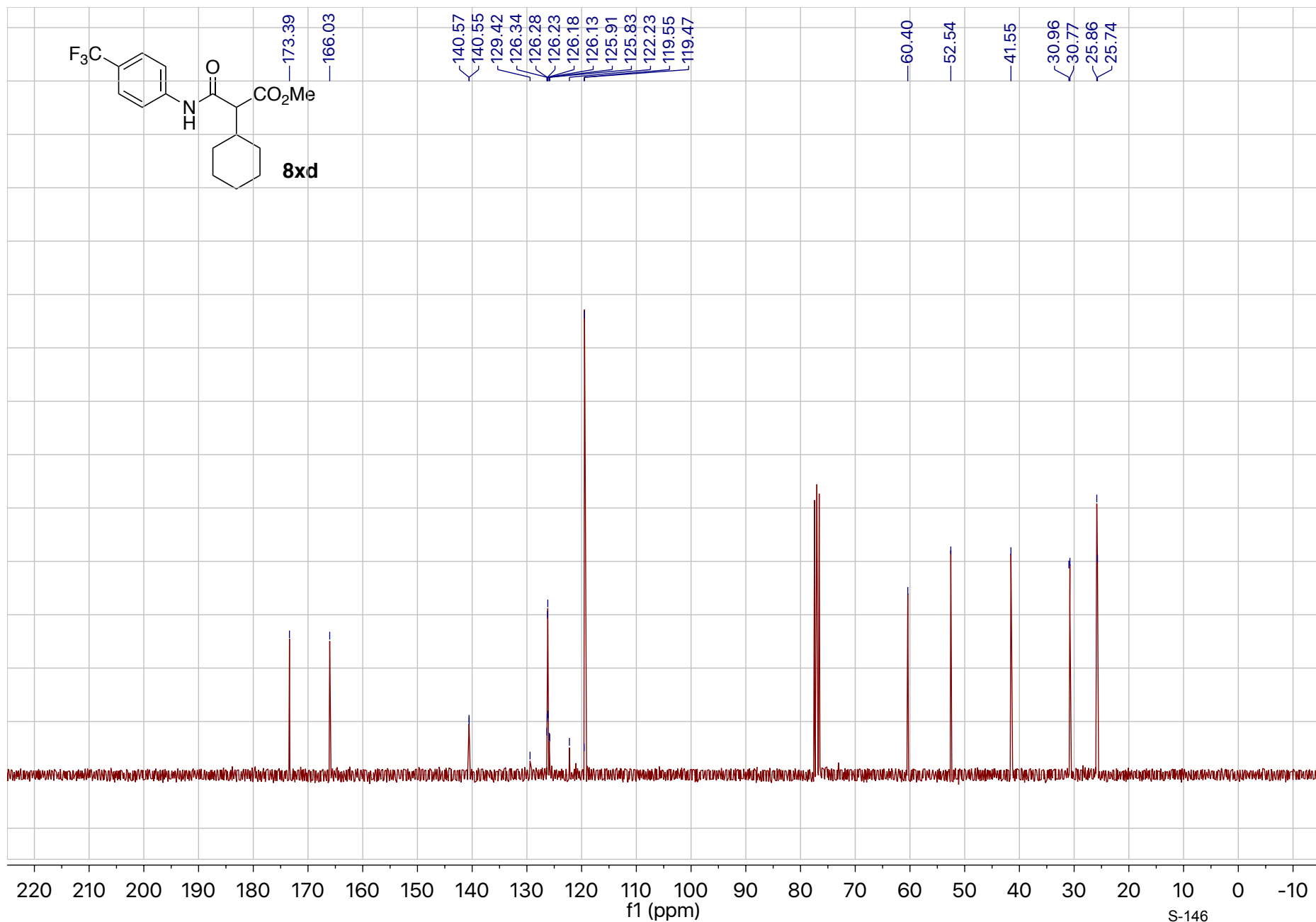
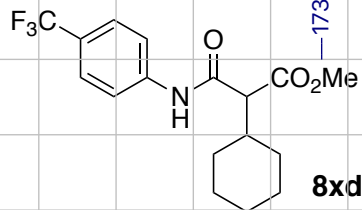
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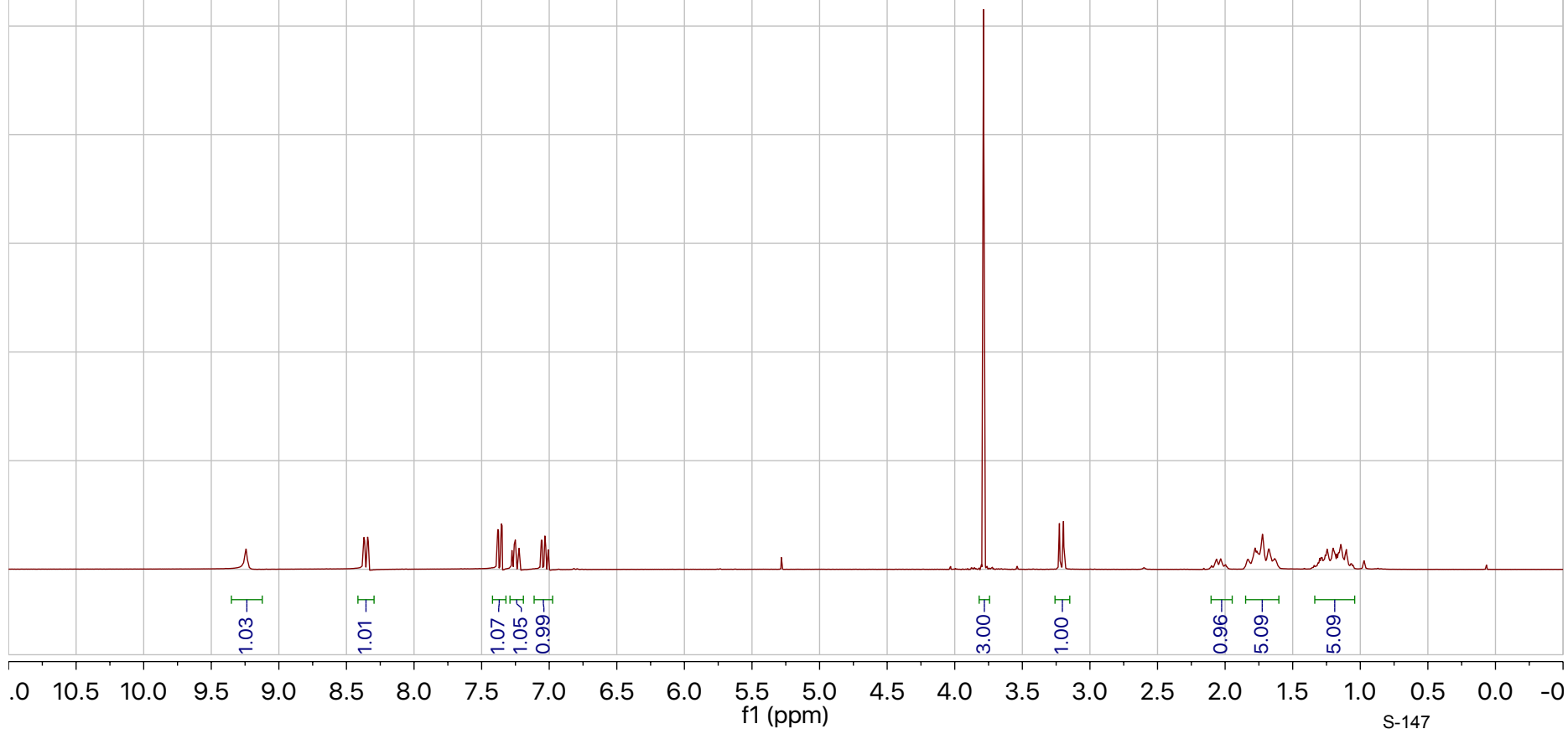
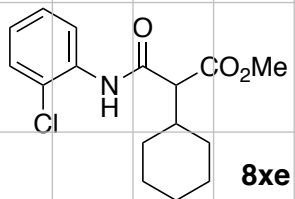
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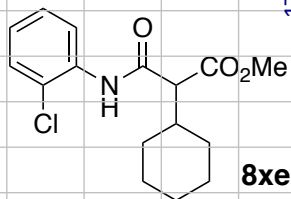
25.78











—172.83

—165.83

134.51

129.09

127.56

124.76

123.29

121.60

—60.86

—52.51

—41.50

31.00

30.75

25.89

25.87

25.80

