Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

of

Sterically Demanding Aryl-Alkyl Suzuki-Miyaura Coupling

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1. General Considerations.

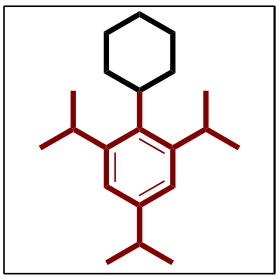
All reactions were carried out under a nitrogen atmosphere unless otherwise specified. Unless otherwise noted, commercialized reagents were used without further purifications. Toluene and xylenes were purchased from Sigma-Aldrich Chemical Co. All other solvents were purified and dried according to standard methods prior to use.

^{1}H NMR, ^{31}P NMR, and ^{13}C NMR data were recorded on a Bruker-Ultrashield PLUS400 NMR or a 500 MHz Agilent spectrometer with $CDCl_3$ as the solvent. ^{1}H chemical shifts were referenced to $CDCl_3$ at 7.26 ppm. ^{13}C chemical shifts were referenced to $CDCl_3$ at 77 ppm and obtained with ^{1}H decoupling. ^{31}P chemical shifts were referenced to 85% H_3PO_4 in D_2O at 0.0 ppm as external standard and obtained with ^{1}H decoupling. Multiplicities are abbreviated as follows: singlet (s), doublet (d), triplet (t), quartet (q), doublet-doublet (dd), quintet (quint), septet (sept), multiplet (m), and broad (br). MS was measured on Agilent 7890A/5975C Series GC/MSD mass spectrometer. HPLC yield were determined on Agilent 1200 Infinity Series.

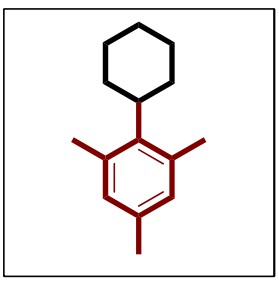
2. General procedures for aryl-alkyl Suzuki-Miyaura couplings.

To a mixture of aryl halide (1 mmol), arylboronic acid (1.5 mmol), potassium phosphate (3 mmol), $Pd(OAc)_2$ (1 mol % Pd), phosphorus ligand (**BI-DIME** or **AntPhos**, 2 mol %, Pd:**L** = 1:2) was charged degassed toluene or xylenes (2 mL). The mixture was pumped and refilled with nitrogen three times. The resulting mixture was stirred at 110℃ under nitrogen for 24 h, and then cooled to room temperature, partioned with water (10 mL) and dichloromethane (10 mL). The organic layer was separated, dried over sodium sulfate, concentrated, and purified by silica gel column chromatography (hexanes/EtOAc as eluent) to provide the coupling product.

2. Analytical data of Suzuki-Miyaura coupling products.

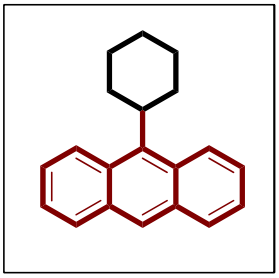


2-Cyclohexyl-1,3,5-triisopropylbenzene： ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.00 (s, 1H), 6.96 (s, 1H), 3.58 (septet, J = 6.75 Hz, 1H), 3.24 (septet, J = 6.80 HZ, 1H), 3.08~3.13 (m, 1H), 2.85 (septet, J = 6.85 HZ, 1H), 1.86~1.94 (m, 4H), 1.72~1.78 (m, 3H), 1.29~1.44 (m, 3H), 1.24~1.26 (m, 18H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.0, 145.5, 145.5, 138.1, 122.8, 120.9, 39.2, 33.8, 32.0, 30.3, 29.5, 27.9, 26.2, 25.0, 24.2, 23.9; EI-MS: *m/z* 286.3 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{21}H_{34}$ (M^+): 286.2661, found: 286.2662.

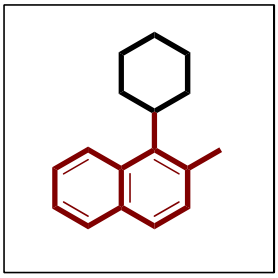


2-Cyclohexyl-1,3,5-trimethylbenzene： ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.85 (s, 2H), 2.97~3.03 (m, 1H), 2.37~2.46 (m, 6H), 2.27 (s, 3H), 1.88~1.99 (m, 4H), 1.80 (d, J = 12.50 Hz, 1H), 1.72 (s, 1H), 1.70 (s, 1H), 1.27~1.45 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.2, 136.1, 134.8, 131.1, 129.2, 41.3, 30.5, 27.8, 26.4,

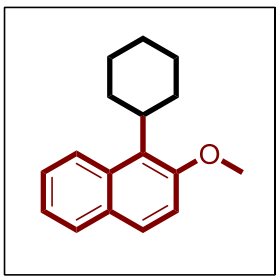
22.1, 21.6, 20.6; EI-MS: *m/z* 202.2 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{15}H_{22}$ (M^+): 202.1722, found: 202.1720.



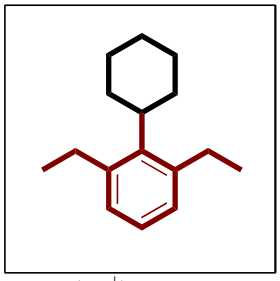
9-Cyclohexylanthracene: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.65 (s, 1H), 8.40 (s, 1H), 8.29 (s, 1H), 7.89 (d, J = 8.08 Hz, 2H), 7.40~7.45 (m, 4H), 4.09~4.15 (m, 1H), 2.52 (m, 2H), 2.01 (d, J = 11.8 Hz, 2H), 1.92 (m, 3H), 1.57~1.65 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 139.4, 131.7, 129.7, 129.6, 128.2, 126.5, 126.3, 125.4, 124.5, 123.9, 40.5, 32.0, 28.0, 26.5; EI-MS: *m/z* 260.1 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{20}H_{20}$ (M^+): 260.1565, found: 260.1563.



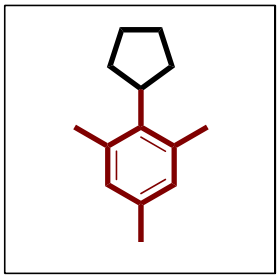
Cyclohexyl-2-methylnaphthalene: ^{1}H NMR (400 MHz, $CDCl_3$, two rotamers) δ 8.44 (d, J = 7.80 Hz, 1H, major), 8.20 (br s, 1H, minor), 7.79 (d, J = 7.96 Hz, 1H), 7.60 (d, J = 8.28 Hz, 1H), 7.37~7.42 (m, 2H), 7.29 (d, J = 7.88 Hz, 1H), 3.69 (br s, 1H, minor), 3.35 (t, J = 13.20 Hz, 1H, major), 2.66 (br s, 3H, minor), 2.53 (s, 3H, major), 2.32~2.41 (m, 2H, major), 2.03~2.13 (m, 2H, minor), 1.95 (s, 2H), 1.83 (t, J = 13.6 Hz, 3H), 1.49 (br s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.1, 133.7, 132.7, 132.1, 129.6, 129.0, 126.3, 126.1, 124.4, 124.0, 41.7, 31.1, 27.8, 26.4, 21.8; EI-MS: *m/z* 224.2 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{17}H_{20}$ (M^+): 224.1565, found: 224.1560.



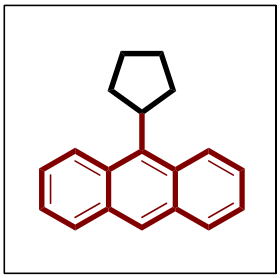
1-Cyclohexyl-2-methoxynaphthalene: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.80 (d, J = 8.05 Hz, 1H), 7.73 (d, J = 8.95 Hz, 1H), 7.48 (m, 1H), 7.34 (t, J = 7.2 Hz, 1H), 7.29 (d, J = 9.00 Hz, 1H), 3.95 (s, 3H), 3.45 (s, 1H), 2.28 (d, J = 11.60 Hz, 2H), 1.91 (d, J = 11.35 Hz, 2H), 1.83 (d, J = 10.50 Hz, 1H), 1.73 (d, J = 10.80 Hz, 2H), 1.40~1.51 (m, 3H); ^{13}C NMR (500 MHz, CDCl3) δ 132.84, 128.73, 127.70, 126.10, 123.05, 122.86, 114.98, 109.97, 56.48, 38.71, 30.48, 27.71, 26.43; EI-MS: *m/z* 240.2 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{17}H_{20}O$ (M^+): 240.1514, found: 240.1512.



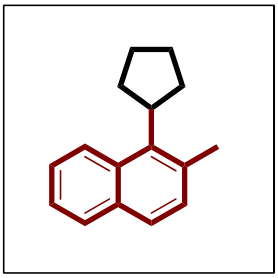
2-Cyclohexyl-1,3-diethylbenzene: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.05~7.10 (m, 2H), 7.00 (d, J = 6.9 Hz, 1H), 2.99~3.04 (m, 1H), 2.85 (dd, J = 14.9, 7.5 Hz, 2H), 2.69 (dd, J = 15.0, 7.5 Hz, 2H), 1.87~1.94 (m, 4H), 1.72~1.80 (m, 3H), 1.30~1.45 (m, 3H), 1.26 (t, J = 7.4 Hz, 3H), 1.20 (t, J = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.4, 142.3, 142.1, 128.8, 127.0, 125.9, 40.7, 31.9, 28.7, 27.8, 26.6, 26.3, 17.3, 16.3; EI-MS: *m/z* 216.2 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{16}H_{24}$ (M^+): 216.1878, found: 216.1874.



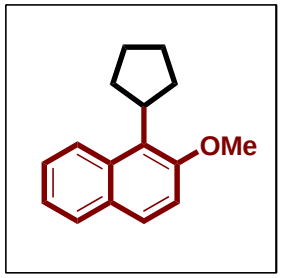
2-Cyclopentyl-1,3,5-trimethylbenzene： ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.89 (s, 2H), 3.53 (quintet, J = 8.80 Hz, 1H), 2.40 (s, 1H), 2.30 (s, 1H), 1.91~1.95 (m, 6H), 1.76 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.5, 136.4, 134.8, 130.0, 40.3, 31.1, 27.1, 21.3, 20.6; EI-MS: *m/z* 188.2 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{14}H_{20}$ (M^+): 188.1565, found: 188.1568.



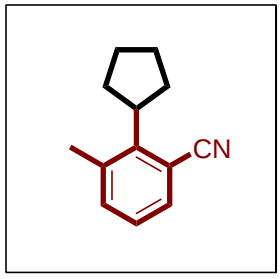
9-Cyclopentylanthracene: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, J = 2.2 Hz, 1H), 8.34 (s, 1H), 8.31 (s, 1H), 7.97~8.00 (m, 2H), 7.40~7.46 (m, 4H), 4.61 (quintet, J = 9.6 Hz, 1H), 2.35~2.44 (m, 2H), 2.17~2.27 (m, 4H), 1.93~2.02 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1, 132.0, 129.7, 129.7, 128.2, 126.3, 126.3, 125.4, 125.0, 124.8, 124.5, 39.6, 33.7, 27.8; EI-MS: *m/z* 246.1 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{19}H_{18}$ (M^+): 246.1409, found: 246.1410.



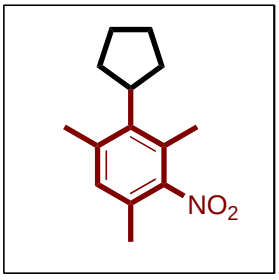
1-Cyclopentyl-2-methylnaphthalene： ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 8.4 Hz, 1H), 7.79 (dd, J= 7.7, 1.6 Hz, 1H), 7.58 (d, J = 8.3 Hz, 1H), 7.34~7.42 (m, 2H), 7.26 (d, J = 8.3 Hz, 1H), 3.88 (quintet, J = 9.4 Hz, 1H), 2.52 (s, 3H), 2.13~2.20 (m, 2H), 2.04~2.10 (m, 4H), 1.81~1.88 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.4, 133.6, 133.5, 131.6, 129.7, 129.2, 126.3, 125.0, 124.8, 124.1, 40.6, 32.2, 27.6, 21.7; EI-MS: *m/z* 210.1 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{16}H_{18}$ (M^+): 210.1409, found: 210.1405.



1-Cyclopentyl-2-methoxynaphthalene: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, J = 10.0 Hz, 1H), 7.80 (d, J = 8.1 Hz, 1H), 7.73 (d, J = 9.0 Hz, 1H), 7.46 (t, J = 7.9 Hz, 1H), 7.34 (t, J = 7.9 Hz, 1H), 7.27~7.30 (m, 1H), 4.05 (quintet, J = 9.3 Hz, 1H), 3.95 (s, 3H), 2.09~2.15 (m, 2H), 1.95~2.03 (m, 4H), 1.79~1.82 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.1, 133.0, 129.7, 128.8, 127.5, 127.3, 125.7, 123.6, 123.0, 114.4, 56.5, 36.7, 31.9, 27.5; EI-MS: *m/z* 226.1 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{16}H_{18}O$ (M^+): 226.1358, found: 226.1359.

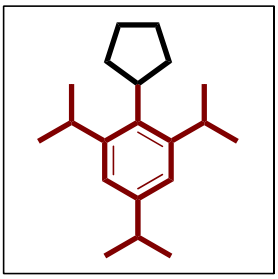


2-Cyclopentyl-3-methylbenzonitrile： ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51， (d, J = 7.6 Hz, 1H), 7.34 (d, J = 7.4 Hz, 1H), 7.15 (t, J = 7.7 Hz, 1H), 3.50 (quintet, J = 8.9 Hz, 1H), 2.41 (s, 3H), 2.02~2.05 (m, 6H), 1.71~1.78 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.9, 137.5, 135.0, 132.7, 125.9, 119.3, 111.2, 41.6, 32.5, 27.0, 20.7; EI-MS: *m/z* 185.1 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{13}H_{15}N$ (M^+): 185.1204, found: 185.1201.

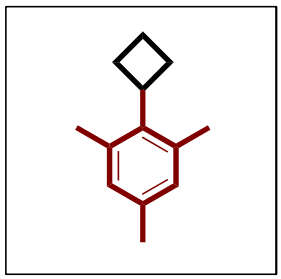


2-Cyclopentyl-1,3,5-trimethyl-4-nitrobenzene： ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.91 (s, 1H), 3.49 (quintet, J = 9.40 Hz, 1H), 2.37 (s, 1H), 2.25 (s, 1H), 2.21 (s, 1H), 1.90~1.94 (m, 4H), 1.79~1.86 (m, 2H), 1.72~1.77 (m, 2H); ^{13}C NMR (125

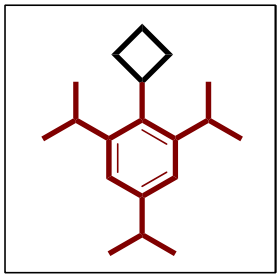
MHz, $CDCl_3$) δ 141.0, 138.5, 131.1, 126.9, 125.5, 40.4, 31.0, 27.0, 21.4, 16.7, 15.1; EI-MS: *m/z* 233.1 $[M]^+$; HRMS (EI) *m/z* calcd for $C_4H_{19}NO_2$ (M^+): 233.1416, found: 233.1415.



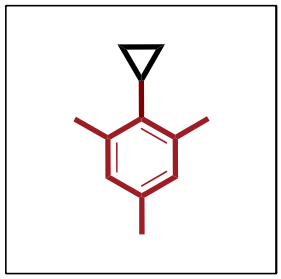
2-Cyclopentyl-1,3,5-triisopropylbenzene： ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.01 (s, 2H), 3.60 (quintet, J = 9.6 Hz, 1H), 3.25 (septet, J = 6.8 Hz, 2H), 2.88 (septet, J = 6.8 Hz, 1H), 1.91~2.03 (m, 4H), 1.73~1.84 (m, 4H), 1.28 (d, J = 6.8 Hz, 12H), 1.28 (d, J = 6.8 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.7, 147.1, 145.7, 136.7, 122.0, 121.8, 38.7, 33.9, 33.5, 29.7, 27.1, 24.6, 24.0; EI-MS: *m/z* 272.3 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{20}H_{32}$ (M^+): 272.2504, found: 272.2509.



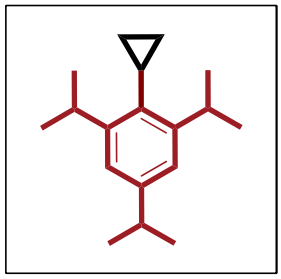
2-Cyclobutyl-1,3,5-trimethylbenzene： ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.79 (s, 2H), 3.86 (quintet, J = 9.6 Hz, 1H), 2.39~2.45 (m, 4H), 2.33 (s, 6H), 2.25 (s, 3H), 1.95 (sextet, J = 10.3 Hz, 1H), 1.82~1.87 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.6, 136.4, 134.7, 129.8, 39.3, 30.7, 21.6, 20.5, 19.0; EI-MS: *m/z* 174.1 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{13}H_{18}$ (M^+): 174.1409, found: 174.1404.



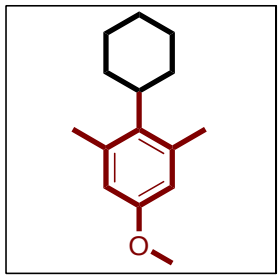
2-Cyclobutyl-1,3,5-triisopropylbenzene: ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.99 (s, 2H), 4.20 (quintet, J = 9.7 Hz, 1H), 3.53 (septet, J = 6.8 Hz, 2H), 2.87 (septet, J = 7.0 Hz, 1H), 2.49 (quintet, J = 9.9 Hz, 2H), 2.35~2.41 (m, 2H), 2.08~2.16 (m, 1H), 1.99~2.05 (m, 1H), 1.28 (d, J = 6.3 Hz, 12H), 1.26 (d, J = 6.9 Hz, 6H); ^{13}C NMR (125 MHz, CDCl3) δ 147.6, 145.9, 135.9, 121.7, 34.9, 34.0, 30.7, 29.4, 24.7, 24.0, 17.7; EI-MS: *m/z* 258.1 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{19}H_{30}$ (M^+): 258.2348, found: 258.2350.



2-Cyclopropyl-1,3,5-trimethylbenzene: ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.88 (s, 2H), 2.45(s, 6H), 2.31 (s, 3H), 1.71 (septet, J = 7.3 Hz, 1H), 1.02~1.05 (m, 2H), 0.55~0.58 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.9, 136.1, 135.6, 128.6, 20.8, 20.5, 11.8, 8.1; EI-MS: *m/z* 160.1 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{12}H_{16}$ (M^+): 160.1252, found: 160.1254.



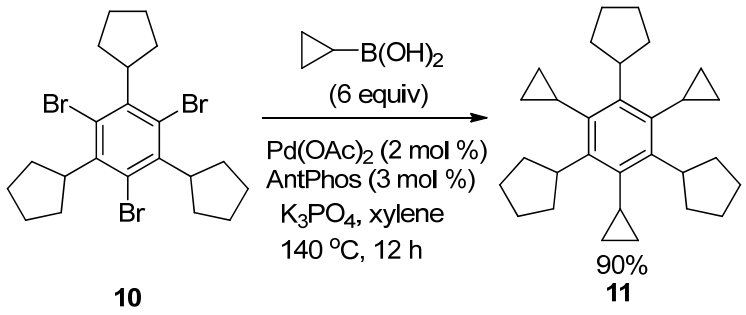
2-Cyclopropyl-1,3,5-triisopropylbenzene： ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.10 (s, 2H), 4.00 (septet, J = 6.9 Hz, 2H), 3.01 (septet, J = 6.9 Hz, 1H), 1.80 (quintet, J = 6.2 Hz, 1H), 1.40 (dd, J = 6.9, 0.9 Hz , 6H), 1.37 (dd, J = 6.9, 0.9 Hz , 12H), 1.16~1.20 (m, 2H), 0.70~0.73 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.5, 146.8, 134.0, 122.0, 34.2, 29.0, 24.6, 24.2, 10.5, 8.6; EI-MS: *m/z* 244.2 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{18}H_{28}$ (M^+): 244.2191, found: 244.2190.



2-Cyclohexyl-5-methoxy-1,3-dimethylbenzene： ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.57 (s, 2H), 3.78 (s, 3H), 2.92~2.98 (m, 1H), 2.46 (s, 3H), 2.37 (s, 3H),

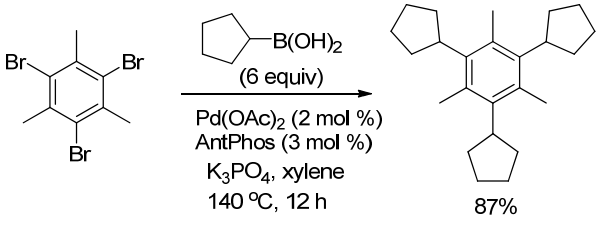
1.87~1.96 (m, 4H), 1.79 (d, J = 12.6 Hz, 1H), 1.69 (d, J = 11.9 Hz, 2H), 1.25~1.43 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.7, 137.6, 135.7, 115.4, 113.9, 55.0, 41.0, 30.8, 27.8, 26.4, 22.3; EI-MS: *m/z* 218.2 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{15}H_{22}$ (M^+): 218.1671, found: 218.1670.

4. Synthesis of hexaalkylbenzenes



10 **11**

To a mixture of 1,3,5-tribromo-2,4,6-tricyclopentylbenzene (**10**, 260 mg, 0.5 mmol, 1 equiv), cyclopropylboronic acid (258 mg, 3 mmol, 6 equiv), potassium phosphate (636 mg, 3 mmol, 6 equiv), $Pd(OAc)_2$ (2.2 mg, 0.01 mmol, 2 mol %), AntPhos (5.6 mg, 0.015 mmol, 3 mol %) was charged degassed *o*-xylene (3 mL). The mixture was pumped and refilled with nitrogen three times. The resulting mixture was stirred at 140℃ under nitrogen for 12 h, and then cooled to room temperature, partioned with water (10 mL) and dichloromethane (10 mL). The organic layer was separated, dried over sodium sulfate, concentrated, and purified by silica gel column chromatography (hexanes as eluent) to provide the coupling product **11** as white solid (90%). 1,3,5-Tricyclopentyl-2,4,6-trimethylbenzene (**11**)：^{1}H NMR (400 MHz, $CDCl_3$) δ 3.93 (quintet, J = 9.3 Hz, 3H), 2.10~2.17 (m, 6H), 1.85~1.97 (m, 9H), 1.65~1.73 (m, 6H), 1.58~1.63 (m, 6H), 0.87~0.92 (m, 6H), 0.39~0.43 (m, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.94, 139.77, 43.84, 32.16, 26.17, 16.10, 11.52; EI-MS: *m/z* 402.0 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{30}H_{42}$ (M^+): 402.3287, found: 402.3290.



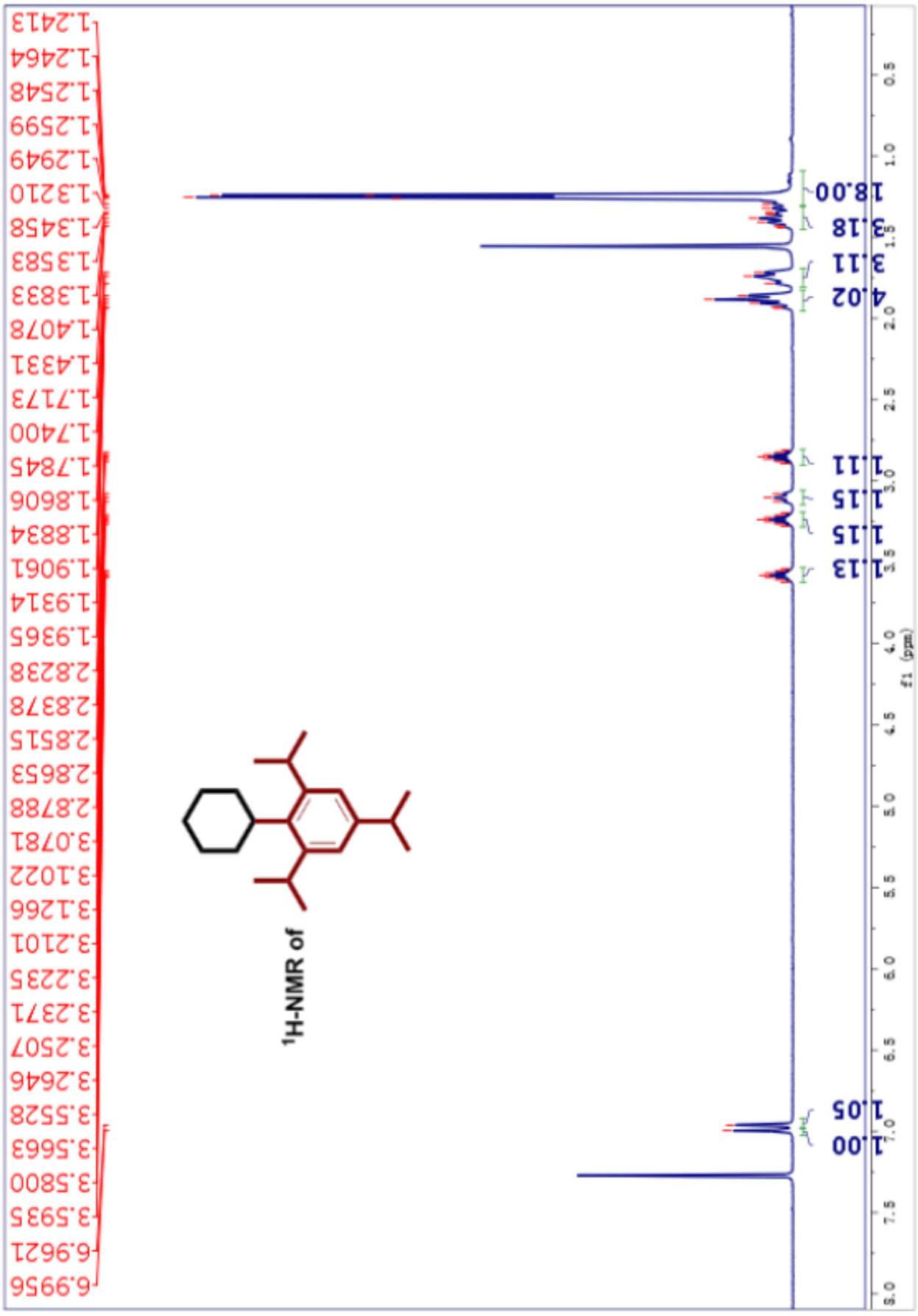
12 **13**

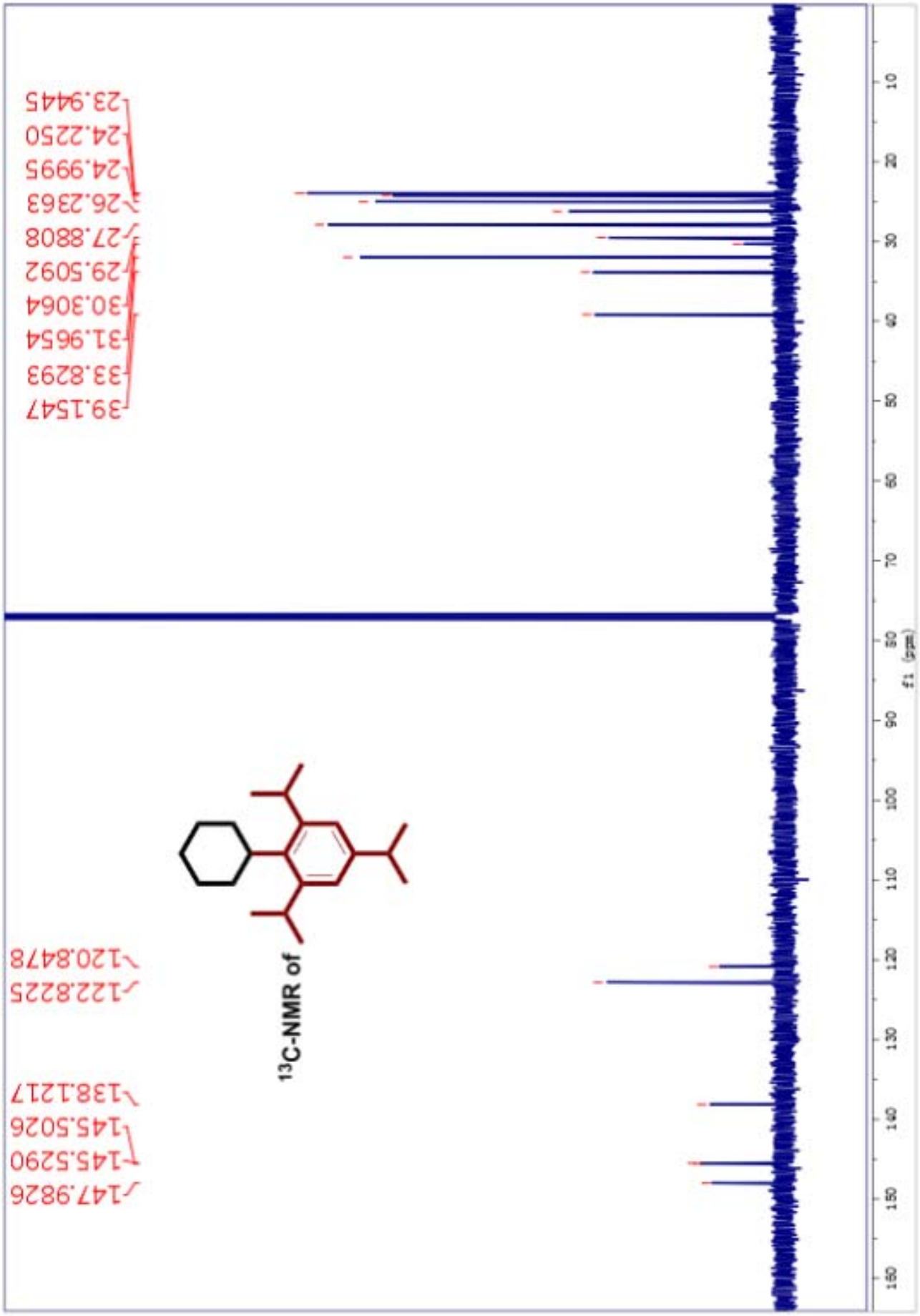
To a mixture of 1,3,5-tribromo-2,4,6-trimethylbenzene (**12**, 179 mg, 0.5 mmol, 1 equiv), cyclopentaneboronic acid (342 mg, 3 mmol, 6 equiv), potassium phosphate (636 mg, 3 mmol, 6 equiv), $Pd(OAc)_2$ (2.2 mg, 0.01 mmol, 2 mol %), AntPhos (5.6 mg, 0.015 mmol, 3 mol %) was charged degassed *o*-xylene (3 mL). The mixture was pumped and refilled with nitrogen three times. The resulting mixture was stirred at 140℃ under nitrogen for 12 h, and then cooled to room temperature, partioned with water (10 mL) and dichloromethane (10 mL). The organic layer was separated, dried over sodium sulfate,

concentrated, and purified by silica gel column chromatography (hexanes as eluent) to provide the coupling product **13** as white solid (87 %). 1,3,5-Tricyclopentyl-2,4,6-trimethylbenzene (**13**)：^{1}H NMR (500 MHz, $CDCl_3$) δ 3.66 (quintet, J = 9.4 Hz, 3H), 2.34 (s, 9H), 1.87~1.95 (m, 18H), 1.74~1.77 (m, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.8，133.3，40.6，31.3，27.3，18.9; EI-MS: *m/z* 324.2 $[M]^+$; HRMS (EI) *m/z* calcd for $C_{24}H_{36}$ (M^+): 324.2817, found: 324.2816.

5. NMR spectra

6.

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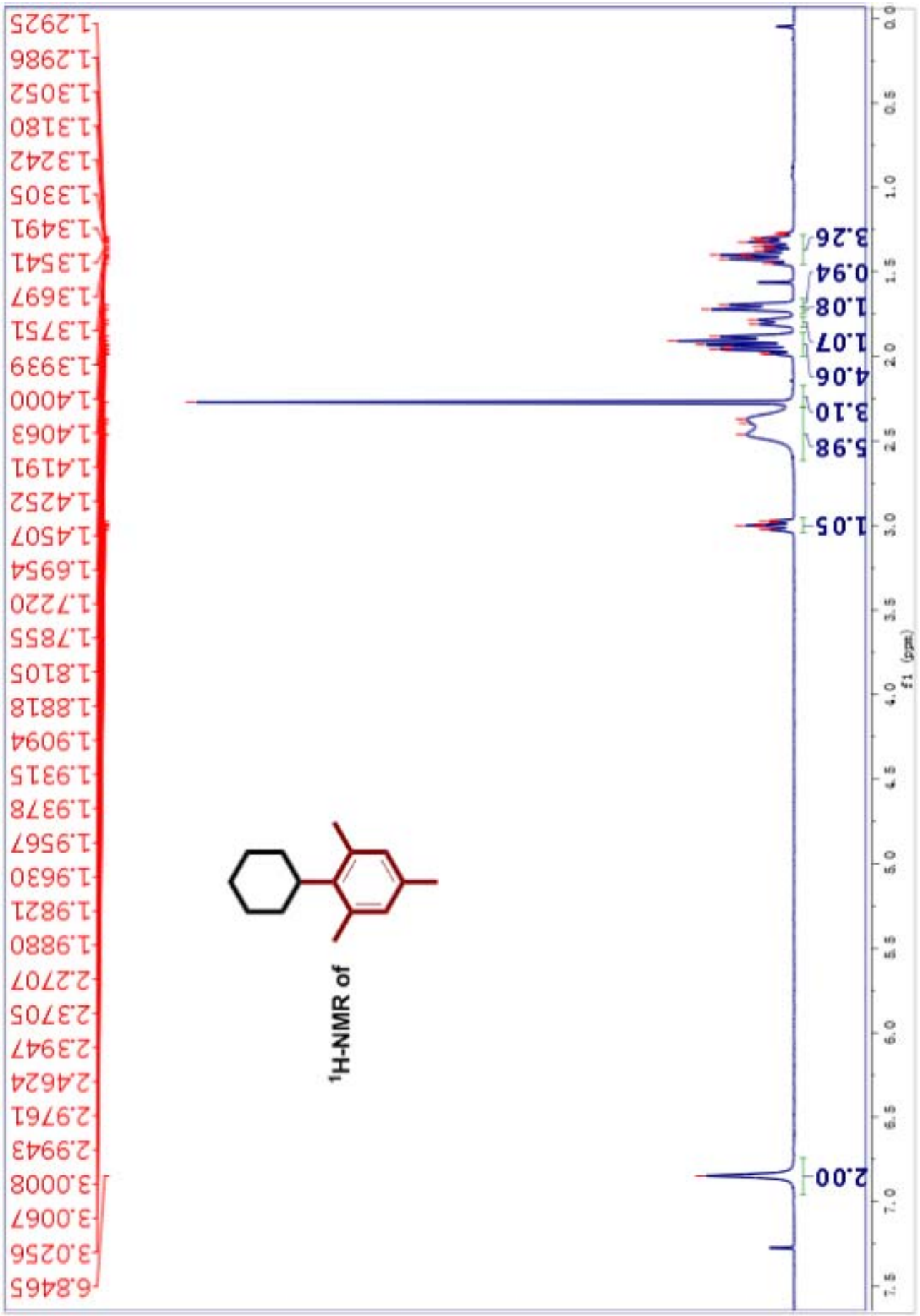
24.9995
26.2363
27.8808
29.5092
30.3064
31.9654
33.8293
39.1547
120.8478
122.8225
138.1217
145.5026
145.5290
147.9826
^{13}C-NMR of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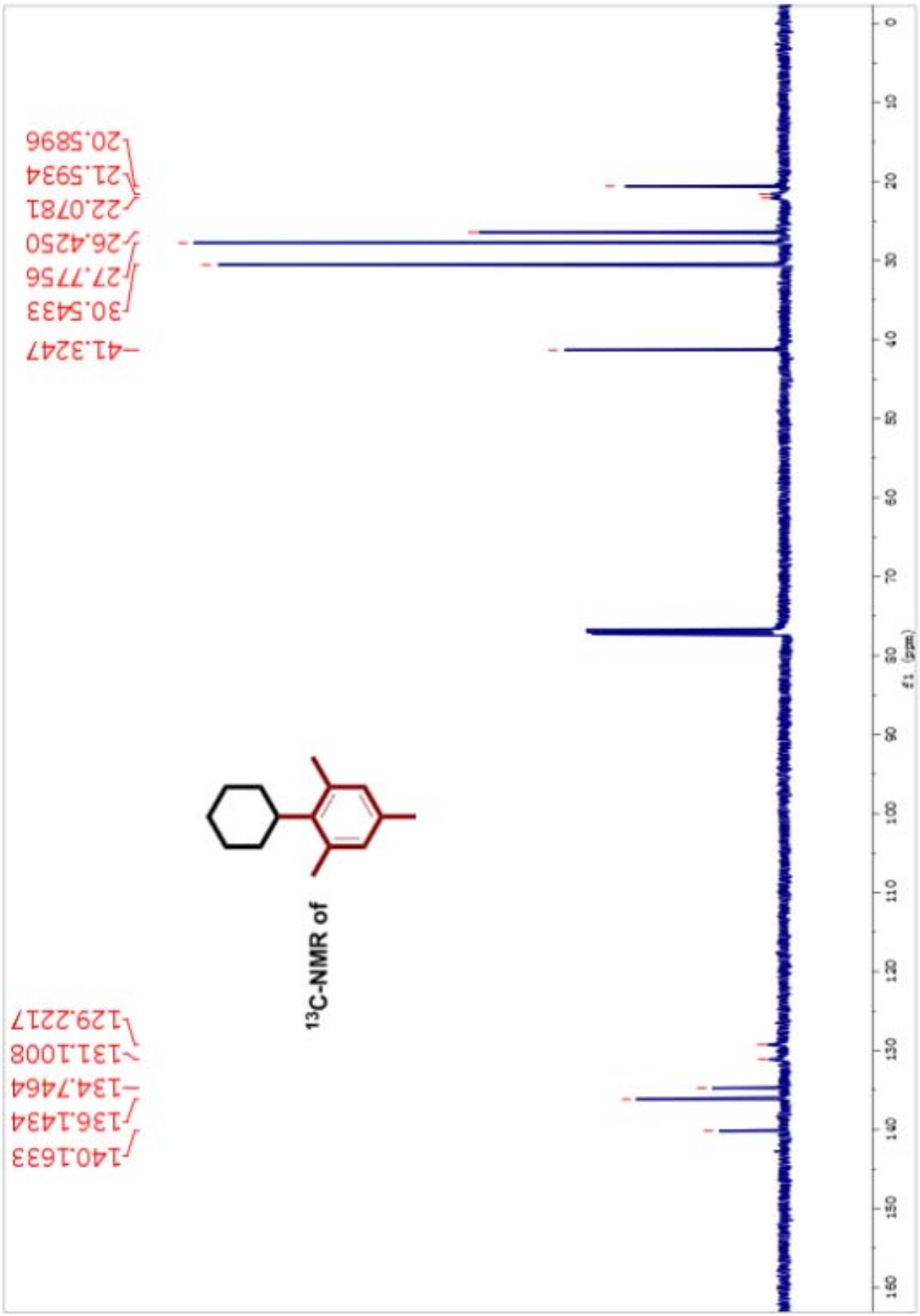
1.3052
1.3180
1.3242
1.3305
1.3491
1.3541
1.3697
1.3751
1.3939
1.4000
1.4063
1.4191
1.4252
1.4507
1.6954
1.7220
1.7855
1.8105
1.8818
1.9094
1.9315
1.9378
1.9567
1.9630
1.9821
1.9880
2.2707
2.3705
2.3947
2.4624
2.9761
2.9943
3.0008
3.0067
3.0256
6.8465
3.26
0.94
1.08
1.07
4.06
3.10
5.98
1.05
2.00
f1 (ppm)
^{1}H-NMR of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134.7464
131.1008
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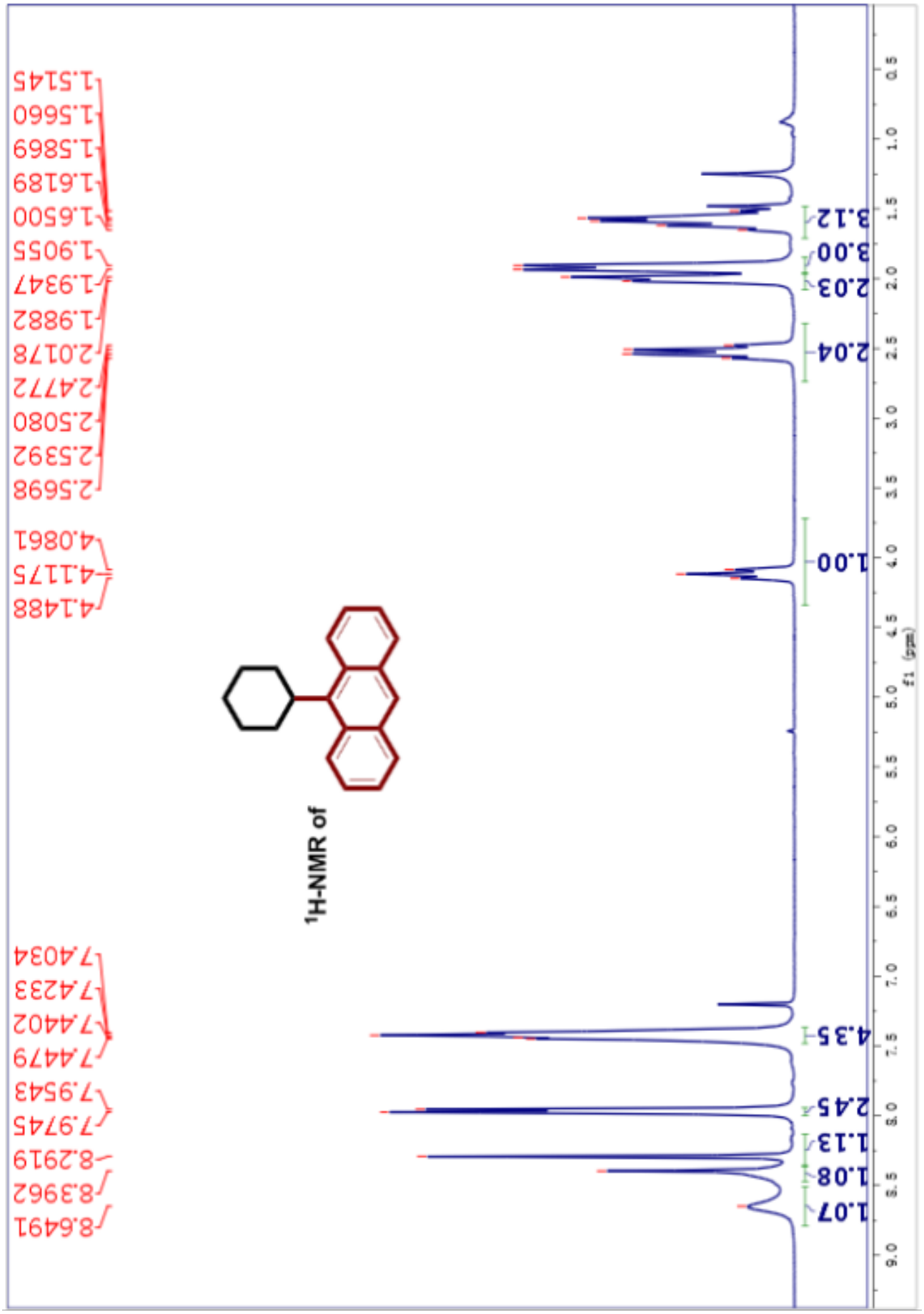
30.5433
27.7756
26.4250
22.0781
21.5934
20.5896
f1 (ppm)
13C-NMR of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1.9347
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2.5080
2.5392
2.5698
4.0861
4.1175
4.1488
7.4034
7.4233
7.4402
7.4479
7.9543
7.9745
8.2919
8.3962
8.6491
3.12
3.00
2.03
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1.00
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2.45
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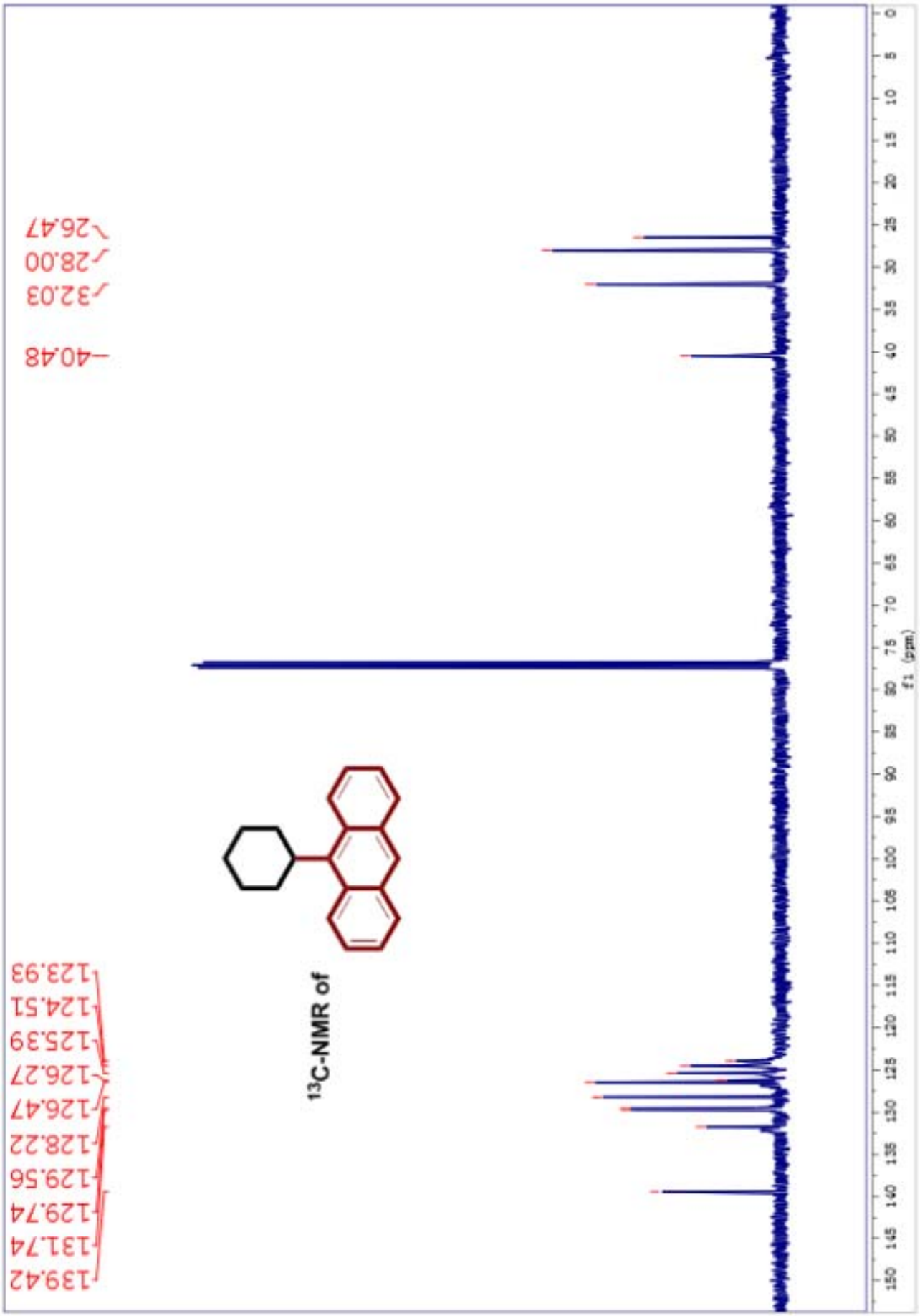
1.08
1.07
f1 (ppm)
^{1}H-NMR of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129.74
129.56
128.22
126.47
126.27
125.39
124.51
123.93
^{13}C-NMR of
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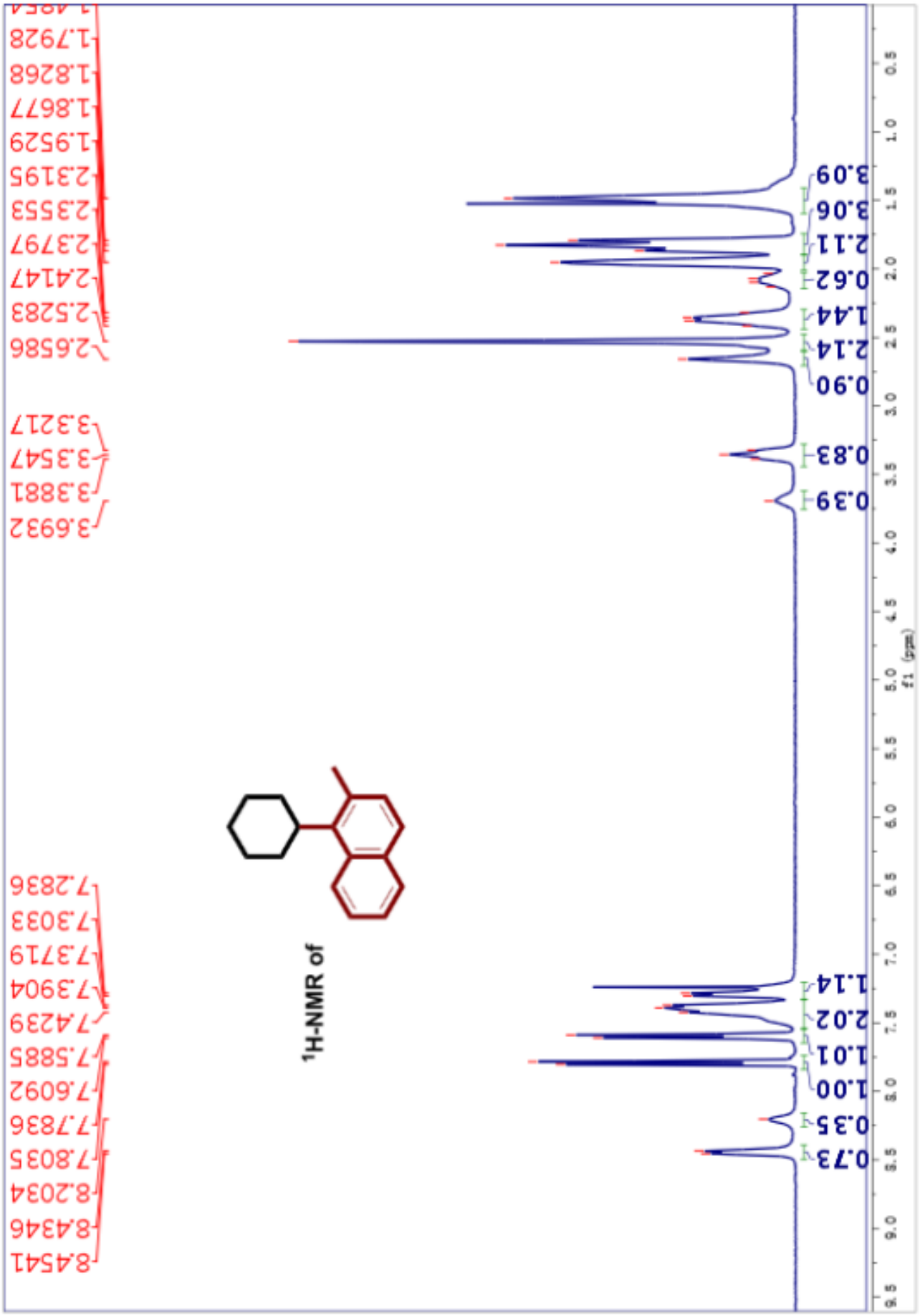
32.03
28.00
26.47
f1 (ppm)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2.4147
2.5283
2.6586
3.3217
3.3547
3.3881
3.6932
7.2836
7.3033
7.3719
7.3904
7.4239
7.5885
7.6092
7.7836
7.8035
8.2034
8.4346
8.4541
0.73
0.35
1.00
1.01
2.02
1.14
0.39
0.83
0.90
2.14
1.44
0.62
2.11
3.06
3.09
f1 (ppm)
1H-NMR of

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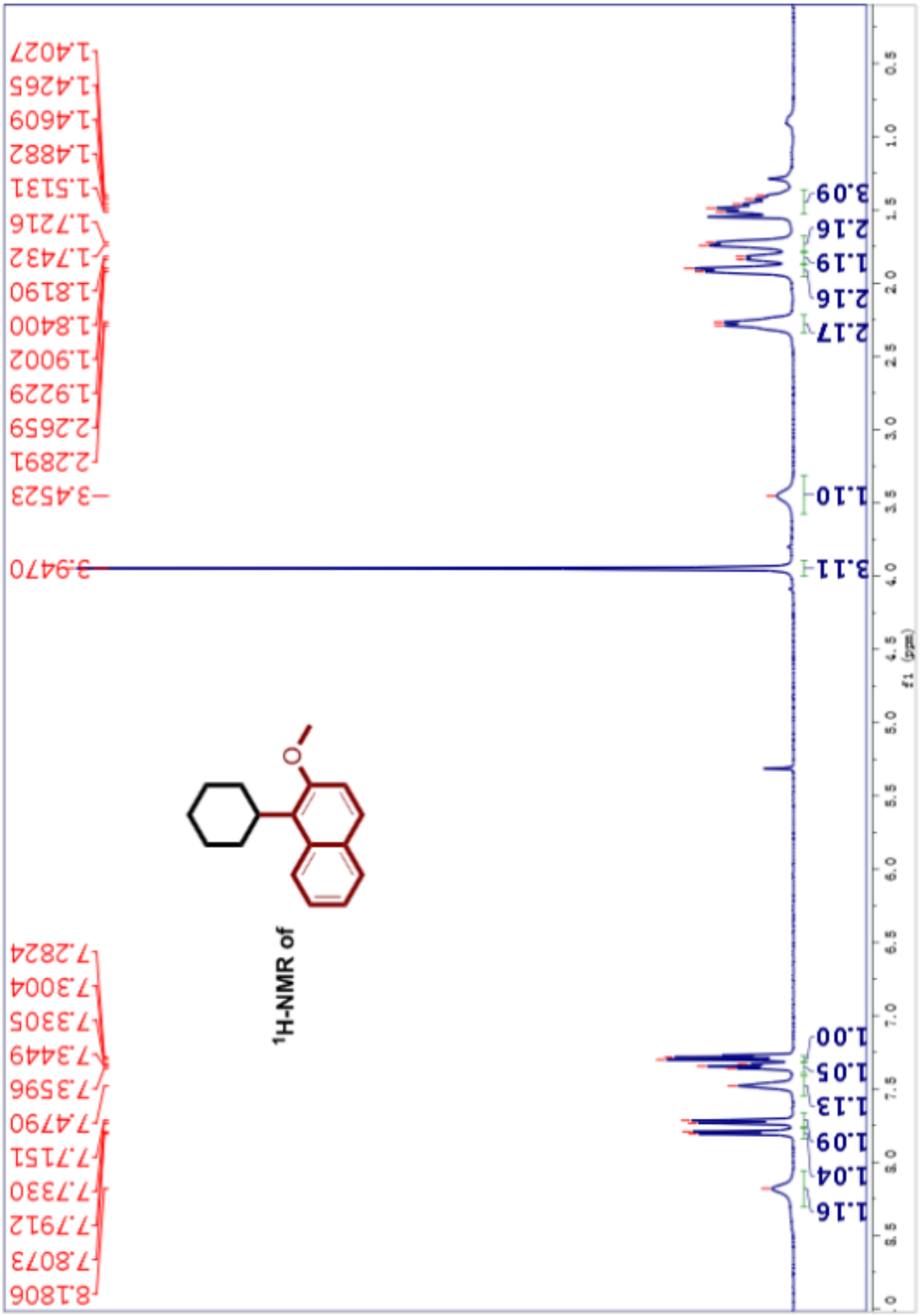
133.7342
132.6710
132.0630
129.6231
128.9895
126.2975
126.1417
124.3718
123.9906
13C-NMR of
41.6464
31.1228
27.8112
26.4014
21.7746
f1 (ppm)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1.8400
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1.9229
2.2659
2.2891
3.4523
3.9470
7.2824
7.3004
7.3305
7.3449
7.3596
7.4790
7.7151
7.7330
7.7912
7.8073
8.1806
3.09
2.16
1.19
2.16
2.17
1.10
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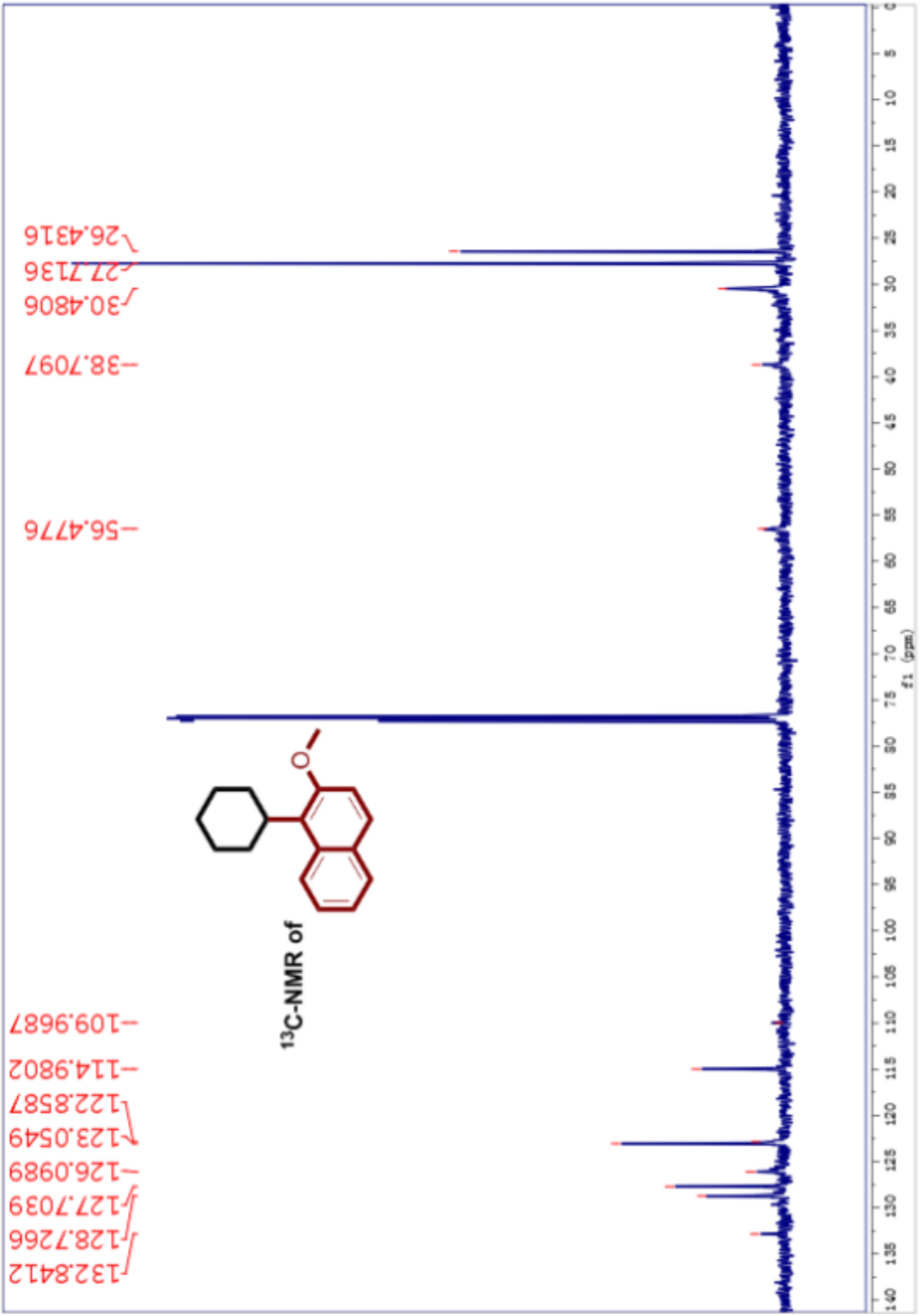
1.00
1.05
1.13
1.09
1.04
1.16
O
1H-NMR of
f1 (ppm)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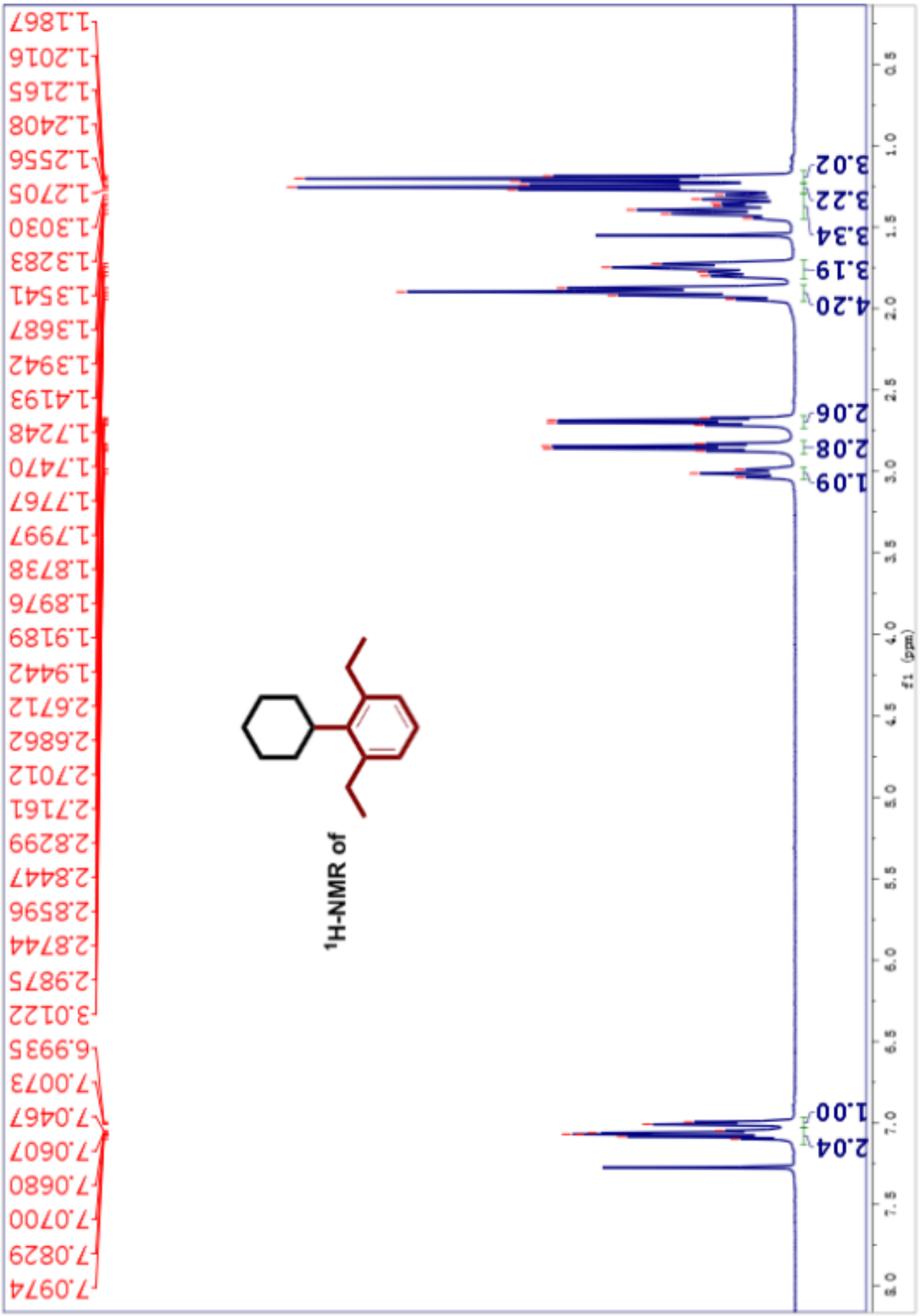
f1 (ppm)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1.7470
1.7767
1.7997
1.8738
1.8976
1.9189
1.9442
2.6712
2.6862
2.7012
2.7161
2.8299
2.8447
2.8596
2.8744
2.9875
3.0122
6.9935
7.0073
7.0467
7.0607
7.0680
7.0700
7.0829
7.0974
3.02
3.22
3.34
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4.20
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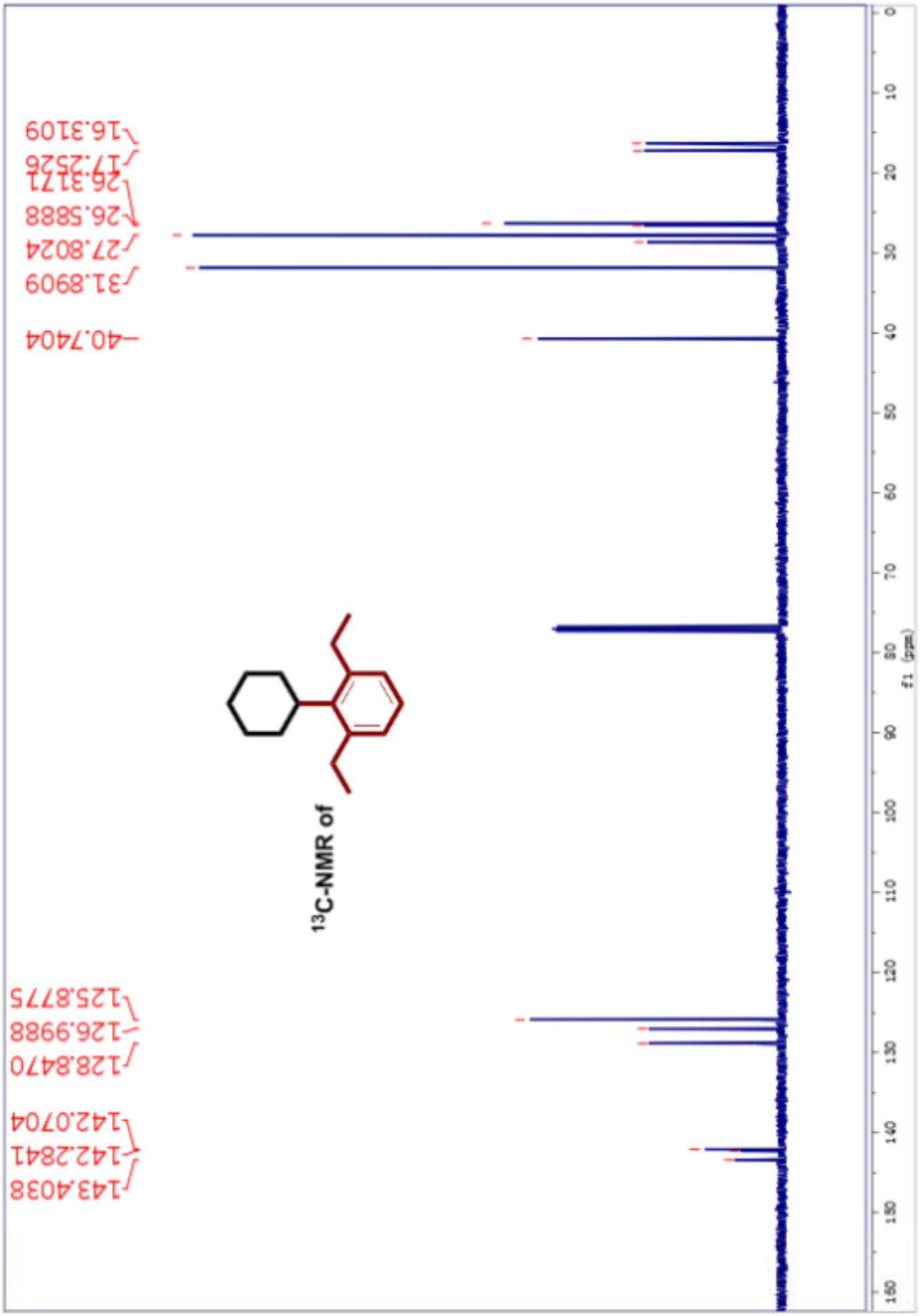
2.08
1.09
1.00
2.04
f1 (ppm)
^{1}H-NMR of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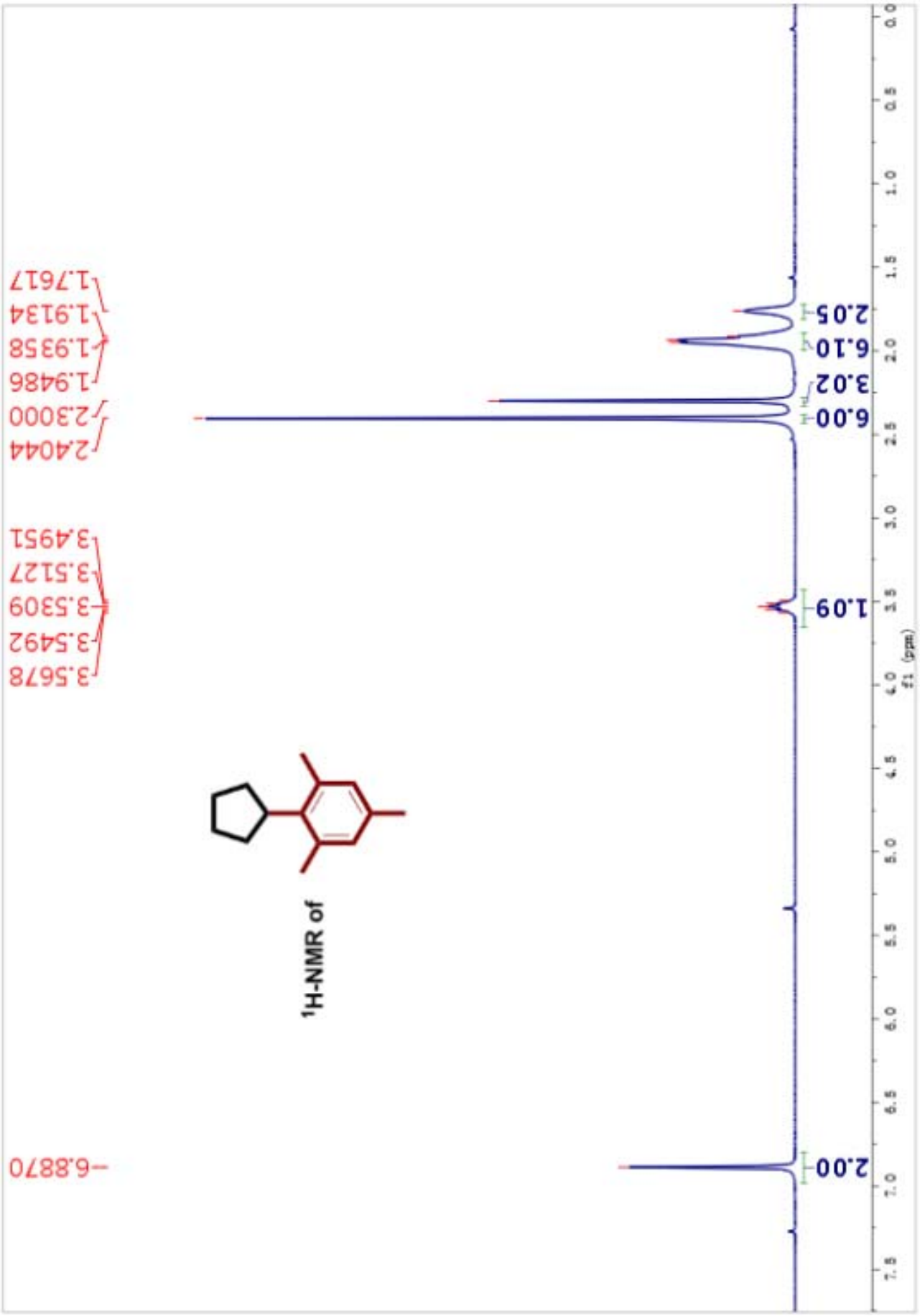
^{13}C-NMR of
f1 (ppm)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3.5492
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6.00
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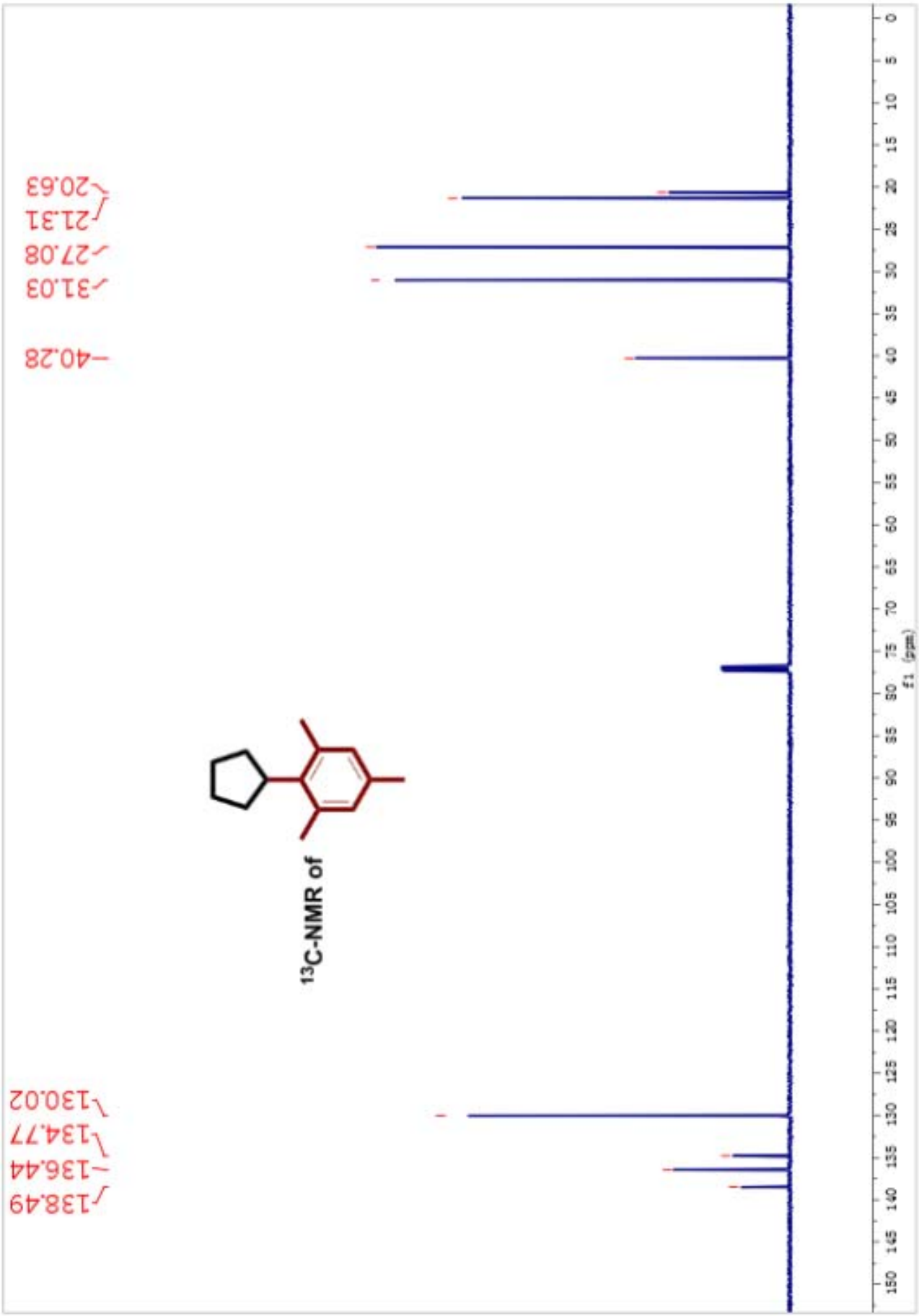
6.10
2.05
f1 (ppm)
^{1}H-NMR of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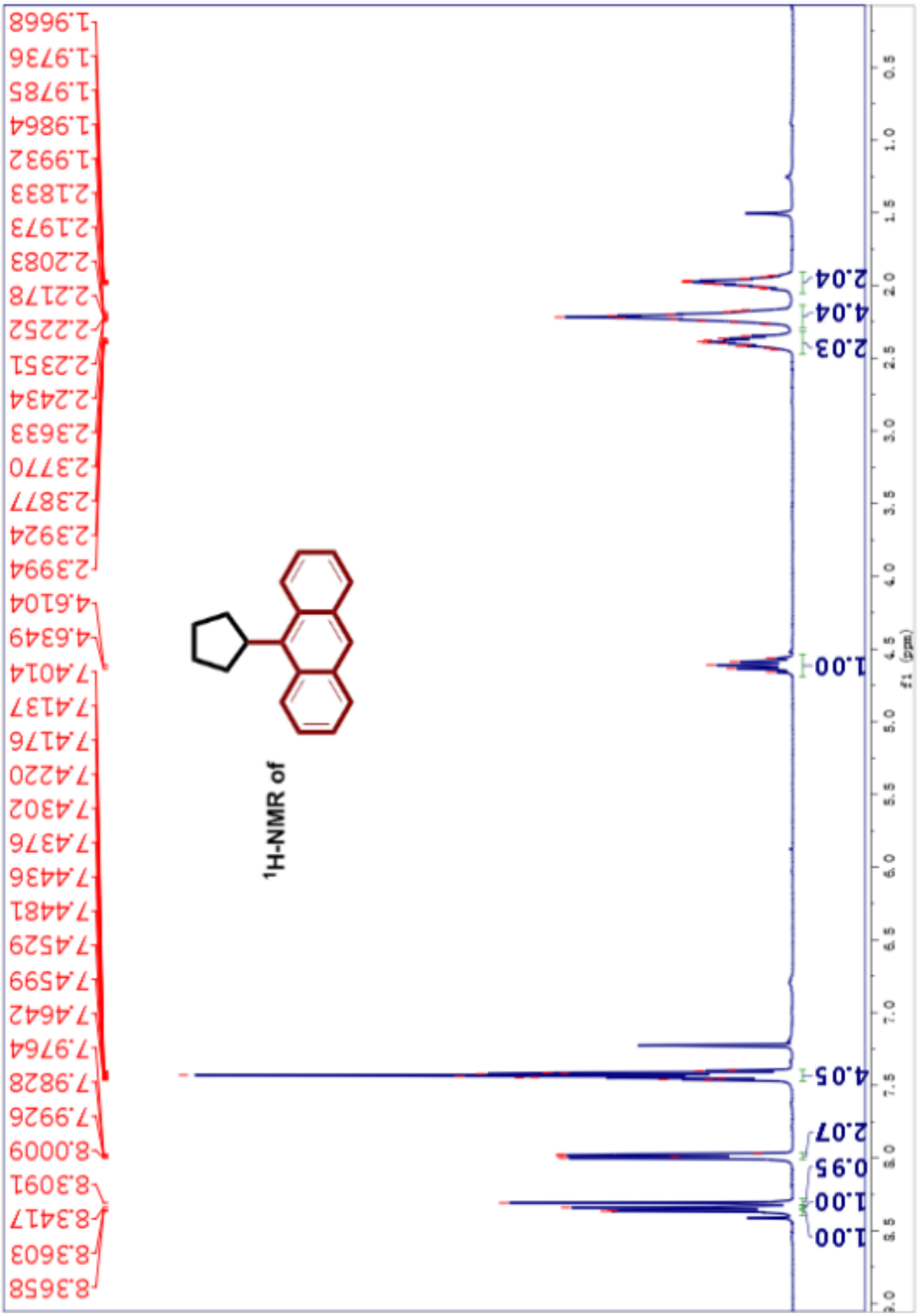
31.03
27.08
21.31
20.63
f1 (ppm)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1.9864
1.9932
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2.2351
2.2434
2.3633
2.3770
2.3877
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4.6349
7.4014
7.4137
7.4176
7.4220
7.4302
7.4376
7.4436
7.4481
7.4529
7.4599
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7.9828
7.9926
8.0009
8.3091
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8.3603
8.3658
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2.07
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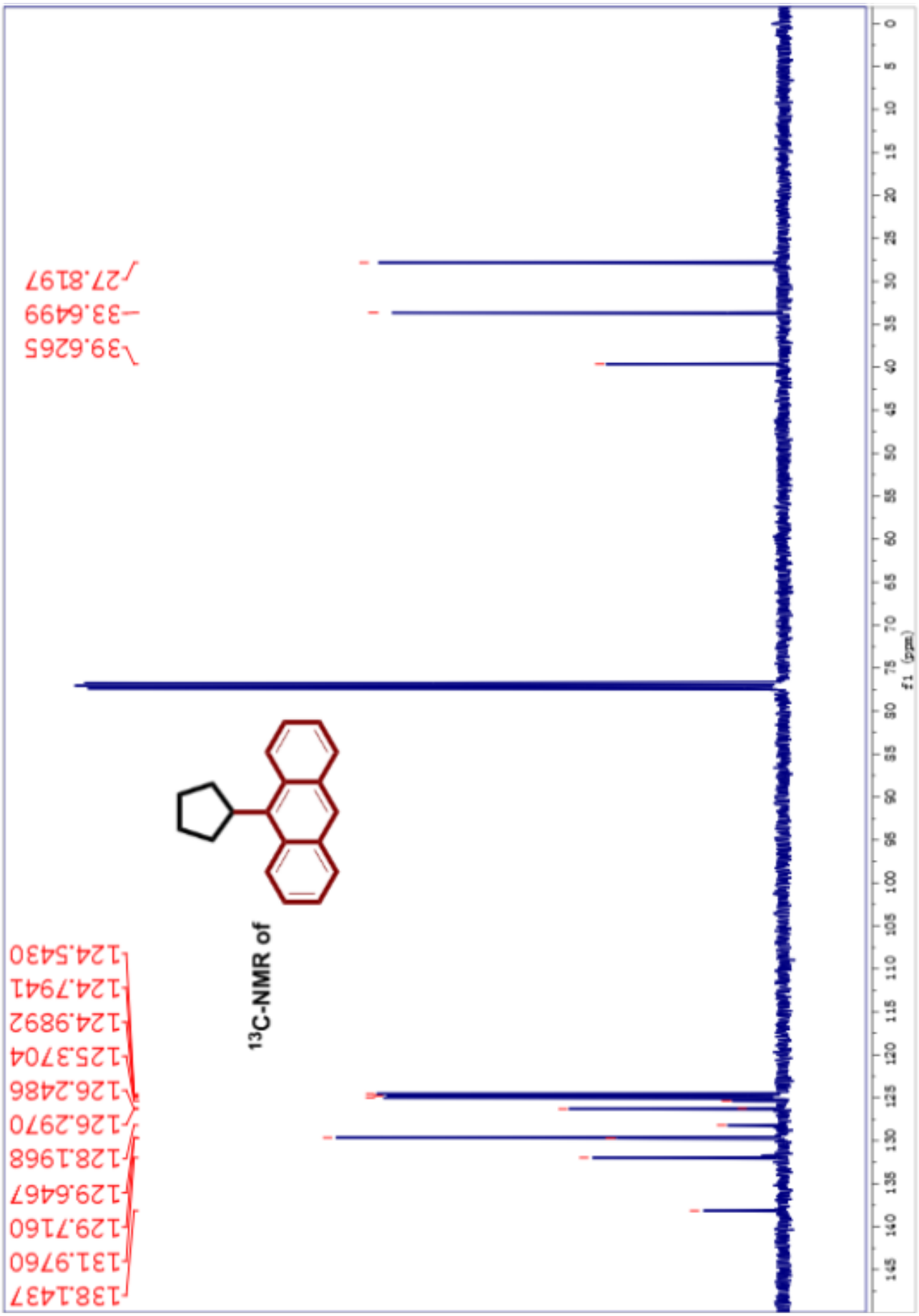
1.00
f1 (ppm)
^{1}H-NMR of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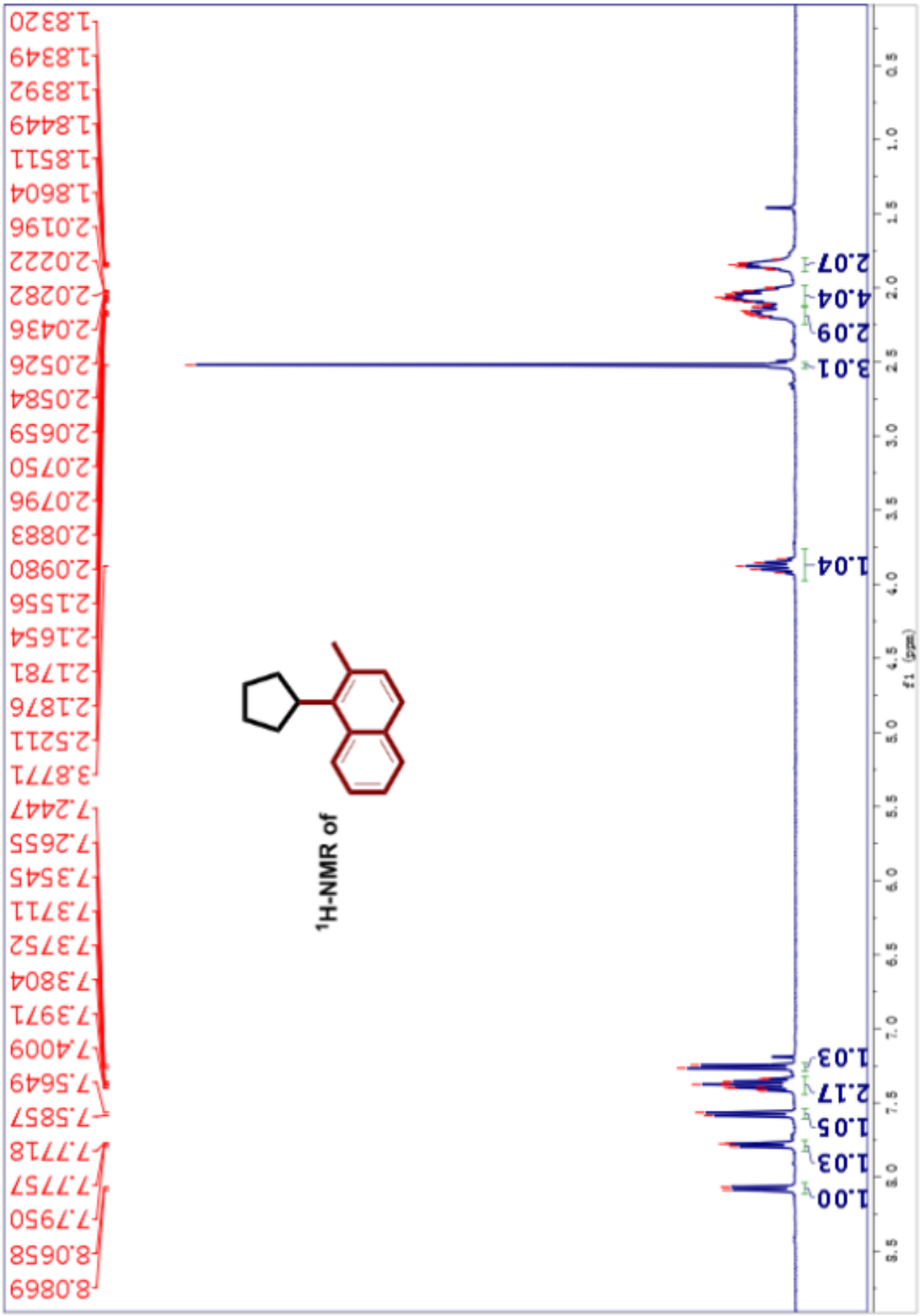
39.6265
33.6499
27.8197
f1 (ppm)


1H-NMR of
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1.05
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1.03
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1.8320
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1.8449
1.8511
1.8604
2.0196
2.0222
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2.0436
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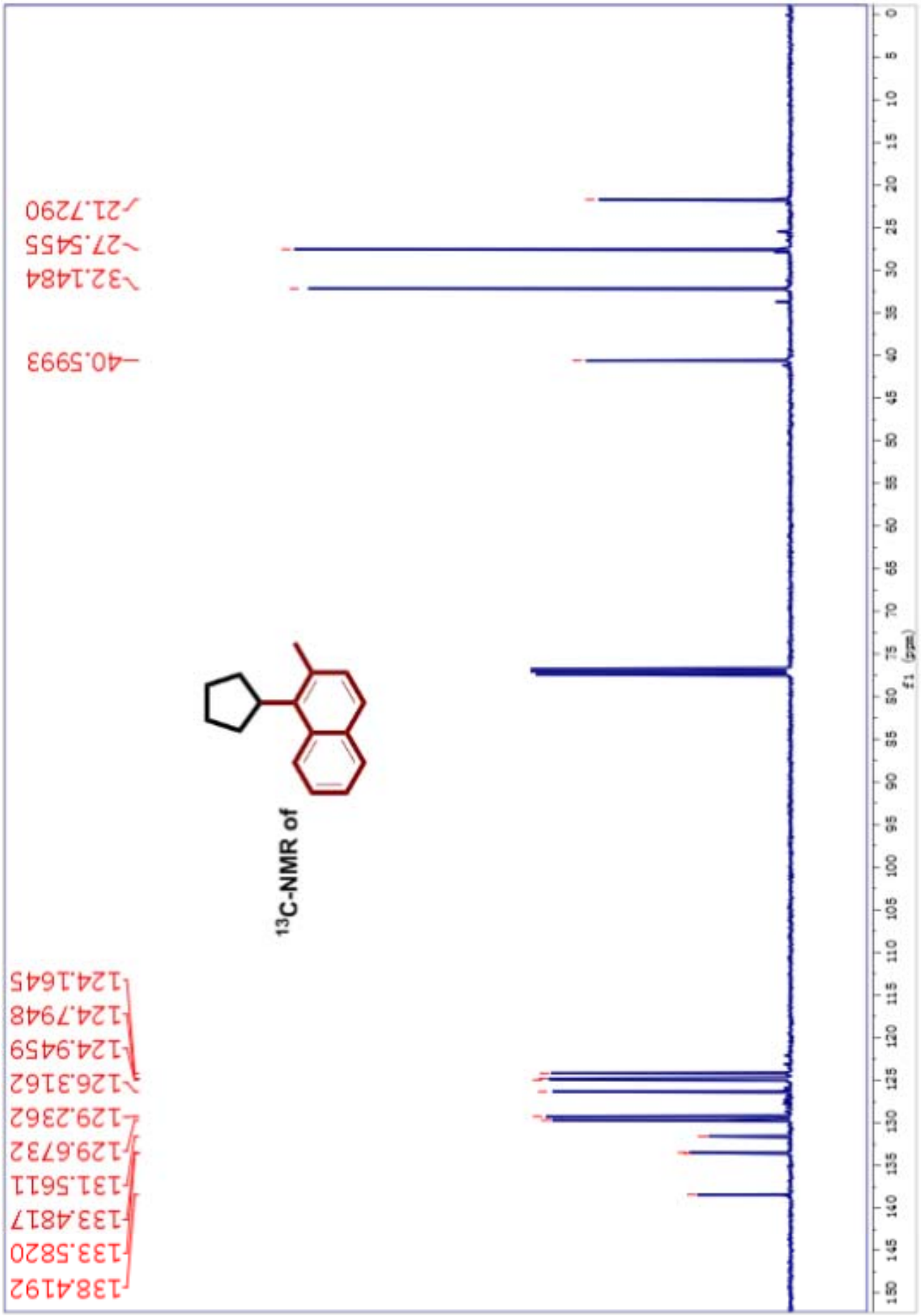
8.0869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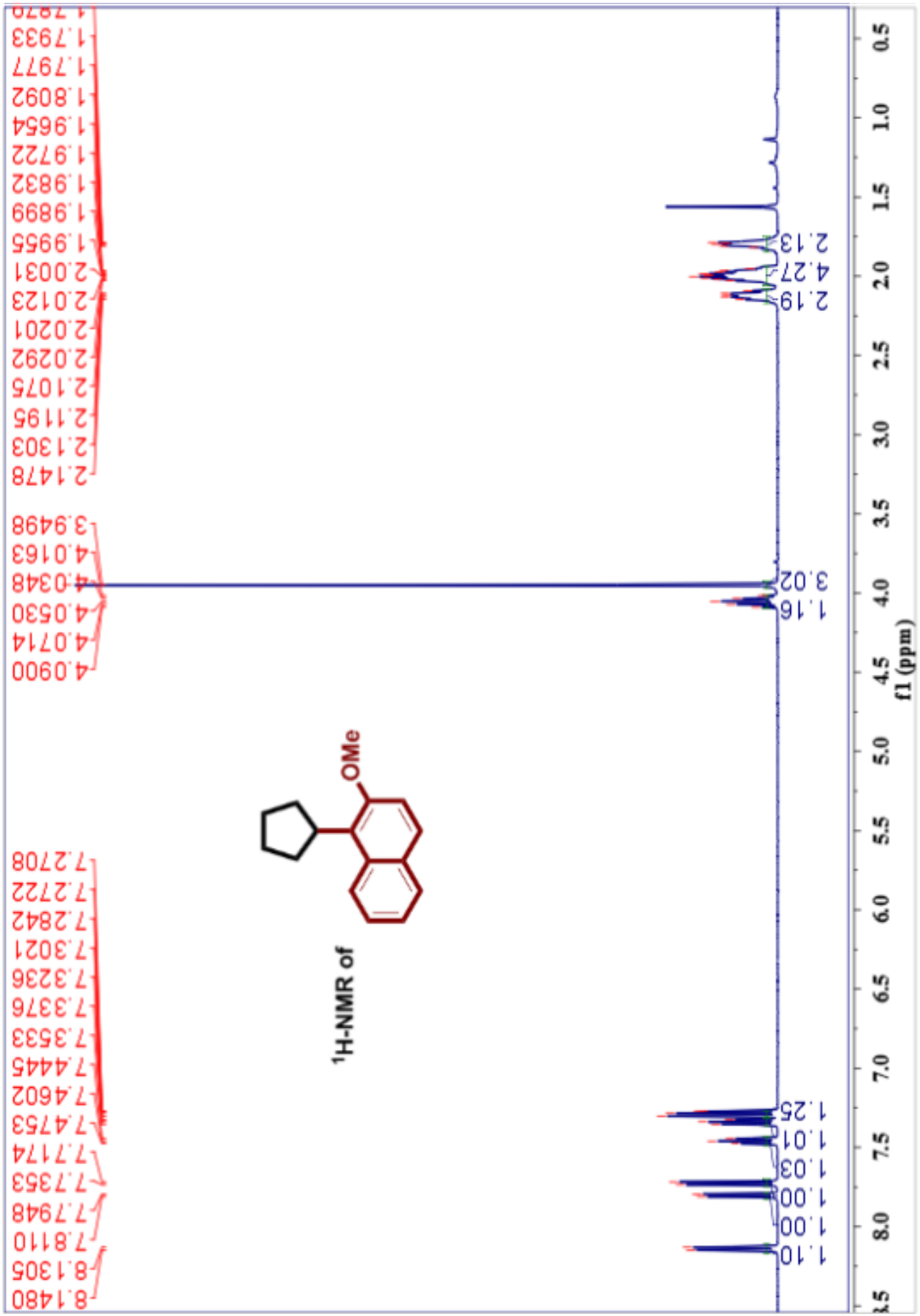
f1 (ppm)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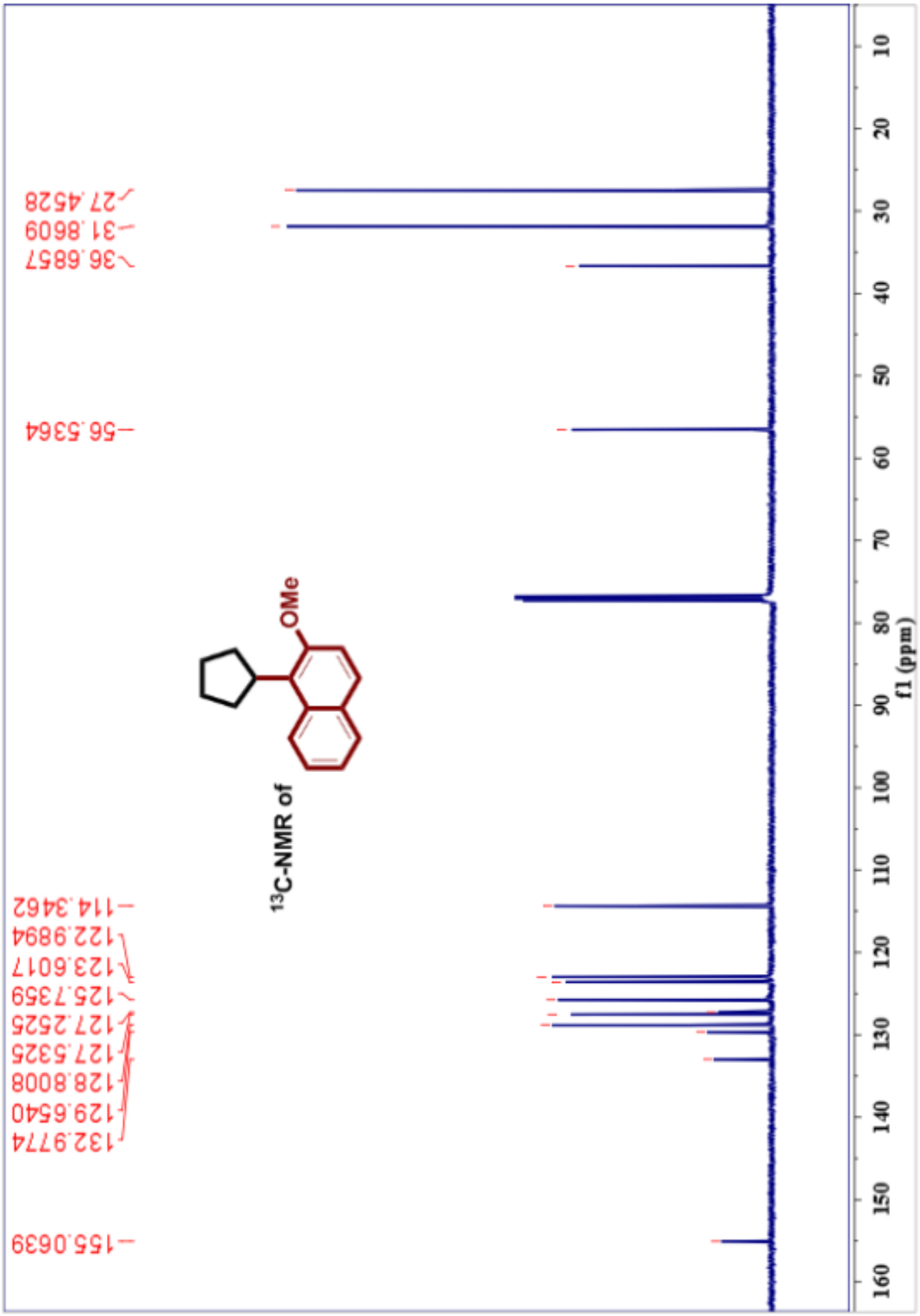
^{1}H-NMR of
f1 (ppm)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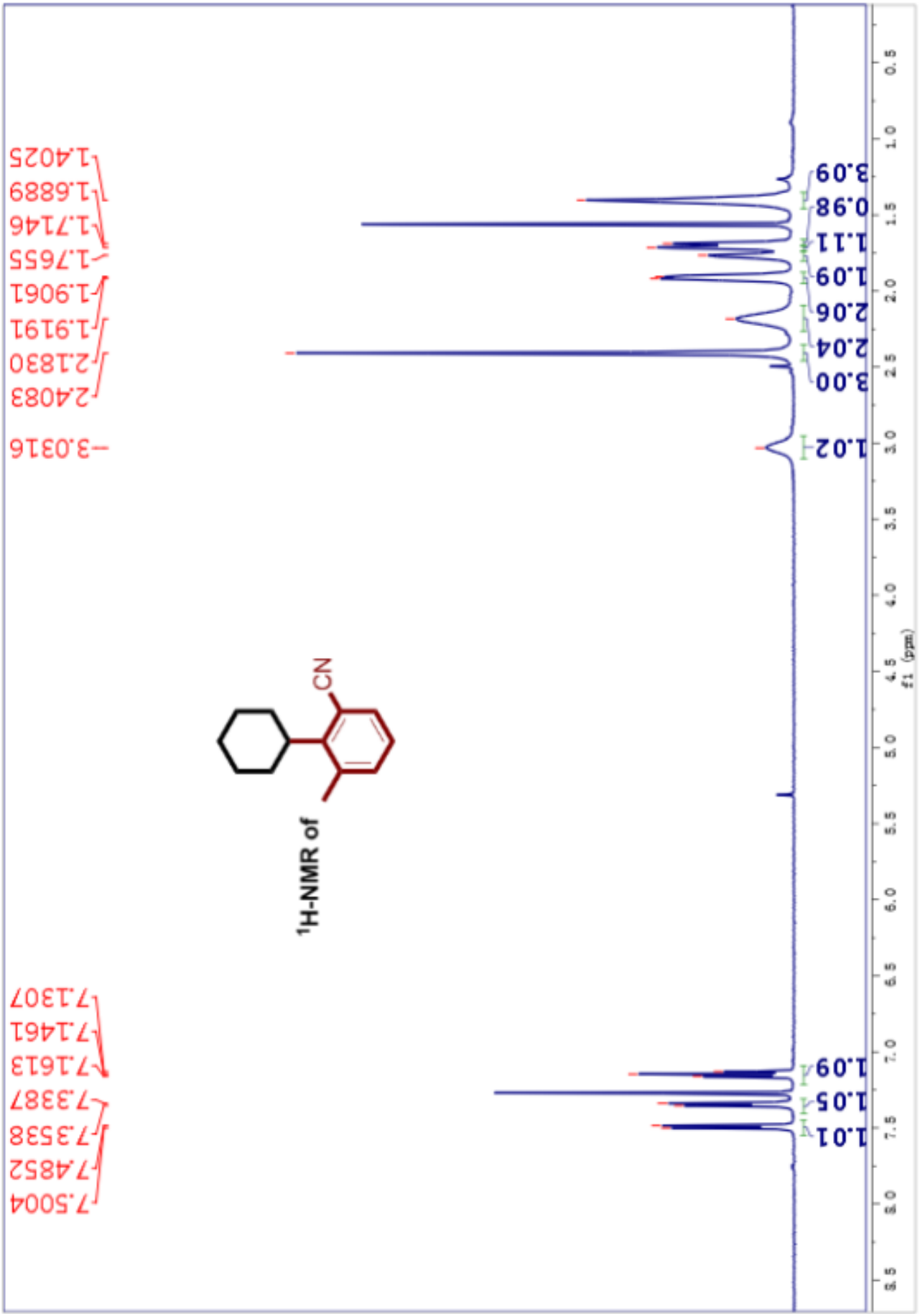
13C-NMR of
f1 (ppm)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7.1613
7.3387
7.3538
7.4852
7.5004
3.09
0.98
1.11
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2.04
3.00
1.02
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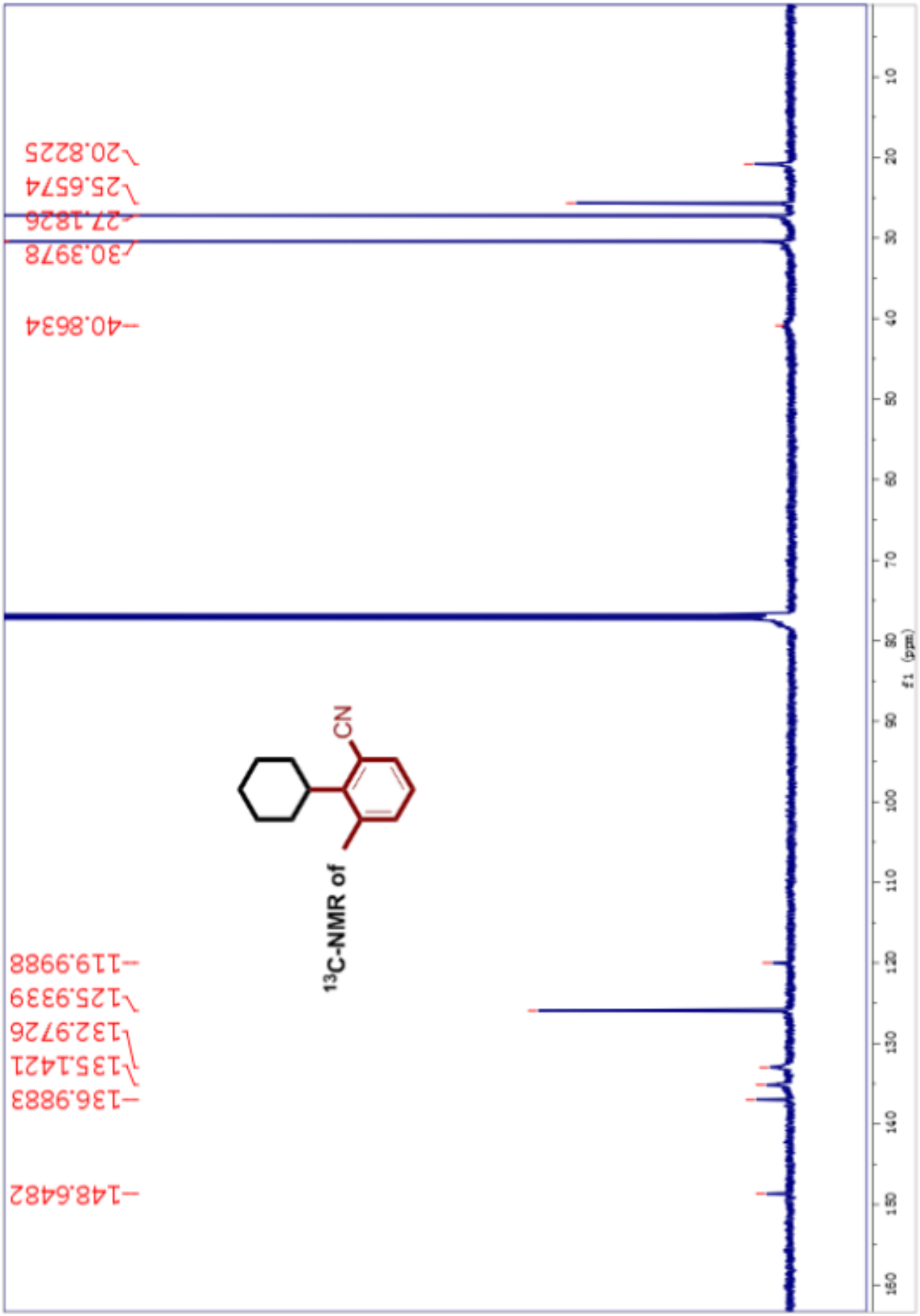
1.05
1.01
CN
^{1}H-NMR of
f1 (ppm)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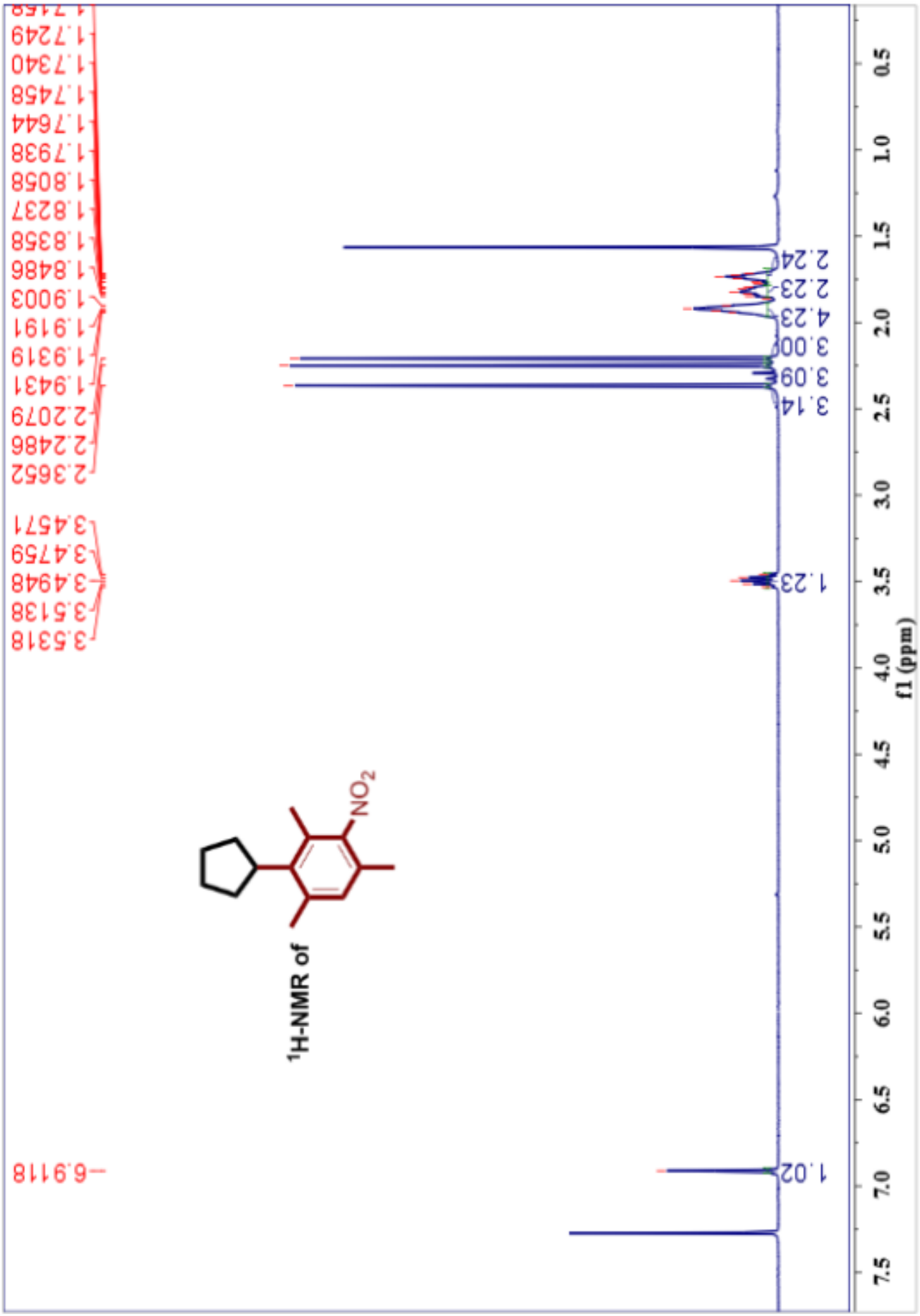
CN
^{13}C-NMR of
f1 (ppm)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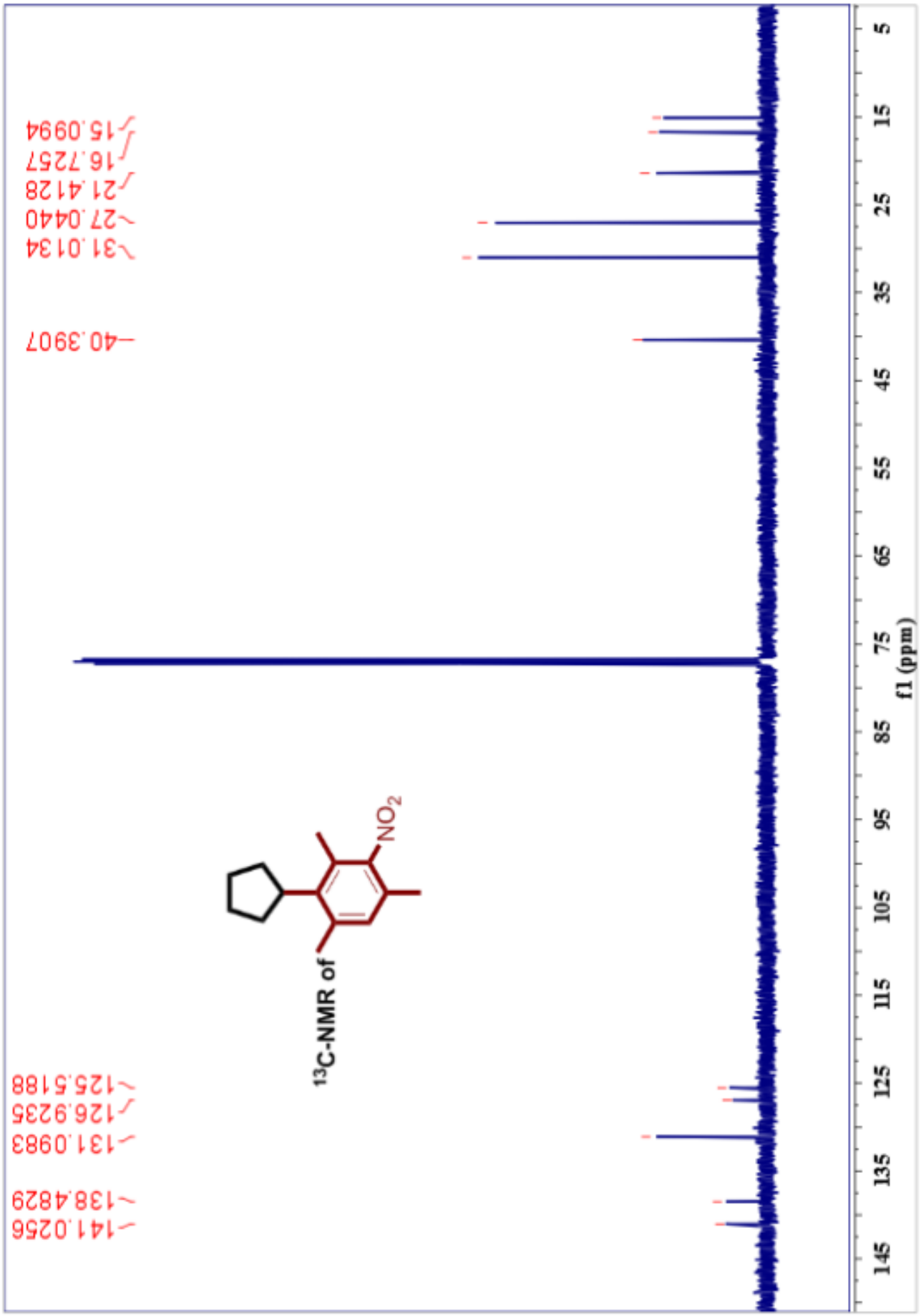
1.9319
1.9431
2.2079
2.2486
2.3652
3.4571
3.4759
3.4948
3.5138
3.5318
6.9118
2.24
2.23
4.23
3.00
3.09
3.14
1.23
1.02
NO2
1H-NMR of
f1 (ppm)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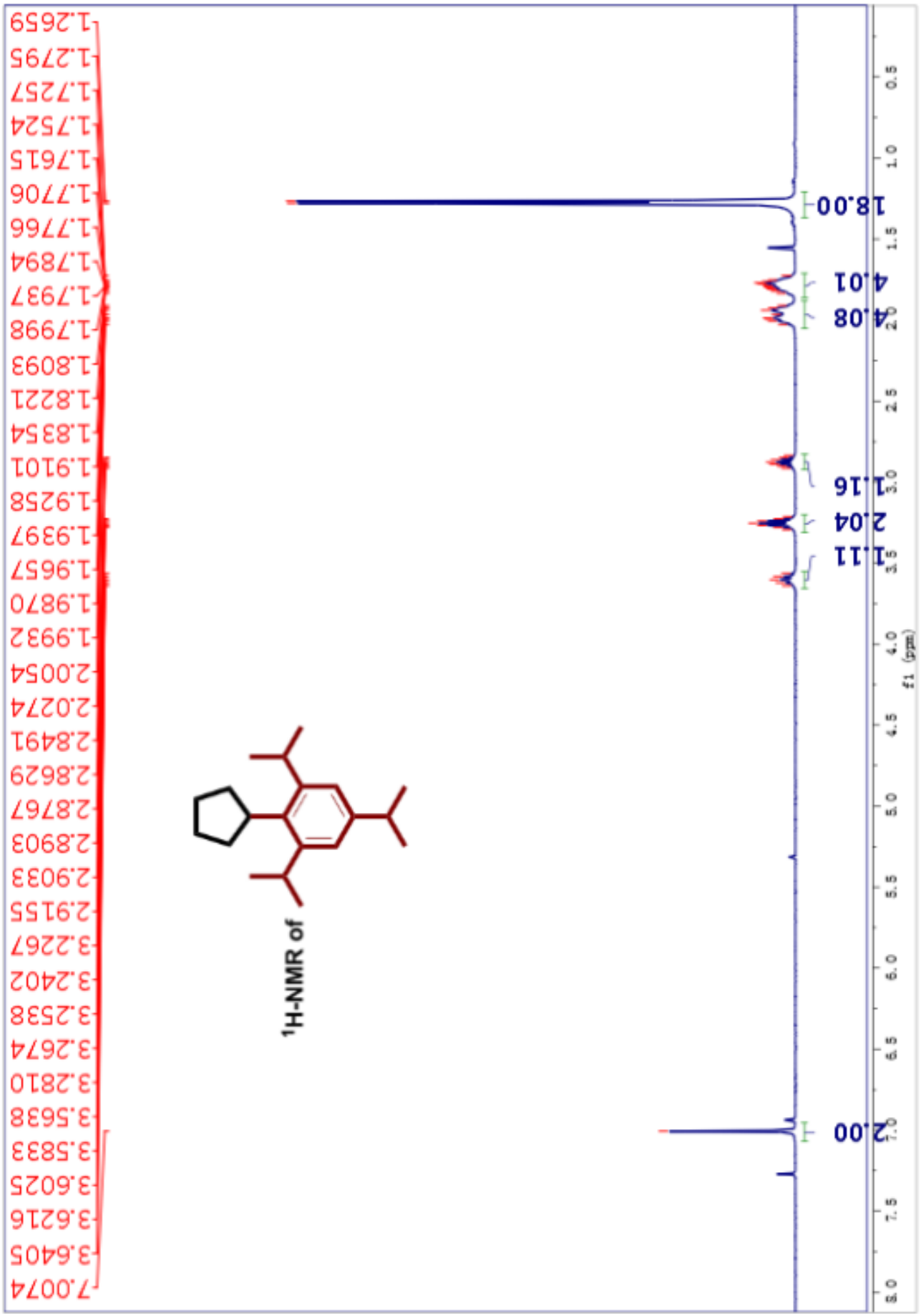
^{13}C-NMR of
NO_2
f1 (ppm)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1.8354
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1.9258
1.9397
1.9657
1.9870
1.9932
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2.8767
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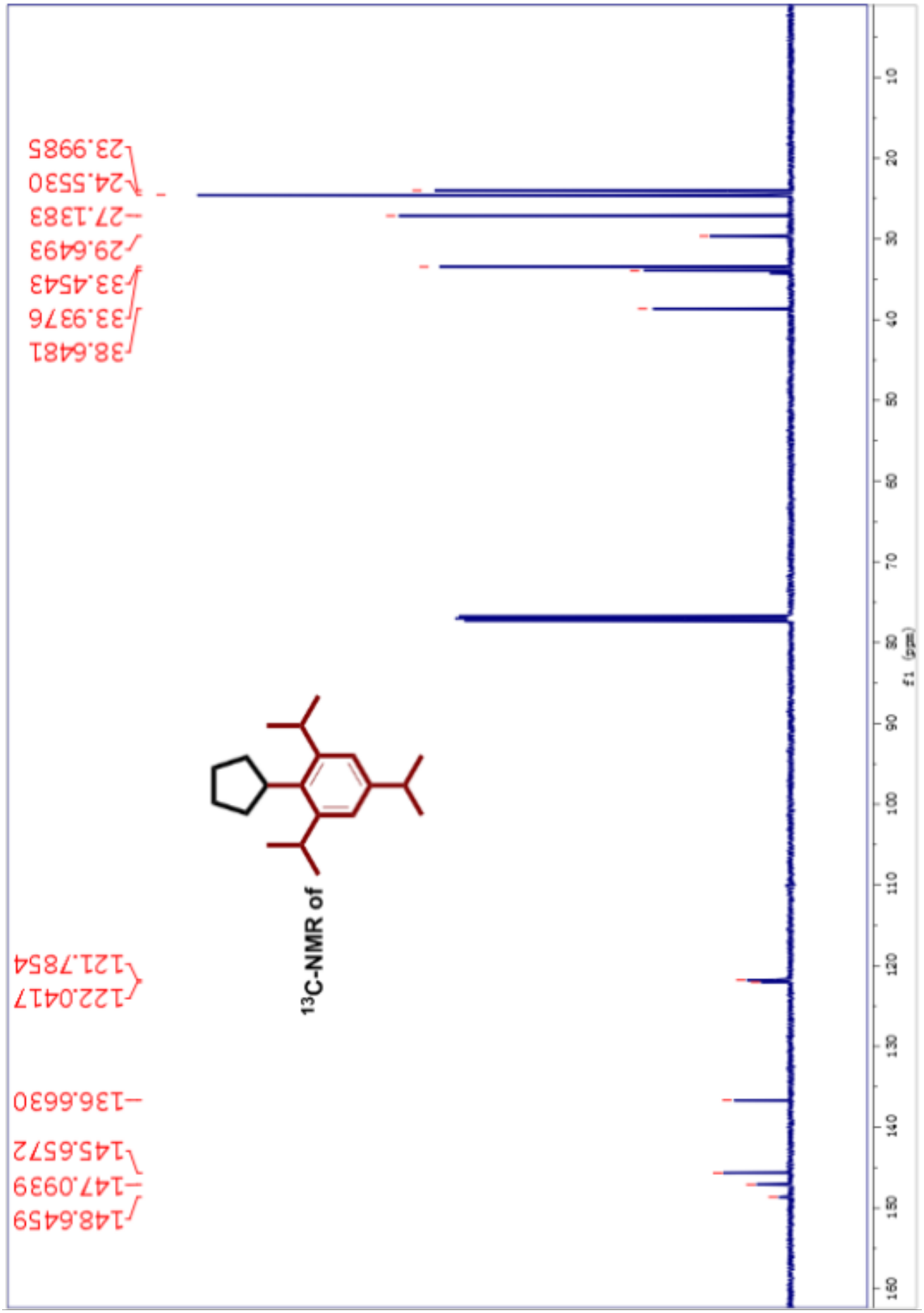
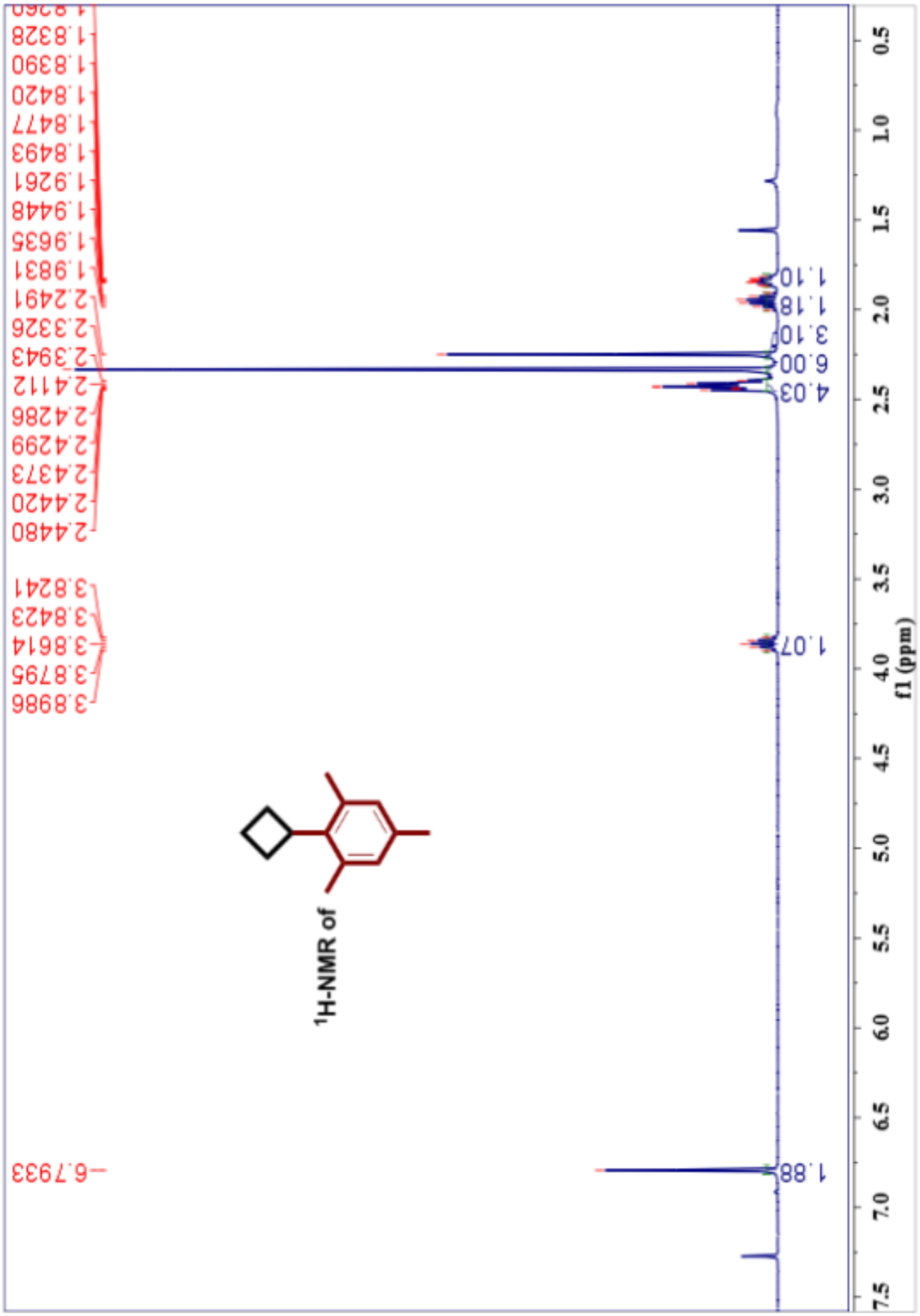
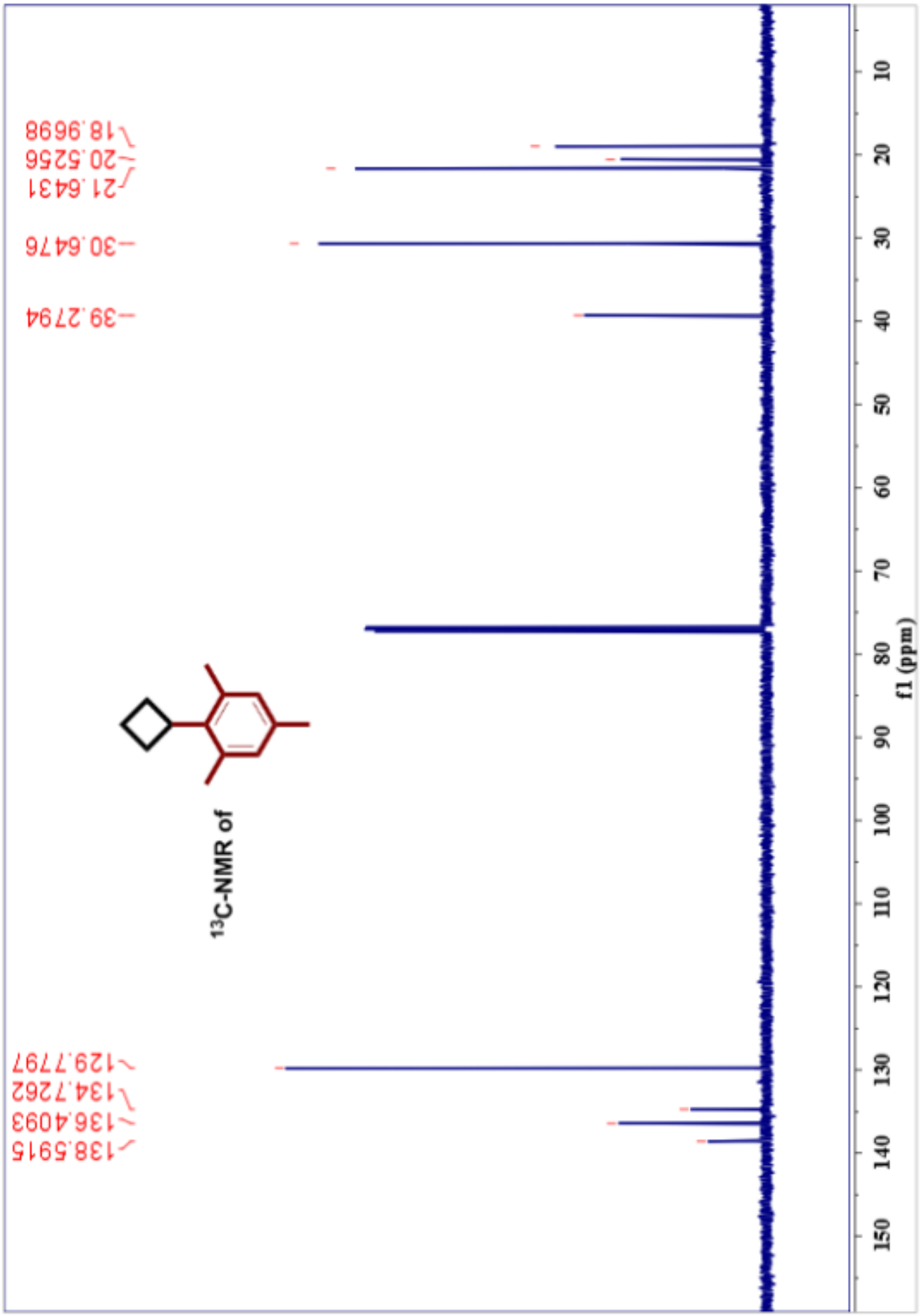
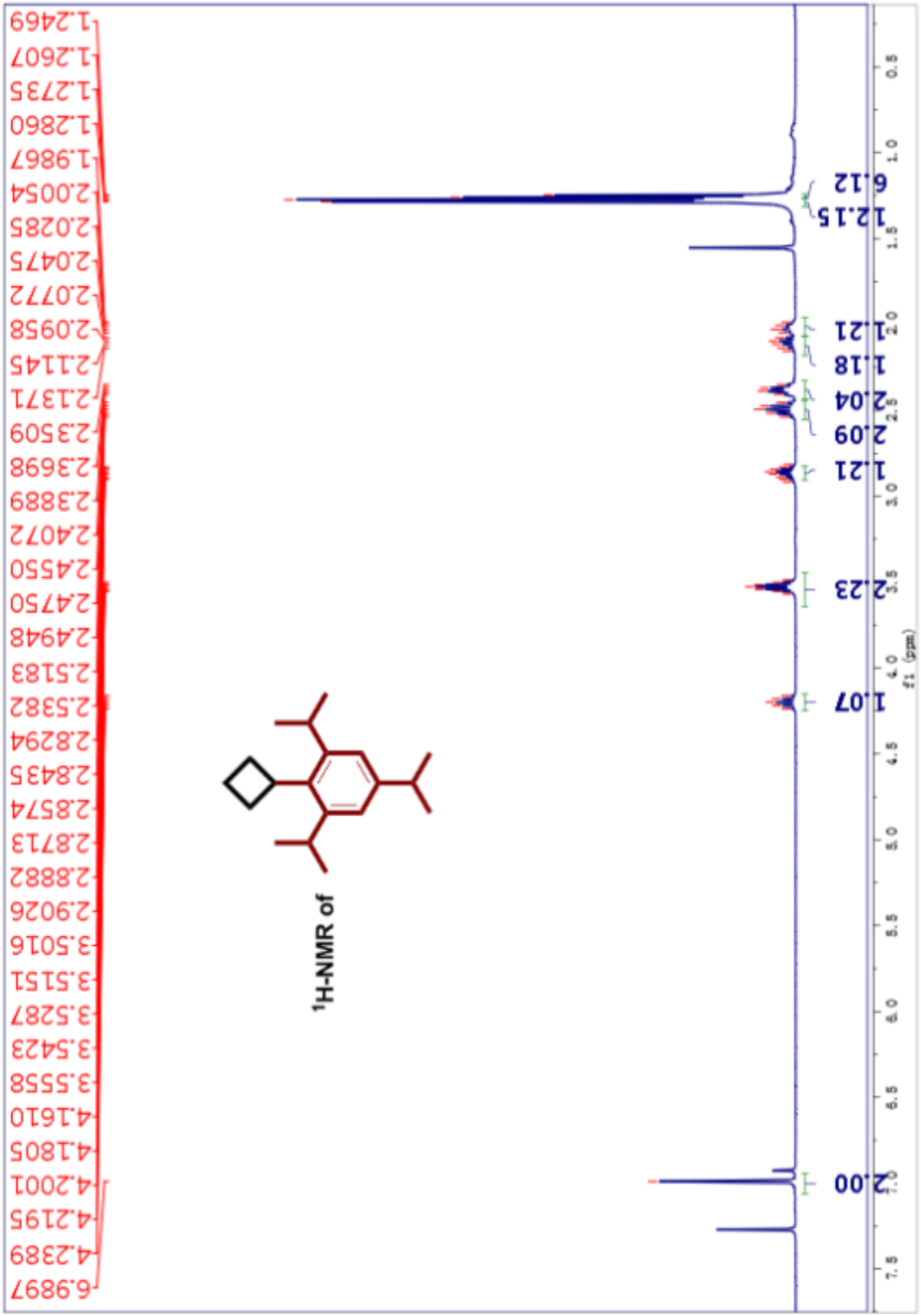
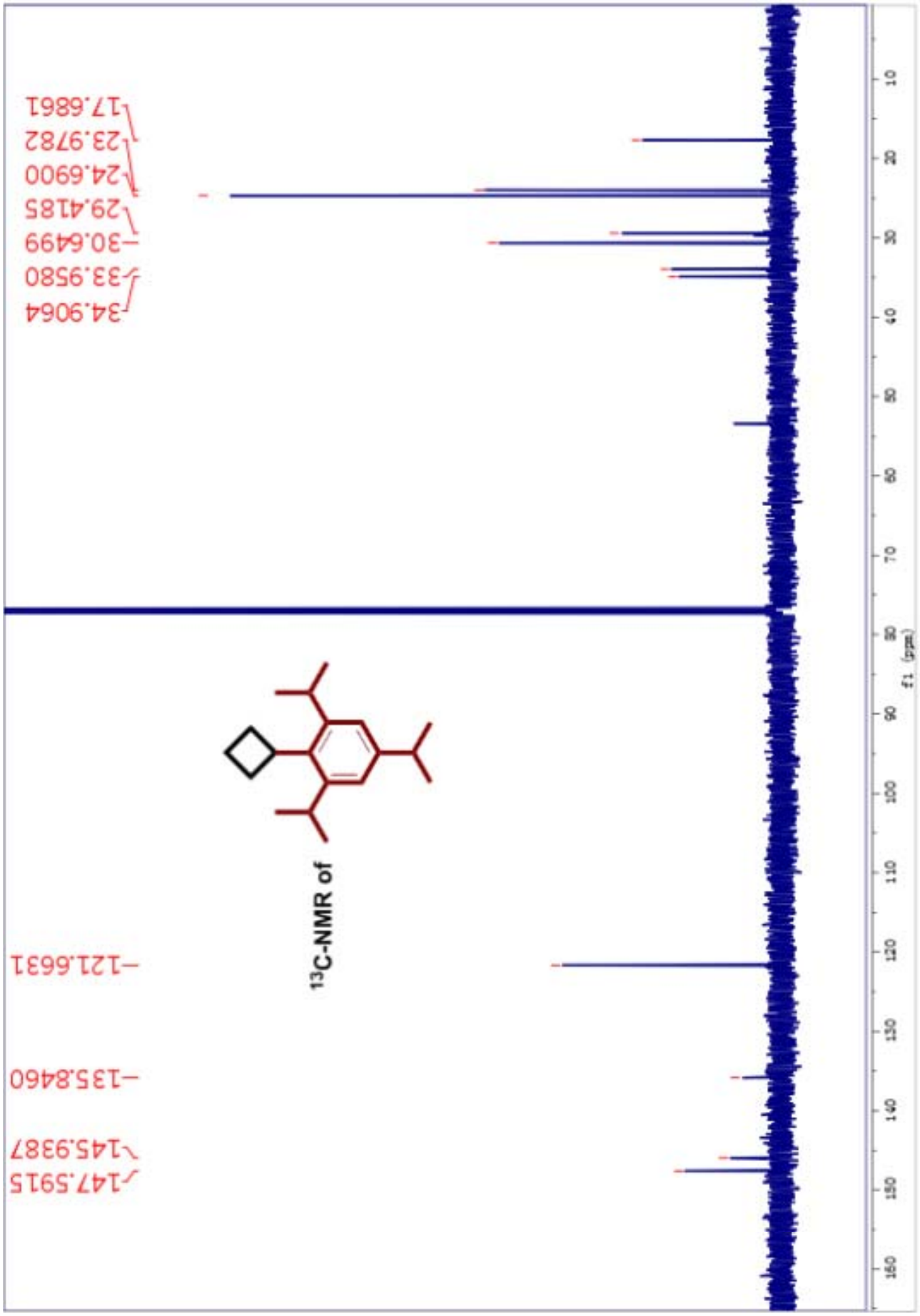
3.6025
3.6216
3.6405
7.0074
18.00
4.01
4.08
1.16
2.04
1.11
2.00
f1 (ppm)
^{1}H-NMR of

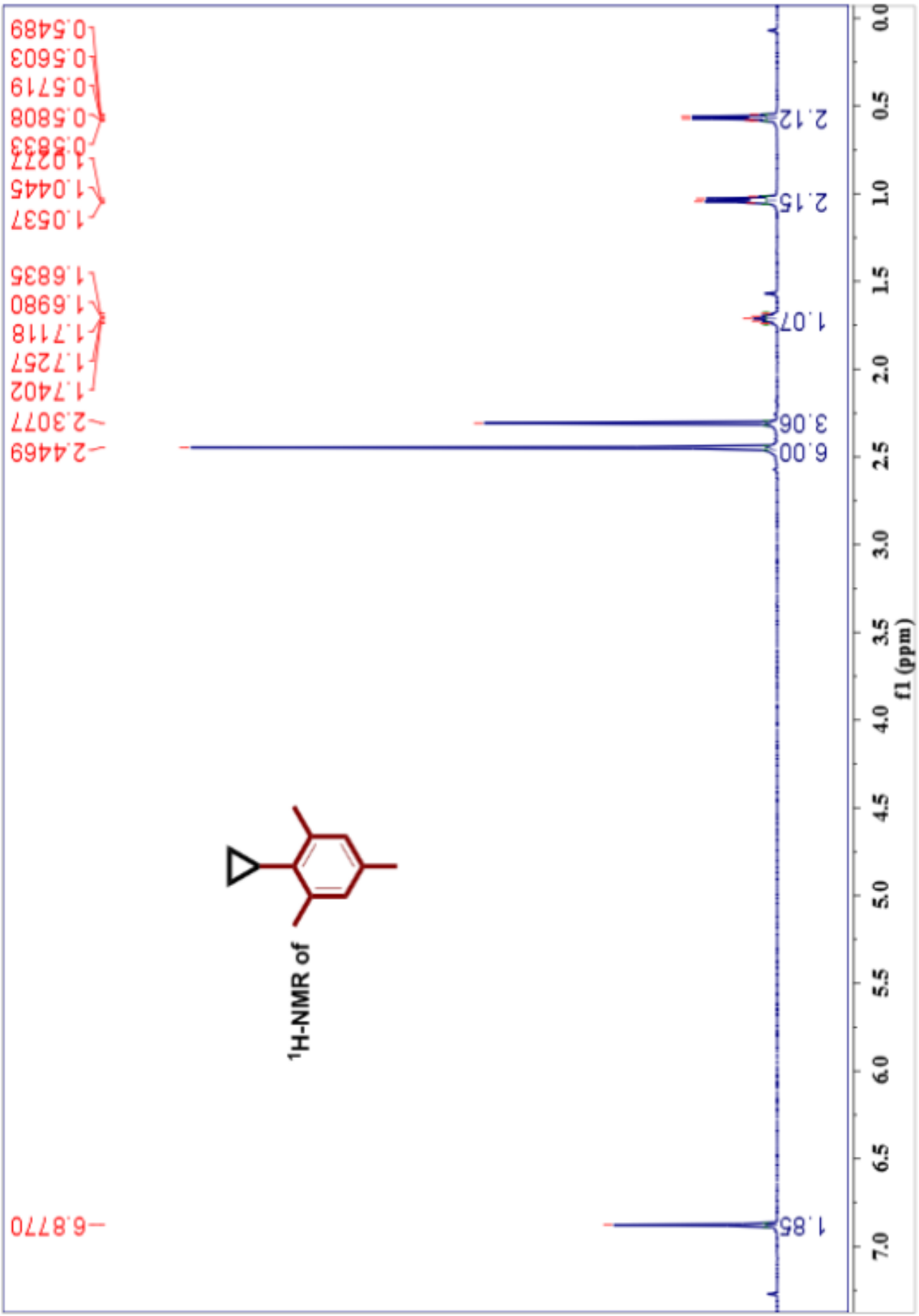

^{13}C-NMR of
148.6459
147.0939
145.6572
136.6630
122.0417
121.7854
38.6481
33.9376
33.4543
29.6493
27.1383
24.5530
23.9985
f1 (ppm)


1.8260
1.8328
1.8390
1.8420
1.8477
1.8493
1.9261
1.9448
1.9635
1.9831
2.2491
2.3326
2.3943
2.4112
2.4286
2.4299
2.4373
2.4420
2.4480
3.8241
3.8423
3.8614
3.8795
3.8986
6.7933
1.10
1.18
3.10
6.00
4.03
1.07
1.88
f1 (ppm)
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
^{1}H-NMR of


138.5915
136.4093
134.7262
129.7797
18.9698
20.5256
21.6431
30.6476
39.2794
f1 (ppm)
13C-NMR of


1H-NMR of
6.12
12.15
1.21
1.18
2.04
2.09
1.21
2.23
1.07
2.00
f1 (ppm)


17.6861
23.9782
24.6900
29.4185
30.6499
33.9580
34.9064
121.6631
135.8460
145.9387
147.5915
13C-NMR of
f1 (ppm)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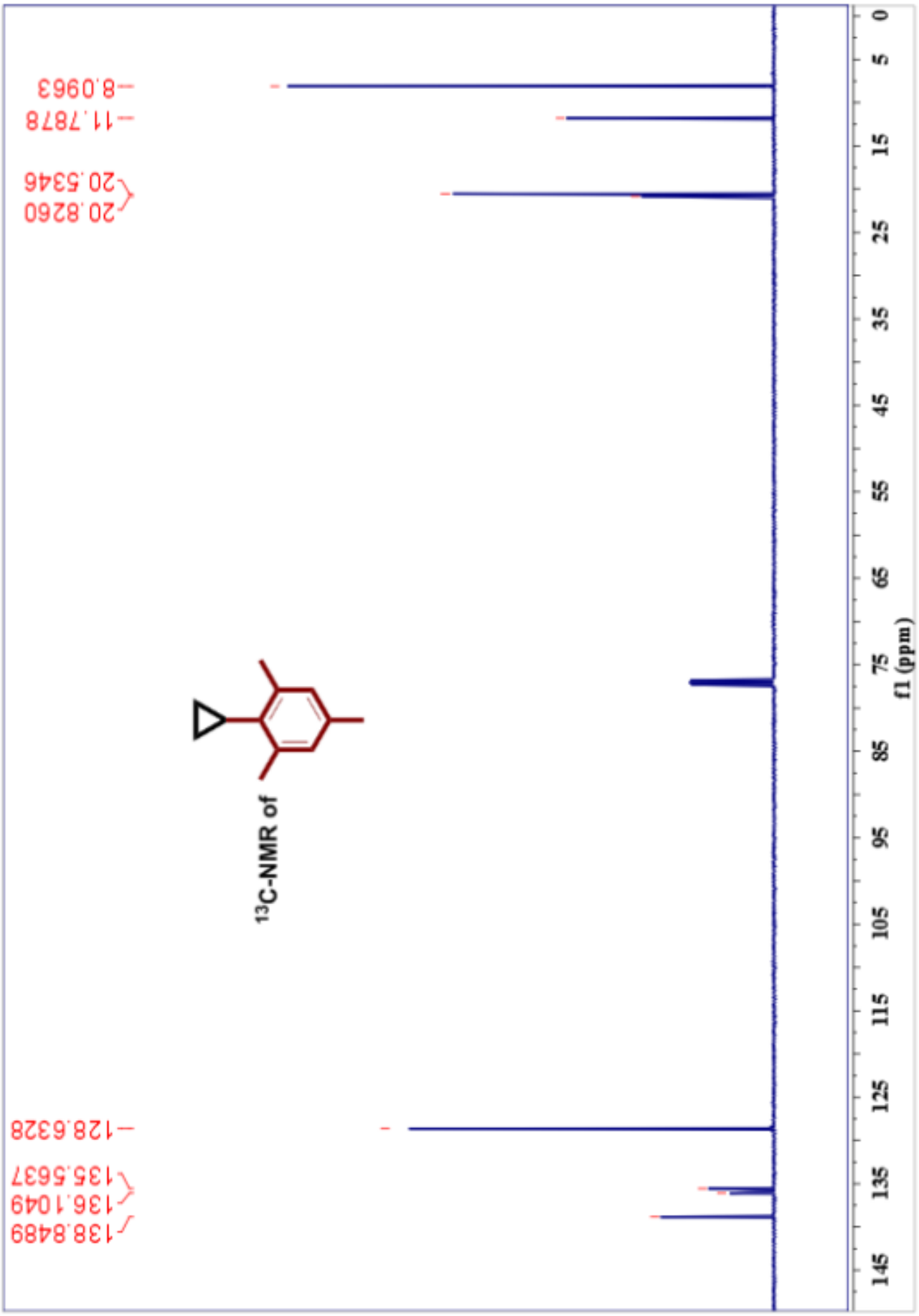
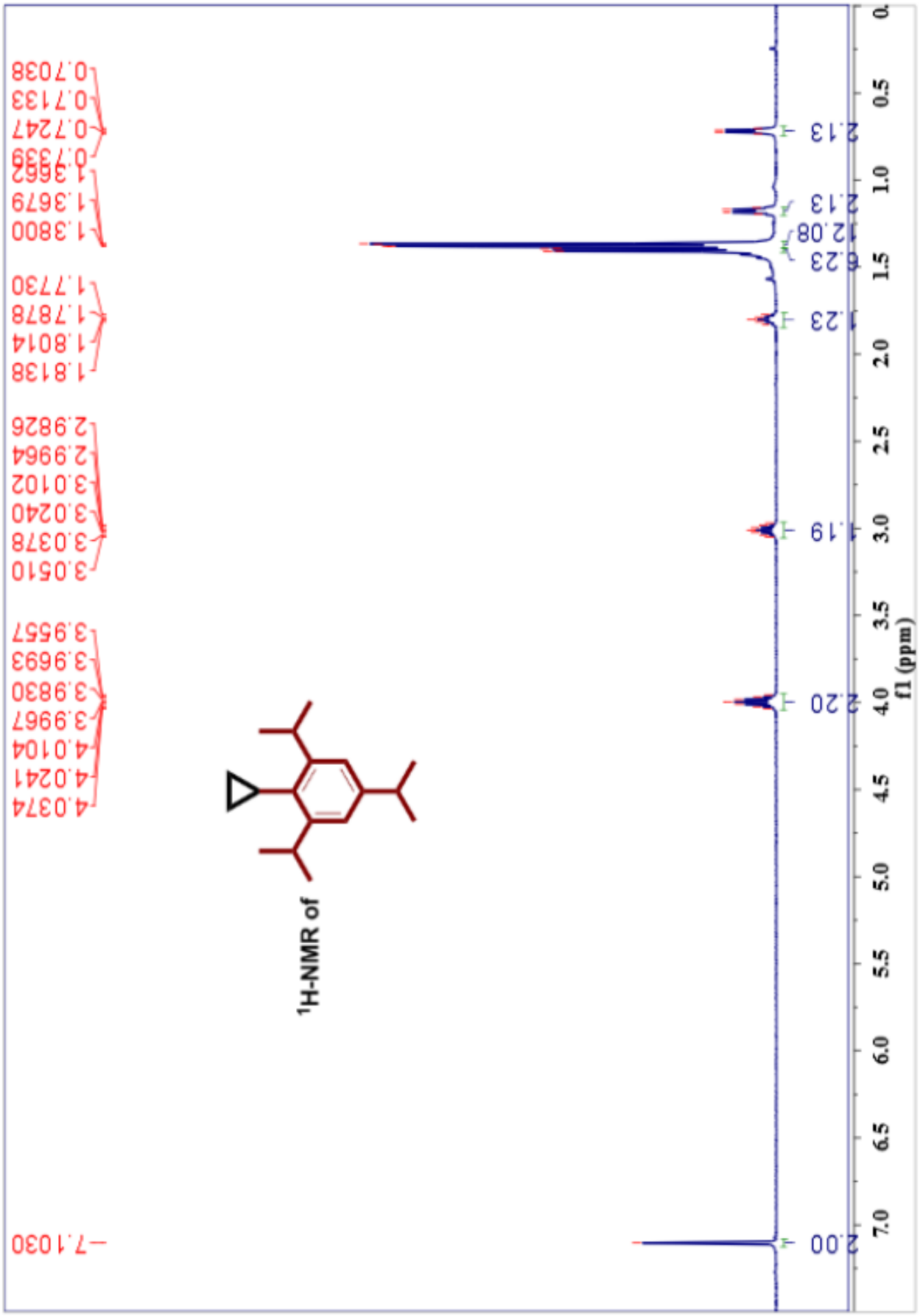
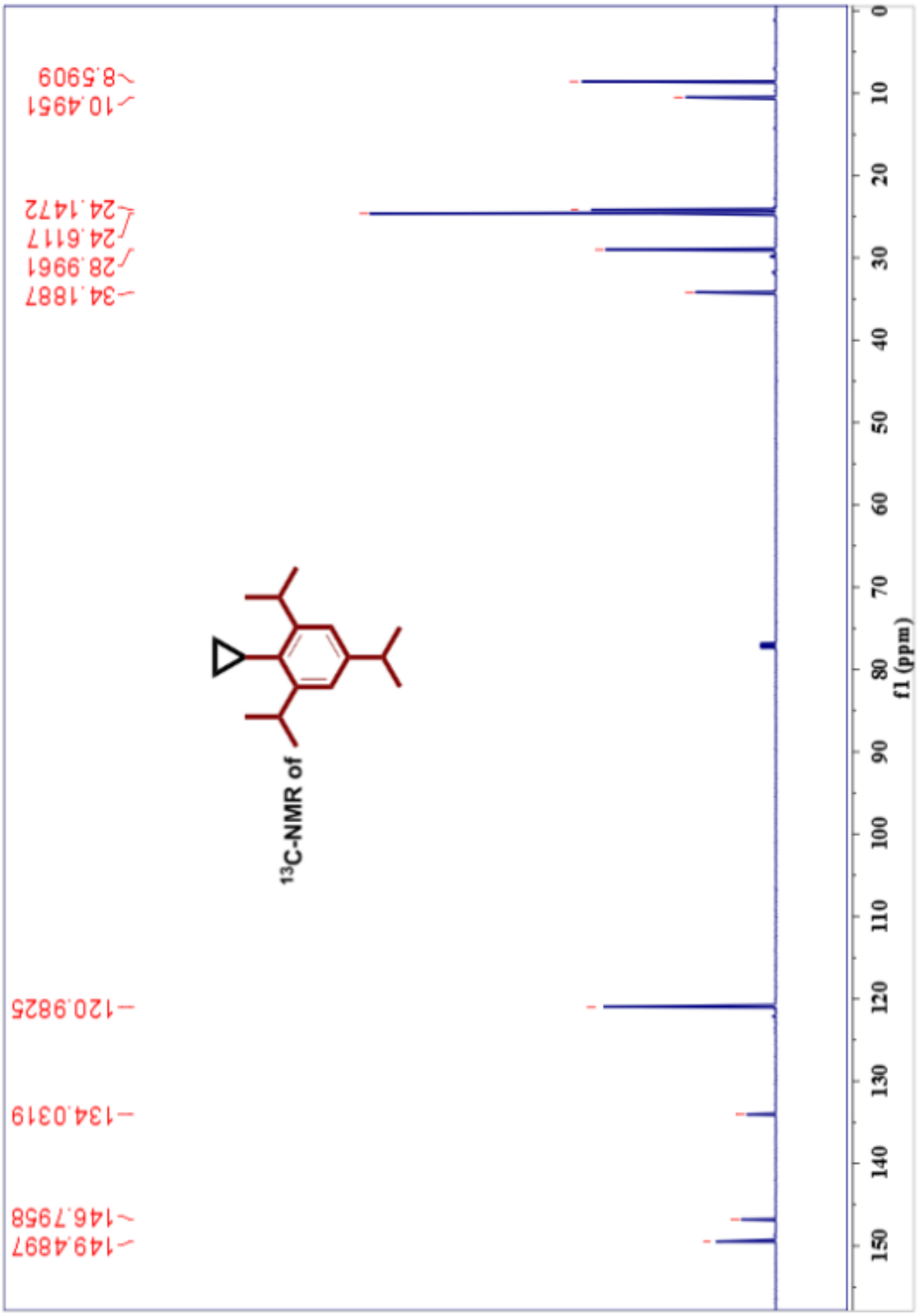
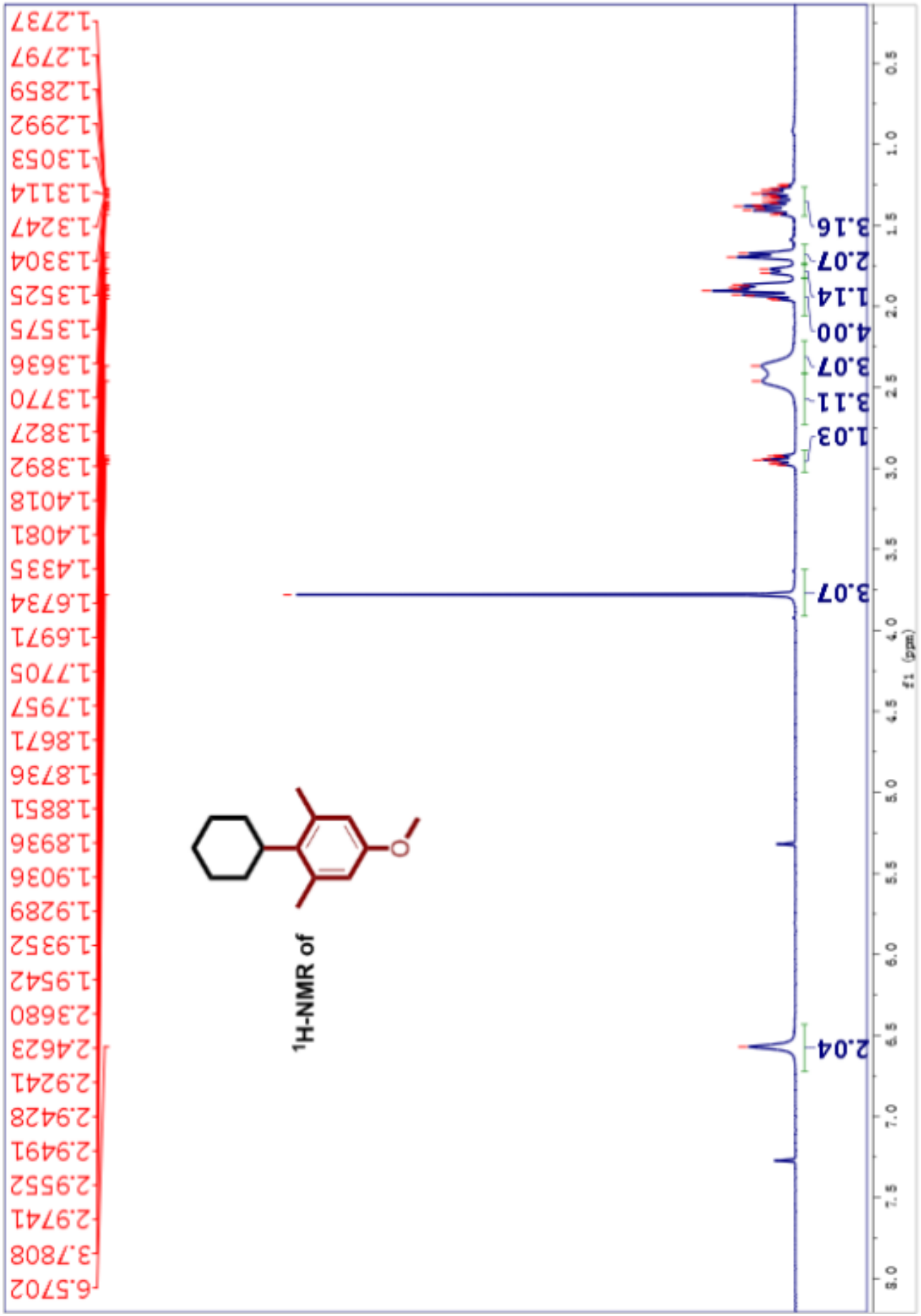
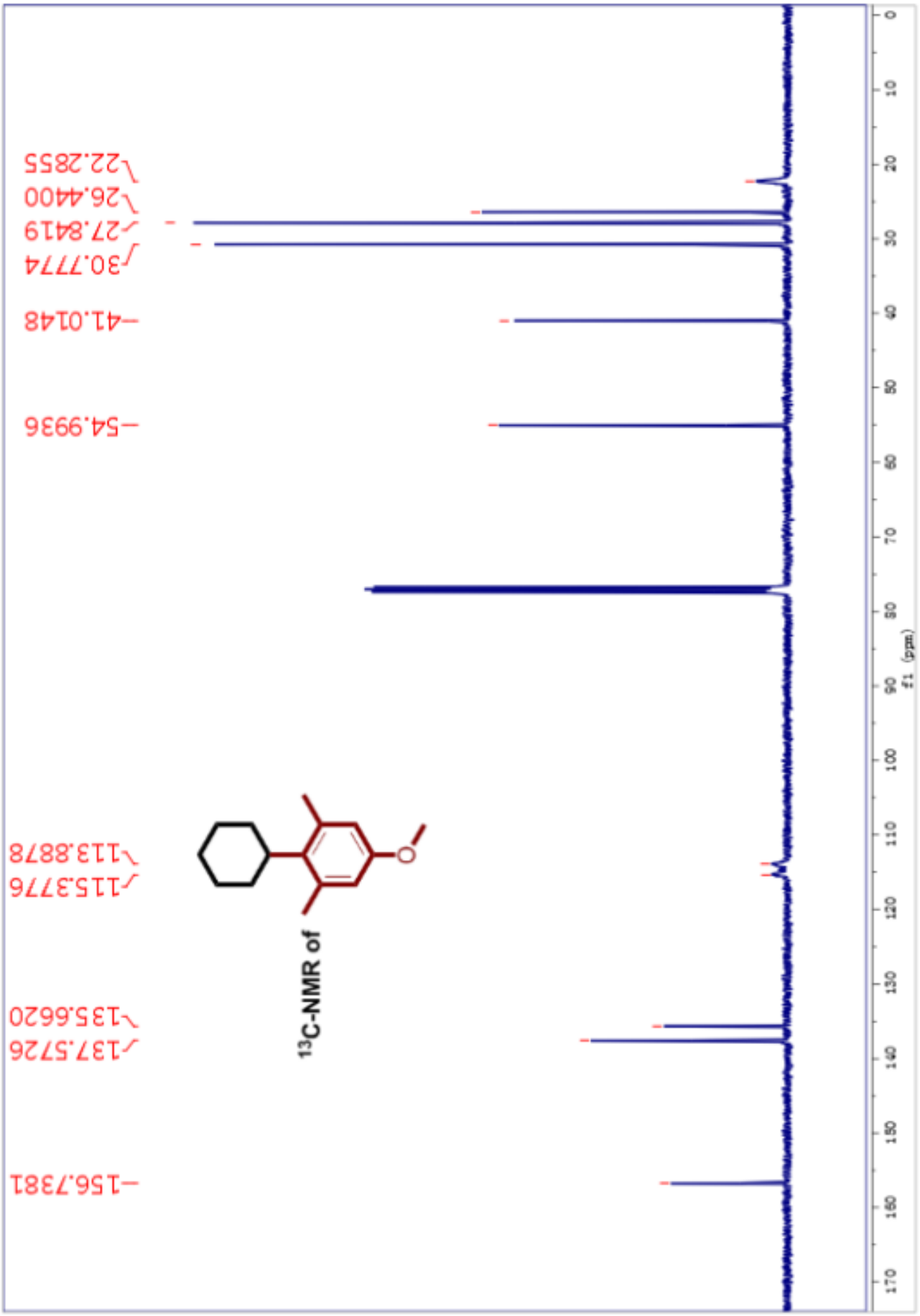
0.5603
0.5719
0.5808
0.5833
1.0272
1.0445
1.0537
1.6835
1.6980
1.7118
1.7257
1.7402
2.3077
2.4469
6.8770
2.12
2.15
1.07
3.06
6.00
1.85
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
f1 (ppm)
^{1}H-NMR of

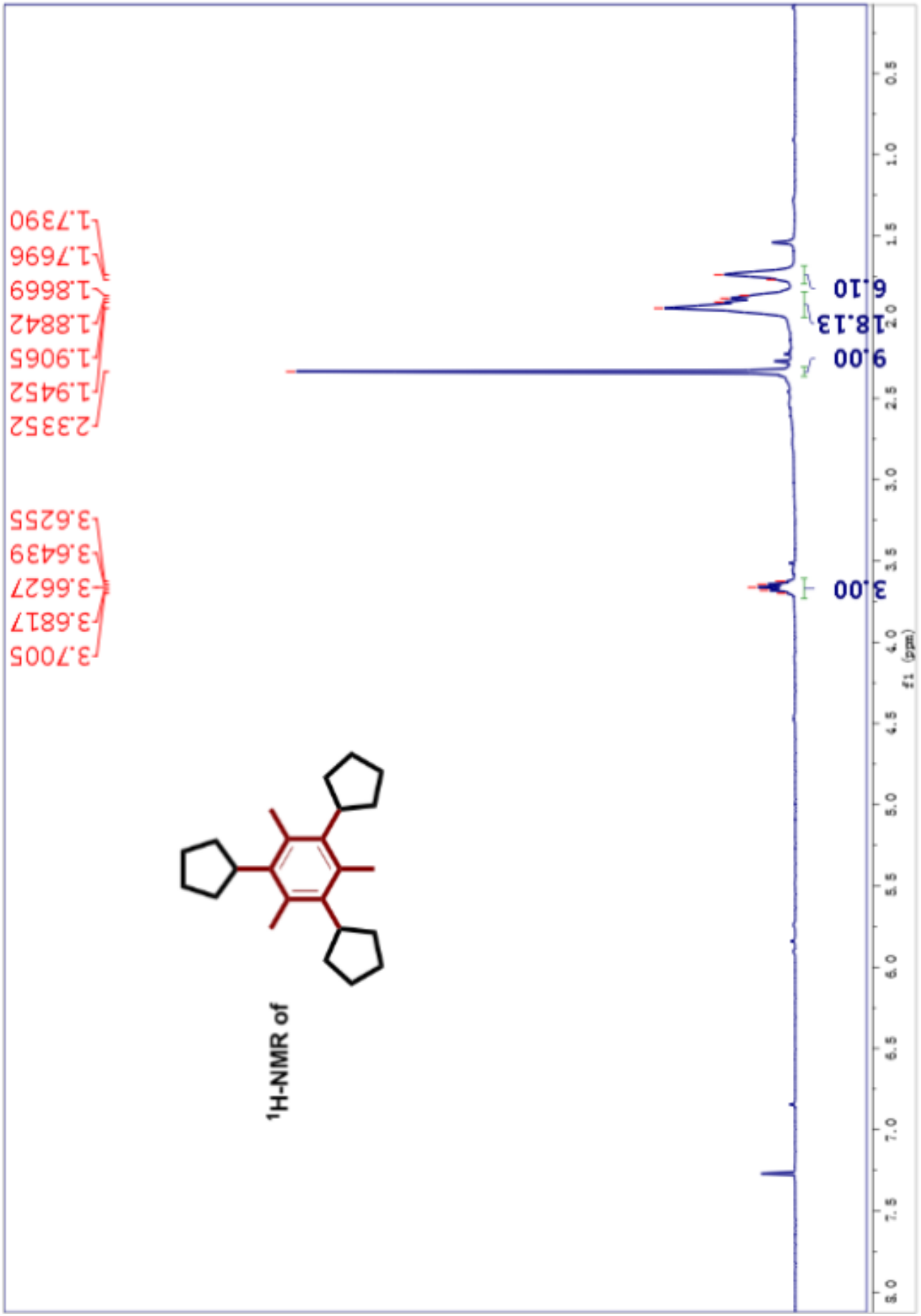

8.0963
11.7878
20.5346
20.8260
128.6328
135.5637
136.1049
138.8489
^{13}C-NMR of
f1 (ppm)


7.1030
4.0374
4.0241
4.0104
3.9967
3.9830
3.9693
3.9557
3.0510
3.0378
3.0240
3.0102
2.9964
2.9826
1.8138
1.8014
1.7878
1.7730
1.3800
1.3679
1.3662
0.7339
0.7247
0.7133
0.7038
2.00
2.20
1.19
2.23
6.23
12.08
2.13
2.13
f1 (ppm)
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
^{1}H-NMR of

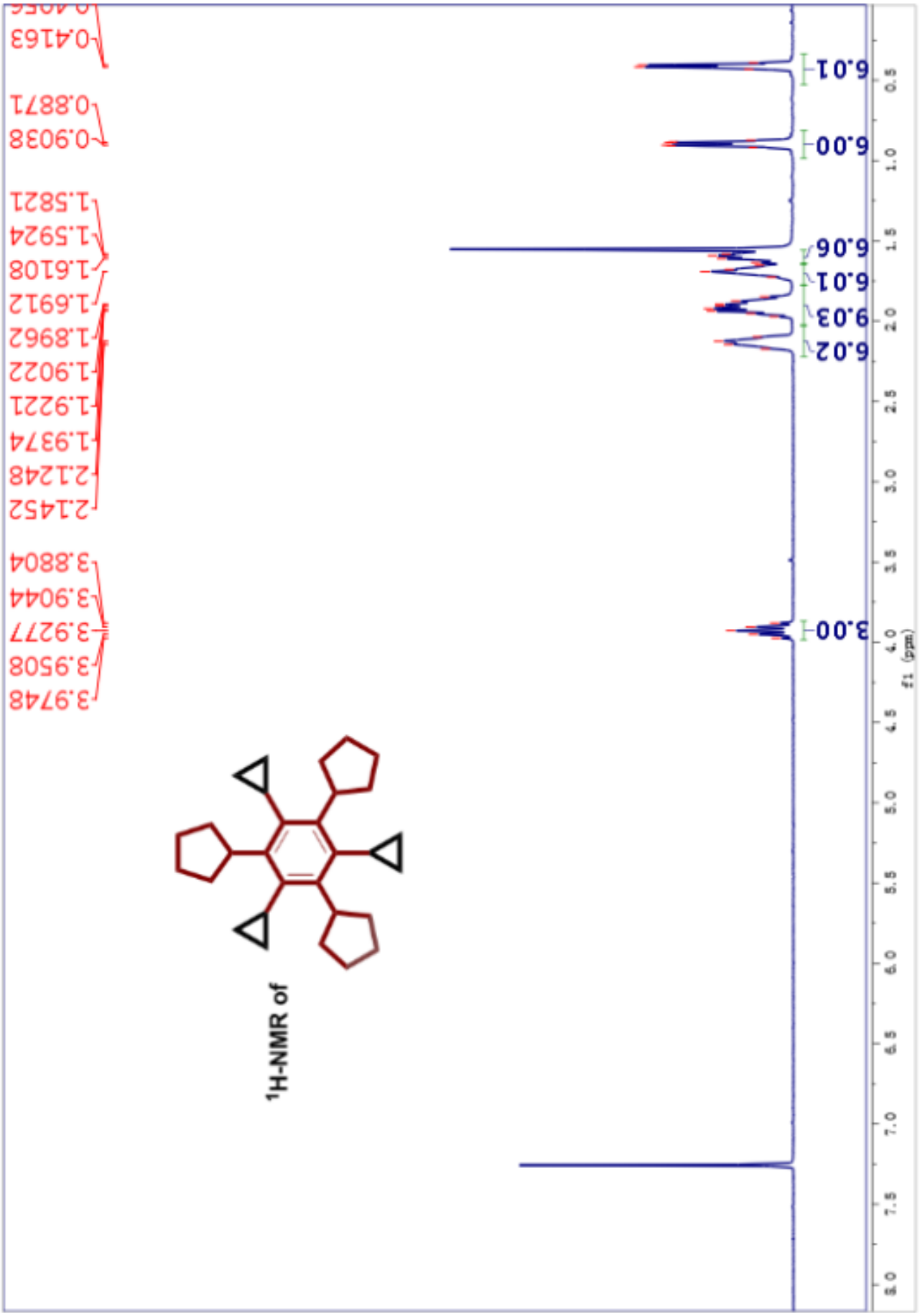

^{13}C-NMR of
8.5909
10.4951
24.1472
24.6117
28.9961
34.1887
120.9825
134.0319
146.7958
149.4897
f1 (ppm)

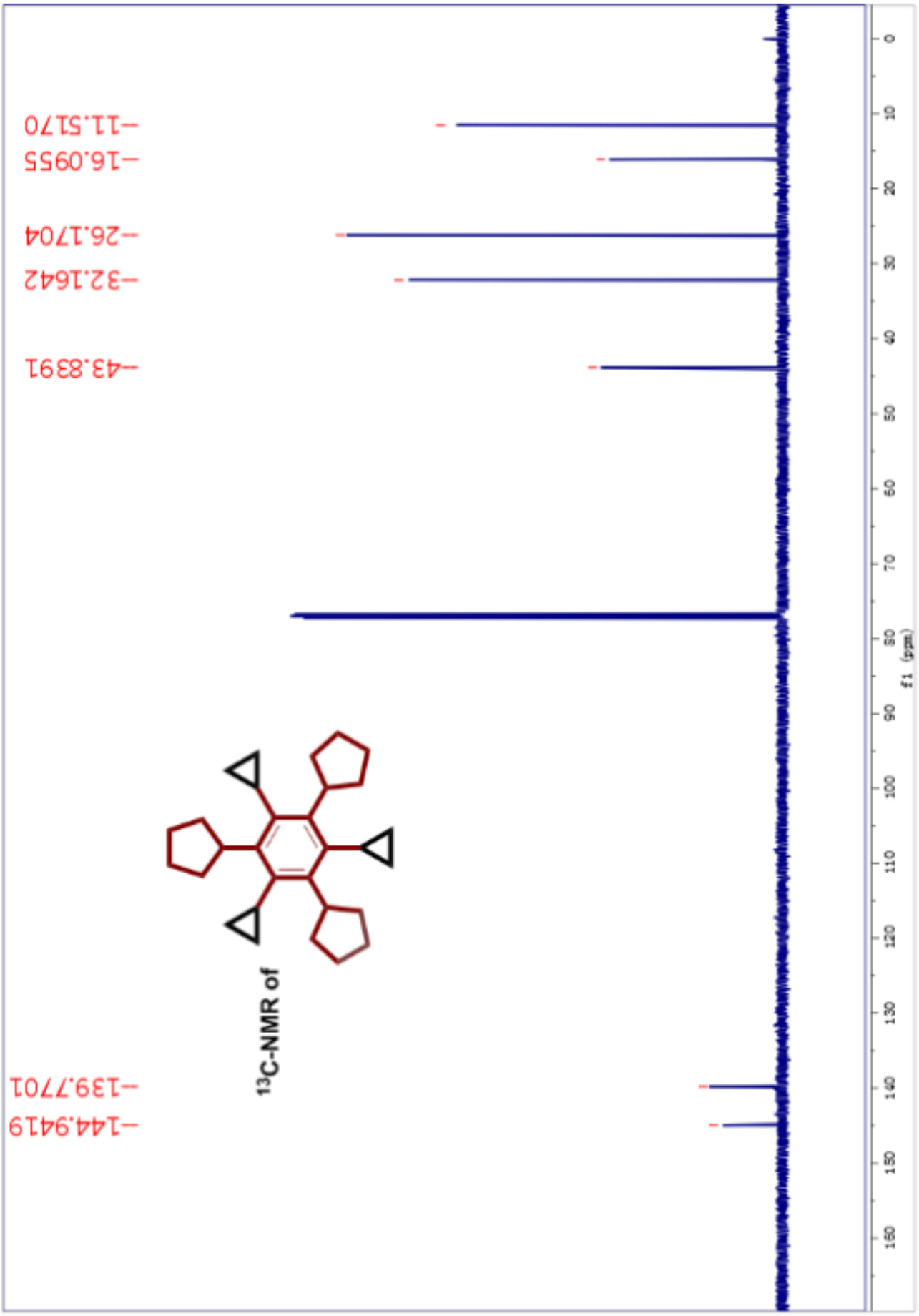

1.2737
1.2797
1.2859
1.2992
1.3053
1.3114
1.3247
1.3304
1.3525
1.3575
1.3636
1.3770
1.3827
1.3892
1.4018
1.4081
1.4335
1.6734
1.6971
1.7705
1.7957
1.8671
1.8736
1.8851
1.8936
1.9036
1.9289
1.9352
1.9542
2.3680
2.4623
2.9241
2.9428
2.9491
2.9552
2.9741
3.7808
6.5702
3.16
2.07
1.14
4.00
3.07
3.11
1.03
3.07
2.04
f1 (ppm)
^{1}H-NMR of


156.7381
137.5726
135.6620
115.3776
113.8878
54.9936
41.0148
30.7774
27.8419
26.4400
22.2855
^{13}C-NMR of
f1 (ppm)


1.7390
1.7696
1.8669
1.8842
1.9065
1.9452
2.3352
3.6255
3.6439
3.6627
3.6817
3.7005
6.10
18.13
9.00
3.00
f1 (ppm)
1H-NMR of

140.7779
133.2525
^{13}C-NMR of
40.5686
31.3386
27.2754
18.9402
f1 (ppm)


0.4163
0.8871
0.9038
1.5821
1.5924
1.6108
1.6912
1.8962
1.9022
1.9221
1.9374
2.1248
2.1452
3.8804
3.9044
3.9277
3.9508
3.9748
6.01
6.00
6.06
6.01
9.03
6.02
3.00
f1 (ppm)
1H-NMR of


11.5170
16.0955
26.1704
32.1642
43.8391
139.7701
144.9419
^{13}C-NMR of
f1 (ppm)