Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Visible-light-induced remote C(sp^3)-H sulfonylvinylation: assembly of cyanoalkylated vinyl sulfones

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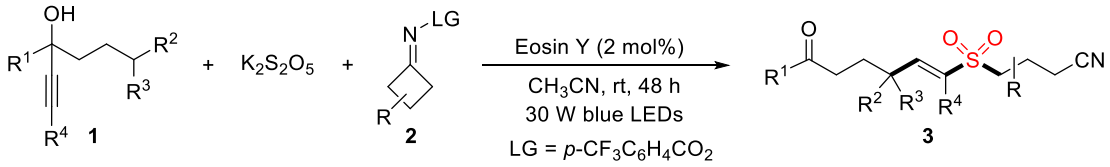
Supporting Information

1. General experimental methods (S2).
2. General experimental procedure and characterization data (S2-S10).
3. ^{1}H and ^{13}C NMR spectra of compounds **3** (S11-S51).

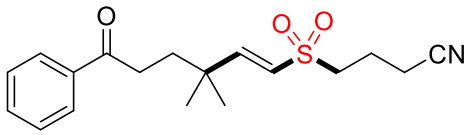
General experimental methods:

Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32-63 µm, standard grade). Analytical thin-layer chromatography was performed using glass plates pre-coated with 0.25 mm 230-400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25-35 °C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument.

*General experimental procedure for the reaction of propargyl alcohols **1**, cycloketone oxime esters **2** and $K_2S_2O_5$*

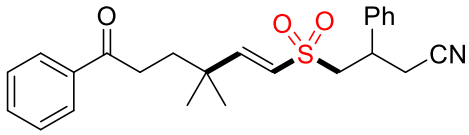


Cycloketone oxime ester **2** (0.3 mmol) was added to a mixture of propargyl alcohol **1** (0.2 mmol), $K_2S_2O_5$ (0.4 mmol) and Eosin Y (0.004 mmol, 2 mol %) in CH_3CN (2.0 mL) under N_2 atmosphere. The mixture was placed around a 30 W blue LEDs and stirred under blue light irradiation for 48 hours at room temperature. After completion of reaction as indicated by TLC, the solvent was evaporated. The residue was diluted with ethyl acetate. The solution was successively washed with a saturated aqueous Na_2CO_3 and brine, and dried over Na_2SO_4. Subsequently, the solvent was concentrated under reduced pressure, and the residue was purified directly by flash column chromatography (*n*-hexane/ethyl acetate = 2:1-1:1) to give the corresponding products **3**.



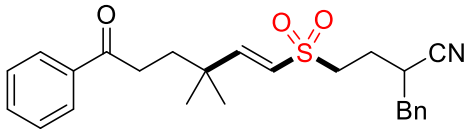
(*E*)-4-((3,3-Dimethyl-6-oxo-6-phenylhex-1-en-1-yl)sulfonyl)butanenitrile (**3a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.8 Hz, 2H), 7.56 (t, *J* = 7.3 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 6.93 (d, *J* = 15.4 Hz, 1H), 6.26 (d, *J* = 15.4 Hz, 1H), 3.10 (t, *J* = 7.4 Hz, 2H), 2.91 (t, *J* = 8.0 Hz, 2H), 2.59 (t, *J* = 7.0 Hz, 2H), 2.21 – 2.10 (m, 2H), 1.91 (t, *J* = 7.2 Hz, 2H), 1.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 158.5, 136.7, 133.3, 128.7, 128.0, 125.6, 118.2, 52.7, 37.1, 35.4, 33.6, 26.1, 18.9, 16.2; HRMS (ESI) calcd for $C_{18}H_{23}NNaO_3S^+$ (M+Na$^+$): 356.1296, found: 356.1302.



(*E*)-4-((3,3-Dimethyl-6-oxo-6-phenylhex-1-en-1-yl)sulfonyl)-3-phenylbutanenitrile (**3b**)

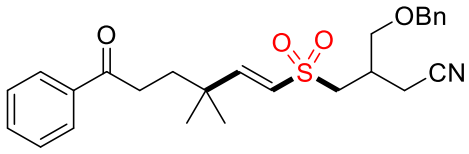
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 7.3 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.40 -7.31 (m, 3H), 7.29 – 7.24 (m, 2H), 6.82 (d, *J* = 15.4 Hz, 1H), 5.88 (d, *J* = 15.4 Hz, 1H), 3.72 – 3.61 (m, 1H), 3.54 – 3.34 (m, 2H), 2.97 – 2.87 (m, 2H), 2.83 (t, *J* = 8.0 Hz, 2H), 1.8 (t, *J* = 8.0 Hz, 2H), 1.02 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 157.7, 139.1, 136.7, 133.3, 129.5, 128.7, 128.6, 128.0, 127.3, 126.3, 117.3, 58.7, 36.9, 36.7, 35.4, 33.6, 26.0, 25.9, 24.7; HRMS (ESI) calcd for $C_{24}H_{27}NNaO_3S^+$ (M+Na$^+$): 432.1609, found: 432.1611.



(*E*)-2-Benzyl-4-((3,3-dimethyl-6-oxo-6-phenylhex-1-en-1-yl)sulfonyl)butanenitrile (**3c**)

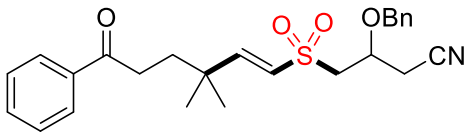
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 –7.89 (m, 2H), 7.60 – 7.54 (m, 1H), 7.51-7.44 (m, 2H), 7.39 – 7.29 (m, 5H), 6.85 (d, *J* = 15.4 Hz, 1H), 6.22 (d, *J* = 15.4 Hz, 1H), 4.73 – 4.57 (m, 2H), 4.37 – 4.27 (m, 1H), 3.40 (dd, *J* = 14.6, 7.1 Hz, 1H), 3.22 (dd, *J* = 14.6, 5.1 Hz, 1H), 2.87 – 2.77 (m, 3H), 2.69 (dd, *J* = 17.1, 4.9 Hz, 1H), 1.87 – 1.76 (m, 2H), 1.03 (d, *J* = 2.6

Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 156.9, 136.7, 136.2, 133.3, 128.8, 128.7, 128.6, 128.3, 128.0, 127.4, 116.1, 72.7, 70.0, 58.6, 36.9, 35.4, 33.6, 26.0, 25.8, 23.0; HRMS (ESI) calcd for $C_{25}H_{29}NNaO_3S^+$ (M+Na^+): 446.1766, found: 446.1761.



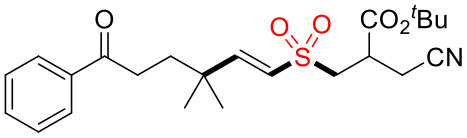
(*E*)-4-(Benzyloxy)-3-(((3,3-dimethyl-6-oxo-6-phenylhex-1-en-1-yl)sulfonyl)methyl)butanenitrile (**3d**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.7 Hz, 2H), 7.59 – 7.53 (m, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.38 – 7.28 (m, 5H), 6.92 (d, *J* = 15.4 Hz, 1H), 6.26 (d, *J* = 15.4 Hz, 1H), 4.52 (s, 2H), 3.64 – 3.54 (m, 2H), 3.16 (dd, *J* = 14.4, 4.8 Hz, 1H), 3.02 (dd, *J* = 14.4, 7.5 Hz, 1H), 2.93 – 2.85 (m, 2H), 2.76 (dd, *J* = 5.9, 2.1 Hz, 2H), 2.72 – 2.63 (m, 1H), 1.89 (t, *J* = 8.0 Hz 2H), 1.16 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 158.1, 137.3, 136.7, 133.3, 128.7, 128.6, 128.1, 128.0, 127.8, 126.1, 117.5, 73.5, 70.1, 54.6, 37.1, 35.4, 33.6, 31.4, 26.1, 26.1, 19.4; HRMS (ESI) calcd for $C_{26}H_{31}NNaO_4S^+$ (M+Na^+): 476.1871, found: 476.1867.



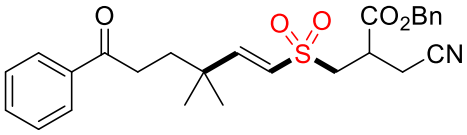
(*E*)-3-(Benzyloxy)-4-((3,3-dimethyl-6-oxo-6-phenylhex-1-en-1-yl)sulfonyl)butanenitrile (**3e**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.6 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.38 – 7.28 (m, 5H), 6.84 (d, *J* = 15.4 Hz, 1H), 6.23 (d, *J* = 15.4 Hz, 1H), 4.63 – 4.56 (m, 2H), 4.35–4.26 (m, 1H), 3.40 (dd, *J* = 14.6, 7.2 Hz, 1H), 3.23 (dd, *J* = 14.6, 5.0 Hz, 1H), 2.85 – 2.79 (m, 3H), 2.69 (dd, *J* = 17.1, 4.9 Hz, 1H), 1.84 – 1.77 (m, 2H), 1.02 (d, *J* = 3.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 156.8, 136.7, 136.3, 133.3, 128.7, 128.5, 128.3, 128.0, 127.5, 116.2, 72.7, 70.0, 58.6, 36.9, 35.4, 33.6, 26.1, 25.8, 23.0; HRMS (ESI) calcd for $C_{25}H_{29}NNaO_4S^+$ (M+Na^+): 462.1715, found: 462.1708.



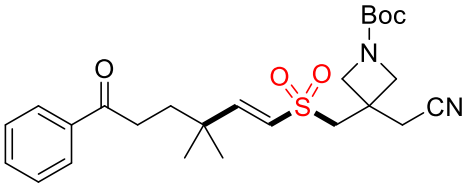
tert-Butyl (*E*)-3-cyano-2-(((3,3-dimethyl-6-oxo-6-phenylhex-1-en-1-yl)sulfonyl)methyl)propanoate (**3f**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.8 Hz, 2H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 6.95 (d, *J* = 15.4Hz, 1H), 6.30 (d, *J* = 15.4 Hz, 1H), 3.61 – 3.52 (m, 1H), 3.27 – 3.16 (m, 2H), 2.92 (dd, *J* = 14.3, 6.7 Hz, 4H), 1.91 (t, *J* = 8.0 Hz, 2H), 1.50 (s, 9H), 1.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 168.4, 158.5, 136.7, 133.3, 128.7, 128.0, 126.1, 116.7, 83.9, 53.9, 37.1, 37.0, 35.4, 33.6, 27.8, 26.1, 26.1, 19.6; HRMS (ESI) calcd for $C_{23}H_{31}NNaO_5S^+$ (M+Na$^+$): 456.1821, found: 456.1825.



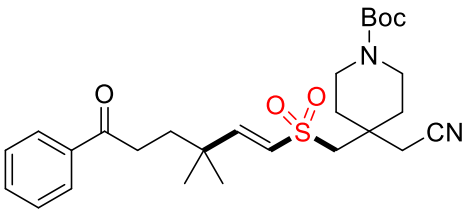
Benzyl (*E*)-3-cyano-2-(((3,3-dimethyl-6-oxo-6-phenylhex-1-en-1-yl)sulfonyl)methyl)propanoate (**3g**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.3 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.36 (s, 5H), 6.93 (d, *J* = 15.4 Hz, 1H), 6.28 (d, *J* = 15.4 Hz, 1H), 5.20 (d, *J* = 1.6 Hz, 2H), 3.60 (dd, *J* = 14.0, 4.4 Hz, 1H), 3.40 – 3.32 (m, 1H), 3.27 (dd, *J* = 14.1, 8.0 Hz, 1H), 2.98 (d, *J* = 5.6 Hz, 2H), 2.93 – 2.85 (m, 2H), 1.94 – 1.83 (m, 2H), 1.15 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 169.4, 158.9, 136.7, 134.5, 133.3, 128.9, 128.8, 128.7, 128.6, 128.0, 125.9, 116.5, 68.4, 53.8, 37.2, 36.5, 35.4, 33.6, 26.1, 19.4; HRMS (ESI) calcd for $C_{26}H_{29}NNaO_5S^+$ (M+Na$^+$): 490.1664, found: 490.1669.



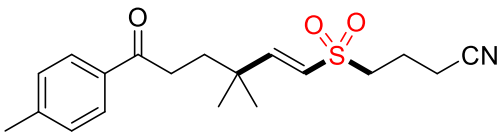
tert-Butyl (*E*)-3-(cyanomethyl)-3-(((3,3-dimethyl-6-oxo-6-phenylhex-1-en-1-yl)sulfonyl)methyl)azetidine-1-carboxylate (**3h**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.2 Hz, 2H), 7.62 – 7.54 (m, 1H), 7.47 (t, *J* = 7.3 Hz, 2H), 6.95 (d, *J* = 15.4 Hz, 1H), 6.31 (d, *J* = 15.4 Hz, 1H), 4.03 (d, *J* = 8.9 Hz, 2H), 3.84 (d, *J* = 9.3 Hz, 2H), 3.39 (s, 2H), 3.12 (s, 2H), 2.92 (t, *J* = 7.2 Hz, 2H), 1.92 (t, *J* = 7.6 Hz, 2H), 1.44 (s, 9H), 1.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 158.4, 155.9, 136.7, 133.3, 128.8, 128.0, 127.1, 116.6, 80.5, 58.6, 37.1, 35.3, 33.5, 28.3, 26.0, 25.8; HRMS (ESI) calcd for $C_{25}H_{34}N_2NaO_5S^+$ (M+Na^+): 497.2086, found: 497.2085.



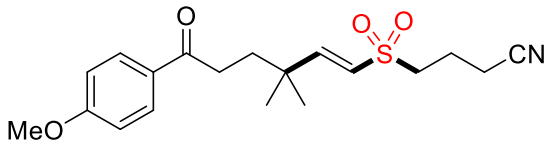
tert-Butyl (*E*)-4-(cyanomethyl)-4-(((3,3-dimethyl-6-oxo-6-phenylhex-1-en-1-yl)sulfonyl)methyl)piperidine-1-carboxylate (**3i**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 6.92 (d, *J* = 15.3 Hz, 1H), 6.33 (d, *J* = 15.3 Hz, 1H), 3.66 – 3.52 (m, 2H), 3.40 – 3.28 (m, 2H), 3.15 (s, 2H), 2.92 (t, *J* = 7.5 Hz, 4H), 1.95 – 1.84 (m, 4H), 1.72 – 1.63 (m, 2H), 1.46 (s, 9H), 1.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 157.4, 154.6, 136.7, 133.3, 128.7, 128.0, 127.8, 117.1, 80.1, 57.9, 37.0, 35.9, 35.4, 34.5, 33.6, 28.4, 26.6, 26.0; HRMS (ESI) calcd for $C_{27}H_{38}N_2NaO_5S^+$ (M+Na^+): 525.2399, found: 525.2403.



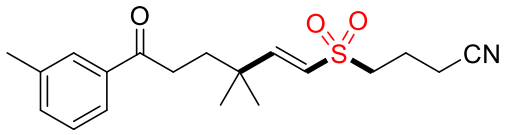
(*E*)-4-((3,3-Dimethyl-6-oxo-6-(*p*-tolyl)hex-1-en-1-yl)sulfonyl)butanenitrile (**3j**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.2 Hz, 2H), 7.31 – 7.23 (m, 2H), 6.93 (d, *J* = 15.4 Hz, 1H), 6.26 (d, *J* = 15.4 Hz, 1H), 3.10 (t, *J* = 7.2 Hz, 2H), 2.93 – 2.83 (m, 2H), 2.59 (t, *J* = 7.0 Hz, 2H), 2.41 (s, 3H), 2.20 – 2.10 (m, 2H), 1.94 – 1.86 (m, 2H), 1.17 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 158. 6, 144.1, 134.2, 129.4, 128.1, 118.2, 52.7, 37.1, 35.5, 33.5, 26.1, 21.7 18.9, 16.2; HRMS (ESI) calcd for $C_{19}H_{25}NNaO_3S^+$ (M+Na^+): 370.1453, found: 370.1452.



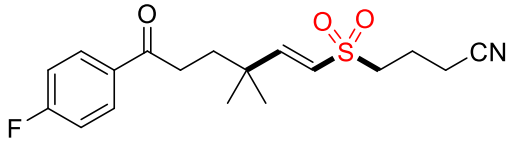
(*E*)-4-((6-(4-Methoxyphenyl)-3,3-dimethyl-6-oxohex-1-en-1-yl)sulfonyl)butanenitrile (**3k**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.85 (m, 2H), 7.00 – 6.87 (m, 3H), 6.27 (d, *J* = 15.4 Hz, 1H), 3.87 (s, 3H), 3.11 (t, *J* = 7.4 Hz, 2H), 2.90 – 2.81 (m, 2H), 2.64 – 2.55 (m, 2H), 2.21 – 2.09 (m, 2H), 1.93 – 1.85 (m, 2H), 1.17 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 163.6, 158.6, 130.3, 129.7, 125.5, 118.3, 113.9, 55.5, 52.7, 37.1, 35.6, 33.2, 26.1, 18.9, 16.2; HRMS (ESI) calcd for $C_{19}H_{25}NNaO_4S^+$ ($M+Na^+$): 386.1402, found: 386.1405.



(*E*)-4-((3,3-Dimethyl-6-oxo-6-(*m*-tolyl)hex-1-en-1-yl)sulfonyl)butanenitrile (**3l**)

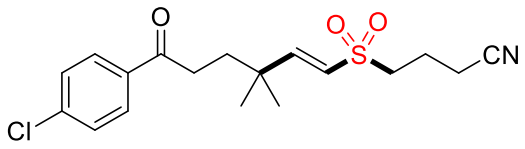
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.7 Hz, 2H), 7.41 – 7.32 (m, 2H), 6.93 (d, *J* = 15.4 Hz, 1H), 6.27 (d, *J* = 15.4 Hz, 1H), 3.11 (t, *J* = 7.2 Hz, 2H), 2.93 – 2.86 (m, 2H), 2.59 (t, *J* = 7.0 Hz, 2H), 2.42 (s, 3H), 2.20 – 2.10 (m, 2H), 1.94 – 1.86 (m, 2H), 1.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 158.5, 138.6, 136.7, 134.1, 128.6, 128.5, 125.5, 125.2, 118.3, 52.7, 37.1, 35.4, 33.7, 26.1, 21.4, 18.9, 16.2; HRMS (ESI) calcd for $C_{19}H_{25}NNaO_3S^+$ ($M+Na^+$): 370.1453, found: 370.1452.



(*E*)-4-((6-(4-Fluorophenyl)-3,3-dimethyl-6-oxohex-1-en-1-yl)sulfonyl)butanenitrile (**3m**)

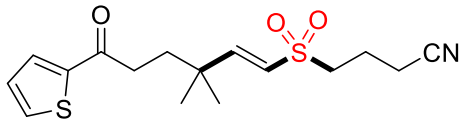
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.93 (m, 2H), 7.14 (t, *J* = 8.2 Hz, 2H), 6.93 (d, *J* = 15.4 Hz, 1H), 6.28 (d, *J* = 15.4 Hz, 1H), 3.13 (t, *J* = 7.2 Hz, 2H), 2.88 (t, *J* = 7.3 Hz, 2H), 2.61 (t, *J* = 6.9 Hz, 2H), 2.22 – 2.12 (m, 2H), 1.90 (t, *J* = 7.5 Hz, 2H), 1.18 (s, 6H); ^{13}C NMR (100

MHz, $CDCl_3$) δ 197.6, 165.8 (d, *J* = 255.0 Hz), 158.4, 133.1 (d, *J* = 3.1 Hz), 130.7 (d, *J* = 9.4 Hz), 125.6, 118.2, 115.8 (d, *J* = 21.9 Hz), 52.7, 37.1, 35.4, 33.5, 26.1, 18.9, 16.3; HRMS (ESI) calcd for $C_{18}H_{22}FNNaO_3S^+$ ($M+Na^+$): 374.1202, found: 374.1198.



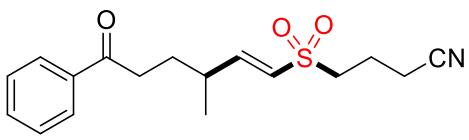
(*E*)-4-((6-(4-Chlorophenyl)-3,3-dimethyl-6-oxohex-1-en-1-yl)sulfonyl)butanenitrile (**3n**)

^1H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.6 Hz, 2H), 7.45 (d, *J* = 8.6 Hz, 2H), 6.93 (d, *J* = 15.4 Hz, 1H), 6.26 (d, *J* = 15.4 Hz, 1H), 3.12 (t, *J* = 7.6 Hz, 2H), 2.92 – 2.83 (m, 2H), 2.62 (t, *J* = 7.0 Hz, 2H), 2.24 – 2.13 (m, 2H), 1.94 – 1.86 (m, 2H), 1.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.0, 158.4, 139.8, 135.0, 129.4, 129.1, 125.7, 118.2, 52.7, 37.1, 35.3, 33.6, 26.1, 18.8, 16.3; HRMS (ESI) calcd for $C_{18}H_{22}ClNO_3S^+$ ($M+Na^+$): 390.0907, found: 390.0903.



(*E*)-4-((3,3-Dimethyl-6-oxo-6-(thiophen-2-yl)hex-1-en-1-yl)sulfonyl)butanenitrile (**3o**)

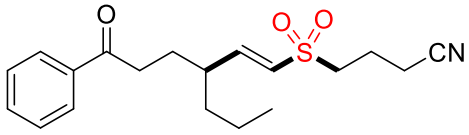
^1H NMR (400 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 23.3, 3.9 Hz, 2H), 7.15 (t, *J* = 4.3 Hz, 1H), 6.92 (d, *J* = 15.4 Hz, 1H), 6.27 (d, *J* = 15.4 Hz, 1H), 3.12 (t, *J* = 7.4 Hz, 2H), 2.84 (t, *J* = 8.0 Hz, 2H), 2.61 (t, *J* = 7.0 Hz, 2H), 2.22 – 2.11 (m, 2H), 1.91 (t, *J* = 8.0 Hz, 2H), 1.17 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.2, 158.3, 143.8, 133.9, 132.0, 128.3, 125.7, 118.3, 52.7, 37.1, 35.6, 34.5, 26.1, 18.9, 16.3; HRMS (ESI) calcd for $C_{16}H_{21}NNaO_3S_2^+$ ($M+Na^+$): 362.0861, found: 362.0861.



(*E*)-4-((3-Methyl-6-oxo-6-phenylhex-1-en-1-yl)sulfonyl)butanenitrile (**3p**)

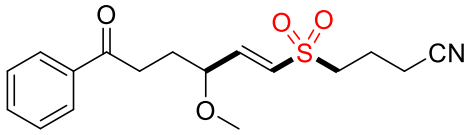
^1H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.90 (m, 2H), 7.63 – 7.54 (m, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 6.91 (dd, *J* = 15.2, 7.8 Hz, 1H), 6.30 (d, *J* = 15.2 Hz, 1H), 3.09 (t, *J* = 7.6 Hz, 2H), 3.00

(t, *J* = 7.2 Hz, 2H), 2.64 – 2.51 (m, 3H), 2.21 – 2.10 (m, 2H), 1.90 (q, *J* = 7.1 Hz, 2H), 1.17 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 154.9, 136.7, 133.3, 128.8, 128.0, 127.0, 118.2, 52.7, 35.7, 35.6, 29.5, 19.1, 18.9, 16.3; HRMS (ESI) calcd for $C_{17}H_{21}NNaO_3S^+$ ($M+Na^+$): 342.1140, found: 342.1141.



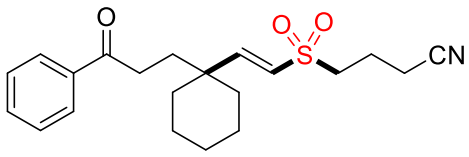
(*E*)-4-((6-Oxo-6-phenyl-3-propylhex-1-en-1-yl)sulfonyl)butanenitrile (**3q**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.3 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 6.78 (dd, *J* = 15.1, 9.4 Hz, 1H), 6.30 (d, *J* = 15.1 Hz, 1H), 3.06 (t, *J* = 7.2 Hz, 2H), 3.02 – 2.92 (m, 2H), 2.58 (t, *J* = 7.0 Hz, 2H), 2.47 –2.35 (m, 1H), 2.18 – 2.09 (m, 2H), 2.08 – 1.97 (m, 1H), 1.87 – 1.77 (m, 1H), 1.60 – 1.49 (m, 1H), 1.48 – 1.36 (m, 1H), 1.36 – 1.25 (m, 2H), 0.92 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 154.0, 136.7, 133.3, 128.8, 128.1, 128.0, 118.2, 52.7, 41.5, 36.2, 35.6, 28.0, 20.3, 18.9, 16.3, 14.0; HRMS (ESI) calcd for $C_{19}H_{25}NNaO_3S^+$ ($M+Na^+$): 370.1453, found: 370.1459.



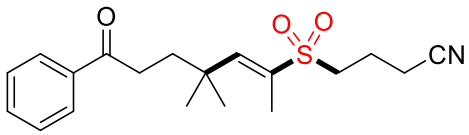
(*E*)-4-((3-Methoxy-6-oxo-6-phenylhex-1-en-1-yl)sulfonyl)butanenitrile (**3r**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.7 Hz, 2H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 6.92 (dd, *J* = 15.1, 4.6 Hz, 1H), 6.56 (d, *J* = 15.1 Hz, 1H), 4.10 – 4.03 (m, 1H), 3.35 (s, 3H), 3.15 – 3.06 (m, 4H), 2.60 (t, *J* = 7.1 Hz, 2H), 2.24 – 2.12 (m, 3H), 2.03 – 1.93 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.1, 149.5, 136.7, 133. 3, 128.7, 128.2, 128.0, 118.1, 78.3, 57.7, 52.6, 33.1, 28.0, 18.8, 16.3; HRMS (ESI) calcd for $C_{17}H_{21}NNaO_4S^+$ ($M+Na^+$): 358.1089, found: 358.1093.



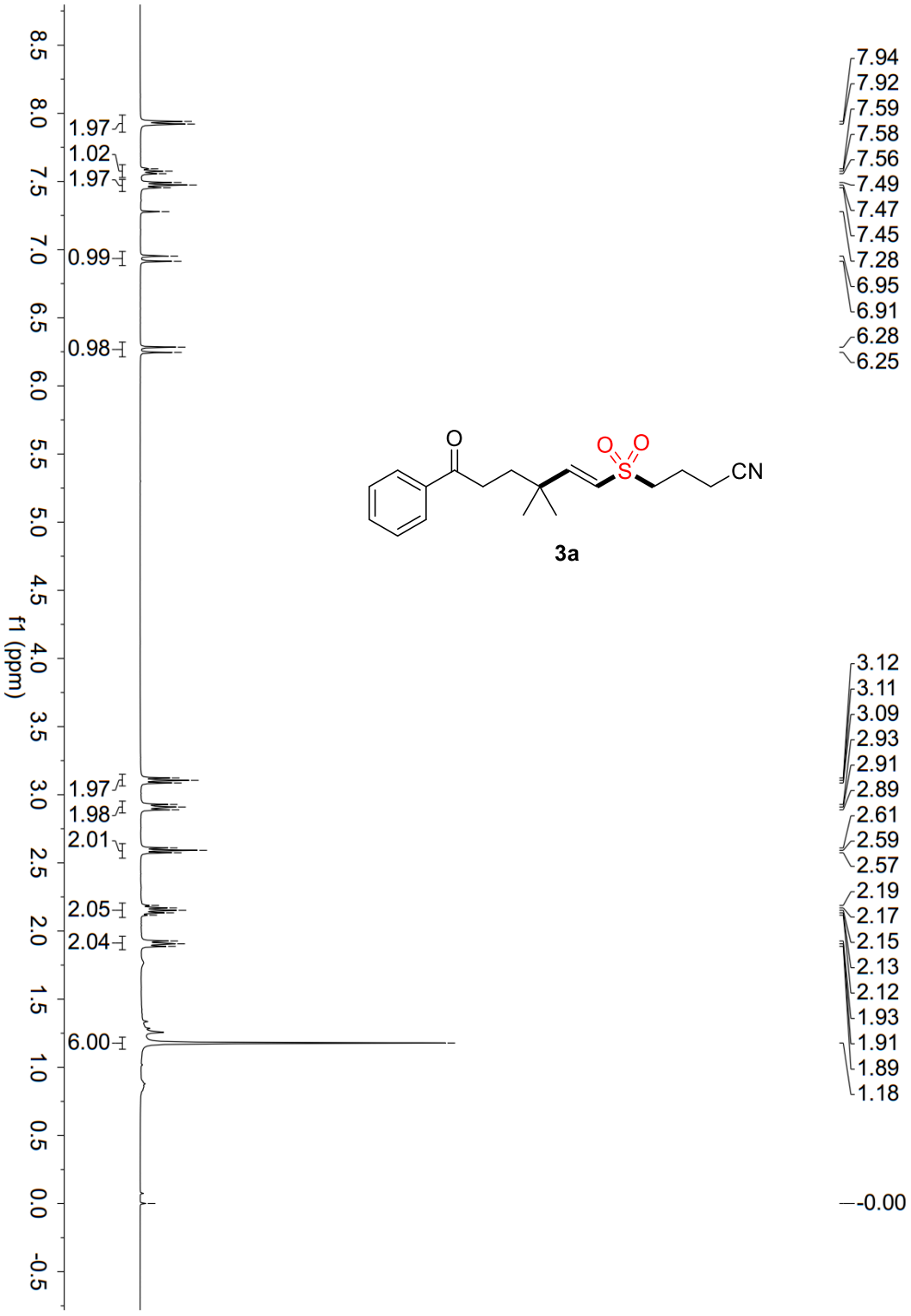
(*E*)-4-((2-(1-(3-Oxo-3-phenylpropyl)cyclohexyl)vinyl)sulfonyl)butanenitrile (**3s**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.5 Hz, 2H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 6.86 (d, *J* = 15.6 Hz, 1H), 6.29 (d, *J* = 15.7 Hz, 1H), 3.11 (t, *J* = 7.3 Hz, 2H), 2.85 (m, *J* = 7.0 Hz, 2H), 2.59 (t, *J* = 7.0 Hz, 2H), 2.22 – 2.11 (m, 2H), 1.92 (t, *J* = 8.0 Hz, 2H), 1.68 – 1.38 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 157.6, 136.7, 133.3, 128.8, 128.0, 127.3, 118.2, 52.8, 40.4, 35.1, 32.7, 25.8, 22.0, 18.9, 16.3; HRMS (ESI) calcd for $C_{21}H_{27}NNaO_3S^+$ (M+Na^+): 396.1609, found: 396.1612.



(*E*)-4-((4,4-Dimethyl-7-oxo-7-phenylhept-2-en-2-yl)sulfonyl)butanenitrile (**3t**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.92 (m, 2H), 7.61 – 7.54 (m, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 6.74 (d, *J* = 1.2 Hz, 1H), 3.05 (t, *J* = 7.6 Hz, 2H), 2.98 – 2.92 (m, 2H), 2.60 (t, *J* = 7.0 Hz, 2H), 2.19 (d, *J* = 1.2 Hz, 3H), 2.18 – 2.09 (m, 2H), 1.99 – 1.93 (m, 2H), 1.27 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 150.4, 136.7, 135.1, 133.3, 128.7, 128.0, 118.3, 49.5, 36.8, 36.7, 34.0, 27.7, 18.8, 16.3, 12.7; HRMS (ESI) calcd for $C_{19}H_{25}NNaO_3S^+$ (M+Na^+): 370.1453, found: 370.1459.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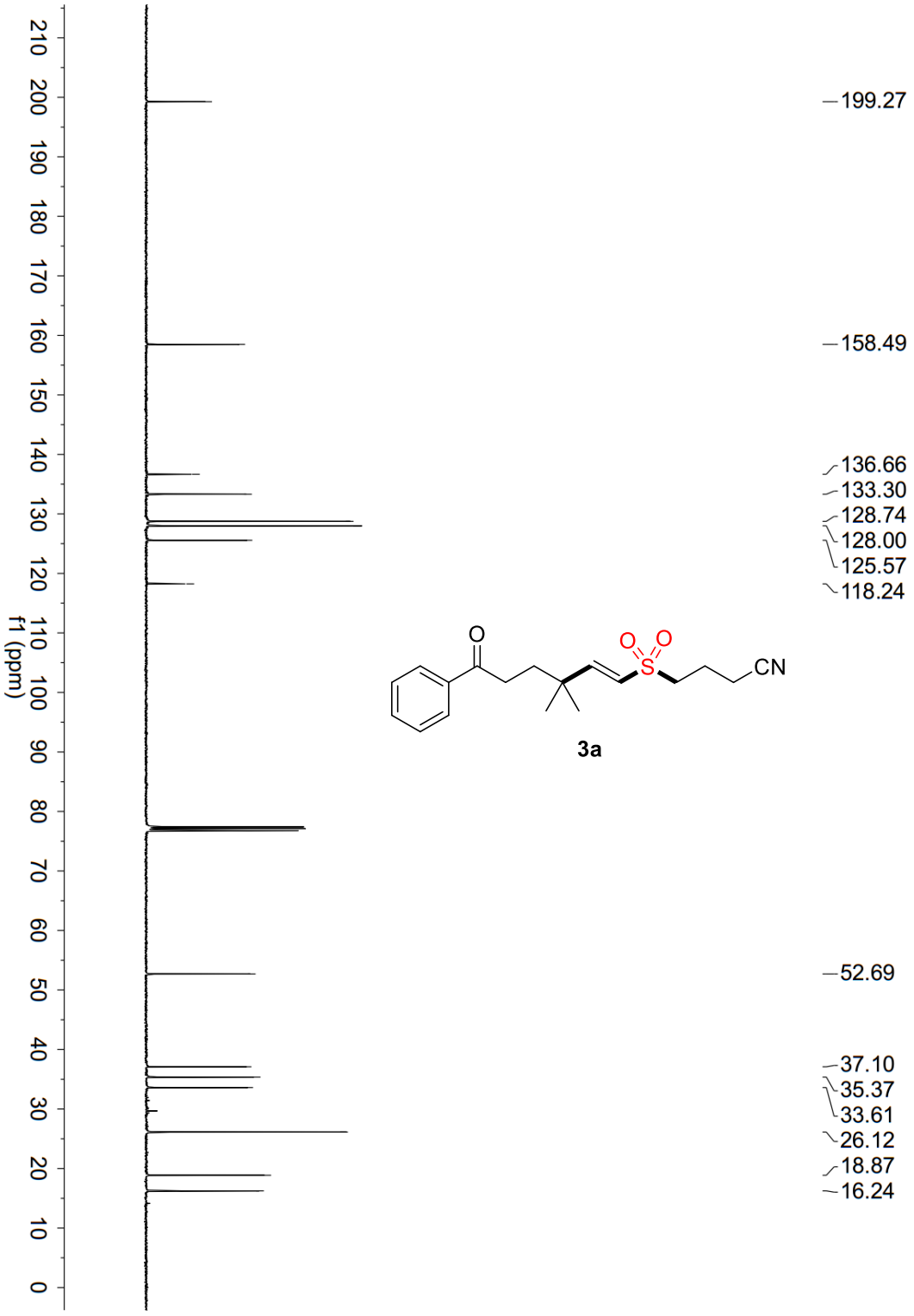
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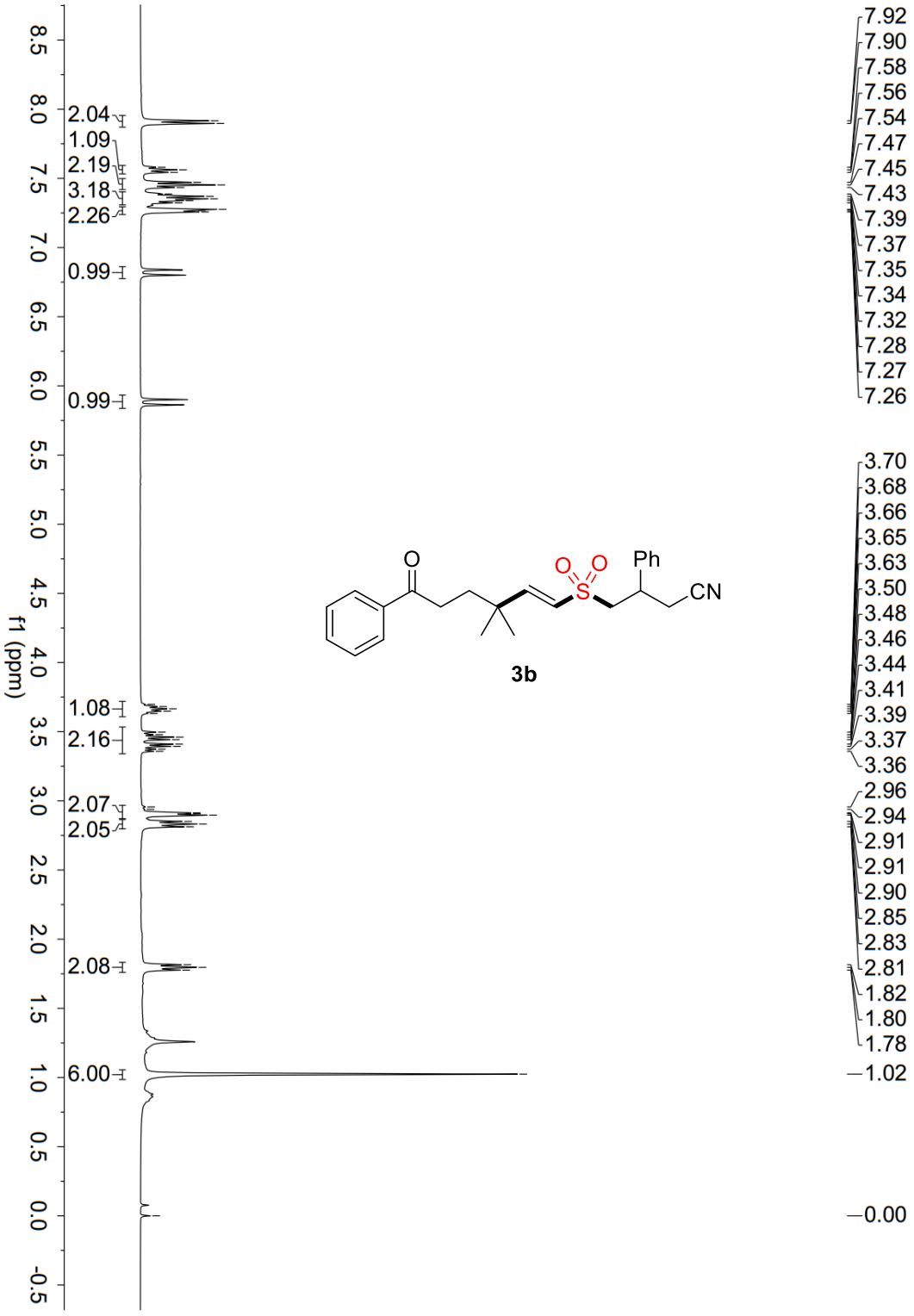
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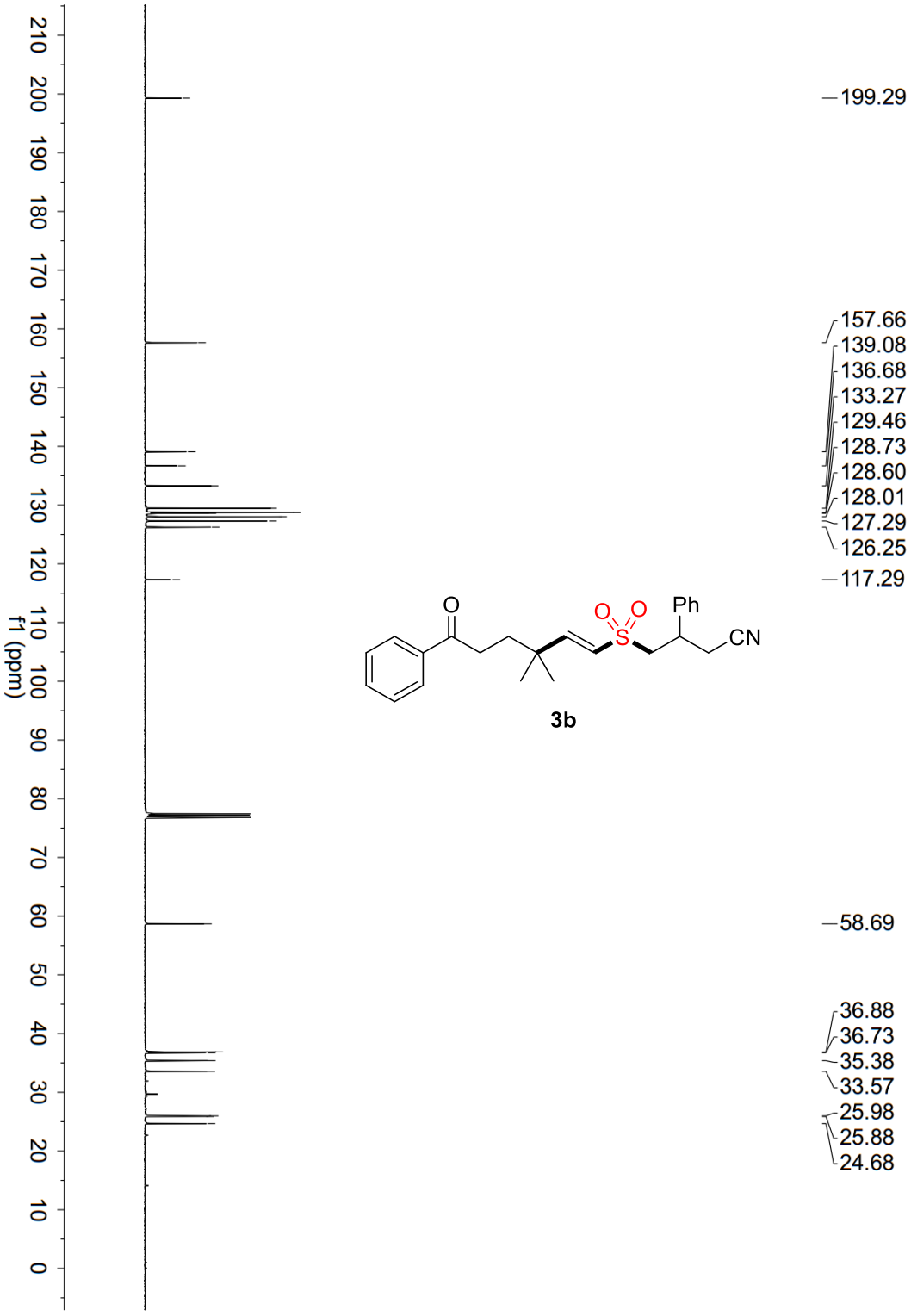
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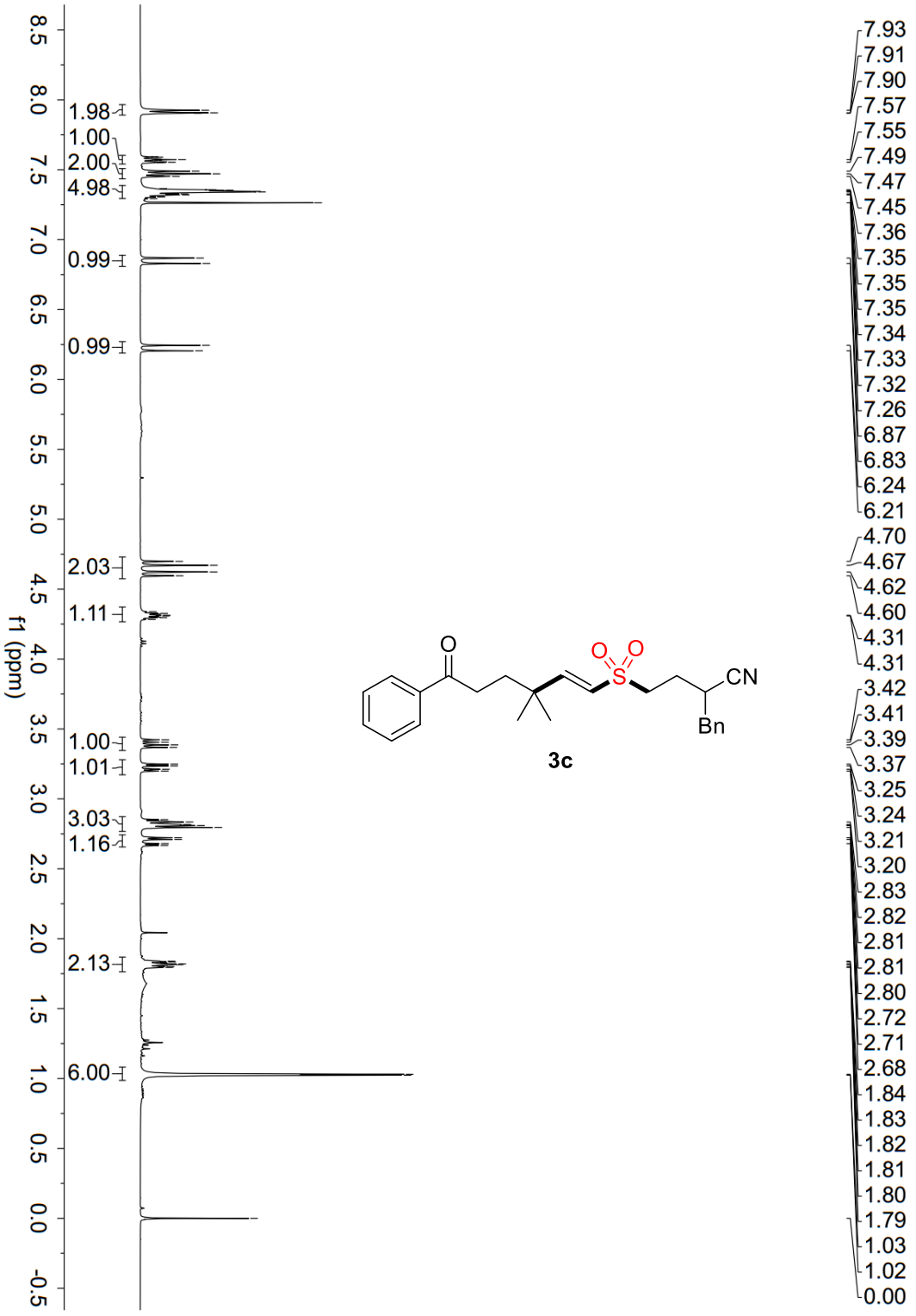
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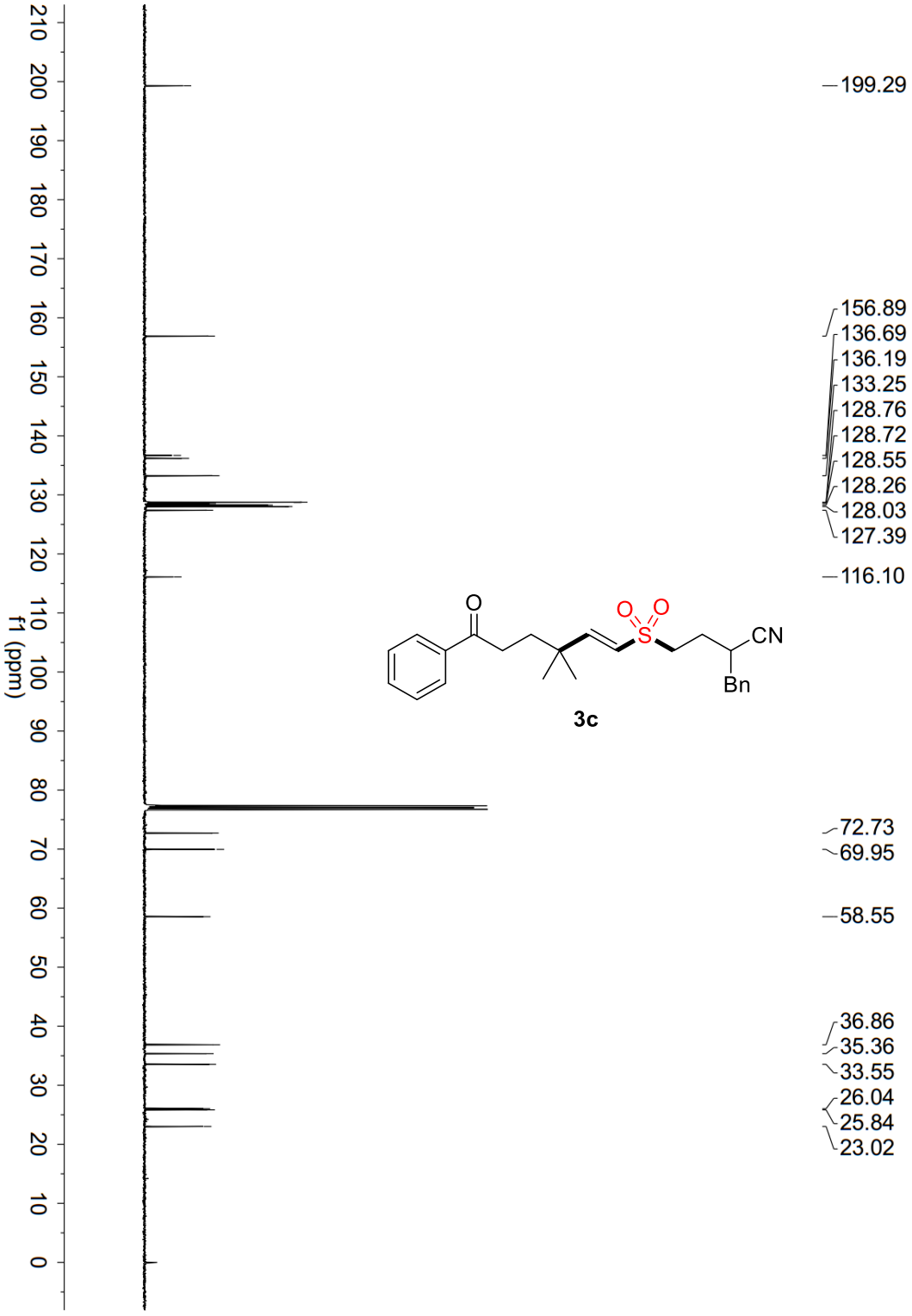
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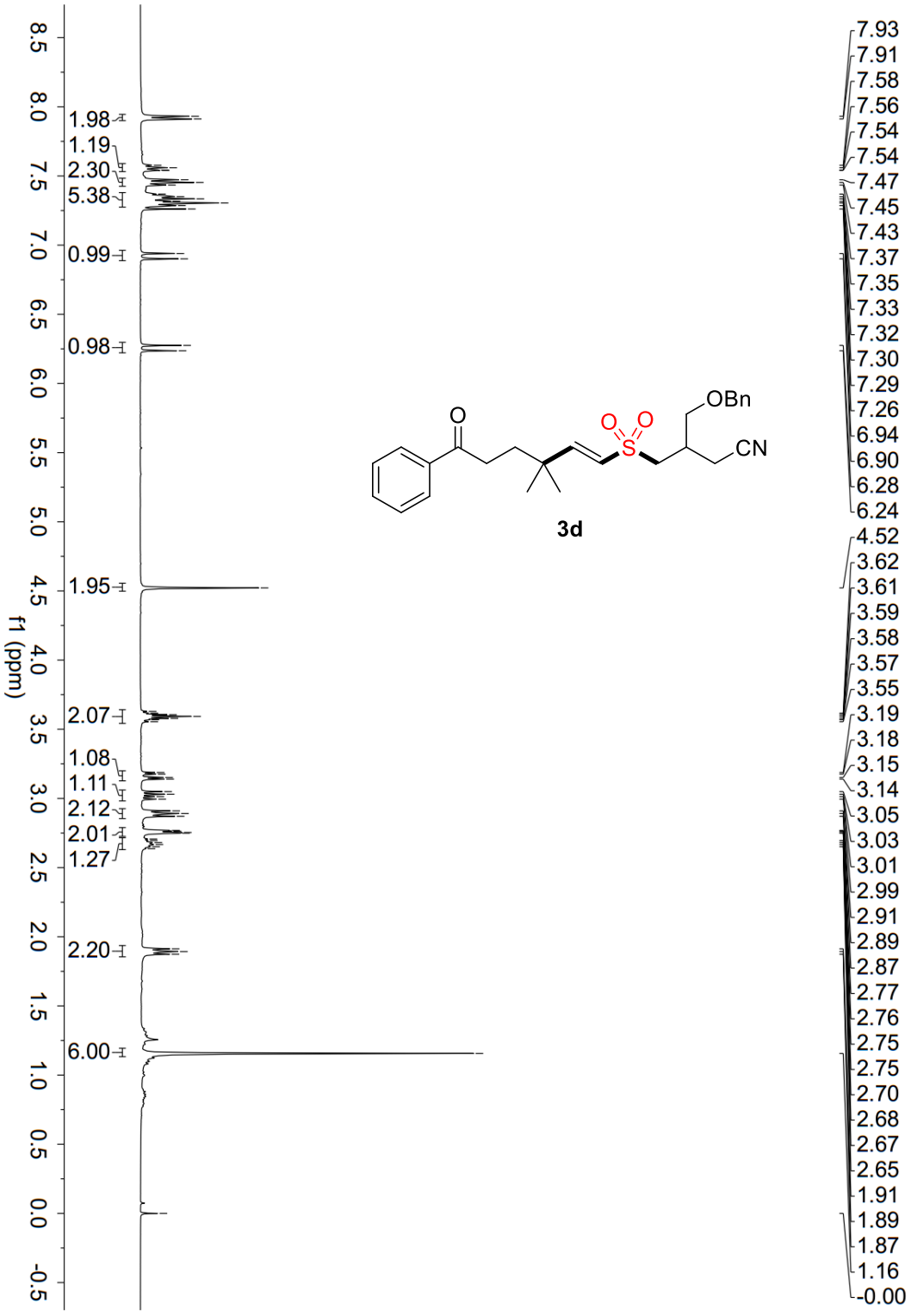
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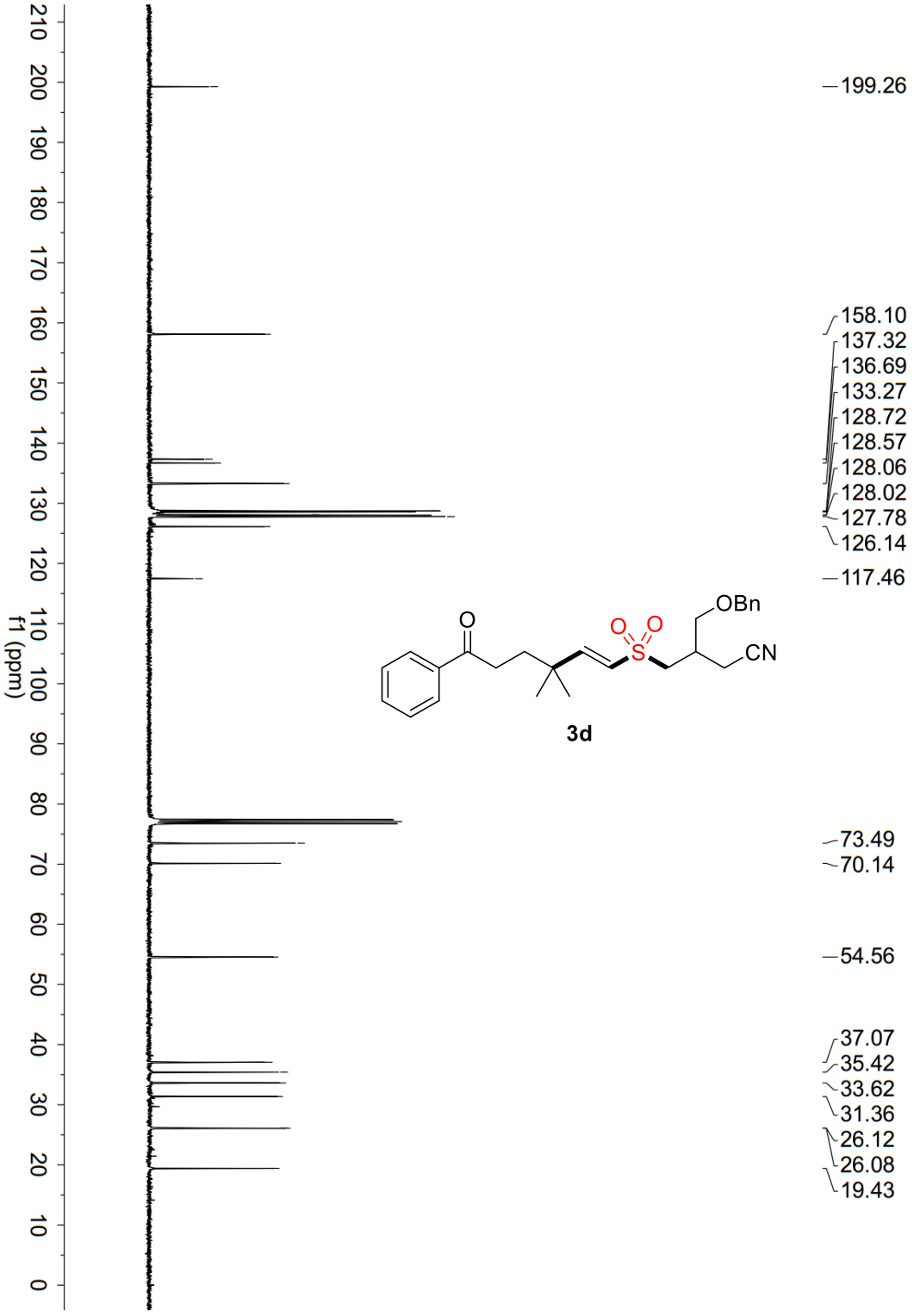
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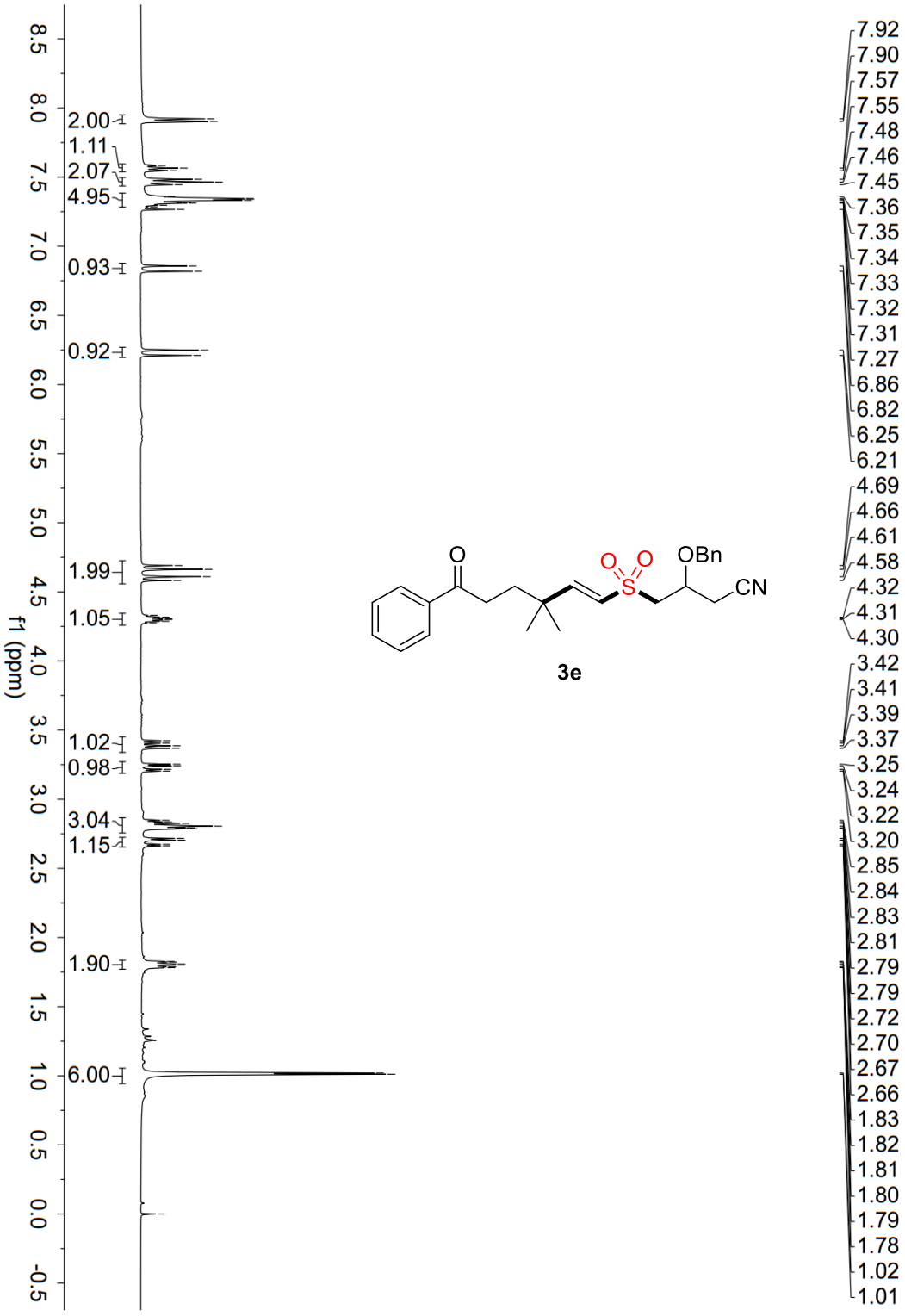
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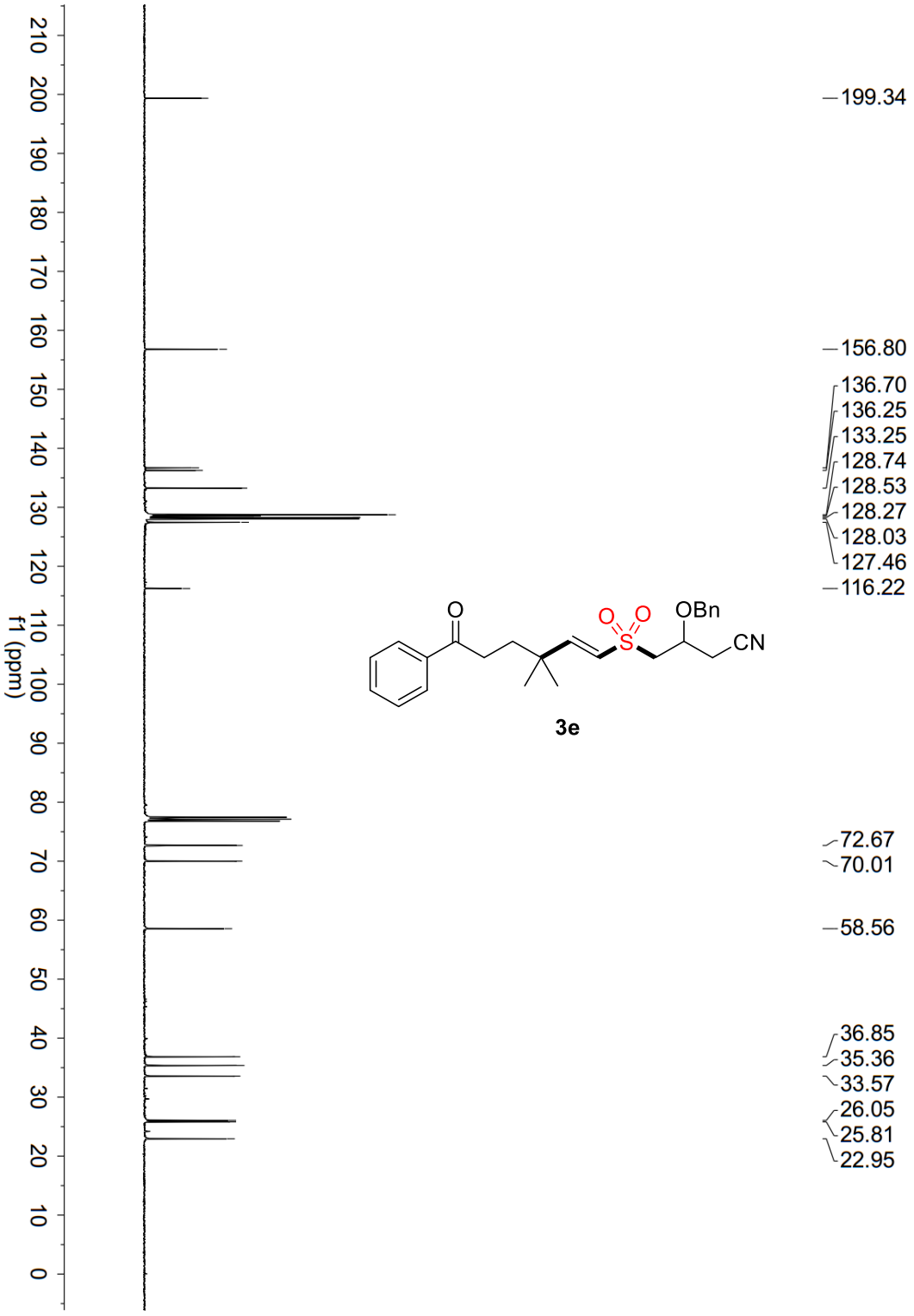
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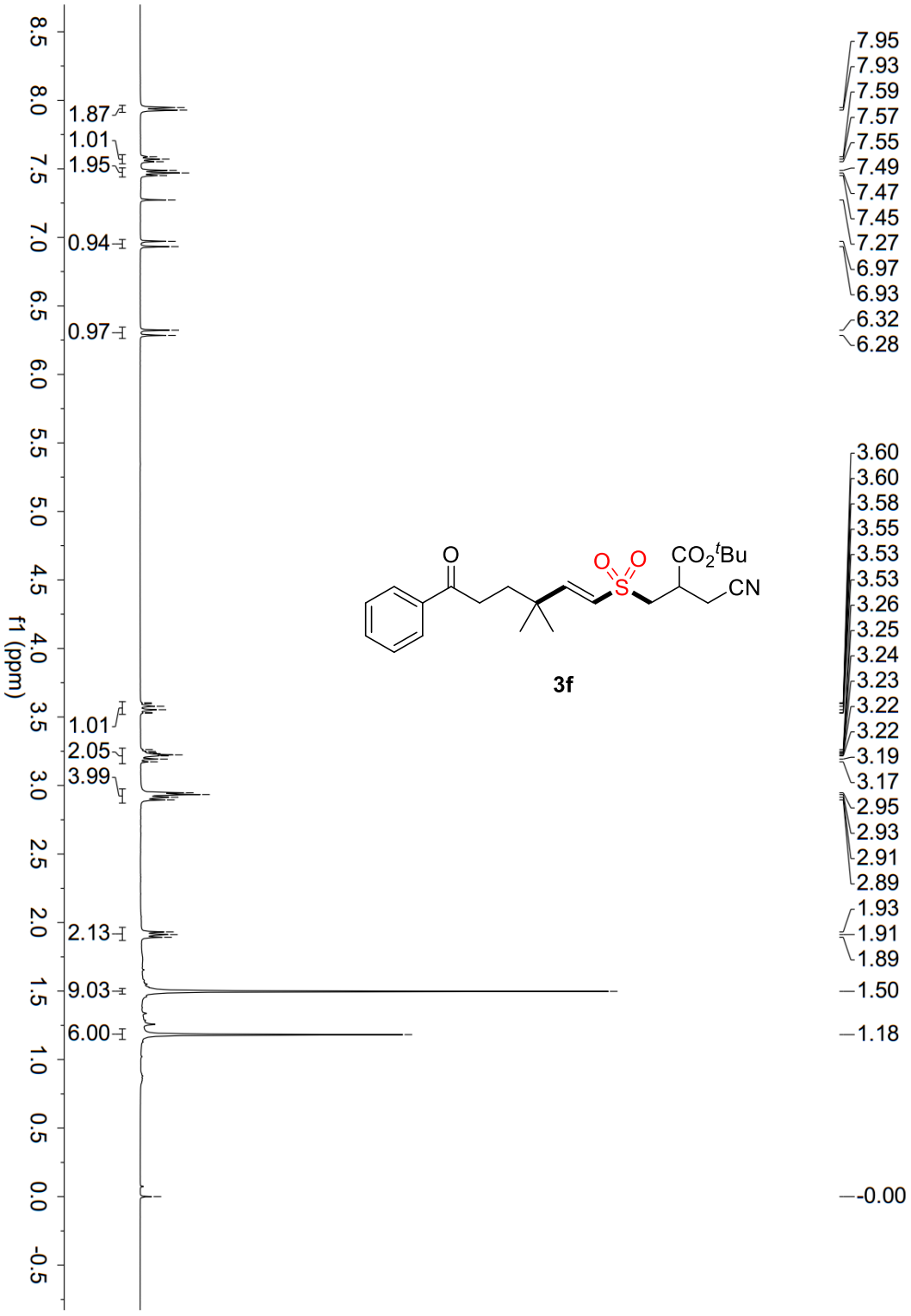
3e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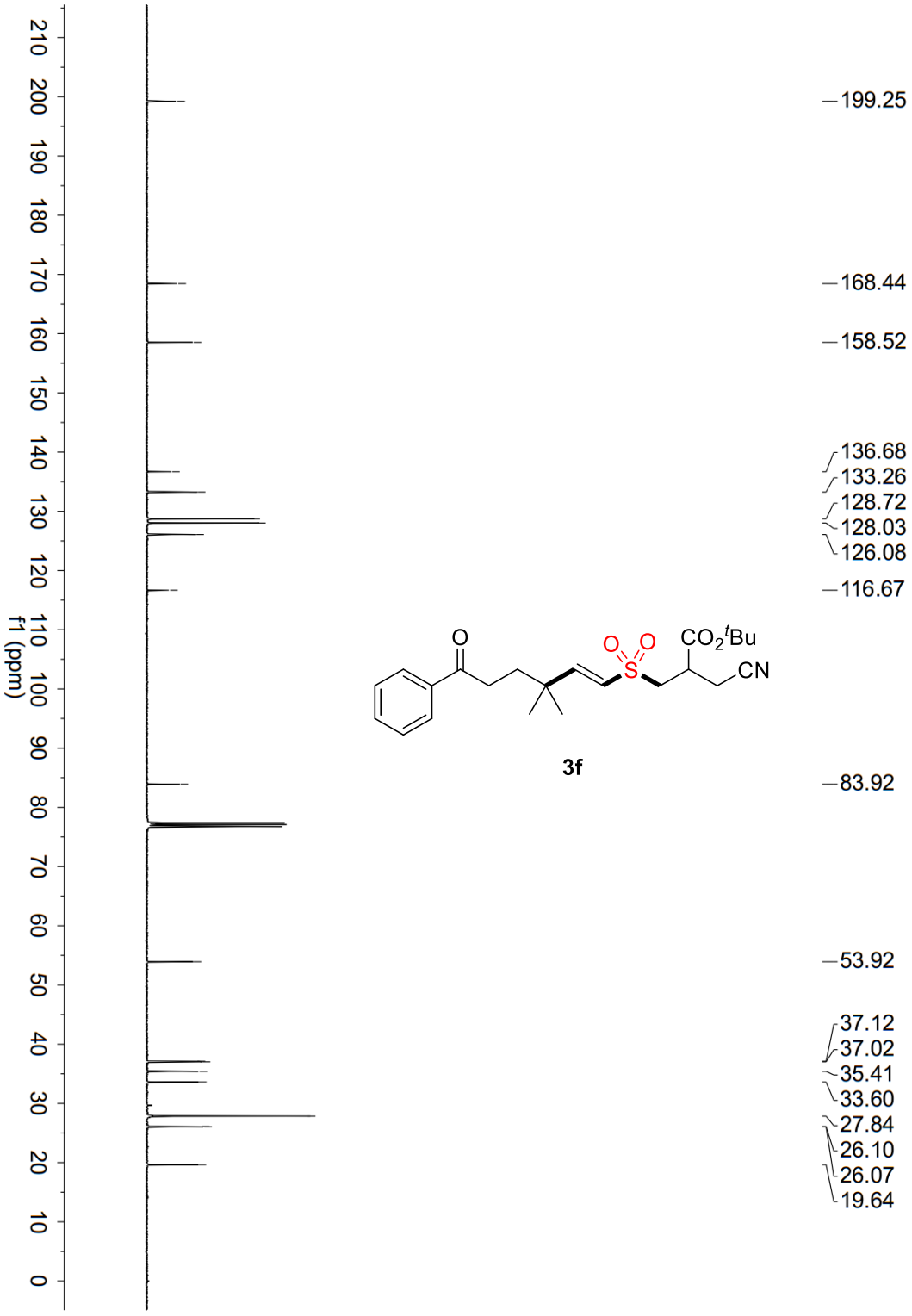
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128.03
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53.92
37.12
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33.60
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26.10
26.07
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O
O
O
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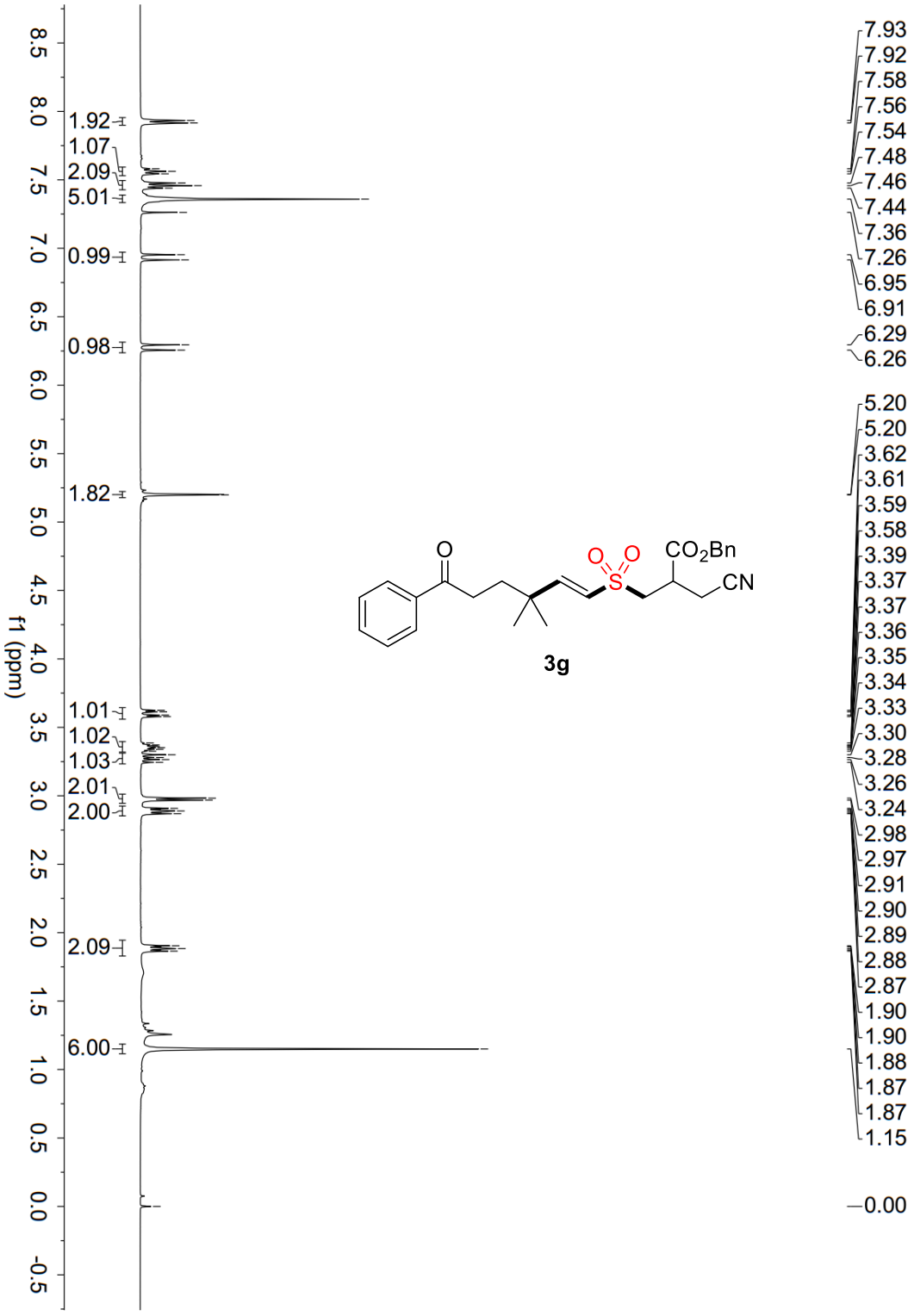
CO2tBu
CN

3f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2.09
5.01
0.99
0.98
1.82
1.01
1.02
1.03
2.01
2.00
2.09
6.00
O
O
O
S
CO2Bn
CN
3g
7.93
7.92
7.58
7.56
7.54
7.48
7.46
7.44
7.36
7.26
6.95
6.91
6.29
6.26
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3.61
3.59
3.58
3.39
3.37
3.37
3.36
3.35
3.34
3.33
3.30
3.28
3.26
3.24
2.98
2.97
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1.88
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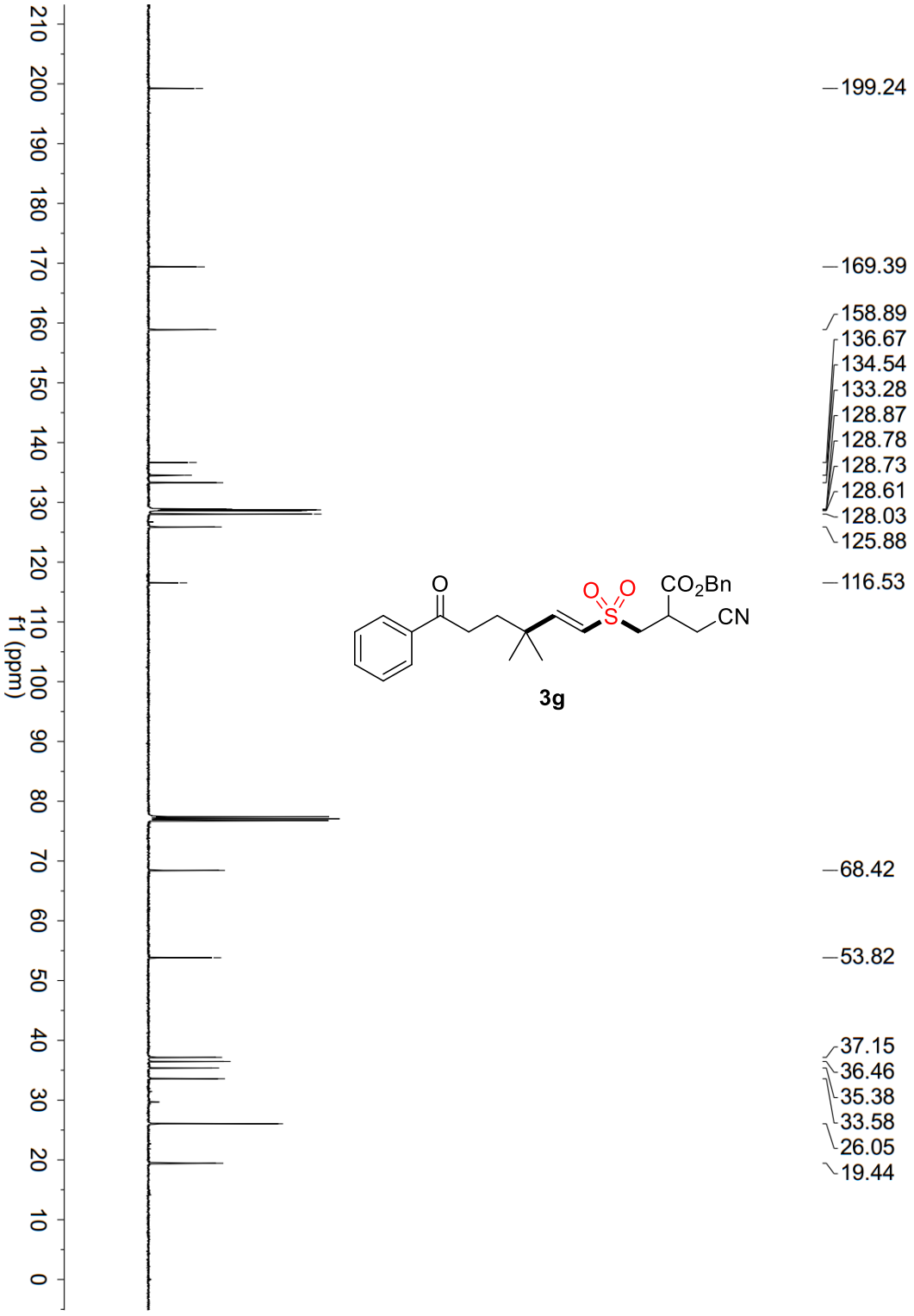
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116.53
68.42
53.82
37.15
36.46
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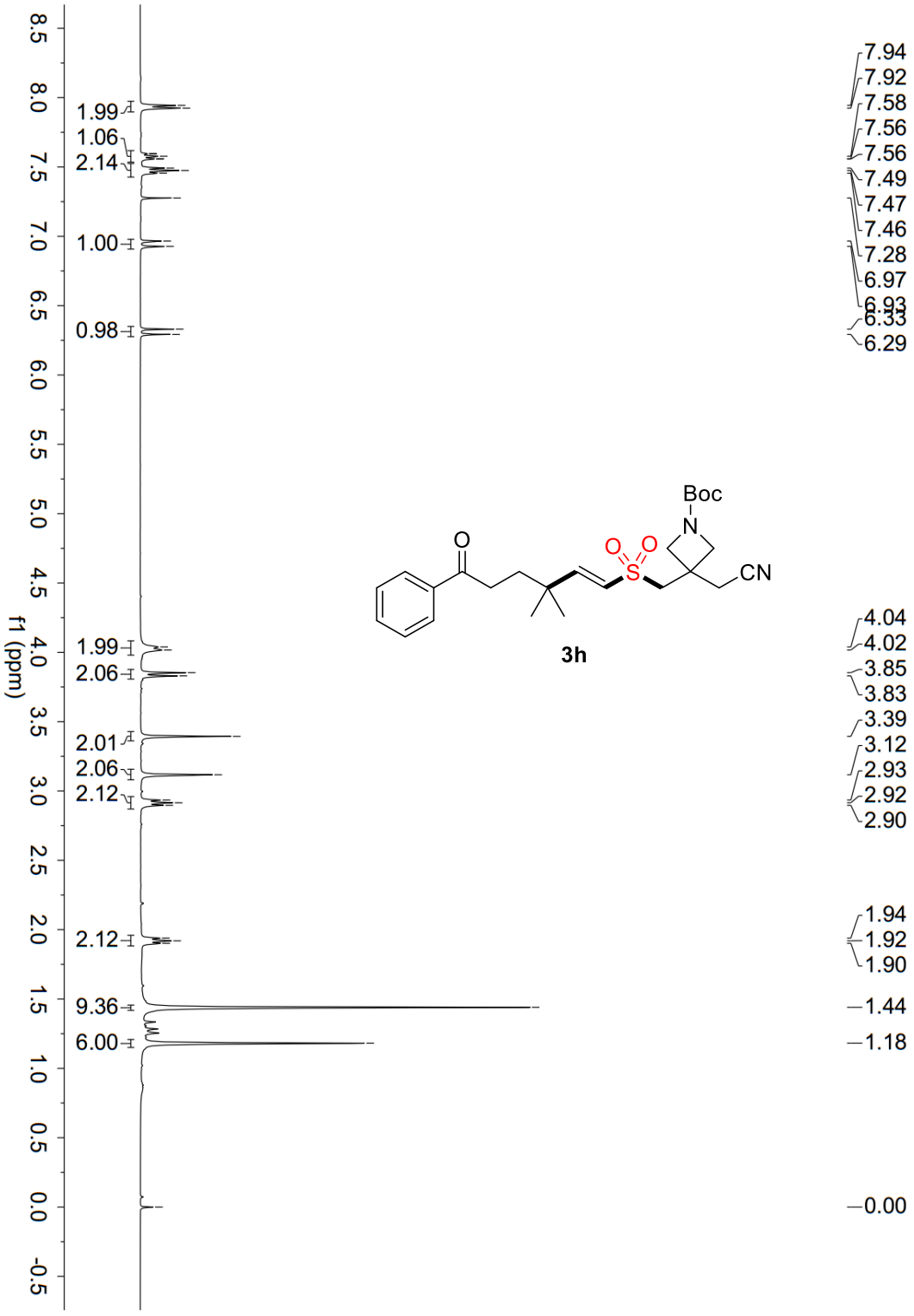
33.58
26.05
19.44
f1 (ppm)
O
O
O
S
CO2Bn
CN
3g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3.0
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1.0
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-0.5
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1.00
0.98
1.99
2.06
2.01
2.06
2.12
2.12
9.36
6.00
7.94
7.92
7.58
7.56
7.56
7.49
7.47
7.46
7.28
6.97
6.93
6.33
6.29
4.04
4.02
3.85
3.83
3.39
3.12
2.93
2.92
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1.90
1.44
1.18
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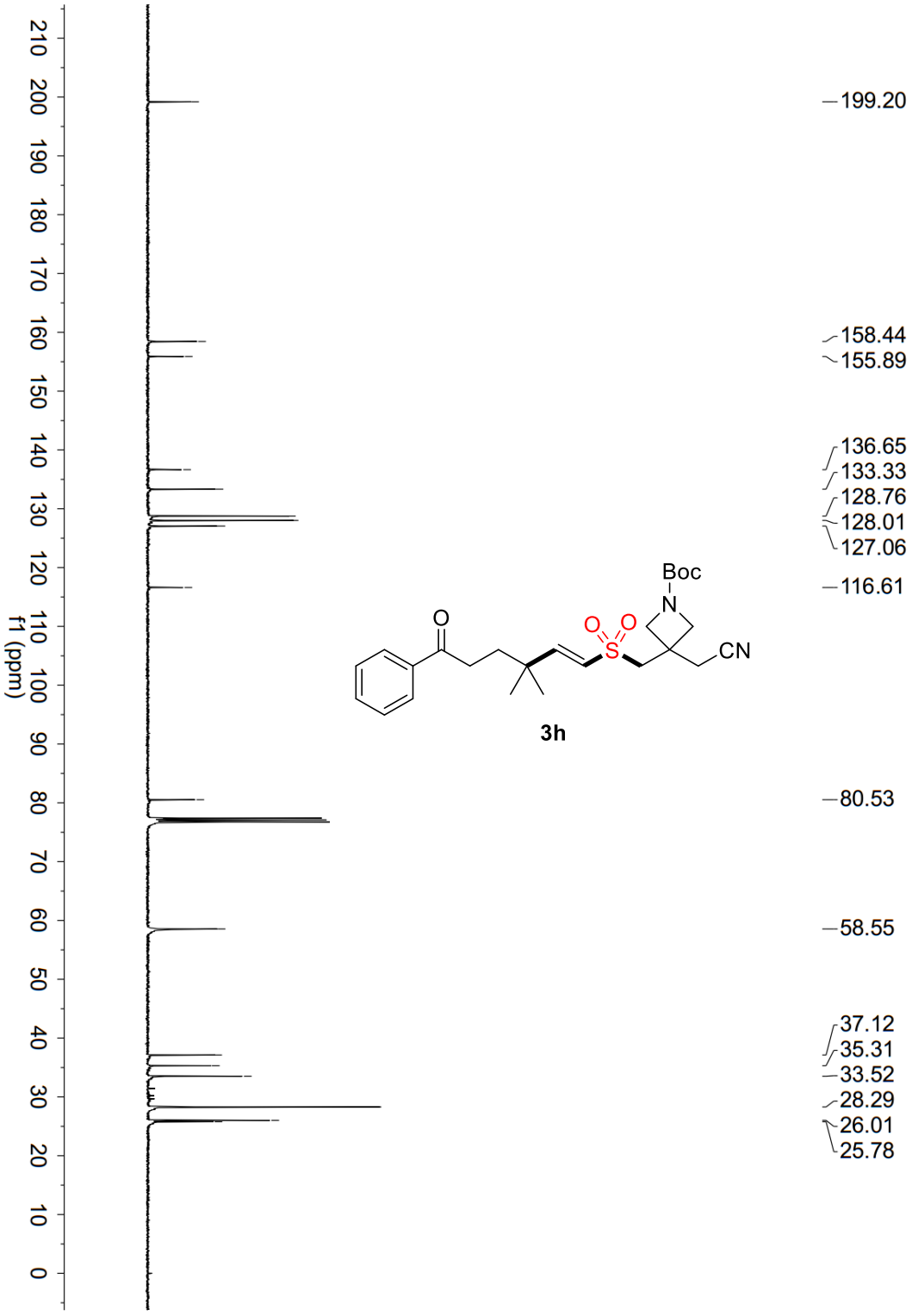
Boc
N
O
O
O
S
CN
3h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199.20
158.44
155.89
136.65
133.33
128.76
128.01
127.06
116.61
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33.52
28.29
26.01
25.78
Boc
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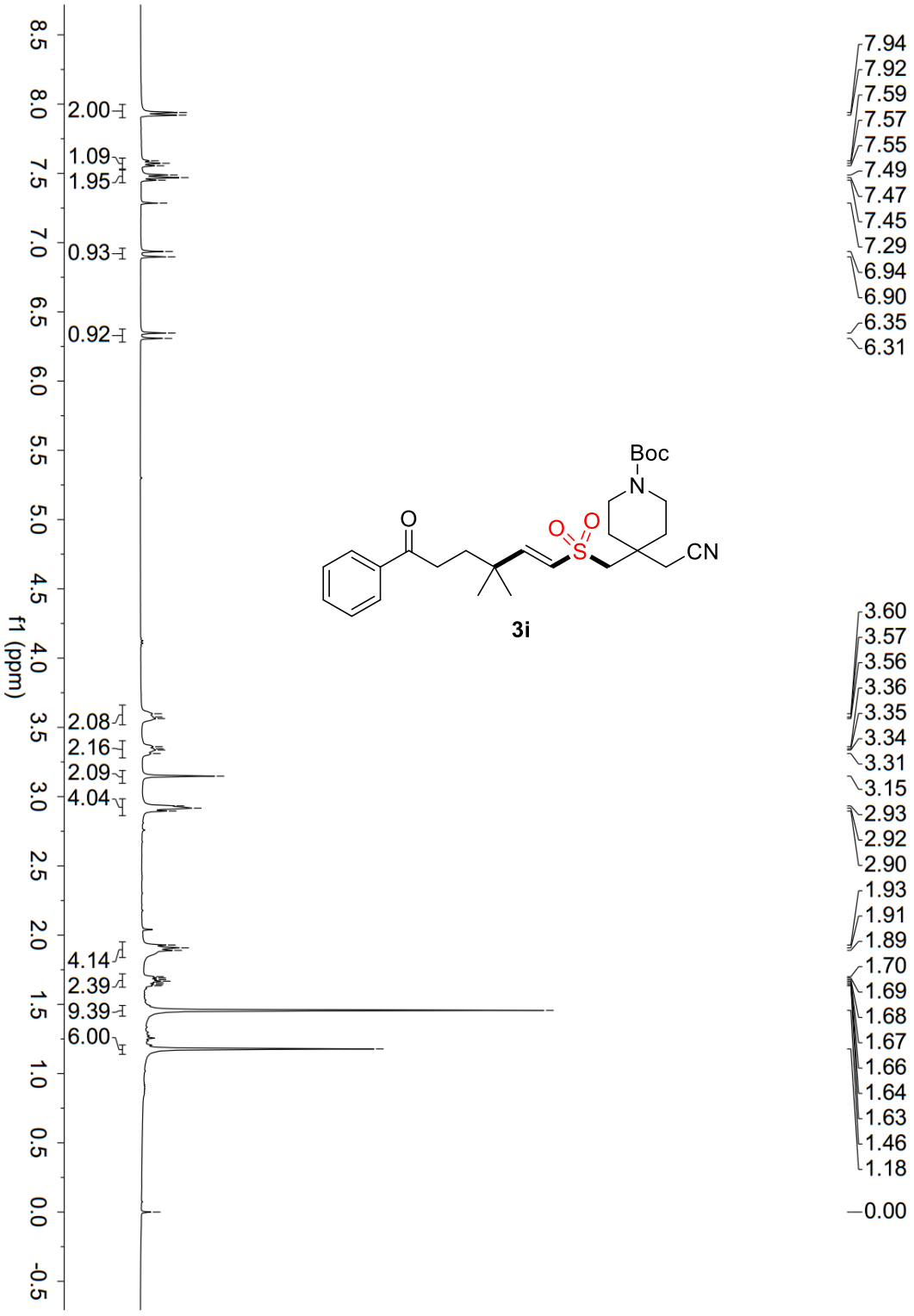
O
O
S
CN

3h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4.0
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3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
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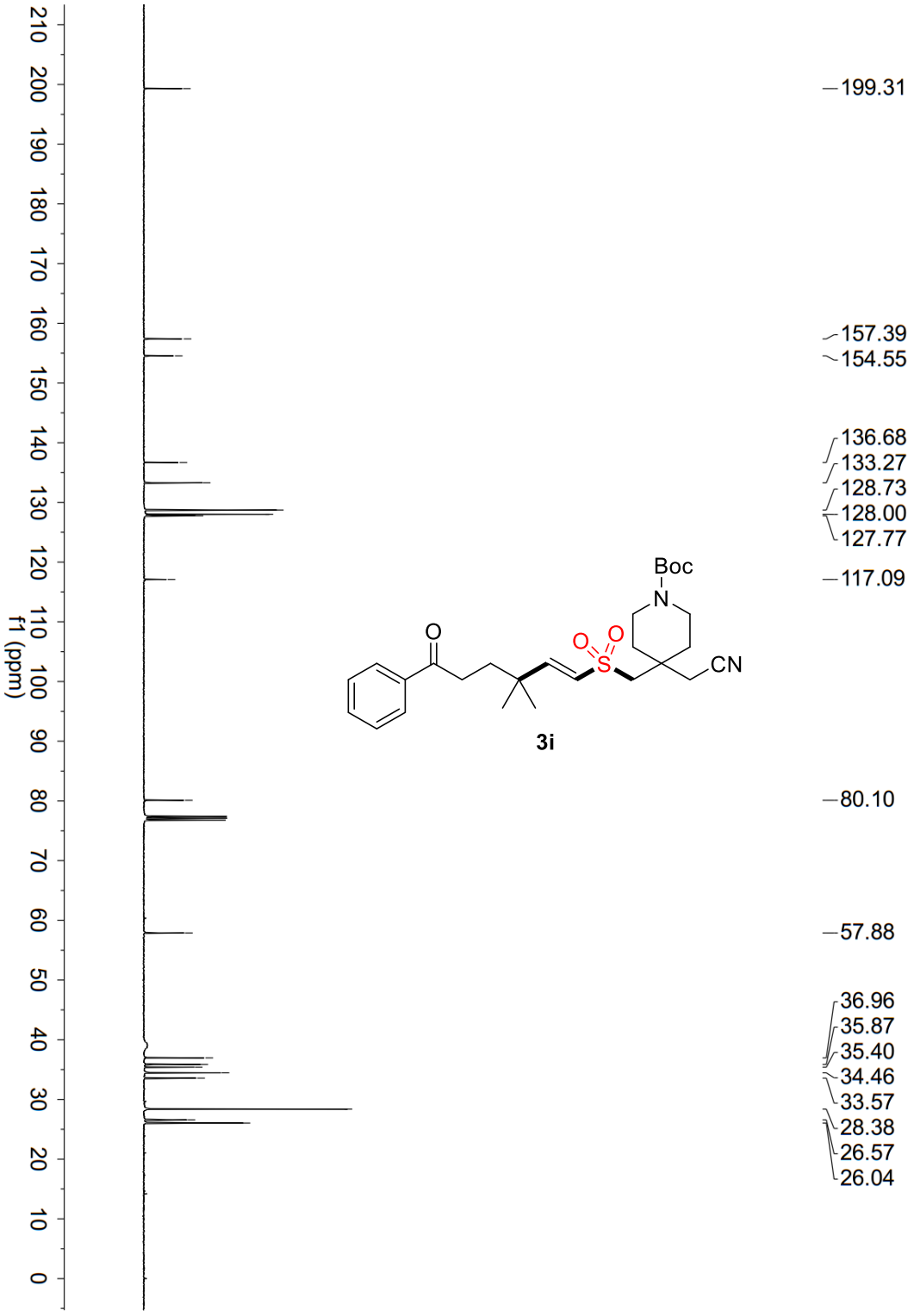
1.09
1.95
0.93
0.92
2.08
2.16
2.09
4.04
4.14
2.39
9.39
6.00
7.94
7.92
7.59
7.57
7.55
7.49
7.47
7.45
7.29
6.94
6.90
6.35
6.31
3.60
3.57
3.56
3.36
3.35
3.34
3.31
3.15
2.93
2.92
2.90
1.93
1.91
1.89
1.70
1.69
1.68
1.67
1.66
1.64
1.63
1.46
1.18
0.00
Boc
N
O
O
O
S
CN

3i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170
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150
140
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120
110
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90
80
70
60
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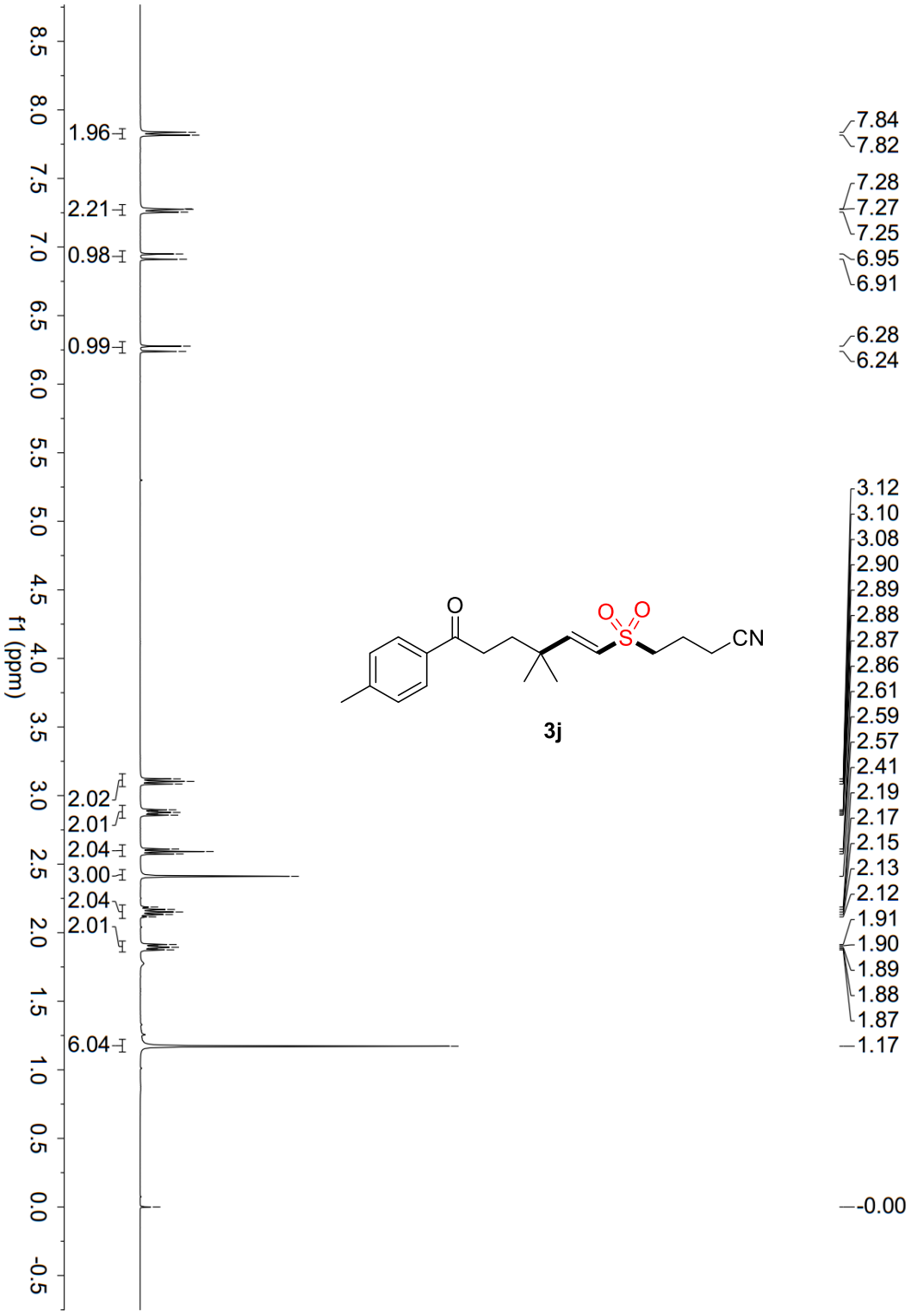
40
30
20
10
0
199.31
157.39
154.55
136.68
133.27
128.73
128.00
127.77
117.09
80.10
57.88
36.96
35.87
35.40
34.46
33.57
28.38
26.57
26.04
Boc
N
O
O
O
S
CN
3i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4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
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2.21
0.98
0.99
2.02
2.01
2.04
3.00
2.04
2.01
6.04
7.84
7.82
7.28
7.27
7.25
6.95
6.91
6.28
6.24
3.12
3.10
3.08
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2.89
2.88
2.87
2.86
2.61
2.59
2.57
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2.17
2.15
2.13
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1.89
1.88
1.87
1.17
-0.00
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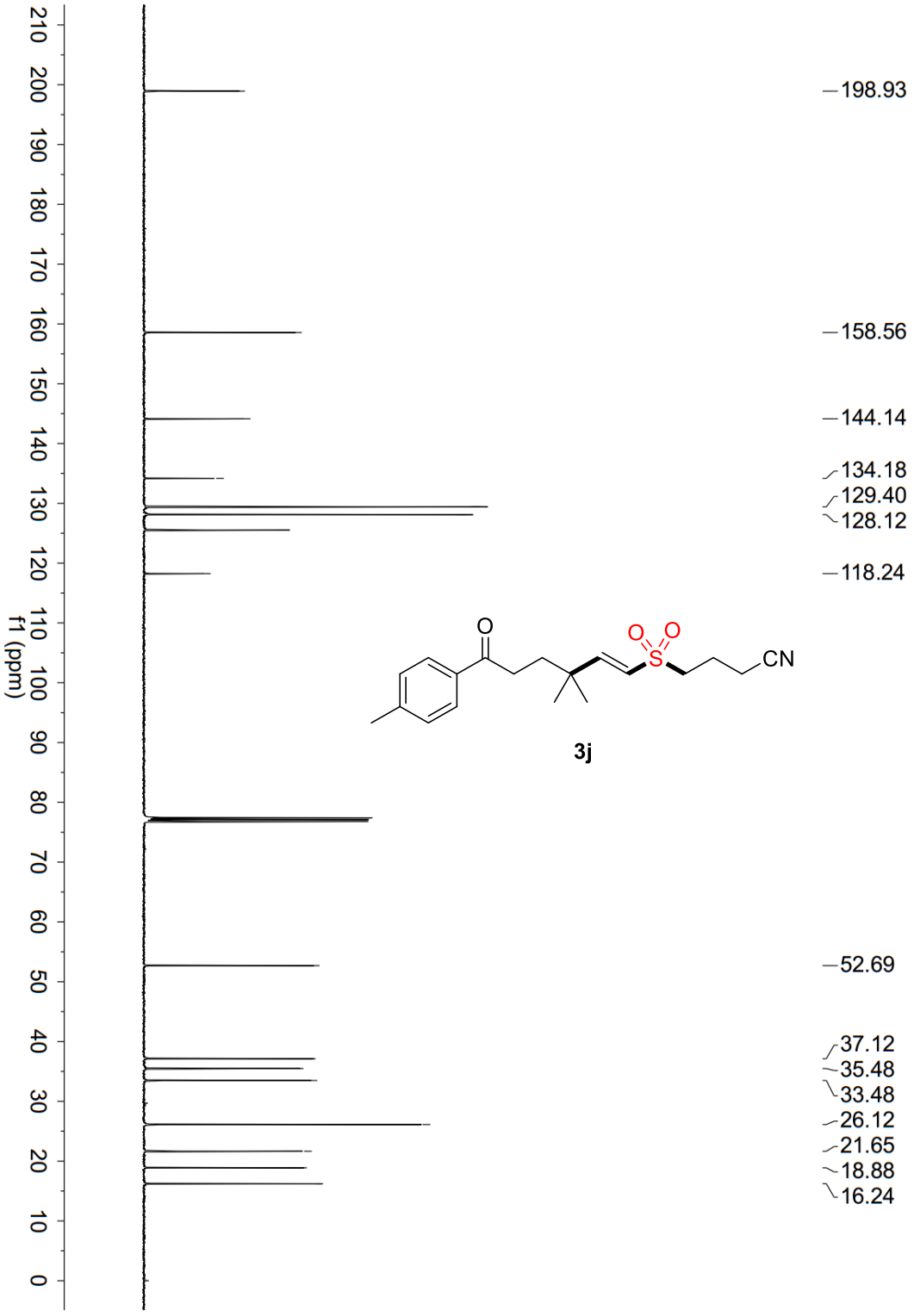
O
O
S
CN

3j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118.24
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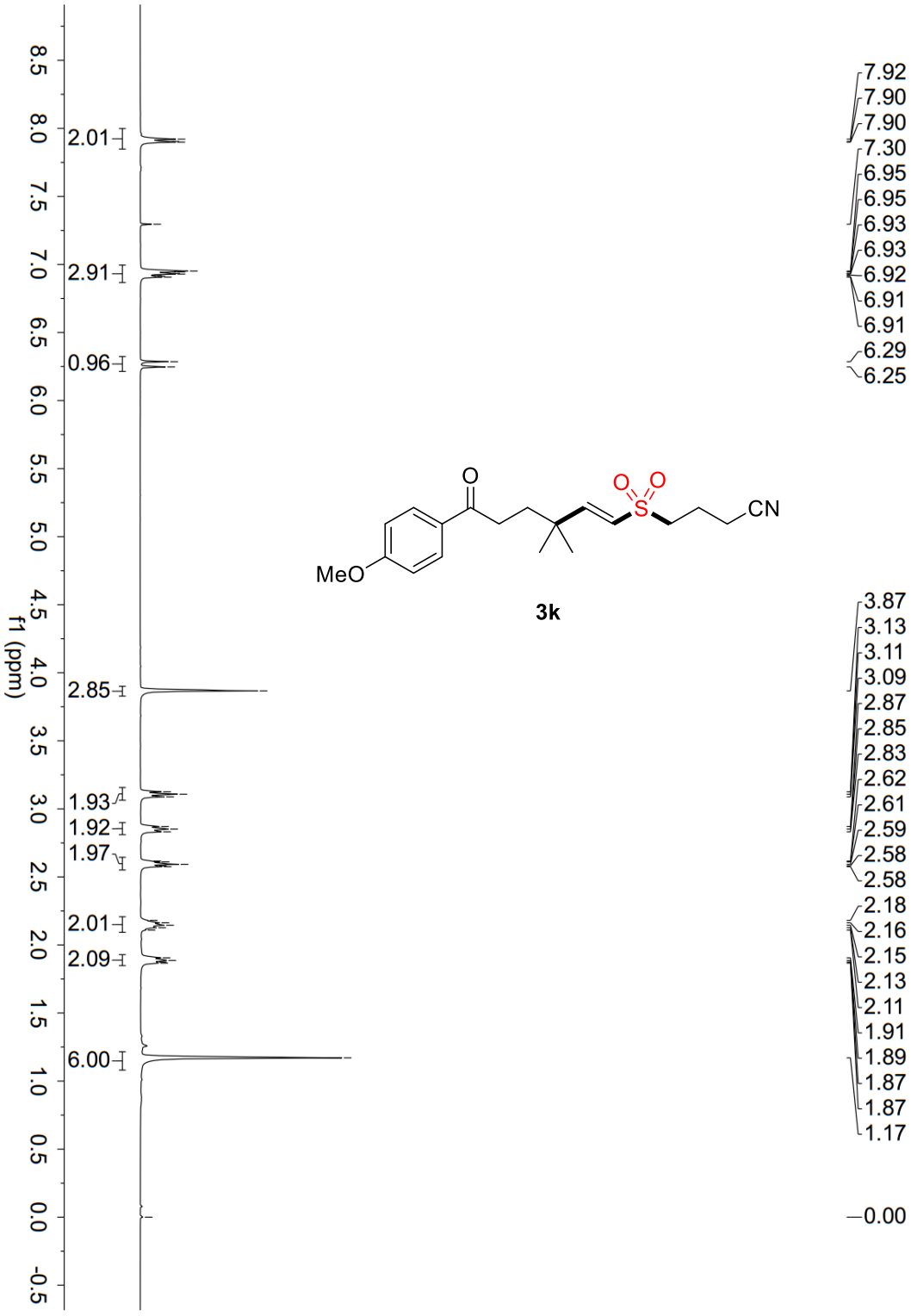
26.12
21.65
18.88
16.24
f1 (ppm)
O
O
O
S
CN
3j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4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
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2.91
0.96
2.85
1.93
1.92
1.97
2.01
2.09
6.00
7.92
7.90
7.90
7.30
6.95
6.95
6.93
6.93
6.92
6.91
6.91
6.29
6.25
3.87
3.13
3.11
3.09
2.87
2.85
2.83
2.62
2.61
2.59
2.58
2.58
2.18
2.16
2.15
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1.89
1.87
1.87
1.17
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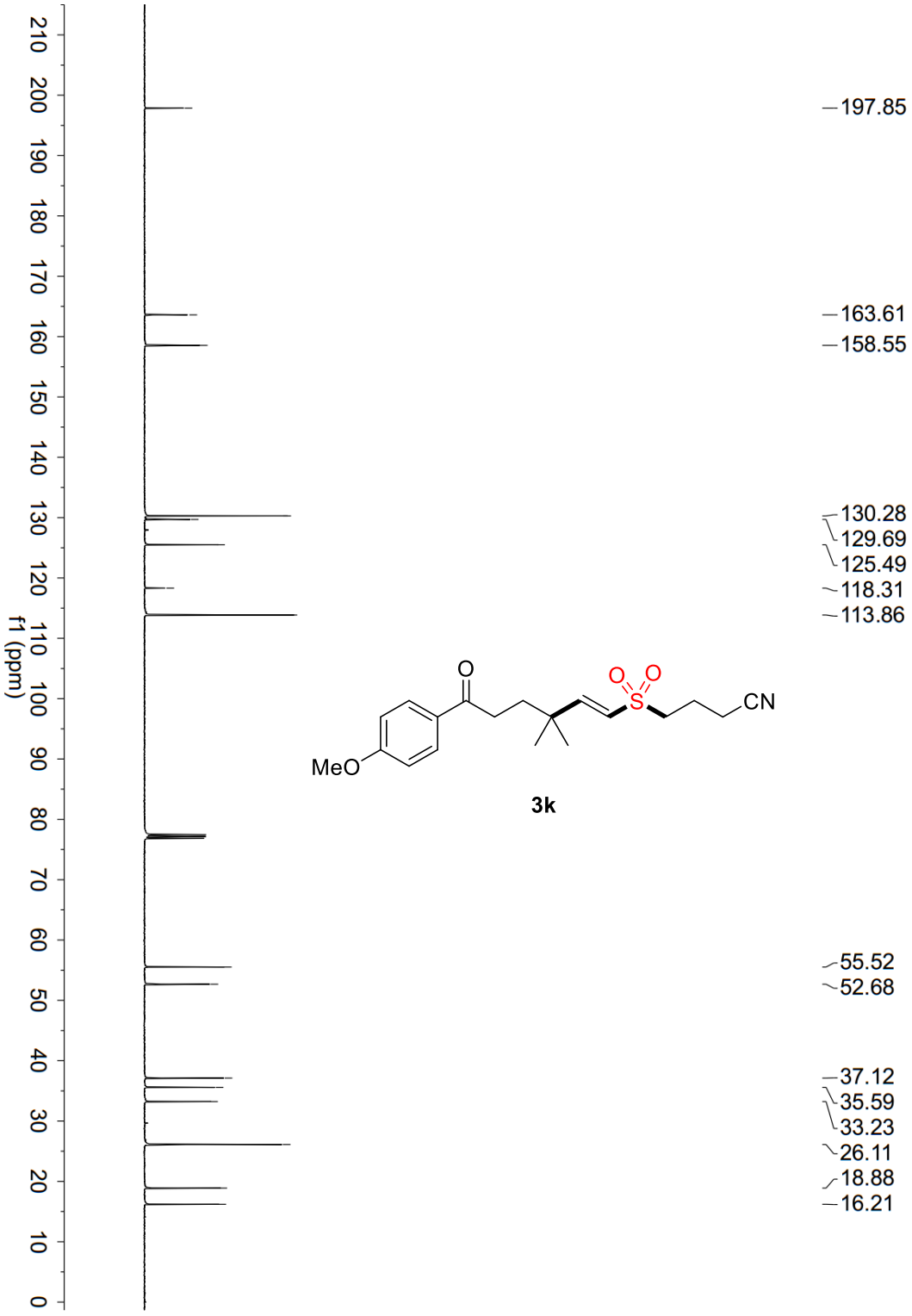
O
O
O
S
CN
MeO

3k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26.11
18.88
16.21
f1 (ppm)
O
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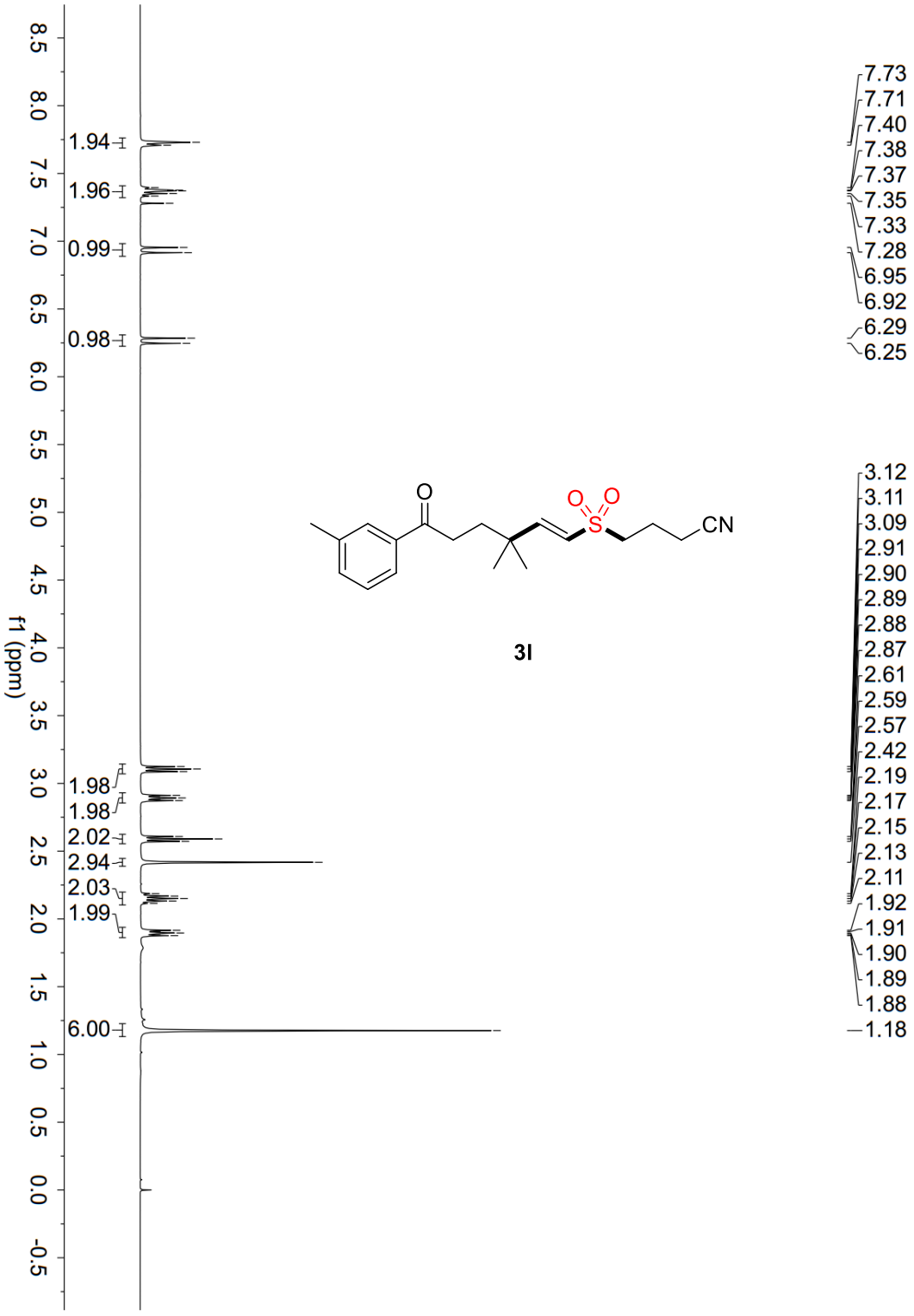
O
S
CN
MeO

3k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4.0
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3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
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1.96
0.99
0.98
1.98
1.98
2.02
2.94
2.03
1.99
6.00
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7.71
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7.37
7.35
7.33
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6.95
6.92
6.29
6.25
3.12
3.11
3.09
2.91
2.90
2.89
2.88
2.87
2.61
2.59
2.57
2.42
2.19
2.17
2.15
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O
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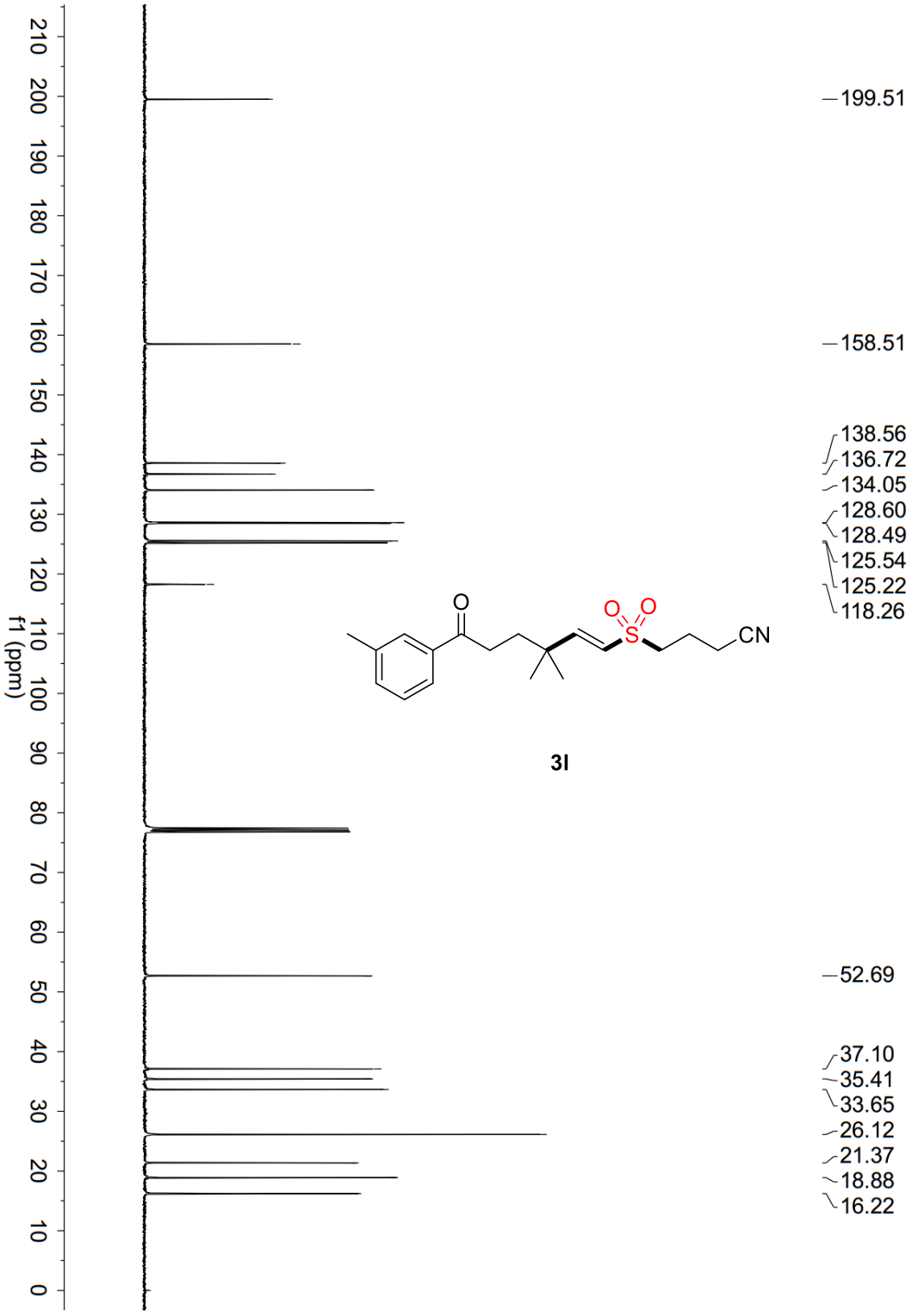
CN

3l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10
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158.51
138.56
136.72
134.05
128.60
128.49
125.54
125.22
118.26
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35.41
33.65
26.12
21.37
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16.22
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O
O
S
CN

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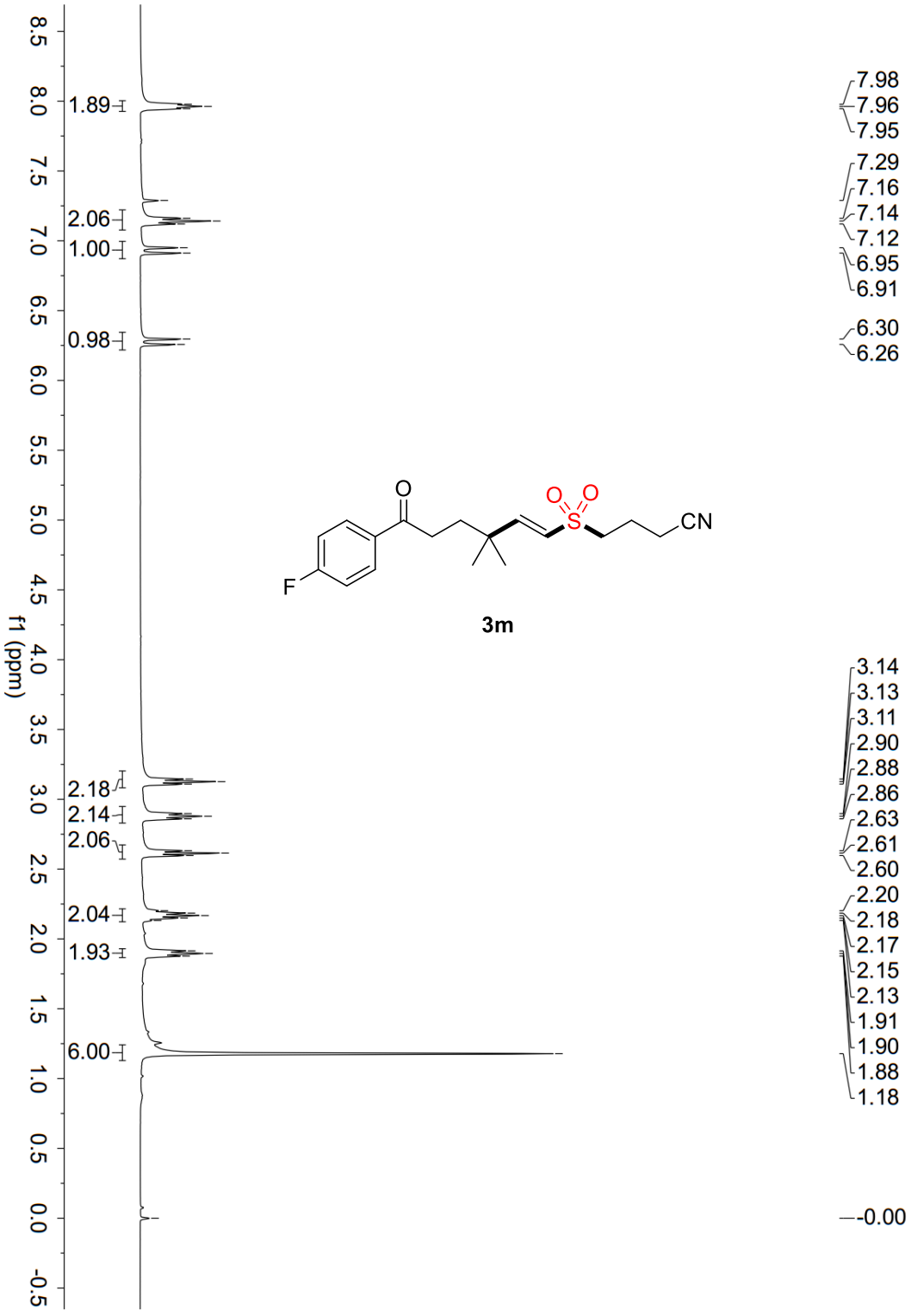
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4.5
4.0
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2.5
2.0
1.5
1.0
0.5
0.0
-0.5
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2.06
1.00
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2.18
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2.06
2.04
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6.00
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7.96
7.95
7.29
7.16
7.14
7.12
6.95
6.91
6.30
6.26
3.14
3.13
3.11
2.90
2.88
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2.60
2.20
2.18
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1.91
1.90
1.88
1.18
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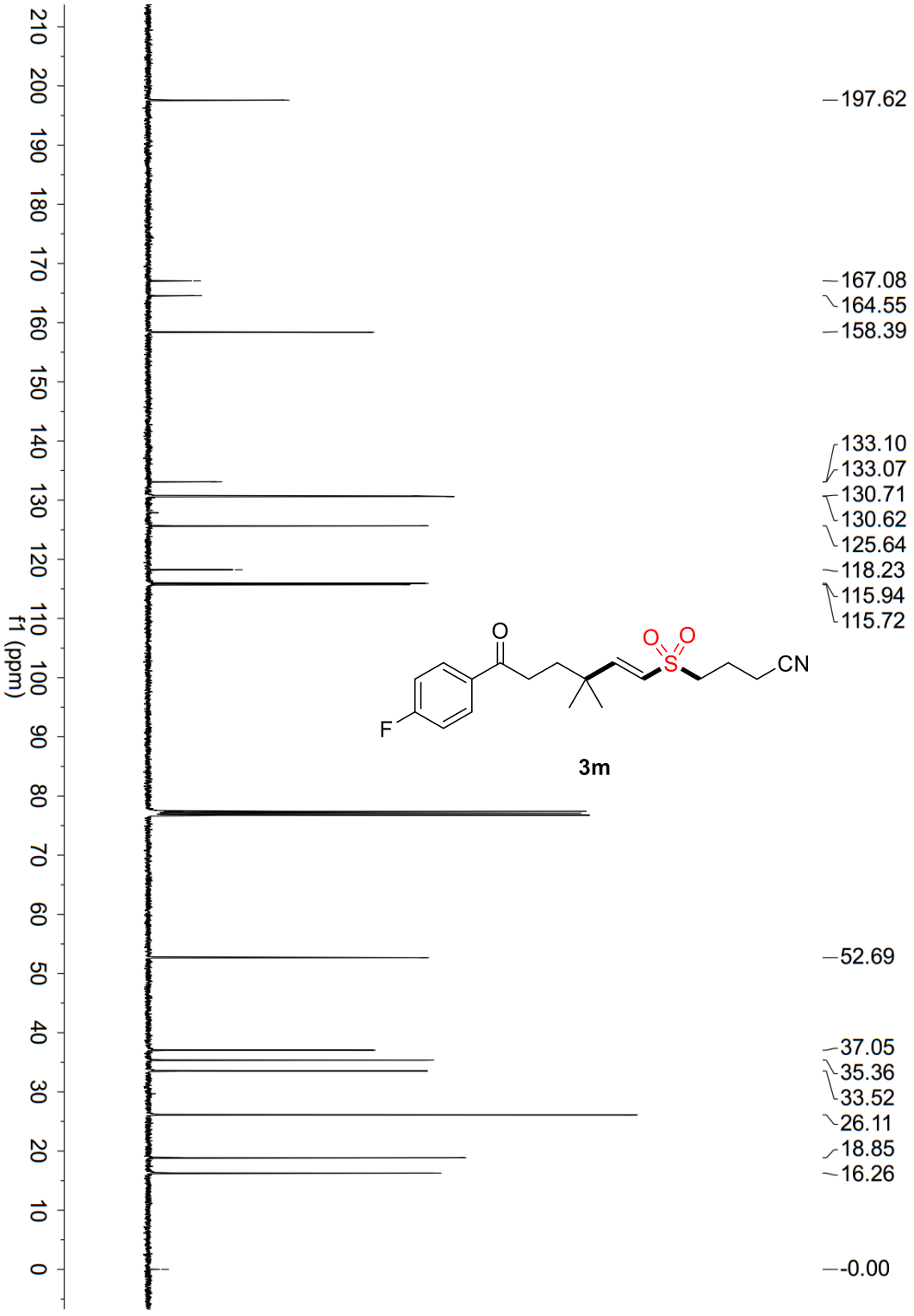
O
O
S
CN
F

3m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80
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30
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10
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167.08
164.55
158.39
133.10
133.07
130.71
130.62
125.64
118.23
115.94
115.72
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33.52
26.11
18.85
16.26
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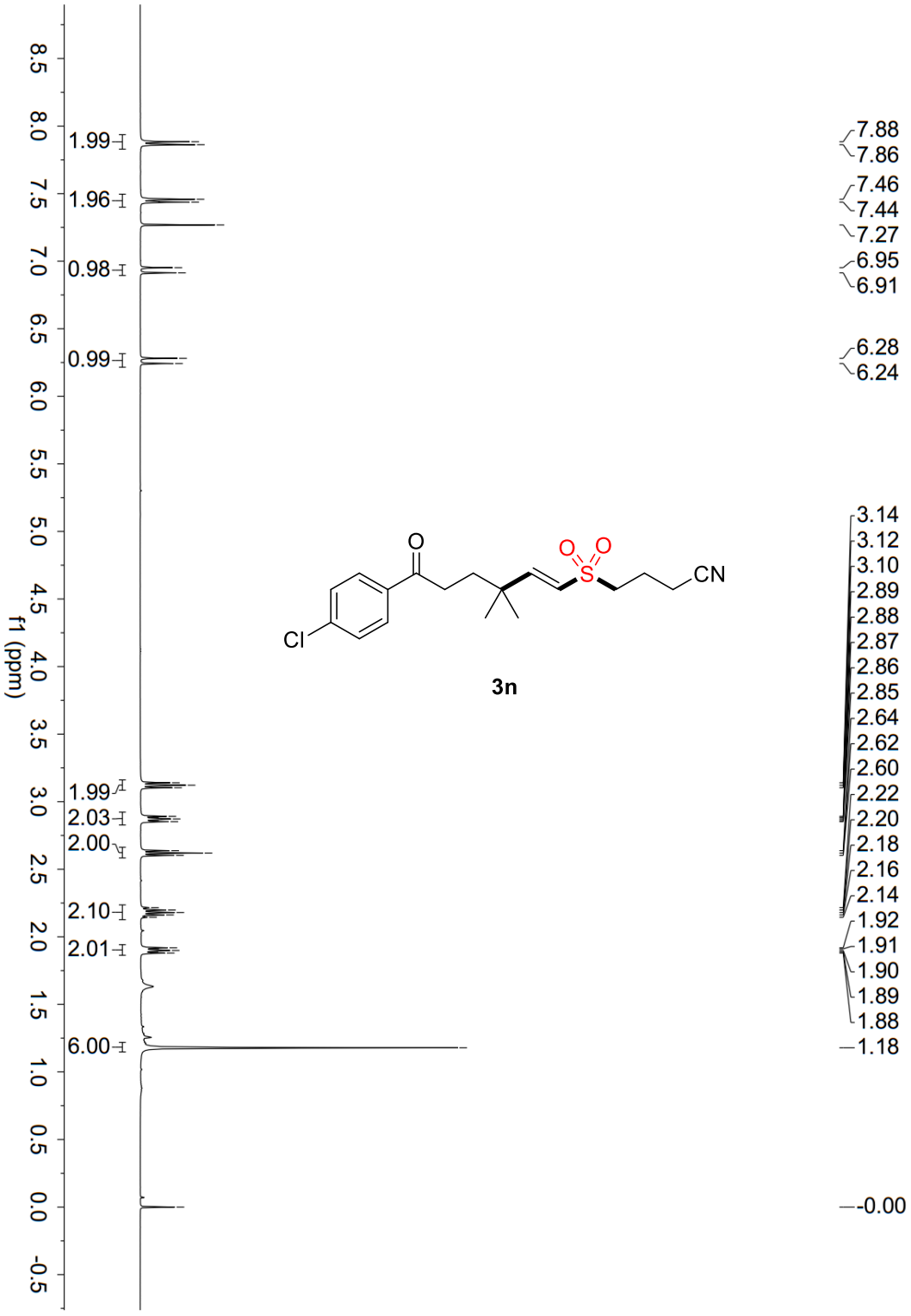
O
O
S
CN
F
3m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3.0
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2.0
1.5
1.0
0.5
0.0
-0.5
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1.96
0.98
0.99
1.99
2.03
2.00
2.10
2.01
6.00
7.88
7.86
7.46
7.44
7.27
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6.91
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3.12
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1.89
1.88
1.18
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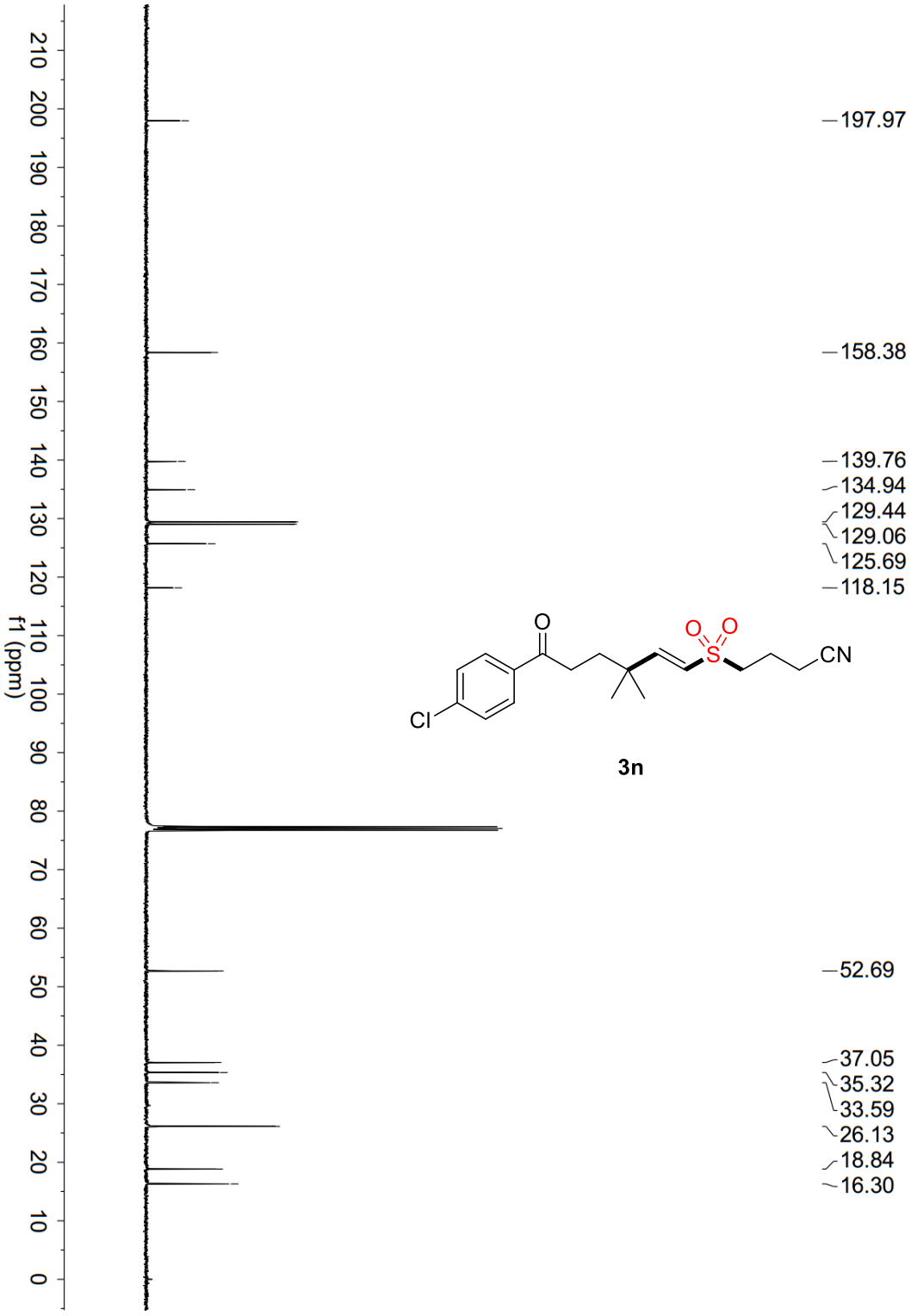
O
O
S
CN
Cl

3n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26.13
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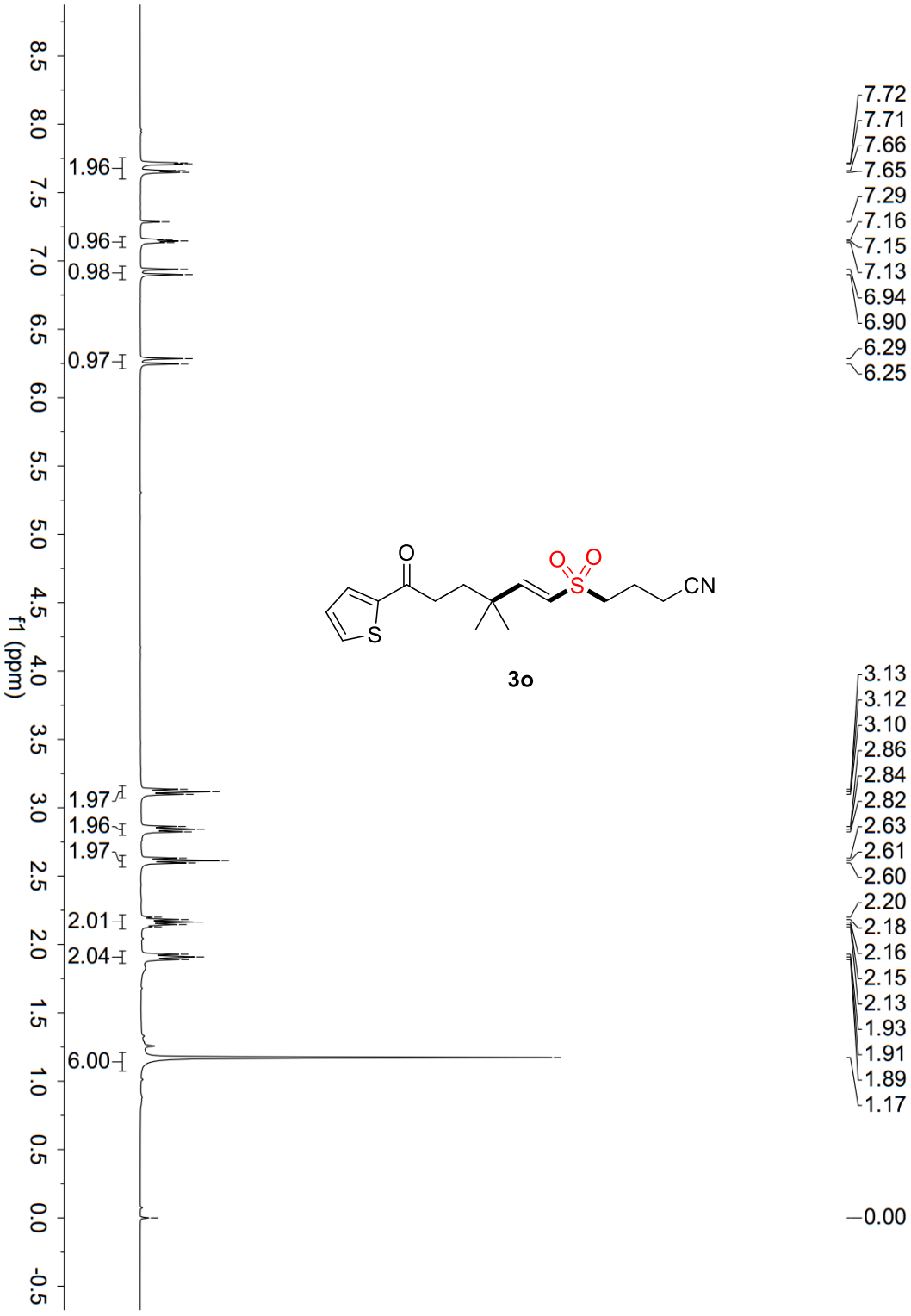
16.30
f1 (ppm)
O
O
O
S
CN
Cl

3n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2.0
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-0.5
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1.96
1.97
2.01
2.04
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3.12
3.10
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S
S
CN

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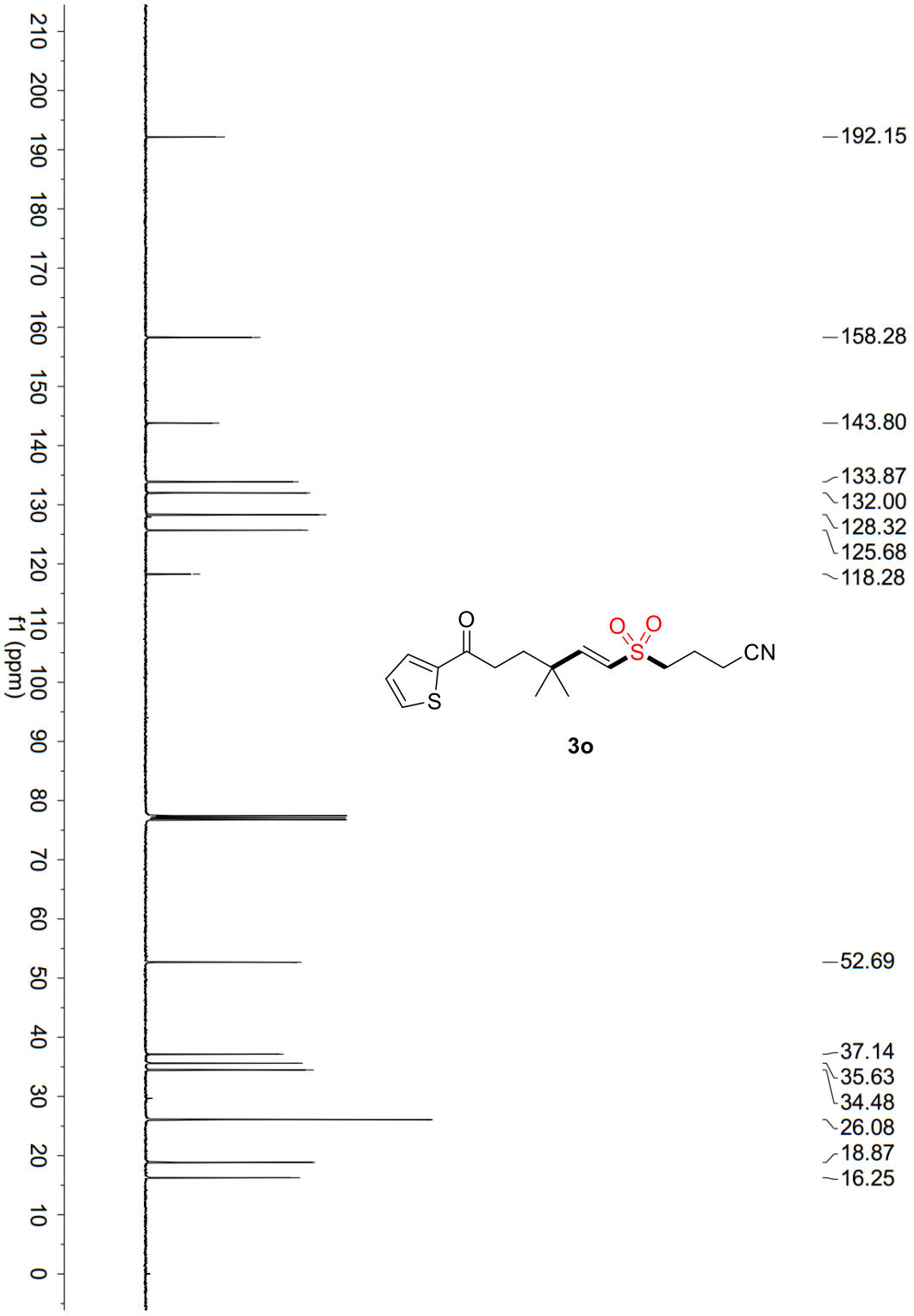
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143.80
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132.00
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125.68
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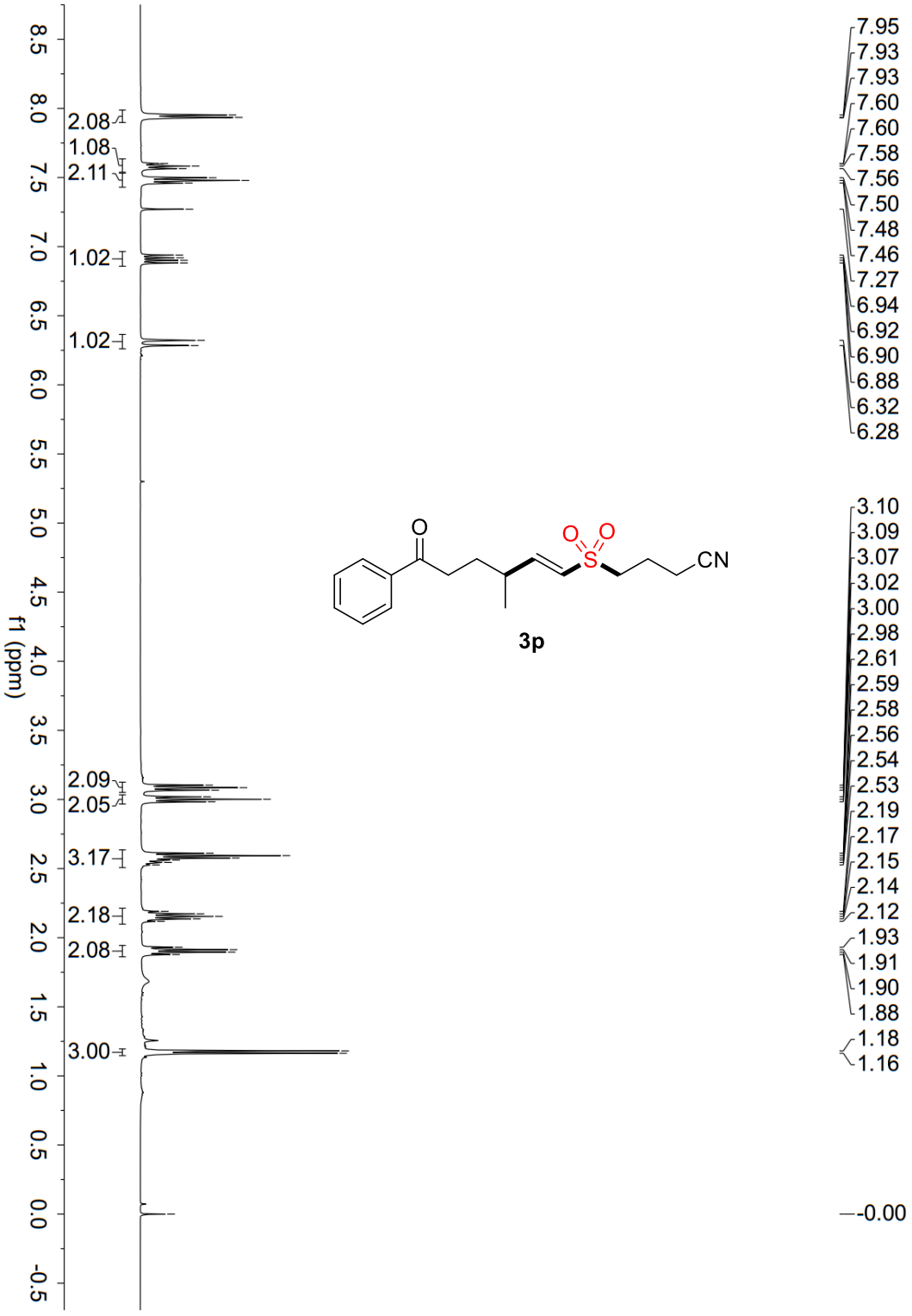
S
CN

3o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3.0
2.5
2.0
1.5
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0.5
0.0
-0.5
2.08
1.08
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1.02
1.02
2.09
2.05
3.17
2.18
2.08
3.00
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O
O
S
CN
3p
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6.28
3.10
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3.07
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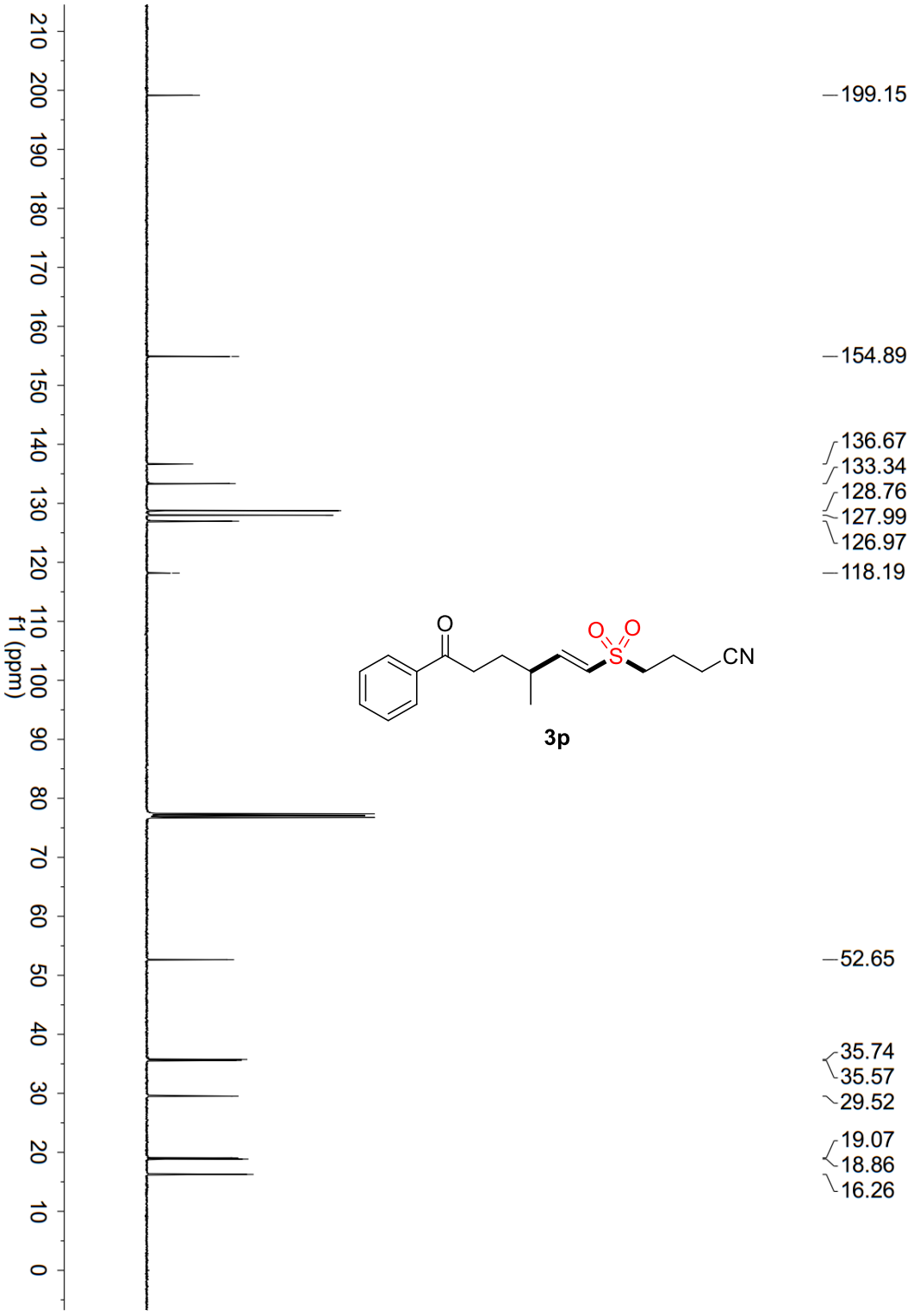
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180
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30
20
10
0
199.15
154.89
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133.34
128.76
127.99
126.97
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35.57
29.52
19.07
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16.26
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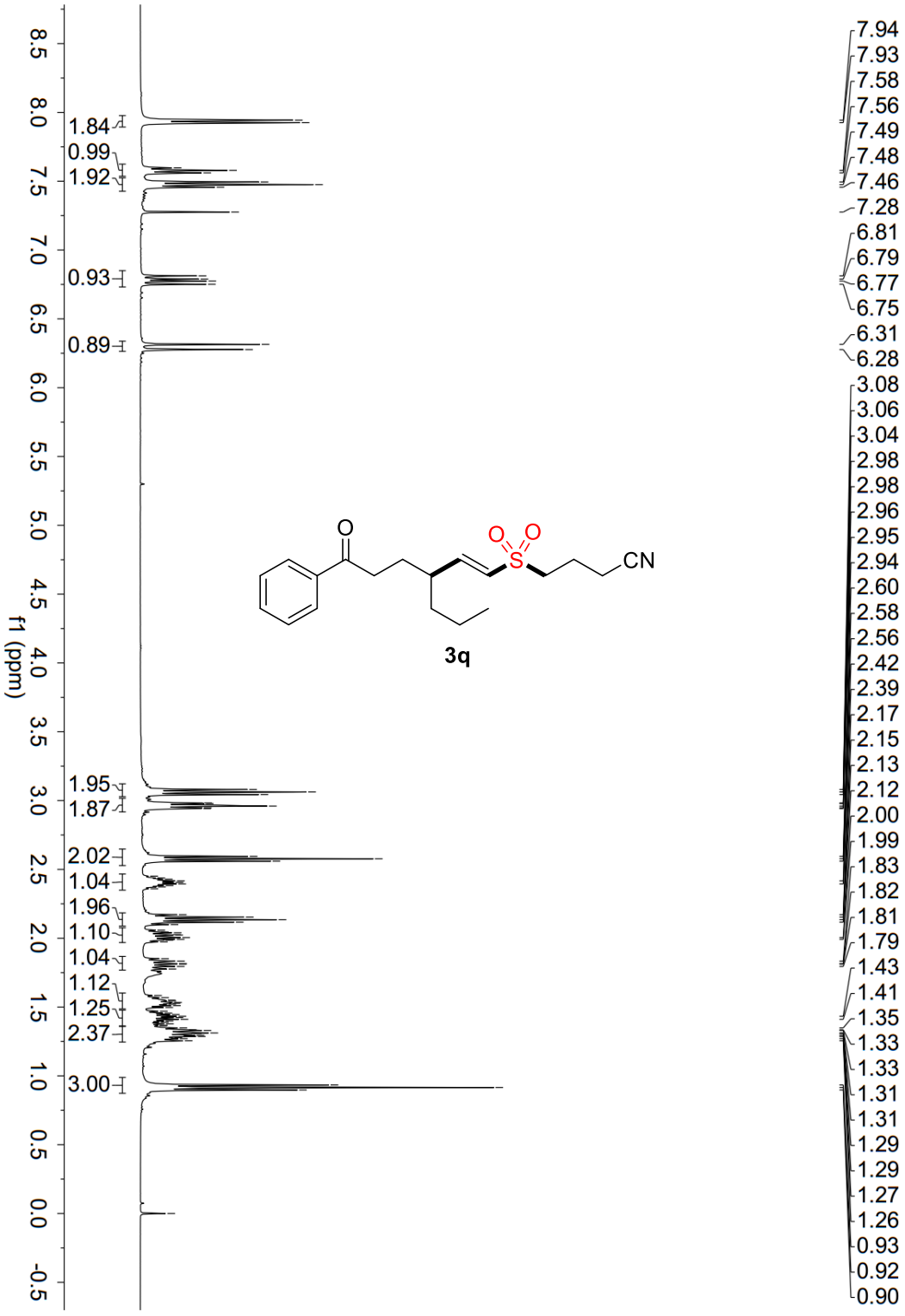
O
O
S
CN

3p


f1 (ppm)
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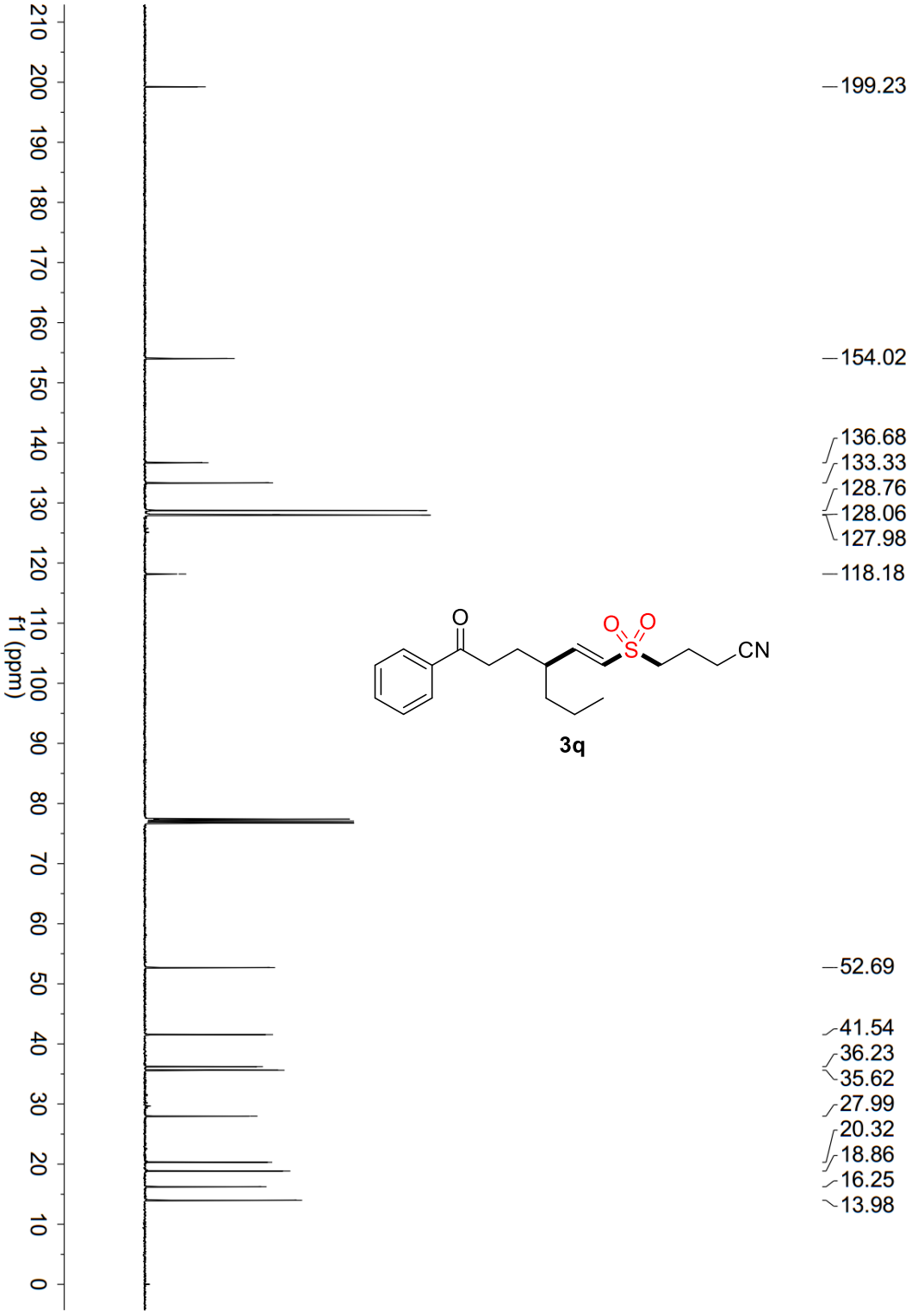
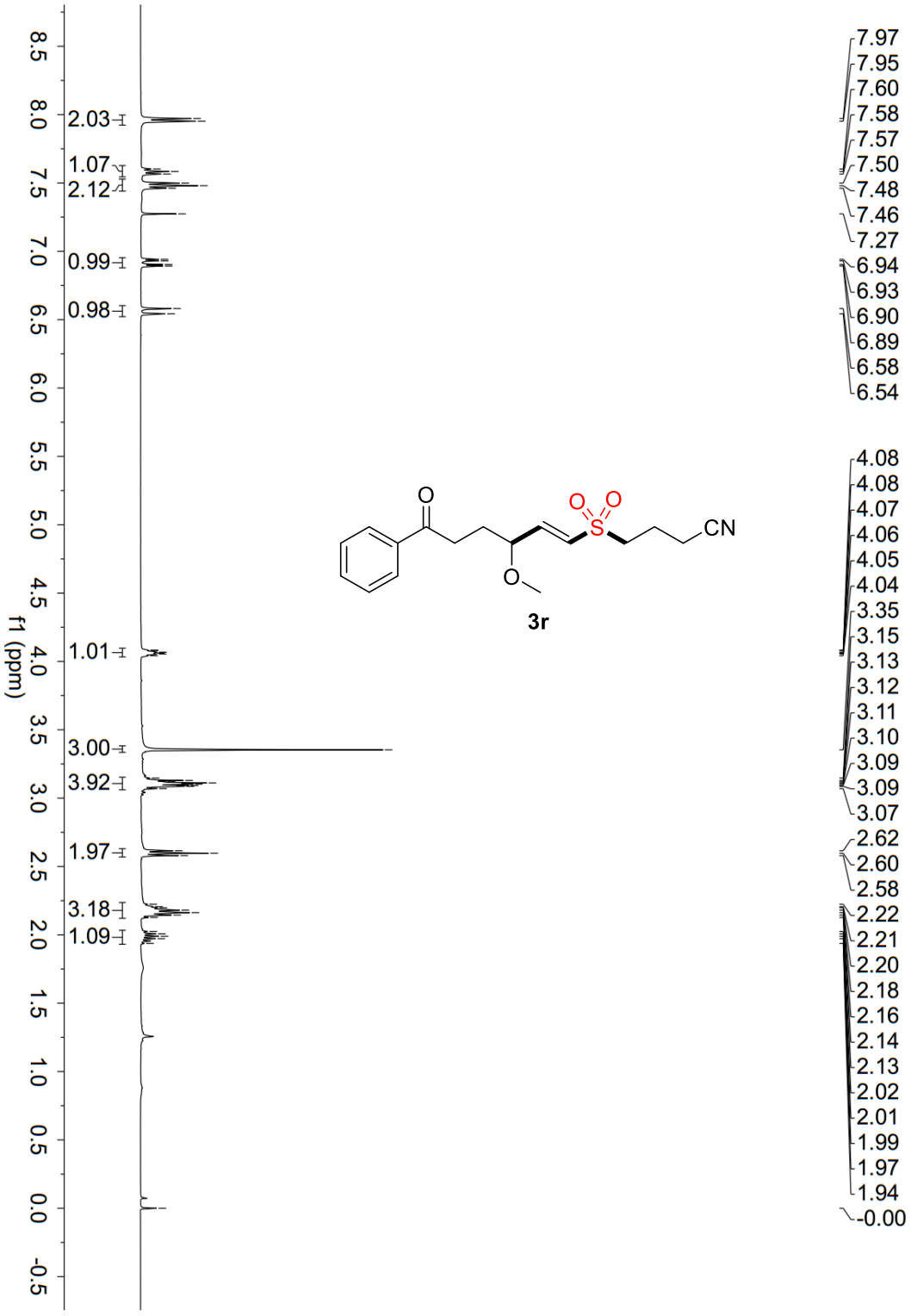
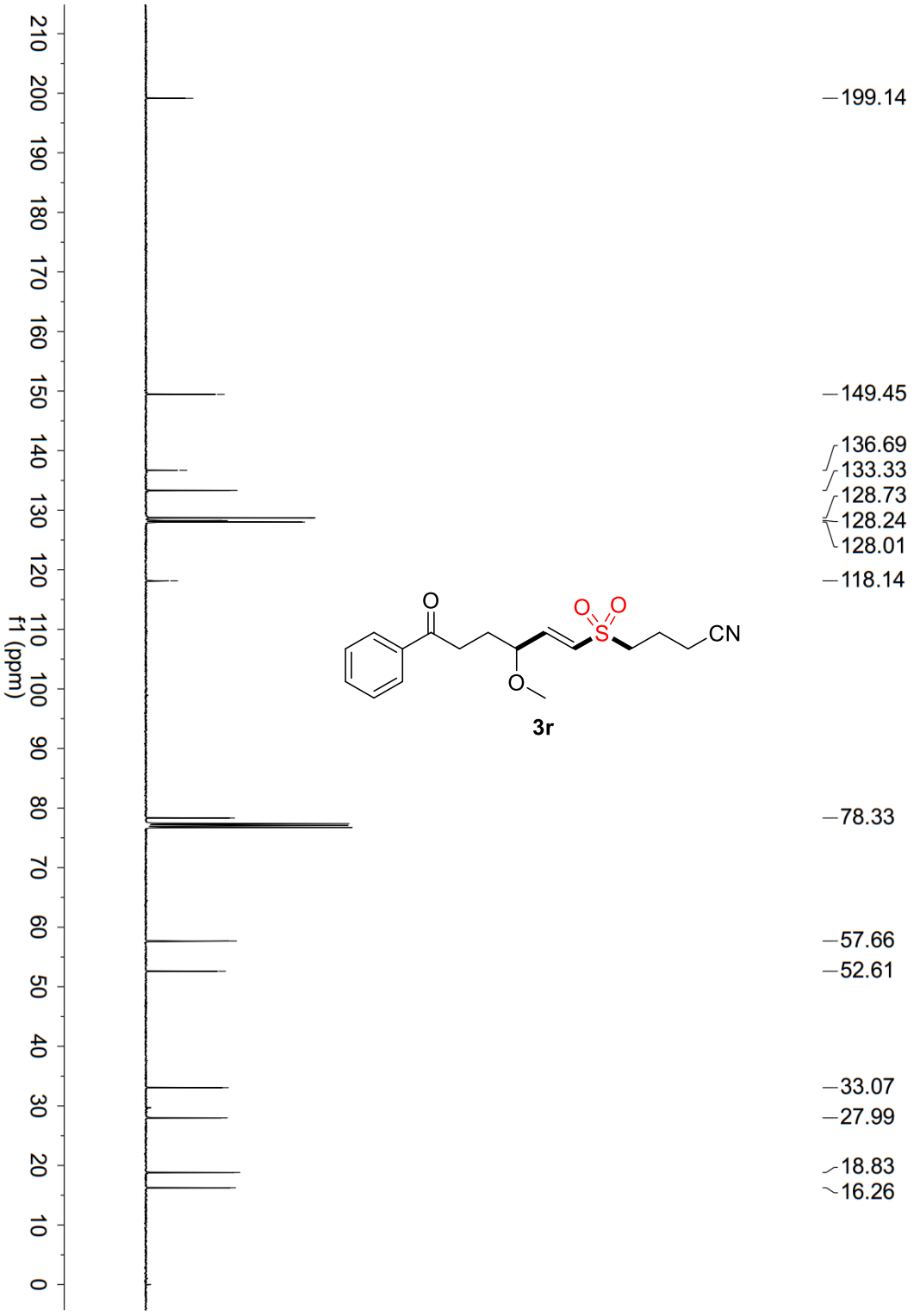
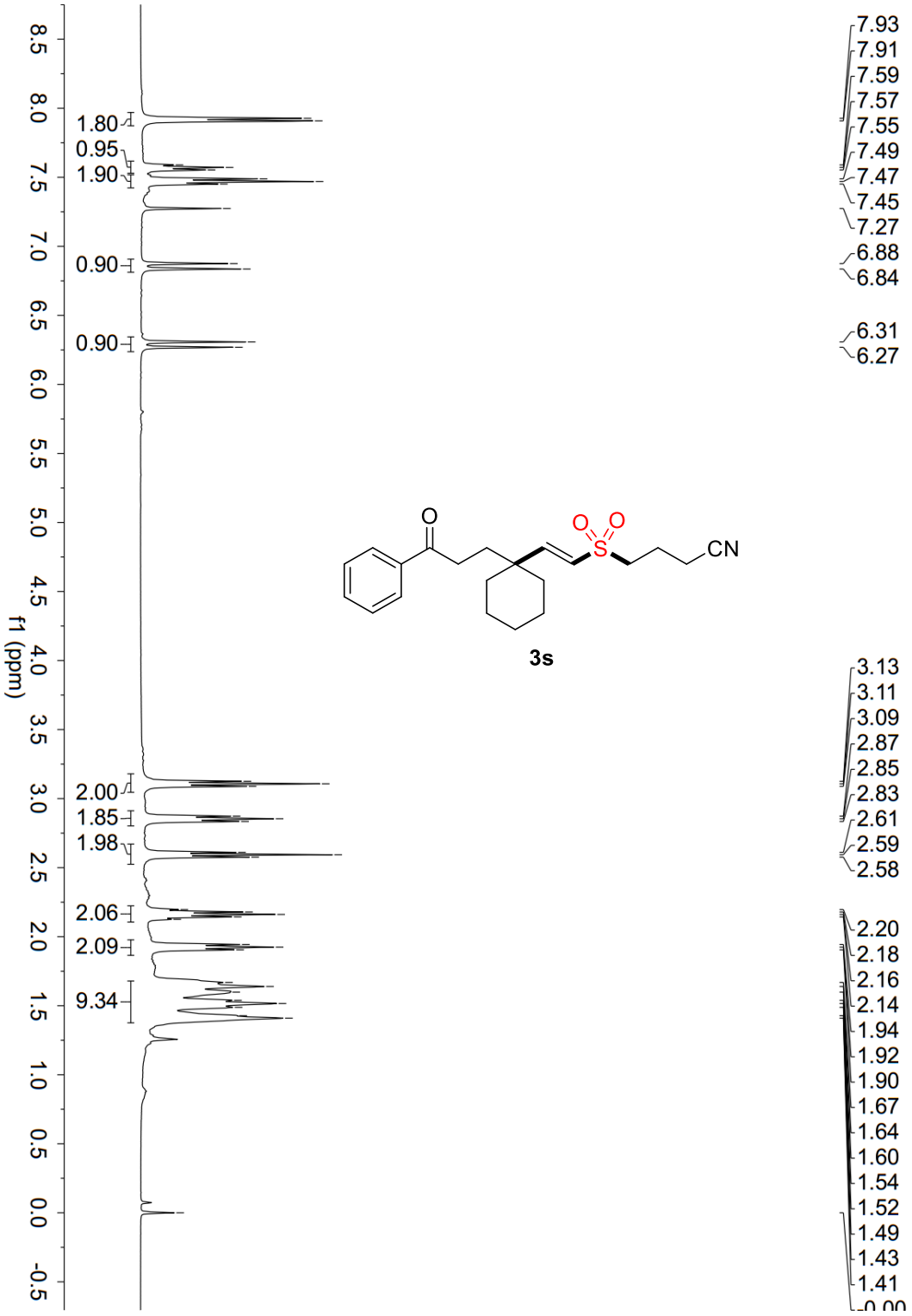
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
1.84
0.99
1.92
0.93
0.89
1.95
1.87
2.02
1.04
1.96
1.10
1.04
1.12
1.25
2.37
3.00
O
O
O
S
CN
3q
7.94
7.93
7.58
7.56
7.49
7.48
7.46
7.28
6.81
6.79
6.77
6.75
6.31
6.28
3.08
3.06
3.04
2.98
2.98
2.96
2.95
2.94
2.60
2.58
2.56
2.42
2.39
2.17
2.15
2.13
2.12
2.00
1.99
1.83
1.82
1.81
1.79
1.43
1.41
1.35
1.33
1.33
1.31
1.31
1.29
1.29
1.27
1.26
0.93
0.92
0.90


f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
199.23
154.02
136.68
133.33
128.76
128.06
127.98
118.18
52.69
41.54
36.23
35.62
27.99
20.32
18.86
16.25
13.98
O
O
O
S
CN

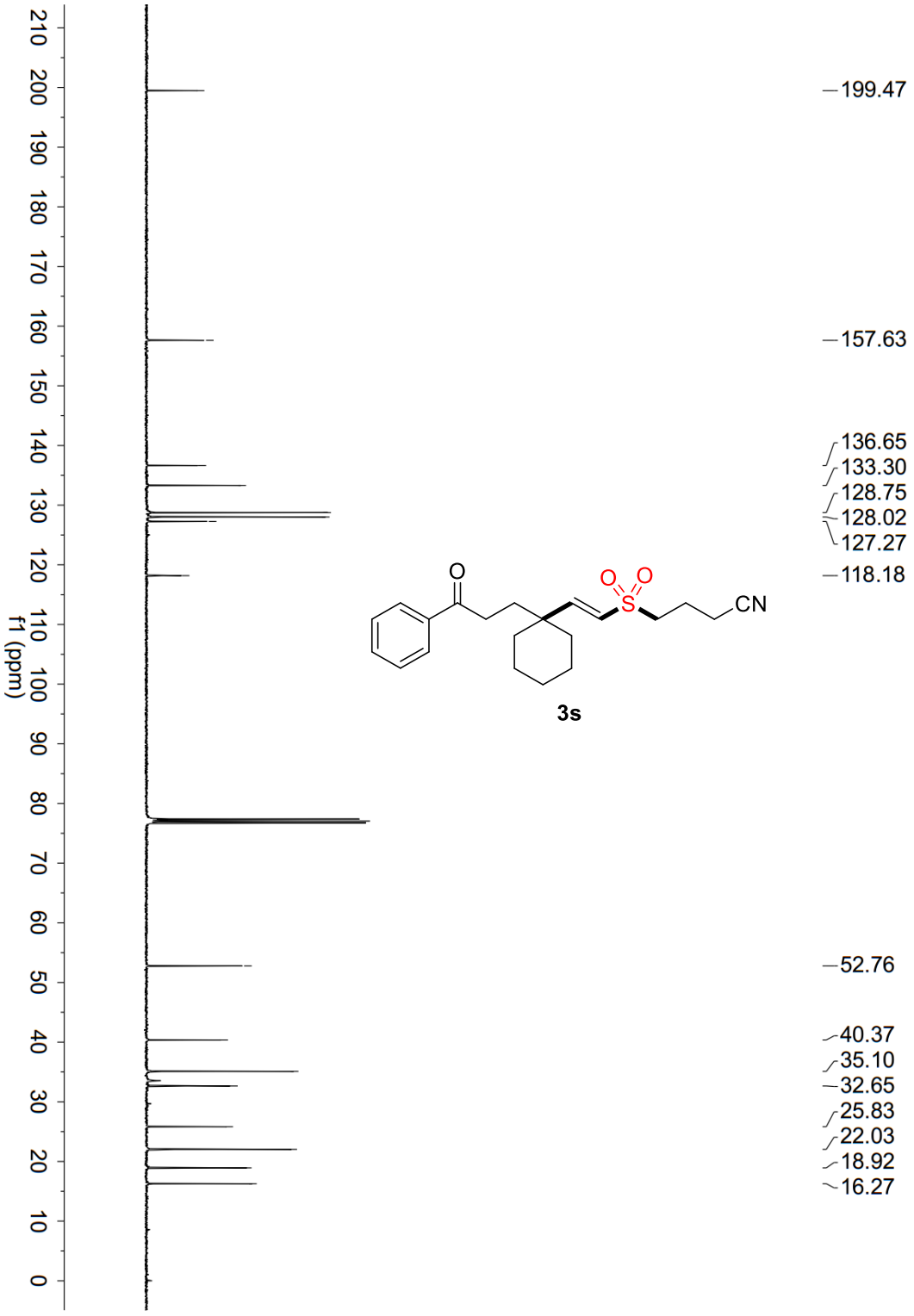
3q

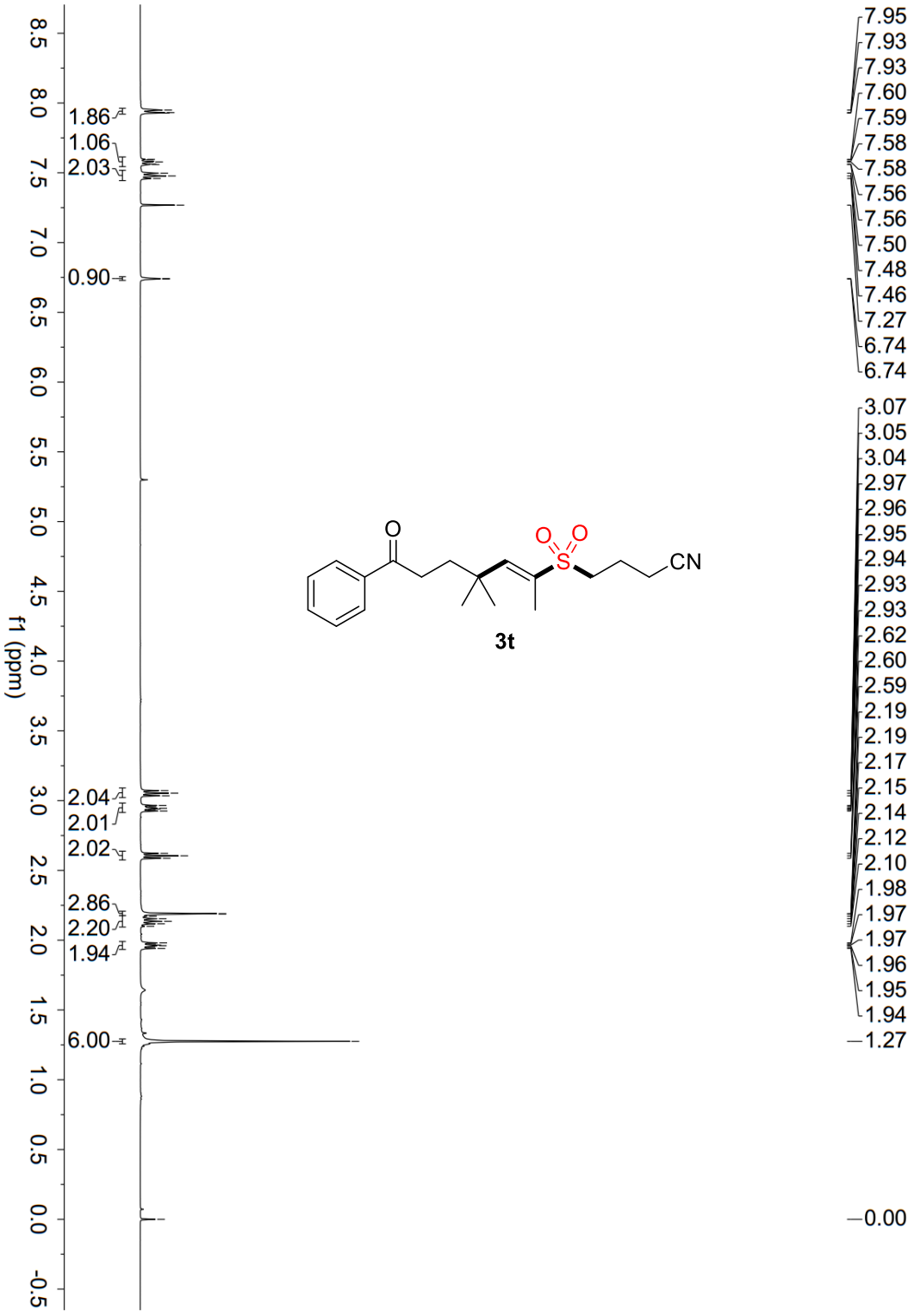

f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
2.03
1.07
2.12
0.99
0.98
1.01
3.00
3.92
1.97
3.18
1.09
O
O
O
S
CN
O
3r
7.97
7.95
7.60
7.58
7.57
7.50
7.48
7.46
7.27
6.94
6.93
6.90
6.89
6.58
6.54
4.08
4.08
4.07
4.06
4.05
4.04
3.35
3.15
3.13
3.12
3.11
3.10
3.09
3.09
3.07
2.62
2.60
2.58
2.22
2.21
2.20
2.18
2.16
2.14
2.13
2.02
2.01
1.99
1.97
1.94
-0.00

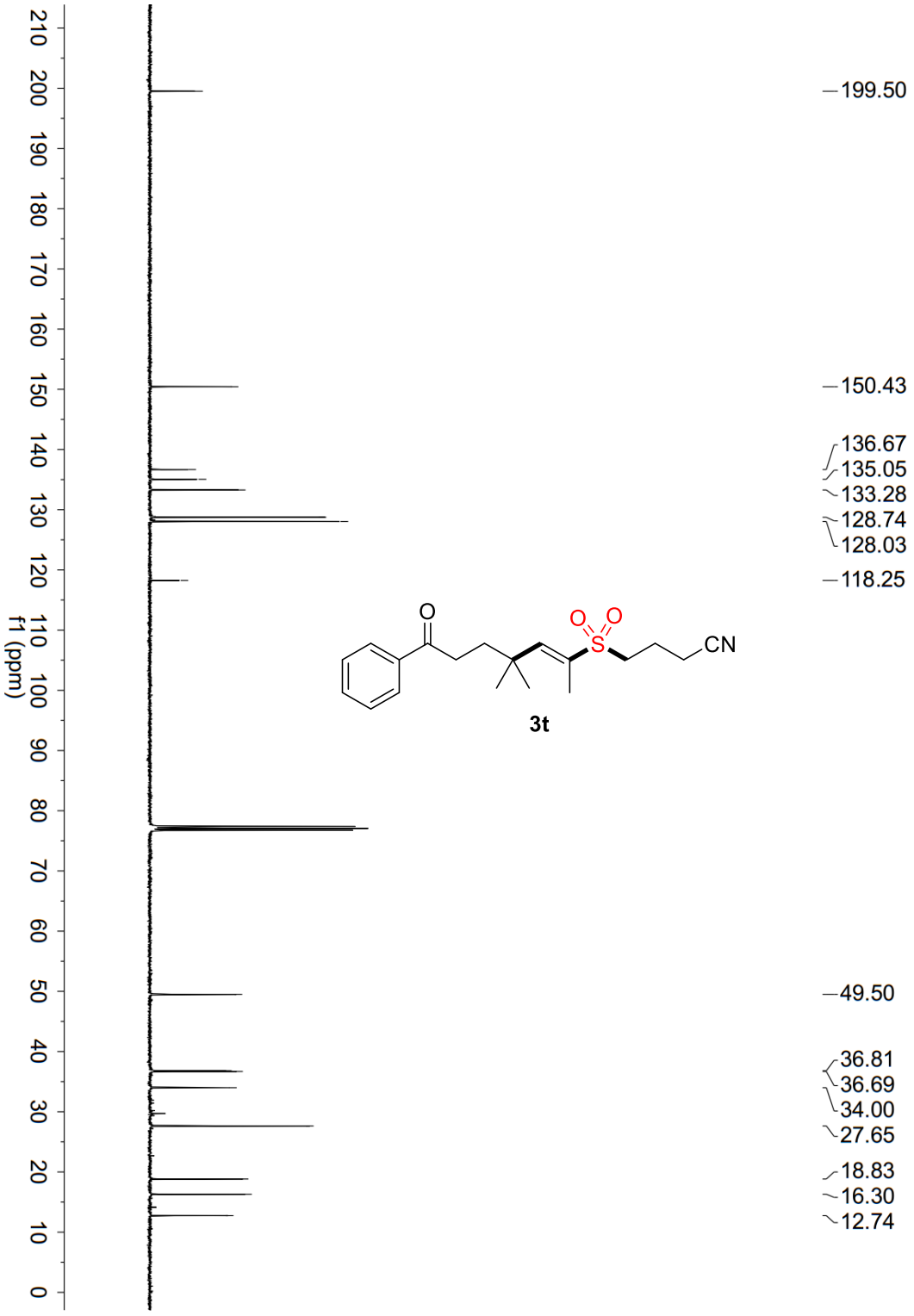

199.14
149.45
136.69
133.33
128.73
128.24
128.01
118.14
78.33
57.66
52.61
33.07
27.99
18.83
16.26
f1 (ppm)
O
O
O
S
CN
O
3r

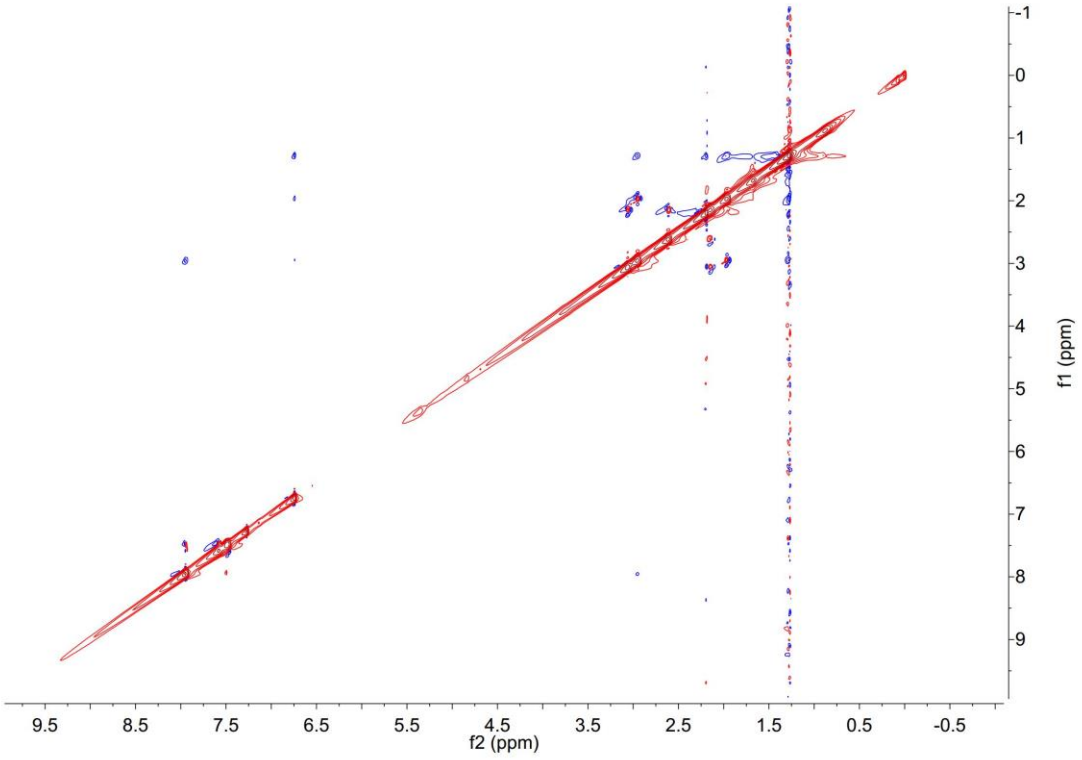

f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
1.80
0.95
1.90
0.90
0.90
2.00
1.85
1.98
2.06
2.09
9.34
7.93
7.91
7.59
7.57
7.55
7.49
7.47
7.45
7.27
6.88
6.84
6.31
6.27
3.13
3.11
3.09
2.87
2.85
2.83
2.61
2.59
2.58
2.20
2.18
2.16
2.14
1.94
1.92
1.90
1.67
1.64
1.60
1.54
1.52
1.49
1.43
1.41
O
O
O
S
CN

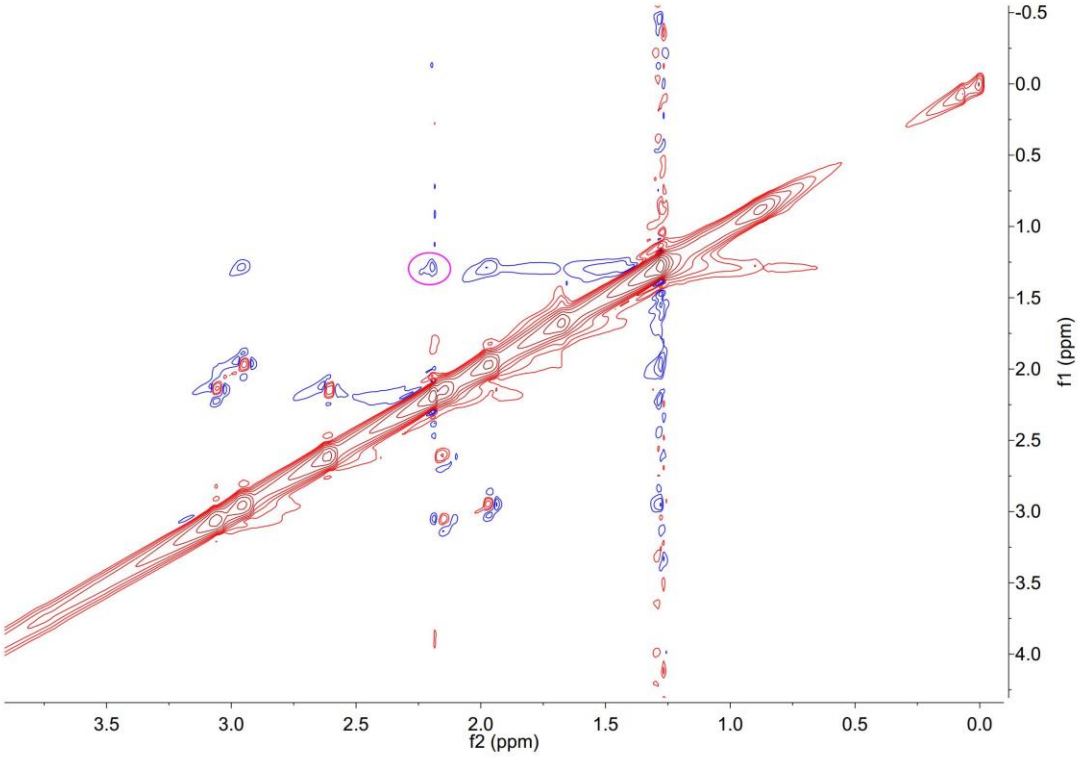
3s


199.47
157.63
136.65
133.30
128.75
128.02
127.27
118.18
52.76
40.37
35.10
32.65
25.83
22.03
18.92
16.27
f1 (ppm)
O
O
O
S
CN
3s


f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
1.86
1.06
2.03
0.90
2.04
2.01
2.02
2.86
2.20
1.94
6.00
O
O
O
S
CN
3t
7.95
7.93
7.93
7.60
7.59
7.58
7.58
7.56
7.56
7.50
7.48
7.46
7.27
6.74
6.74
3.07
3.05
3.04
2.97
2.96
2.95
2.94
2.93
2.93
2.62
2.60
2.59
2.19
2.19
2.17
2.15
2.14
2.12
2.10
1.98
1.97
1.97
1.96
1.95
1.94
1.27
0.00


199.50
150.43
136.67
135.05
133.28
128.74
128.03
118.25
49.50
36.81
36.69
34.00
27.65
18.83
16.30
12.74
f1 (ppm)
O
O
O
S
CN
3t


-1
0
1
2
3
4
5
6
7
8
9
f1 (ppm)
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f2 (ppm)


-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
f1 (ppm)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (ppm)