Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

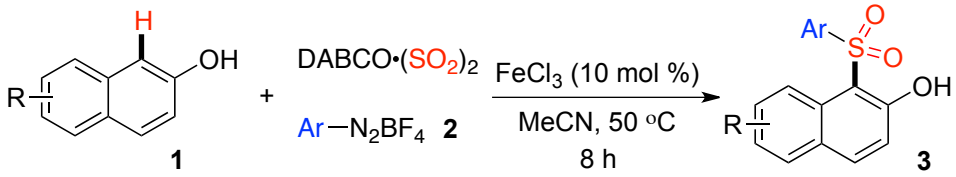
Supporting Information

1. General experimental methods (S2).
2. General experimental procedure and characterization data (S3-S10).
3. ^{1}H and ^{13}C NMR spectra of compounds **3** (S11–S56).

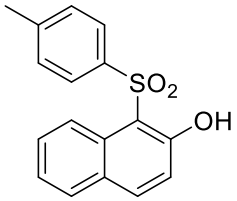
General experimental methods:

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, 32–63µm, 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 synthesis of sulfonated naphthols through a three-component reaction of naphthols ***1****, sulfur dioxide, and aryldiazonium tetrafluoroborates* ***2***

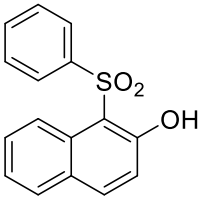


2-Naphthol **1** (0.2 mmol), $DABCO{\cdot}(SO_2)_2$ (0.16 mmol), aryldiazonium tetrafluoroborate **2** (0.3 mmol) and $FeCl_3$ (10 mol %) were combined in a test tube. The test tube was evacuated and backfilled with N_2 three times before the addition of MeCN (4.0 mL). The mixture was then placed in oil bath and stirred for 8 hours at 50 °C. After the conversion was completed as indicated by TLC, the solvent was evaporated under reduced pressure. The residue was purified directly by flash column chromatography (EtOAc/*n*-hexane, 1:8) to give the corresponding product **3**.



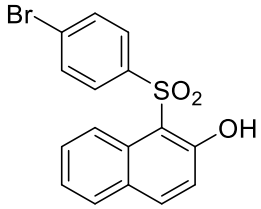
1-tosylnaphthalen-2-ol (**3a**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.10 (s, 1H), 8.30 (d, *J* = 8.7 Hz, 1H), 7.88 (d, *J* = 9.0 Hz, 1H), 7.80 (d, *J* = 7.8 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.22 (s, 2H), 7.14 (d, J = 9.0 Hz, 1H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 158.9, 144.8, 137.6, 130.1, 129.7, 129.3, 129.0, 128.9, 126.8, 124.5, 123.2, 121.6, 120.4, 115.2, 21.8.



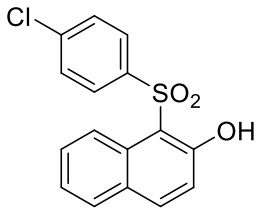
1-(phenylsulfonyl)naphthalen-2-ol (**3b**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.09 (s, 1H), 8.31 (d, *J* = 8.7 Hz, 1H), 7.93 (t, *J* = 7.9 Hz, 3H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.57 – 7.50 (m, 1H), 7.50 - 7.41 (m, 3H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.17 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.2, 142.3, 137.8, 133.8, 129.7, 129.5, 129.3, 129.0, 128.96, 126.7, 124.6, 123.2, 120.4, 111.9.



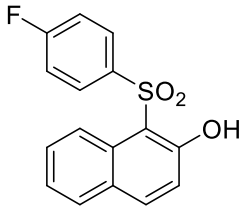
1-((4-bromophenyl)sulfonyl)naphthalen-2-ol (**3c**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 10.99 (s, 1H), 8.26 (d, *J* = 8.7 Hz, 1H), 7.93 (d, *J* = 9.0 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 7.9 Hz, 2H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.17 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.0, 141.0, 137.9, 132.5, 129.2, 129.0, 128.74, 128.73, 128.0, 125.1, 124.5, 122.7, 120.2.



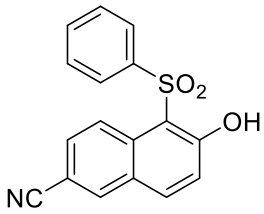
1-((4-chlorophenyl)sulfonyl)naphthalen-2-ol (**3d**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.00 (s, 1H), 8.27 (d, *J* = 8.7 Hz, 1H), 7.93 (d, *J* = 9.0 Hz, 1H), 7.87 (d, *J* = 7.6 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 7.3 Hz, 1H), 7.43 (d, *J* = 8.5 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.17 (d, *J* = 8.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.2, 140.7, 140.4, 138.1, 129.8, 129.5, 129.5, 129.2, 129.0, 128.2, 124.7, 122.9, 120.4.



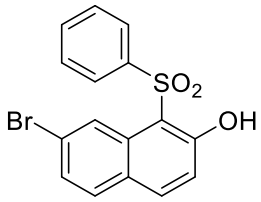
1-((4-fluorophenyl)sulfonyl)naphthalen-2-ol (**3e**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.03 (s, 1H), 8.29 (d, *J* = 8.7 Hz, 1H), 8.00 – 7.89 (m, 3H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.19 – 7.11 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.0, 164.4, 159.1, 138.0, 129.7, 129.6 (d, *J* = 3.9 Hz), 129.4, 129.1, 129.0, 124.7, 123.0, 120.4, 116.8 (d, *J* = 23 Hz), 111.8.



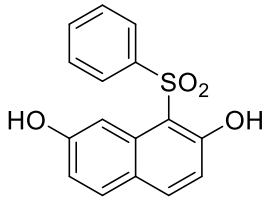
6-hydroxy-5-(phenylsulfonyl)-2-naphthonitrile (**3f**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.32 (s, 1H), 8.43 (d, *J* = 9.0 Hz, 1H), 8.06 (d, *J* = 1.2 Hz, 1H), 7.98 - 7.90 (m, 3H), 7.63 – 7.55 (m, 2H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 9.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.9, 156.9, 141.4, 137.3, 134.3, 134.1, 129.6, 129.5, 129.4, 127.9, 126.5, 124.1, 122.4, 118.4. HRMS (ESI) calcd for $C_{17}H_{11}N_1O_3S$: 332.0352 ($M + Na^+$), found: 332.0352.



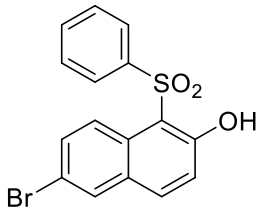
7-bromo-1-(phenylsulfonyl)naphthalen-2-ol (**3g**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.11 (s, 1H), 8.54 (s, 1H), 7.94 (d, *J* = 7.8 Hz, 2H), 7.86 (d, *J* = 9.0 Hz, 1H), 7.60 - 7.47 (m, 4H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.17 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.3, 137.2, 136.6, 133.9, 130.4, 129.4, 128.8, 127.9, 127.5, 127.2, 126.6, 125.5, 123.7, 120.6.



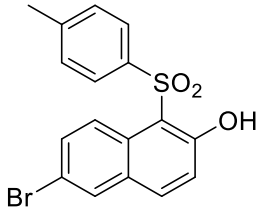
1-(phenylsulfonyl)naphthalene-2,7-diol (**3h**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.00 (s, 1H), 7.92 (d, *J* = 7.7 Hz, 2H), 7.83 (d, *J* = 8.9 Hz, 1H), 7.70 (s, 1H), 7.60 (d, *J* = 8.7 Hz, 1H), 7.57 - 7.43 (m, 4H), 7.00 (d, *J* = 9.0 Hz, 1H), 6.91 (d, *J* = 8.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.9, 156.4, 142.1, 137.6, 133.8, 131.4, 129.5, 126.6, 124.1, 120.6, 117.6, 115.7, 106.8.



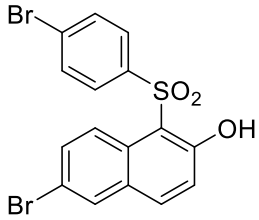
6-bromo-1-(phenylsulfonyl)naphthalen-2-ol (**3i**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.07 (s, 1H), 8.21 (d, *J* = 9.2 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 2H), 7.86 – 7.79 (m, 2H), 7.58 – 7.44 (m, 4H), 7.19 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.2, 142.0, 136.6, 134.0, 132.1, 131.2, 130.2, 129.6, 128.3, 126.7, 124.9, 121.7, 118.5, 112.4.



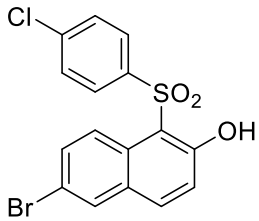
6-bromo-1-tosylnaphthalen-2-ol (**3j**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.09 (s, 1H), 8.21 (d, *J* = 9.2 Hz, 1H), 7.83 (s, 1H), 7.81 – 7.75 (m, 3H), 7.49 (d, *J* = 9.2 Hz, 1H), 7.25 (d, *J* = 8.6 Hz, 2H), 7.17 (d, *J* = 9.1 Hz, 1H), 2.35 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 158.9, 145.1, 139.0, 136.4, 132.0, 131.1, 130.2, 130.2, 128.3, 126.8, 125.0, 121.7, 118.4, 112.8, 21.8. HRMS (ESI) calcd for $C_{17}H_{13}BrO_3S$: 398.9661 ($M + Na^+$), found: 398.9669.



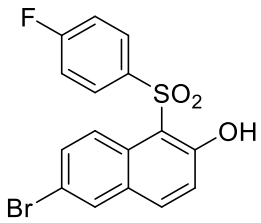
6-bromo-1-((4-bromophenyl)sulfonyl)naphthalen-2-ol (**3k**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 10.97 (s, 1H), 8.17 (d, *J* = 9.2 Hz, 1H), 7.89 – 7.80 (m, 2H), 7.76 (d, *J* = 8.1 Hz, 2H), 7.60 (d, *J* = 7.7 Hz, 2H), 7.52 (d, *J* = 9.2 Hz, 1H), 7.19 (d, *J* = 9.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.2, 140.9, 136.9, 132.9, 132.3, 131.3, 130.2, 129.3, 128.2, 124.7, 121.7, 120.7, 118.6, 112.0. HRMS (ESI) calcd for $C_{16}H_{10}Br_2O_3S$: 462.8610 ($M + Na^+$), found: 462.8633.



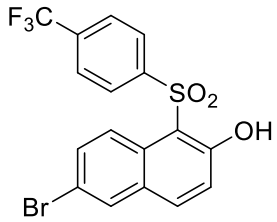
6-bromo-1-((4-chlorophenyl)sulfonyl)naphthalen-2-ol (**3l**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 10.98 (s, 1H), 8.17 (d, *J* = 9.2 Hz, 1H), 7.87 - 7.80 (m, 4H), 7.52 (d, *J* = 9.2 Hz, 1H), 7.44 (d, *J* = 7.4 Hz, 2H), 7.19 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.2, 140.7, 140.4, 136.9, 132.3, 131.3, 130.3, 129.9, 128.2, 124.7, 121.7, 118.6, 112.0. HRMS (ESI) calcd for $C_{16}H_{10}BrClO_3S$: 418.9115 ($M + Na^+$), found: 418.9081.



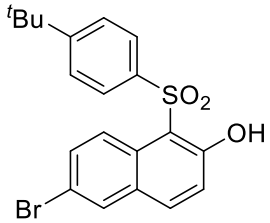
6-bromo-1-((4-fluorophenyl)sulfonyl)naphthalen-2-ol (**3m**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 10.98 (s, 1H), 8.17 (d, *J* = 9.2 Hz, 1H), 7.83 (dd, *J* = 9.2, 4.2 Hz, 4H), 7.52 (d, *J* = 9.2 Hz, 1H), 7.44 (d, *J* = 7.4 Hz, 2H), 7.19 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.2, 140.5, 136.9, 132.3, 131.3, 130.2, 129.9, 128.2, 124.7, 121.7, 118.6, 112.0. HRMS (ESI) calcd for $C_{16}H_{10}BrFO_3S$: 402.9410 (M + Na^+), found: 402.9426.



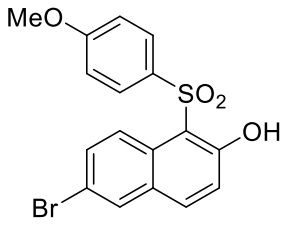
6-bromo-1-((4-(trifluoromethyl)phenyl)sulfonyl)naphthalen-2-ol (**3n**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 10.95 (s, 1H), 8.18 (d, *J* = 9.2 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 2H), 7.86 (d, *J* = 9.7 Hz, 2H), 7.74 (d, *J* = 8.0 Hz, 2H), 7.53 (d, *J* = 9.2 Hz, 1H), 7.21 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.6, 145.4, 140.5, 137.2, 135.6 (t, *J* = 33 Hz), 132.5, 131.4, 130.3, 128.1, 127.3, 126.8, 124.5, 121.7, 118.4 111.4. HRMS (ESI) calcd for $C_{17}H_{11}BrF_3O_3S^+$: 428.9402 (M-H^+), found: 428.9405.



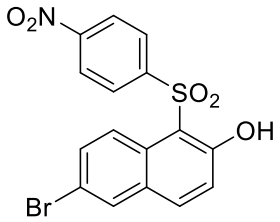
6-bromo-1-((4-(*tert*-butyl)phenyl)sulfonyl)naphthalen-2-ol (**3o**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.10 (s, 1H), 8.27 (d, *J* = 9.2 Hz, 1H), 7.85 – 7.78 (m, 4H), 7.52 (d, *J* = 9.2 Hz, 1H), 7.47 (d, *J* = 7.7 Hz, 2H), 7.18 (d, *J* = 9.0 Hz, 1H), 1.26 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.0, 158.0, 138.9, 136.4, 132.0, 131.1, 130.3, 128.4, 126.6, 126.6, 125.1, 121.7, 118.4, 112.8, 35.5, 31.2. HRMS (ESI) calcd for $C_{20}H_{20}BrO_3S^+$: 419.0311 (M + H^+), found: 419.0325.



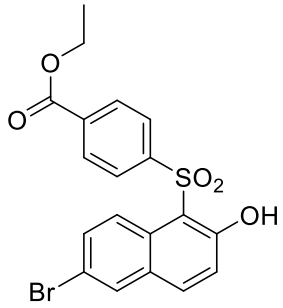
6-bromo-1-((4-methoxyphenyl)sulfonyl)naphthalen-2-ol (**3p**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.11 (s, 1H), 8.24 (d, *J* = 9.2 Hz, 1H), 7.87 - 7.82 (m, 3H), 7.78 (d, *J* = 9.1 Hz, 1H), 7.53 - 7.48 (m, 1H), 7.17 (d, *J* = 9.1 Hz, 1H), 6.94 – 6.89 (m, 2H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 163.9, 158.7, 136.2, 133.5, 131.9, 131.1, 130.3, 129.0, 128.2, 124.9, 121.7, 118.4, 114.7, 113.2, 55.9. HRMS (ESI) calcd for $C_{17}H_{13}BrO_4S$: 392.9791 ($M + H^+$), found: 392.9796.



6-bromo-1-((4-nitrophenyl)sulfonyl)naphthalen-2-ol (**3q**)

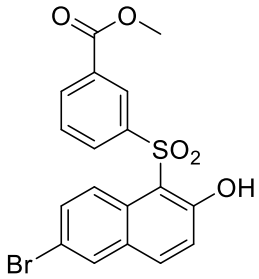
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 10.87 (s, 1H), 8.30 (d, *J* = 7.7 Hz, 2H), 8.16 (d, *J* = 9.2 Hz, 1H), 8.08 (d, *J* = 7.7 Hz, 2H), 7.91 – 7.85 (m, 2H), 7.54 (d, *J* = 9.2 Hz, 1H), 7.22 (d, *J* = 9.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.8, 147.3, 137.6, 132.6, 131.6, 130.3, 128.0, 126.0, 124.9, 124.3, 121.7, 118.9, 117.2, 110.9. HRMS (ESI) calcd for $C_{16}H_{10}BrN_1O_5S$: 405.9379 ($M-H^+$), found: 405.9391.



ethyl 4-((6-bromo-2-hydroxynaphthalen-1-yl)sulfonyl)benzoate (**3r**)

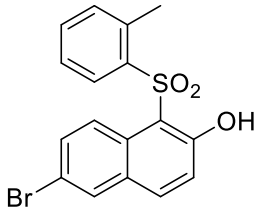
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 10.98 (s, 1H), 8.19 - 8.09 (m, 3H), 7.96 (d, *J* = 7.7 Hz, 2H), 7.84 (d, *J* = 9.8 Hz, 2H), 7.50 (d, *J* = 9.2 Hz, 1H), 7.20 (d, *J* = 9.1 Hz, 1H), 4.35 (q, *J* = 7.0 Hz, 2H), 1.35 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 164.9,

159.5, 145.5, 137.0, 135.4, 132.3, 131.3, 130.7, 130.2, 128.2, 126.7, 124.7, 121.7, 118.7, 111.7, 62.0, 14.4. HRMS (ESI) calcd for $C_{19}H_{16}BrO_5S^+$: 434.9896 ($M + H^+$), found: 434.9873.



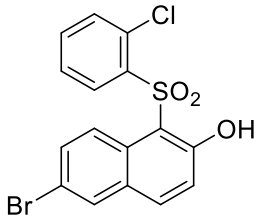
methyl 3-((6-bromo-2-hydroxynaphthalen-1-yl)sulfonyl)benzoate (**3s**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 10.99 (s, 1H), 8.56 (s, 1H), 8.23 - 8.16 (m, 2H), 8.06 (d, *J* = 7.6 Hz, 1H), 7.84 (d, *J* = 10.1 Hz, 2H), 7.60 – 7.49 (m, 2H), 7.21 (d, *J* = 9.2 Hz, 1H), 3.92 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 165.2, 159.5, 142.7, 137.0, 134.9, 132.3, 131.9, 131.4, 130.7, 130.3, 129.9, 127.8, 124.7, 121.8, 118.6, 53.0. HRMS (ESI) calcd for $C_{18}H_{13}BrO_5S$: 442.9559 ($M + Na^+$), found: 442.9557.



6-bromo-1-(*o*-tolylsulfonyl)naphthalen-2-ol (**3t**)

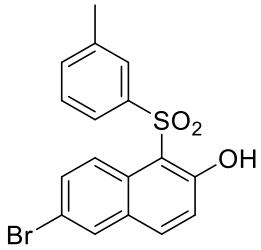
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.09 (s, 1H), 8.25 (d, *J* = 7.6 Hz, 1H), 7.96 (d, *J* = 9.1 Hz, 1H), 7.84 (d, *J* = 9.3 Hz, 2H), 7.49 - 7.41 (m, 3H), 7.22 - 7.16 (m, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.6, 140.0, 138.2, 136.6, 134.1, 133.3, 131.9, 131.2, 130.2, 128.9, 126.7, 124.8, 121.7, 118.4, 19.3. HRMS (ESI) calcd for $C_{17}H_{13}BrO_3S$: 398.9661 ($M + Na^+$), found: 398.9658.



6-bromo-1-((2-chlorophenyl)sulfonyl)naphthalen-2-ol (**3u**)

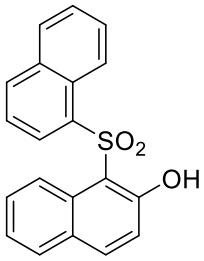
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 10.91 (s, 1H), 8.48 (d, *J* = 7.2 Hz, 1H), 7.93 (d, *J* =

9.2 Hz, 1H), 7.84 (d, *J* = 9.0 Hz, 2H), 7.59 – 7.48 (m, 2H), 7.46 - 7.37 (m, 2H), 7.18 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.6, 139.0, 136.9, 135.1, 132.5, 131.9, 131.3, 130.9, 130.1, 127.9, 127.4, 124.4, 121.7, 118.2, 115.0. HRMS (ESI) calcd for $C_{16}H_{10}BrClO_3S$: 418.9115 ($M + Na^+$), found: 418.9101.



6-bromo-1-(m-tolylsulfonyl)naphthalen-2-ol (**3v**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 11.08 (s, 1H), 8.21 (d, *J* = 9.2 Hz, 1H), 7.86 - 7.79 (m, 2H), 7.70 (d, *J* = 5.5 Hz, 2H), 7.53 - 7.48 (m, 1H), 7.35 (d, *J* = 4.7 Hz, 2H), 7.19 (d, *J* = 9.1 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.1, 141.8, 140.0, 136.5, 134.9, 132.0, 131.2, 130.2, 129.4, 128.3, 126.9, 125.0, 123.9, 121.7, 118.4, 21.6. HRMS (ESI) calcd for $C_{17}H_{13}BrO_3S$: 398.9661 ($M + Na^+$), found: 398.9644.

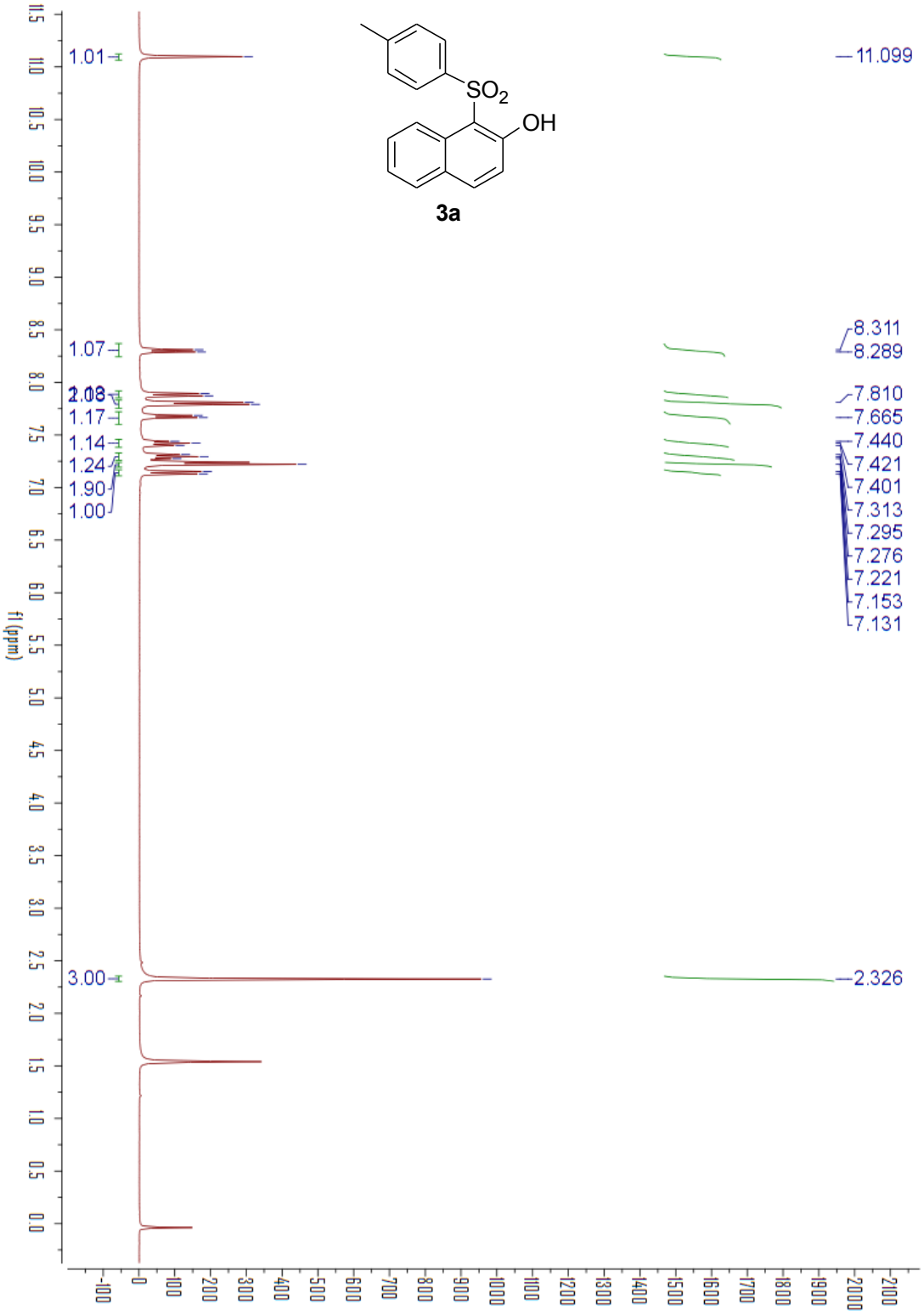


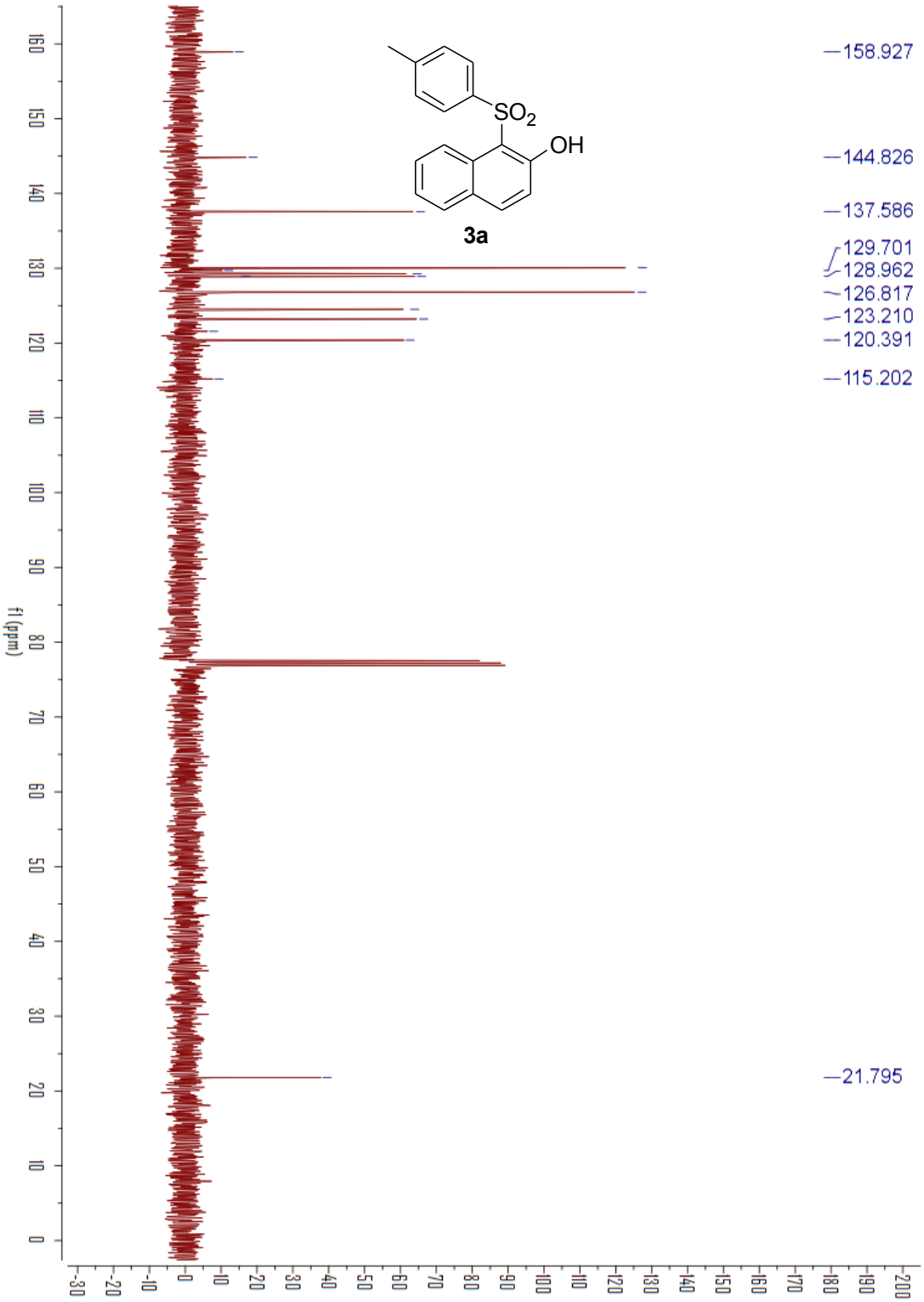
1-(naphthalen-1-ylsulfonyl)naphthalen-2-ol (**3w**)

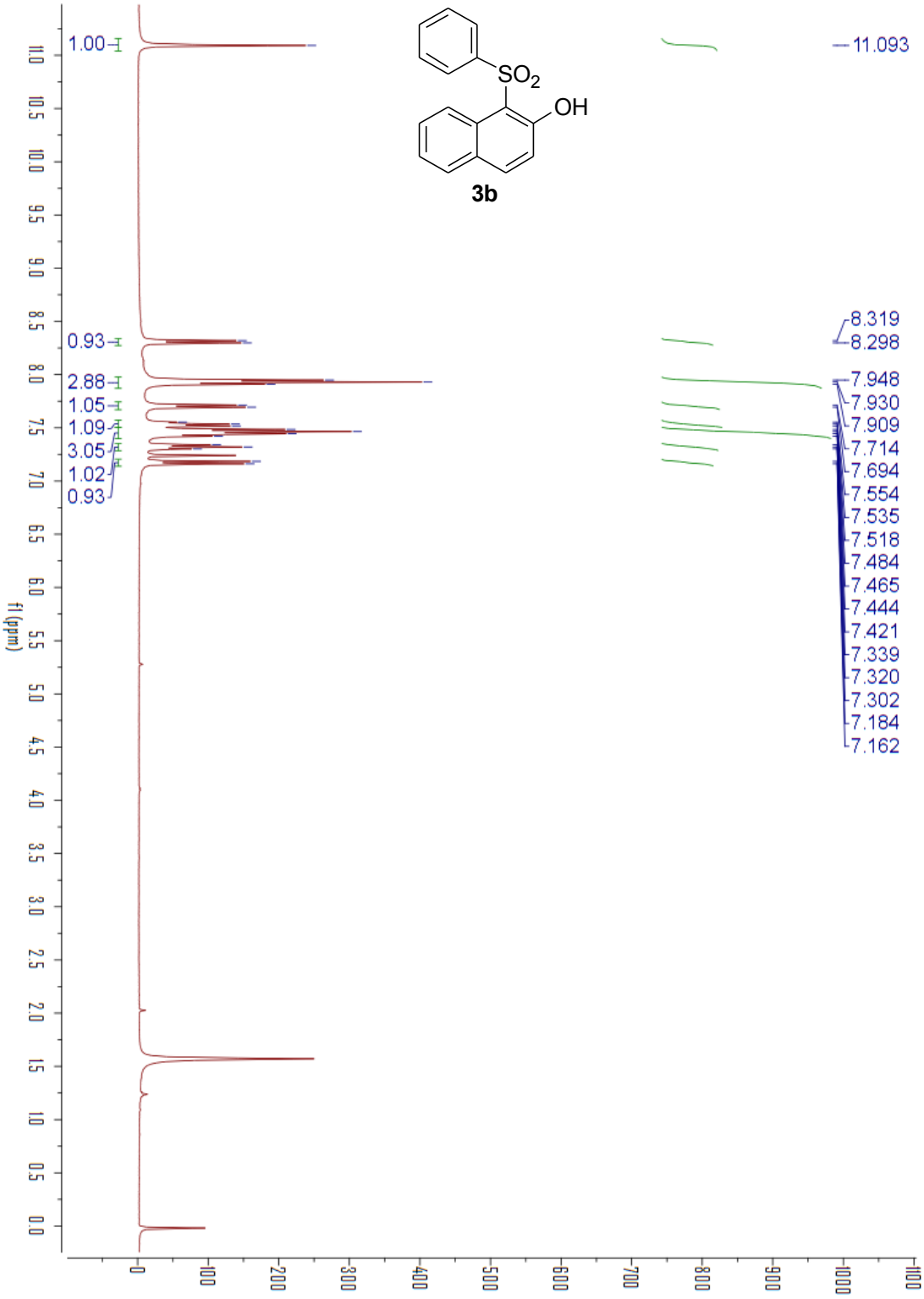
^{1}H NMR (400 MHz, $CDCl_3$) δ = 11.30 (s, 1H), 8.48 (d, *J* = 7.4, 1H), 8.38 (d, *J* = 8.6, 1H), 8.18 (d, *J* = 8.7, 1H), 8.04 (d, *J* = 8.2, 1H), 7.91 (d, *J* = 9.1, 1H), 7.85 (d, *J* = 8.1, 1H), 7.65 (d, *J* = 8.0, 1H), 7.61 – 7.54 (m, 2H), 7.49 (t, *J* = 7.5, 1H), 7.33 (t, *J* = 7.8, 1H), 7.25 (t, *J* = 8.4, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 159.1, 137.8, 137.0, 135.5, 134.5, 129.7, 129.5, 129.3, 129.0, 128.9, 128.8, 128.6, 127.2, 124.5, 124.2, 123.3, 123.3, 120.5, 112.4. HRMS (ESI) calcd for $C_{20}H_{14}O_3S$: 335.0736 ($M + H^+$), found: 335.0736.

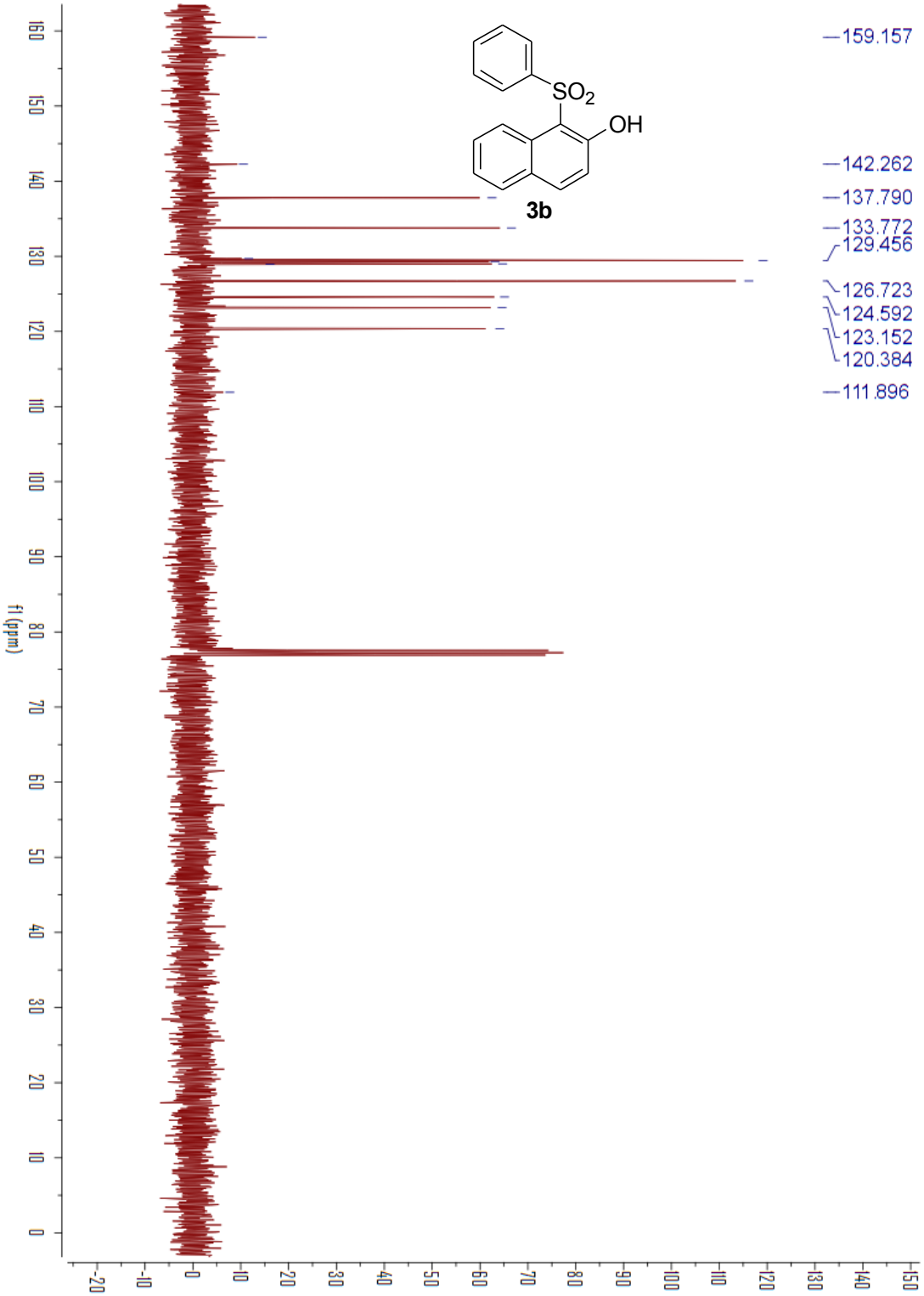
Reference：

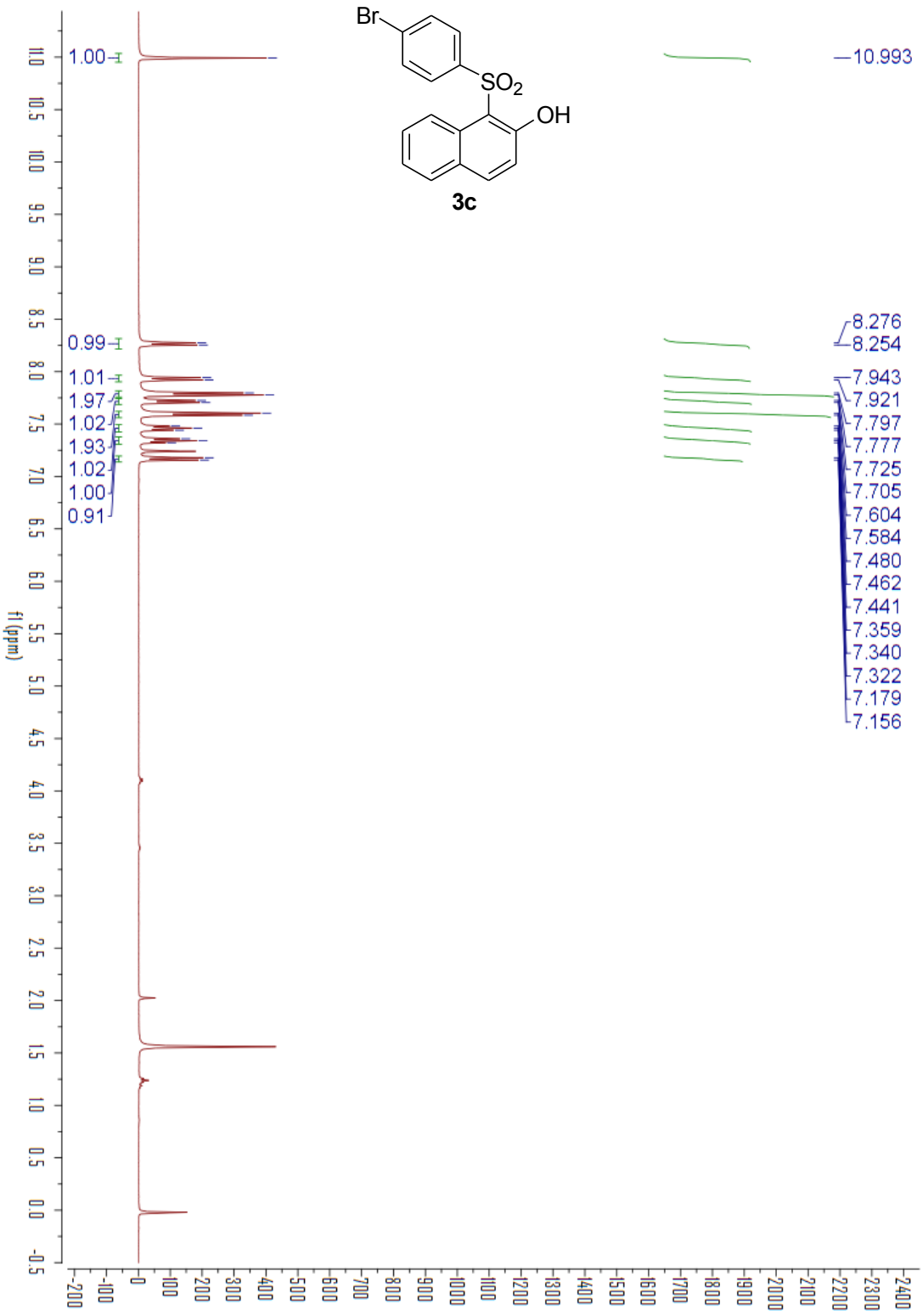
(1) F. Xiao, S. Chen, J. Tian, H. Huang, Y. Liu and G. Deng, *Green Chem.* 2016, **18**, 1538.

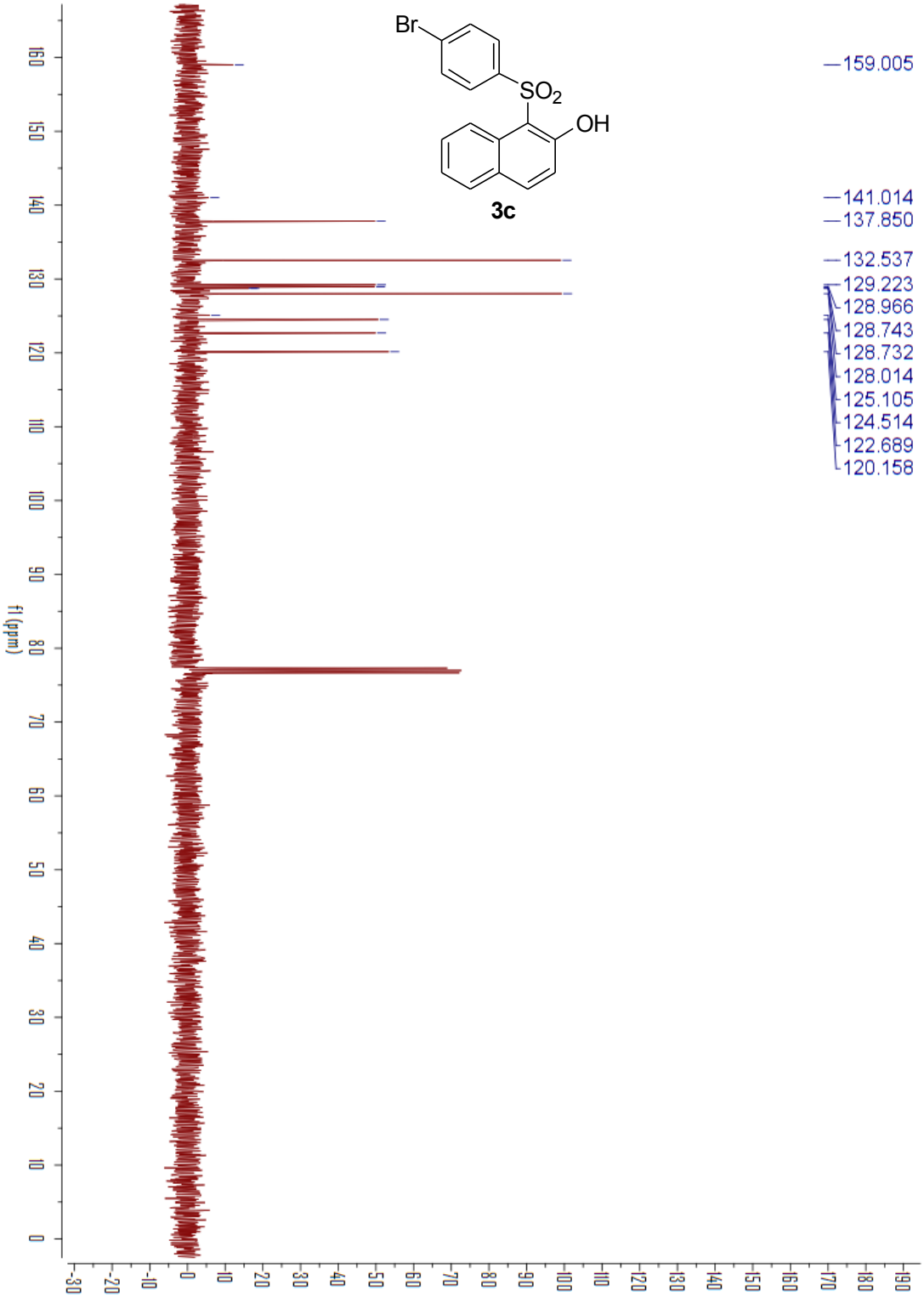

SO2
OH
3a
1.01
1.07
2.08
1.17
1.14
1.24
1.90
1.00
3.00
11.099
8.311
8.289
7.810
7.665
7.440
7.421
7.401
7.313
7.295
7.276
7.221
7.153
7.131
2.326
f1 (ppm)

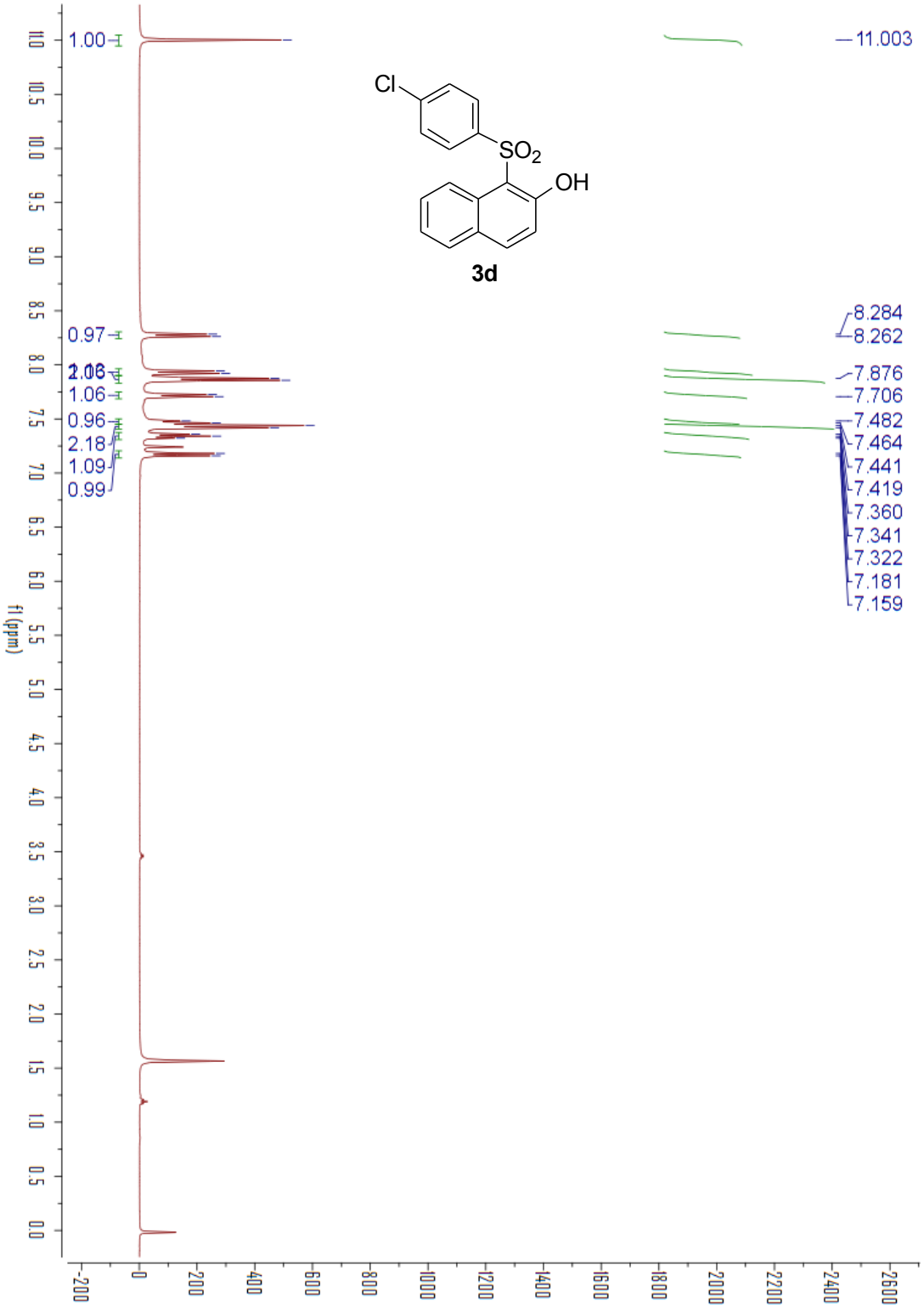

158.927
144.826
137.586
129.701
128.962
126.817
123.210
120.391
115.202
21.795
SO2
OH
3a
f1 (ppm)

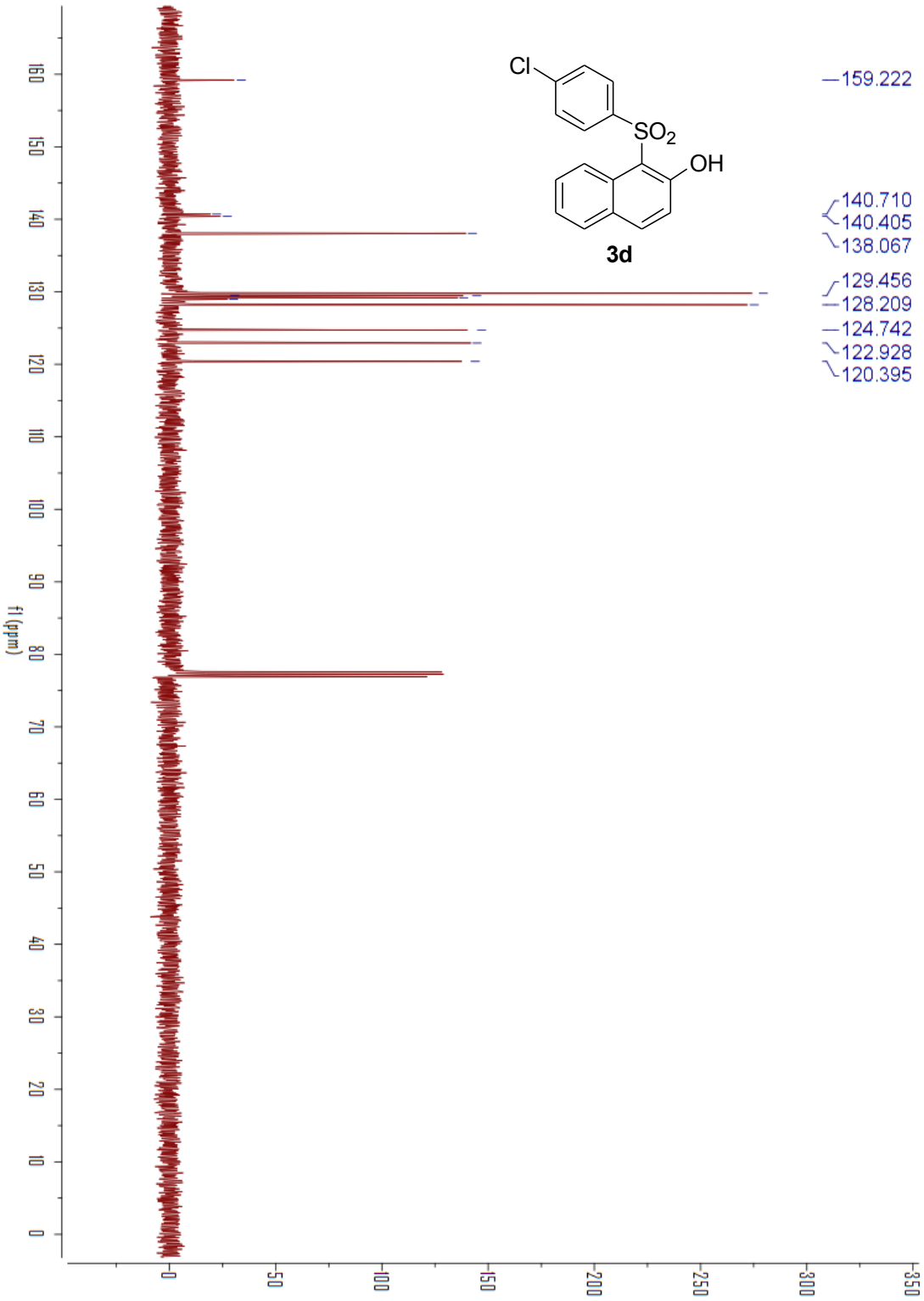

1.00
0.93
2.88
1.05
1.09
3.05
1.02
0.93
11.093
8.319
8.298
7.948
7.930
7.909
7.714
7.694
7.554
7.535
7.518
7.484
7.465
7.444
7.421
7.339
7.320
7.302
7.184
7.162
SO2
OH
3b
f1 (ppm)

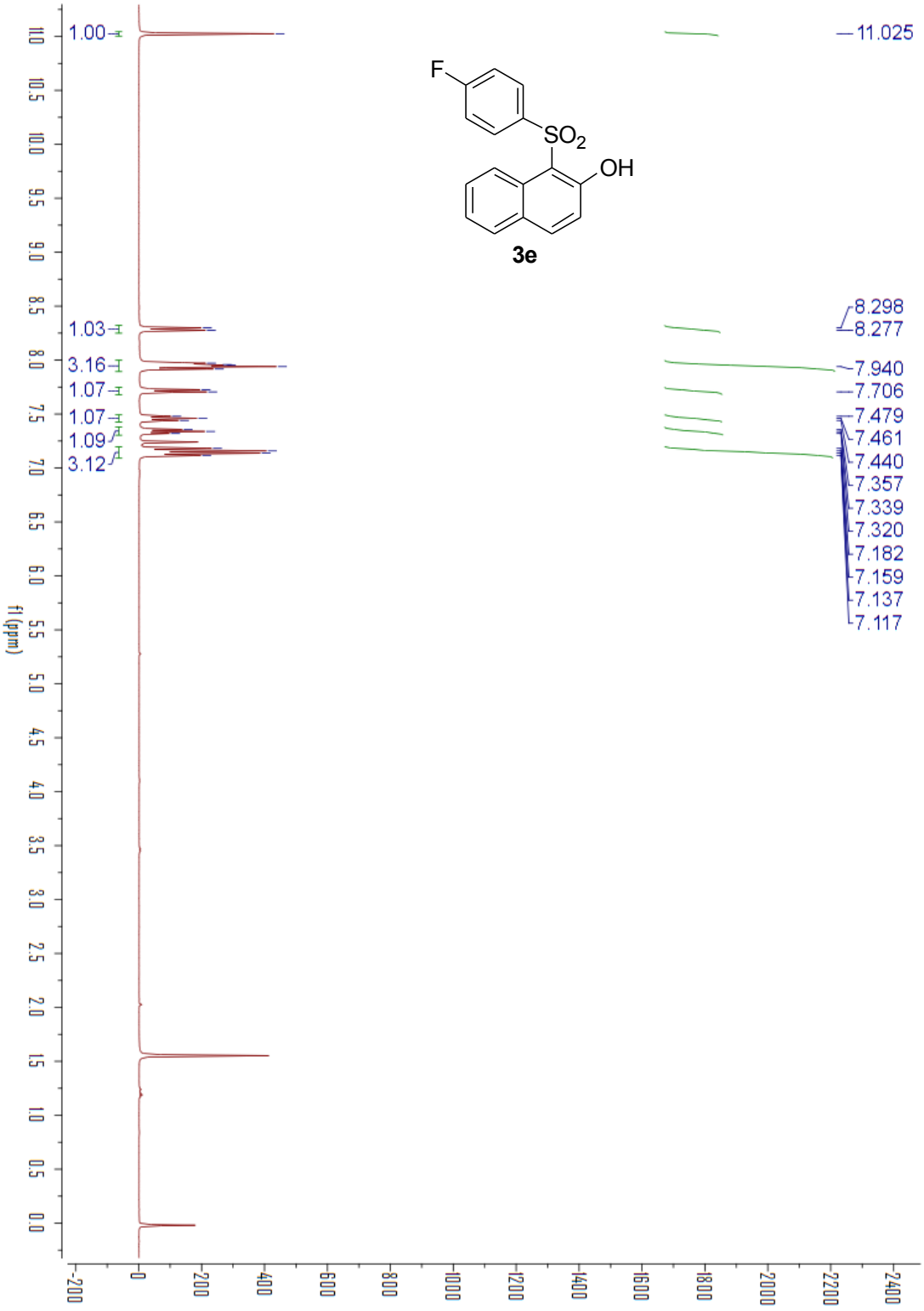

159.157
142.262
137.790
133.772
129.456
126.723
124.592
123.152
120.384
111.896
SO2
OH
3b
f1 (ppm)

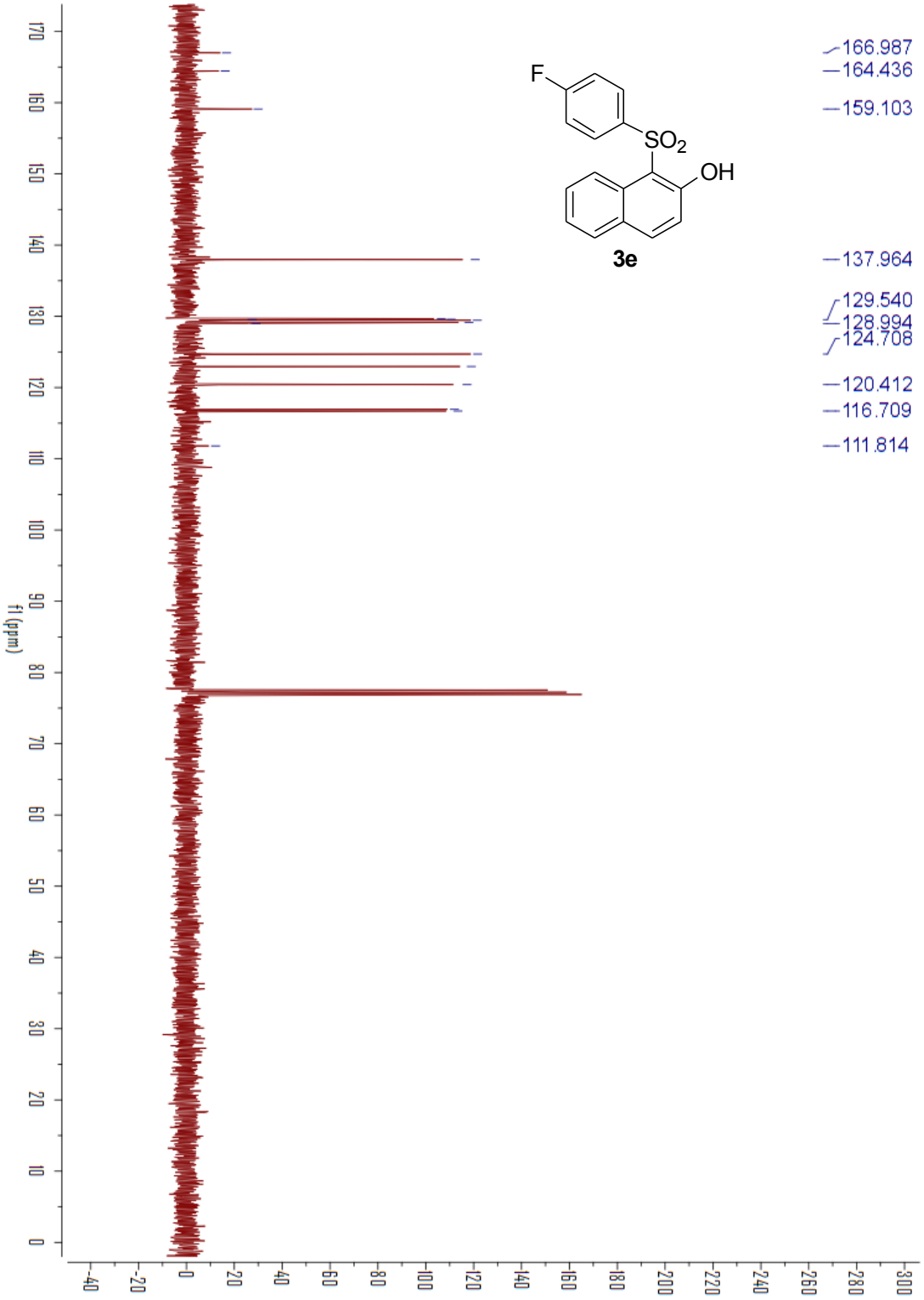

Br
SO2
OH
3c
1.00
0.99
1.01
1.97
1.02
1.93
1.02
1.00
0.91
10.993
8.276
8.254
7.943
7.921
7.797
7.777
7.725
7.705
7.604
7.584
7.480
7.462
7.441
7.359
7.340
7.322
7.179
7.156
f1 (ppm)

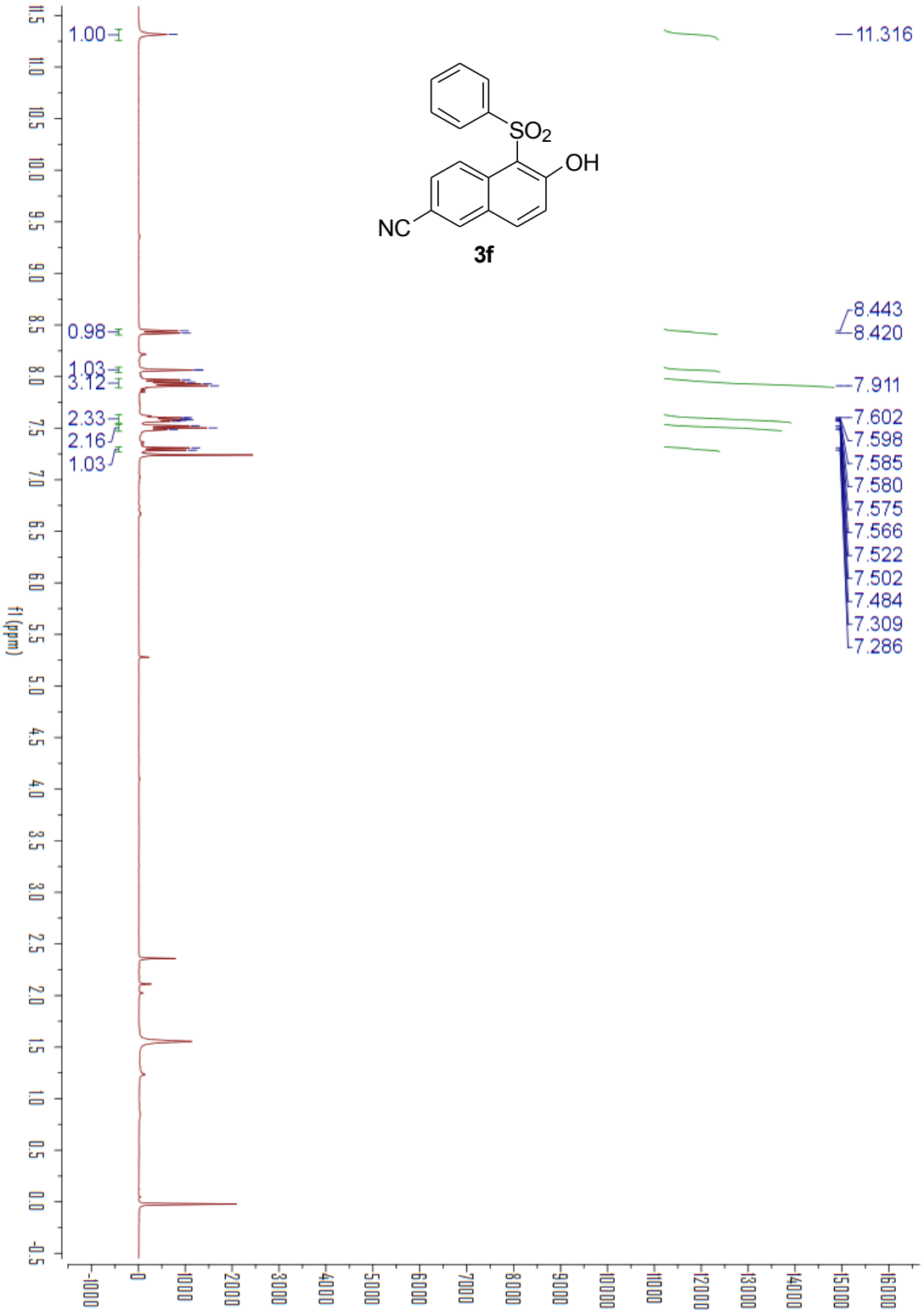

Br
SO2
OH
3c
159.005
141.014
137.850
132.537
129.223
128.966
128.743
128.732
128.014
125.105
124.514
122.689
120.158
f1 (ppm)

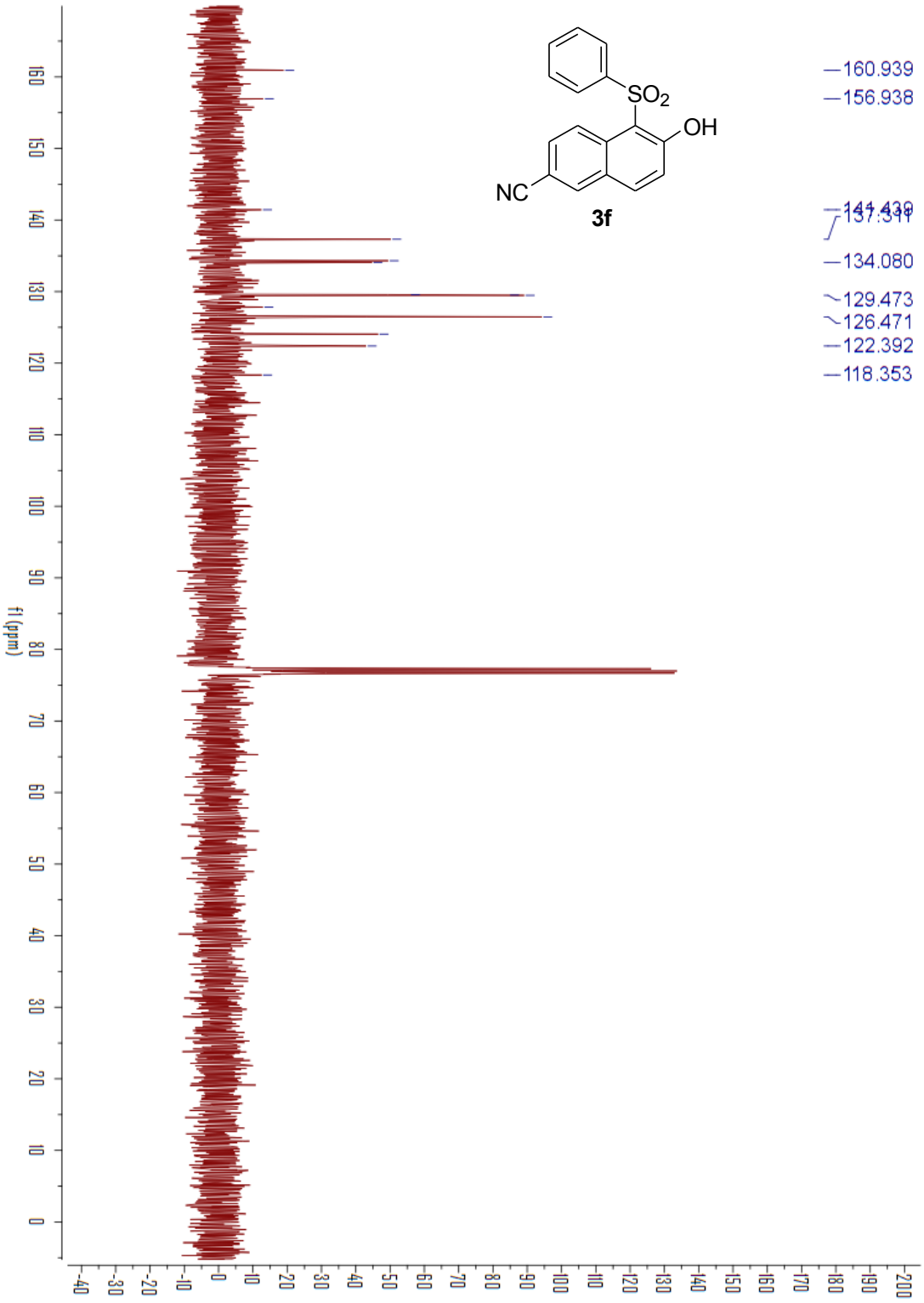

Cl
SO2
OH
3d
11.003
8.284
8.262
7.876
7.706
7.482
7.464
7.441
7.419
7.360
7.341
7.322
7.181
7.159
1.00
0.97
2.06
1.06
0.96
2.18
1.09
0.99
f1 (ppm)

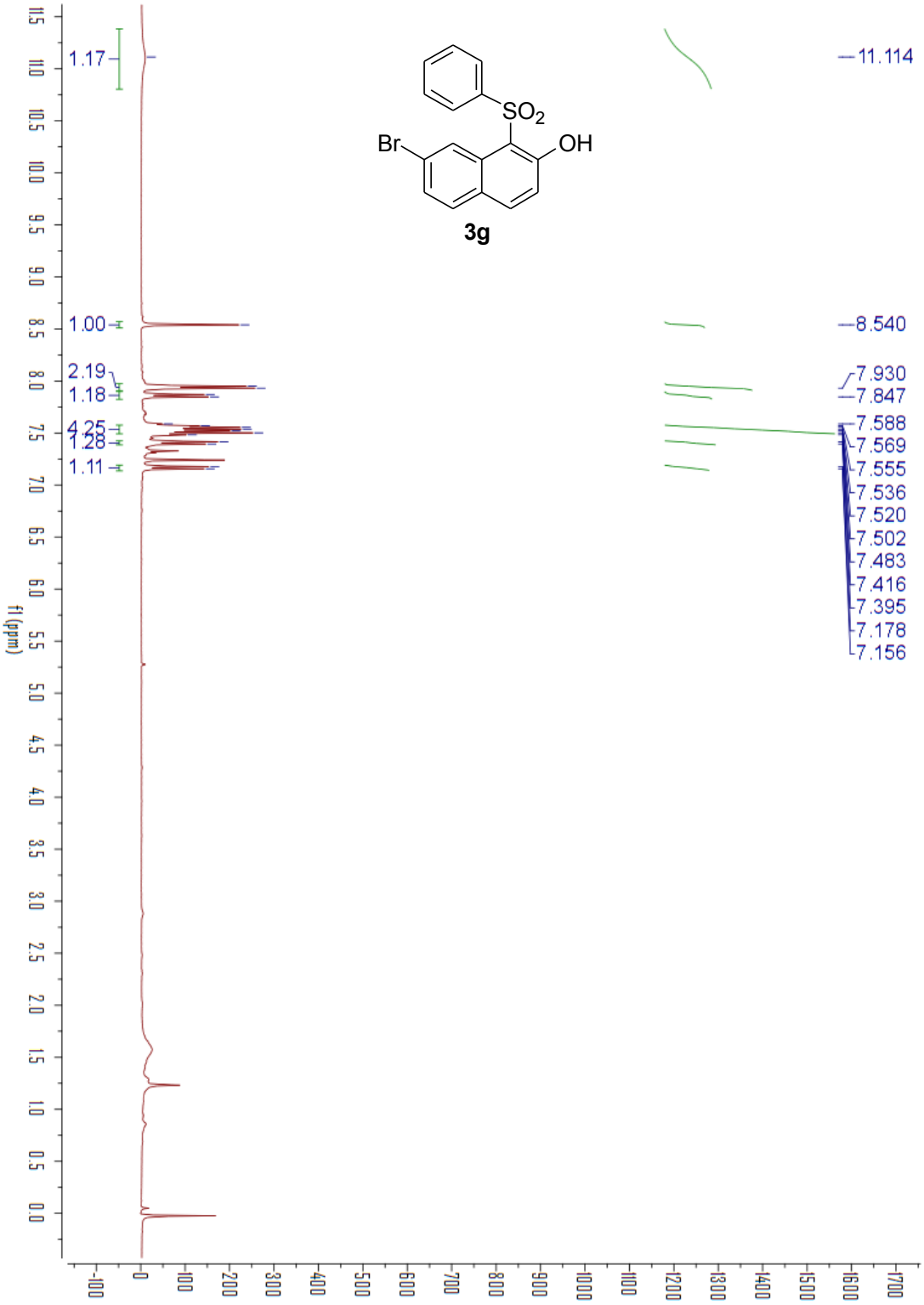

Cl
SO2
OH
3d
159.222
140.710
140.405
138.067
129.456
128.209
124.742
122.928
120.395
f1 (ppm)


F
SO2
OH
3e
11.025
8.298
8.277
7.940
7.706
7.479
7.461
7.440
7.357
7.339
7.320
7.182
7.159
7.137
7.117
1.00
1.03
3.16
1.07
1.07
1.09
3.12
f1 (ppm)


F
SO2
OH
3e
166.987
164.436
159.103
137.964
129.540
128.994
124.708
120.412
116.709
111.814
f1 (ppm)

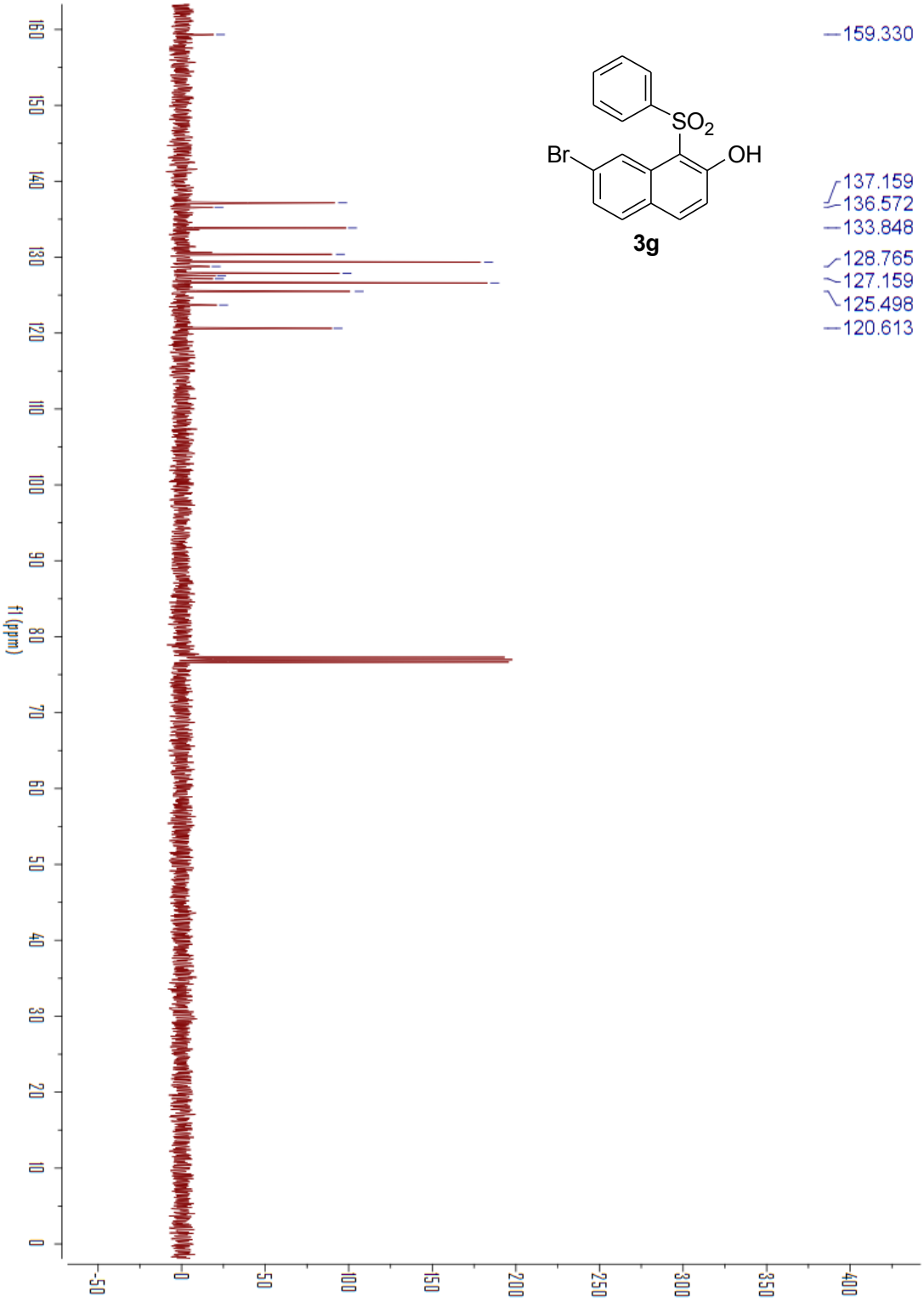

1.00
0.98
1.03
3.12
2.33
2.16
1.03
11.316
8.443
8.420
7.911
7.602
7.598
7.585
7.580
7.575
7.566
7.522
7.502
7.484
7.309
7.286
SO2
OH
NC
3f
f1 (ppm)

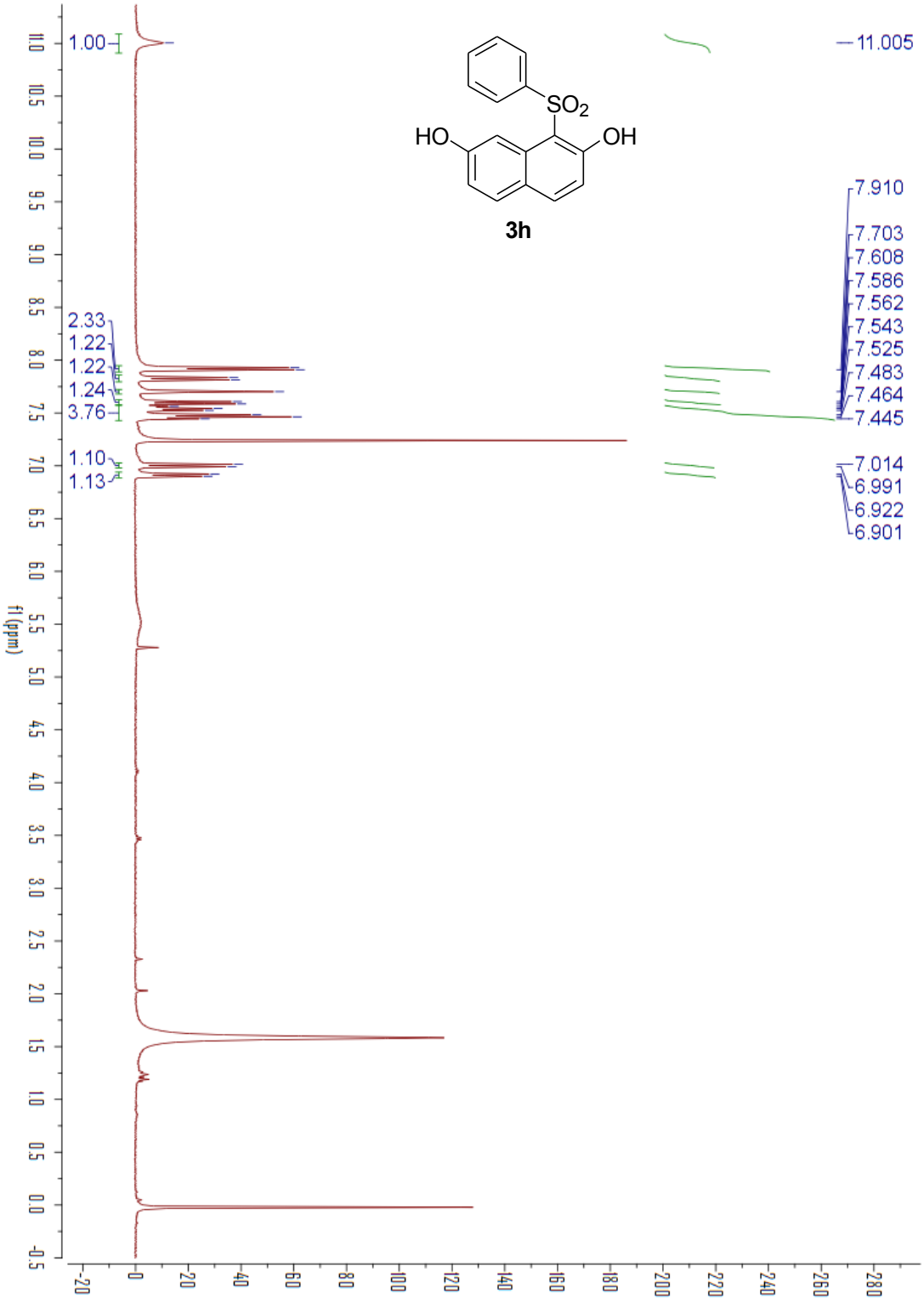

SO2
OH
NC
3f
160.939
156.938
144.439
137.311
134.080
129.473
126.471
122.392
118.353
f1 (ppm)

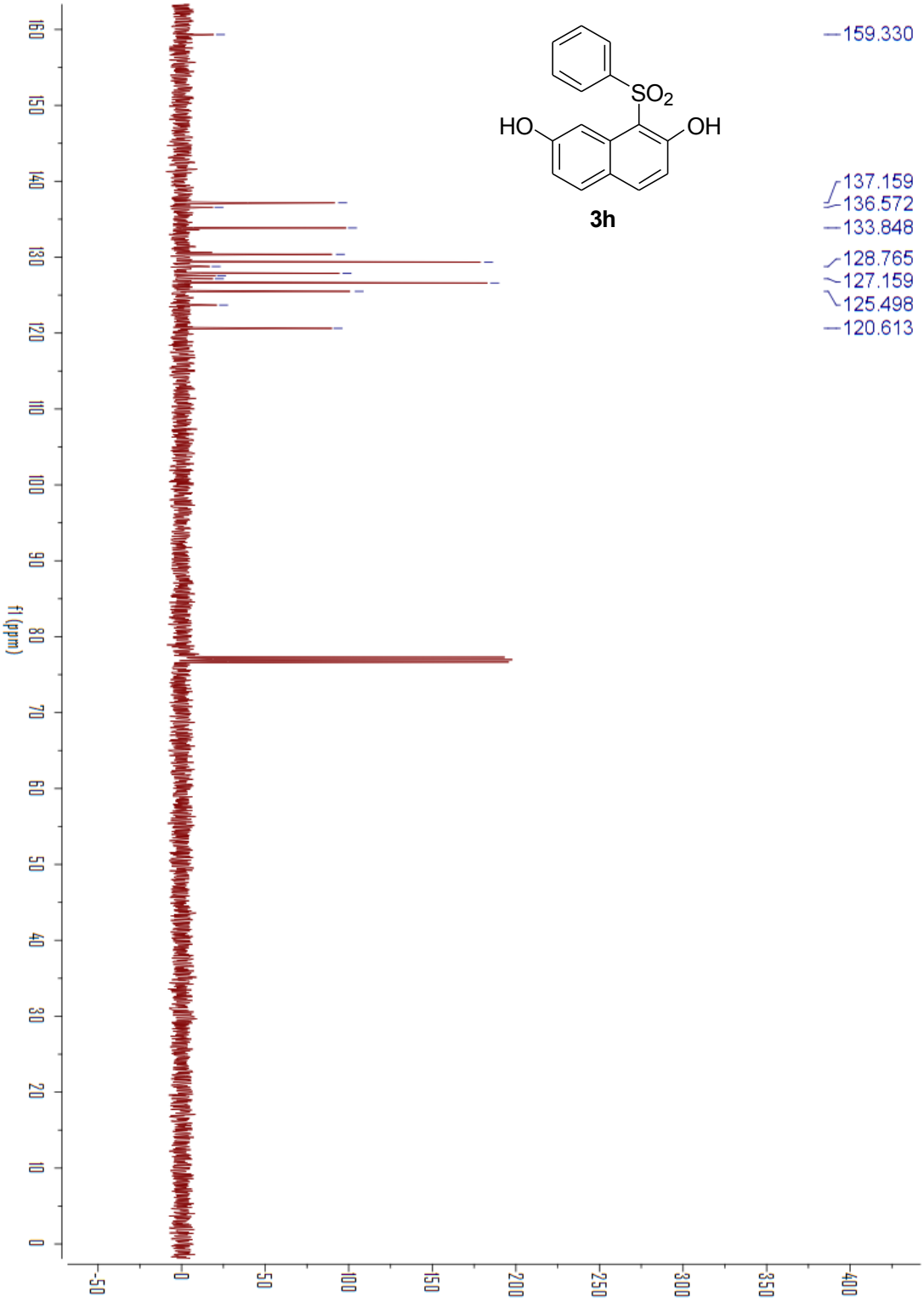

1.17
1.00
2.19
1.18
4.25
1.28
1.11
11.114
8.540
7.930
7.847
7.588
7.569
7.555
7.536
7.520
7.502
7.483
7.416
7.395
7.178
7.156
f1 (ppm)

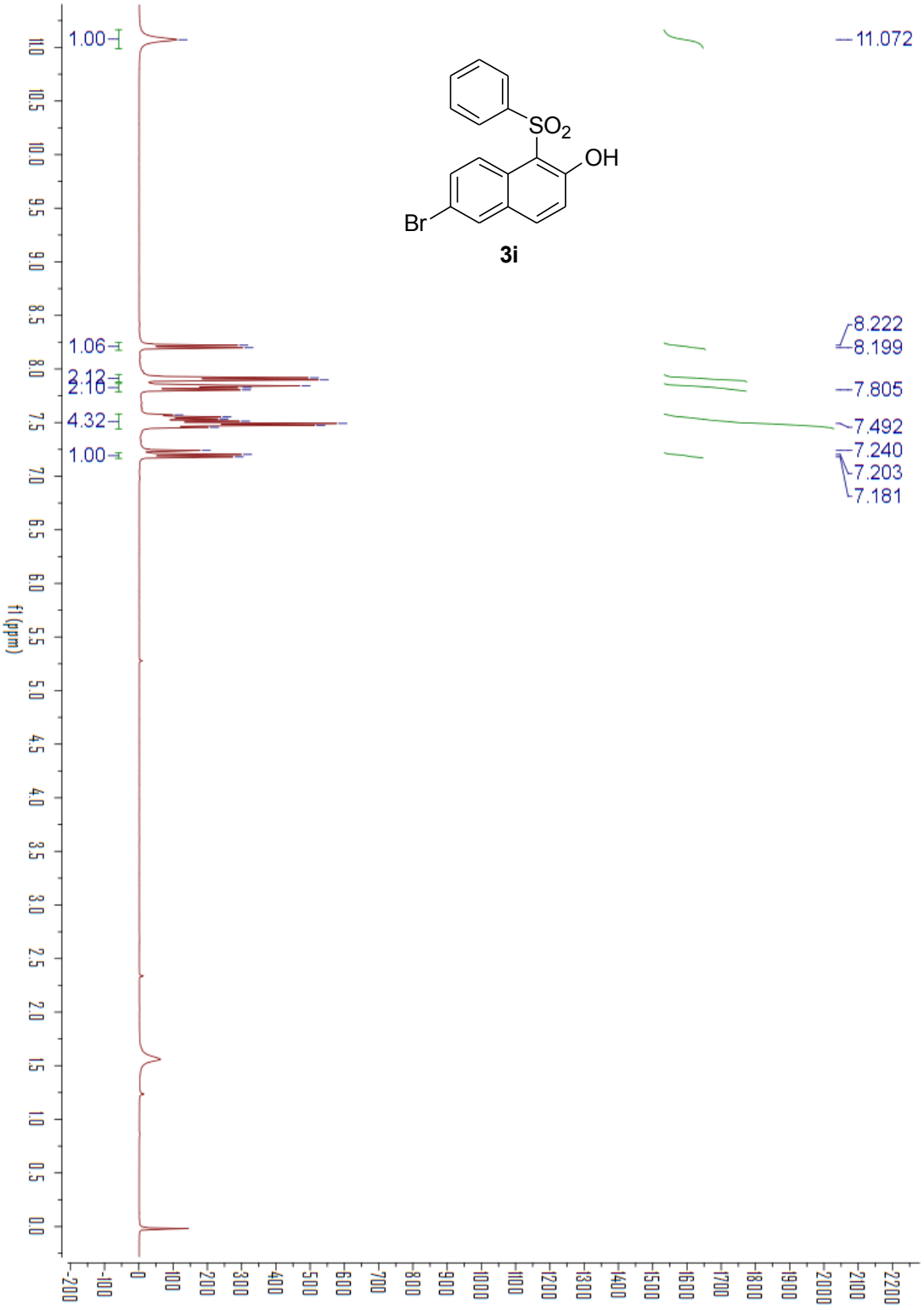
SO2
Br
OH

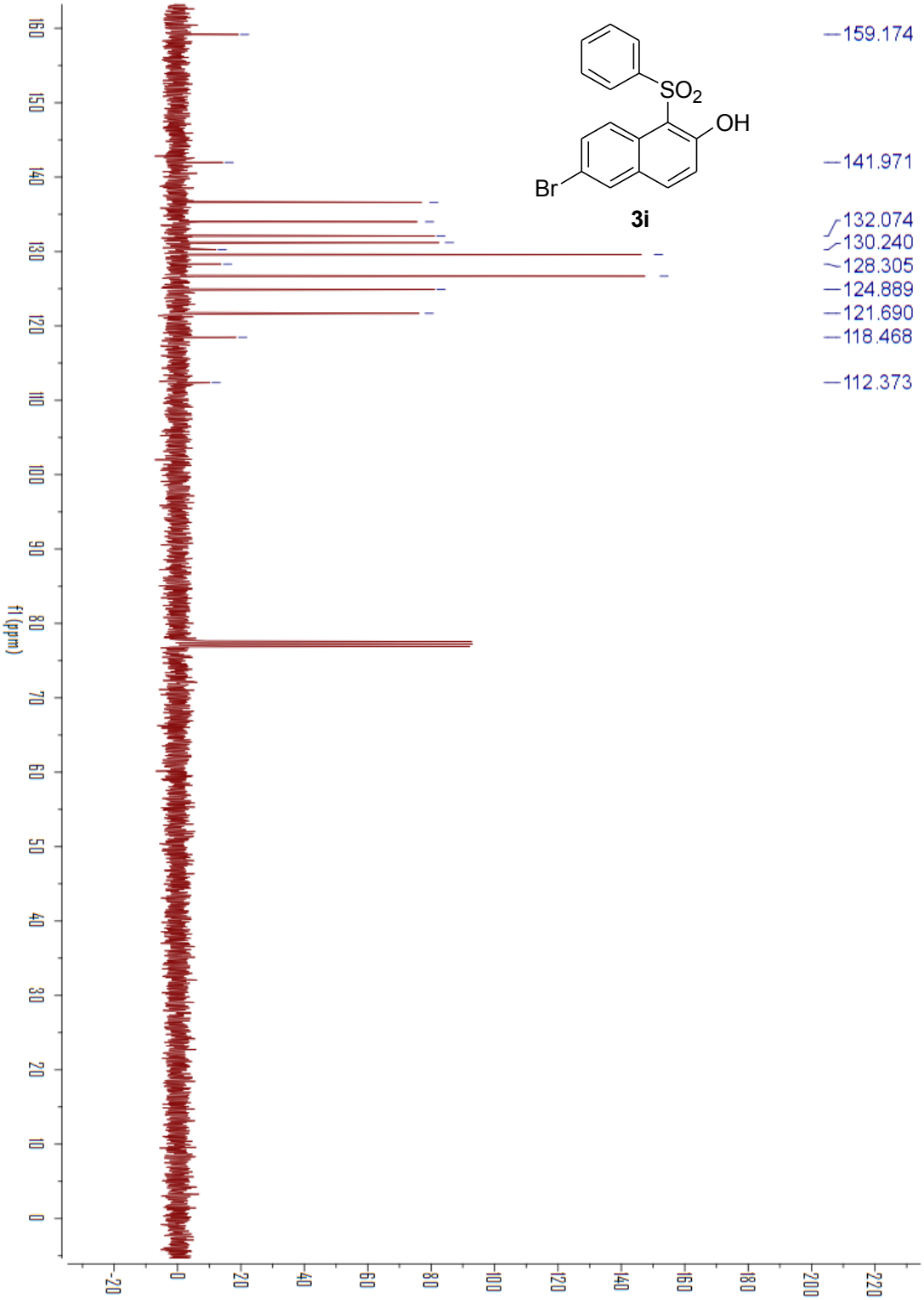
3g

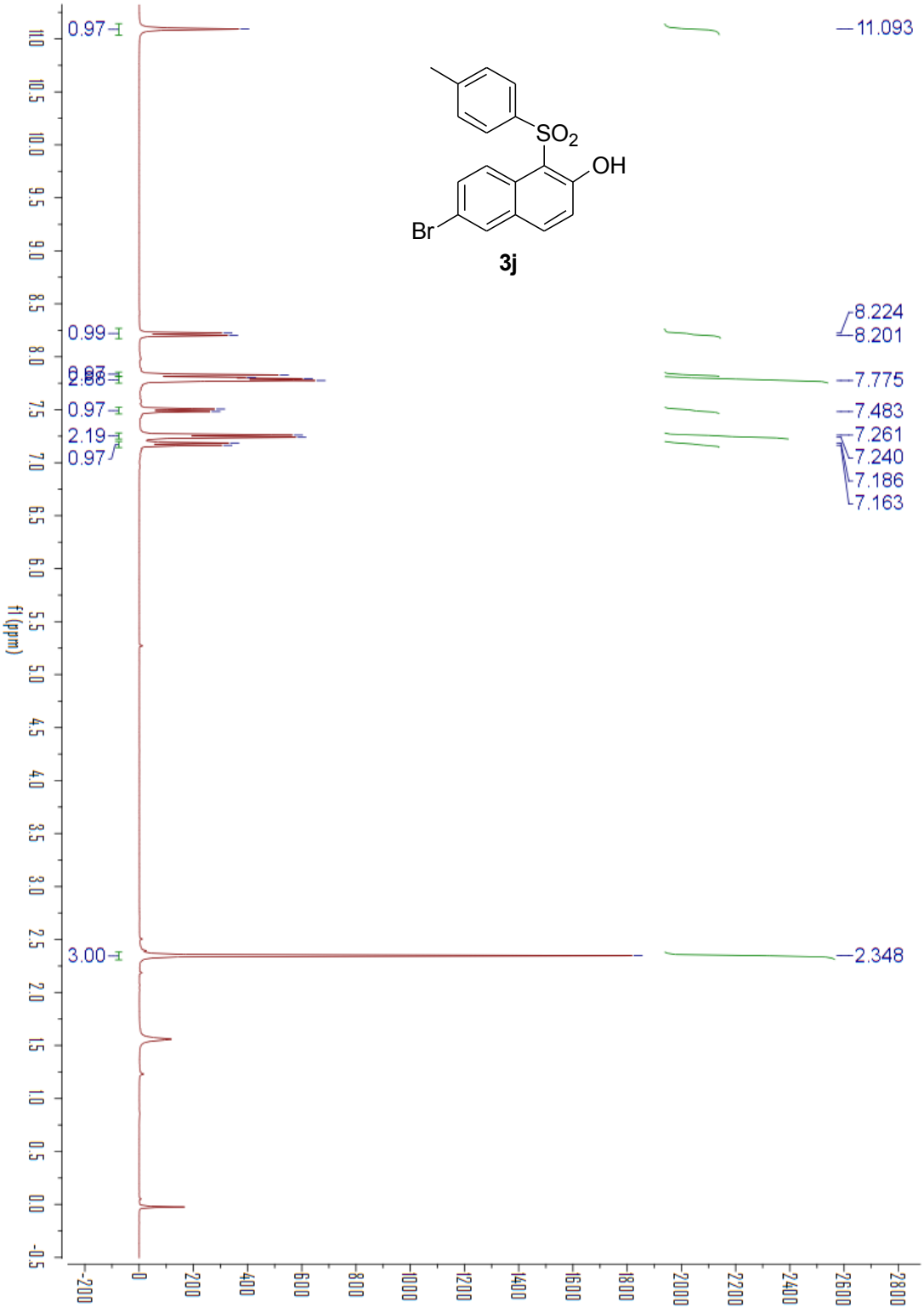

159.330
137.159
136.572
133.848
128.765
127.159
125.498
120.613
SO2
Br
OH
3g
f1 (ppm)

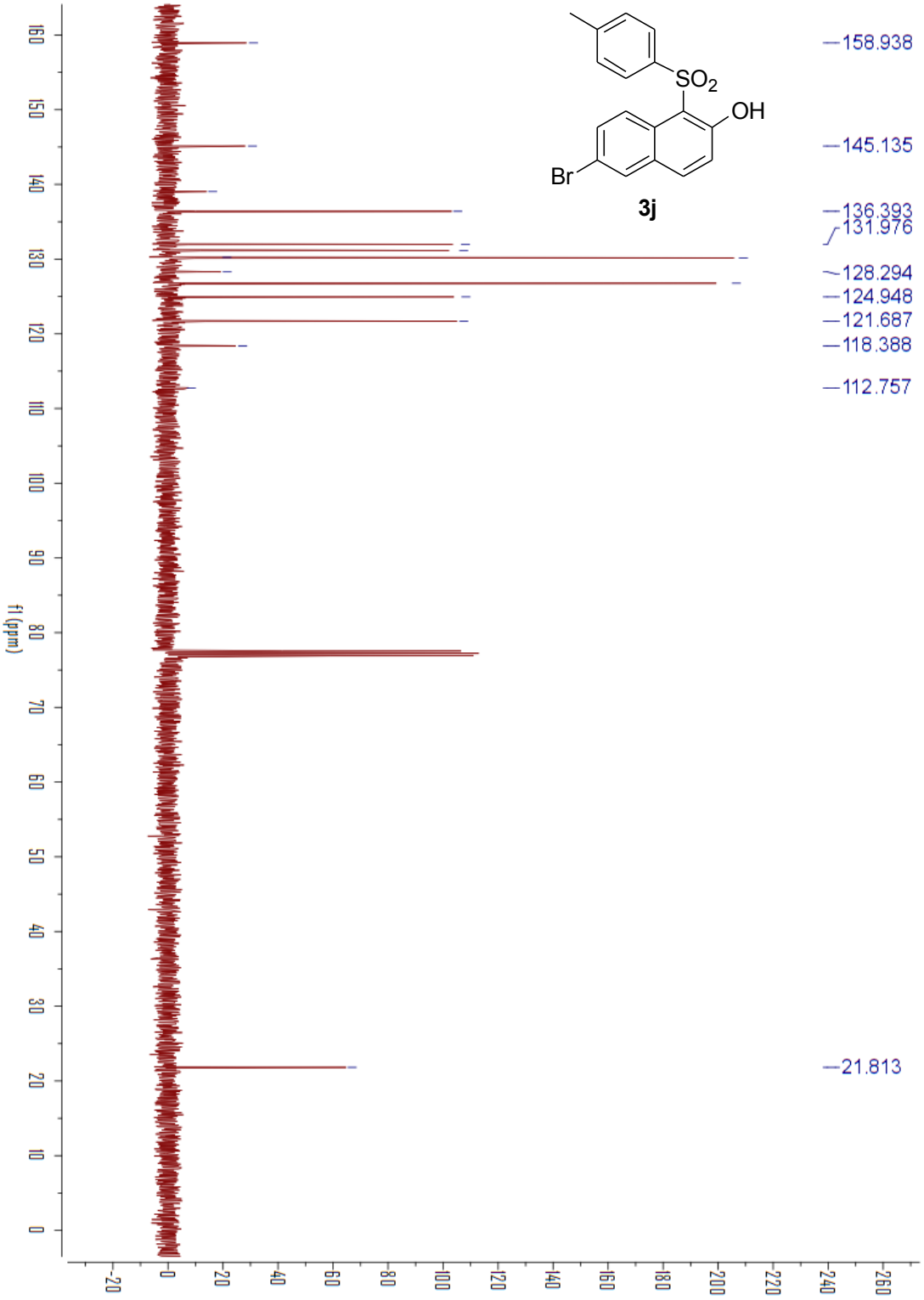

1.00
2.33
1.22
1.22
1.24
3.76
1.10
1.13
11.005
7.910
7.703
7.608
7.586
7.562
7.543
7.525
7.483
7.464
7.445
7.014
6.991
6.922
6.901
SO2
HO
OH
3h
f1 (ppm)

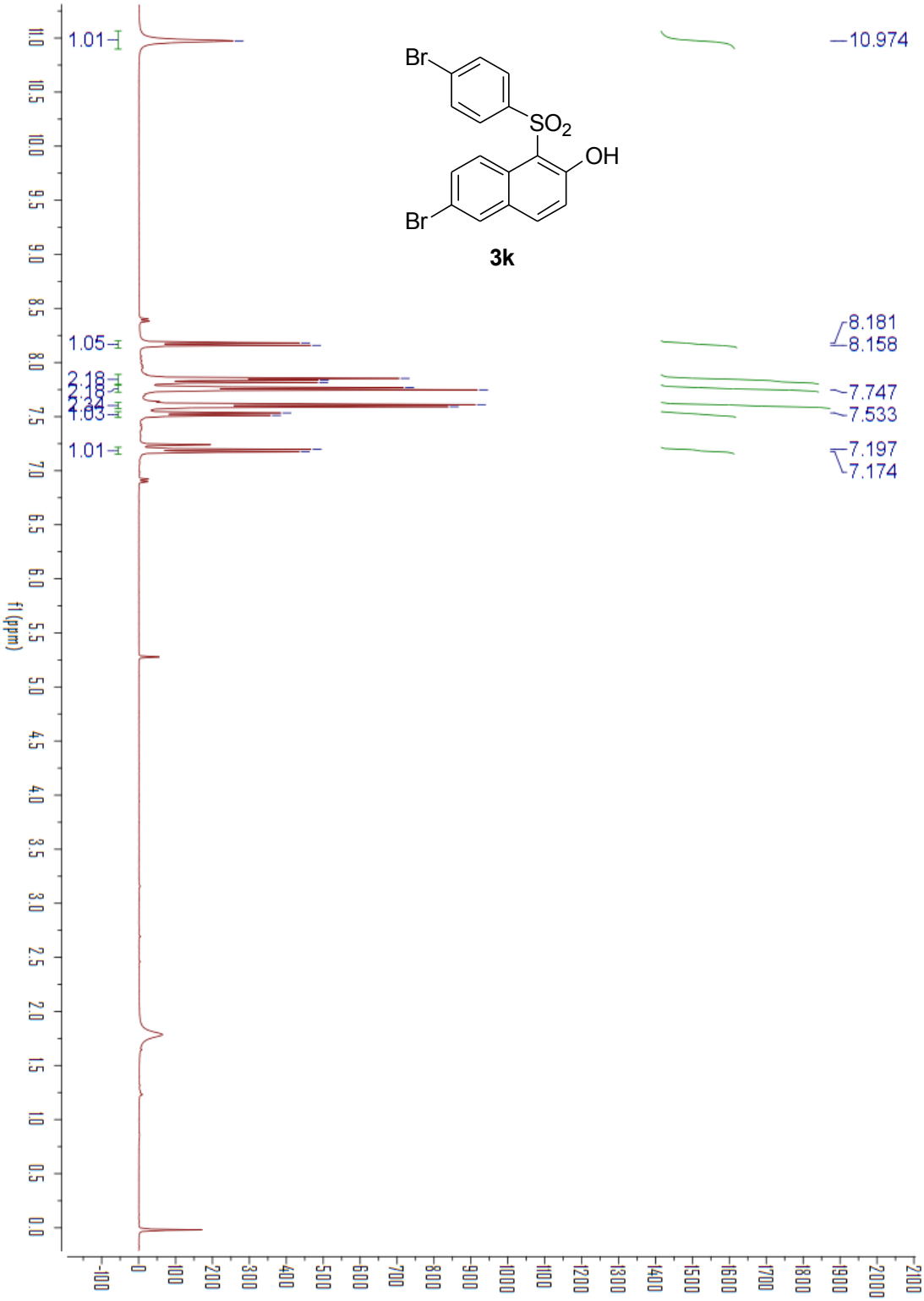

159.330
137.159
136.572
133.848
128.765
127.159
125.498
120.613
SO2
HO
OH
3h
f1 (ppm)

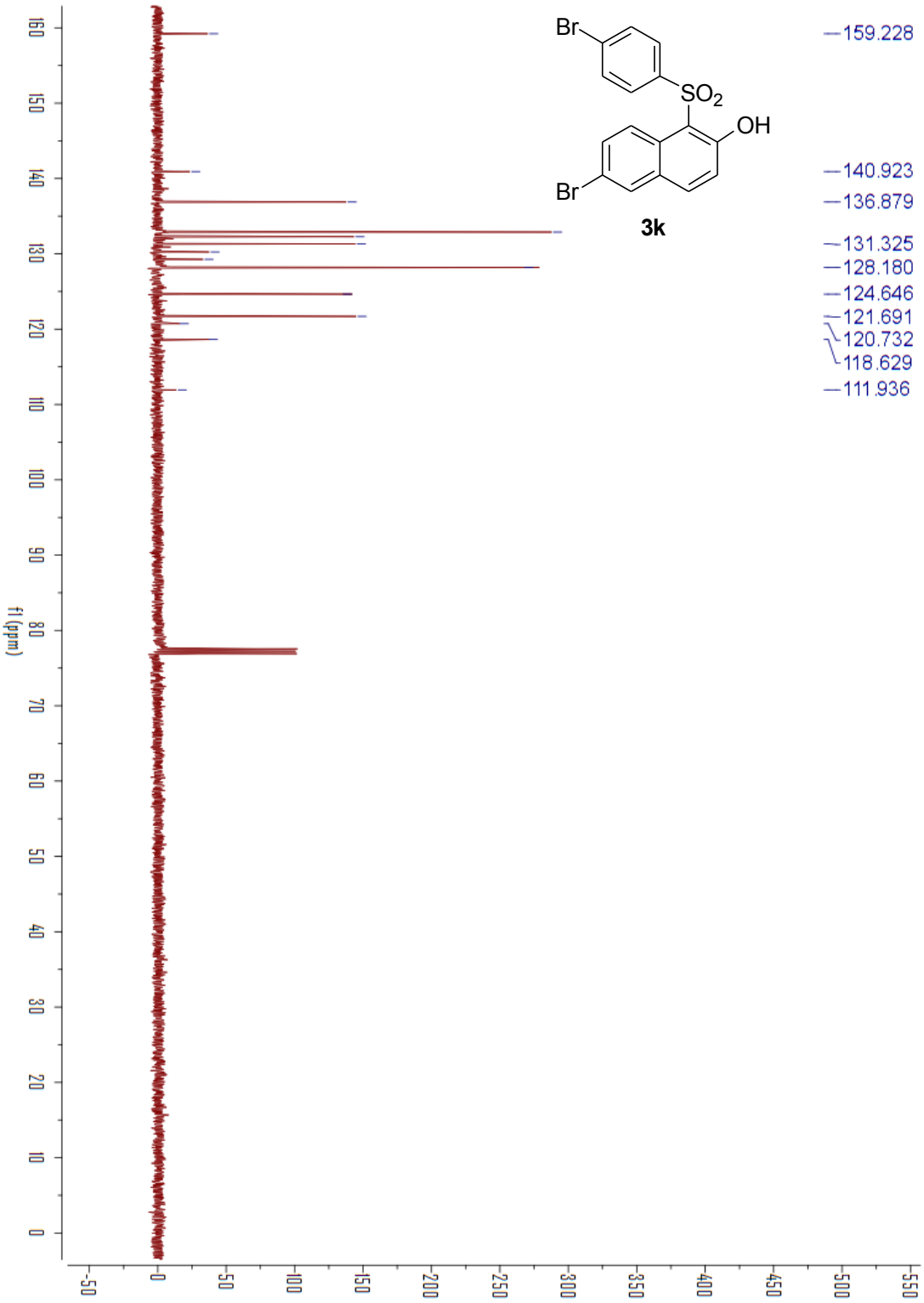

1.00
1.06
2.12
2.10
4.32
1.00
11.072
8.222
8.199
7.805
7.492
7.240
7.203
7.181
SO2
OH
Br
3i
f1 (ppm)

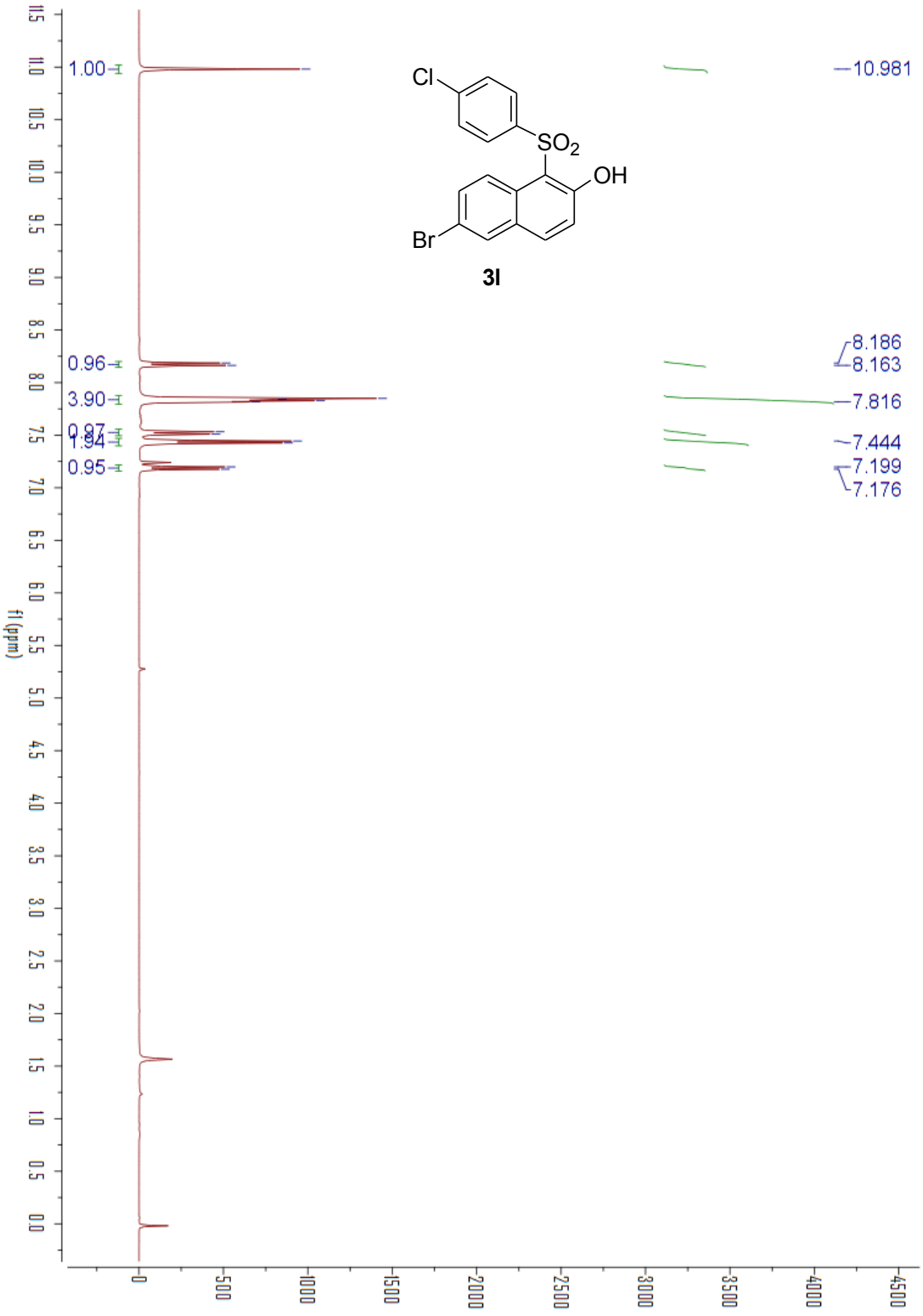

159.174
141.971
132.074
130.240
128.305
124.889
121.690
118.468
112.373
SO2
OH
Br
3i
f1 (ppm)

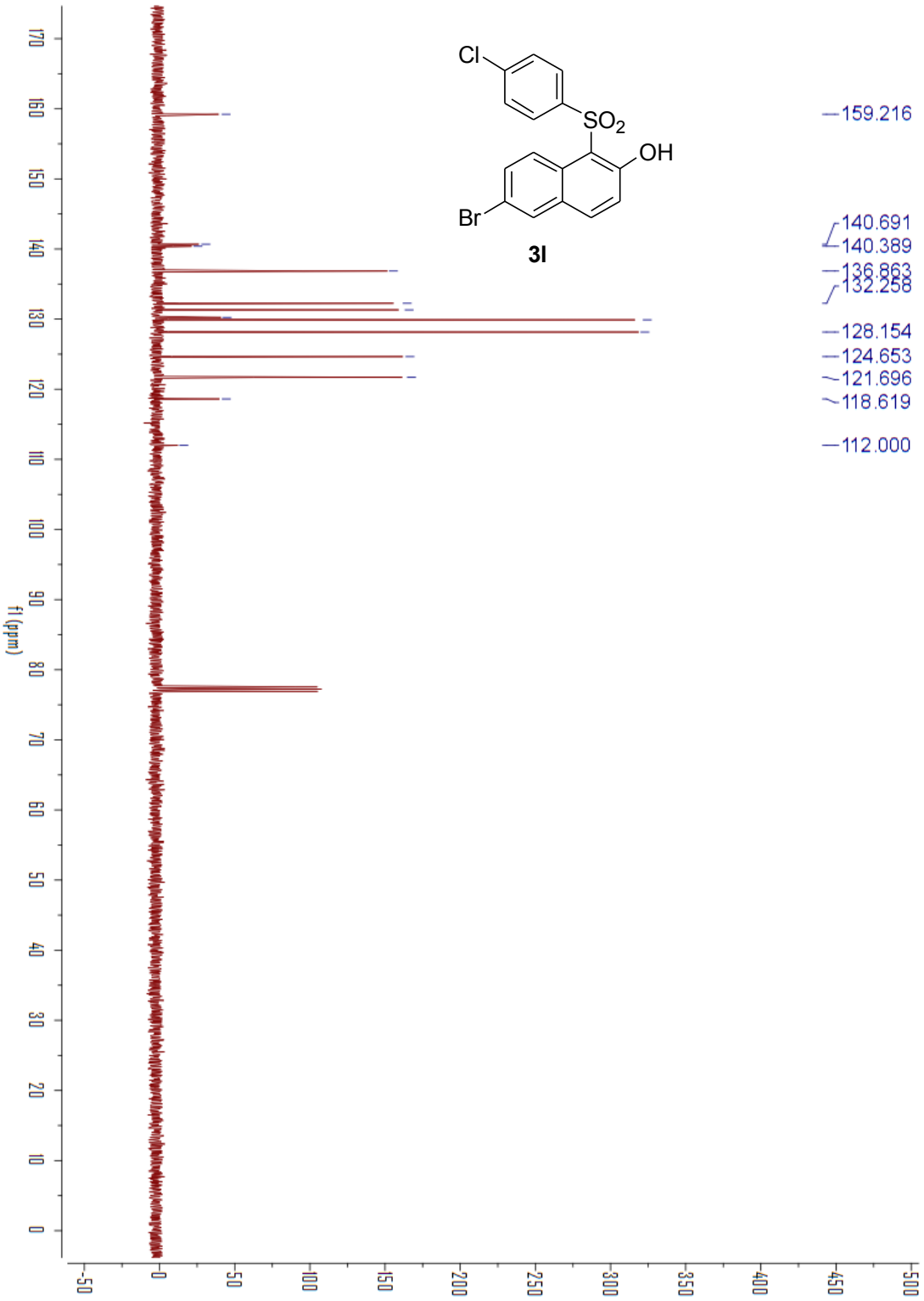

0.97
0.99
2.88
0.97
2.19
0.97
3.00
11.093
8.224
8.201
7.775
7.483
7.261
7.240
7.186
7.163
2.348
SO2
OH
Br
3j
f1 (ppm)

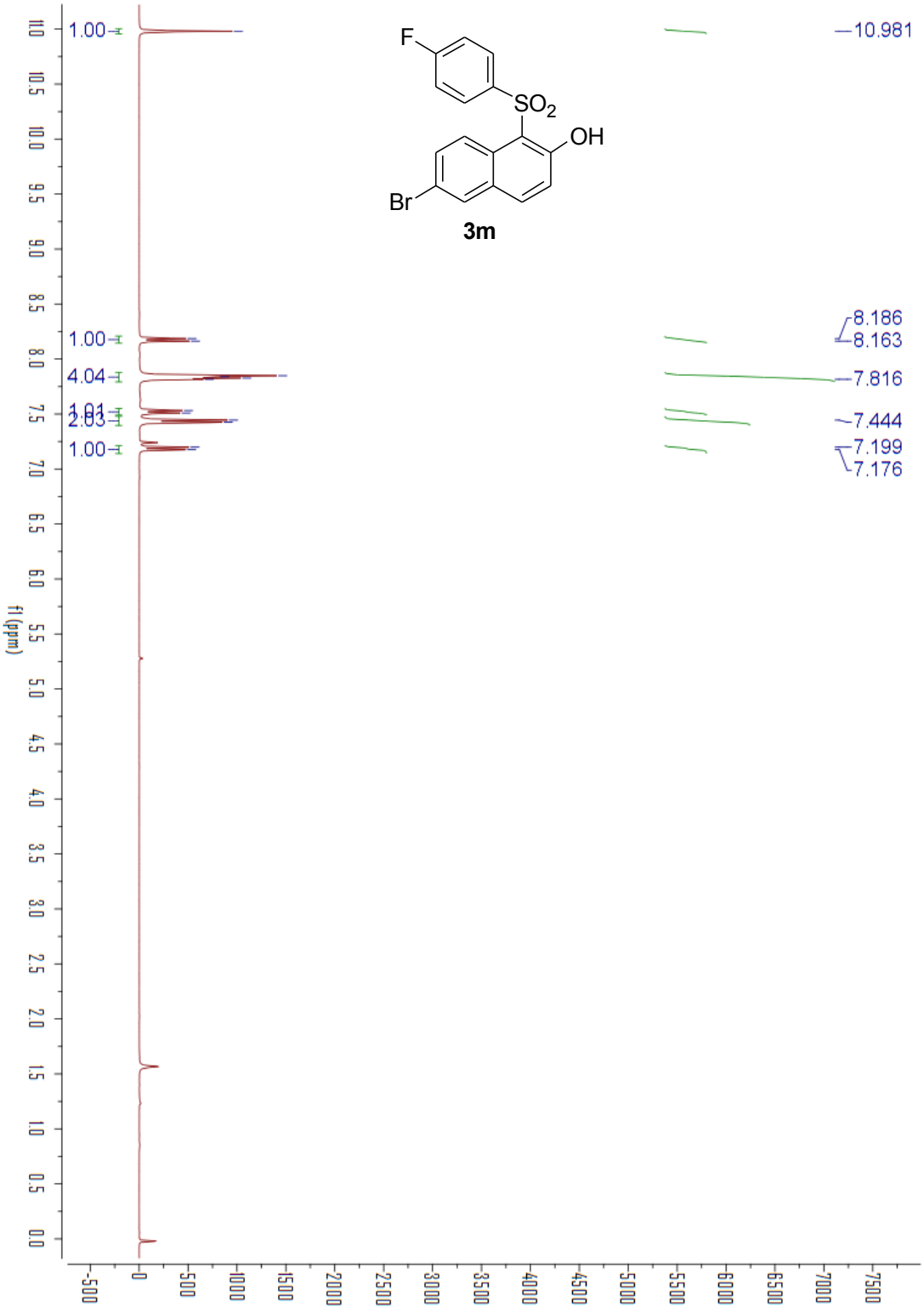

158.938
145.135
136.393
131.976
128.294
124.948
121.687
118.388
112.757
21.813
SO2
OH
Br
3j
f1 (ppm)

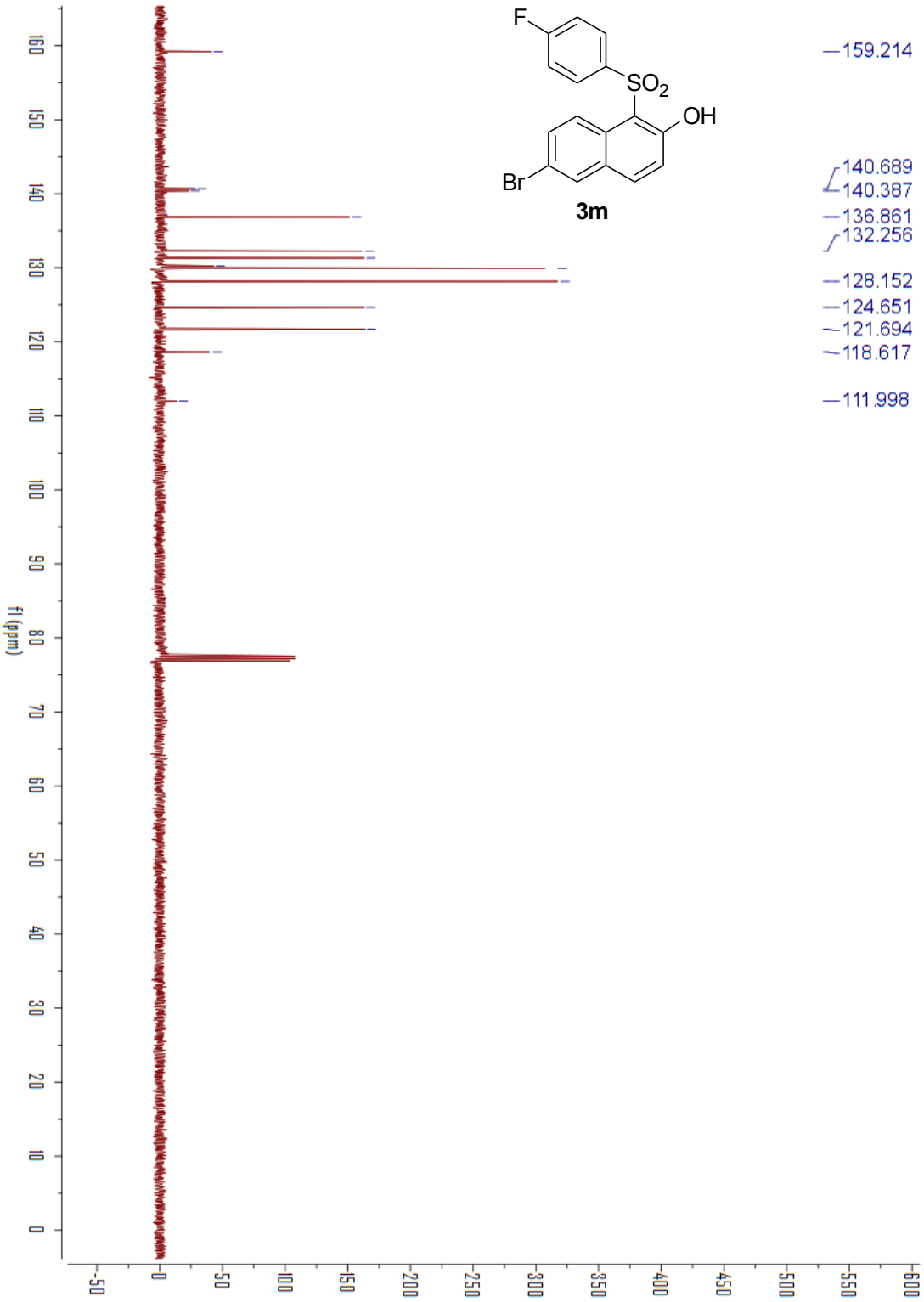

Br
SO2
OH
Br
3k
1.01
1.05
2.18
2.18
2.34
1.03
1.01
10.974
8.181
8.158
7.747
7.533
7.197
7.174
f1 (ppm)

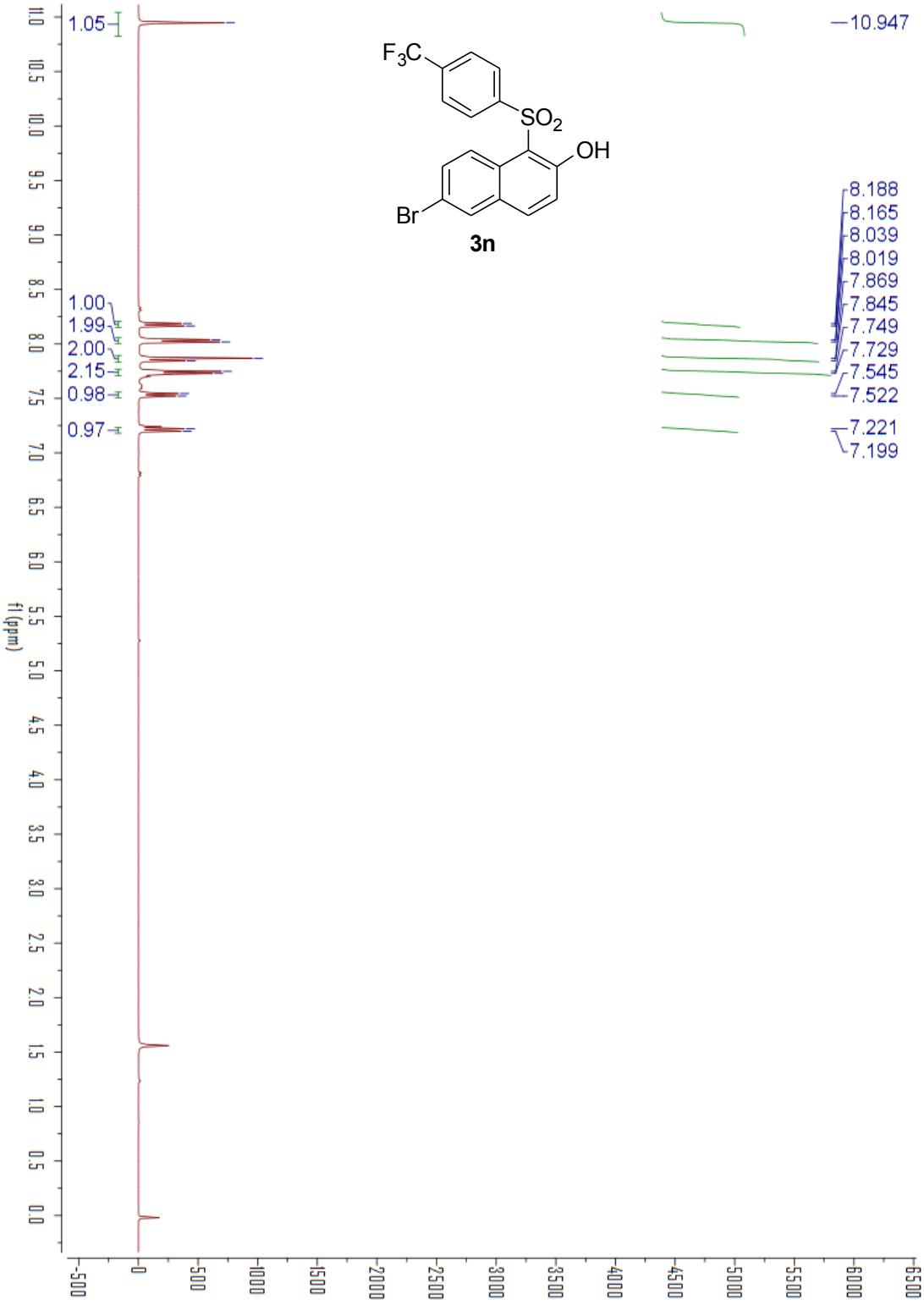

Br
SO2
OH
Br
3k
159.228
140.923
136.879
131.325
128.180
124.646
121.691
120.732
118.629
111.936
f1 (ppm)

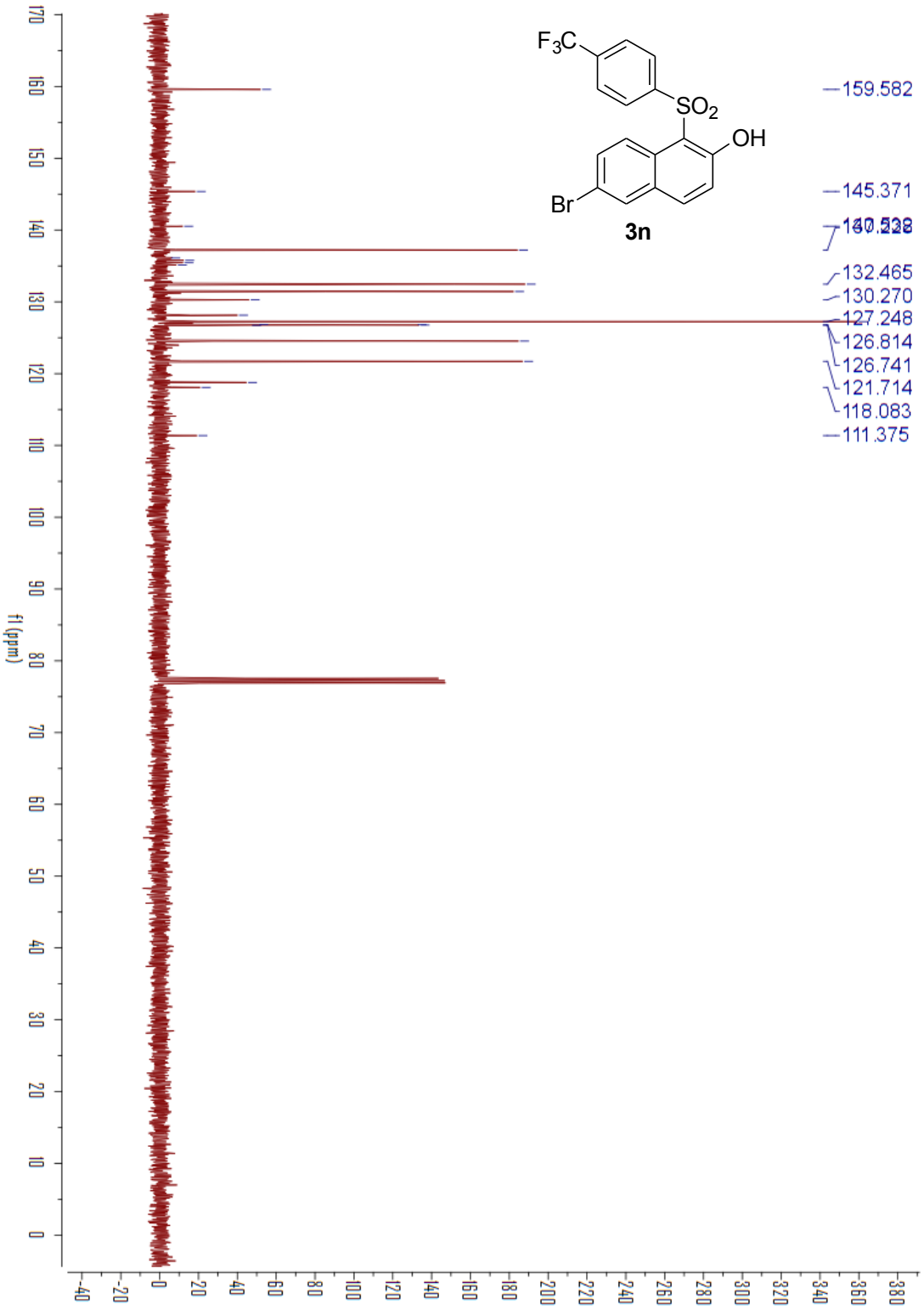

Cl
SO2
OH
Br
3l
10.981
8.186
8.163
7.816
7.444
7.199
7.176
1.00
0.96
3.90
0.97
1.94
0.95
f1 (ppm)

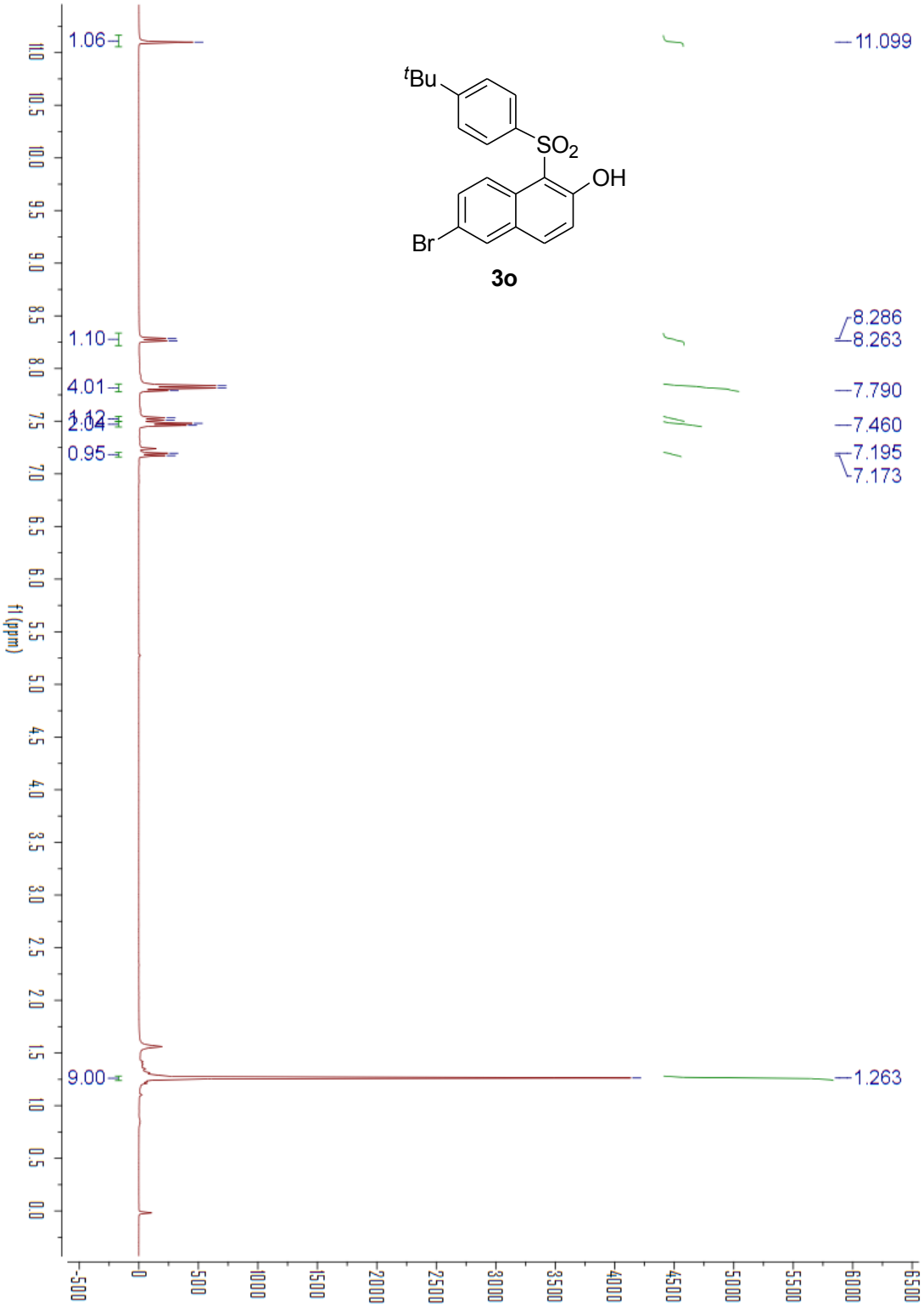

Cl
SO2
OH
Br
3l
159.216
140.691
140.389
136.863
132.258
128.154
124.653
121.696
118.619
112.000
f1 (ppm)

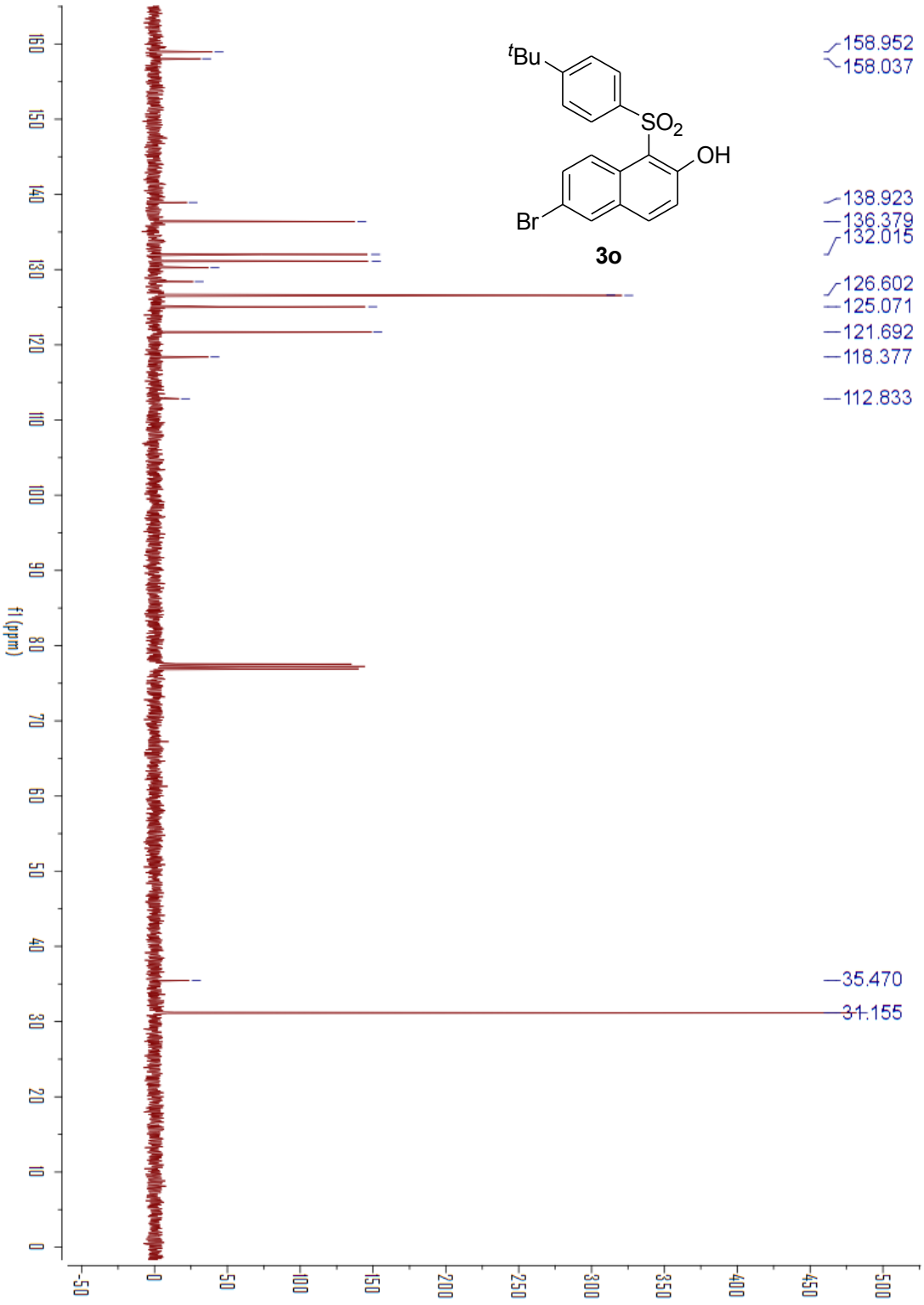

F
SO2
OH
Br
3m
1.00
1.00
4.04
1.01
2.03
1.00
10.981
8.186
8.163
7.816
7.444
7.199
7.176
f1 (ppm)

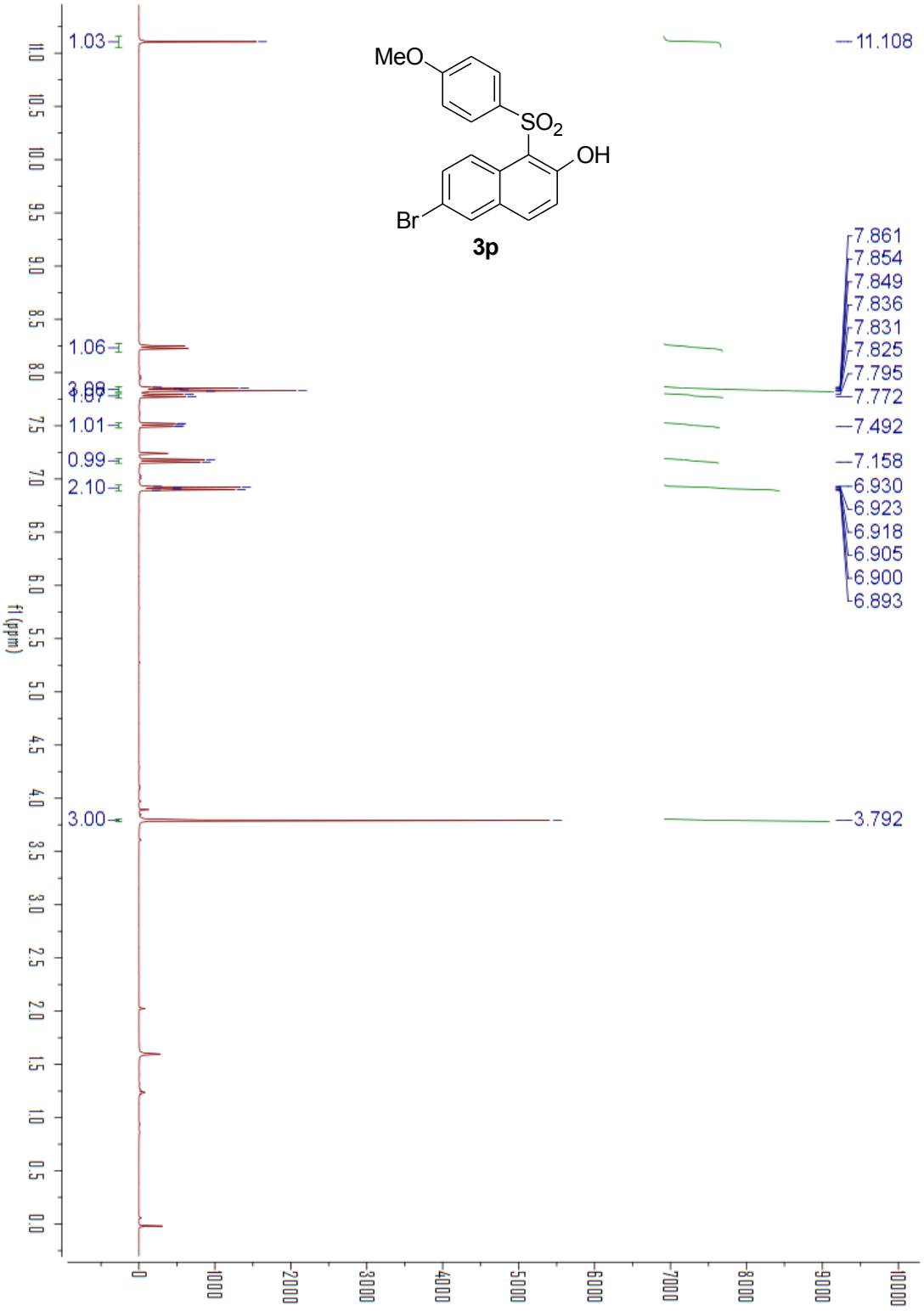

F
SO2
OH
Br
3m
159.214
140.689
140.387
136.861
132.256
128.152
124.651
121.694
118.617
111.998
f1 (ppm)

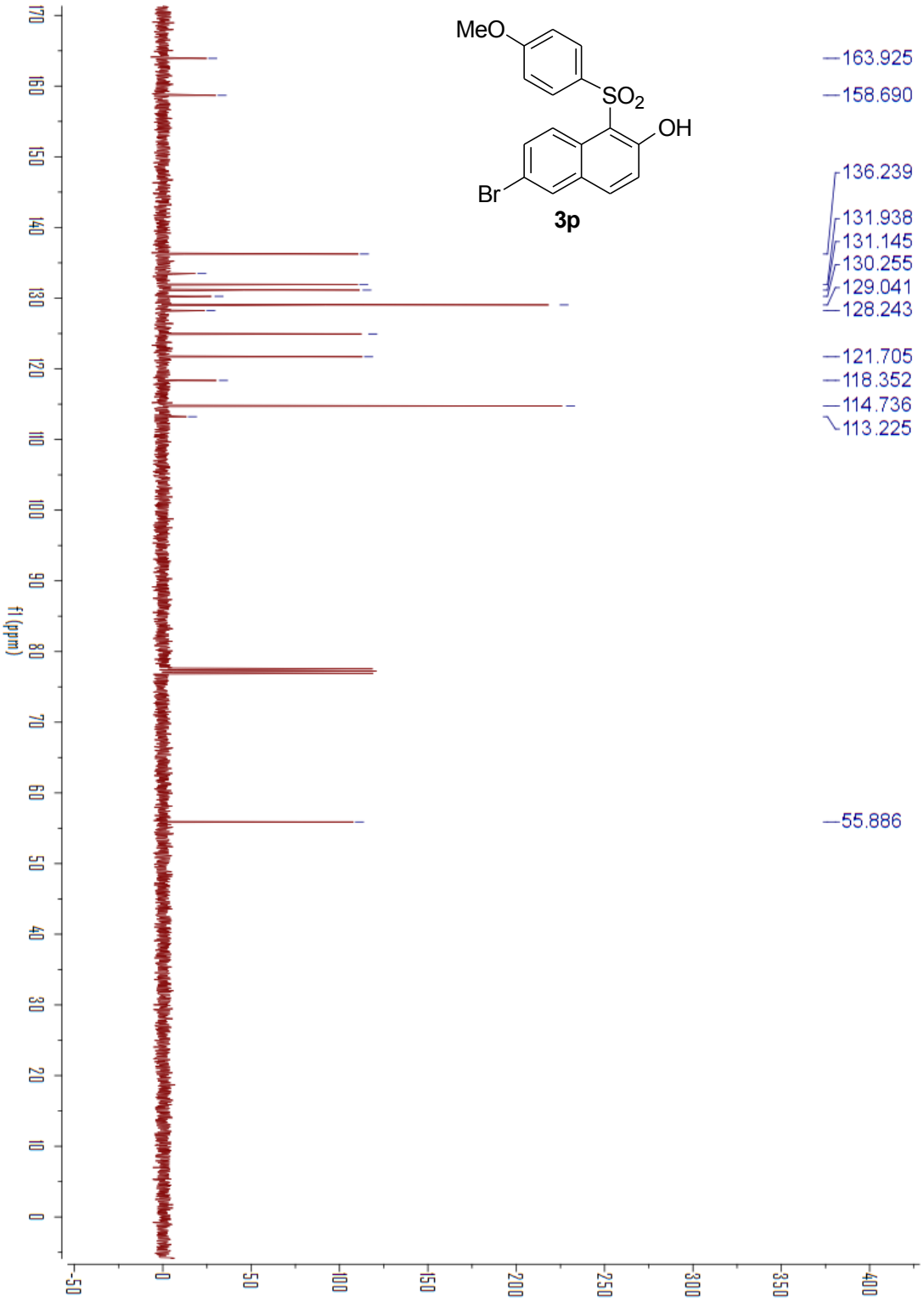

F3C
SO2
OH
Br
3n
1.05
1.00
1.99
2.00
2.15
0.98
0.97
10.947
8.188
8.165
8.039
8.019
7.869
7.845
7.749
7.729
7.545
7.522
7.221
7.199
f1 (ppm)

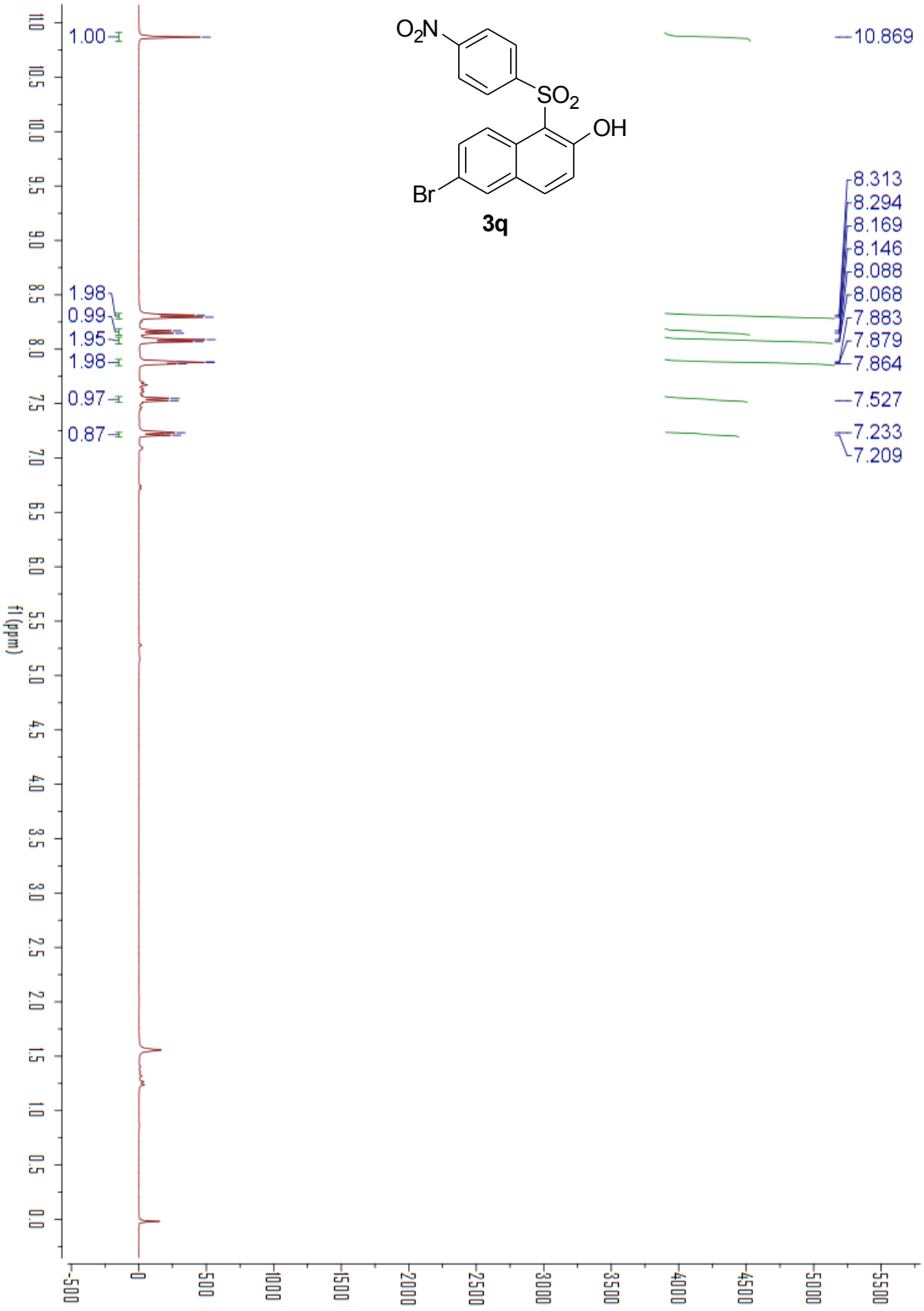

F3C
SO2
OH
Br
3n
159.582
145.371
132.465
130.270
127.248
126.814
126.741
121.714
118.083
111.375
f1 (ppm)

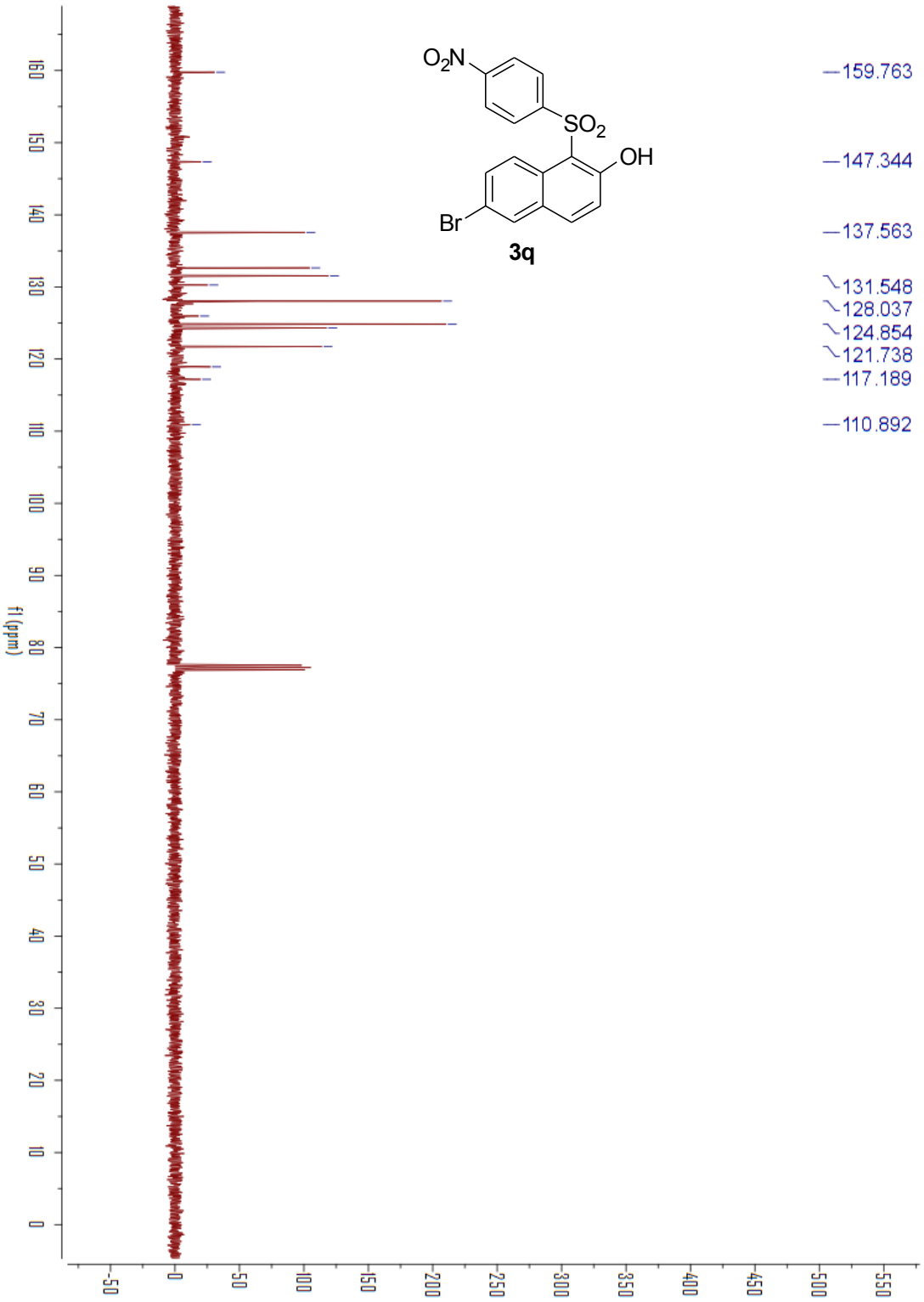

1.06
1.10
4.01
1.12
2.04
0.95
9.00
11.099
8.286
8.263
7.790
7.460
7.195
7.173
1.263
f1 (ppm)
tBu
SO2
OH
Br
3o

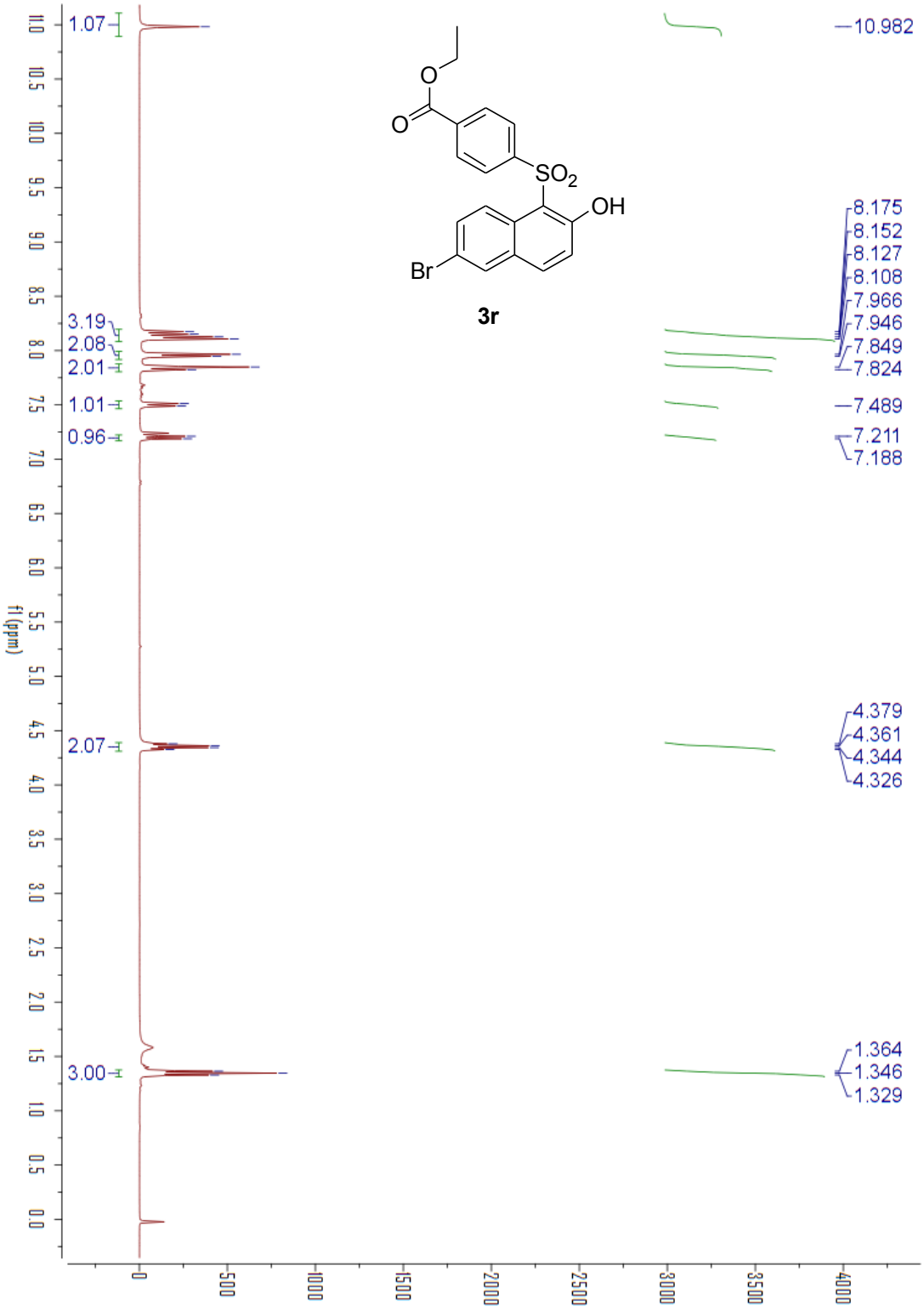

tBu
SO2
OH
Br
3o
158.952
158.037
138.923
136.379
132.015
126.602
125.071
121.692
118.377
112.833
35.470
31.155
f1 (ppm)

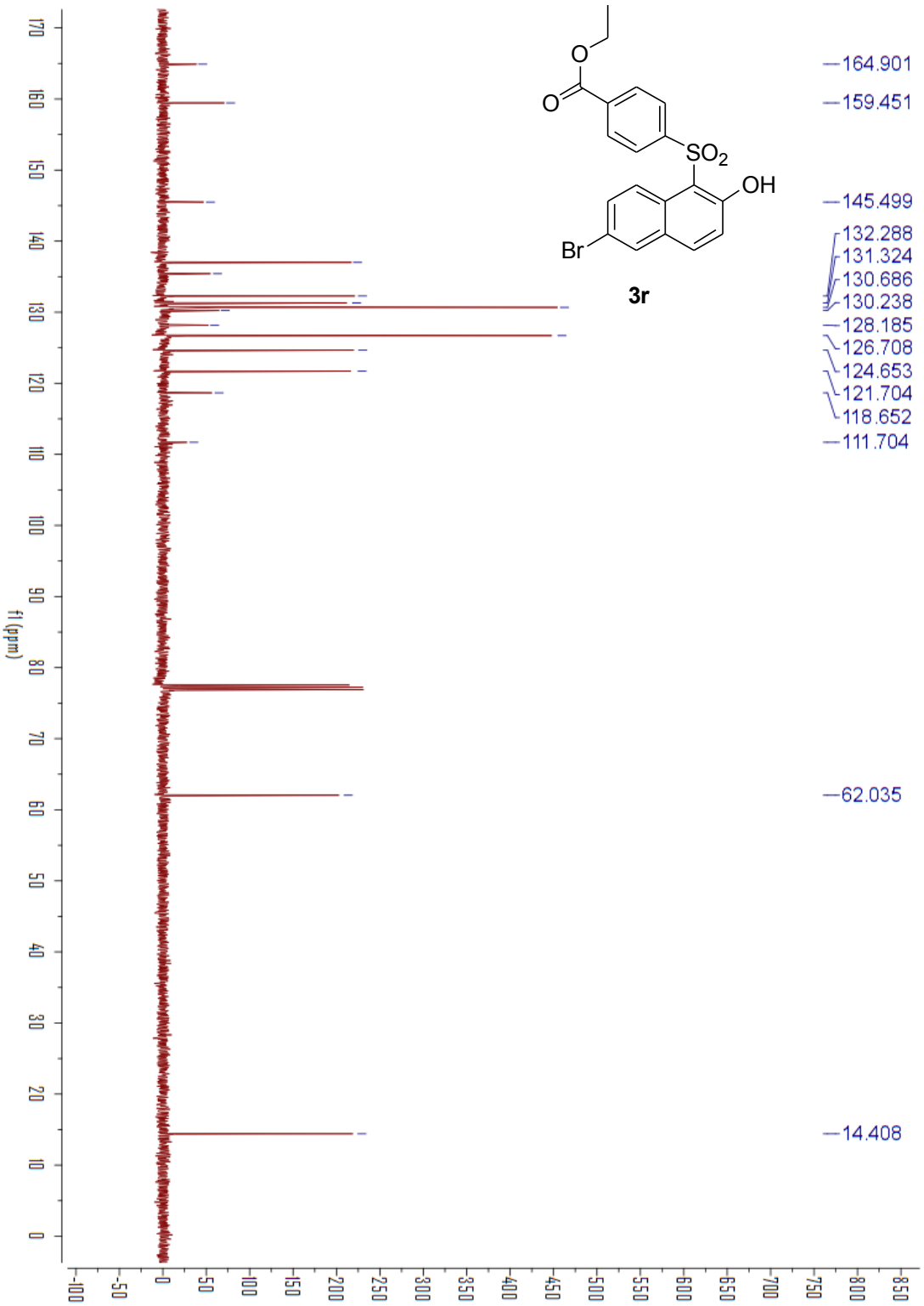

MeO
SO2
OH
Br
3p
1.03
1.06
2.08
1.87
1.01
0.99
2.10
3.00
11.108
7.861
7.854
7.849
7.836
7.831
7.825
7.795
7.772
7.492
7.158
6.930
6.923
6.918
6.905
6.900
6.893
3.792
f1 (ppm)

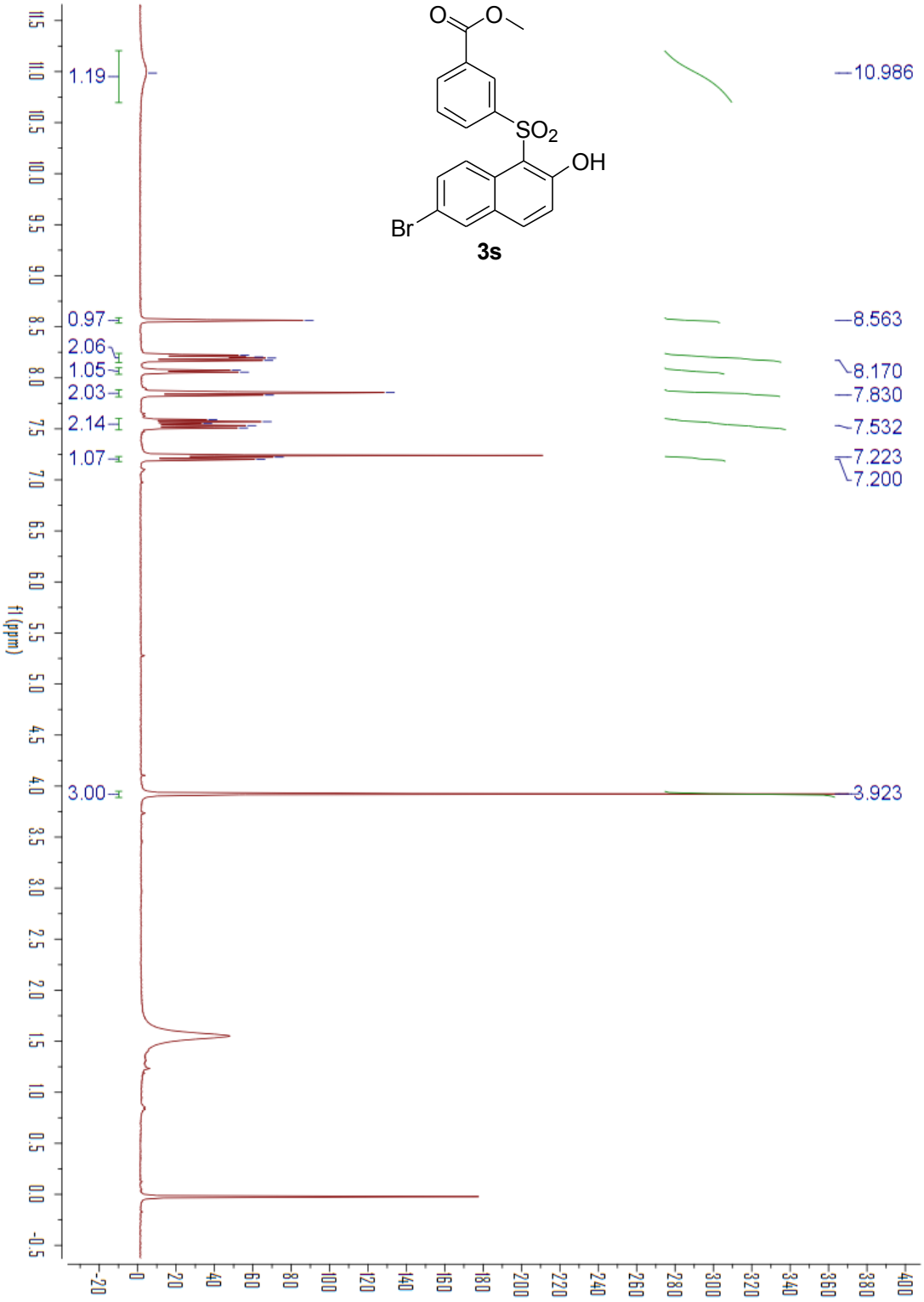

MeO
SO2
OH
Br
3p
163.925
158.690
136.239
131.938
131.145
130.255
129.041
128.243
121.705
118.352
114.736
113.225
55.886
f1 (ppm)

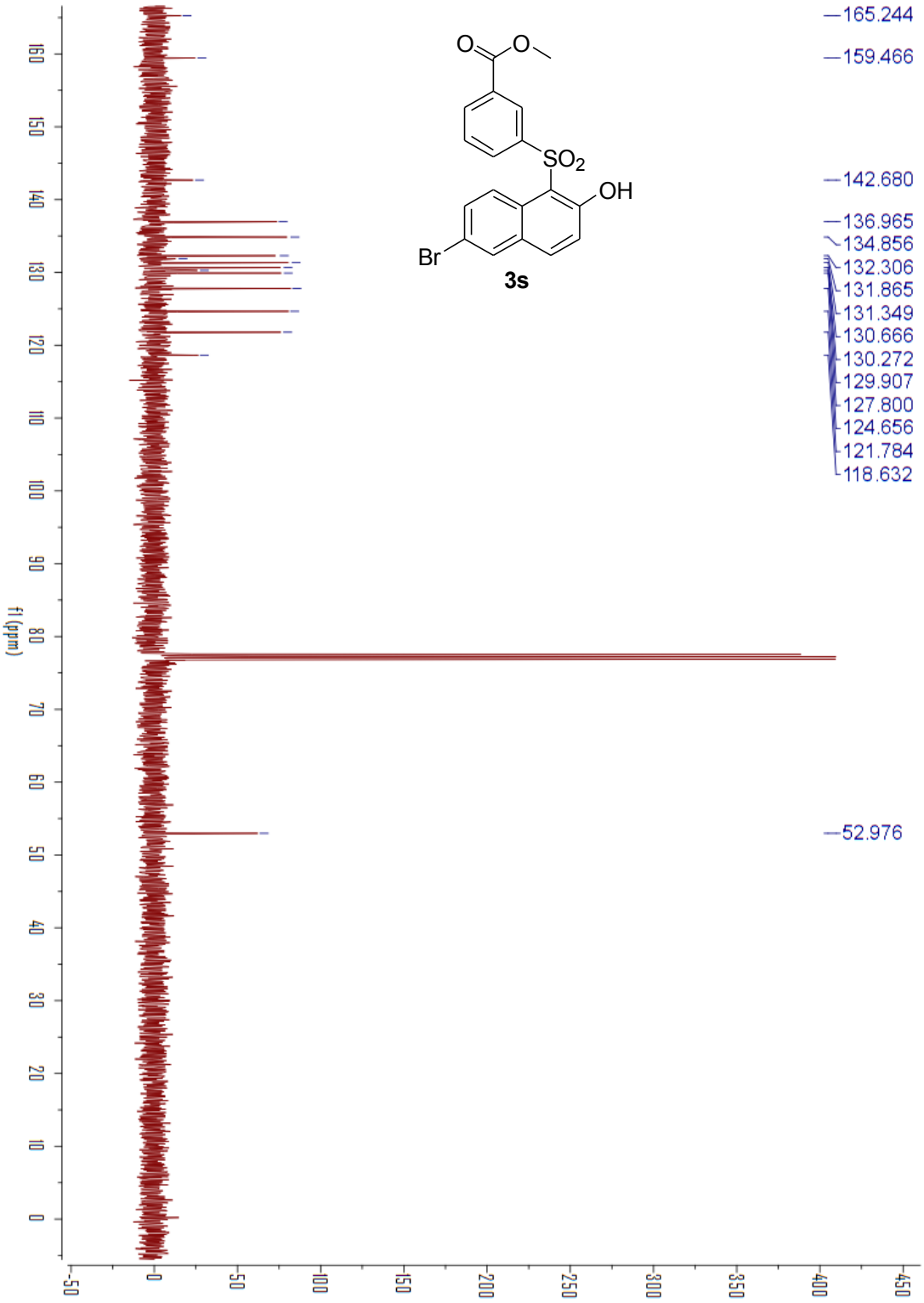

O2N
SO2
OH
Br
3q
1.00
1.98
0.99
1.95
1.98
0.97
0.87
10.869
8.313
8.294
8.169
8.146
8.088
8.068
7.883
7.879
7.864
7.527
7.233
7.209
f1 (ppm)

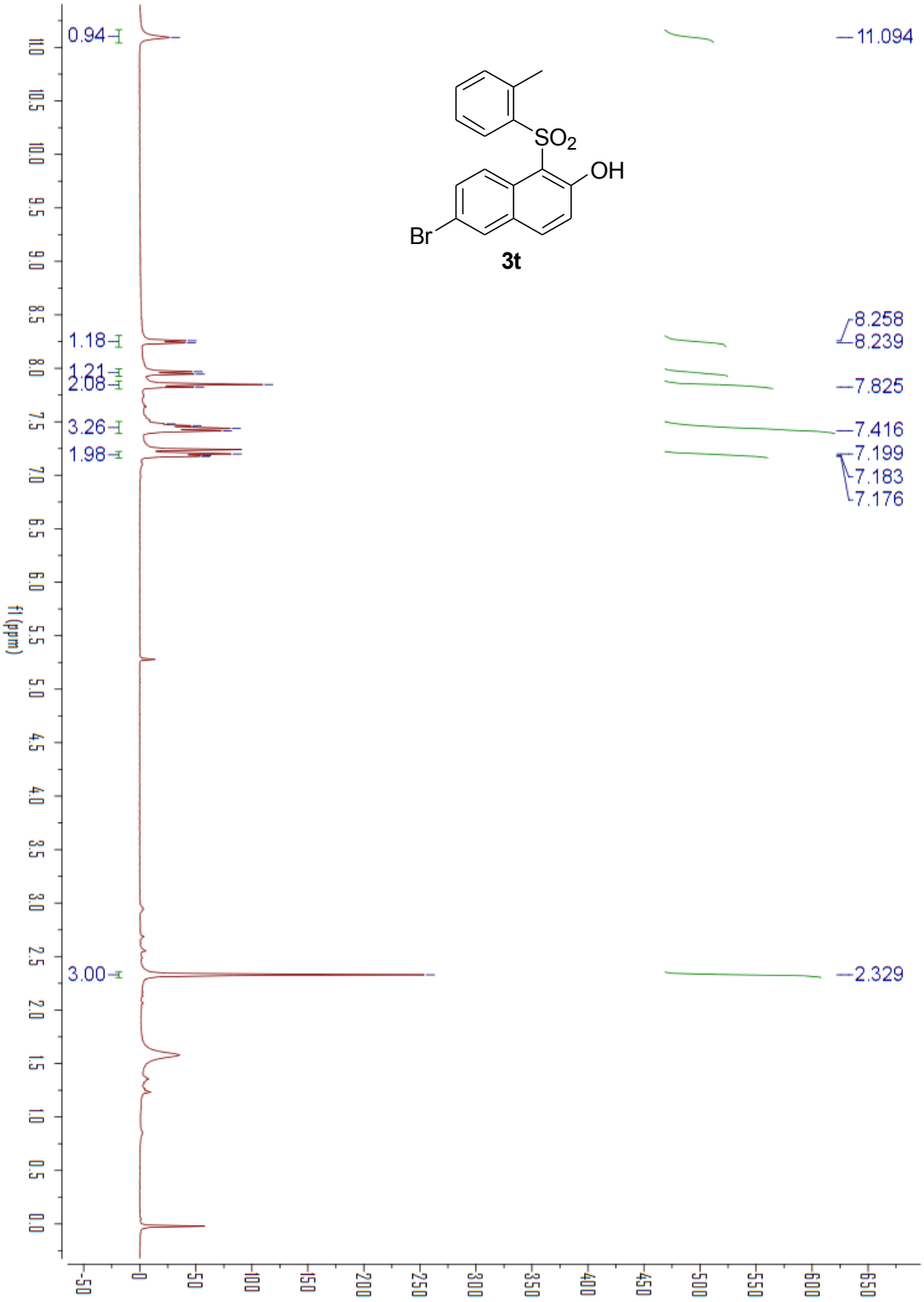

O2N
SO2
OH
Br
3q
159.763
147.344
137.563
131.548
128.037
124.854
121.738
117.189
110.892
f1 (ppm)

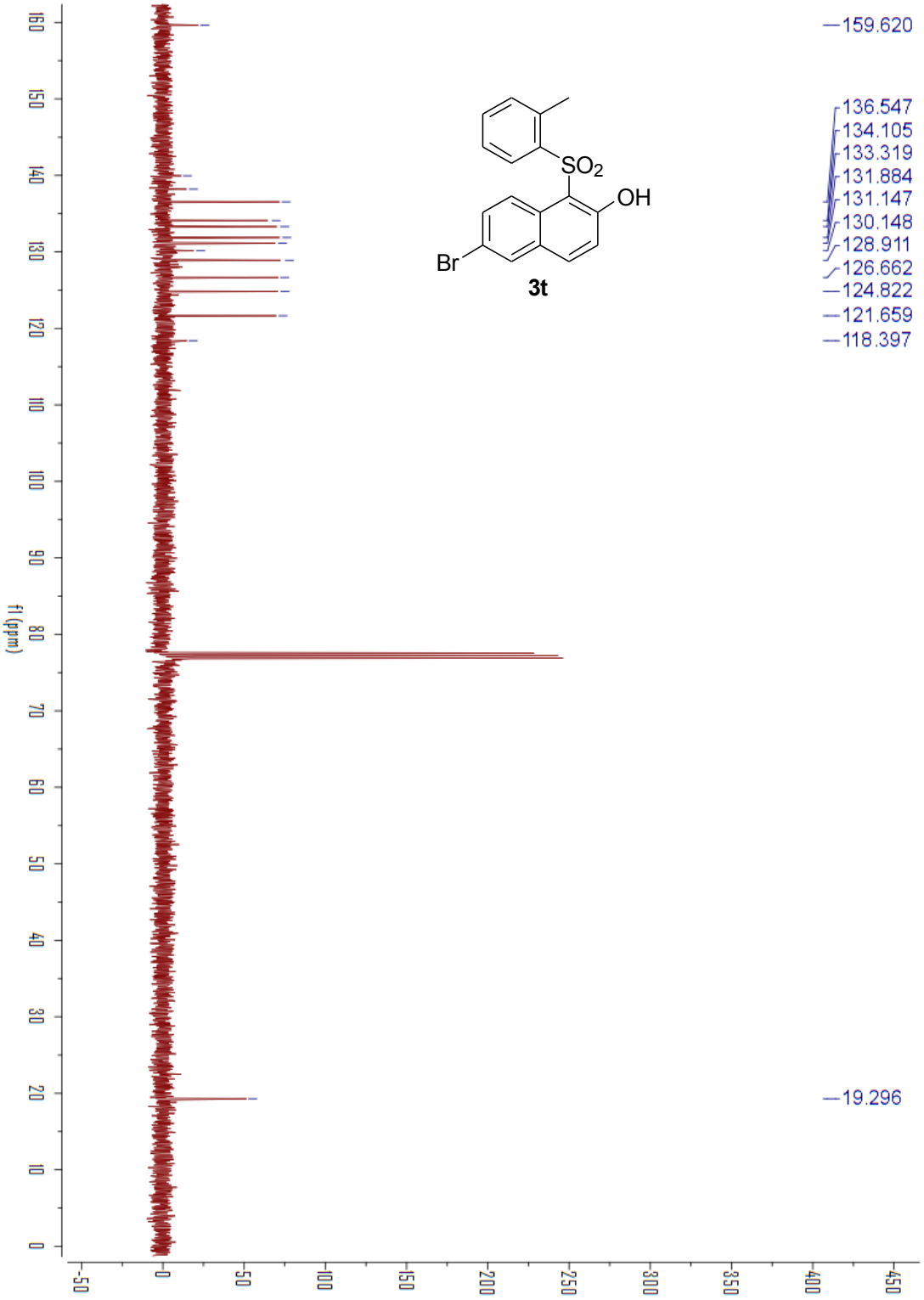

1.07
3.19
2.08
2.01
1.01
0.96
2.07
3.00
f1 (ppm)
O
O
SO2
OH
Br
3r
10.982
8.175
8.152
8.127
8.108
7.966
7.946
7.849
7.824
7.489
7.211
7.188
4.379
4.361
4.344
4.326
1.364
1.346
1.329

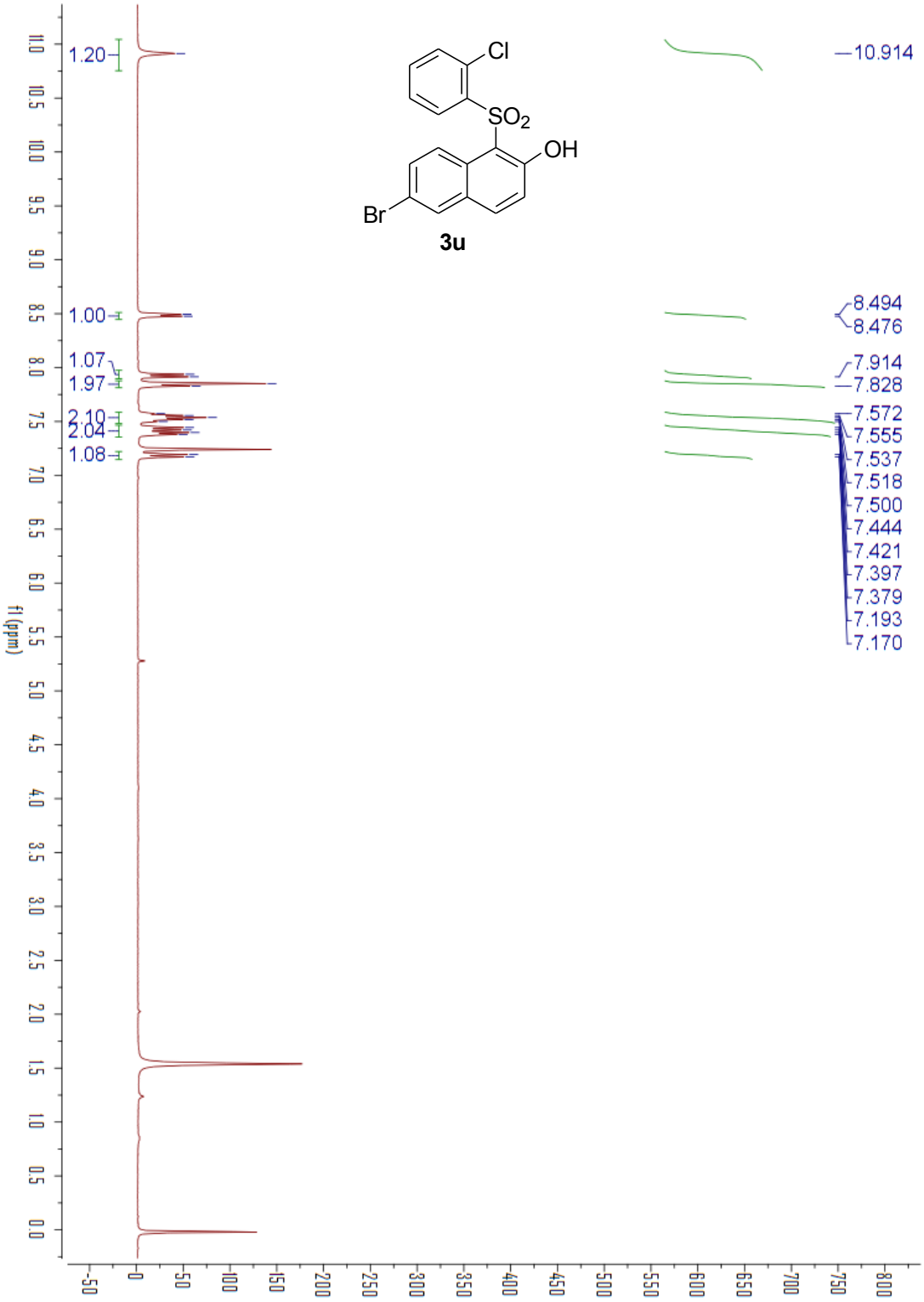

O
O
SO2
OH
Br
3r
164.901
159.451
145.499
132.288
131.324
130.686
130.238
128.185
126.708
124.653
121.704
118.652
111.704
62.035
14.408
f1 (ppm)

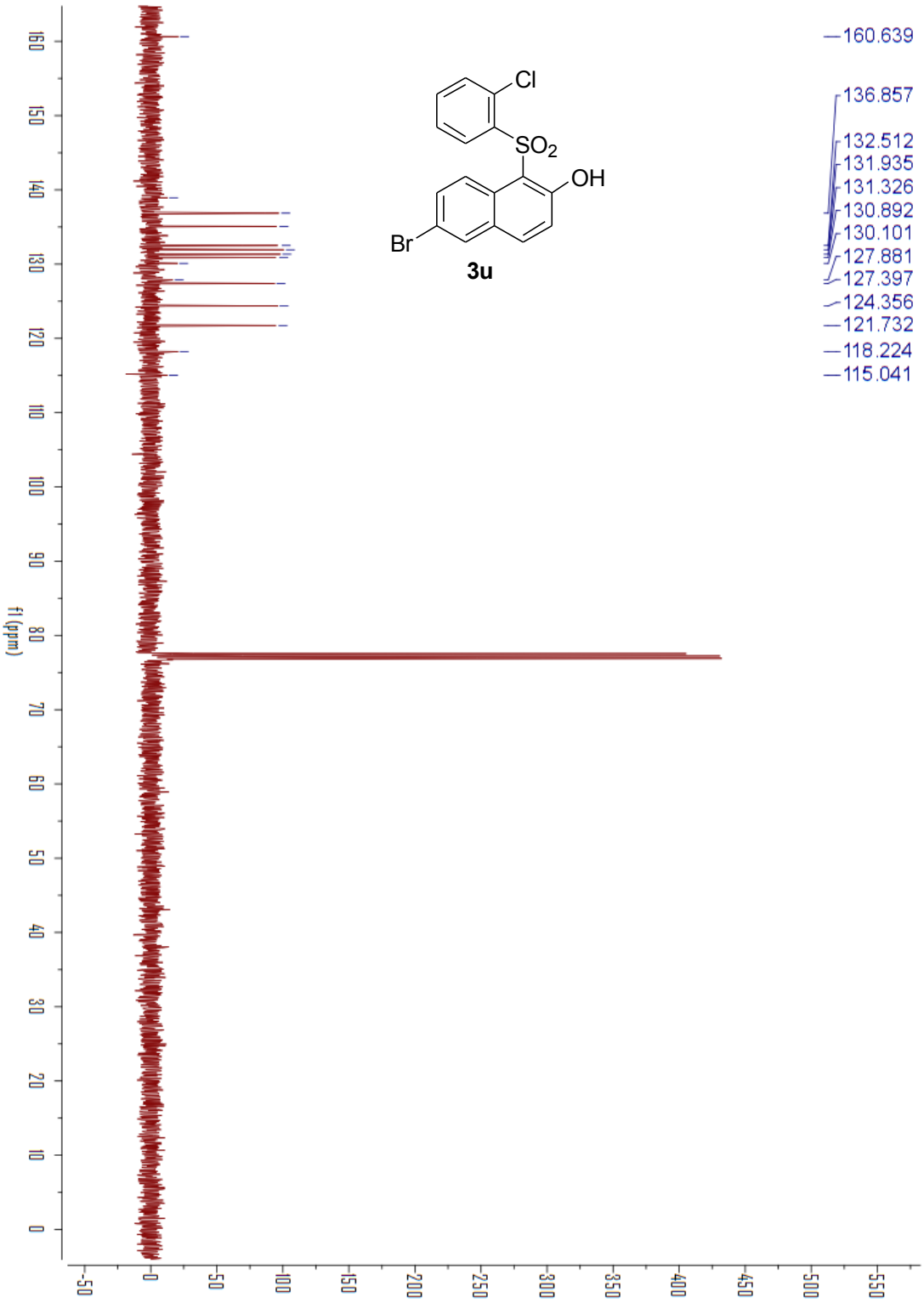

O
O
SO2
OH
Br
3s
1.19
0.97
2.06
1.05
2.03
2.14
1.07
3.00
10.986
8.563
8.170
7.830
7.532
7.223
7.200
3.923
f1 (ppm)

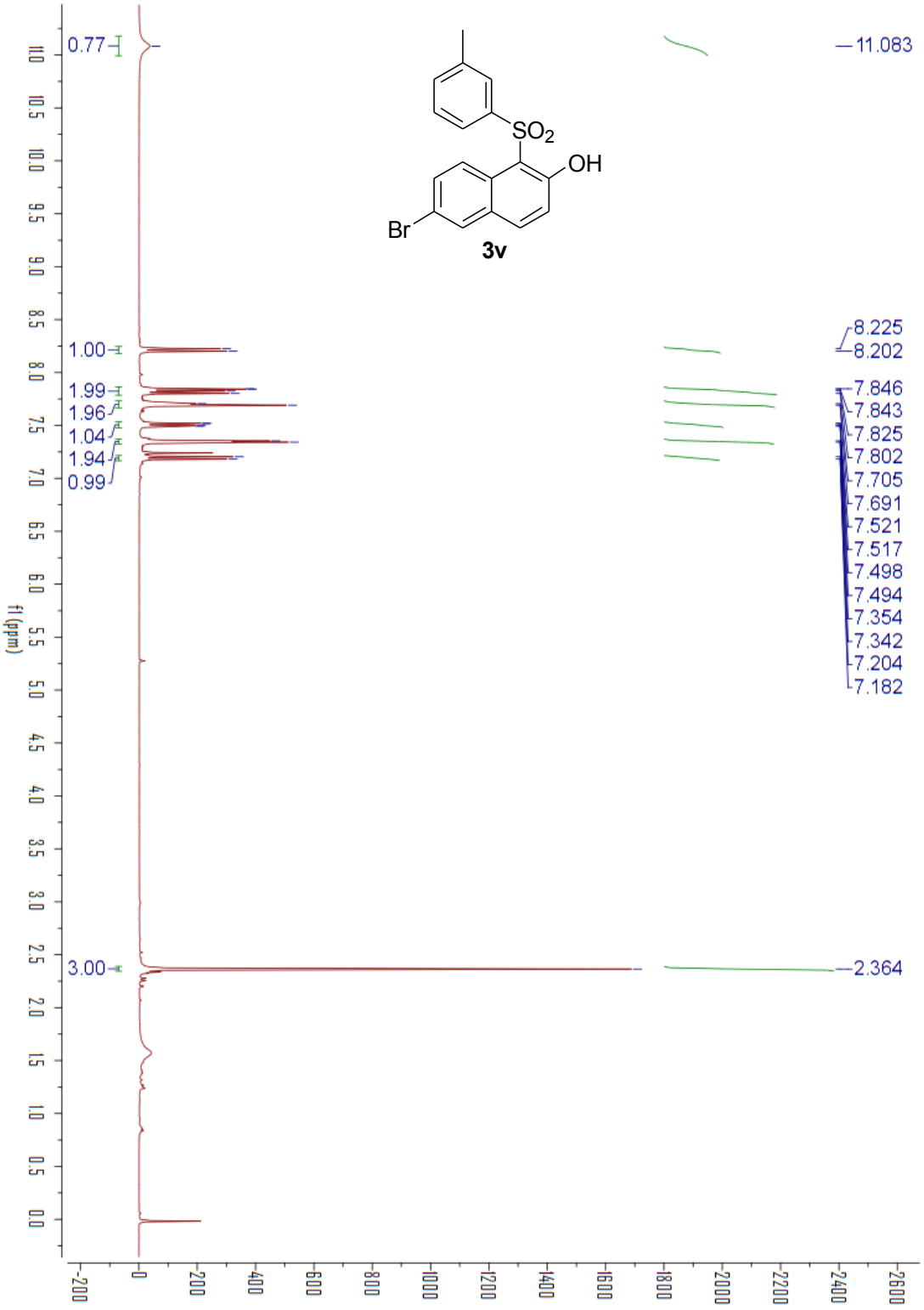

O
O
SO2
OH
Br
3s
165.244
159.466
142.680
136.965
134.856
132.306
131.865
131.349
130.666
130.272
129.907
127.800
124.656
121.784
118.632
52.976
f1 (ppm)

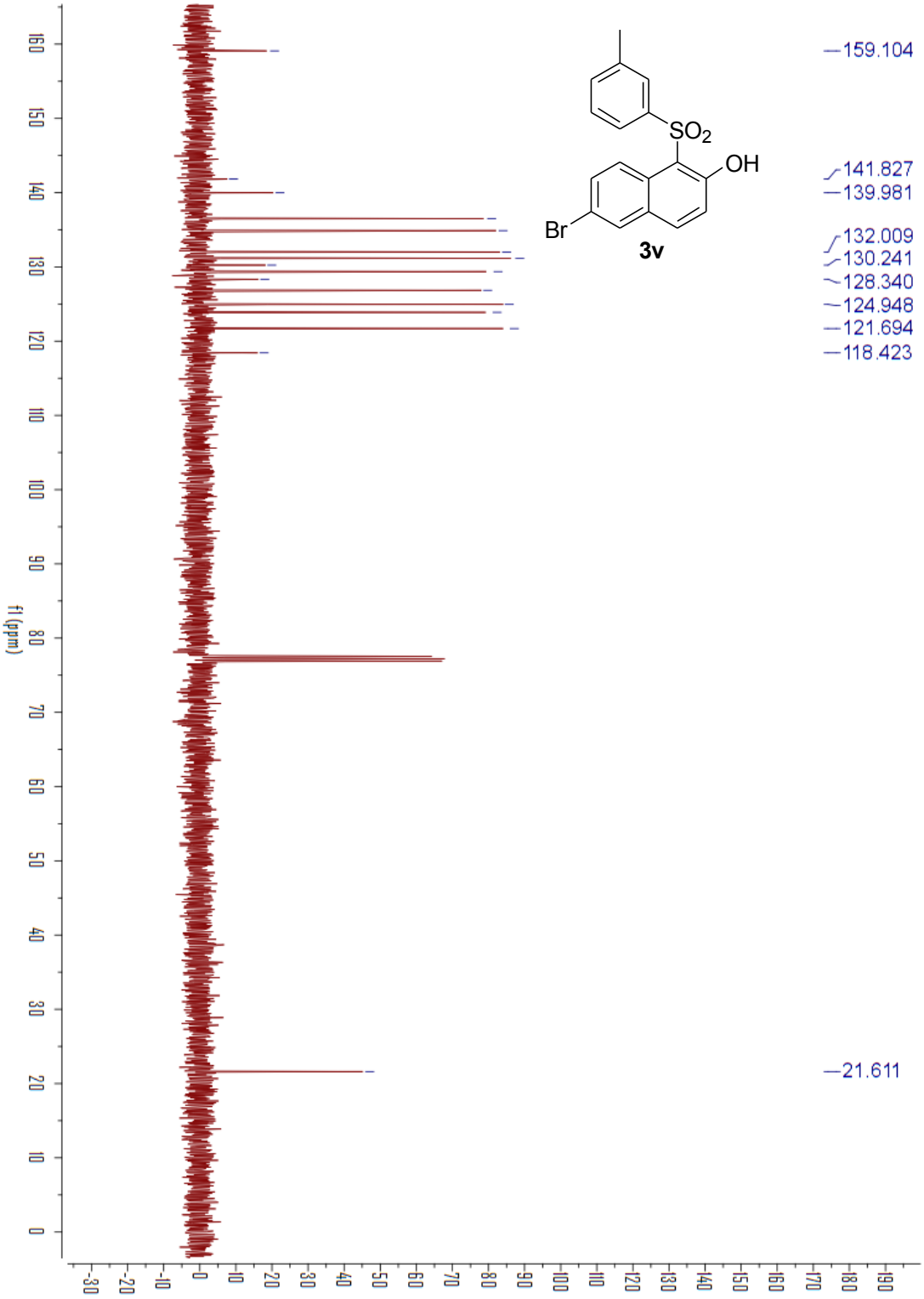

0.94
1.18
1.21
2.08
3.26
1.98
3.00
11.094
8.258
8.239
7.825
7.416
7.199
7.183
7.176
2.329
SO2
OH
Br
3t
f1 (ppm)

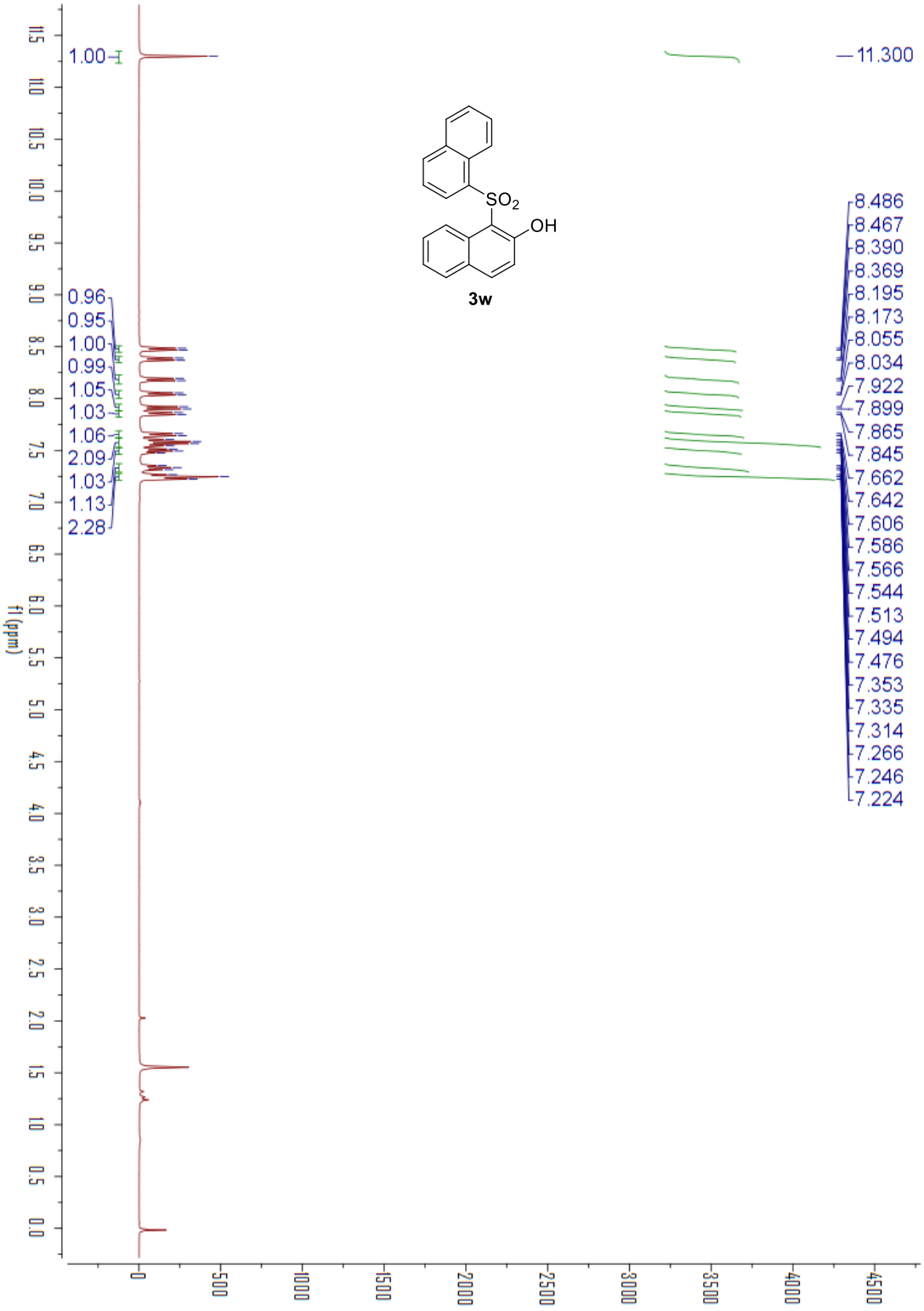

159.620
136.547
134.105
133.319
131.884
131.147
130.148
128.911
126.662
124.822
121.659
118.397
19.296
SO2
OH
Br
3t
f1 (ppm)

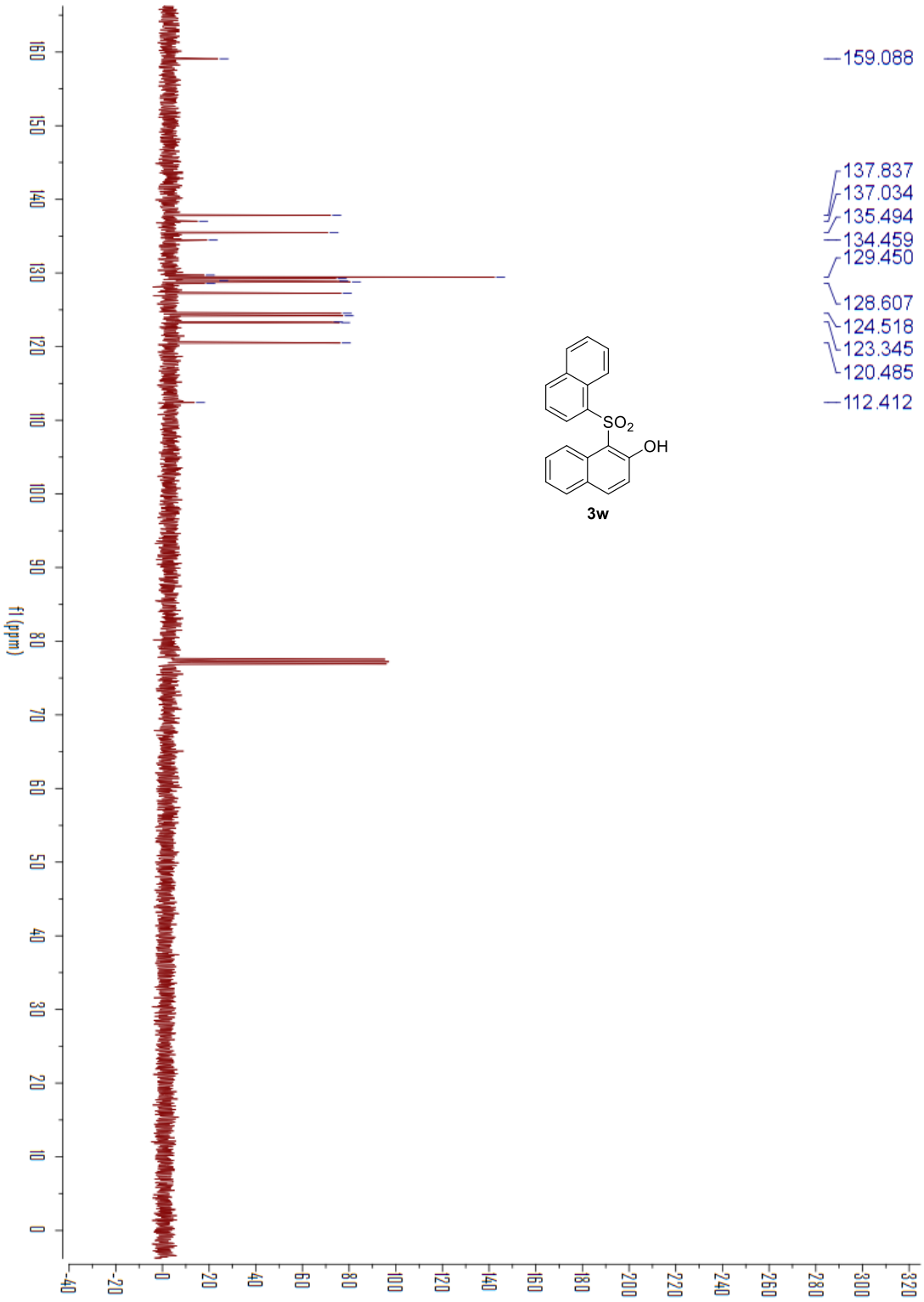

Cl
SO2
OH
Br
3u
1.20
1.00
1.07
1.97
2.10
2.04
1.08
10.914
8.494
8.476
7.914
7.828
7.572
7.555
7.537
7.518
7.500
7.444
7.421
7.397
7.379
7.193
7.170
f1 (ppm)


Cl
SO2
OH
Br
3u
160.639
136.857
132.512
131.935
131.326
130.892
130.101
127.881
127.397
124.356
121.732
118.224
115.041
f1 (ppm)


0.77
1.00
1.99
1.96
1.04
1.94
0.99
3.00
11.083
8.225
8.202
7.846
7.843
7.825
7.802
7.705
7.691
7.521
7.517
7.498
7.494
7.354
7.342
7.204
7.182
2.364
SO2
OH
Br
3v
f1 (ppm)


159.104
141.827
139.981
132.009
130.241
128.340
124.948
121.694
118.423
21.611
SO2
OH
Br
3v
f1 (ppm)


1.00
0.96
0.95
1.00
0.99
1.05
1.03
1.06
2.09
1.03
1.13
2.28
11.300
8.486
8.467
8.390
8.369
8.195
8.173
8.055
8.034
7.922
7.899
7.865
7.845
7.662
7.642
7.606
7.586
7.566
7.544
7.513
7.494
7.476
7.353
7.335
7.314
7.266
7.246
7.224
SO2
OH
3w
f1 (ppm)


159.088
137.837
137.034
135.494
134.459
129.450
128.607
124.518
123.345
120.485
112.412
SO2
OH
3w
f1 (ppm)