Supporting Information

Generation of Thioethers via Direct C-H Functionalization with Sodium Benzenesulfinate as Sulfur Source

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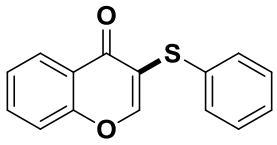
General experimental procedures

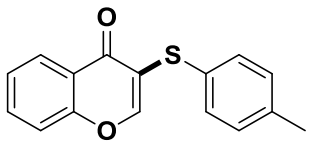
All reactions were carried out in sealed tubes; stirring was achieved with an oven-dried magnetic stirring bar. Solvents were purified by standard methods unless otherwise noted. Commercially available reagents were purchased from Aladdin Company in China and used throughout without further purification other than those detailed below. Flash column chromatography was performed on silica gel (200-300 mesh). All reactions were monitored by TLC analysis. Deuterated solvents were purchased from Cambridge Isotope laboratories. ^{1}H- and ^{13}C-NMR spectra were recorded on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz respectively. HRMS spectrometry (LC-HRMS) was recorded on a LXQ Spectrometer (Thermo Scientific) operating on ESI-TOF (MeOH as a solvent). Flavones derivatives were synthesized according to the literature.

3-(Phenylthio)-4H-chromen-4-one (3a)



FTIR: 3058, 2925, 1653, 1612, 1464, 1309, 1113, 760 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.28 (dd, *J*=8.0, 1.6 Hz, 1H), 8.18 (s, 1H), 7.74-7.70 (m, 1H), 7.51-7.40 (m, 4H), 7.33-7.22 (m, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 175.1, 157.4, 156.4, 134.0, 129.9, 129.2, 127.1, 126.5, 125.8, 123.7, 120.0, 118.2; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_{10}NaO_2S^+$ 277.0294 $(M+Na)^+$, found 277.0296.

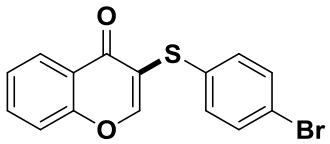
3-(*p*-Tolylthio)-4H-chromen-4-one (3b)



FTIR: 3075, 2923, 2359, 1647, 1464, 1114, 758 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.26 (dd, *J*=8.0, 1.6 Hz, 1H), 8.07 (s, 1H), 7.72-7.68 (m, 1H), 7.49-7.42 (m, 2H), 7.37 (d, *J*=8.0 Hz, 2H), 7.13 (d, *J*=8.0 Hz, 2H), 2.33 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 175.1, 156.3, 156.2, 137.6, 133.9, 131.0, 130.1, 129.8, 126.4, 125.4, 123.6,

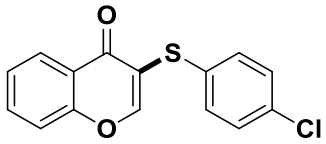
121.1, 118.1, 21.1; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{12}NaO_2S^+$ 291.0450 $(M+Na)^+$, found 291.0447.

3-((4-Bromophenyl)thio)-4H-chromen-4-one (3c)



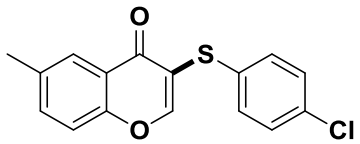
FTIR: 3061, 2925, 1641, 1463, 1086, 901, 798 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.26(dd, *J*=7.2, 4.8 Hz, 2H), 7.76-7.71 (m, 1H), 7.52-7.45 (m, 2H), 7.41 (dd, *J*=6.8, 2.0 Hz, 2H), 7.26 (dd, *J*=8.8, 6.8 Hz, 2H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 174.9, 158.1, 156.4, 134.2, 133.6, 132.2, 131.0, 126.5, 126.0, 123.7, 121.0, 119.0, 118.2; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_9BrNaO_2S^+$ 354.9399 $(M+Na)^+$, found 354.9394.

3-((4-Chlorophenyl)thio)-4H-chromen-4-one (3d)



FTIR: 3051, 1648, 1478，1465, 1313, 1091, 827, 758 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.25 (m, 2H), 7.75-7.71 (m, 1H), 7.52-7.45 (m, 2H), 7.35-7.25 (m, 4H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 175.0, 157.9, 156.4, 134.2, 133.1, 132.8, 130.9, 129.3, 126.5, 125.9, 123.7, 119.2, 118.2; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_9ClNaO_2S^+$ 310.9904 $(M+Na)^+$, found 310.9894.

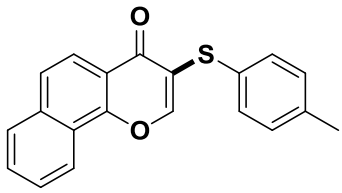
3-((4-Chlorophenyl)thio)-6-methyl-4H-chromen-4-one (3e)



FTIR: 3053, 2922, 1639, 1478, 1311, 1091, 812, 789 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.24 (s, 1H), 8.03 (d, *J*=1.2 Hz, 1H), 7.53 (dd, *J*=8.4, 2.0 Hz, 1H), 7.40 (d, *J*=8.8 Hz, 1H), 7.33-7.22 (m, 4H), 2.47 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ

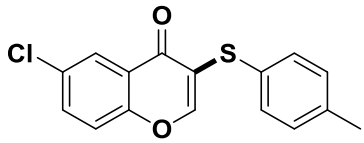
175.1, 158.1, 154.7, 136.1, 135.4, 133.1, 132.9, 130.7, 129.2, 125.7, 123.4, 118.8, 118.0, 21.0; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{11}ClNaO_2S^+$ 325.0060 $(M+Na)^+$, found 325.0049.

3-(*p*-Tolylthio)-4H-benzo[h]chromen-4-one (3f)



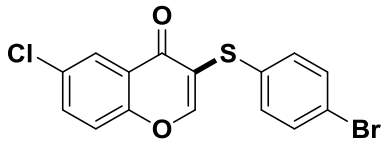
FTIR: 3057, 2920, 2361, 1650, 1633, 1384, 1113, 886, 765 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.40 (d, *J*=8.0 Hz, 1H), 8.16 (d, *J*=8.8 Hz, 1H), 8.08 (s, 1H), 7.91 (d, *J*=7.6 Hz, 1H), 7.77-7.64 (m, 3H), 7.43 (d, *J*=8.0 Hz, 2H), 7.16 (d, *J*=8.0 Hz, 2H), 2.35 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 174.8, 154.3, 153.7, 138.0, 135.8, 131.7, 130.2, 129.5, 129.1, 128.1, 127.3, 125.7, 123.8, 123.4, 122.2, 121.0, 119.6, 21.2; **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{14}NaO_2S^+$ 341.0607 $(M+Na)^+$, found 341.0603.

6-Chloro-3-(p-tolylthio)-4H-chromen-4-one (3g)



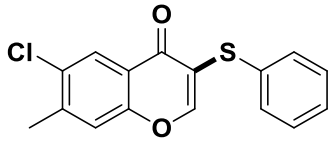
FTIR: 3065, 2923, 1658, 1468, 1305, 1112, 818, 735 cm^{-1}; **^{1}H-NMR** (CDCl3, 400 MHz): δ 8.20 (d, *J*= 2.6 Hz, 1H), 8.00 (s, 1H), 7.63 (dd, *J*=9.2, 2.8 Hz, 1H), 7.43 (d, *J*=9.2 Hz, 1H), 7.38-7.35 (m, 2H), 7.14 (d, *J*=8.0 Hz, 2H), 2.34 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 174.0, 155.8, 154.6, 138.0, 134.1, 131.5, 131.4, 130.2, 129.2, 125.7, 124.3, 121.7, 120.0, 21.1; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{11}ClNaO_2S^+$ 325.0060 $(M+Na)^+$, found 325.0059.

3-((4-Bromophenyl)thio)-6-chloro-4H-chromen-4-one (3h)



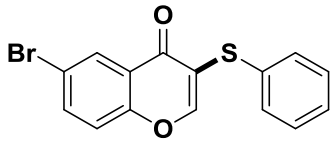
FTIR: 3055, 2923, 1653, 1468, 1303, 1122, 908, 765 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.22 (s, 1H), 8.21 (d, *J*=2.4 Hz, 1H), 7.67 (dd, *J*=8.8, 2.4 Hz, 1H), 7.47 (d, *J* =8.8 Hz, 1H), 7.43-7.41 (m, 2H), 7.27 (d, *J*=8.8 Hz, 2H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 173.8, 157.7, 154.7, 134.4, 132.9, 132.3, 131.9, 131.4, 125.8, 124.6, 121.4, 119.9, 119.6; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_8BrClNaO_2S^+$ 388.9009 $(M+Na)^+$, found 388.8993.

6-Chloro-7-methyl-3-(phenylthio)-4H-chromen-4-one (3i)



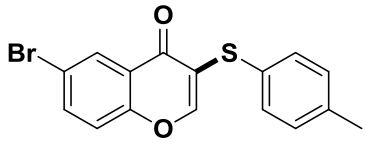
FTIR: 3065, 2922, 1656, 1432, 1107, 918, 796 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.19 (s, 1H), 8.10 (s, 1H), 7.42-7.39 (m, 2H), 7.37 (d, *J*=0.8 Hz, 1H), 7.33-7.28 (m, 2H), 7.27-7.23 (m, 1H), 2.51 (d, *J*=0.8 Hz, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 173.9, 157.0, 154.6, 143.4, 133.7, 132.4, 130.0, 129.2, 127.3, 125.9, 122.6, 120.1, 119.9, 20.9; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{11}ClNaO_2S^+$ 325.0060 $(M+Na)^+$, found 325.0058.

6-Bromo-3-(phenylthio)-4H-chromen-4-one (3j)



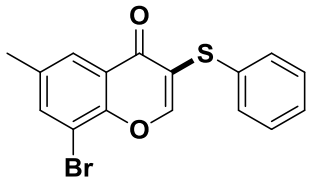
FTIR: 3058, 2923, 1652, 1548, 1462, 1121, 908, 818, 735 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.38 (d, *J*=2.4 Hz, 1H), 8.12 (s, 1H), 7.78 (q, *J*=2.4, 1H), 7.43-7.38 (m, 3H), 7.34-7.24 (m, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 173.8, 157.0, 155.1, 137.0, 133.4, 130.3, 129.3, 129.0, 127.5, 124.8, 120.6, 120.2, 119.2; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_9BrNaO_3S^+$ 354.9399 $(M+Na)^+$, found 354.9394.

6-Bromo-3-(*p*-tolylthio)-4H-chromen-4-one (3k)



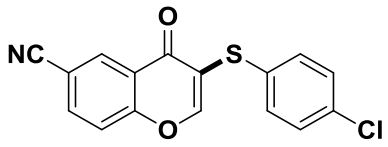
FTIR : 3052, 2913, 1657, 1548, 1465, 1122, 908, 818, 735 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.37 (d, *J*=2.4 Hz, 1H), 8.00 (s, 1H), 7.76 (dd, *J*=8.8, 2.4 Hz, 1H), 7.37 (d, *J*=8.4 Hz, 3H), 7.14 (m, *J*=8.0 Hz, 3H), 2.34 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 173.8, 155.8, 155.1, 138.0, 136.9, 131.5, 130.2, 129.1, 128.9, 124.7, 121.9, 120.1, 119.0, 119, 21.1; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{11}BrNaO_2S^+$ 368.9555 $(M+Na)^+$, found 368. 9531.

8-Bromo-6-methyl-3-(phenylthio)-4H-chromen-4-one (3l)



FTIR: 3054, 2925, 2360, 1660, 1463, 1299, 1090, 785, 691 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.11 (s, 1H), 7.98 (d, *J*=1.2 Hz, 1H), 7.75 (d, *J*=2.0 Hz, 1H), 7.43 (dd, *J*=3.6, 1.6 Hz, 2H), 7.34-7.24 (m, 3H), 2.45 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 174.5, 156.4, 151.2, 138.5, 136.8, 133.2, 130.5, 129.3, 127.5, 125.3, 124.3, 120.8, 111.2, 20.8; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{11}BrNaO_2S^+$ 368.9555 $(M+Na)^+$, found 368. 9553.

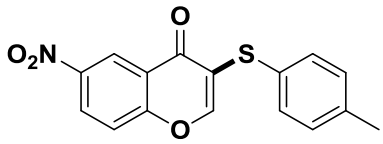
3-((4-Chlorophenyl)thio)-4-oxo-4H-chromene-6-carbonitrile (3m)



FTIR: 3054, 2924, 2361, 1654, 1475, 1313, 815, 670 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.58 (d, *J*=2.0 Hz, 1H), 8.16 (s, 1H), 7.94 (dd, *J*=8.8, 2.0 Hz, 1H), 7.62 (d, *J*=8.4 Hz, 1H), 7.40 (d, *J*=8.4 Hz, 2H), 7.30 (d, *J*=8.4 Hz, 2H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 173.2, 158.0, 156.7, 136.3, 134.1, 132.2, 132.1, 131.1, 129.6, 123.9,

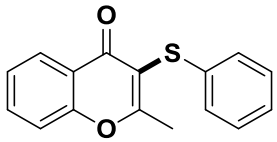
121.7, 120.0, 117.2, 110.2; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_8ClNNaO_2S^+$ 335.9856 $(M+Na)^+$, found 335.9853.

6-Nitro-3-(p-tolylthio)-4H-chromen-4-one (3n)



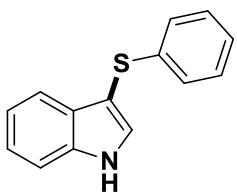
FTIR: 3062, 2342, 1658, 1524, 1336, 1115, 819, 765 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 9.13 (d, *J*=2.8 Hz, 1H), 8.52 (dd, *J*=9.2, 2.8 Hz,1H), 7.91 (s, 1H), 7.62 (d, *J*=9.2 Hz, 1H), 7.44-7.42 (m, 2H), 7.20-7.18 (m, 2H), 2.37 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 173.6, 158.9, 154.5, 145.0, 138.9, 132.5, 130.4, 128.1, 127.8, 123.8, 123.2, 123.1, 120.0, 21.2; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{11}NNaO_4S^+$ 336.0301 $(M+Na)^+$, found 336.0302.

2-Methyl-3-(phenylthio)-4H-chromen-4-one (3p)



FTIR: 3050, 2924, 1647, 1465, 1120, 982, 764, 691 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.23 (dd, *J*=8.0, 1.6 Hz, 1H), 7.71-7.67 (m, 1H), 7.47-7.40 (m, 2H), 7.28-7.22 (m, 4H), 7.17-7.12 (m, 1H), 2.74 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 175.3, 171.5, 155.6, 135.7, 133.8, 129.3, 129.0, 127.5, 126.6, 126.0, 125.5, 122.9, 117.7, 115.3, 20.8; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{12}NaO_2S^+$ 291.0450 $(M+Na)^+$, found 291.0451.

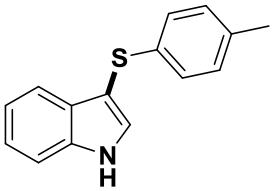
3-(Phenylthio)-1H-indole (4a) [1]



^{1}H-NMR ($CDCl_3$, 400 MHz): δ 8.45 (s, 1H), 7.66 (d, *J*=8.0 Hz, 1H), 7.50-7.46 (m,

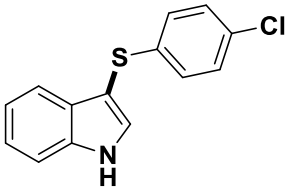
2H), 7.33-7.29 (m, 1H), 7.23-7.14 (m, 5H), 7.12-7.08 (m, 1H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 139.3, 136.5, 130.8, 129.1, 128.7, 125.9, 124.8, 123.1, 119.7, 111.7, 102.7.

3-(*p*-Tolylthio)-1H-indole (4b) [1]



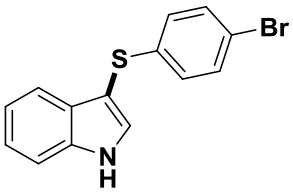
^{1}H-NMR ($CDCl_3$, 400 MHz): δ 8.23 (s, 1H), 7.74 (d, *J*=7.6 Hz, 1H), 7.45-7.43 (m, 2H), 7.38-7.34 (m, 1H), 7.29-7.25 (m, 1H), 7.15 (d, *J*=8.0 Hz, 1H), 7.08 (d, *J*=8.0 Hz, 1H), 2.35 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 136.5, 135.6, 134.9, 130.7, 129.7, 129.2, 126.4, 123.1, 120.9, 119.7, 111.8, 103.2, 21.0.

3-((4-Chlorophenyl)thio)-1H-indole (4c) [1]



^{1}H-NMR ($CDCl_3$, 400 MHz): δ 8.45 (s, 1H), 7.61 (d, *J*=8.0 Hz, 1H), 7.51-7.46 (m, 2H), 7.34-7.30 (m, 1H), 7.24-7.20 (m, 1H), 7.07-7.04 (m, 2H), 7.24-7.20 (m, 1H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 137.8, 136.5, 130.8, 130.6, 128.8, 128.7, 127.1, 123.2, 121.1, 119.5, 111.7, 103.4.

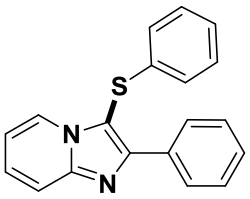
3-((4-Bromophenyl)thio)-1H-indole (4d) [1]



^{1}H-NMR ($CDCl_3$, 400 MHz): δ 8.60 (s, 1H), 7.60 (d, *J*=8.0 Hz, 1H), 7.50-7.46 (m, 2H), 7.33-7.27 (m, 3H), 7.23-7.19 (m, 1H), 7.00-6.98 (m, 2H); **^{13}C-NMR** ($CDCl_3$,

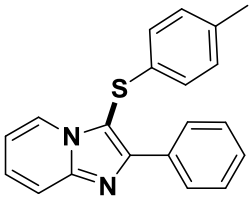
100 MHz): δ 138.6, 136.6, 131.7, 130.9, 128.8, 127.4, 123.2, 121.0, 119.5, 118.3 111.8, 102.0.

2-phenyl-3-(phenylthio)imidazo[1,2-a]pyridine (5a) [2]



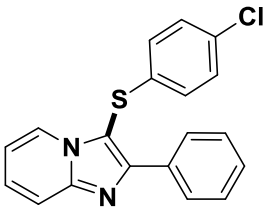
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.30 (dt, *J*=6.9, 1.2 Hz, 1H), 8.26–8.21 (m, 2H), 7.77 (dt, *J*=9.0, 1.1 Hz, 1H), 7.50–7.43 (m, 2H), 7.43–7.35 (m, 2H), 7.27–7.19 (m, 2H), 7.15 (ddt, *J* = 8.5, 6.7, 2.5 Hz, 1H), 7.06 – 6.99 (m, 2H), 6.89 (td, *J* = 6.8, 1.2 Hz, 1H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 151.3, 147.1, 135.2, 133.3, 129.5, 128.6, 128.4, 128.4, 126.7, 126.1, 125.6, 124.5, 117.7, 113.1, 106.4.

2-Phenyl-3-(p-tolylthio)imidazo[1,2-a]pyridine (5b) [2]



^{1}H-NMR ($CDCl_3$, 400 MHz): δ 8.29-8.26 (m, 3H), 7.74 (d, *J*=9.2 Hz, 1H), 7.48-7.45 (m, 2H), 7.39 (t, *J*=7.2 Hz, 4H), 7.31-7.27 (m, 1H), 7.02 (d, *J*=8.0 Hz, 2H), 6.93 (d, *J*=8.4 Hz, 2H), 6.82 (t, *J*=6.8 Hz, 1H), 2.26 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 151.1, 147.0, 136.0, 133.4, 131.5, 130.2, 128.4, 128.4, 128.4, 126.6, 125.8, 124.5, 117.6, 113.0, 106.9, 20.9.

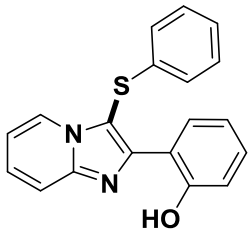
3-((4-Chlorophenyl)thio)-2-phenylimidazo[1,2-a]pyridine (5c) [2]



^{1}H-NMR ($CDCl_3$, 400 MHz): δ 8.28-8.24 (m, 1H), 8.21-8.18 (m, 1H), 7.77 (dd, *J*=8.8,

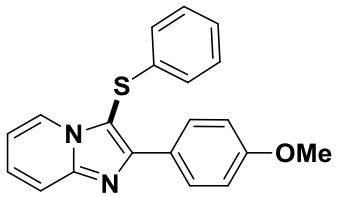
1.2 Hz, 1H), 7.49-7.45 (m, 2H), 7.43-7.36 (m, 2H), 7.22-7.19 (m, 2H), 6.96-6.90 (m, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 151.6, 147.2, 133.7, 133.1, 132.1, 129.6, 128.8, 128.5, 128.3, 126.9, 126.8, 124.3, 117.8, 113.3, 105.7.

2-(3-(Phenylthio)imidazo[1,2-a]pyridin-2-yl)phenol (5d)



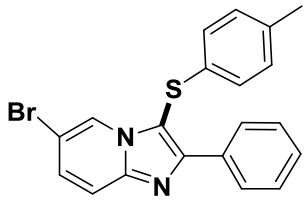
^{1}H-NMR ($CDCl_3$, 400 MHz): δ 13.13 (s, 1H), 8.64 (dd, *J*=8.0, 2.0 Hz, 1H), 8.39 (d, *J*=6.8 Hz, 1H), 7.70 (d, *J*=8.8 Hz, 1H), 7.44-7.39 (m, 1H), 7.33-7.29 (m, 1H), 7.27-7.22 (m, 2H), 7.20-7.16 (m, 1H), 7.12-7.06 (m, 3H), 6.98-6.95 (m, 1H), 6.92-6.87 (m, 1H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 158.4, 149.5, 144.7, 134.4, 130.6, 129.6, 127.8, 127.5, 126.4, 125.9, 124.2, 118.9, 117.8, 116.7, 116.1, 113.8, 105.5; **HRMS (**ESI-TOF) m/z calculated for $C_{19}H_{15}N_2OS^+$ 319.0900 $(M+H)^+$, found 319.0902.

2-(4-Methoxyphenyl)-3-(phenylthio)imidazo[1,2-a]pyridine (5e) [2]



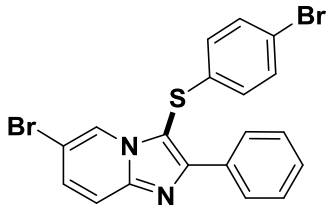
^{1}H-NMR ($CDCl_3$, 400 MHz): δ 8.27 (d, *J*=6.8 Hz, 1H), 8.22-8.18 (m, 2H), 7.73 (d, *J*=9.2 Hz, 1H), 7.35-7.31 (m, 1H), 7.25-7.20 (m, 2H), 7.16-7.12 (m, 1H), , 7.036-6.97 (m, 4H), 3.85 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 160.0, 151.3, 147.1, 135.3, 129.7, 129.4, 126.6, 126.0, 125.9, 125.5, 124.4, 117.4, 113.9, 112.9, 105.3, 55.3.

6-bromo-2-phenyl-3-(p-tolylthio)imidazo[1,2-a]pyridine(5f) [3]



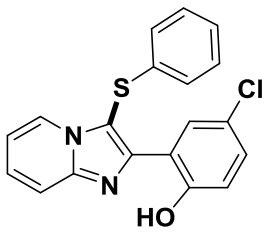
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.45 (s, 1H), 8.23 (d, *J* = 7.0 Hz, 14H), 7.63 (dd, *J* = 9.4, 0.8 Hz, 14H), 7.46 (dd, *J* = 8.2, 6.4 Hz, 27H), 7.43 – 7.38 (m, 25H), 7.07 (d, *J* = 8.0 Hz, 28H), 6.94 (d, *J* = 8.2 Hz, 24H), 2.30 (s, 41H). **^{13}C NMR** (($CDCl_3$, 100 MHz): δ 151.7, 145.3, 136.4, 132.9, 130.9, 130.4, 130.1, 128.8, 128.5, 128.3, 126.0, 124.7, 118.3, 108.0, 20.91

6-bromo-3-((4-bromophenyl)thio)-2-phenylimidazo[1,2-a]pyridine(5g)



^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.42 (s, 1H), 8.18 (d, *J* = 6.6 Hz, 15H), 7.51 – 7.41 (m, 52H), 7.38 (d, *J* = 8.5 Hz, 23H), 6.89 (d, *J* = 8.6 Hz, 22H). **^{13}C NMR** (($CDCl_3$, 100 MHz):151.7, 147.7, 133.6, 130.8, 129.7, 128.8, 128.3, 128.3, 126.7, 126.5, 125.6, 117.5, 113.1. **HRMS (**ESI-TOF) m/z calculated for $C_{19}H_{12}N_2NaS^+$ 480.8980 $(M+Na)^+$, found 480.8981.

5-chloro-2-(3-(phenylthio)imidazo[1,2-a]pyridin-2-yl)phenol(5h)



^{1}H NMR ($CDCl_3$, 400 MHz): δ 13.15 (s, 1H), 8.72 – 8.61 (m, 1H), 8.39 (d, *J* = 6.8 Hz, 1H), 7.73 – 7.65 (m, 1H), 7.49 – 7.39 (m, 1H), 7.28 – 7.13 (m, 4H), 7.10 – 7.05 (m, 2H), 7.04 – 6.93 (m, 2H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 157.1, 147.8, 144.5, 133.9, 130.3, 129.6, 127.7, 126.3, 124.3, 119.0, 118.3, 117.1, 116.8, 116.7, 114.0, 113.9,

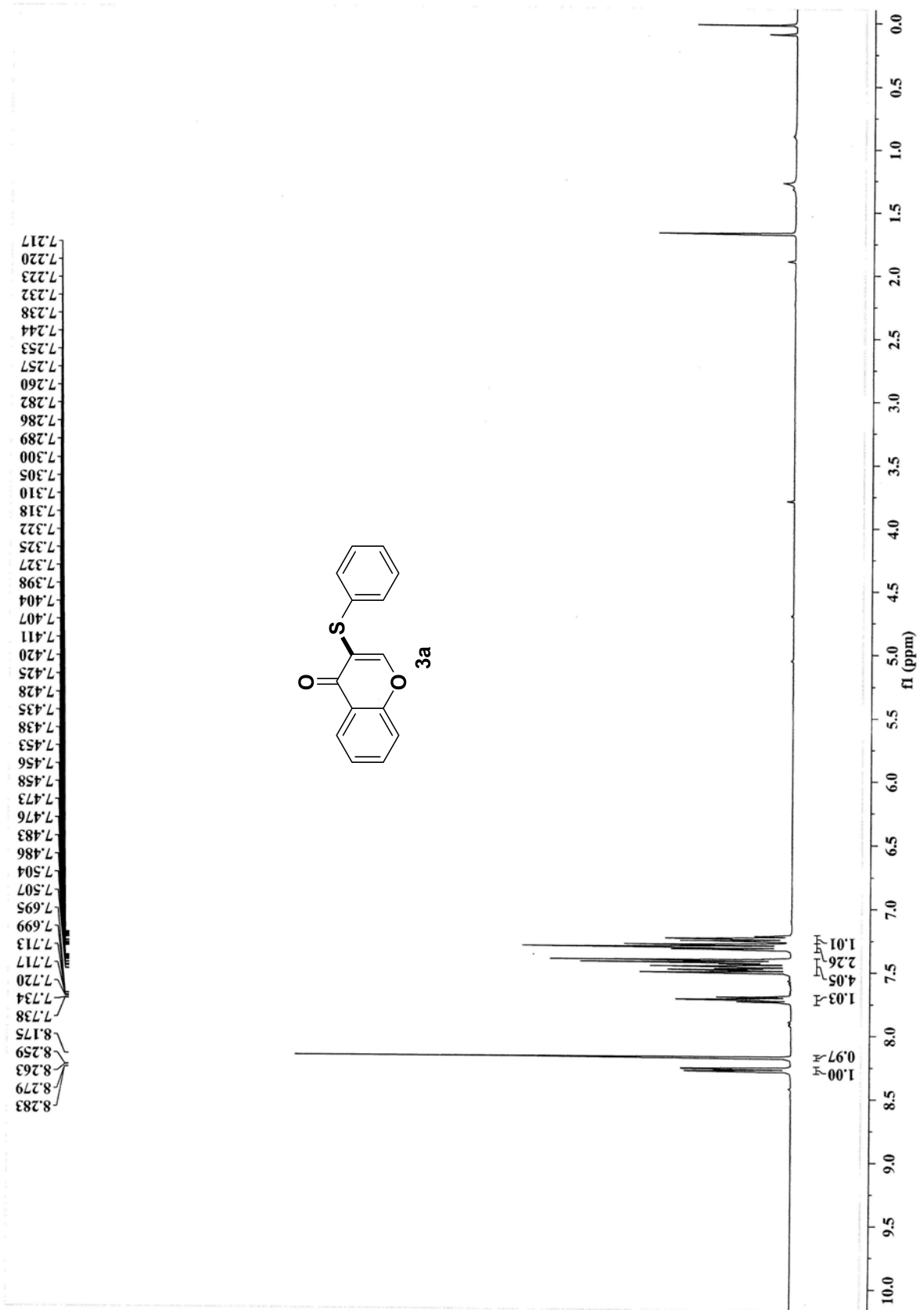
106.4. **HRMS (**ESI-TOF) m/z calculated for $C_{19}H_{13}ClN_2NaOS^+$ 375.0329 $(M+Na)^+$, found 375.0327.

Reference

[1] F. L. Yang, S. K. Tian, *Angew. Chem.* **2013**, *125*, 5029; *Angew. Chem. Int. Ed.* **2013,** *52*, 4929.

[2] X. Huang, S. Wang, B. Li, X. Wang, Z. Ge, R. Li, *RSC Adv.*, **2015**, *5*, 22654.

[3] H. Marie-Aude, S. Bertina-Raboin, *Green Chem.*, **2015**,***17***, 937


3a
S
O
O
f1 (ppm)
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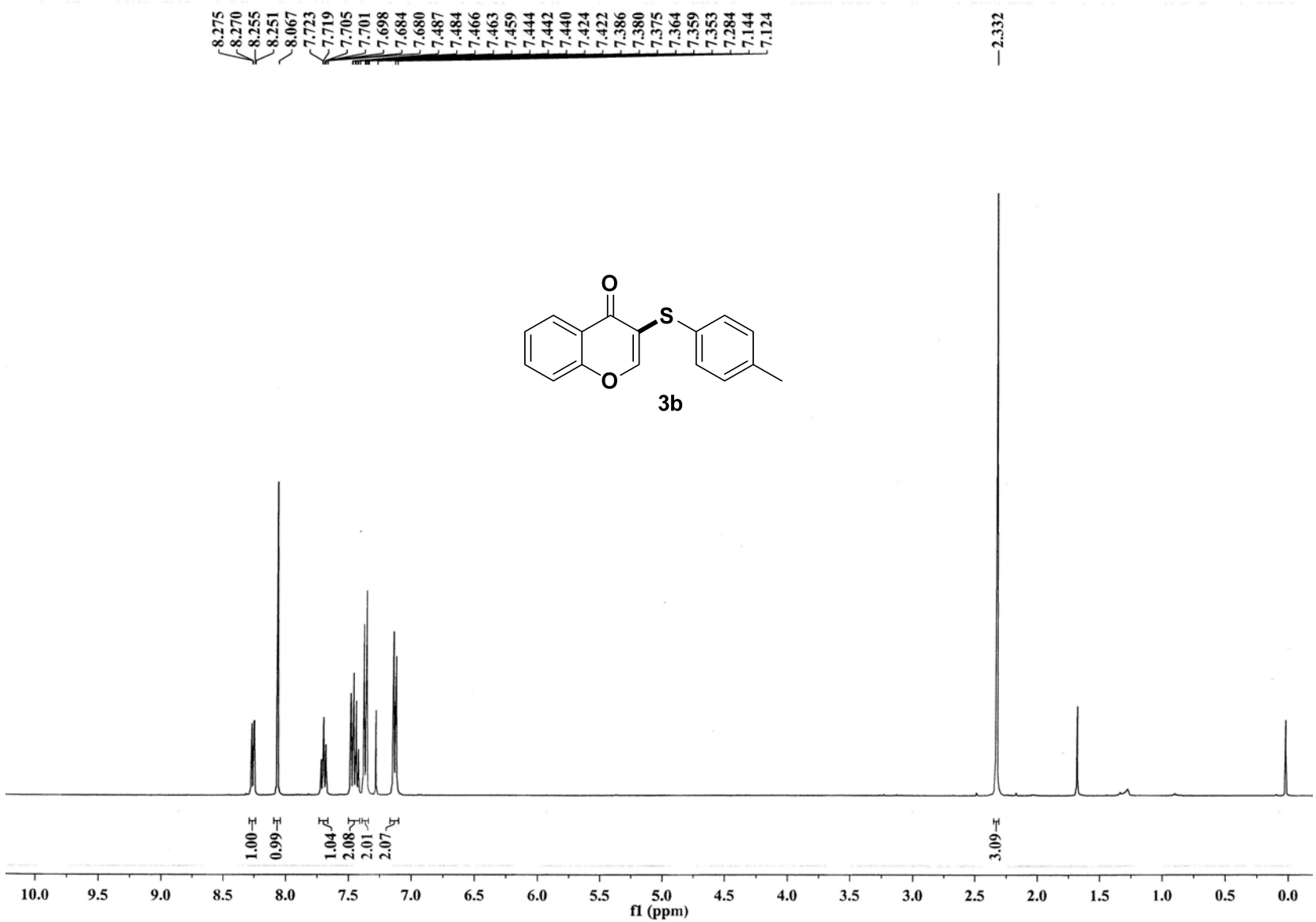
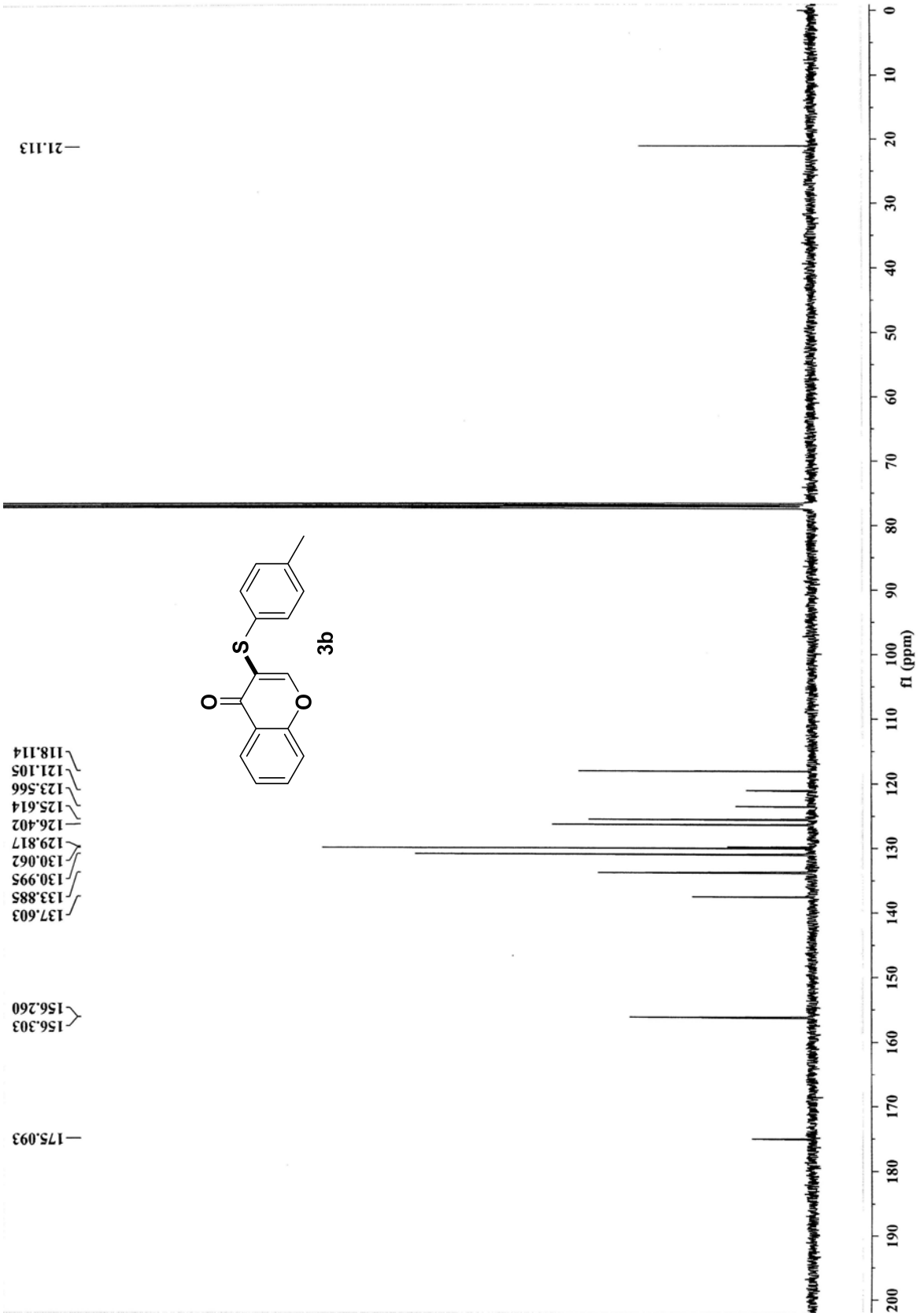
0.97
1.03
4.05
2.26
1.01
7.217
7.220
7.223
7.232
7.238
7.244
7.253
7.257
7.260
7.282
7.286
7.289
7.300
7.305
7.310
7.318
7.322
7.325
7.327
7.398
7.404
7.407
7.411
7.420
7.425
7.428
7.435
7.438
7.453
7.456
7.458
7.473
7.476
7.483
7.486
7.504
7.507
7.695
7.699
7.713
7.717
7.720
7.734
7.738
8.175
8.259
8.263
8.279
8.283

175.073
157.361
156.348
134.019
134.002
129.847
129.803
129.201
127.124
126.467
125.749
123.680
119.950
118.160
S
O
O
3a
f1 (ppm)


8.275
8.270
8.255
8.251
8.067
7.723
7.719
7.705
7.701
7.698
7.684
7.680
7.487
7.484
7.466
7.463
7.459
7.444
7.442
7.440
7.424
7.422
7.386
7.380
7.375
7.364
7.359
7.353
7.284
7.144
7.124
2.332
O
S
O
3b
1.00
0.99
1.04
2.08
2.01
2.07
3.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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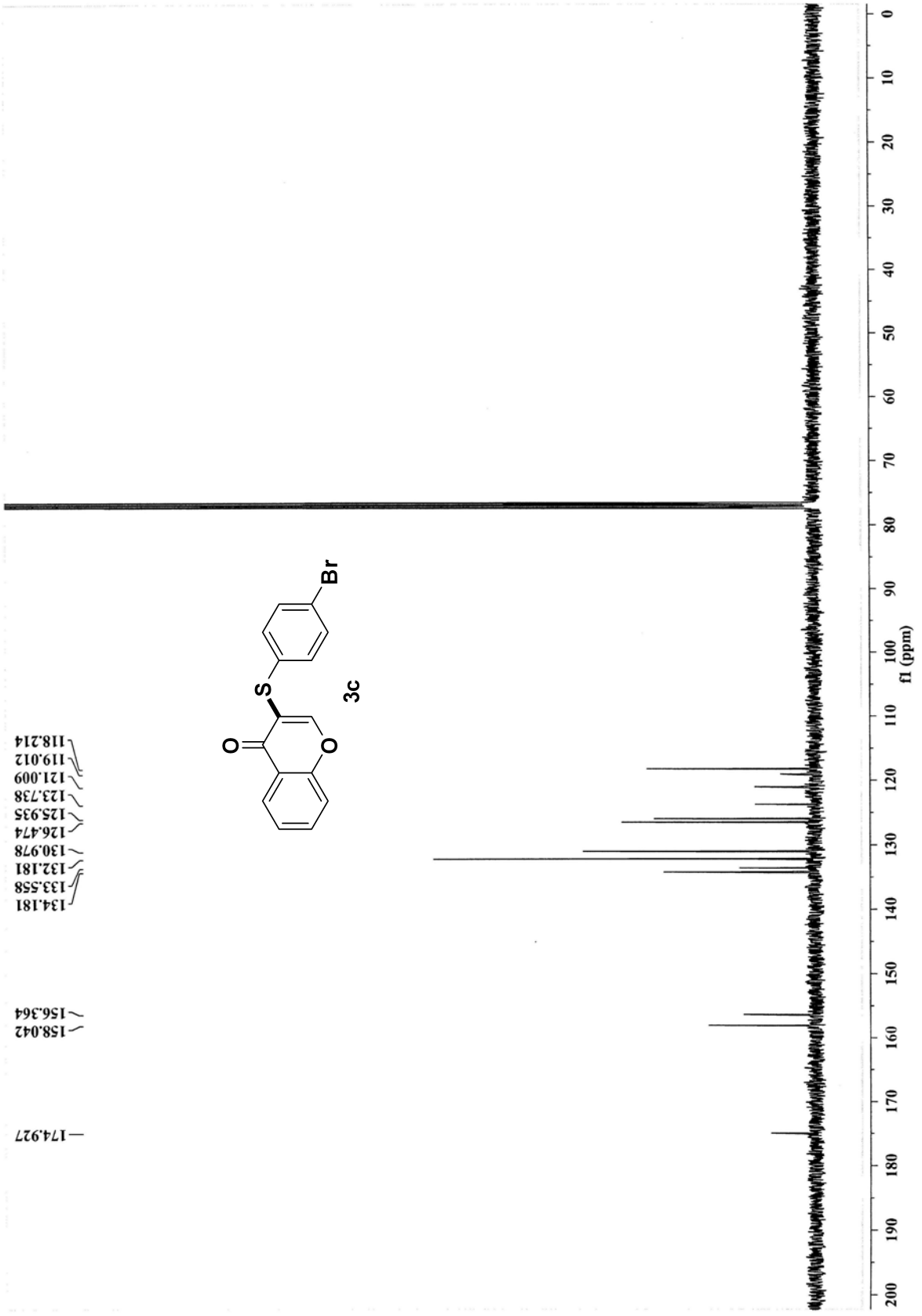
118.114
121.105
123.566
125.614
126.402
129.817
130.062
130.995
133.885
137.603
156.260
156.303
175.093
3b
S
O
O
f1 (ppm)

8.268
8.257
8.251
8.246
7.756
7.752
7.738
7.734
7.730
7.717
7.713
7.524
7.522
7.503
7.500
7.491
7.488
7.473
7.471
7.468
7.453
7.450
7.417
7.412
7.400
7.395
7.283
7.274
7.269
7.252
Br
S
O
O
3c
2.00
1.11
2.15
1.98
1.91
f1 (ppm)


Br
S
O
O
3c
174.927
158.042
156.364
134.181
133.558
132.181
130.978
126.474
125.935
123.738
121.009
119.012
118.214
f1 (ppm)

8.266
8.262
8.255
8.246
8.242
7.750
7.746
7.732
7.728
7.725
7.711
7.707
7.525
7.516
7.495
7.484
7.482
7.464
7.447
7.444
7.347
7.342
7.331
7.326
7.319
7.284
7.273
7.266
7.261
7.250
7.245
1.92
1.00
2.03
1.99
2.04
f1 (ppm)
3d

174.953
157.915
156.355
134.171
133.101
132.802
130.877
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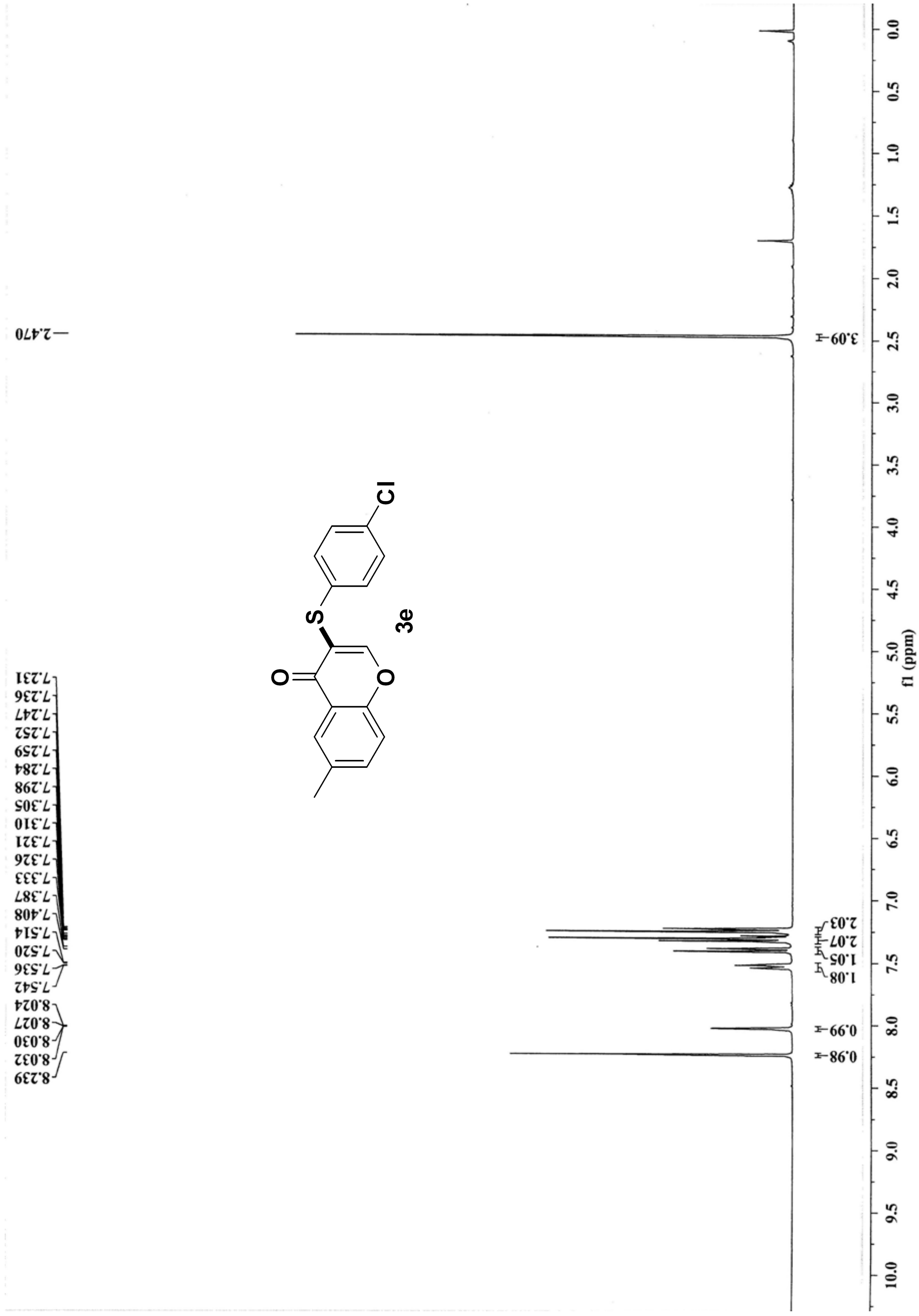
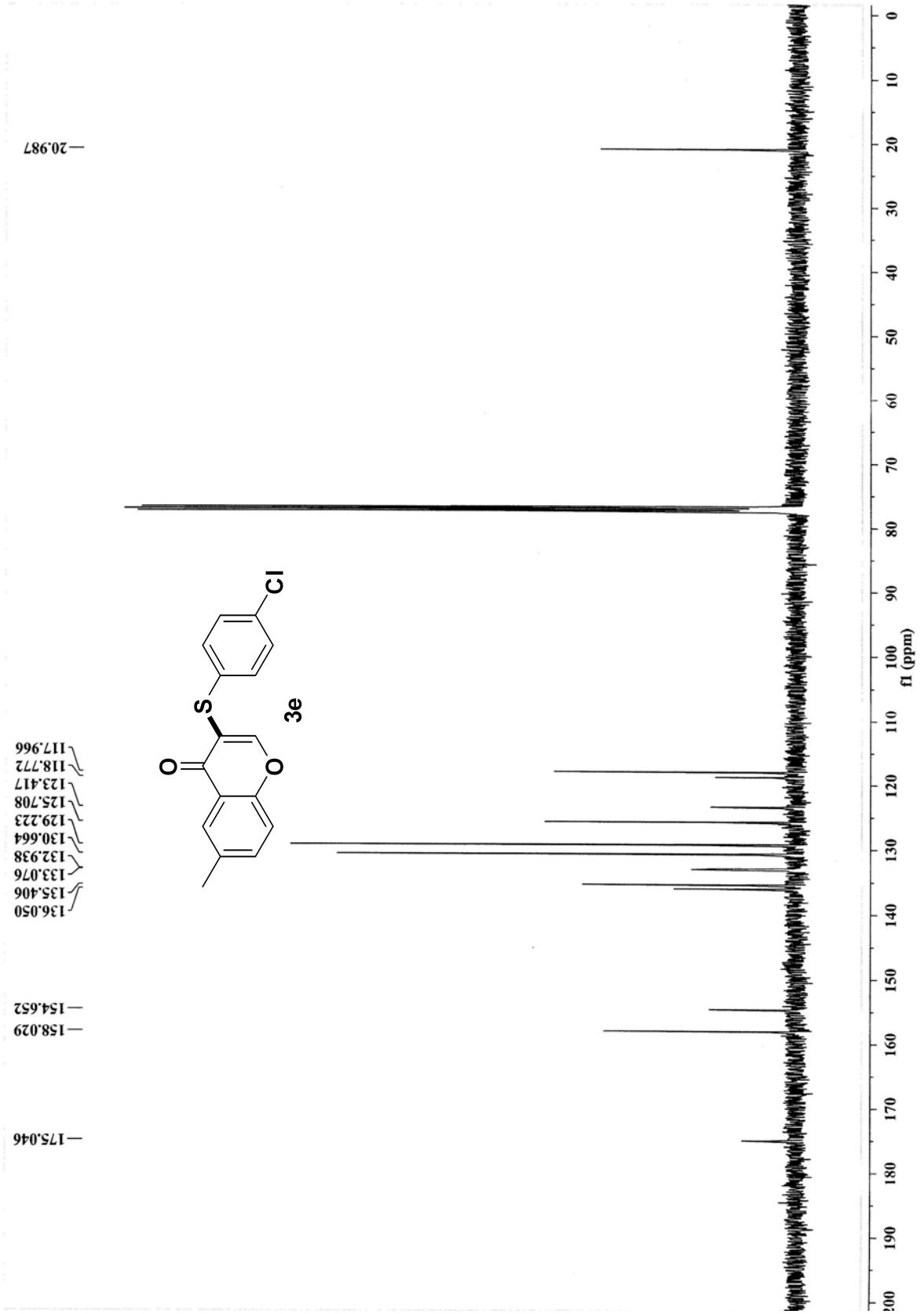
126.449
125.913
123.722
119.225
118.211
O
S
O
Cl
3d
f1 (ppm)


2.470
7.231
7.236
7.247
7.252
7.259
7.284
7.298
7.305
7.310
7.321
7.326
7.333
7.387
7.408
7.514
7.520
7.536
7.542
8.024
8.027
8.030
8.032
8.239
O
S
Cl
O
3e
3.09
2.03
2.07
1.05
1.08
0.99
0.98
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
7.5
8.0
8.5
9.0
9.5
10.0
f1 (ppm)


20.987
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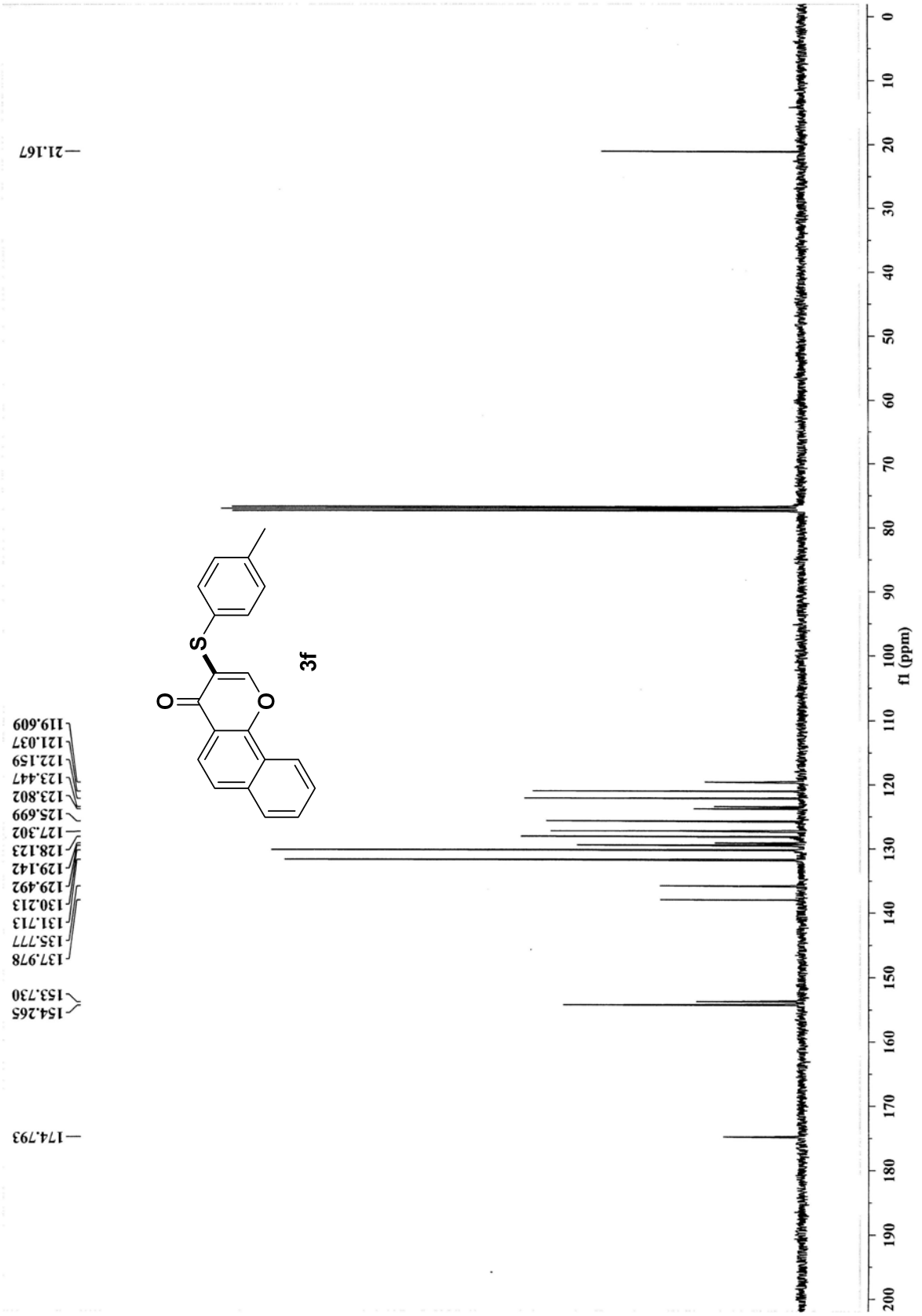
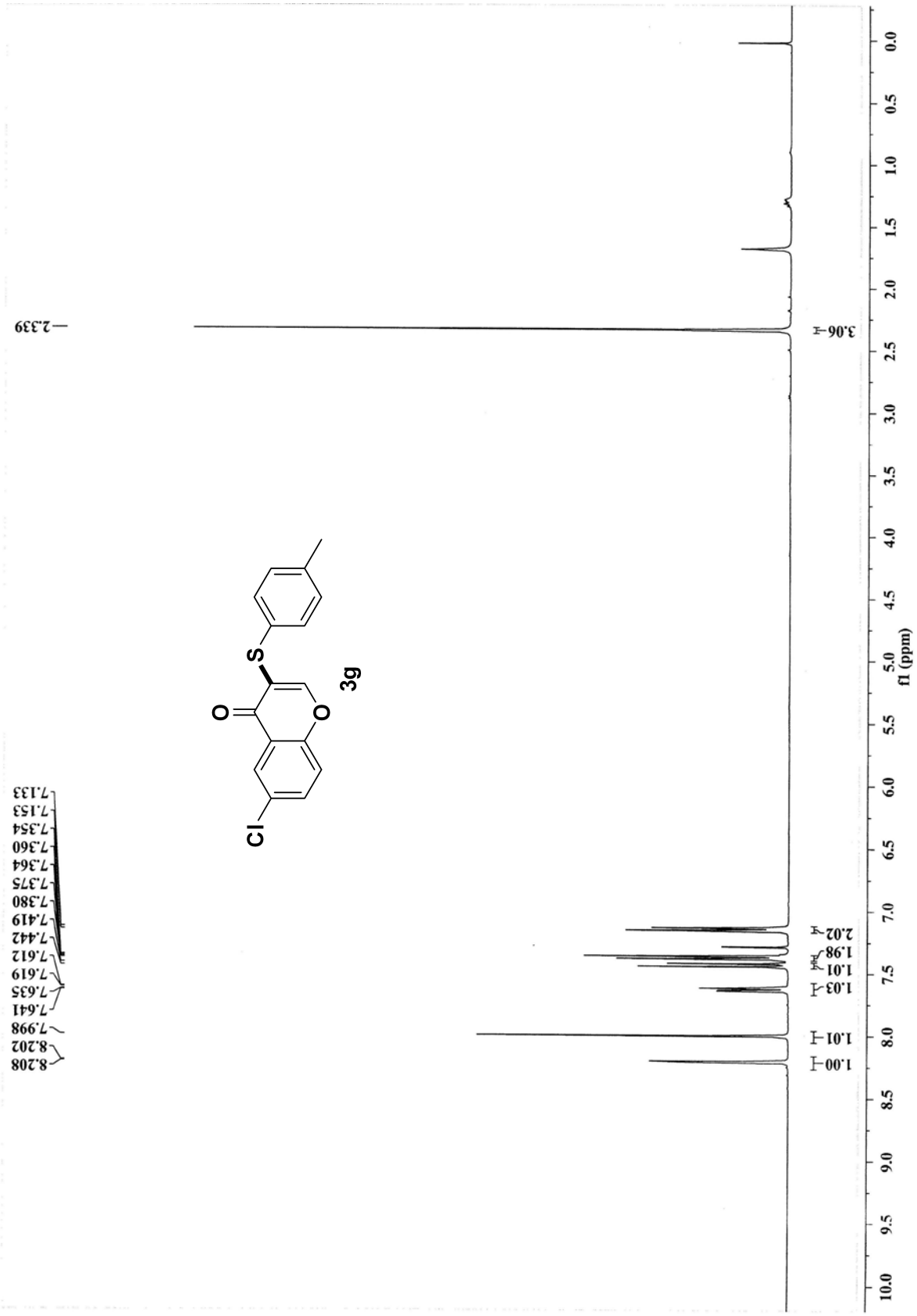
118.772
123.417
125.708
129.223
130.664
132.938
133.076
135.406
136.050
154.652
158.029
175.046
O
S
Cl
O
3e
f1 (ppm)

8.417
8.413
8.396
8.393
8.171
8.149
8.082
7.928
7.925
7.909
7.905
7.766
7.744
7.732
7.729
7.715
7.711
7.708
7.695
7.691
7.684
7.680
7.666
7.663
7.660
7.646
7.642
7.442
7.438
7.427
7.422
7.174
7.154
2.347
3.01
1.00
1.00
0.97
1.03
3.06
1.96
2.00
S
O
O
3f
f1 (ppm)


21.167
174.793
154.265
153.730
137.978
135.777
131.713
130.213
129.492
129.142
128.123
127.302
125.699
123.802
123.447
122.159
121.037
119.609
3f
O
O
S
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
f1 (ppm)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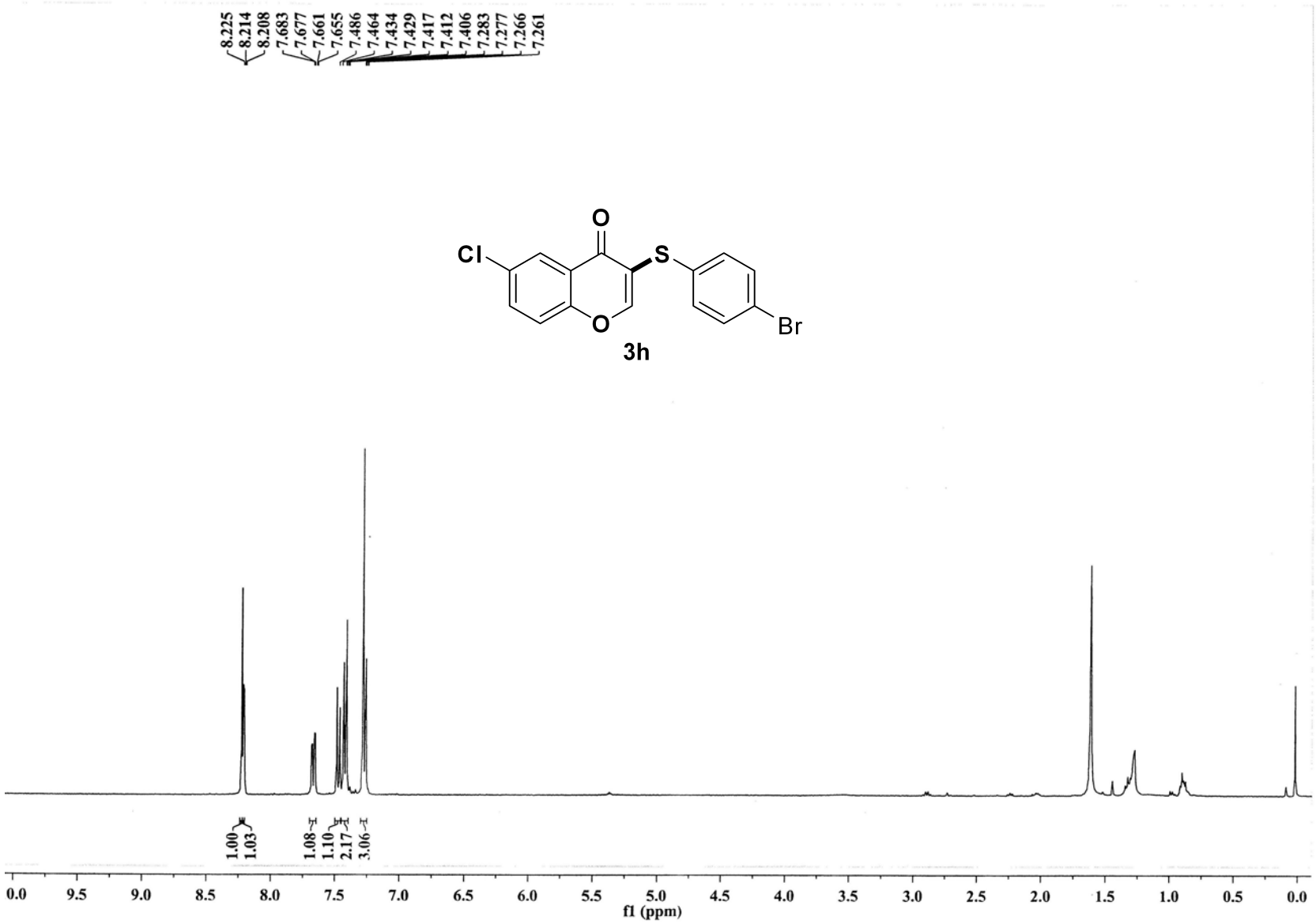
7.619
7.612
7.442
7.419
7.380
7.375
7.364
7.360
7.354
7.153
7.133
2.339
3.06
1.00
1.01
1.03
1.01
1.98
2.02
3g
O
S
O
Cl
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

21.128
173.973
155.823
154.604
137.983
134.105
131.542
131.421
130.162
129.160
125.681
124.345
121.719
119.876
S
O
O
Cl
3g
f1 (ppm)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8.214
8.208
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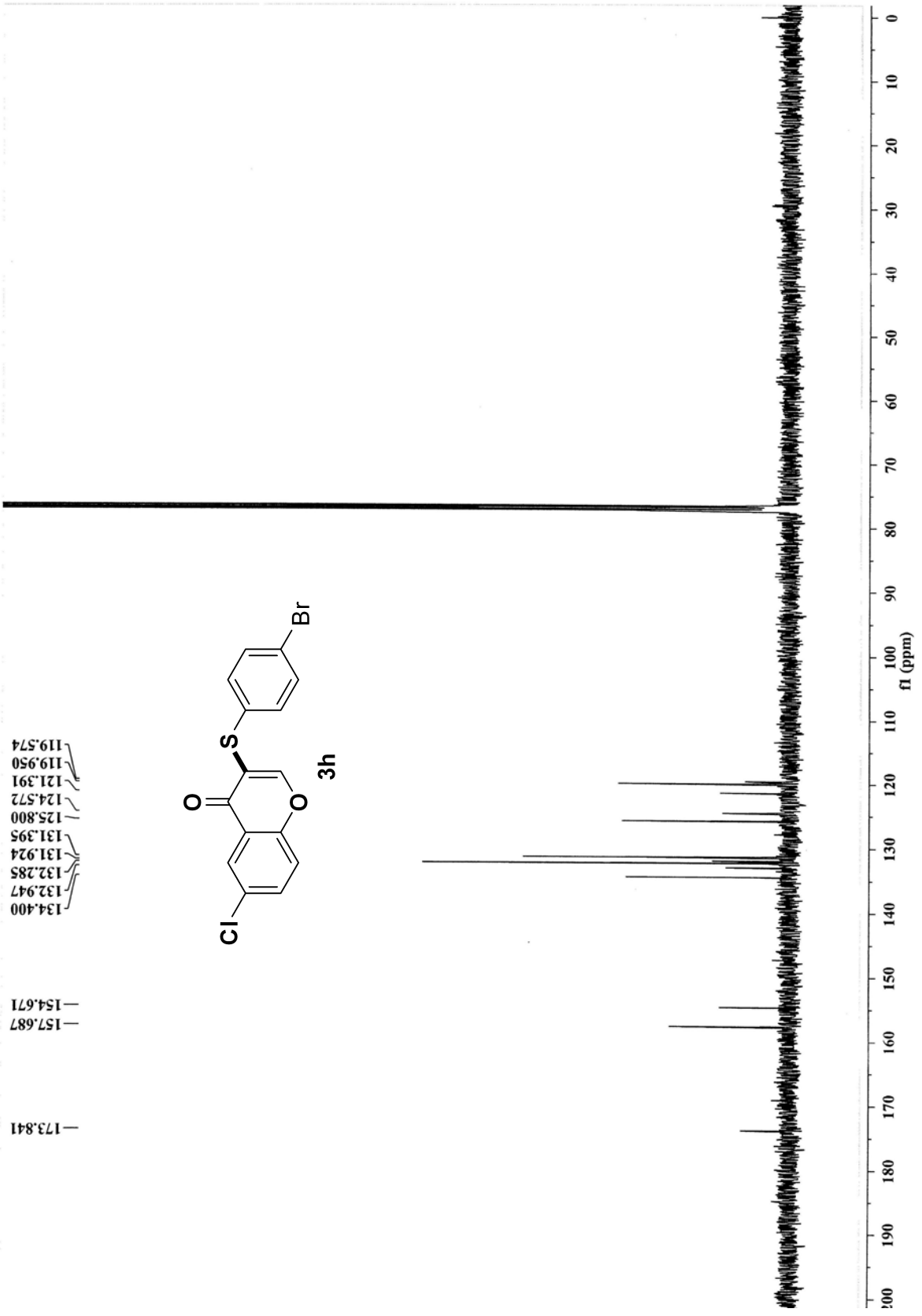
7.677
7.661
7.655
7.486
7.464
7.434
7.429
7.417
7.412
7.406
7.283
7.277
7.266
7.261
O
Cl
S
O
Br
3h
1.00
1.03
1.08
1.10
2.17
3.06
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Br
S
O
O
Cl
3h
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157.687
154.671
134.400
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132.285
131.924
131.395
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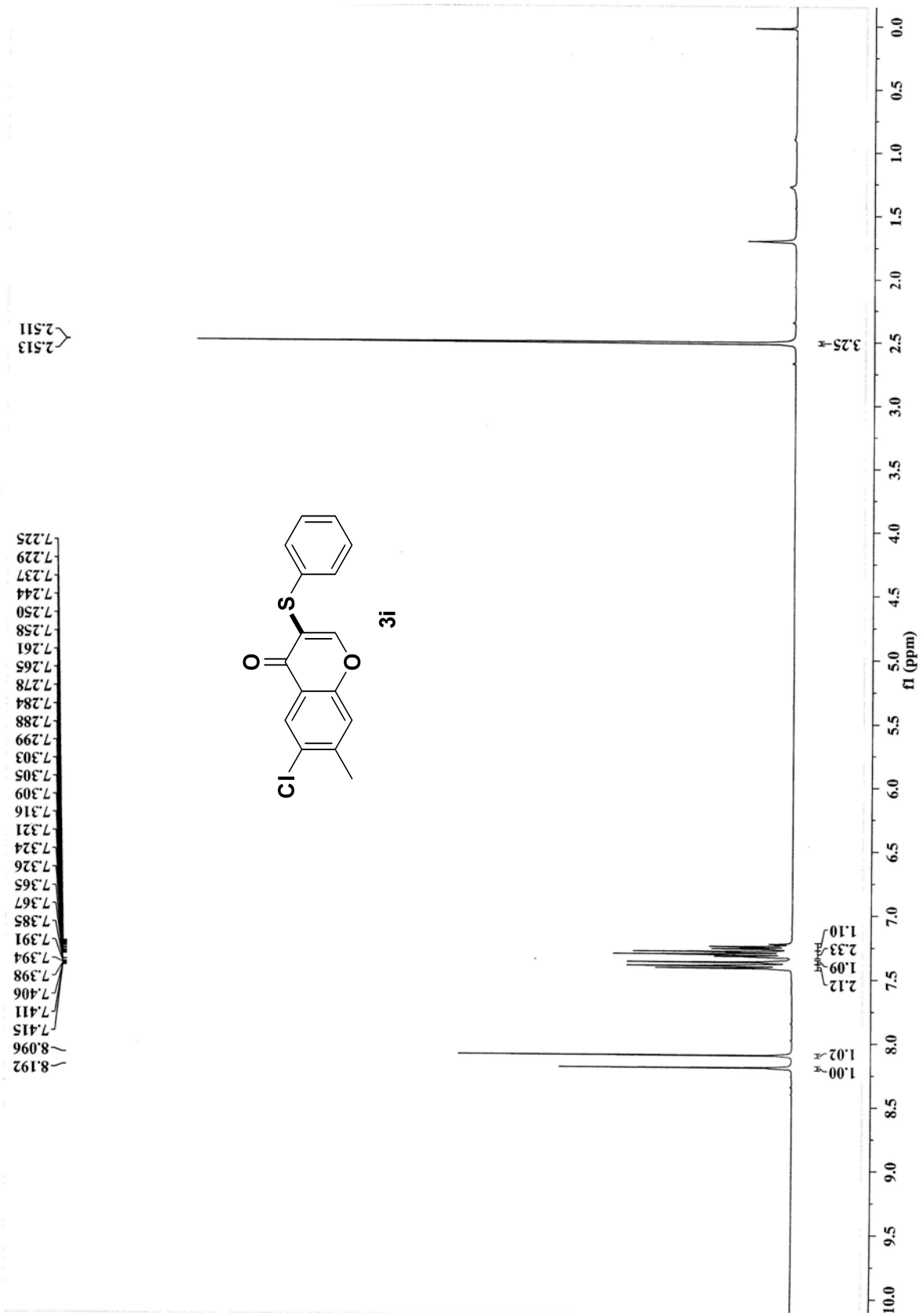
124.572
121.391
119.950
119.574
f1 (ppm)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8.096
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7.411
7.406
7.398
7.394
7.391
7.385
7.367
7.365
7.326
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7.237
7.229
7.225
2.513
2.511
3.25
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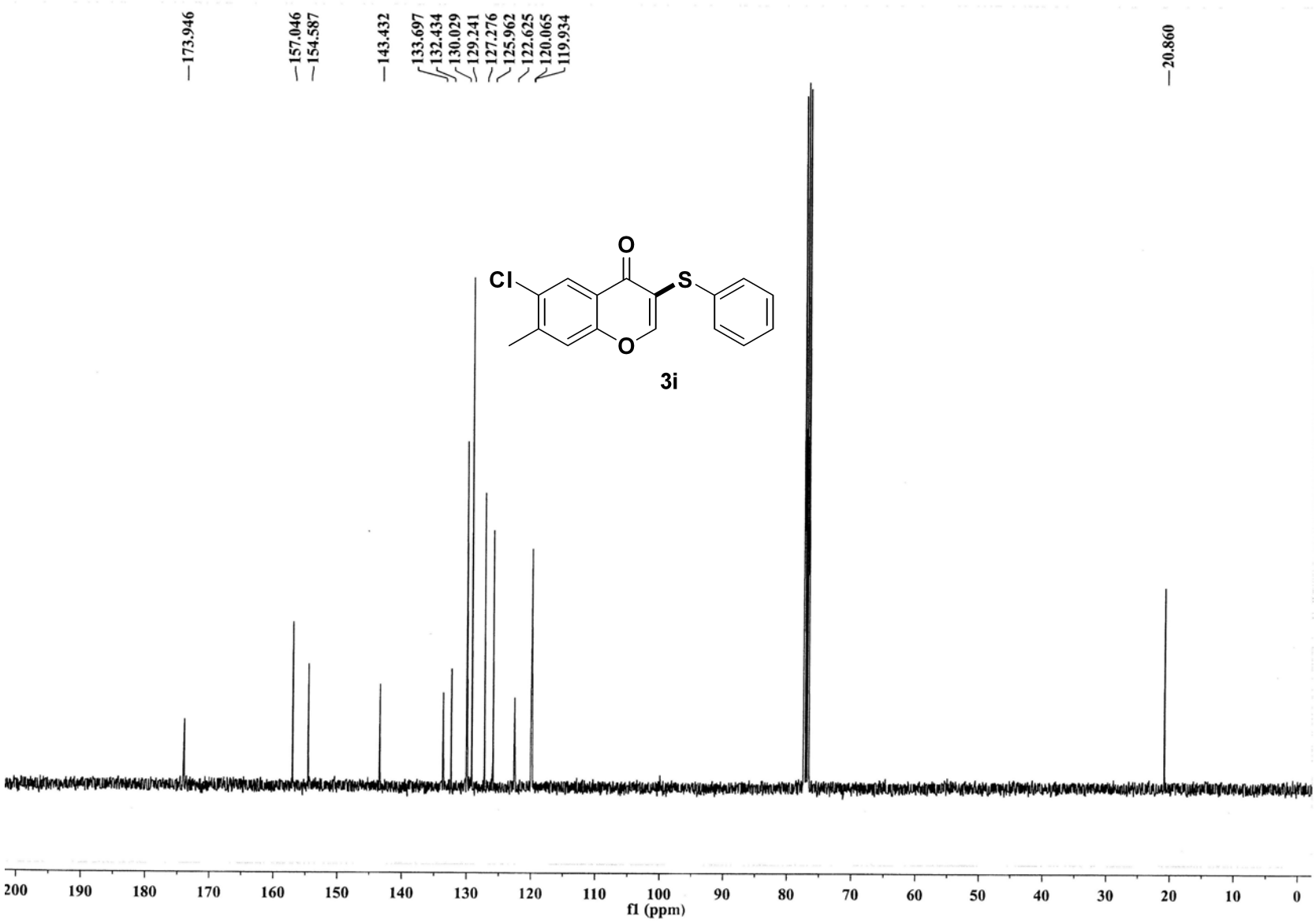
1.02
2.12
1.09
2.33
1.10
O
O
S
Cl
3i
f1 (ppm)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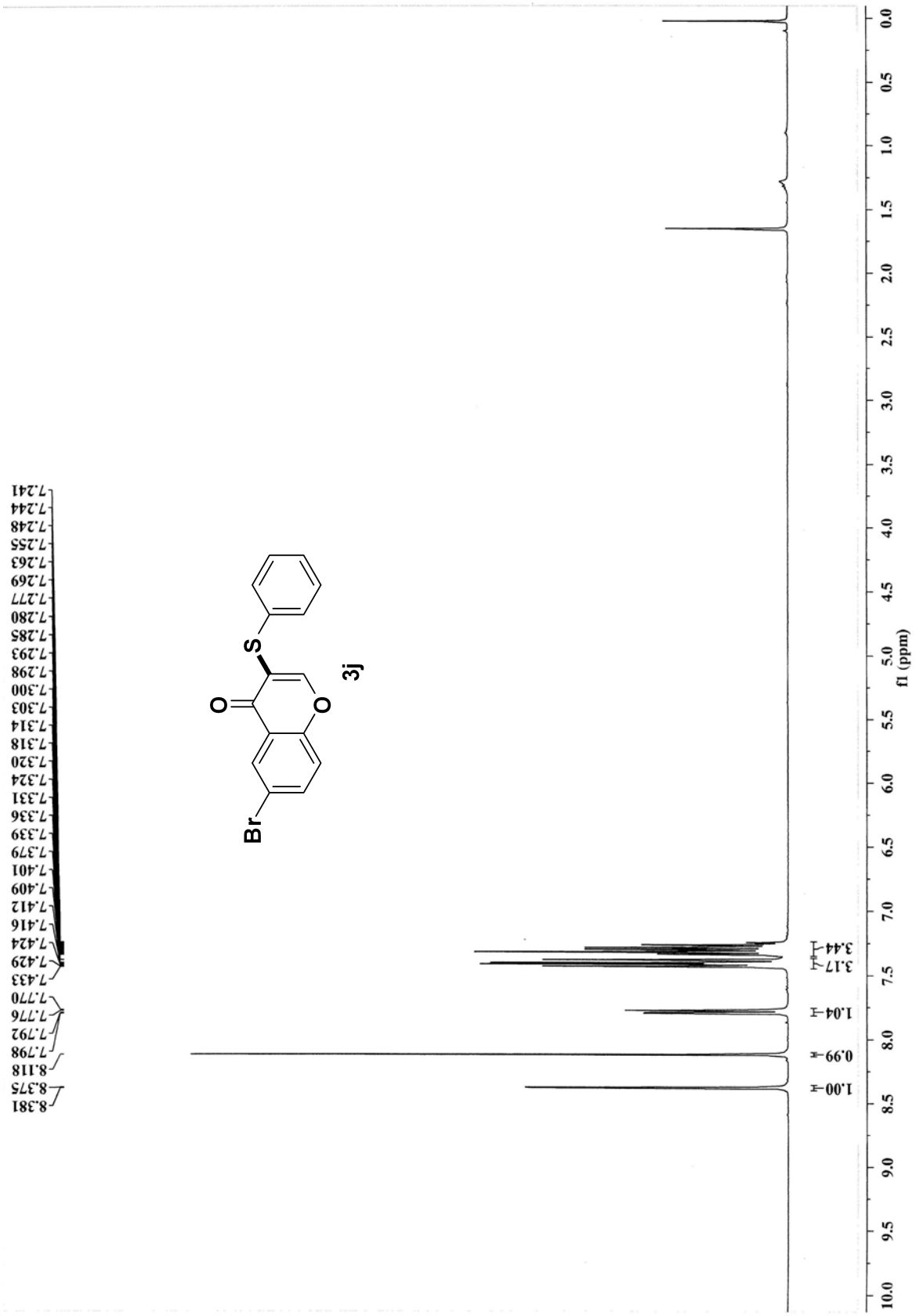
129.241
127.276
125.962
122.625
120.065
119.934
20.860
O
Cl
S
O
3i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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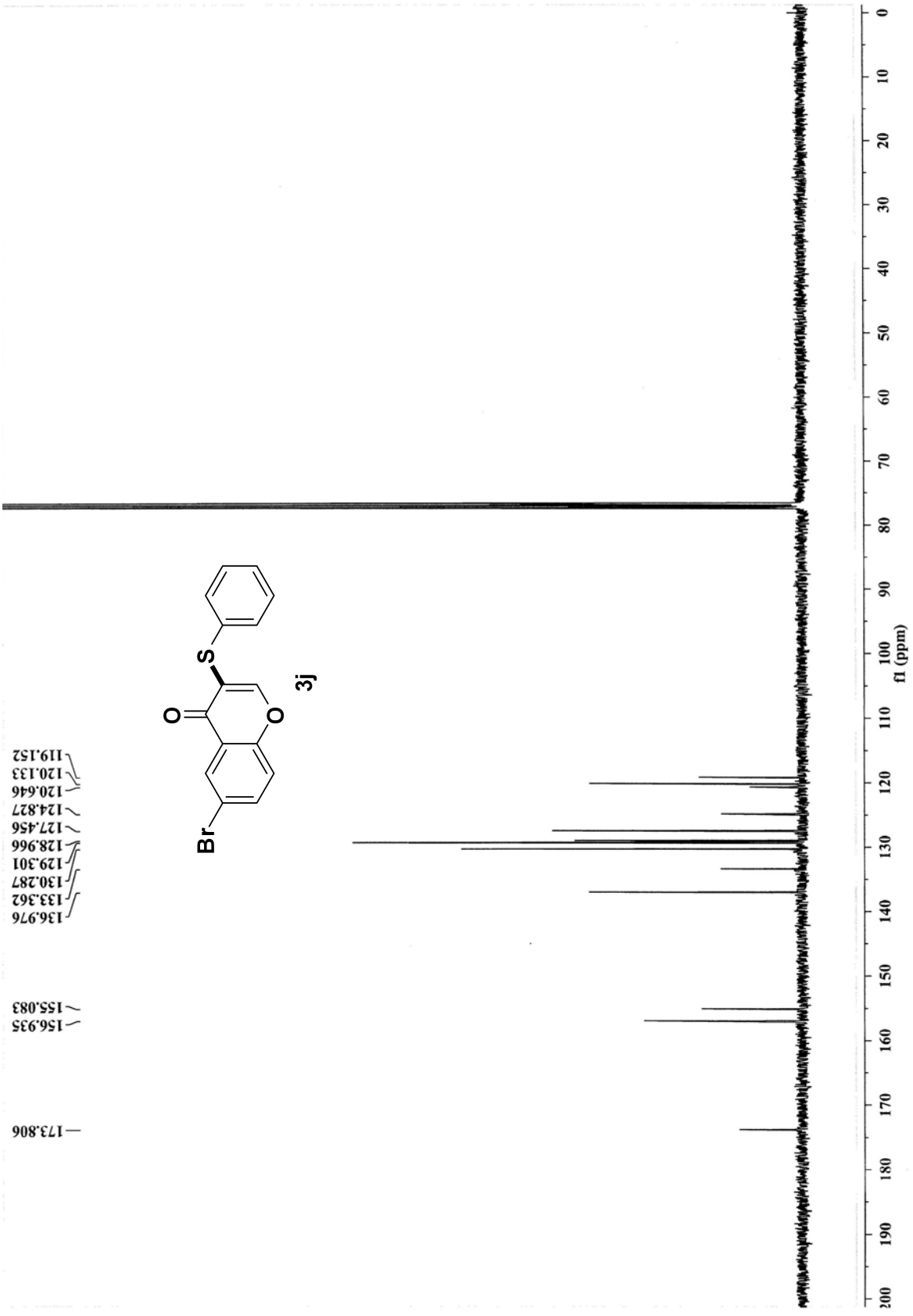
8.118
7.798
7.792
7.776
7.770
7.433
7.429
7.424
7.416
7.412
7.409
7.401
7.379
7.339
7.336
7.331
7.324
7.320
7.318
7.314
7.303
7.300
7.298
7.293
7.285
7.280
7.277
7.269
7.263
7.255
7.248
7.244
7.241
O
S
O
Br
3j
1.00
0.99
1.04
3.17
3.44
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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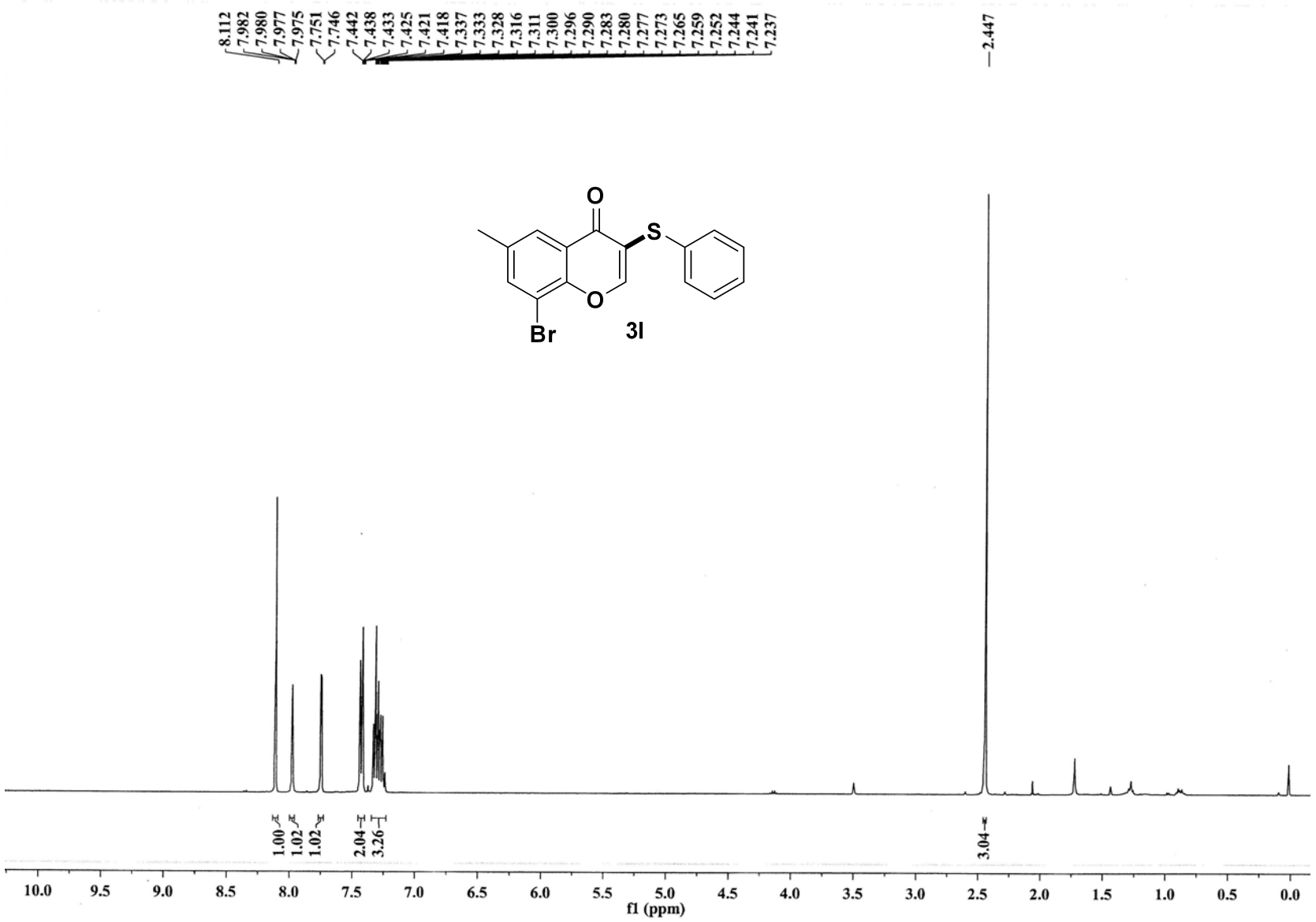
156.935
155.083
136.976
133.362
130.287
129.301
128.966
127.456
124.827
120.646
120.133
119.152
O
S
O
Br
3j
f1 (ppm)

8.375
8.369
7.999
7.783
7.777
7.761
7.755
7.381
7.360
7.156
7.136
2.341
1.00
0.98
1.03
3.09
2.05
3.02
3k
Br
O
O
S
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

21.129
173.819
155.782
155.040
138.001
136.856
131.444
130.165
129.133
128.906
124.708
121.849
120.076
118.997
O
S
O
Br
3k
f1 (ppm)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7.980
7.977
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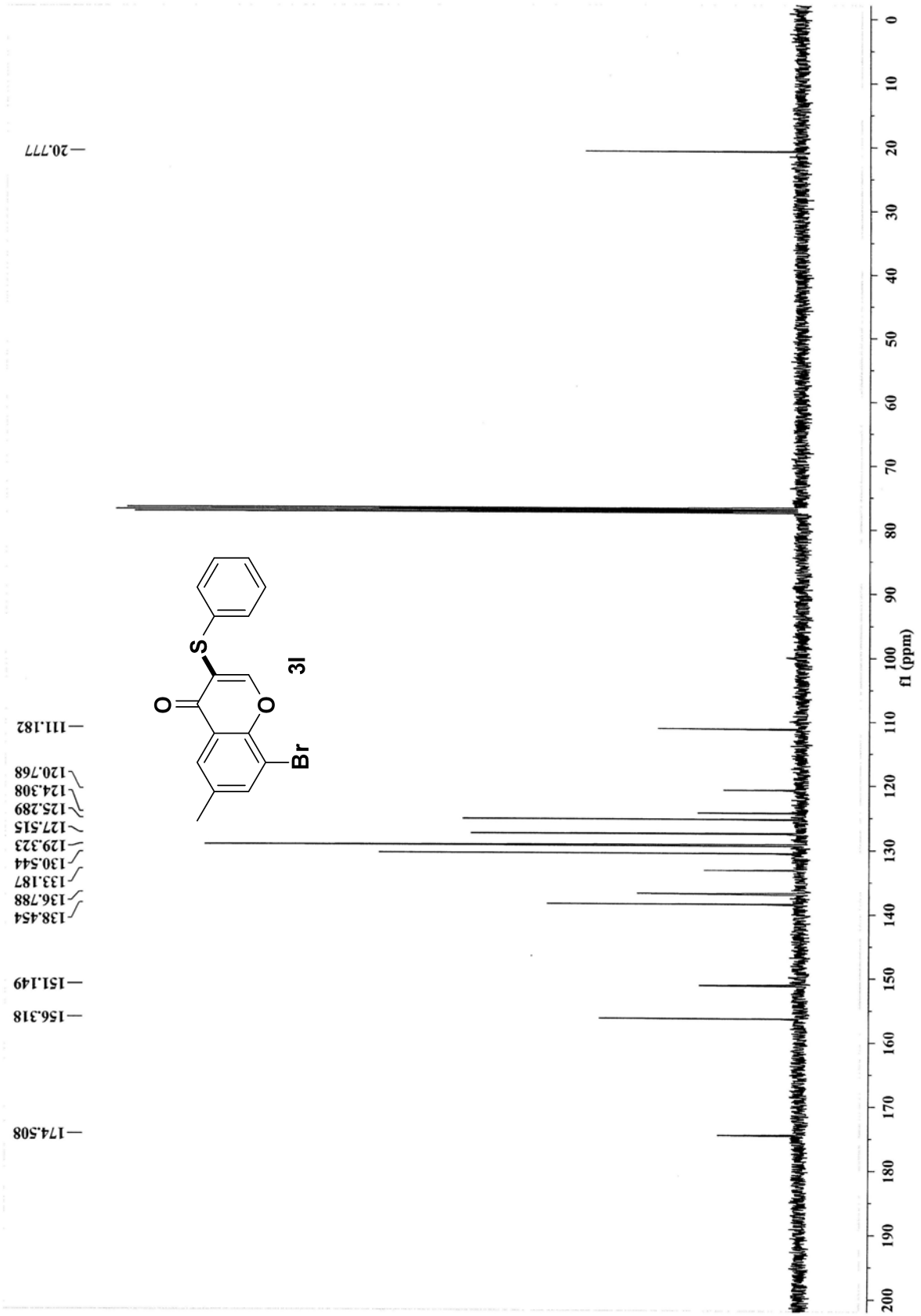
7.751
7.746
7.442
7.438
7.433
7.425
7.421
7.418
7.337
7.333
7.328
7.316
7.311
7.300
7.296
7.290
7.283
7.280
7.277
7.273
7.265
7.259
7.252
7.244
7.241
7.237
2.447
O
S
O
Br
3l
1.00
1.02
1.02
2.04
3.26
3.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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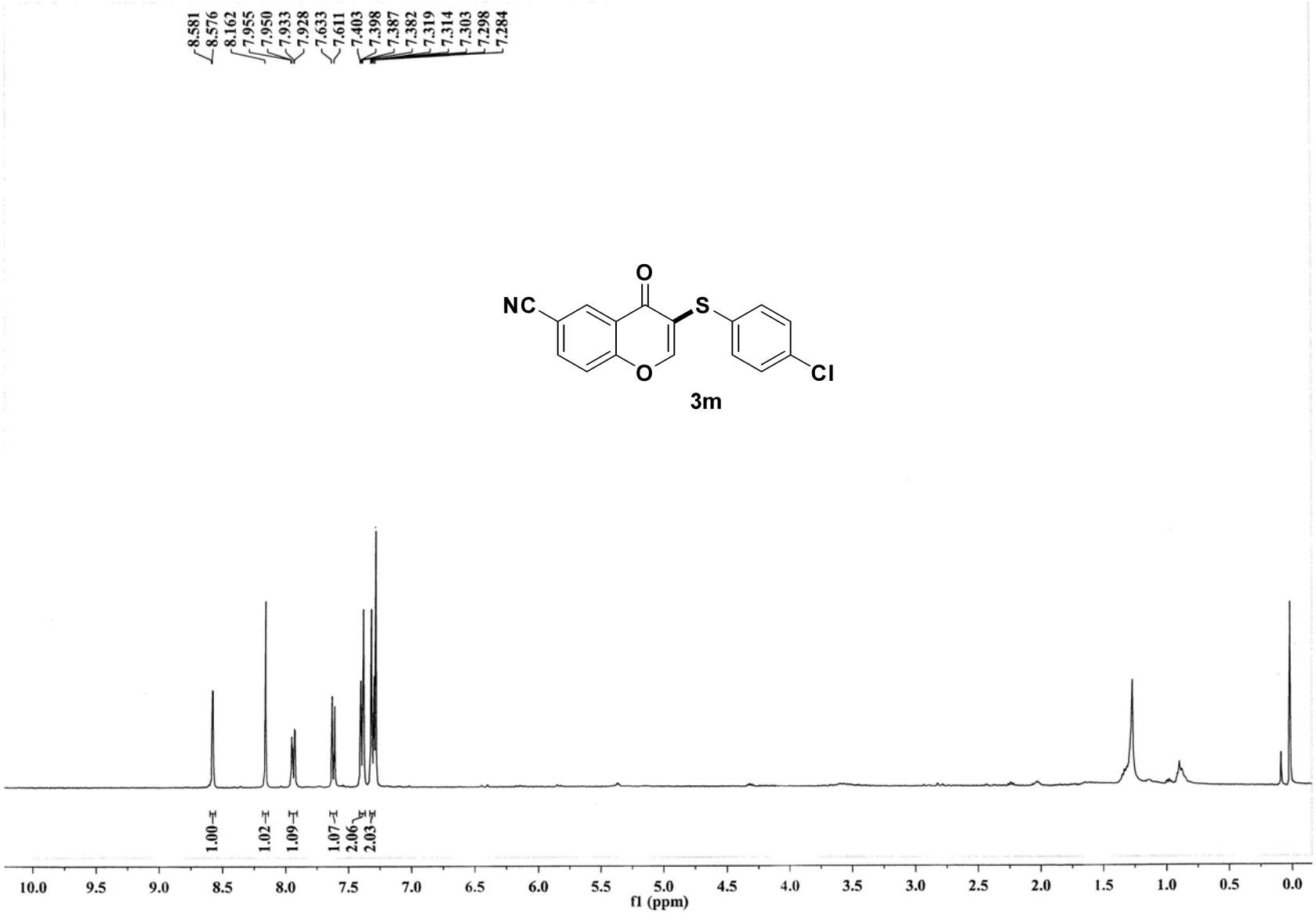
111.182
120.768
124.308
125.289
127.515
129.323
130.544
133.187
136.788
138.454
151.149
156.318
174.508
O
S
O
Br
3l
f1 (ppm)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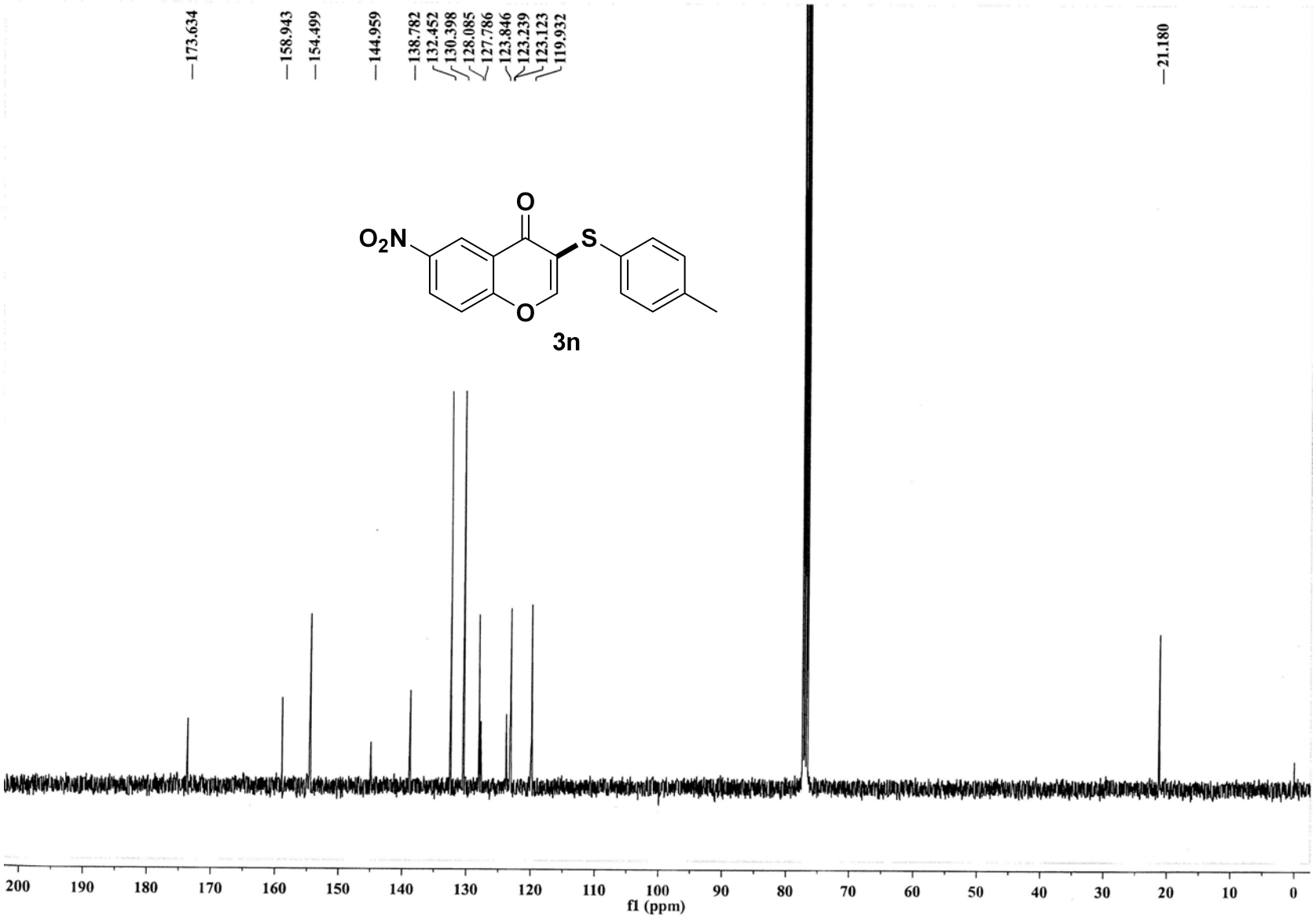
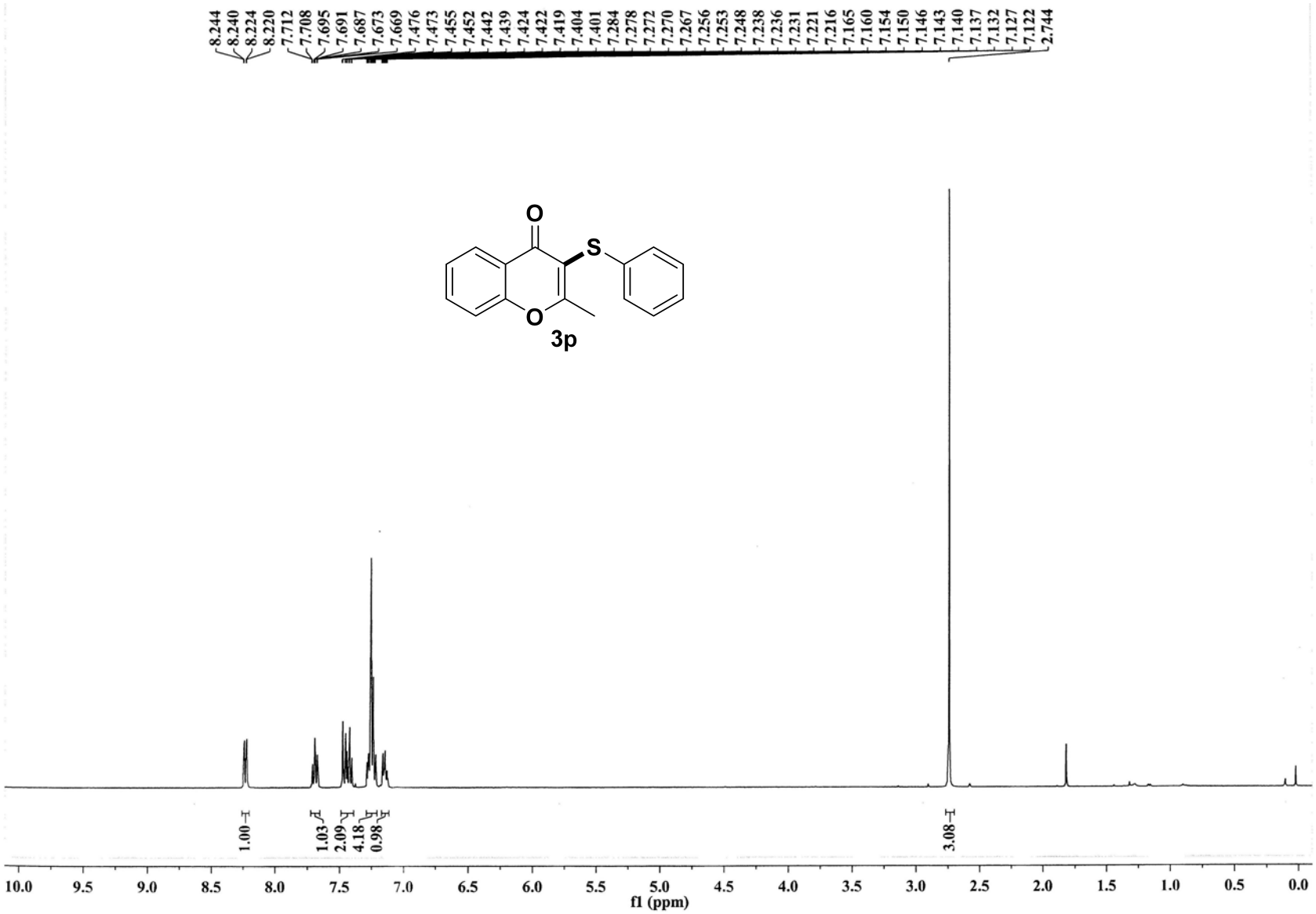
8.576
8.162
7.955
7.950
7.933
7.928
7.633
7.611
7.403
7.398
7.387
7.382
7.319
7.314
7.303
7.298
7.284
NC
O
S
O
Cl
3m
1.00
1.02
1.09
1.07
2.06
2.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

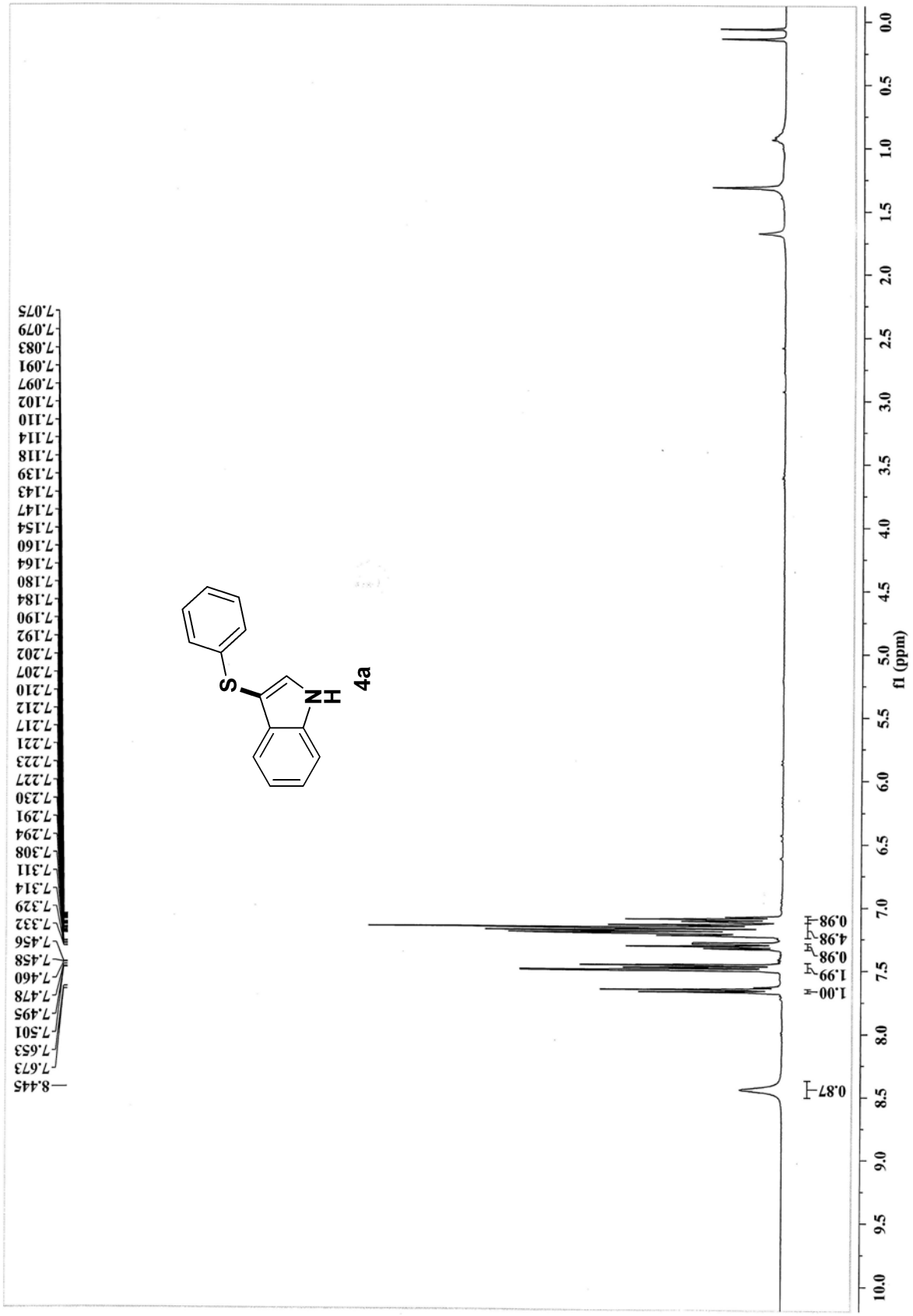
173.191
157.947
156.676
136.295
134.126
132.151
132.054
131.104
129.577
123.859
121.706
119.948
117.201
110.169
3m
S
O
O
Cl
NC
f1 (ppm)

9.129
9.122
8.532
8.525
8.509
8.502
7.910
7.634
7.611
7.435
7.430
7.420
7.415
7.284
7.200
7.198
7.194
7.184
7.178
2.365
3.01
1.00
1.08
1.03
1.05
2.05
2.12
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
O
S
O
O2N
3n


173.634
158.943
154.499
144.959
138.782
132.452
130.398
128.085
127.786
123.846
123.239
123.123
119.932
21.180
O
O2N
S
O
3n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.244
8.240
8.224
8.220
7.712
7.708
7.695
7.691
7.687
7.673
7.669
7.476
7.473
7.455
7.452
7.442
7.439
7.424
7.422
7.419
7.404
7.401
7.284
7.278
7.272
7.270
7.267
7.256
7.253
7.248
7.238
7.236
7.231
7.221
7.216
7.165
7.160
7.154
7.150
7.146
7.143
7.140
7.137
7.132
7.127
7.122
2.744
O
S
O
3p
1.00
1.03
2.09
4.18
0.98
3.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

175.272
171.513
155.565
135.693
133.831
128.998
127.489
127.465
126.587
125.945
125.516
122.935
117.721
115.322
20.766
3p
O
S
O
f1 (ppm)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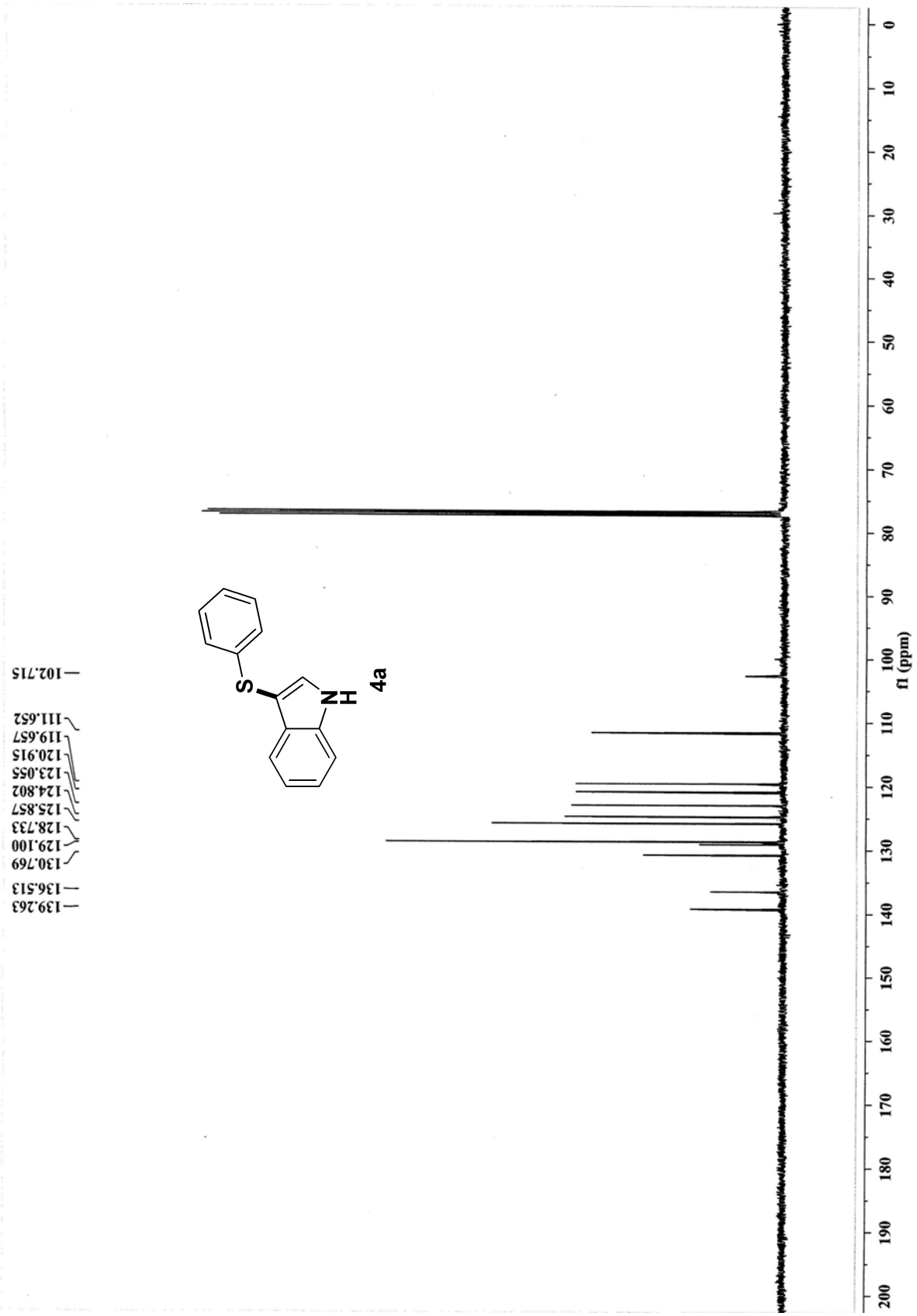
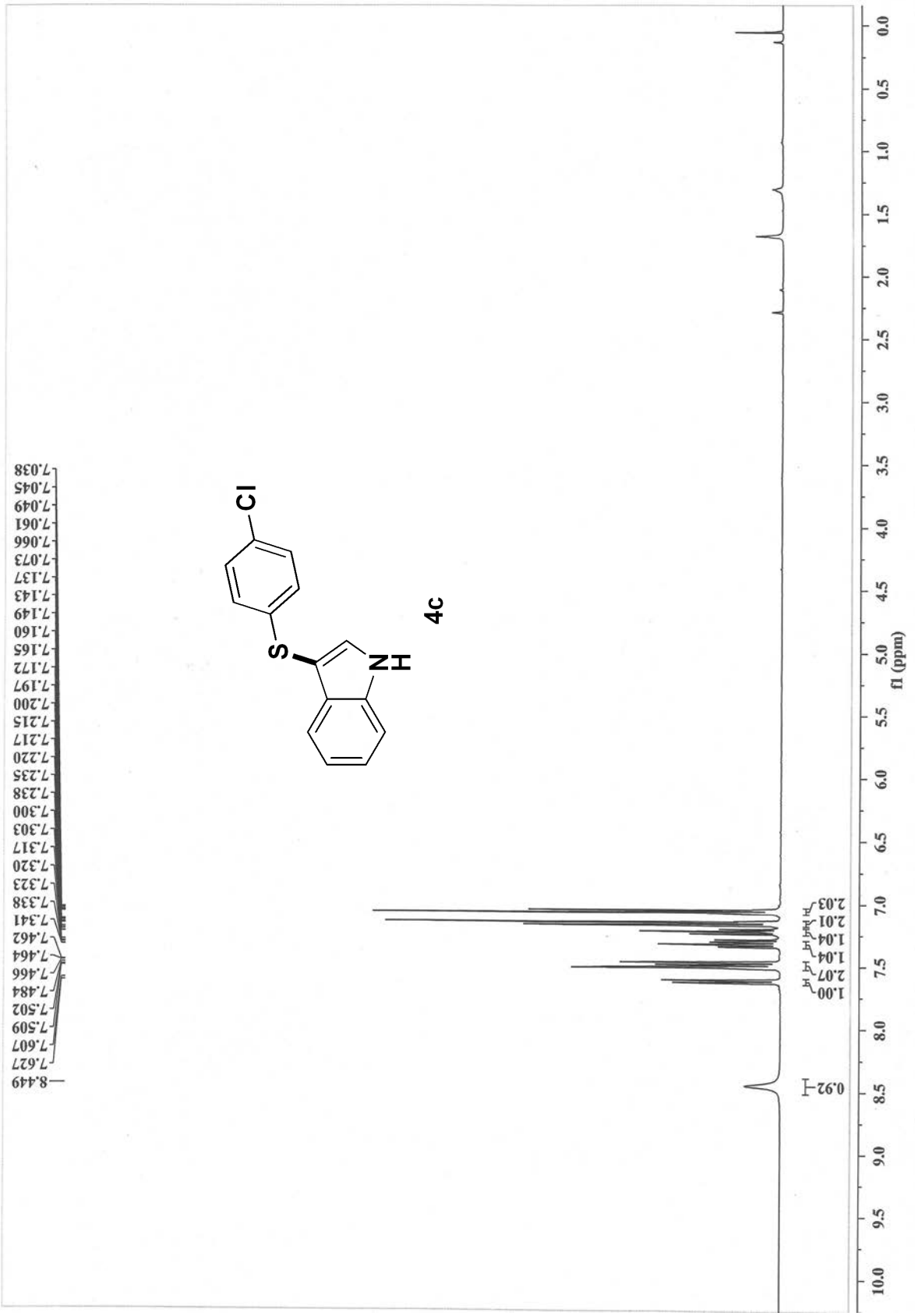
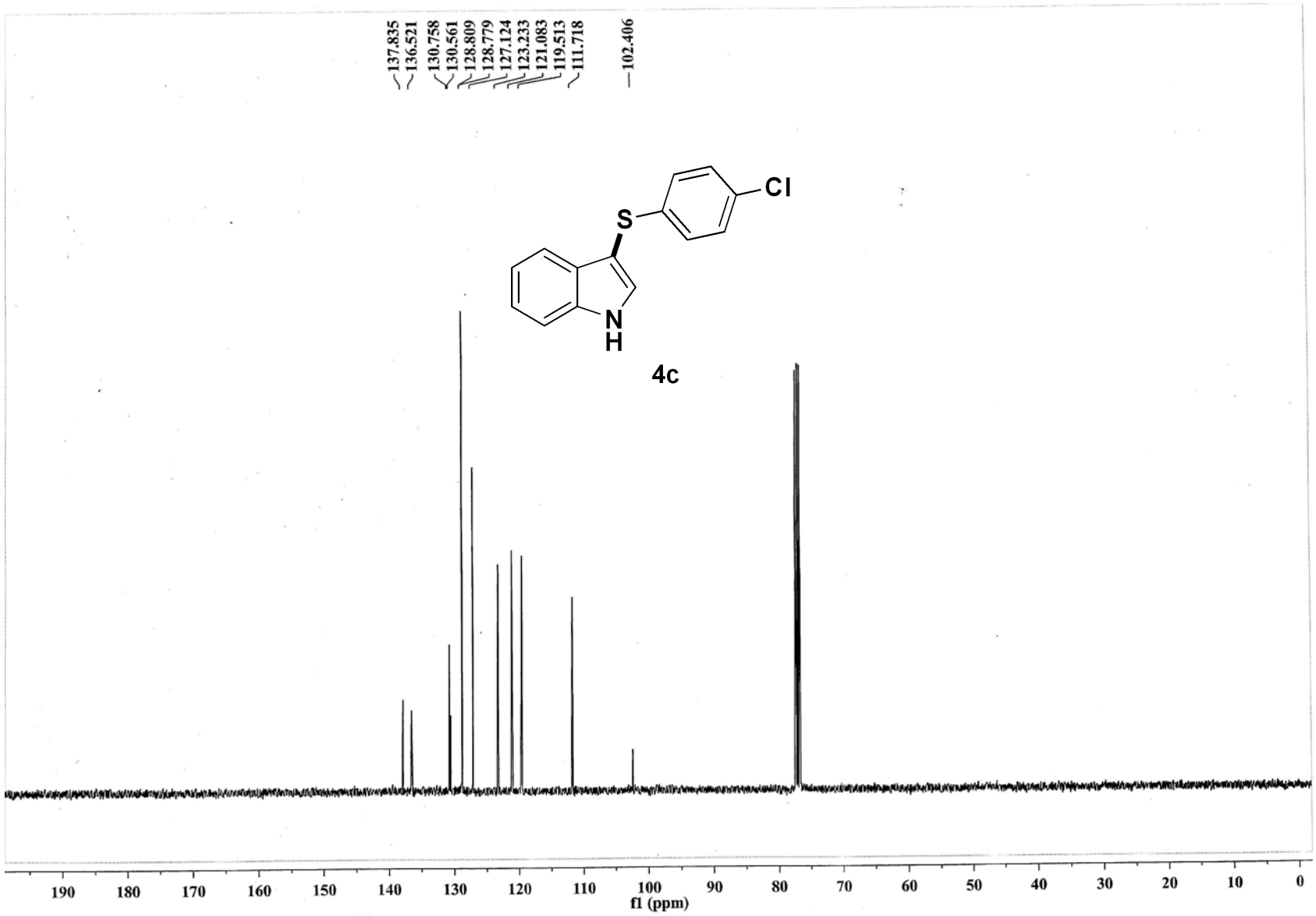
7.673
7.653
7.501
7.495
7.478
7.460
7.458
7.456
7.332
7.329
7.314
7.311
7.308
7.294
7.291
7.230
7.227
7.223
7.221
7.217
7.212
7.210
7.207
7.202
7.192
7.190
7.184
7.180
7.164
7.160
7.154
7.147
7.143
7.139
7.118
7.114
7.110
7.102
7.097
7.091
7.083
7.079
7.075
S
NH
4a
0.87
1.00
1.99
0.98
4.98
0.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

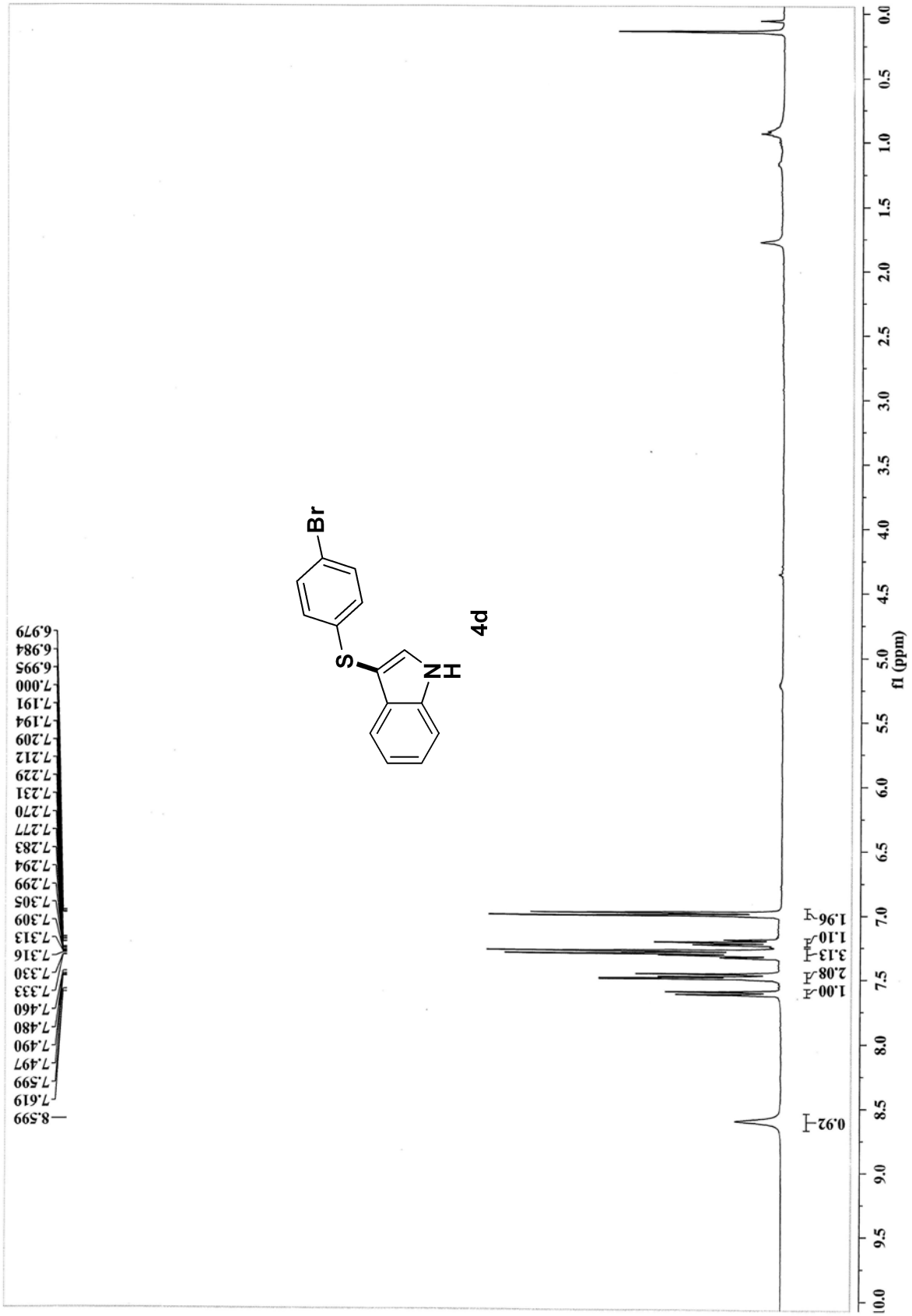

102.715
111.652
119.657
120.915
123.055
124.802
125.857
128.733
129.100
130.769
136.513
139.263
S
N
H
4a
f1 (ppm)

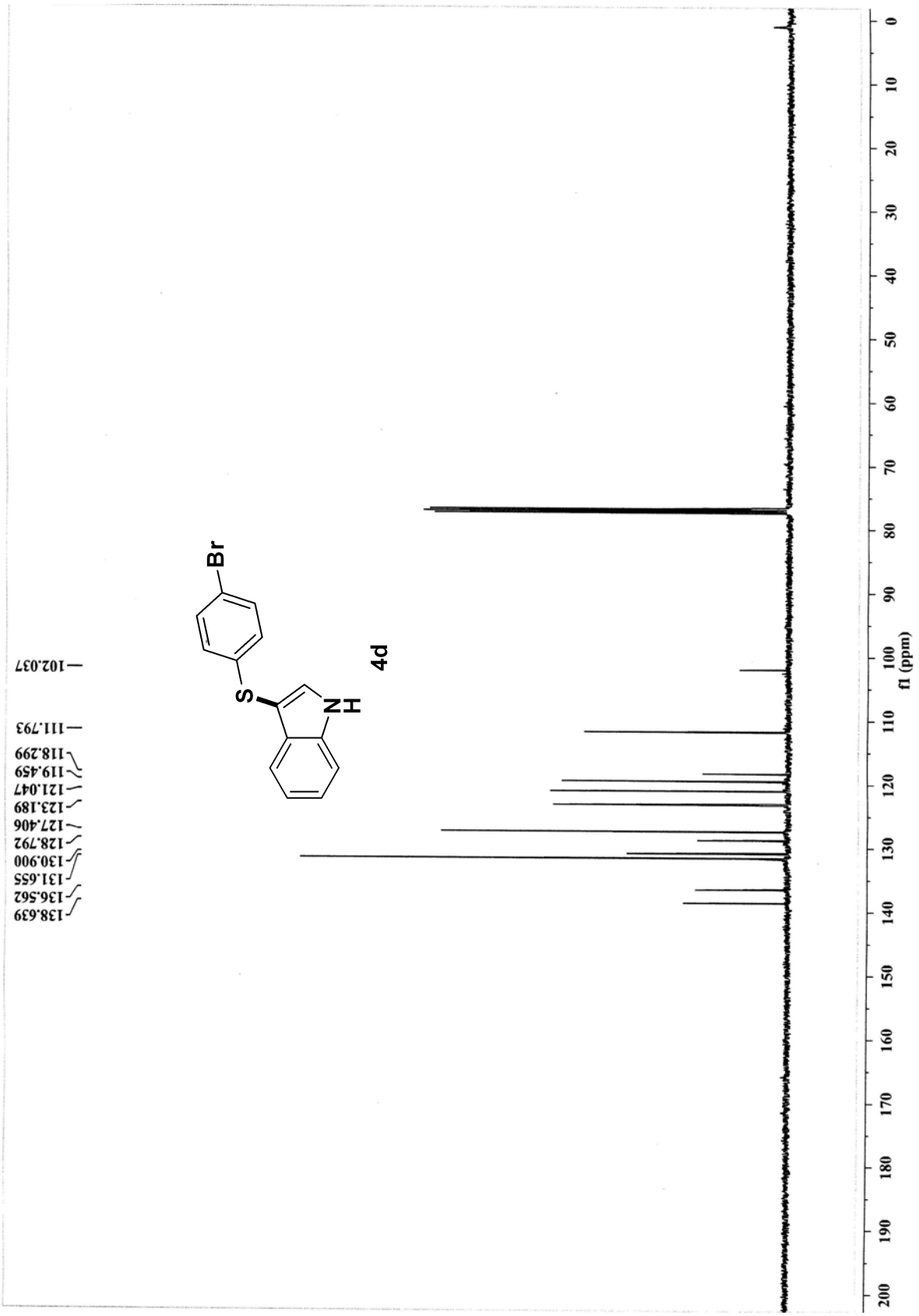
8.232
7.757
7.738
7.736
7.453
7.433
7.426
7.380
7.377
7.363
7.360
7.343
7.339
7.291
7.288
7.274
7.271
7.268
7.253
7.251
7.169
7.164
7.153
7.148
7.090
7.070
2.352
3.03
1.00
1.08
2.05
1.11
1.17
2.09
1.95
S
NH
4b
f1 (ppm)

20.980
103.235
111.777
119.697
120.937
123.067
126.363
129.150
129.671
130.685
134.843
135.562
136.528
4b
S
NH
f1 (ppm)


Cl
S
N
H
4c
8.449
7.627
7.607
7.509
7.502
7.484
7.466
7.464
7.462
7.341
7.338
7.323
7.320
7.317
7.303
7.300
7.238
7.235
7.220
7.217
7.215
7.200
7.197
7.172
7.165
7.160
7.149
7.143
7.137
7.073
7.066
7.061
7.049
7.045
7.038
0.92
1.00
2.07
1.04
1.04
2.01
2.03
f1 (ppm)


137.835
136.521
130.758
130.561
128.809
128.779
127.124
123.233
121.083
119.513
111.718
102.406
Cl
S
N
H
4c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Br
S
N
H
4d
8.599
7.619
7.599
7.497
7.490
7.480
7.460
7.333
7.330
7.316
7.313
7.309
7.305
7.299
7.294
7.283
7.277
7.270
7.231
7.229
7.212
7.209
7.194
7.191
7.000
6.995
6.984
6.979
0.92
1.00
2.08
3.13
1.10
1.96
f1 (ppm)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119.459
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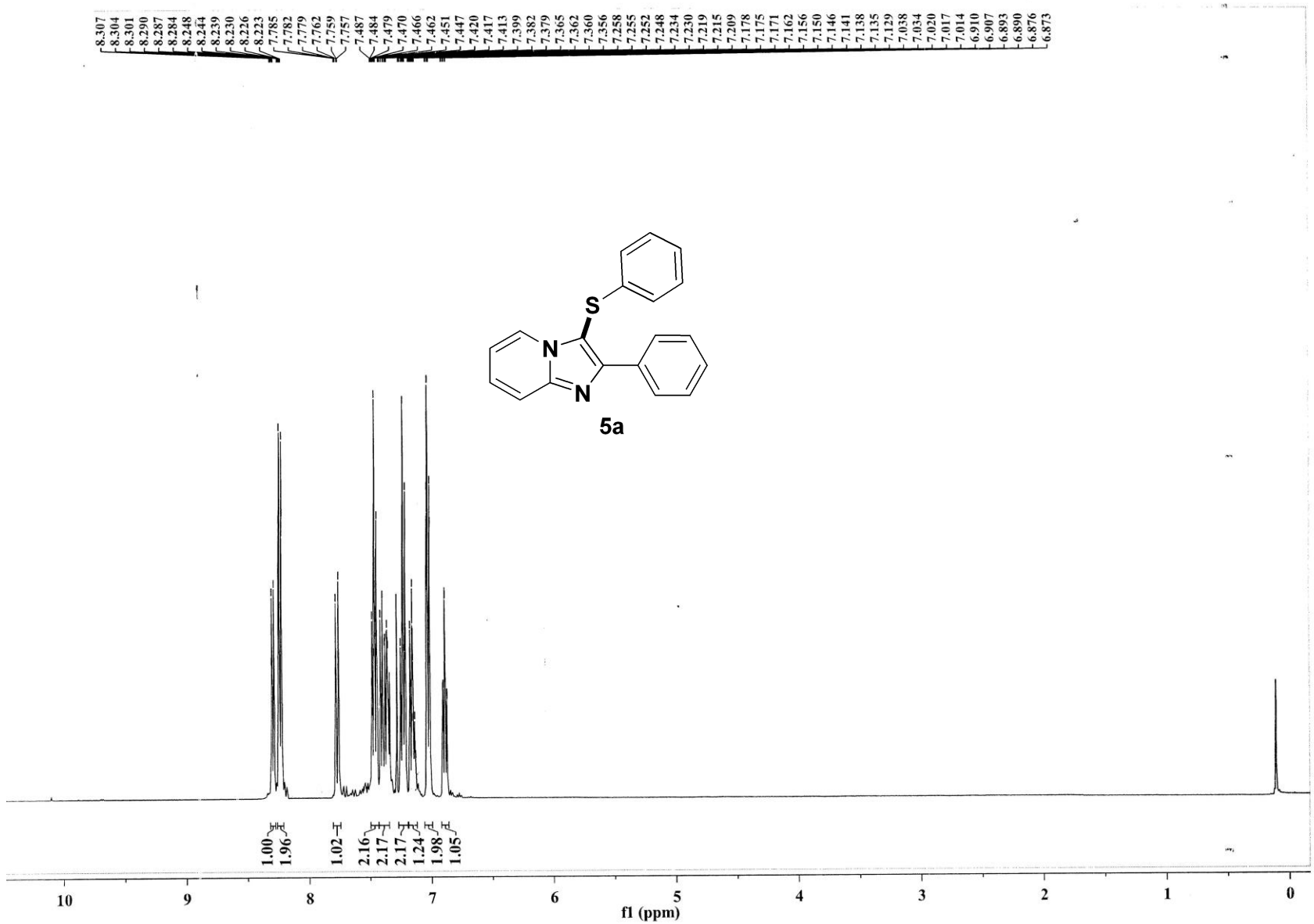
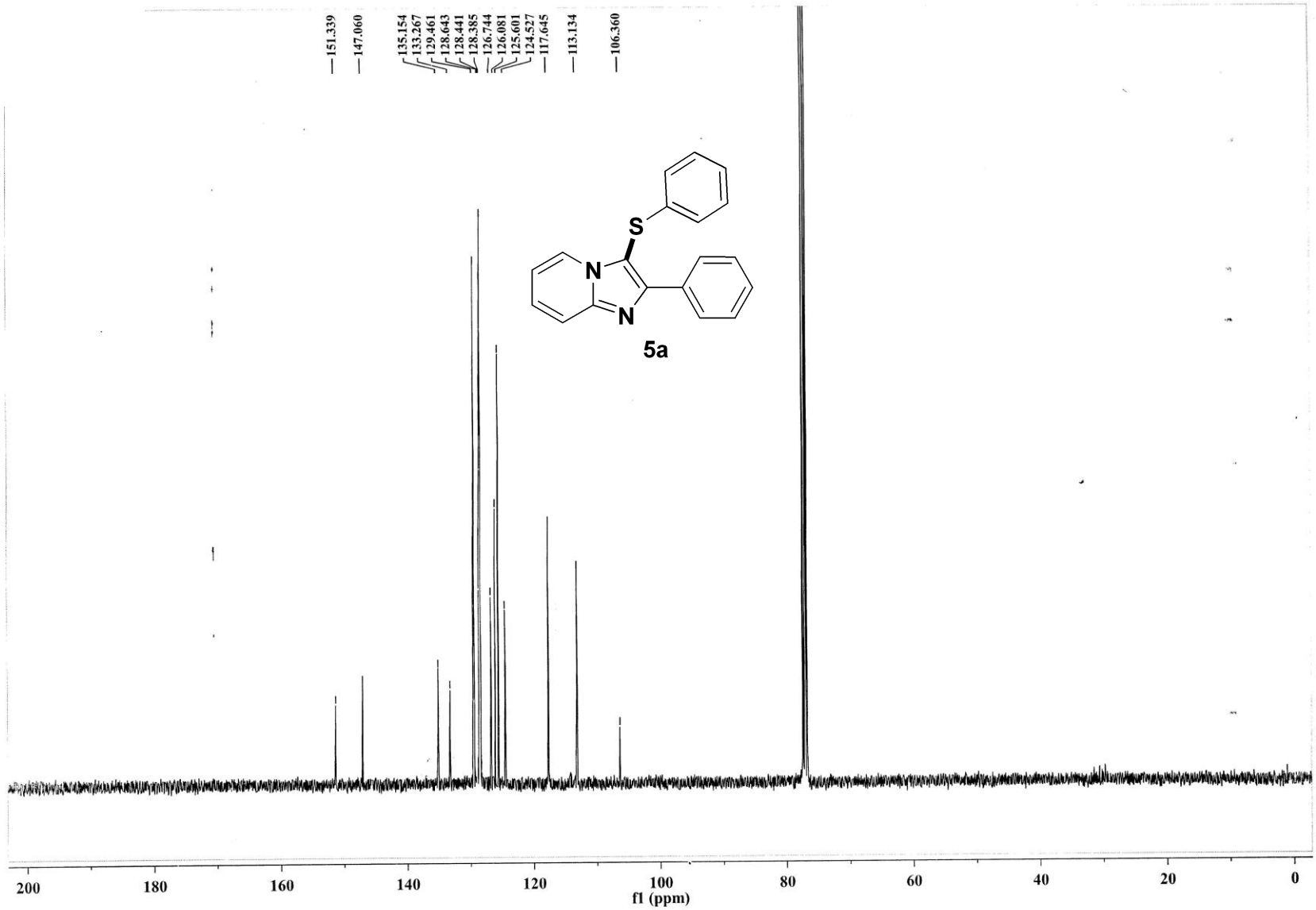
123.189
127.406
128.792
130.900
131.655
136.562
138.639
Br
S
NH
4d
f1 (ppm)


8.307
8.304
8.301
8.290
8.287
8.284
8.248
8.244
8.239
8.230
8.226
8.223
7.785
7.782
7.779
7.762
7.759
7.757
7.487
7.484
7.479
7.470
7.466
7.462
7.451
7.447
7.420
7.417
7.413
7.399
7.382
7.379
7.365
7.362
7.360
7.356
7.258
7.255
7.252
7.248
7.234
7.230
7.219
7.215
7.209
7.178
7.175
7.171
7.162
7.156
7.150
7.146
7.141
7.138
7.135
7.129
7.038
7.034
7.020
7.017
7.014
6.910
6.907
6.893
6.890
6.876
6.873
S
N
N
5a
1.00
1.96
1.02
2.16
2.17
2.17
1.24
1.98
1.05
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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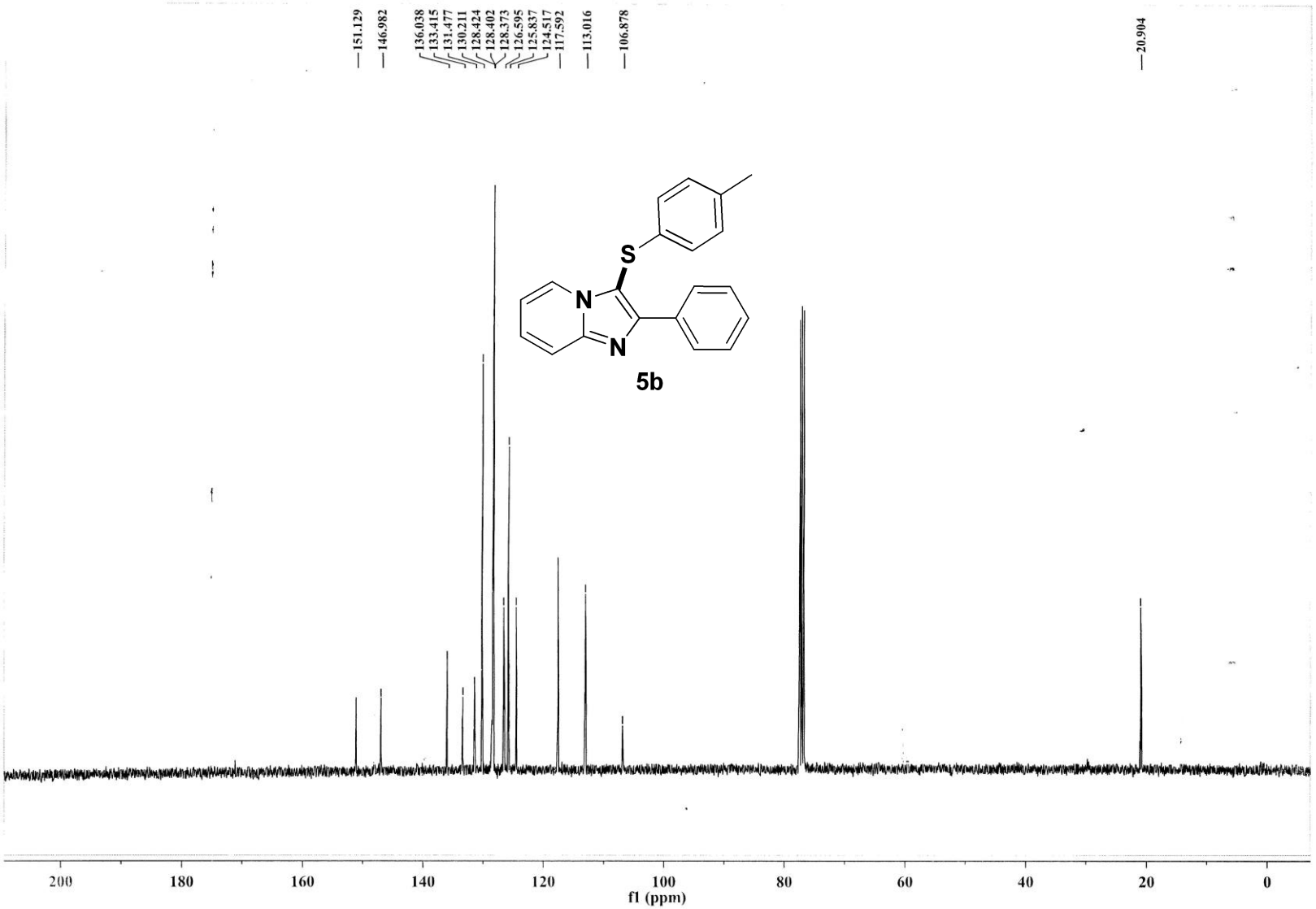
128.441
128.385
126.744
126.081
125.601
124.527
117.645
113.134
106.360
S
N
N
5a
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

2.255
3.06
3.04
1.00
2.08
1.05
1.09
2.06
2.03
1.03
8.298
8.294
8.280
8.276
8.274
8.259
7.753
7.750
7.730
7.727
7.487
7.484
7.466
7.462
7.451
7.447
7.409
7.405
7.402
7.393
7.387
7.381
7.369
7.315
7.312
7.298
7.294
7.289
7.276
7.272
7.032
7.012
6.945
6.940
6.924
6.833
6.830
6.816
6.813
6.799
6.796
S
N
N
5b
f1 (ppm)


151.129
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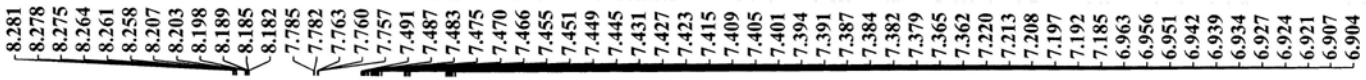
136.038
133.415
131.477
130.211
128.424
128.402
128.373
126.595
125.837
124.517
117.592
113.016
106.878
20.904
S
N
N
5b
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


8.281
8.278
8.275
8.264
8.261
8.258
8.207
8.203
8.198
8.189
8.185
8.182
7.785
7.782
7.763
7.760
7.757
7.491
7.487
7.483
7.475
7.470
7.466
7.455
7.451
7.449
7.445
7.431
7.427
7.423
7.415
7.409
7.405
7.401
7.394
7.391
7.387
7.384
7.382
7.379
7.365
7.362
7.220
7.213
7.208
7.197
7.192
7.185
6.963
6.956
6.951
6.942
6.939
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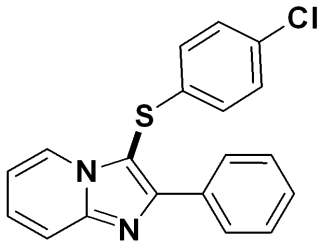
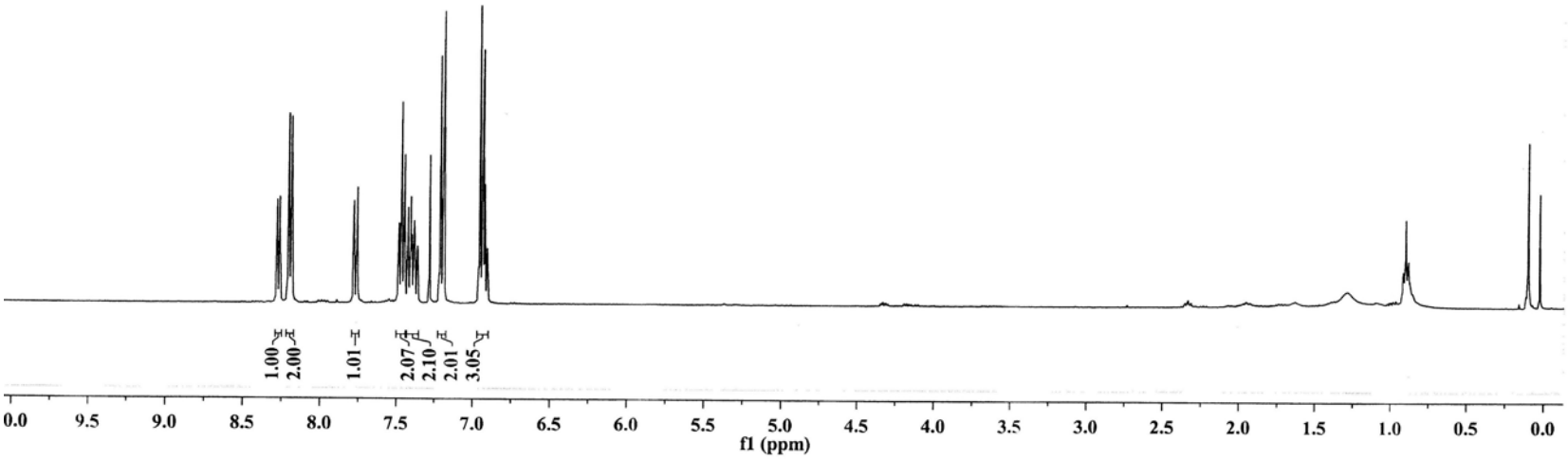
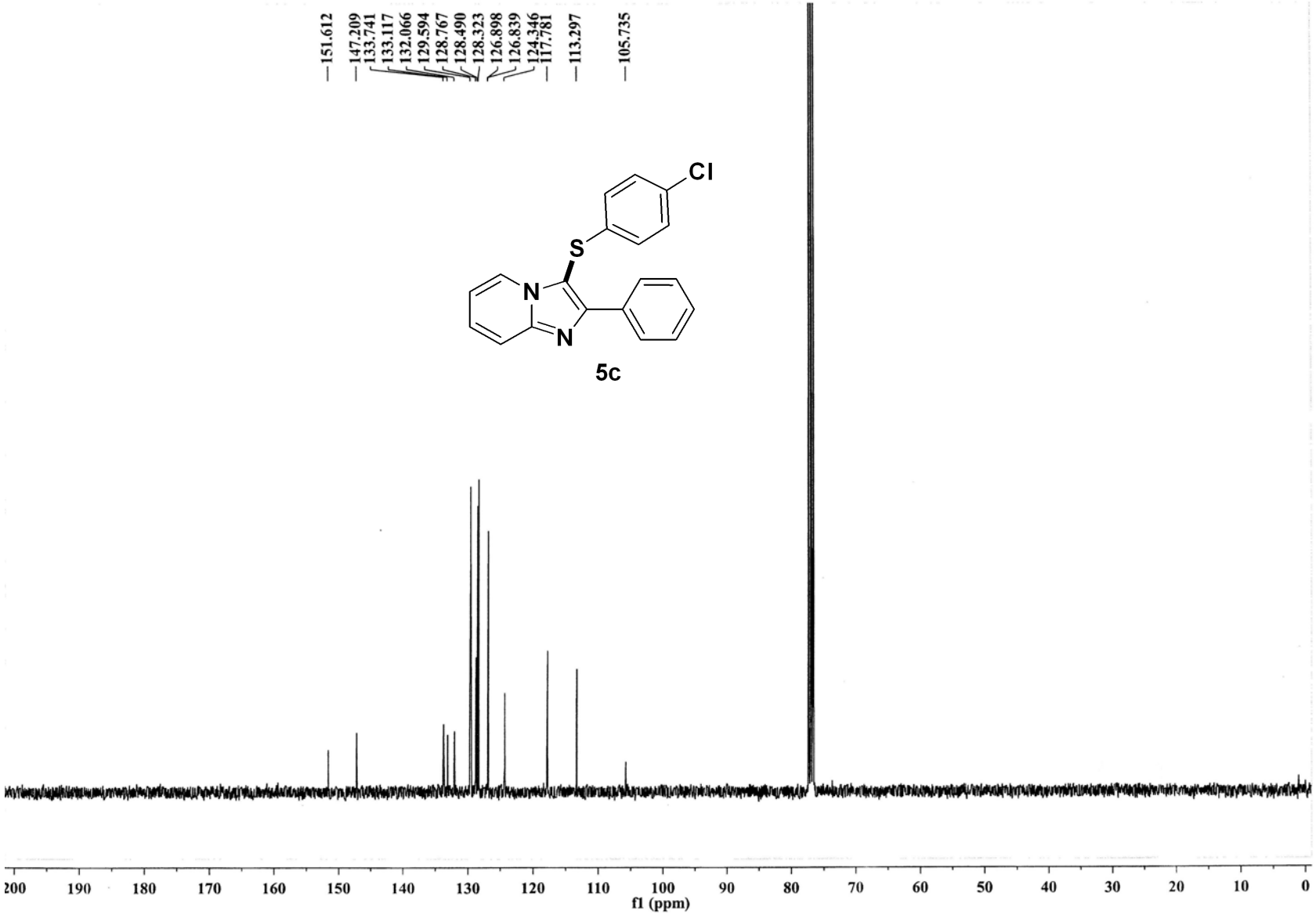
6.927
6.924
6.921
6.907
6.904


Cl
S
N
N

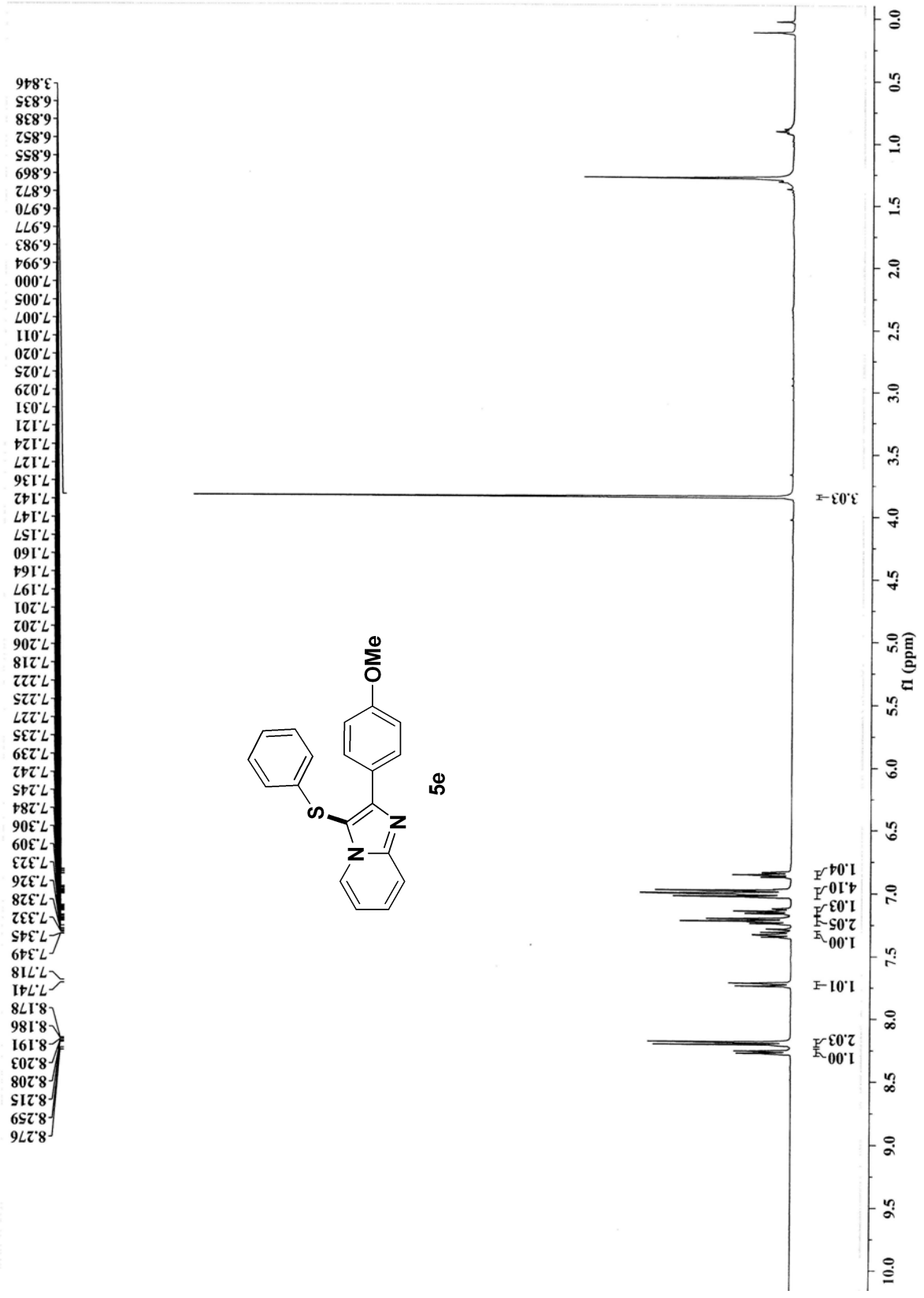
5c

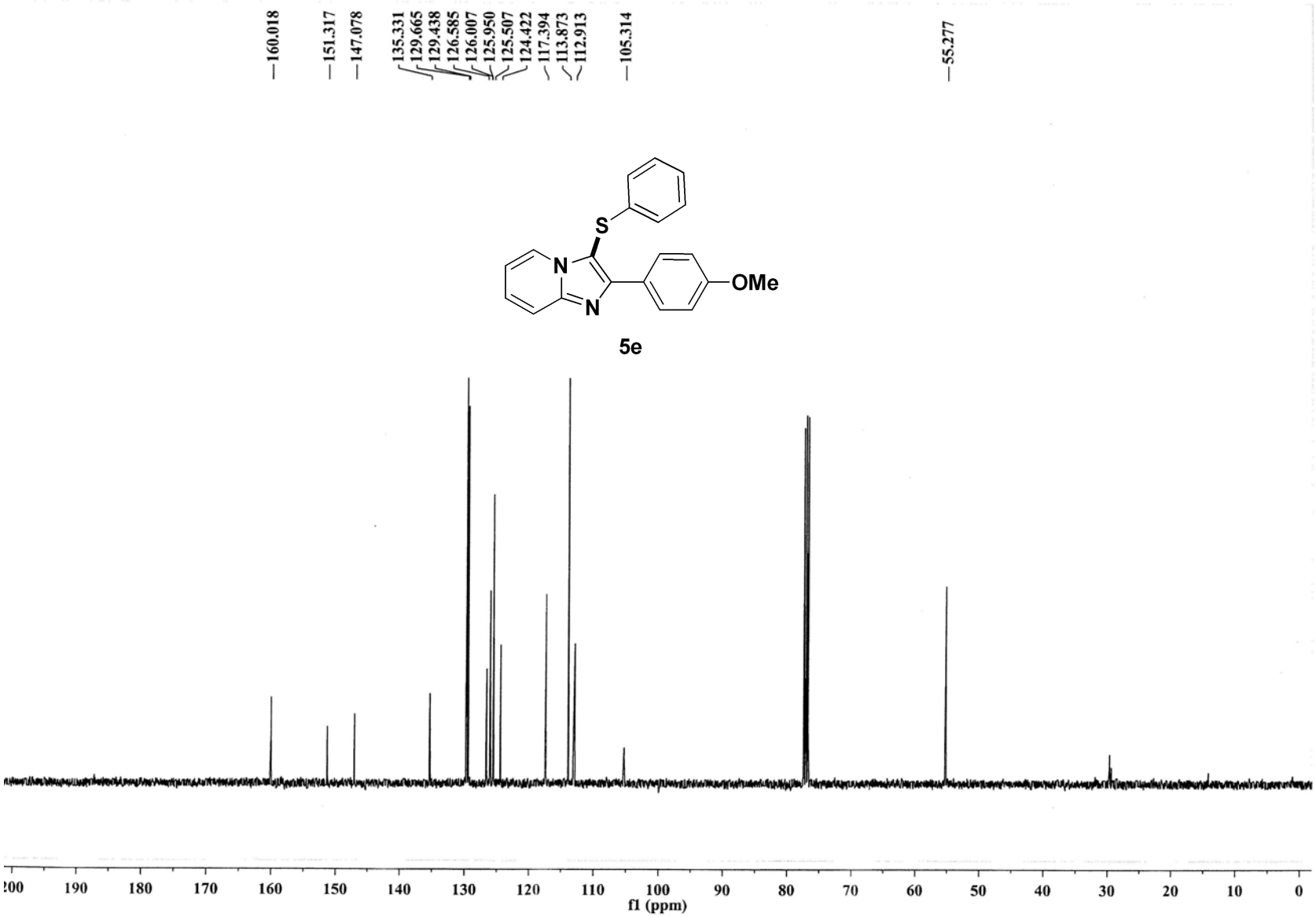

1.00
2.00
1.01
2.07
2.10
2.01
3.05
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


151.612
147.209
133.741
133.117
132.066
129.594
128.767
128.490
128.323
126.898
126.839
124.346
117.781
113.297
105.735
Cl
S
N
N
5c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

13.134
8.655
8.650
8.635
8.631
8.400
8.383
7.714
7.692
7.437
7.434
7.420
7.417
7.415
7.398
7.310
7.307
7.303
7.290
7.286
7.284
7.264
7.246
7.242
7.231
7.227
7.225
7.193
7.190
7.175
7.117
7.114
7.097
7.094
7.087
7.085
7.081
7.067
7.064
7.061
6.983
6.980
6.966
6.963
6.915
6.912
6.897
6.895
6.892
HO
S
N
N
5d
0.90
1.02
1.00
1.01
1.05
1.19
2.08
1.09
3.11
1.07
1.07
f1 (ppm)

158.438
149.452
144.662
134.406
130.631
129.558
127.754
127.477
126.390
125.851
124.238
118.879
117.725
116.701
116.132
113.809
105.466
S
N
N
HO
5d
f1 (ppm)


OMe
S
N
N
5e
f1 (ppm)


160.018
151.317
147.078
135.331
129.665
129.438
126.585
126.007
125.950
125.507
124.422
117.394
113.873
112.913
105.314
55.277
S
N
N
OMe
5e
f1 (ppm)

8.453
8.236
8.219
7.646
7.644
7.623
7.621
7.484
7.480
7.463
7.458
7.448
7.444
7.426
7.422
7.419
7.414
7.410
7.404
7.395
7.390
7.077
7.057
6.952
6.931
2.297
3.09
1.00
2.06
2.00
2.05
2.06
2.10
1.04
Br
S
N
N
5f
f1 (ppm)

20.907
107.959
118.254
124.691
125.973
128.316
128.486
128.827
130.098
130.350
130.903
132.912
136.397
145.383
151.668
S
N
N
Br
5f
f1 (ppm)

8.416
8.186
8.170
7.485
7.468
7.464
7.461
7.449
7.441
7.437
7.433
7.426
7.419
7.386
7.379
7.373
7.370
7.365
6.900
6.879
Br
S
N
N
Br
5g
1.00
2.00
4.08
2.72
2.02
f1 (ppm)

151.733
147.690
133.645
130.844
129.685
128.793
128.301
128.260
126.699
126.540
125.618
117.494
113.066
Br
S
N
N
Br
5g
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
f1 (ppm)

Cl
HO
N
N
5h
f1 (ppm)
0.87
1.00
1.04
1.07
1.17
4.08
2.09
2.07
13.147
8.663
8.656
8.648
8.399
8.382
7.703
7.700
7.697
7.681
7.678
7.675
7.448
7.444
7.430
7.427
7.422
7.408
7.405
7.267
7.262
7.249
7.245
7.237
7.230
7.224
7.215
7.208
7.203
7.199
7.185
7.177
7.078
7.074
7.069
7.060
7.056
7.054
7.022
7.000
6.996
6.982
6.979
6.968
6.965
6.963

157.119
147.792
144.497
133.885
130.293
129.623
127.709
126.266
124.250
119.039
118.273
117.143
116.766
116.667
114.037
113.886
106.444
Cl
HO
N
N
5h
f1 (ppm)