Supporting Information

Cu-catalyzed sulfenylation of imidazol[1,2-α]pyridine via C-H functionalization using a combination of $Na_2S_2O_3$ and halides

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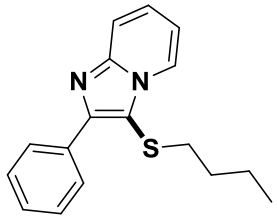
General experimental procedures

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.

General procedure for the synthesis of compounds 2a-x.

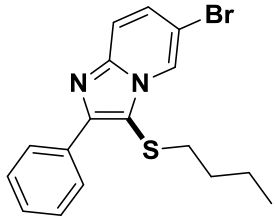
2-phenylimidazo[1,2-α]pyridine (0.5 mmol, 1.0 equiv.), $Na_2S_2O_3$(1.25 equiv.) and Butyl chloride (2.0 equiv.) were added to a dried flask with DMF (0.5 mL) , followed by the addition of CuI (0.2 equiv.). The mixture was stirred at 120 ^{o}C. After 12 h, the reaction was cooled down to room temperature, diluted with ethyl acetate, washed with brine, dried over anhydrous Na_2SO_4 and concentrated under vacuum. The residue was purified by flash chromatography (Petroleum ether: EtOAc =30:1) on silica gel to give the desired product **2a** as a colorless oil in an 75% yield. The same procedure was applied to the production of other compounds **2a-x**.

3-(Butylthio)-2-phenylimidazo[1,2-α]pyridine (2a)



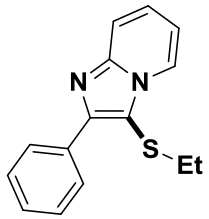
FTIR: 2975, 2913, 2365, 2341, 1345, 1051, 669 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.53 (d, *J*=6.9 Hz, 1H), 8.35 (dd, *J*=8.4, 1.3 Hz, 2H), 7.67 (dd, *J*=9.0, 1.2 Hz, 1H), 7.49 (t, *J*=7.6 Hz, 2H), 7.41-7.30 (m, 1H), 7.28 (ddd, *J*=9.0, 6.8, 1.3 Hz, 1H), 6.91 (td, *J*=6.8, 1.2 Hz, 1H), 2.66 (t, *J*=7.2 Hz, 2H), 1.45-1.39 (m, 2H), 1.32 (dt, *J*=8.6, 7.1 Hz, 2H), 0.77 (t, *J*=7.3 Hz, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 149.5, 146.4, 133.9, 128.4, 128.3, 128.1, 125.9, 124.4, 117.5, 112.6, 110.4, 35.5, 31.5, 21.7, 13.5. **HRMS (**ESI-TOF) m/z calculated for $C_{17}H_{19}N_2S^+$ 283.1263 $(M+H)^+$, found 283.1265.

6-Bromo-3-(butylthio)-2-phenylimidazo[1,2-α]pyridine (2b)



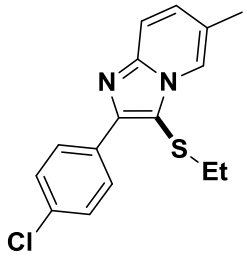
FTIR: 3004, 2928, 2345, 1310, 1080, 679 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.32 (dd, *J*=2.0, 0.8 Hz, 1H), 8.31-8.30 (m, 2H), 7.58 (dd, *J*=9.4, 0.8 Hz, 1H), 7.56-7.48 (m, 2H), 7.47–7.40 (m, 1H), 7.35 (dd, *J*=9.4, 2.0 Hz, 1H), 2.67 (t, *J*=7.1 Hz, 2H), 1.47–1.41 (m, 2H), 1.39-1.30 (m, 2H), 0.79 (t, *J*=7.2 Hz, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 150.0, 144.7, 133.4, 129.3, 128.5, 128.4, 128.3, 124.6, 118.2, 111.2, 111.15, 107.6, 35.5, 31.5, 21.7, 13.5. **HRMS (**ESI-TOF) m/z calculated for $C_{17}H_{18}BrN_2S^+$ 361.0369 $(M+H)^+$, found 361.0346.

3-(Ethylthio)-2-phenylimidazo[1,2-α]pyridine (2c)



FTIR: 3064, 2922, 2364, 1345, 7563, 694 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.36 (dt, J=6.8, 1.2 Hz, 1H), 7.71-7.69 (m, 2H), 7.50 (dt, J=9.0, 1.2 Hz, 1H), 7.41-7.38 (m, 2H), 7.33-7.30 (m, 1H), 7.00-6.93 (m, 1H), 6.94 (td, J=6.8, 1.2 Hz, 1H), 2.71 (q, J=7.4 Hz, 2H), 1.14 (t, J=7.4 Hz, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 149.4, 146.3, 133.8, 128.4, 128.3, 128.3, 126.0, 124.4, 117.5, 112.7, 110.1, 29.9, 14.8. **HRMS** (ESI-TOF) m/z calculated for $C_{15}H_{15}N_2S^+$ 255.0950 $(M+H)^+$, found 255.0951.

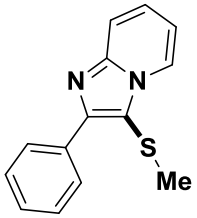
2-(4-Chlorophenyl)-3-(ethylthio)-6-methylimidazo[1,2-α]pyridine (2d)



FTIR: 3060, 2919, 2361, 1388, 917, 723,cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.32 – 8.30 (m, 3H), 7.59 (d, *J*=9.2 Hz, 1H), 7.45-7.43 (m, 2H), 7.17 (dd, *J*=9.1, 1.8 Hz, 1H), 2.69 (q, *J*=7.4 Hz, 2H), 2.42 (d, J=1.1 Hz, 3H), 1.12 (t, *J*=7.4 Hz, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 148.1, 145.4, 134.0, 132.5, 129.5, 129.4, 128.5, 122.7, 122.1, 116.9, 29.8, 18.5, 14.7. **HRMS** (ESI-TOF) m/z calculated for $C_{27}H_{22}ClN_2S^+$ 441.1187

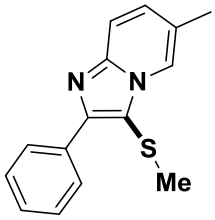
$(M+H)^+$, found 441.1189.

3-(Methylthio)-2-phenylimidazo[1,2-α]pyridine (2e)



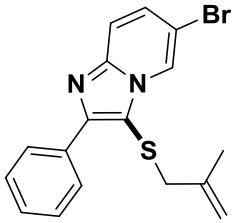
FTIR: 3066, 2920, 2364, 1345, 756, 695 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.51 (d, *J*=6.8 Hz, 1H), 8.32-8.30 (m, 2H), 7.70 (dt, *J*=9.0, 1.1 Hz, 1H), 7.53-7.49 (m, 2H), 7.43-7.40 (m, 1H), 7.34-7.28 (m, 1H), 6.96 (td, *J*=6.8, 1.2 Hz, 1H), 2.28 (s, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 148.7, 146.3, 133.7, 128.4, 128.30, 128.3, 126.0, 124.3, 117.6, 112.8, 111.5, 18.2. **HRMS** (ESI-TOF) m/z calculated for $C_{14}H_{13}N_2S^+$ 241.0794 $(M+H)^+$, found 241.07880.

6-Methyl-3-(methylthio)-2-phenylimidazo[1,2-α]pyridine (2f)



FTIR: 3057, 2920, 2360, 1338, 816, 776 699 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.31-8.29 (m, 3H), 7.60 (dd, *J*=9.1, 0.9 Hz, 1H), 7.52-7.50 (m, 2H), 7.48-7.38 (m, 1H), 7.17 (dd, *J*=9.1, 1.7 Hz, 1H), 2.43 (s, 3H), 2.28 (s, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 148.5, 145.3, 133.9, 129.1, 128.4, 128.2, 122.6, 122.0, 116.9, 111.0, 18.5, 18.2. **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_{15}N_2S^+$ 255.0950 $(M+H)^+$, found 255.0950.

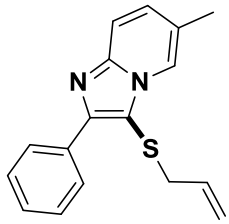
6-Bromo-3-((2-methylallyl)thio)-2-phenylimidazo[1,2-α]pyridine (2g)



FTIR: 2922, 2851, 2362, 2340, 699 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.64 (d, *J*=1.8 Hz, 1H), 8.27-8.25 (m, 2H), 7.56 (dd, *J*=9.0, 2.6 Hz, 1H), 7.49 (t, *J*=7.4 Hz, 2H), 7.45-7.40 (m, 1H), 7.36 (dd, *J*=9.4, 1.9 Hz, 1H), 4.54 (t, *J*=1.5 Hz, 1H), 4.37 (s, 1H), 3.24 (s, 2H), 1.74 (s, 3H), 1.28(s, 2). **^{13}C-NMR** ($CDCl_3$, 100 MHz) δ 150.7, 144.8, 133.3, 129.4, 128.5, 128.4, 128.4, 124.8, 118.2, 115.4, 110.7, 107.5, 43.1, 30.2, 22.7, 20.8. **HRMS (**ESI-TOF) m/z calculated for $C_{17}H_{16}BrN_2S^+$ 359.0212 $(M+H)^+$,

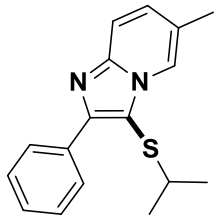
found 359.0209.

3-(Allylthio)-6-methyl-2-phenylimidazo[1,2-α]pyridine (3h)



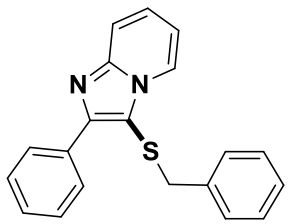
FTIR: 3061, 2919, 2361, 1345, 915, 753 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.33-8.31 (m, 3H), 7.61 (d, *J*=9.0 Hz, 1H), 7.49 (t, *J*=7.6 Hz, 2H), 7.44-7.35 (m, 1H), 7.17 (dd, *J*=9.0, 1.8 Hz, 1H), 5.74 (ddt, *J*=17.3, 10.0, 7.4 Hz, 1H), 4.89-4.73 (m, 2H), 3.31 (d, *J*=7.4 Hz, 2H), 2.42 (d, *J*=1.1 Hz, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 149.4, 145.2, 133.6, 132.8, 129.5, 128.8, 128.3, 128.3, 122.6, 122.3, 118.5, 116.7, 109.2, 38.9, 18.5. **HRMS** (ESI-TOF) m/z calculated for $C_{17}H_{17}N_2S^+$ 281.1107 $(M+H)^+$, found 281.1118.

3-(Isopropylthio)-6-methyl-2-phenylimidazo[1,2-α]pyridine (2i)



FTIR: 3021, 2989, 2366, 2355, 1606, 1025, 831cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.35-8.33 (m, 3H), 7.58 (dd, *J*=9.0, 0.9 Hz, 1H), 7.49-7.45 (m, 2H), 7.39-7.35 (m, 1H), 7.14 (dd, *J*=9.1, 1.8 Hz, 1H), 3.18 (hept, *J*=6.7 Hz, 1H), 2.40 (d, *J*=1.1 Hz, 3H), 1.16 (d, *J*=6.7 Hz, 6H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 149.7, 145.4, 134.1, 129.1, 128.3, 128.2, 128.0, 122.3, 116.8, 109.8, 40.5, 23.1, 18.5. **HRMS (**ESI-TOF) m/z calculated for $C_{17}H_{18}N_2NaS^+$ 305.1083 $(M+H)^+$, found 305.1080.

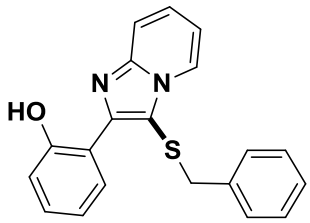
3-(Benzylthio)-2-phenylimidazo[1,2-α]pyridine (2j)



FTIR: 3024, 2925, 2362, 2341, 1453, 1143, 737cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.28-8.26 (m, 2H), 8.09 (d, *J*=6.9 Hz, 1H), 7.62 (d, *J*=9.0 Hz, 1H), 7.51-7.44 (m, 2H), 7.43-7.37 (m, 1H), 7.21 (ddd, *J*=9.0, 6.7, 1.3 Hz, 1H), 7.14-7.04 (m, 3H), 6.97-6.89 (m, 2H), 6.69 (td, *J*=6.8, 1.2 Hz, 1H), 3.83 (s, 2H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ

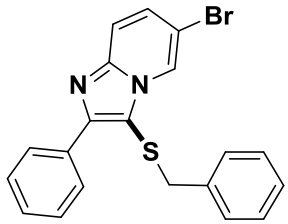
150.1, 146.4, 137.1, 133.7, 129.4, 128.7, 128.5, 128.3, 128.3, 127.3, 126.0, 124.2, 117.2, 112.3, 109.4, 40.6. **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{17}N_2S^+$ 317.1107 $(M+H)^+$, found 317.1113.

2-(3-(Benzylthio)imidazo[1,2-α]pyridin-2-yl)phenol (2k)



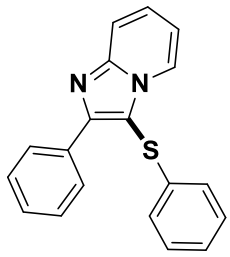
FTIR: 3329, 2974, 2926, 2362, 2341, 1509, 1051, 692 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 13.22 (s, 1H), 8.86 (dd, *J*=7.9, 1.7 Hz, 1H), 8.09 (dd, *J*=6.8, 1.2 Hz, 1H), 7.52 (dt, *J*=8.9, 1.1 Hz, 1H), 7.33 (ddd, *J*=8.6, 7.2, 1.6 Hz, 1H), 7.23 (ddd, *J*=8.9, 6.8, 1.3 Hz, 1H), 7.15-7.04 (m, 4H), 7.02-6.92 (m, 3H), 6.70 (td, *J*=6.8, 1.2 Hz, 1H), 3.88 (s, 2H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 158.4, 148.1, 143.9, 137.0, 130.3, 128.7, 128.5, 127.5, 127.5, 126.8, 123.9, 118.7, 117.7, 116.6, 116.2 , 112.9, 108.4, 40.5. **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{17}N_2OS^+$ 333.1056 $(M+H)^+$, found 333.1064.

3-(Benzylthio)-6-bromo-2-phenylimidazo[1,2-α]pyridine (2l)



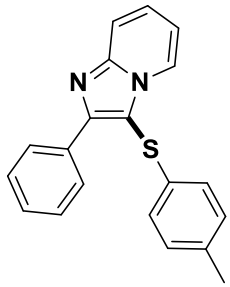
FTIR: 3053, 2966, 2364, 2355, 1603, 1029, 801cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.29-8.27 (m, 2H), 8.04 (d, *J*=2.0 Hz, 1H), 7.55-7.38 (m, 4H), 7.22 (dd, *J*=9.4, 1.9 Hz, 1H), 7.17-7.04 (m, 3H), 6.96-6.88 (m, 2H), 3.83 (s, 2H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 150.7, 144.7, 137.1, 133.3, 129.4, 128.6, 128.6, 128.5, 128.4, 128.2, 127.7, 124.6, 117.7, 110.0, 107.1, 41.0. **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{16}BrN_2S^+$ 395.0212 $(M+H)^+$, found 395.0210.

2-Phenyl-3-(phenylthio)imidazo[1,2-α]pyridine (2m)



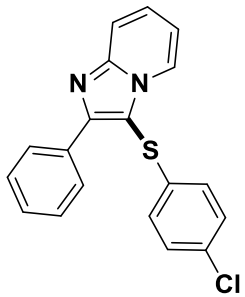
FTIR: 2979, 2921, 2338, 1591, 1463, 1047, 684 cm^{-1}**; ^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.30 (dt, *J*=6.9, 1.2 Hz, 1H), 8.26-8.21 (m, 2H), 7.77 (dt, *J*=9.0, 1.1 Hz, 1H), 7.50-7.43 (m, 2H), 7.43-7.35 (m, 2H), 7.27-7.19 (m, 2H), 7.15 (ddt, *J*=8.5, 6.7, 2.5 Hz, 1H), 7.06-6.99 (m, 2H), 6.89 (td, *J*=6.8, 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. **HRMS (**ESI-TOF) m/z calculated for $C_{19}H_{15}N_2S^+$ 303.0950 $(M+H)^+$, found 303.0941.

2-Phenyl-3-(p-tolylthio)imidazo[1,2-α]pyridine (2n)



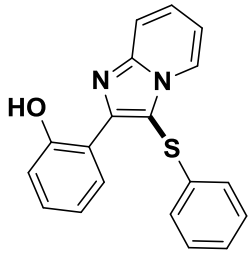
FTIR: 2975, 2927, 1343, 1090, 1463, 1050, 882 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.29-8.26 (m, 3H), 7.74 (d, *J*=9.2 Hz, 1H), 7.48-7.45 (m, 2H), 7.39 (t, *J*=7.2 Hz, 4H), 7.31-7.27 (m, 1H), 7.02 (d, *J*=8.0 Hz, 2H), 6.93 (d, *J*=8.4 Hz, 2H), 6.82 (t, *J*=6.8 Hz, 1H), 2.26 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 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, 20.90.. **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{17}N_2S^+$ 317.1107 $(M+H)^+$, found 317.1113.

3-((4-Chlorophenyl)thio)-2-phenylimidazo[1,2-α]pyridine (2o)



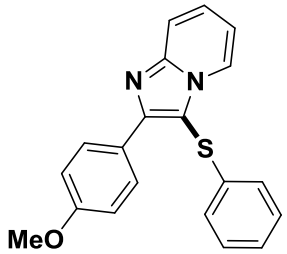
FTIR: 3038, 2924, 2857, 1470, 1345, 1086, 692 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.28-8.24 (m, 1H), 8.21-8.18 (m, 1H), 7.77 (dd, *J*=8.8, 1.2 Hz, 1H), 7.49-7.45 (m, 2H), 7.43-7.36 (m, 2H), 7.22-7.19 (m, 2H), 6.96-6.90 (m, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 151.6, 147.2, 133.7, 133.1, 132.1, 129.6, 128.8, 128.5, 128.3, 126.9, 126.8, 124.3, 117.8, 113.3, 105.7. **HRMS (**ESI-TOF) m/z calculated for $C_{19}H_{14}ClN_2S^+$ 337.0561 $(M+H)^+$, found 337.0550.

2-(3-(Phenylthio)imidazo[1,2-α]pyridin-2-yl)phenol (2p)



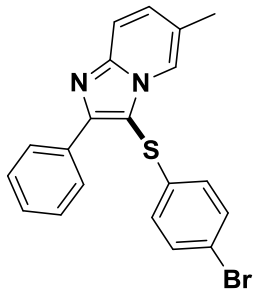
FTIR: 3328, 3053, 3018, 2358, 1457, 1349, 1098, 734 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 13.13 (s, 1H), 8.64 (dd, *J*=8.0, 2.0 Hz, 1H), 8.39 (d, *J*=6.8 Hz, 1H), 7.70 (d, *J*=8.8 Hz, 1H), 7.44-7.39 (m, 1H), 7.33-7.29 (m, 1H), 7.27-7.22 (m, 2H), 7.20-7.16 (m, 1H), 7.12-7.06 (m, 3H), 6.98-6.95 (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-α]pyridine (2q)



FTIR: 2920, 2847, 2357, 1469, 1249, 1035, 744 cm^{-1}; **^{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. **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{17}N_2OS^+$ 333.1056 $(M+H)^+$, found 333.1064.

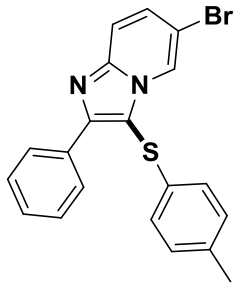
2-(4-bromophenyl)-6-methyl-3-(phenylthio)imidazo[1,2-α]pyridine (2r)



FTIR: 3028, 2929, 2857, 1470, 1345, 1086, 796 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.22-8.13 (m, 2H), 8.10-8.03 (m, 1H), 7.70 (d, *J*=9.1 Hz, 1H), 7.46 (dd, *J*=8.3, 6.4 Hz, 2H), 7.42-7.39 (m, 1H), 7.39-7.33 (m, 2H), 7.25 (dd, *J*=9.2, 1.7 Hz, 1H), 6.88 (d,

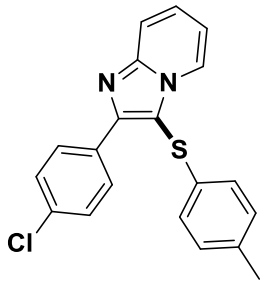
J=8.6 Hz, 2H), 2.36 (s, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 151.2, 146.1, 134.7, 133.0, 132.5, 130.3, 128.7, 128.5, 128.2, 127.0, 123.4, 122.1, 119.8, 117.0, 105.1, 18.4 . **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{16}BrN_2S^+$ 395.0212$(M+H)^+$, found 395.0210.

6-bromo-2-phenyl-3-(p-tolylthio)imidazo[1,2-α]pyridine (2s)



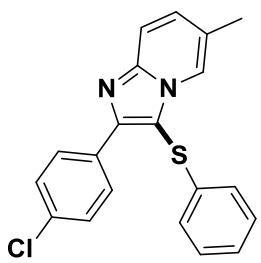
FTIR: 3026, 2928, 2869, 1478, 1349, 1080, 783 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.45 (s, 1H), 8.23 (d, *J*=7.0 Hz, 14H), 7.63 (dd, *J*=9.4, 0.8 Hz, 14H), 7.46 (dd, *J*=8.2, 6.4 Hz, 27H), 7.43-7.38 (m, 25H), 7.07 (d, *J*=8.0 Hz, 28H), 6.94 (d, *J*=8.2 Hz, 24H), 2.30 (s, 41H). **^{13}C-NMR** ($CDCl_3$, 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, 107.7, 20.91. **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{16}BrN_2S^+$ 395.0212 $(M+H)^+$, found 395.0210.

2-(4-chlorophenyl)-3-(p-tolylthio)imidazo[1,2-α]pyridine (2t)



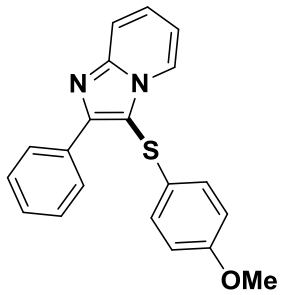
FTIR: 3025, 2928, 2863, 1479, 1345, 1083, 786 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.30 (dt, *J*=6.8, 1.2 Hz, 1H), 8.25-8.18 (m, 2H), 7.77-7.72 (m, 1H), 7.46-7.40 (m, 2H), 7.36 (ddd, *J*=9.0, 6.8, 1.3 Hz, 1H), 7.08-7.01 (m, 2H), 6.96-6.85 (m, 3H), 2.28 (s, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 149.8, 147.0, 136.3, 134.6, 131.8, 131.1, 130.3, 129.6, 128.7, 126.9, 125.9, 124.6, 117.6, 113.2, 107.2, 20.9. **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{16}ClN_2S^+$ 351.0717 $(M+H)^+$, found 351.0710.

2-(4-chlorophenyl)-6-methyl-3-(phenylthio)imidazo[1,2-α]pyridine (2u)



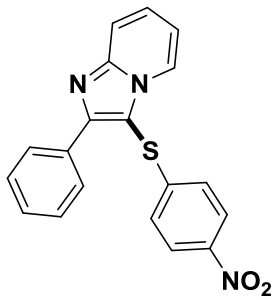
FTIR: 3025, 2927, 2863, 1478, 1346, 1085, 786 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.18-8.16 (m, 2H), 8.09 (t, *J*=1.4 Hz, 1H), 7.65 (d, *J*=9.1 Hz, 1H), 7.46-7.35 (m, 2H), 7.27-7.12 (m, 4H), 7.05-6.96 (m, 2H), 2.33 (s, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 149.9, 146.1, 135.2, 134.4, 132.0, 130.1, 129.5, 129.5, 128.6, 126.1, 125.5, 123.2, 122.2, 117.0, 106.0, 18.4. **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{16}ClN_2S^+$ 351.0717 $(M+H)^+$, found 351.0709.

3-((4-methoxyphenyl)thio)-2-phenylimidazo[1,2-α]pyridine (2v)



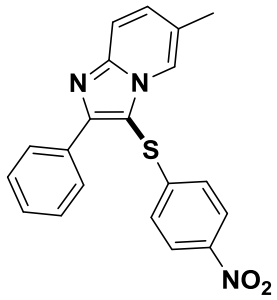
FTIR: 3027, 2928, 2857, 1460, 1345, 1086, 798 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz):δ 8.34 (d, *J*=6.8 Hz, 1H), 8.26 (dd, *J*=7.2, 1.8 Hz, 2H), 7.77 (d, *J*=9.0 Hz, 1H), 7.48 (t, *J*=7.4 Hz, 2H), 7.46-7.31 (m, 2H), 7.06–6.97 (m, 2H), 6.91 (td, *J*=6.8, 1.1 Hz, 1H), 6.83-6.75 (m, 2H), 3.75 (s, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 158.6, 150.6, 146.7, 133.2, 128.6, 128.5, 128.0, 126.7, 125.4, 124.5, 117.5, 115.2, 114.1, 113.1, 107.9, 55.3. **HRMS** (ESI-TOF) m/z calculated for $C_{20}H_{17}N_2OS^+$ 333.1056$(M+H)^+$, found 333.1042.

3-((4-nitrophenyl)thio)-2-phenylimidazo[1,2-α]pyridine (2w)



FTIR: 3025, 2920, 2837, 1460, 1333, 1080, 770 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.23 (dt, *J*=6.9, 1.2 Hz, 1H), 8.19-8.04 (m, 4H), 7.87-7.76 (m, 1H), 7.54-7.36 (m, 4H), 7.17-7.04 (m, 2H), 6.96 (td, *J*=6.8, 1.2 Hz, 1H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 152.3, 147.6, 146.1, 145.0, 132.7, 129.1, 128.6, 128.3, 127.4, 125.3, 124.6, 124.1, 118.0, 113.8, 103.6. **HRMS (**ESI-TOF) m/z calculated for $C_{19}H_{14}N_3O_2S^+$ 348.0801$(M+H)^+$, found 348.0800.

6-methyl-3-((4-nitrophenyl)thio)-2-phenylimidazo[1,2-α]pyridine (2x)



FTIR: 3023, 2921, 2835, 1467, 1335, 1079, 778 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.14-8.08 (m, 3H), 8.02 (d, *J*=1.8 Hz, 1H), 7.79-7.73 (m, 1H), 7.50-7.36 (m, 3H), 7.30 (d, *J*=12.7 Hz, 2H), 7.17-7.07 (m, 2H), 2.37 (d, *J*=1.1 Hz, 3H). **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 146.4, 146.1, 145.1, 132.6, 130.7, 129.0, 128.6, 128.2, 125.2, 124.7, 124.5, 124.0, 121.8, 117.3, 103.2, 22.7. **HRMS** (ESI-TOF) m/z calculated for $C_{20}H_{16}N_3O_2S^+$ 362.0958$(M+H)^+$, found 362.0956.

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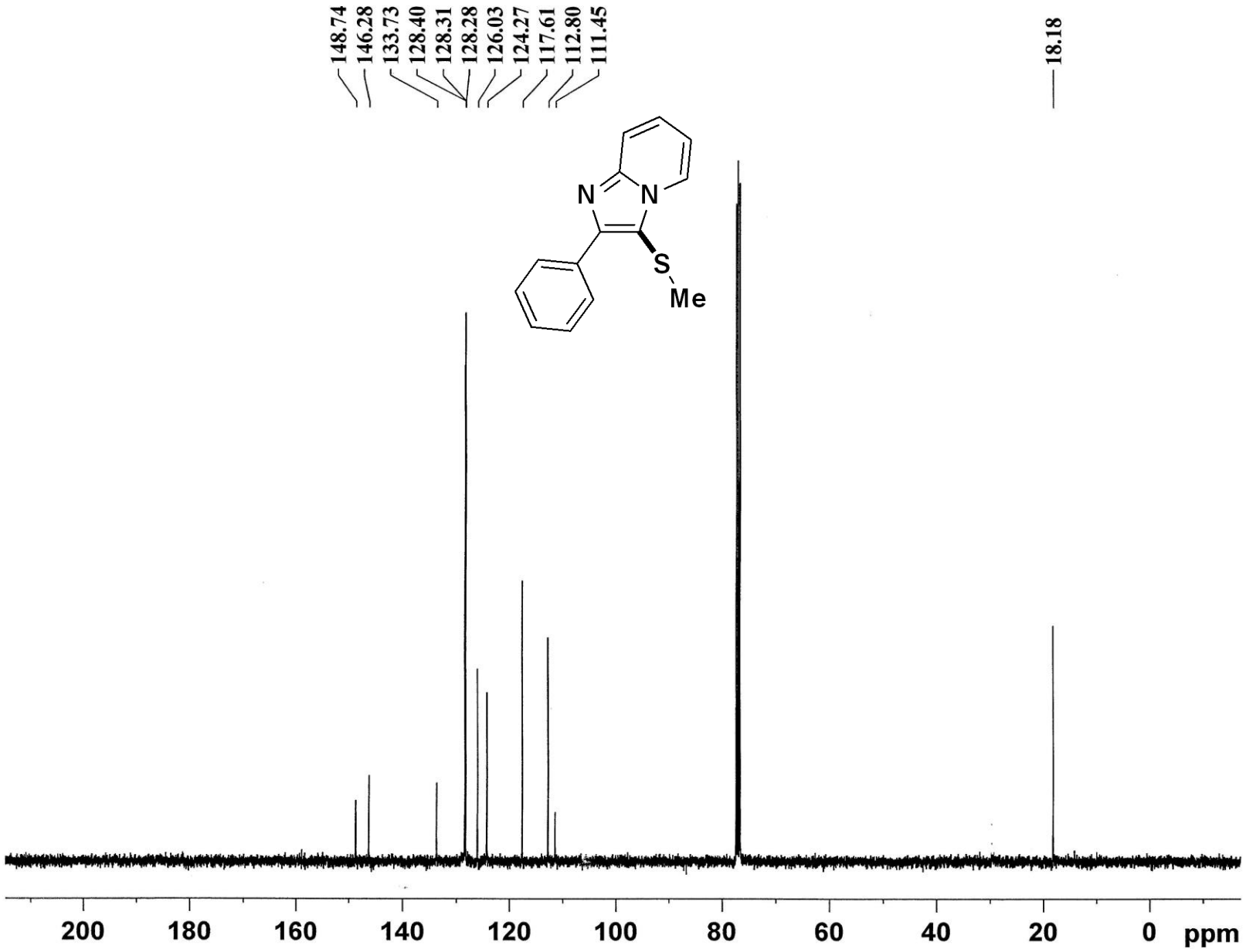
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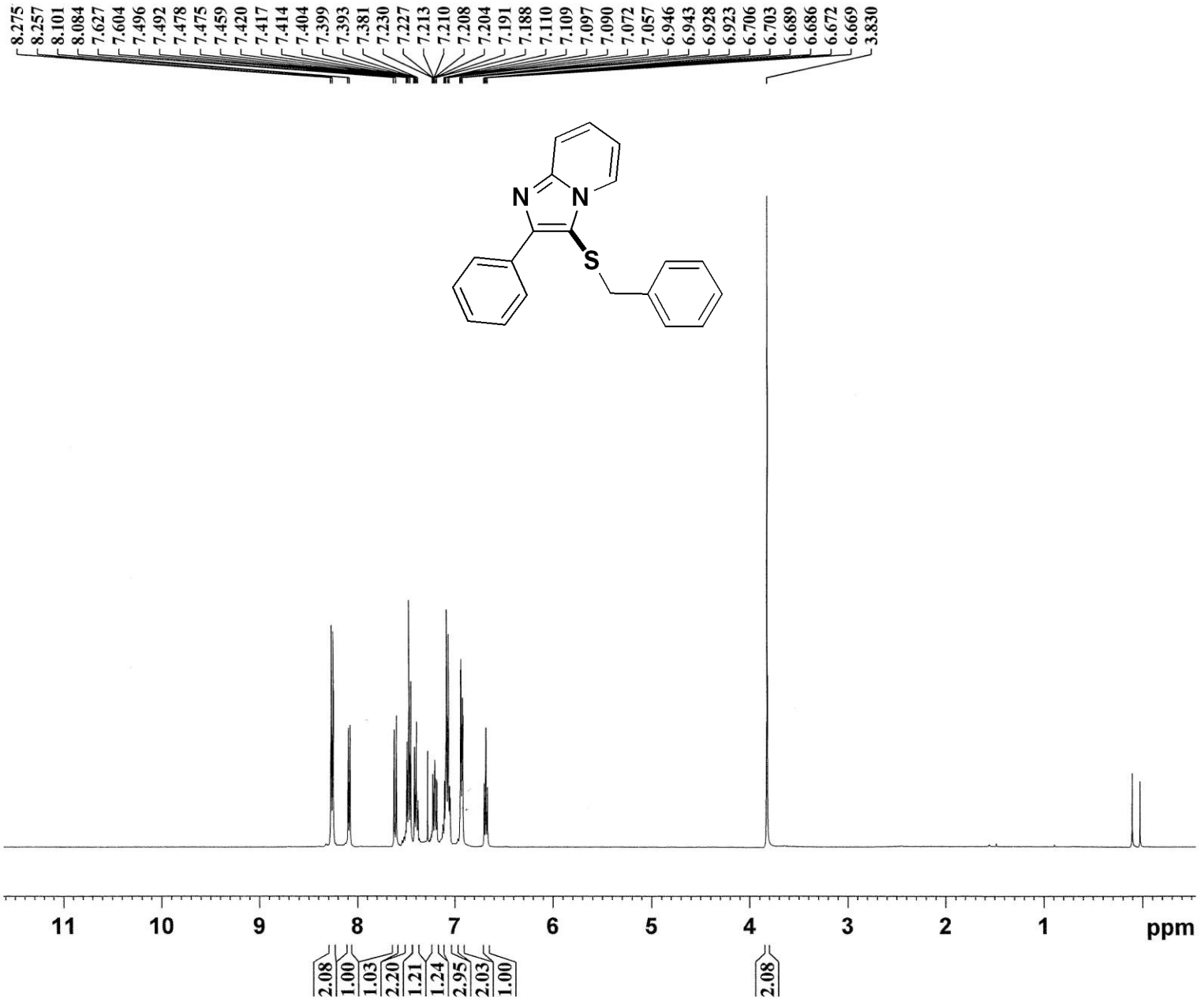
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6.684
6.682
3.885
N
N
S
HO
ppm
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2.00
0.99
1.06
1.26
1.17
4.35
3.20
1.01

40.48
108.37
112.87
116.17
116.56
117.71
118.74
123.90
126.78
127.45
127.50
128.49
128.68
130.28
136.93
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180
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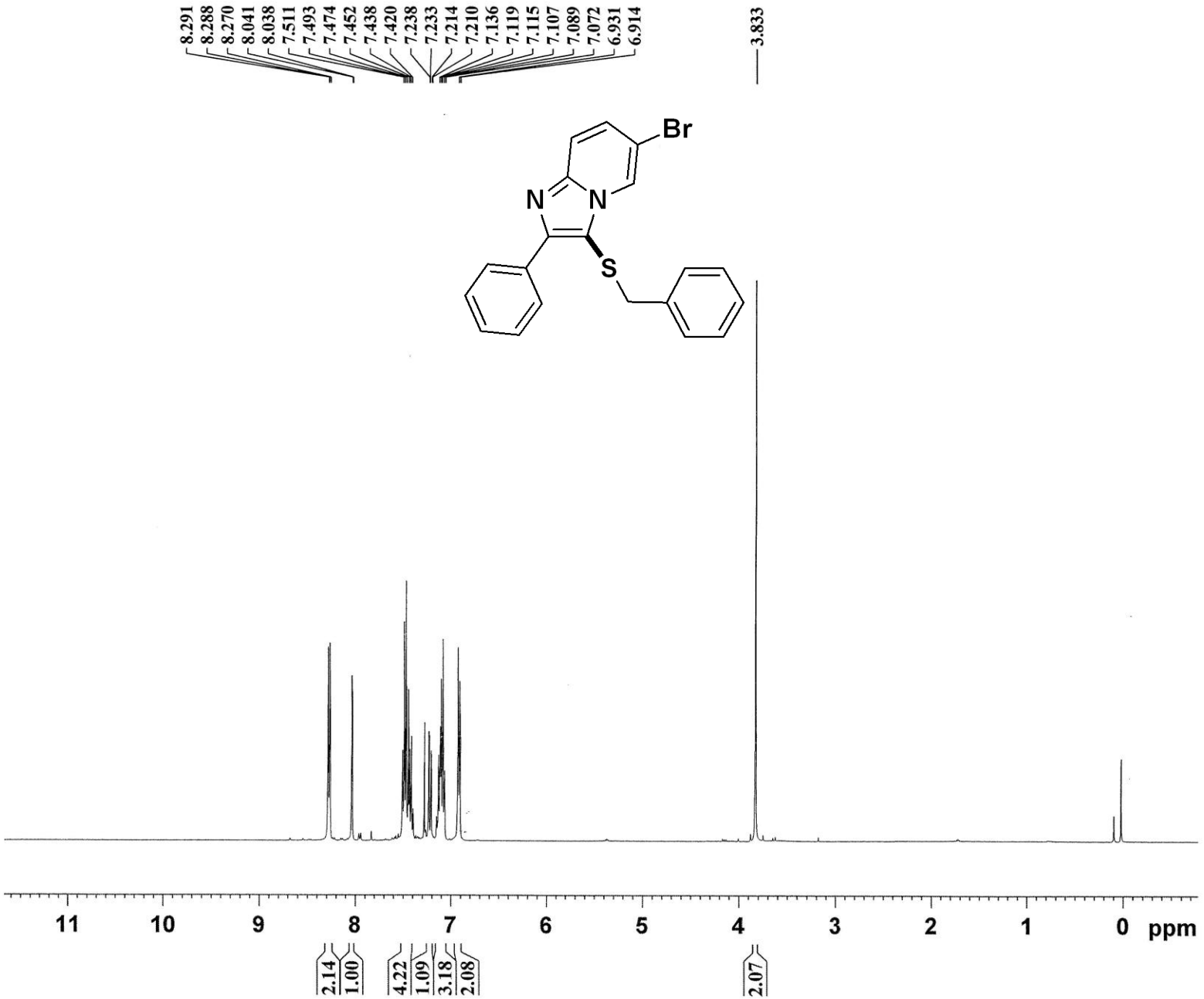
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7.233
7.214
7.210
7.136
7.119
7.115
7.107
7.089
7.072
6.931
6.914
3.833
Br
N
N
S
11
10
9
8
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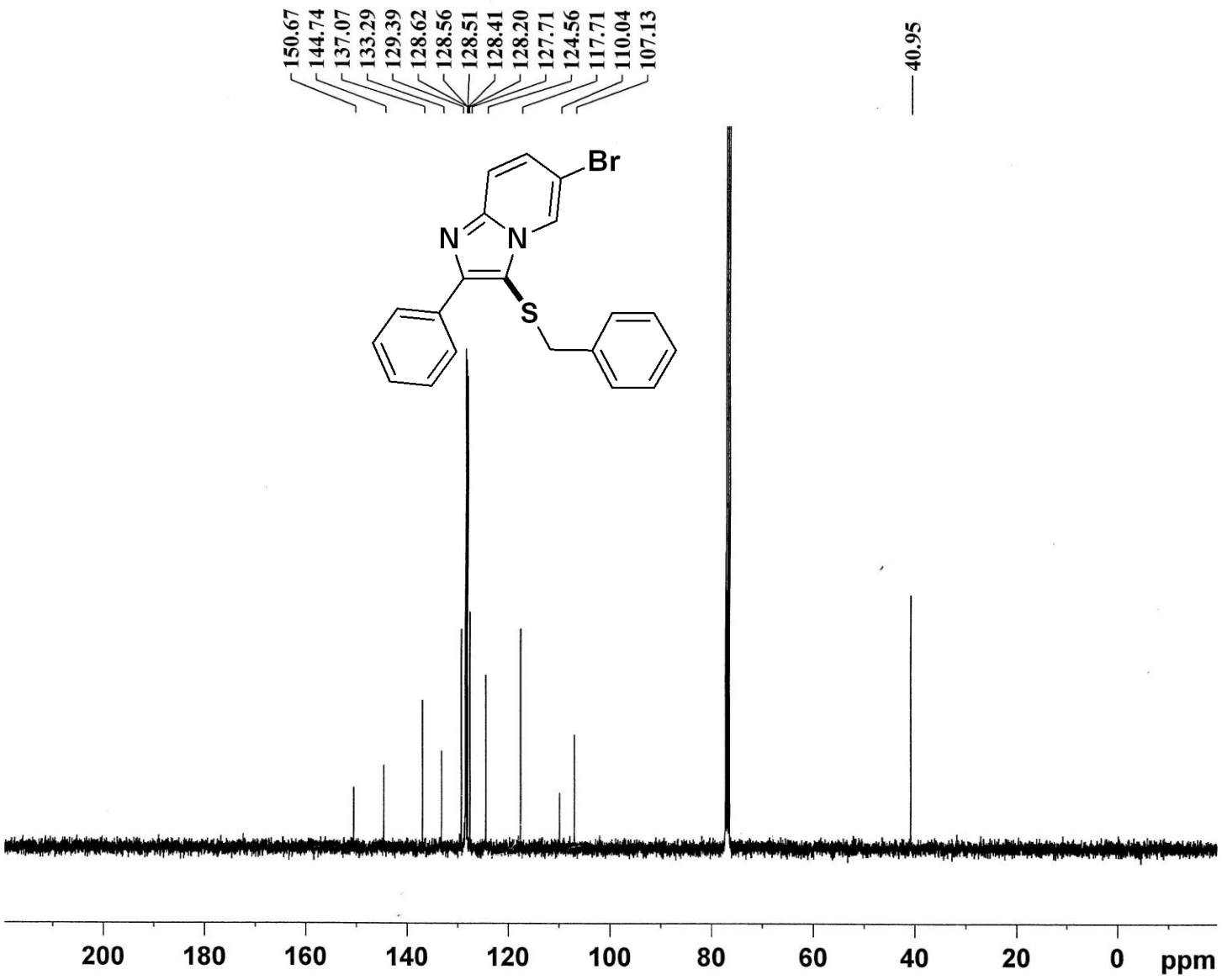
2.07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128.51
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128.20
127.71
124.56
117.71
110.04
107.13
40.95
Br
N
N
S
200
180
160
140
120
100
80
60
40
20
0
ppm

8.280
8.263
8.220
8.202
7.758
7.735
7.464
7.446
7.427
7.396
7.378
7.357
7.337
7.318
7.265
7.232
7.214
7.194
7.154
7.136
7.014
6.995
6.884
6.867
6.850
N
N
S
0.98
2.00
1.05
2.06
2.56
2.07
1.22
1.97
1.08
ppm

105.80
113.37
117.75
124.37
126.86
127.00
128.34
128.51
128.81
129.61
132.10
133.04
133.71
147.16
151.54
N
N
S
200
180
160
140
120
100
80
60
40
20
0
ppm

8.294
8.276
8.259
7.753
7.730
7.484
7.466
7.447
7.405
7.387
7.369
7.314
7.312
7.294
7.290
7.284
7.275
7.273
7.032
7.012
6.945
6.924
6.831
6.814
6.797
2.255
N
N
S
ppm
0
1
2
3
4
5
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7
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9
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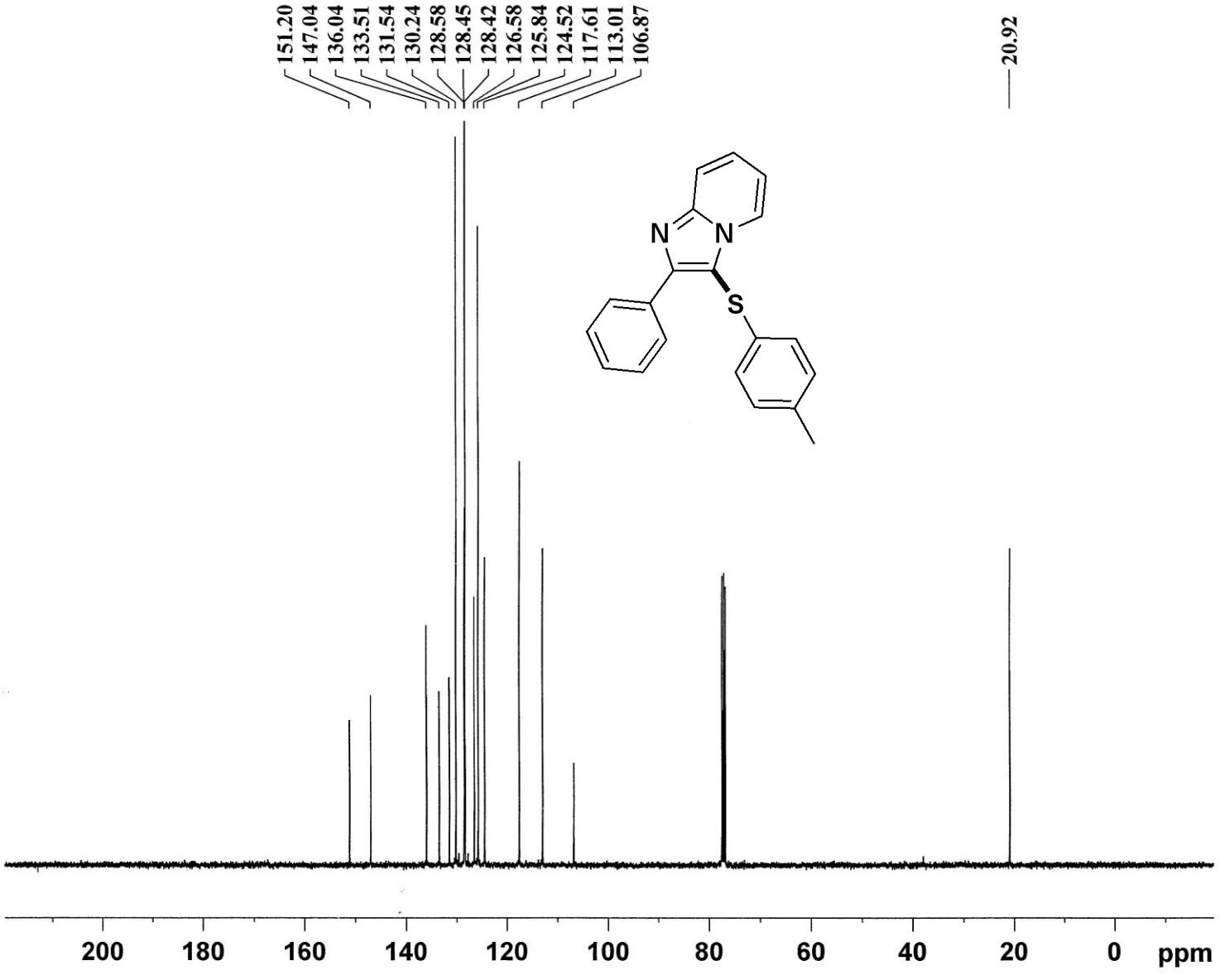
1.00
2.01
1.01
1.05
2.00
1.98
1.00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124.52
117.61
113.01
106.87
20.92
N
N
S
200
180
160
140
120
100
80
60
40
20
0
ppm

ppm
0
1
2
3
4
5
6
7
8
9
10
1.03
2.00
1.02
2.09
2.11
2.01
3.03
7.782
7.762
7.760
7.490
7.487
7.483
7.470
7.466
7.454
7.451
7.430
7.427
7.423
7.415
7.409
7.404
7.401
7.394
7.390
7.387
7.384
7.382
7.379
7.365
7.362
7.220
7.213
7.208
7.196
7.191
7.185
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6.939
6.934
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6.907
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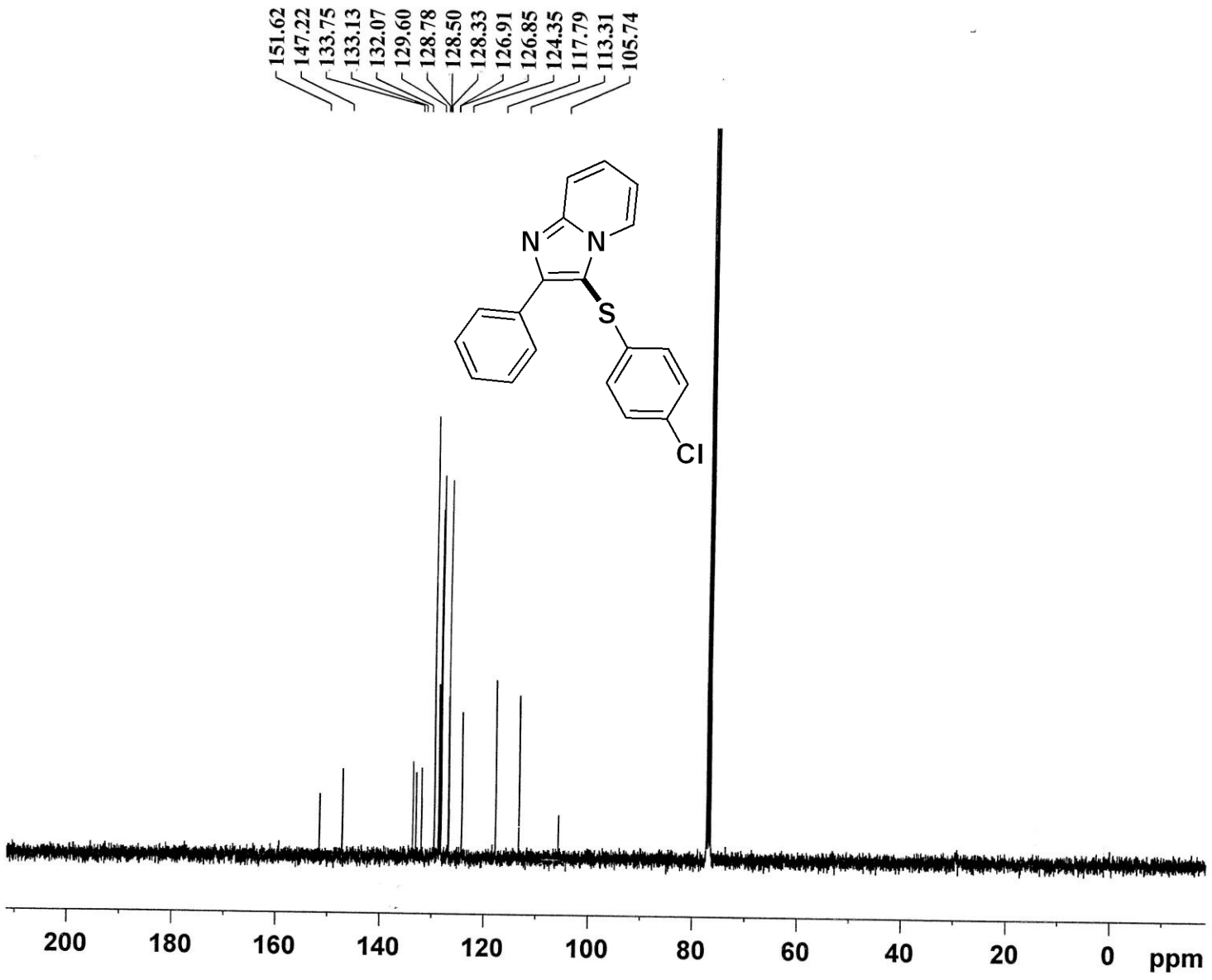
N
S
Cl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133.13
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128.50
128.33
126.91
126.85
124.35
117.79
113.31
105.74
N
N
S
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

8.654
8.650
8.634
8.630
8.402
8.399
8.397
8.385
8.382
8.380
7.716
7.714
7.712
7.694
7.692
7.689
7.437
7.434
7.420
7.417
7.415
7.411
7.397
7.394
7.310
7.307
7.303
7.290
7.285
7.284
7.263
7.246
7.242
7.230
7.227
7.196
7.193
7.190
7.175
7.117
7.114
7.097
7.094
7.085
7.081
7.076
7.063
6.982
6.980
6.965
6.963
6.948
6.946
6.915
6.912
6.894
6.877
6.874
N
N
S
HO
0 ppm
1 2 3 4 5 6 7 8 9 10 11 12 13 14
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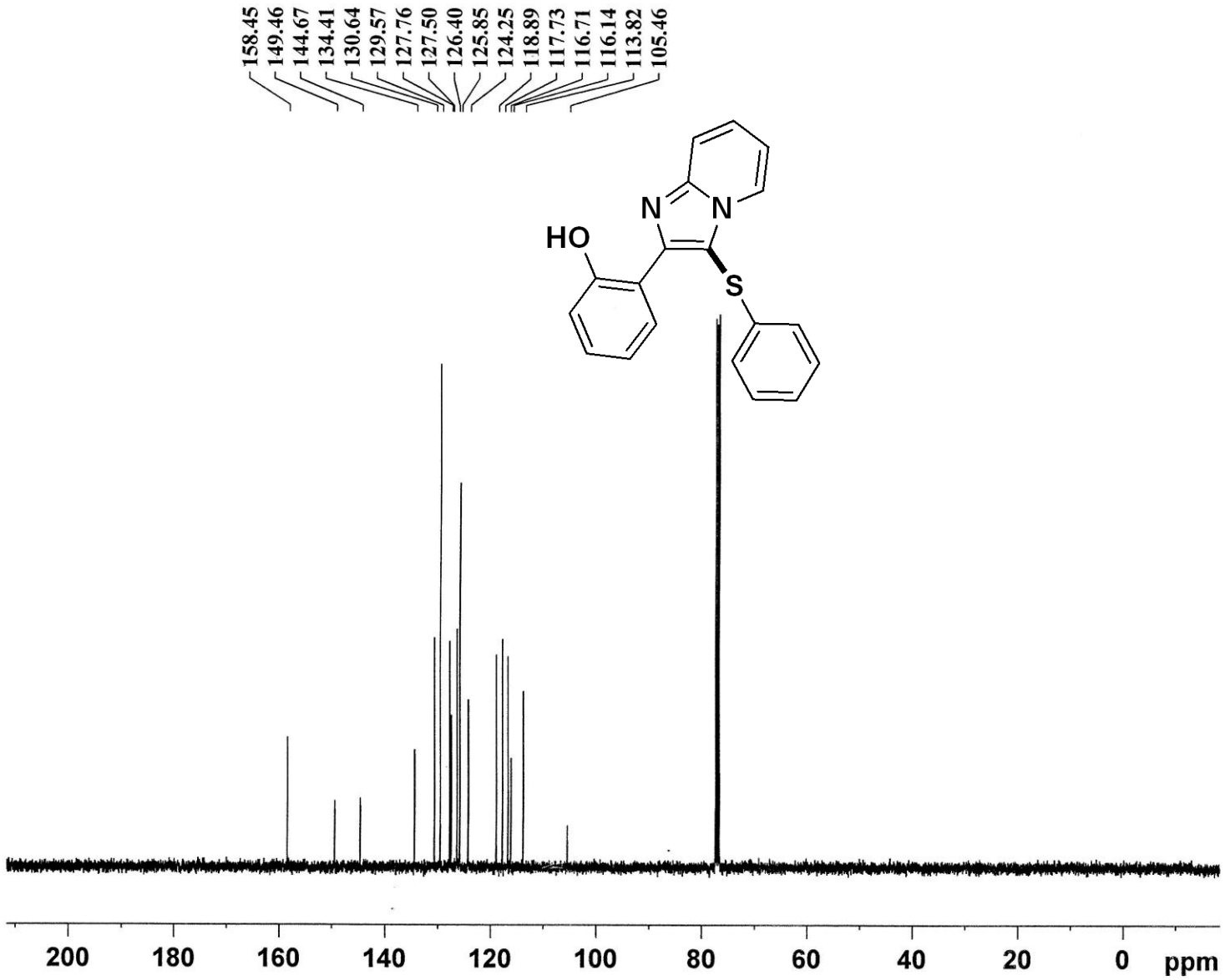
1.04
1.04
1.08
1.08
3.34
1.10
3.16
1.08
1.09
0.91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129.57
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127.50
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125.85
124.25
118.89
117.73
116.71
116.14
113.82
105.46
HO
N
N
S
200
180
160
140
120
100
80
60
40
20
0
ppm

3.846
6.835
6.838
6.852
6.855
6.870
6.872
6.970
6.977
6.982
6.994
7.000
7.005
7.007
7.020
7.025
7.028
7.121
7.123
7.127
7.136
7.142
7.147
7.157
7.160
7.163
7.197
7.202
7.206
7.218
7.221
7.235
7.239
7.242
7.306
7.309
7.323
N
N
S
MeO
ppm
0
1
2
3
4
5
6
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8
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3.03
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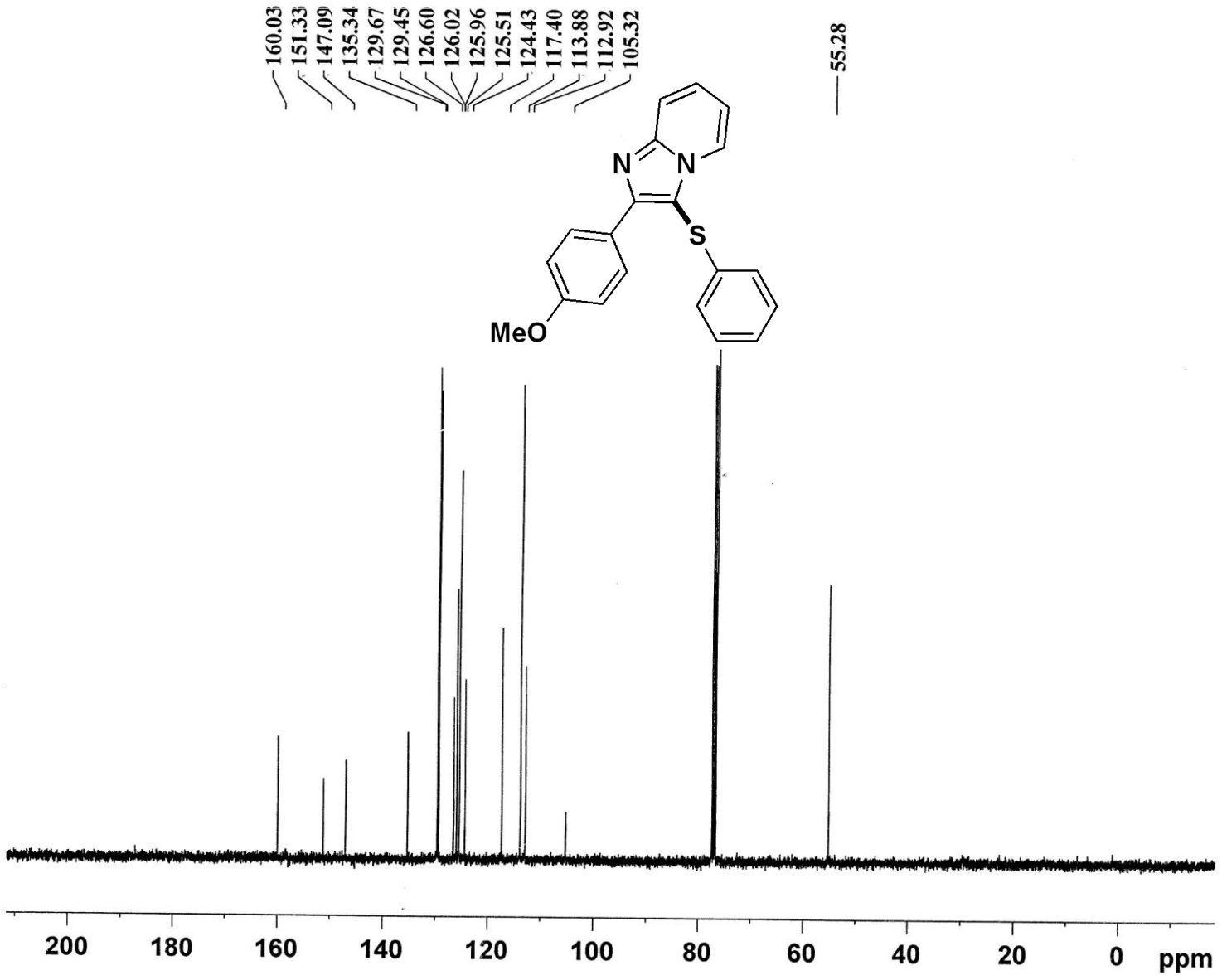
1.02
1.02
2.05
1.03
4.08
1.03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151.33
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126.02
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125.51
124.43
117.40
113.88
112.92
105.32
55.28
N
N
S
MeO
200
180
160
140
120
100
80
60
40
20
0
ppm

2.363
8.184
8.180
8.162
8.059
7.714
7.691
7.474
7.457
7.438
7.415
7.397
7.367
7.363
7.350
7.264
7.260
7.241
7.237
6.895
6.873
Br
S
N
N
ppm
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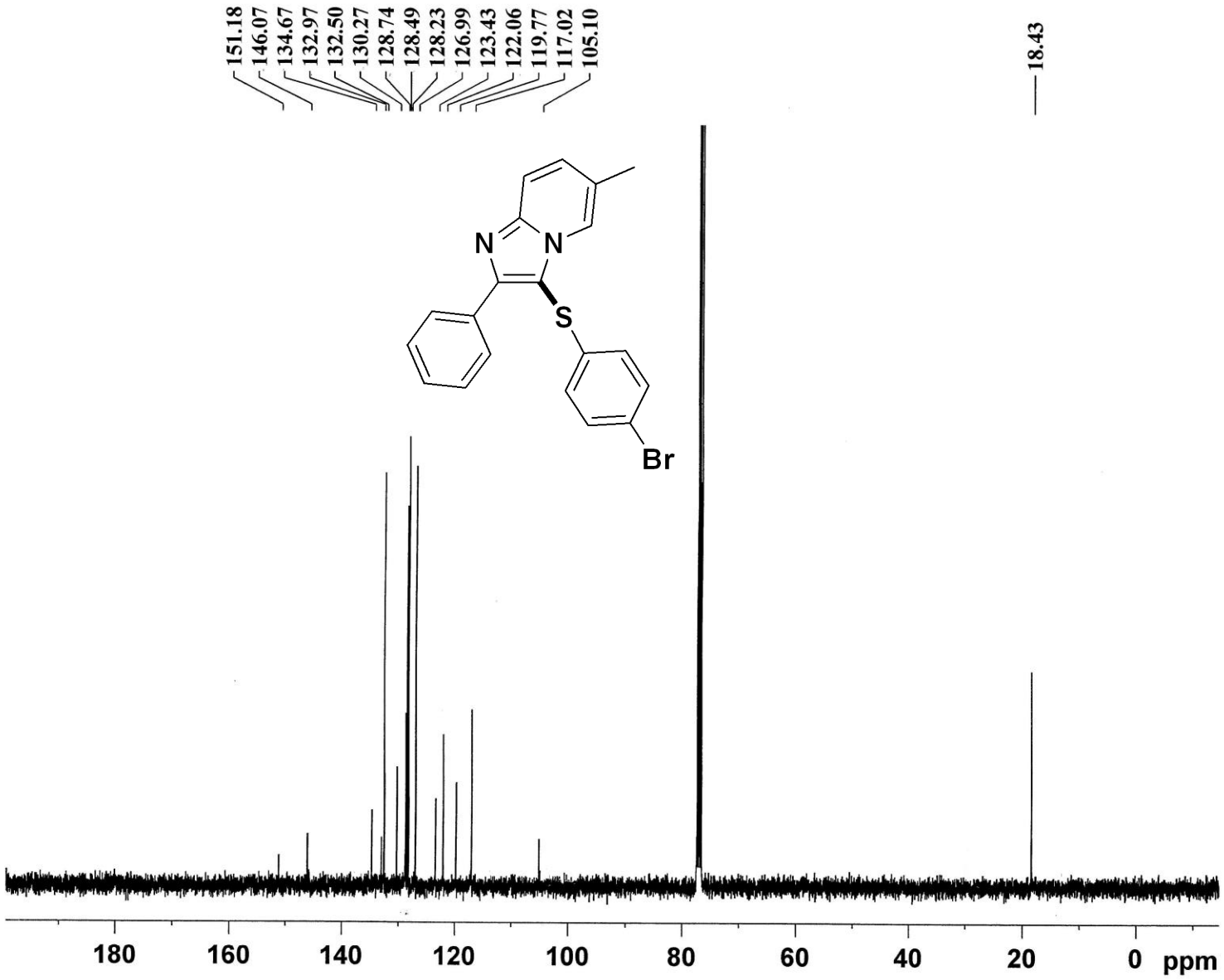
2
3
4
5
6
7
8
9
2.09
1.01
1.04
5.33
1.05
2.00
3.26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130.27
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128.49
128.23
126.99
123.43
122.06
119.77
117.02
105.10
18.43
N
N
S
Br
180
160
140
120
100
80
60
40
20
0
ppm

2.297
Br
N
S
N
6.931
6.952
7.056
7.077
7.284
7.390
7.395
7.404
7.414
7.419
7.421
7.444
7.463
7.476
7.480
7.483
7.622
7.646
8.219
8.236
8.240
8.451
8.454
ppm
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1
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8
9
10
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2.06
4.21
1.05
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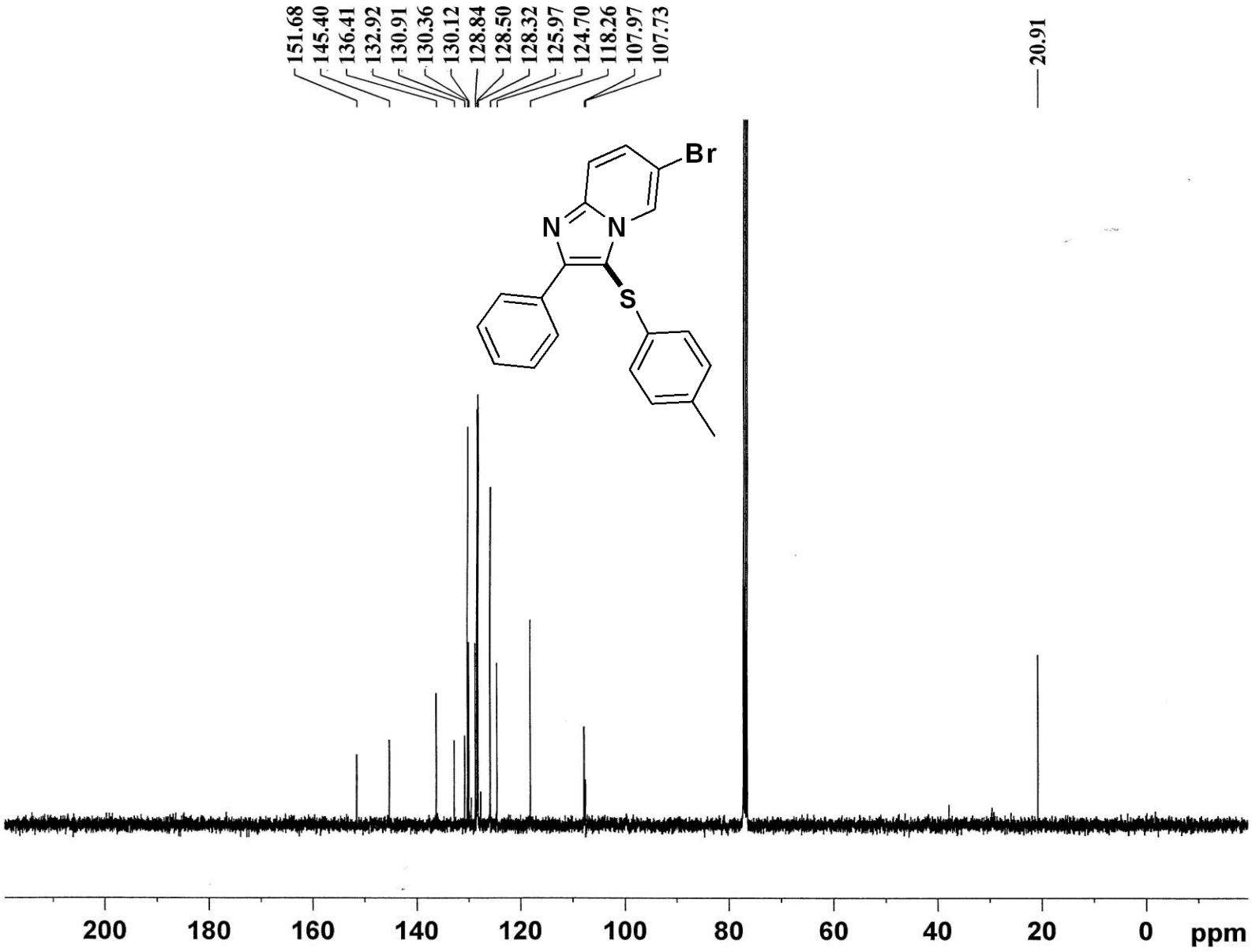
1.00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130.36
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128.84
128.50
128.32
125.97
124.70
118.26
107.97
107.73
20.91
Br
N
N
S
200
180
160
140
120
100
80
60
40
20
0
ppm

2.280
8.293
8.219
8.214
8.202
8.197
7.753
7.731
7.441
7.434
7.430
7.418
7.413
7.407
7.383
7.380
7.366
7.362
7.361
7.357
7.343
7.340
7.054
7.034
6.925
6.919
6.915
6.904
6.898
6.884
6.881
N
N
S
Cl
ppm
0
1
2
3
4
5
6
7
8
9
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3.00
1.98
1.06
2.02
0.98
1.95
1.00

20.89
149.82
146.95
136.28
134.58
131.83
131.12
130.29
129.60
128.65
126.89
125.87
124.55
117.60
113.24
107.16
N
N
S
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

8.179
8.158
8.087
7.657
7.634
7.412
7.390
7.256
7.252
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7.219
7.201
7.178
7.160
7.144
7.142
7.013
7.010
6.992
2.331
3.19
2.07
1.00
1.04
2.05
4.12
2.03
ppm
S
N
N
Cl

18.39
105.96
116.98
122.21
123.21
125.45
126.12
128.60
129.48
129.51
130.08
131.96
134.45
135.20
146.13
149.94
N
N
S
Cl
ppm
200
180
160
140
120
100
80
60
40
20
0

8.268
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7.763
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7.461
7.427
7.409
7.391
7.378
7.375
7.358
7.338
7.336
7.028
7.006
6.999
6.923
6.907
6.891
6.793
6.771
3.745
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S
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1.02
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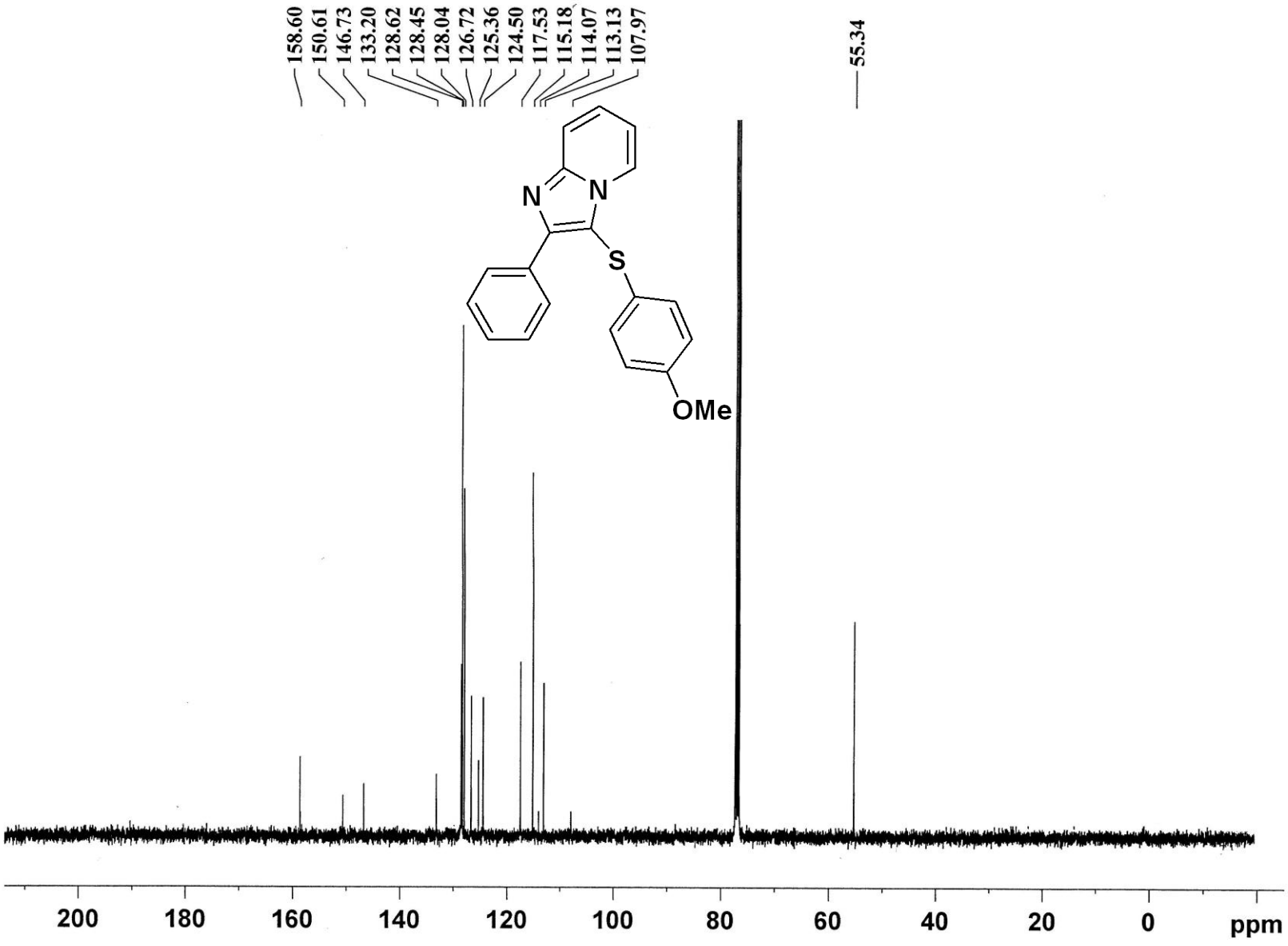
2.09
2.07
1.02
1.90
3.00
ppm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126.72
125.36
124.50
117.53
115.18
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113.13
107.97
55.34
N
N
S
OMe
200
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160
140
120
100
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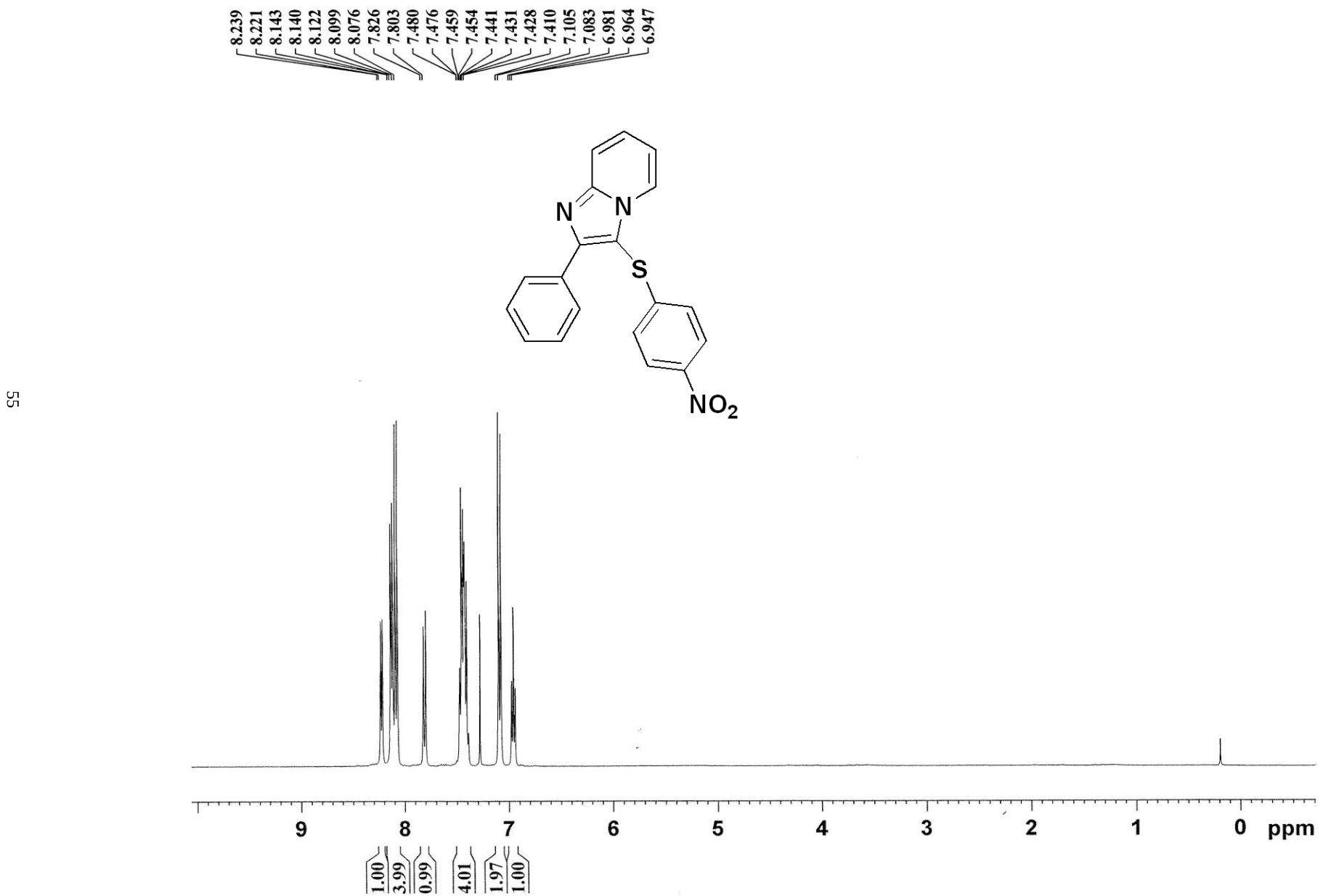
60
40
20
0
ppm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7.480
7.476
7.459
7.454
7.441
7.431
7.428
7.410
7.105
7.083
6.981
6.964
6.947
N
N
S
NO2
9
8
7
6
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4
3
2
1
0
ppm
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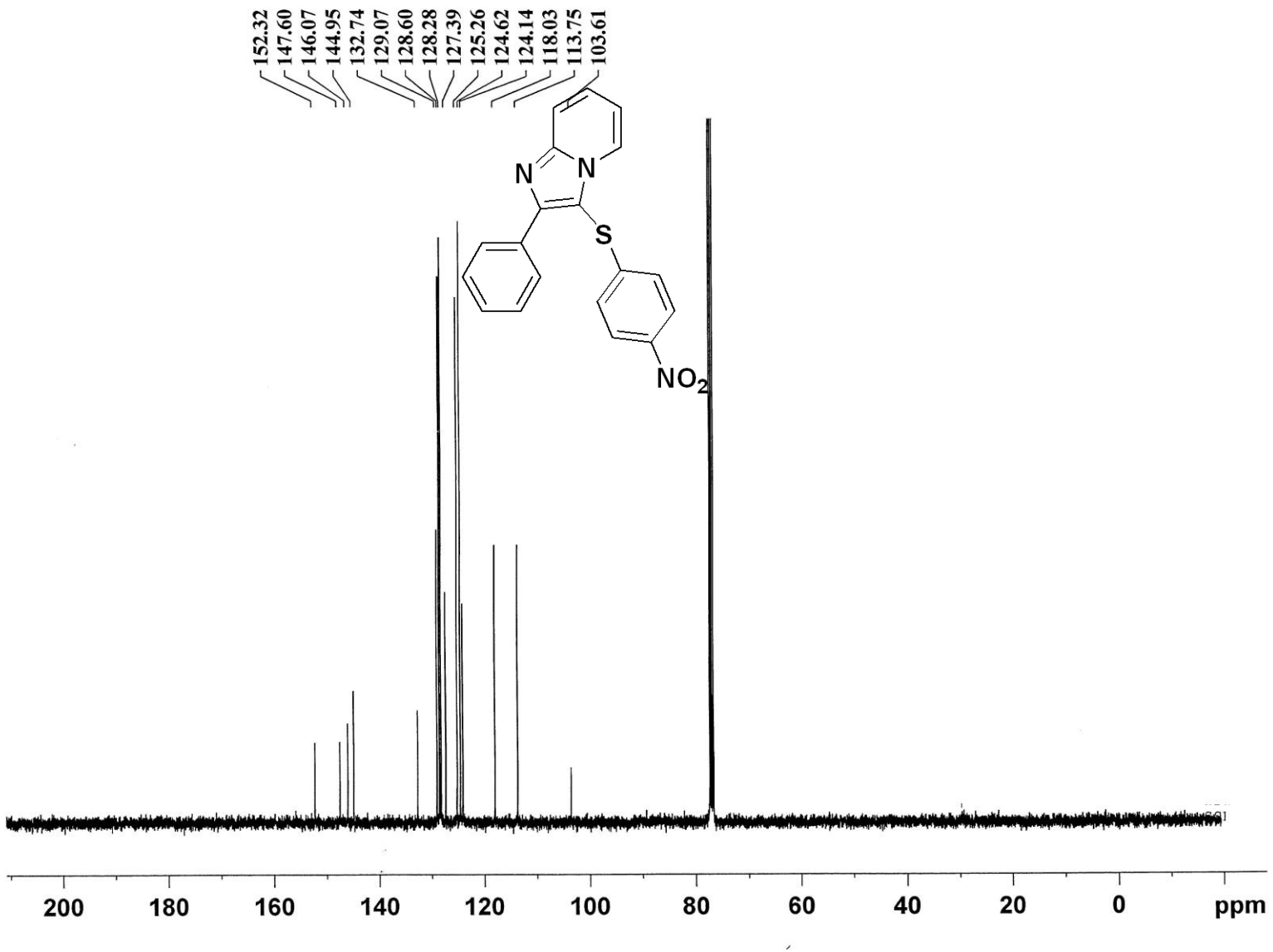
3.99
0.99
4.01
1.97
1.00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132.74
129.07
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128.28
127.39
125.26
124.62
124.14
118.03
113.75
103.61
N
N
S
NO2
200
180
160
140
120
100
80
60
40
20
0
ppm

2.372
7.476
7.472
7.455
7.436
7.428
7.424
7.413
7.407
7.388
7.383
7.378
7.373
7.315
7.312
7.284
7.163
7.157
7.141
7.135
7.118
7.095
N
N
S
NO2
3.48
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1.00
3.09
2.06
2.16
3.00
ppm

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121.83
123.97
124.47
124.65
125.20
128.21
128.59
129.03
130.71
132.58
145.10
146.09
146.41
N
N
S
NO2
200
180
160
140
120
100
80
60
40
20
0
ppm