Supporting Information

Palladium-catalyzed decarboxylative *ortho*-arylation of sulfoxides with aryl acyl peroxides

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Contents:

1. General methods.

All reactions involving air- and moisture-sensitive reagents were carried out under an argon atmosphere. Toluene, DMF, AcOH, DME, 1, 4- dioxane and CH_3CN were distilled from appropriate drying agents prior to use. All chemicals were purchased from Aldrich and used without further purification. Thin-layer chromatography (TLC) was performed using 60 mesh silica gel plates visualized with short-wavelength UV light (254 nm). Silica gel 60 (230~400 mesh) was used for column chromatography. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker INOVA-400. NMR Spectrums were recorded on a 400 instrument (400 MHz for ^{1}H and 100 MHz for ^{13}C). Chemical shifts (δ) were measured in ppm relative to

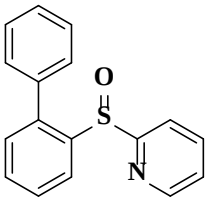
TMS δ = 0 for ^{1}H, or to chloroform δ = 77.0 for ^{13}C as internal standard. Data are reported as follows: Chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), Coupling constants, *J*, are reported in hertz. Mass data were measured with Thermo Scientific DSQ II mass spectrometer.

Sulfoxides and aryl acyl peroxides were easily prepared according to the corresponding literatures.[1,2]

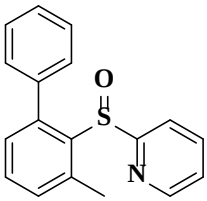
General Catalytic Procedure for *Ortho*-arylation of 2-(phenylsulfinyl)pyridine with BPO.

A mixture of 2-(phenylsulfinyl)pyridine (40.6 mg, 0.2 mmol, 1.0 equiv), AcOH (96.1mg, 1.6 mmol, 8 equiv), BPO (96.8 mg, 0.4 mmol, 2.0 equiv) and $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol %) in MeCN (1 mL) was stirred under argon at 80 ^{o}C for 16 h followed by cooling to room temperature. The volatiles removed under reduced pressure. The contents were subjected to flash chromatography to give the corresponding product (77%) as a white solid. The purified material was dried under an oil-pump vacuum.

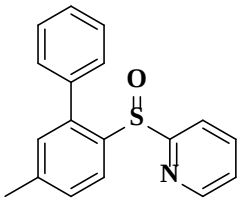
2. Characterization of the Products



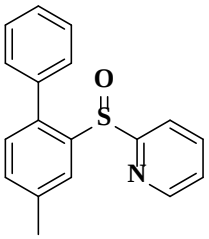
3aa: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.50 (d, *J* = 4 Hz, 1H), 7.85-7.78 (m, 3H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.44-7.37 (m, 5H,), 7.38 (d, *J* = 8.0 Hz, 1H), 7.26 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.61, 149.83, 142.97, 142.62, 138.15, 137.63, 131.15, 130.44, 130.35, 128.60, 128.10, 128.01, 126.35, 124.32, 120.07. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{17}H_{13}NOSNa^+$: 302.0616, Found: 302.0582.



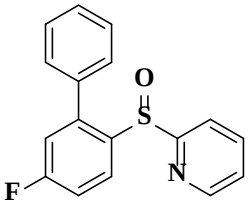
3ba: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.52 (d, *J* = 4.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.79 (t, *J* = 8.0 Hz, 1H), 7.53 (s, 2H), 7.41 (t, *J* = 3.6 Hz, 1H), 7.34 (t, *J* = 2.8 Hz, 3H), 7.24 (t, *J* = 4.0 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 1H) , 2.35(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.84, 149.44, 145.79, 140.39, 139.44, 139.08, 136.85, 131.79, 131.42, 130.41, 128.89, 127.52, 123.41, 121.30, 18.71. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{18}H_{15}NOSNa^+$: 316.0772, Found: 316.0740.



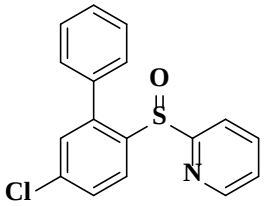
3ca: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.52 (d, *J* = 4.0 Hz, 1H), 7.89 (d, *J* = 4.0 Hz, 1H), 7.84 (t, *J* = 8.0 Hz ,1H), 7.67-7.62 (m, 3H,), 7.47-7.40 (m, 3H), 7.28 (d, *J* = 4.0 Hz, 2H), 7.22 (s, 1H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.84, 149.77, 142.69, 141.67, 139.91, 138.28, 137.57, 131.12, 130.30, 129.42, 128.02, 127.88, 126.61, 124.17, 119.98, 21.37. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{18}H_{15}NOSNa^+$: 316.0772, Found: 316.0742.



3da: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.52 (d, *J* = 4.0 Hz, 1H), 7.83-7.81 (m, 2H), 7.82 (t, *J* = 2.0 Hz, 2H), 7.58 (d, *J* = 1.6 Hz, 1H), 7.45-7.42 (m, 3H), 7.31 (d, *J* = 1.2 Hz, 1H), 7.29 (s, 1H), 7.27 (m, 1H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.64, 149.85, 142.46, 139.85, 138.76, 138.20, 137.60, 132.18, 130.39, 128.07, 127.81, 126.34, 124.29, 120.13, 21.14. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{18}H_{15}NOSNa^+$: 316.0772, Found: 316.0741.

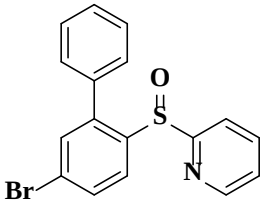


3ea: Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ : 8.51 (d, *J* = 4.0 Hz, 1H), 7.85 (q, *J* = 1.4 Hz, 2H), 7.76 (q, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 4.0 Hz, 2H), 7.44 (d, *J* = 4.0 Hz, 3H), 7.29 (t, *J* = 4.0 Hz, 1H), 7.17-7.08 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.20 (d, *J* = 40.0 Hz), 162.52, 149.89, 145.29 (d, *J* = 9.0 Hz), 138.75, 137.39 (d, *J* = 74.0 Hz), 130.17, 129.20 (d, *J* = 10.0 Hz), 128.49, 128.23, 124.43, 119.96, 117.22 (d, *J* = 22.0 Hz), 116.00 (d, *J* = 22.0 Hz). HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{17}H_{12}FNOSNa^+$: 320.0521, Found: 320.0489.

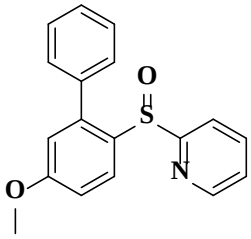


3fa: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.50 (d, *J* = 4.0 Hz, 1H), 7.81 (s, 2H), 7.74 (d, *J* = 8.0 Hz, 1H),7.58 (d, *J* = 4.0 Hz, 2H), 7.44 (s, 4H), 7.38 (s, 1H), 7.29 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz,

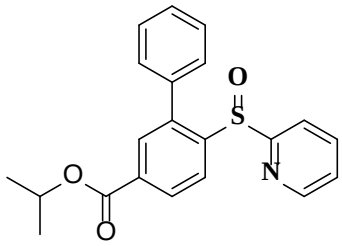
$CDCl_3$) δ: 165.21, 149.94, 144.01, 141.54, 137.78, 137.22, 136.87, 130.29, 130.16, 128.77, 128.50, 128.27, 127.91, 124.53, 120.07. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{17}H_{12}ClNOSNa^+$: 336.0226, Found: 336.0196.



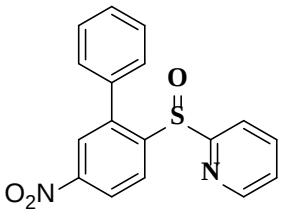
3ga: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.50 (d, *J* = 8.0 Hz, 1H), 7.80 (t, *J* = 8.0 Hz, 2H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.58-7.53 (m, 4H), 7.43 (t, *J* = 3.2 Hz, 3H), 7.28 (t, *J* = 1.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.12, 149.94, 144.09, 142.13, 137.77, 136.78, 133.20, 131.67, 130.16, 128.51, 128.27, 127.95, 125.65, 124.55, 120.08. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{17}H_{12}BrNOSNa^+$: 379.9721, Found: 379.9691.



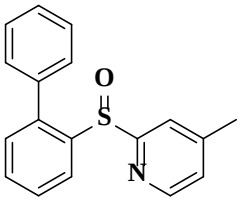
3ha: Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.51 (q, *J* = 8.0 Hz, 1H), 7.92 (d, *J* = 8.9 Hz, 1H), 7.85-7.80 (m, 1H), 7.64-7.60 (m, 3H), 7.46-7.40 (m, 3H), 7.27-7.24 (m, 1H), 6.95 (q, *J* = 8.0 Hz, 1H), 6.86 (d, *J* = 4.0 Hz, 1H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.95, 161.50, 149.75, 144.96, 138.15, 137.58, 134.49, 130.26, 128.90, 128.08, 128.04, 124.10, 119.88, 115.17, 114.83, 55.48. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{18}H_{15}NO_2SNa^+$: 332.0721, Found: 332.0690.



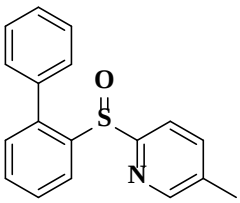
3ia: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.40 (d, *J* = 4.0 Hz, 1H), 8.06-8.03 (m, 1H), 7.95 (d, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.72-7.667 (m, 2H), 7.50 (q, *J* = 8.0 Hz, 2H), 7.37 (t, *J* = 4.0 Hz, 3H), 7.19 (t, *J* = 8.0 Hz, 1H), 5.18 (m, 1H), 1.27 (d, *J* = 2.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.99, 164.96, 149.95, 147.29, 142.25, 137.75, 137.44, 133.21, 131.41, 130.21, 129.27, 128.36, 128.28, 126.13, 124.63, 120.28, 69.04, 21.84.HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{21}H_{19}NNaO_3SNa^+$: 388.0983, Found: 388.0960.



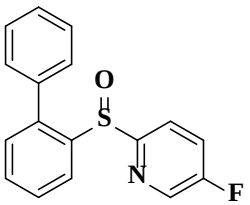
3ja: Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.48 (d, *J* = 4 Hz, 1H), 8.30 (dd, *J* = 2.4 Hz, *J* = 8 Hz, 1H), 8.21 (d, *J* = 2 Hz, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 7.83-7.78 (m, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.57-7.54 (m, 2H), 7.48-7.45 (m, 3H), 7.31-7.28 (m, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.26, 150.17, 149.82, 149.11, 143.43, 137.96, 136.11, 129.99, 129.05, 128.59, 127.44, 125.14, 125.03, 123.04, 120.56.HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{17}H_{12}N_2O_3SNa^+$: 347.0466, Found: 347.0481.



3ka: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.34 (d, *J* = 4.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.63 (s, 1H), 7.59 (d, *J* = 4.0 Hz, 2H), 7.48 (t, *J* = 8.0 Hz, 2H) , 7.43 (d, *J* = 8.0 Hz, 3H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.05 (d, *J* = 4.0 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.07, 149.60, 149.37, 143.00, 142.61, 138.19, 131.10, 130.43, 130.38, 128.57, 128.06, 127.94, 126.43, 125.26, 120.76, 21.19. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{18}H_{15}NOSNa^+$: 316.0772, Found: 316.0735.

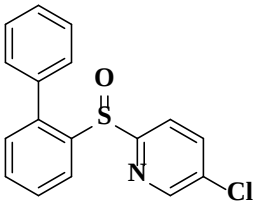


3la: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.32 (s, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 8.0 Hz, 3H), 7.47-7.42 (m, 5H), 7.36 (d, *J* = 8.0 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 162.30, 150.36, 143.09, 142.43, 138.17, 137.93, 134.48, 131.01, 130.35, 130.28, 128.54, 128.06, 127.95, 126.15, 119.72, 18.21. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{18}H_{15}NOSNa^+$: 316.0772, Found: 316.0724.

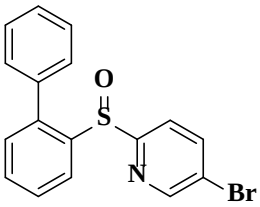


3ma: Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.34 (d, *J* = 4.0 Hz, 2H), 7.83-7.78 (m, 2H), 7.52-7.49 (m, 5H), 7.42 (d, *J* = 4.0 Hz, 2H), 7.37 (t, *J* = 4.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 160.75 (d, *J* = 5.0 Hz), 158.23, 142.55 (d，*J* = 28.0 Hz), 138.53 (d，*J* = 25.0 Hz), 138.05, 131.29, 130.53, 130.19, 128.62, 128.16, 128.08, 126.03, 124.24 (d, *J* = 20.0 Hz), 121.74 (d, *J* = 6.0 Hz). HRMS (ESI) ($[M+Na]^+$) Calcd.

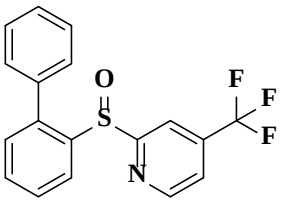
for $C_{17}H_{12}FNOSNa^+$: 320.0521, Found: 320.0511.



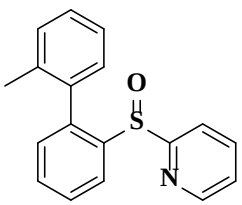
3na: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.44 (d, *J* = 2.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 3H), 7.57-7.54 (m, 2H), 7.49 (m, 2H), 7.43 (m, 3H), 7.38 (q, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.62, 148.69, 142.57, 142.53, 138.00, 137.25, 133.04, 131.36, 130.56, 130.25, 128.65, 128.14, 128.08, 126.14, 120.96. HRMS (ESI) ([M+Na]$^+$) Calcd. for $C_{17}H_{12}ClNOSNa^+$: 336.0226, Found: 336.0190.



3oa: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.53 (d, *J* = 4.0 Hz, 1H), 7.93 (q, *J* = 8.0 Hz, 1H), 7.80-7.77 (m, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.57-7.55 (m, 2H), 7.49 (m, 2H), 7.44-7.42 (m, 3H) , 7.38 (q, *J* =4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.21, 150.81, 142.56, 142.52, 140.14, 137.99, 131.37, 130.56, 130.26, 128.65, 128.13, 128.08, 126.16, 121.82, 121.35. HRMS (ESI) ([M+Na]$^+$) Calcd. for $C_{17}H_{12}BrNOSNa^+$: 379.9721, Found: 379.9681.

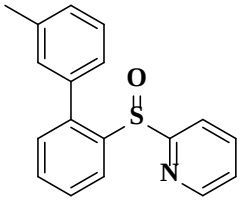


3pa: Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.75 (s, 1H), 8.08-8.04 (m, 2H), 7.76 (q, *J* = 4.0 Hz, 1H), 7.61-7.59 (m, 2H), 7.51 (q, *J* = 12.0 Hz, 1H), 7.49 (q, *J* =8.0 Hz, 1H), 7.46-7.43 (m, 3H), 7.40 (q, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.22, 146.60 (q, *J* = 6.0 Hz), 142.58 (d, *J* = 50.0 Hz), 137.96, 134.90 (d, *J* = 4.0 Hz), 131.17 (d, *J* = 76.0 Hz), 130.32, 129.27, 128.70, 128.13, 127.00 (d, *J* = 33.0 Hz), 126.46, 124.49 (d, *J* = 46.0 Hz), 121.53, 119.85. HRMS (ESI) ([M+Na]$^+$) Calcd. for $C_{17}H_{12}F_3NOSNa^+$: 370.0489, Found: 370.0460.

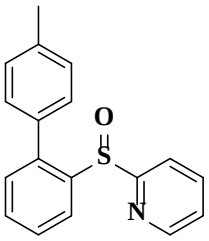


3ab[3]: white solid. This compound was obtained as a 1:1 mixture of diastereoisomers. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.47 (d, *J* = 4.0 Hz, 1H), 8.44 (d, *J* = 4.0 Hz, 1H), 7.94-7.90 (m, 2H), 7.76-7.67 (m, 2H), 7.60

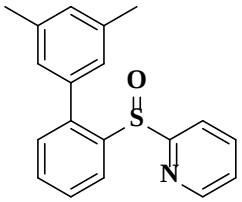
(d, *J* = 8.0 Hz, 1H), 7.54-7. 45 (m, 5H), 7.36-7.13 (m, 11H), 7.09 (d, *J* = 8.0 Hz, 1H), 2.21 (s, 3H), 1.82 (s, 3H) ^{13}C NMR (100 MHz, $CDCl_3$) ^{13}C NMR (101 MHz, $CDCl_3$) δ: 164.97, 164.27, 150.02, 149.86, 142.87, 142.67, 141.28, 141.08, 137.46, 137.38, 137.27, 136.87, 135.88, 131.31, 131.13, 130.60, 130.36, 130.16, 130.10, 129.94, 128.56, 128.51, 128.43, 128.29, 125.71, 125.68, 125.51, 125.18, 124.69, 124.53, 120.75, 120.40, 20.27, 20.02. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{18}H_{15}NOSNa^+$: 316.0772, Found: 316.0740.



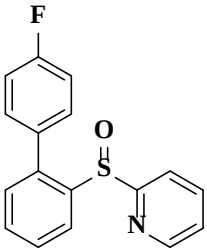
3ac: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.54 (d, *J* = 4.0 Hz, 1H), 7.84 (q, *J* = 12.0 Hz, 3H), 7.53-7.45 (m, 3H), 7.42-7.35 (m, 3H), 7.31-7.28 (m, 2H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.60, 149.80, 142.93, 142.72, 138.07, 137.76, 137.53, 131.06, 130.90, 130.36, 128.71, 128.47, 127.95, 127.47, 126.29, 124.28, 120.17, 21.40. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{18}H_{15}NOSNa^+$: 316.0772, Found: 316.0738.



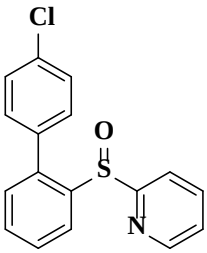
3ad: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.50 (d, *J* = 4.0 Hz, 1H), 7.89 (m, 2H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.51-7.42 (m, 4H), 7.36 (d, *J* = 4.0 Hz, 1H), 7.25 (d, *J* = 4.0 Hz, 3H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.74, 149.79, 142.98, 142.68, 137.86, 137.63, 135.27, 131.11, 130.44, 130.23, 128.84, 128.39, 126.28, 124.29, 120.01, 21.24. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{18}H_{15}NOSNa^+$: 316.0772, Found: 316.0742.



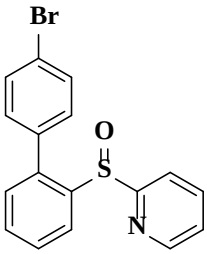
3ae: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.49 (d, *J* = 4.0 Hz, 1H), 7.77 (s, 3H), 7.43 (d, *J* = 4.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.24 (s, 1H), 7.14 (s, 2H), 7.03 (s, 1H), 2.34 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.48, 149.84, 142.79, 138.00, 137.64, 137.47, 131.03, 130.31, 129.60, 128.40, 128.07, 126.25, 124.30, 120.33. 21.31. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{19}H_{17}NOSNa^+$: 330.0929, Found: 330.0896.



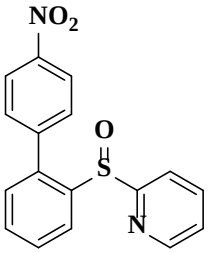
3af: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.49 (d, *J* = 4.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.86 (t, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.60 (q, *J* = 8.0 Hz, 2H), 7.51-7.44 (m, 2H), 7.35 (d, *J* = 4.0 Hz, 1H), 7.29 (t, *J* = 4.0 Hz, 1H), 7.13 (t, *J* = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.69, 162.75 (d, *J* = 250.0 Hz), 149.74, 143.12, 141.68, 137.82, 133.15 (d, *J* = 200 Hz), 132.17 (d, *J* = 15 Hz), 131.26, 130.49, 128.76, 126.54, 124.38, 119.89, 115.06 (d, *J* = 20 Hz), 114.95. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{17}H_{12}FOSNa^+$: 320.0521, Found: 320.0490.



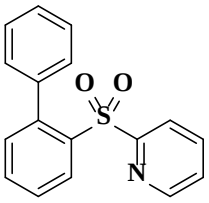
3ag: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.48 (d, *J* = 4.0 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.86 (m, 1H), 7.76 (dd, *J* = 2.0 Hz, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.49-7.44 (m, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.35 (dd, *J* = 4.0 Hz, *J* = 8.0 Hz, 1H), 7.28 (t, *J* = 4.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.69, 149.75, 143.12, 141.47, 137.82, 136.57, 134.29, 131.74, 131.30, 130.35, 128.92, 128.28, 126.55, 124.37, 119.80. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{17}H_{12}ClNOSNa^+$: 336.0226, Found: 336.0193.



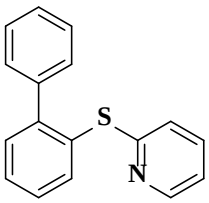
3ah: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.49 (d, *J* = 4.0 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.86 (m, 1H), 7.76 (d, *J* = 4.0 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.53-7.46 (m, 4H), 7.34 (dd, *J* = 2.0 Hz, *J* = 6.0 Hz, 1H) , 7.28 (t, *J* = 4.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.61, 149.75, 143.00, 141.49, 137.84, 137.04, 132.05, 131.34, 131.24, 130.29, 128.95, 126.60, 124.39, 122.56, 119.83. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{17}H_{12}BrNOSNa^+$:379.9721, Found: 379.9689.



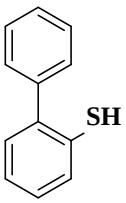
3aj: Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.49 (s, 1H), 8.31 (d, *J* = 8.0 Hz, 2H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.89 (t, *J* = 8.0 Hz, 3H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 3.2 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.73, 149.71, 147.55, 144.80, 143.38, 140.42, 138.06, 131.54, 131.51, 130.21, 129.81, 126.66, 124.50, 123.23, 119.48. HRMS (ESI) ($[M+Na]^+$) Calcd. for $C_{17}H_{12}N_2O_3SNa^+$: 347.0466, Found: 347.0431.



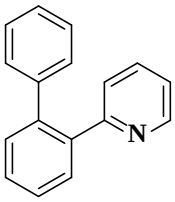
4[1]: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.45-8.41 (m, 2H), 7.57-7.54 (m, 2H), 7.43-7.39 (m, 1H), 7.22-7.19 (m, 2H), 7.15-7.11 (m, 2H), 7.01 (t, *J* = 8 Hz, 2H), 6.84 (q, *J* = 8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.01, 149.64, 141.78, 137.95, 137.68, 137.04, 133.23, 132.09, 129.80, 129.27, 127.83, 127.43, 127.12, 126.26, 122.63.



5[1]: Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.34 (d, *J* = 4.0 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.44 (q, *J* = 8.0 Hz, 2H), 7.41-7.35 (m, 4H), 7.30 (t, *J* = 8.0 Hz, 3H) , 6.94 (q, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.13, 149.51, 146.20, 140.65, 136.45, 136.21, 131.16, 129.90, 129.30, 129.22, 128.38, 127.76, 127.34, 121.99, 119.80.

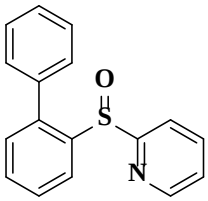


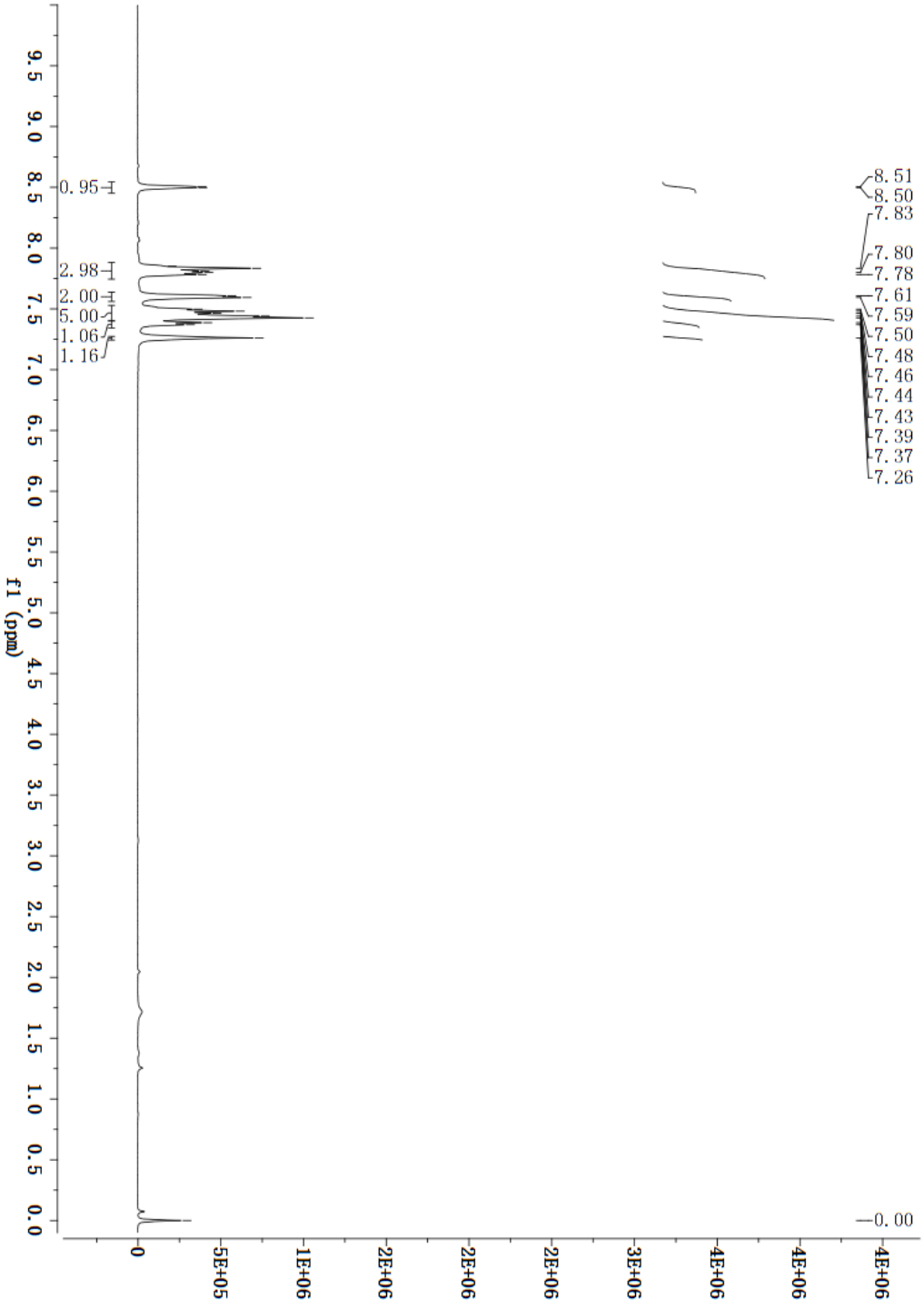
6[1]: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.52-7.49 (m, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.31-7.28 (m, 3H), 7.19-7.16 (m, 1H), 7.15 (t, *J* = 4.0 Hz, 1H), 7.13 (t, *J* = 4.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.15, 139.63, 134.90, 130.07, 129.51, 128.21, 128.19, 127.78, 127.01, 126.50.



7[4]: white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.64-8.62 (m, 1H), 7.71-7.69 (m, 1H), 7.47 (t, *J* = 4.0 Hz, 1H), 7.46-7.43 (m, 2H), 7.40-7.36 (m, 1H), 7.24-7.22 (m, 3H), 7.17-7.15 (m, 2H), 7.12-7.08 (m, 1H), 6.88 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.21, 149.39, 141.31, 140.58, 139.43, 135.17, 130.47, 130.45, 129.68, 128.50, 128.03, 127.62, 126.67, 125.38, 121.32.

3. NMR Charts


O
S
N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2.98
2.00
5.00
1.06
1.16
8.51
8.50
7.83
7.80
7.78
7.61
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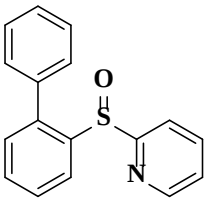
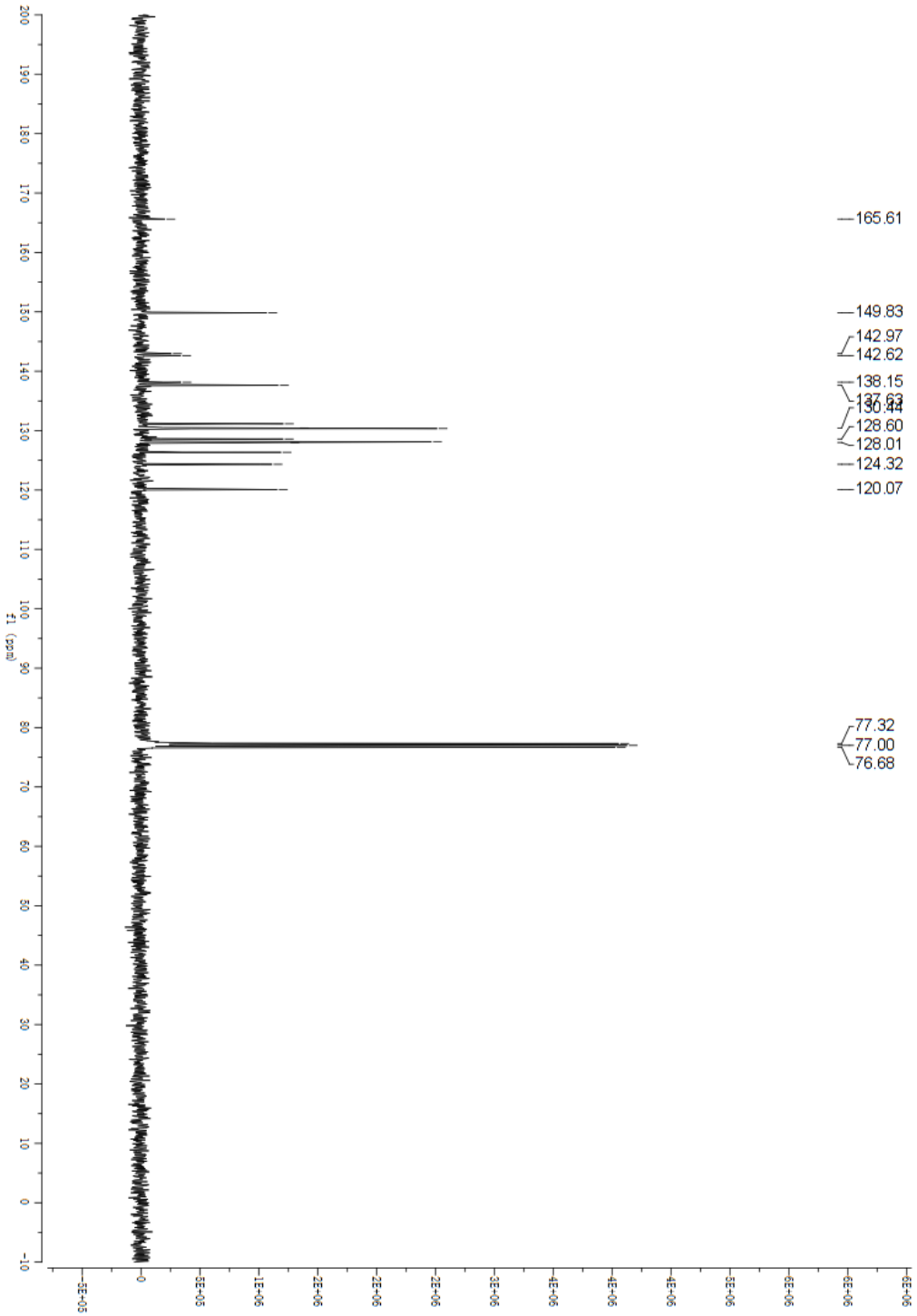
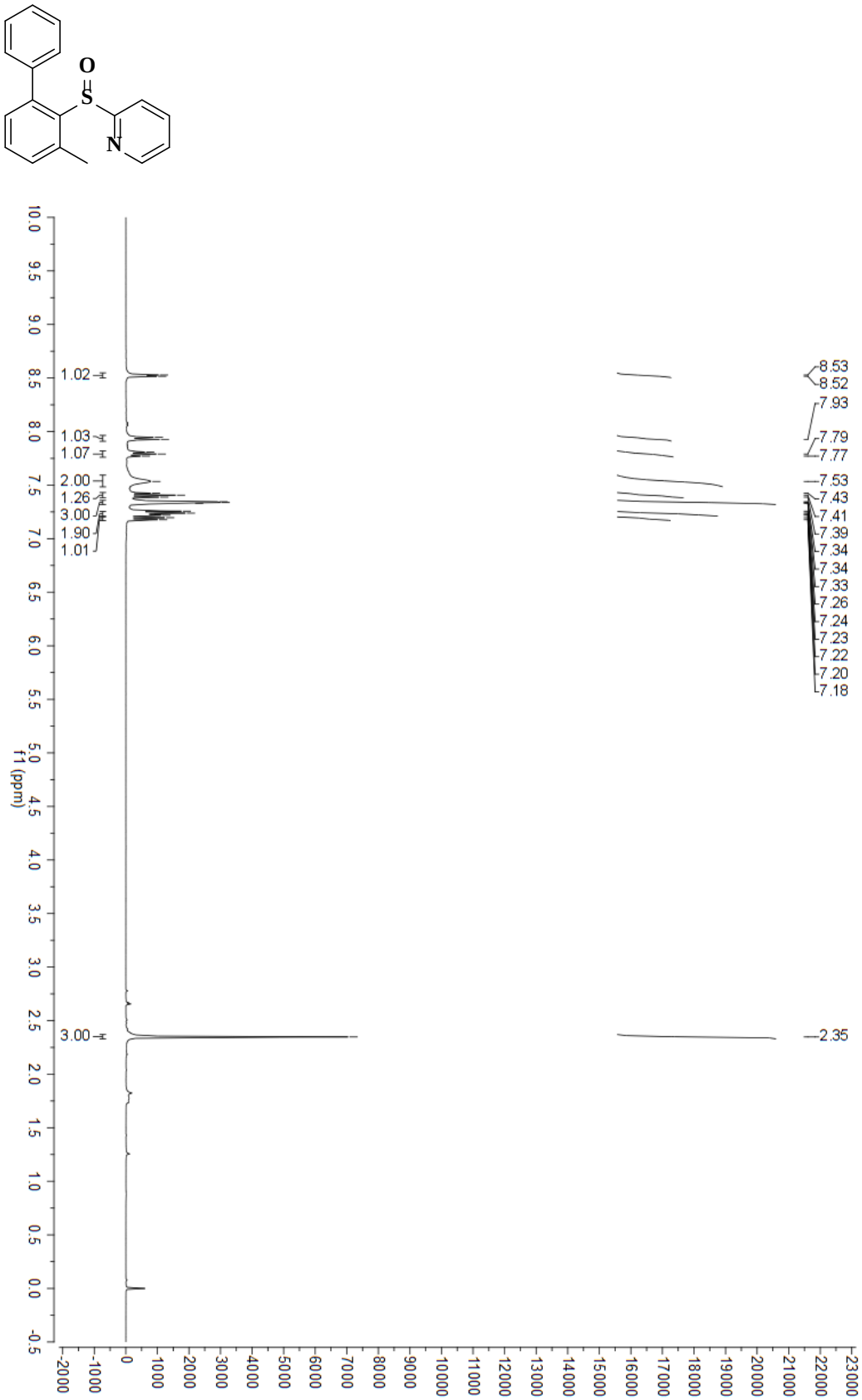
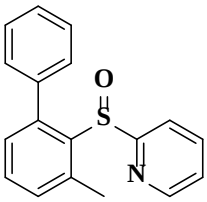
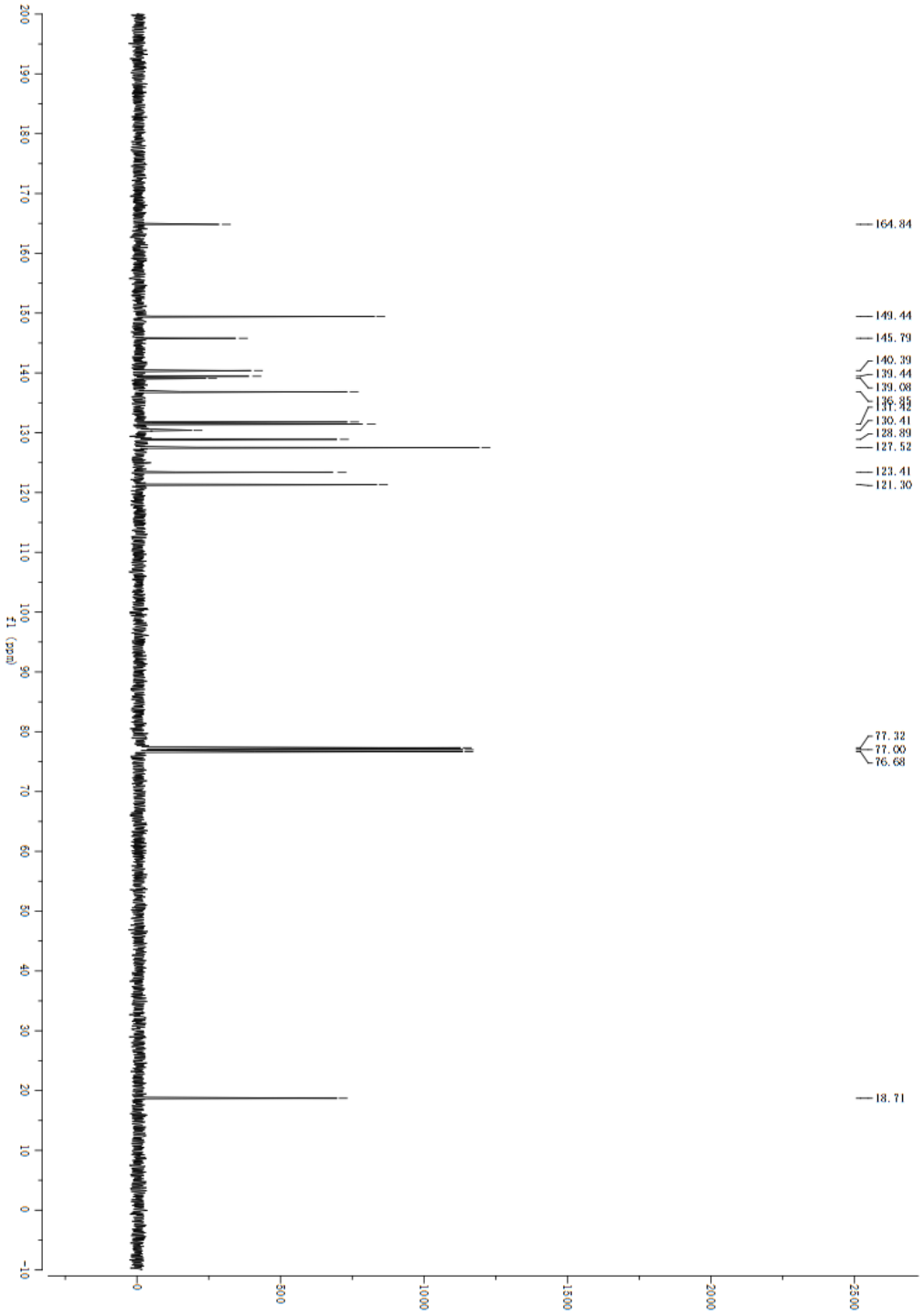
7.39
7.37
7.26
0.00
f1 (ppm)


O
S
N


165.61
149.83
142.97
142.62
138.15
137.63
130.44
128.60
128.01
124.32
120.07
77.32
77.00
76.68
f1 (ppm)


O
S
N
1.02
1.03
1.07
2.00
1.26
3.00
1.90
1.01
3.00
8.53
8.52
7.93
7.79
7.77
7.53
7.43
7.41
7.39
7.34
7.34
7.33
7.26
7.24
7.23
7.22
7.20
7.18
2.35
f1 (ppm)


O
S
N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149.44
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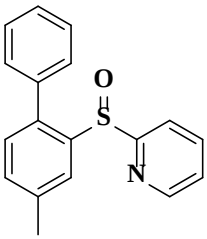
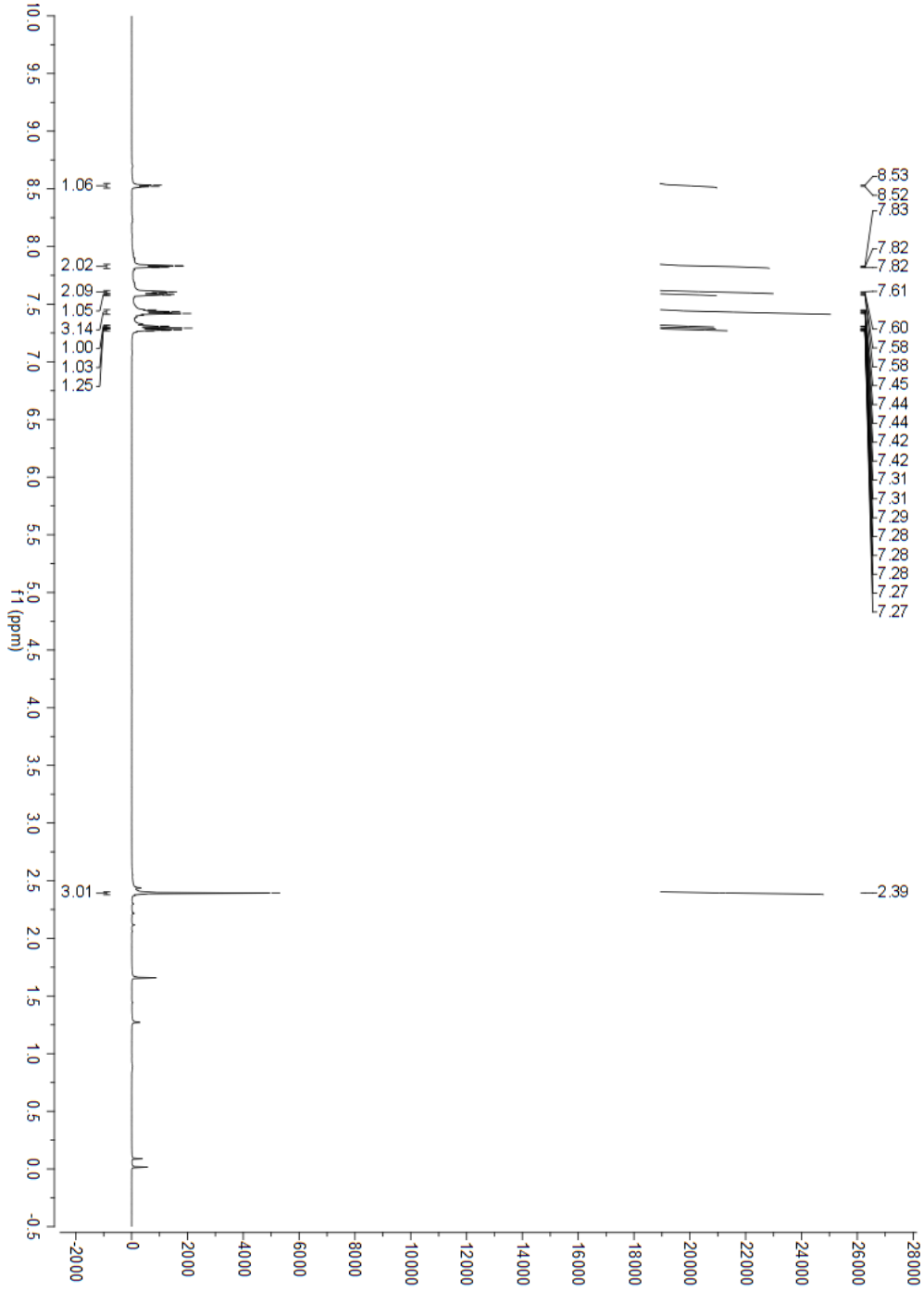
140.39
139.44
139.08
136.85
131.42
130.41
128.89
127.52
123.41
121.30
77.32
77.00
76.68
18.71
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
0
500
1000
1500
2000
2500


O
S
N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2.09
1.05
3.14
1.00
1.03
1.25
3.01
8.53
8.52
7.83
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7.82
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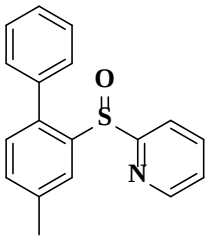
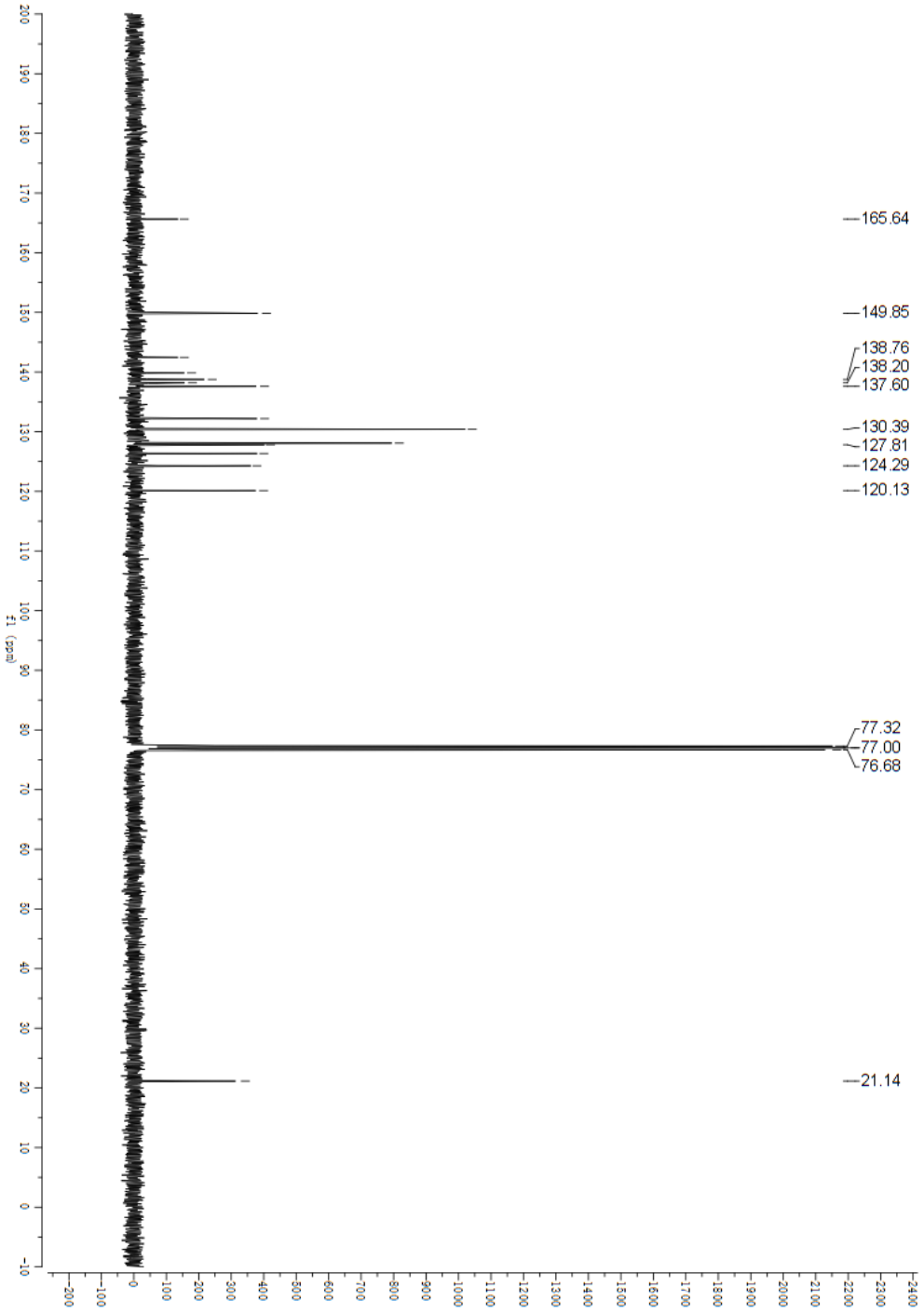
7.28
7.27
7.27
2.39
f1 (ppm)


O
S
N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138.20
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130.39
127.81
124.29
120.13
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77.00
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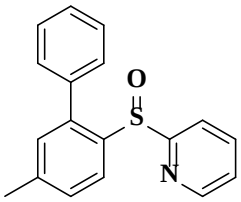
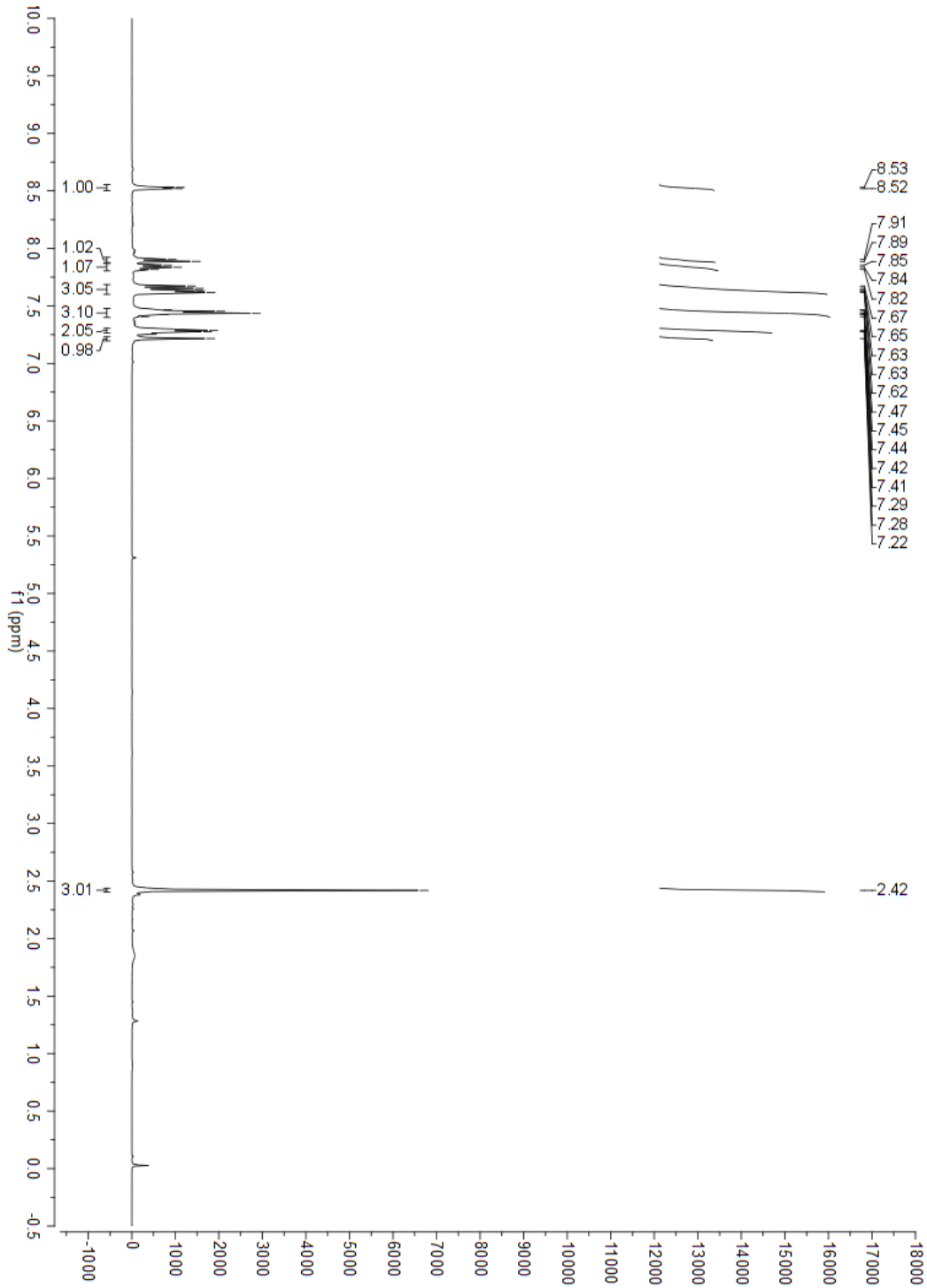
21.14
f1 (ppm)


O
S
N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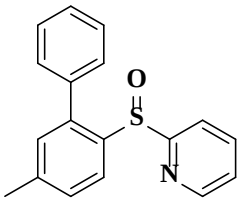
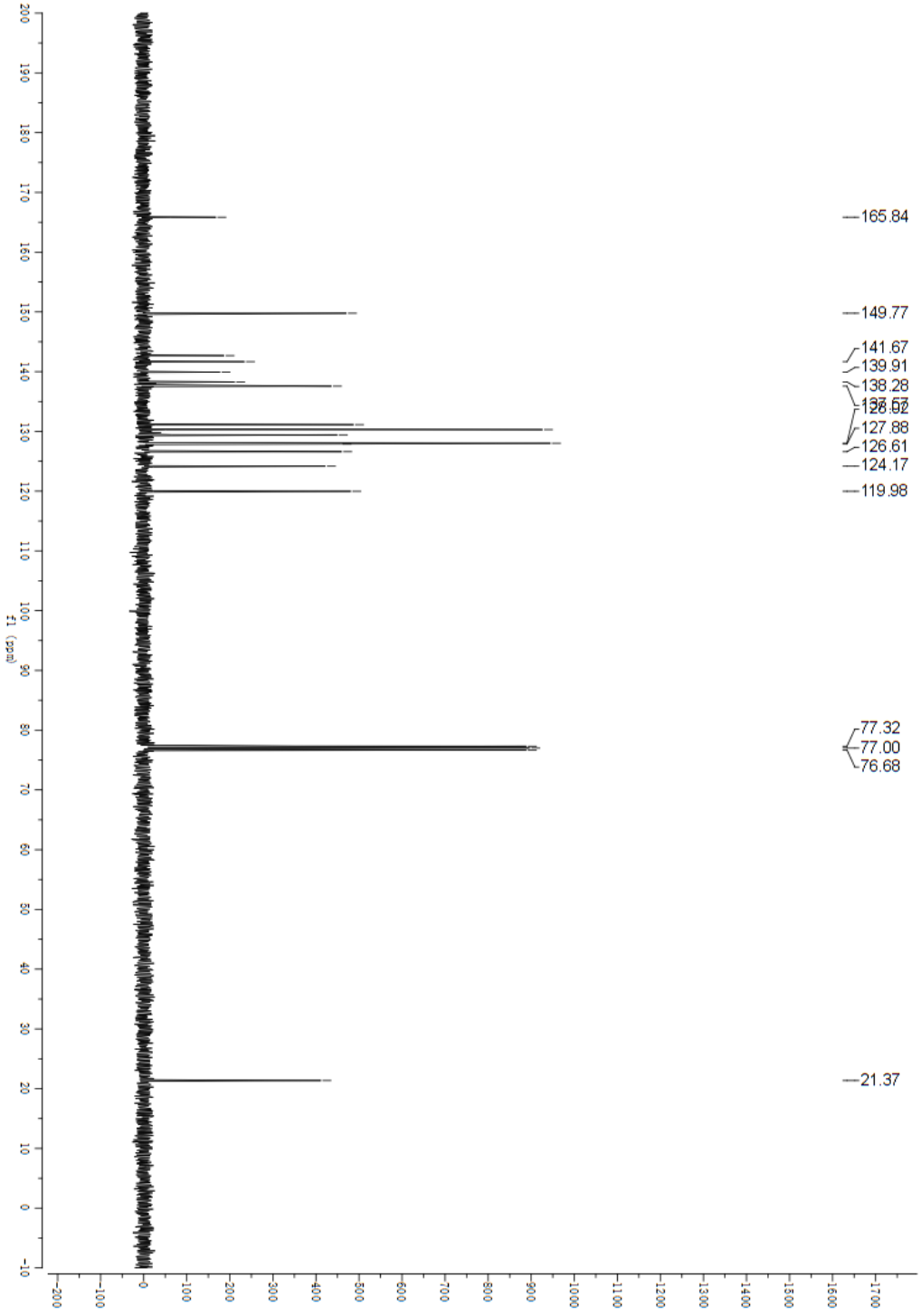
1.07
3.05
3.10
2.05
0.98
3.01
8.53
8.52
7.91
7.89
7.85
7.84
7.82
7.67
7.65
7.63
7.63
7.62
7.47
7.45
7.44
7.42
7.41
7.29
7.28
7.22
2.42
f1 (ppm)


O
S
N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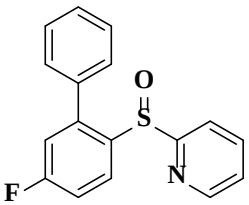
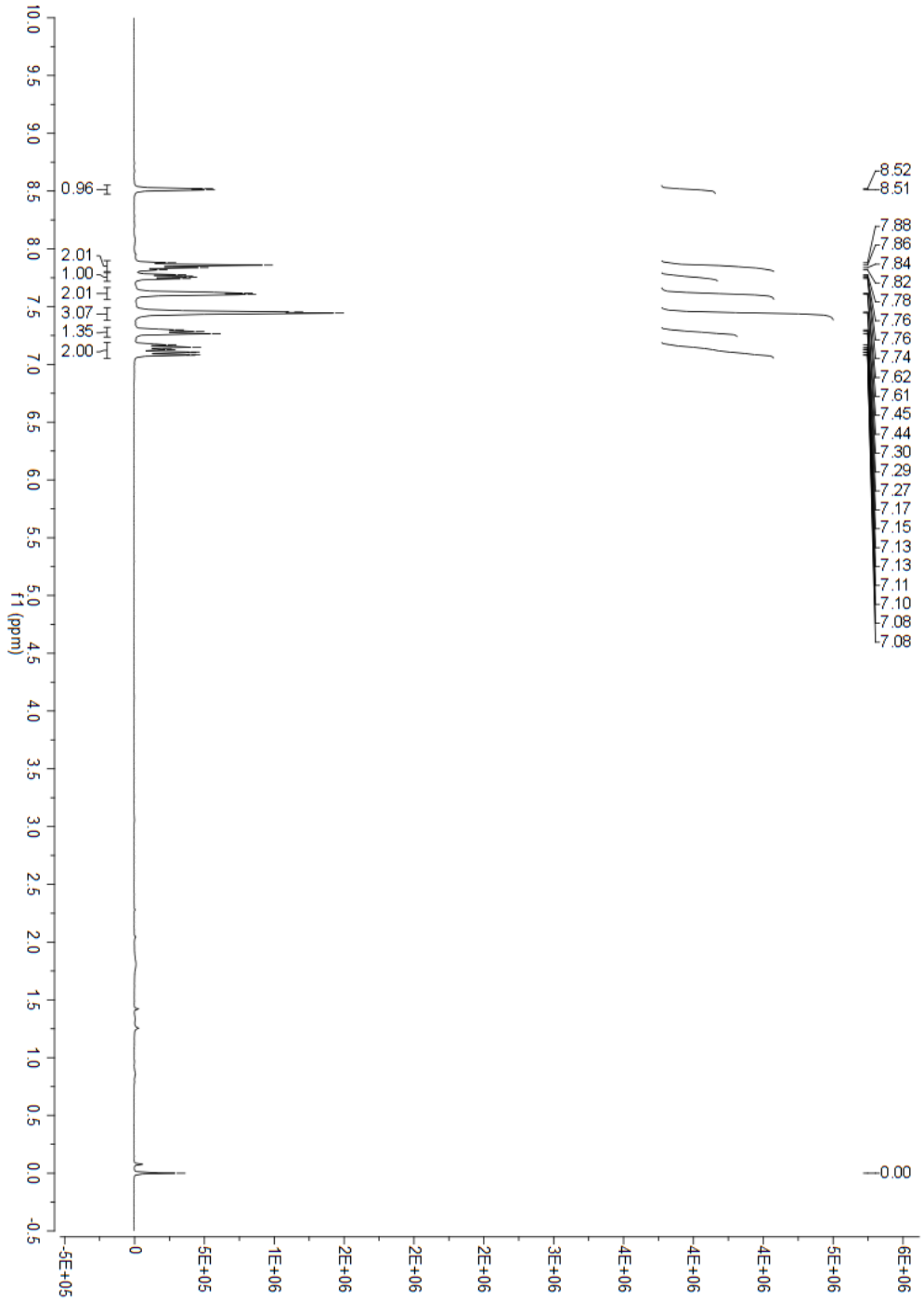
139.91
138.28
128.92
127.88
126.61
124.17
119.98
77.32
77.00
76.68
21.37
f1 (ppm)


O
S
N
F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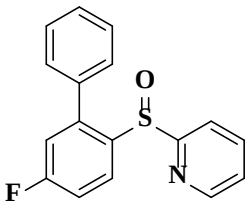
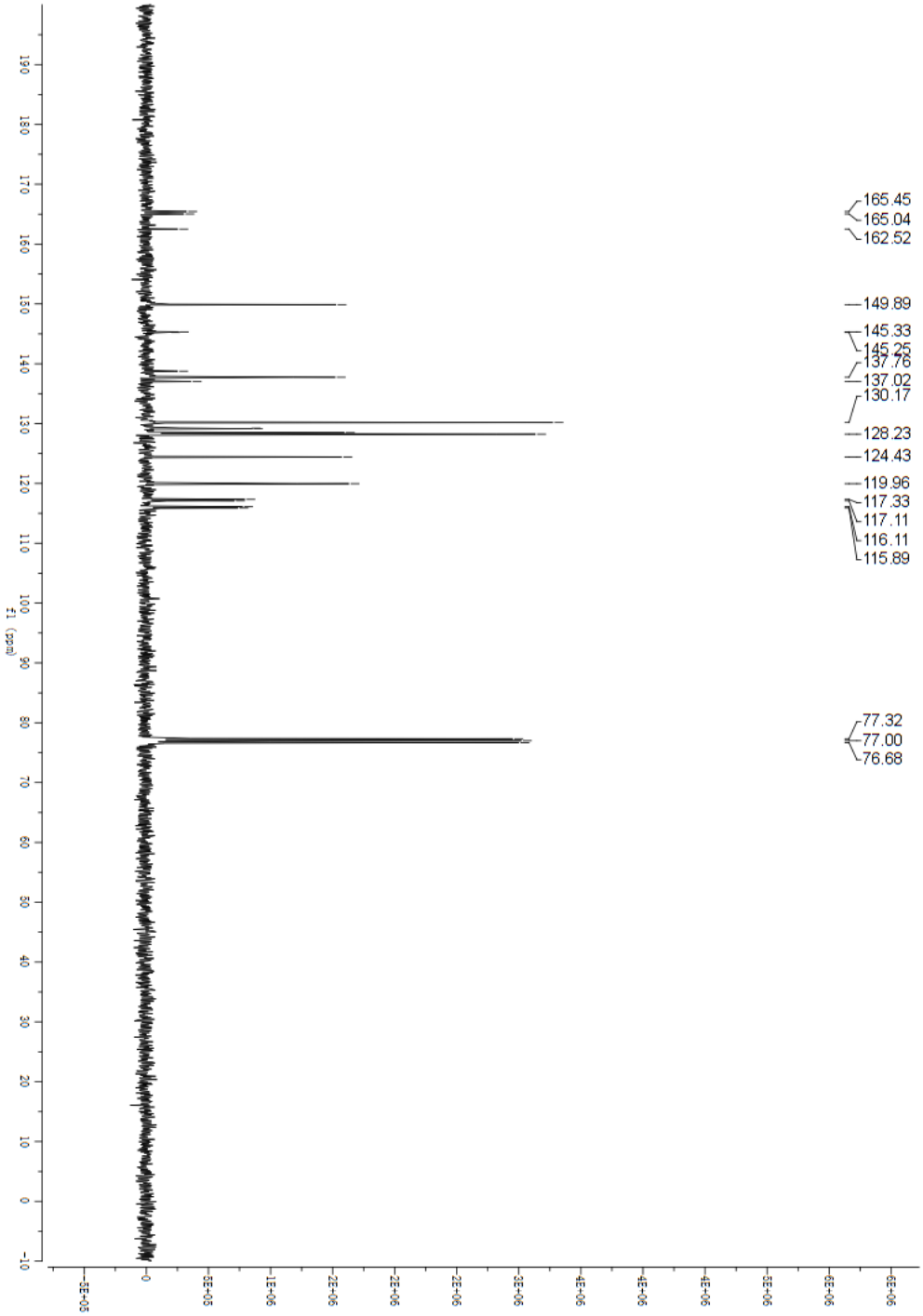
2.01
3.07
1.35
2.00
8.52
8.51
7.88
7.86
7.84
7.82
7.78
7.76
7.76
7.74
7.62
7.61
7.45
7.44
7.30
7.29
7.27
7.17
7.15
7.13
7.13
7.11
7.10
7.08
7.08
0.00
f1 (ppm)


O
S
N
F


165.45
165.04
162.52
149.89
145.33
145.25
137.76
137.02
130.17
128.23
124.43
119.96
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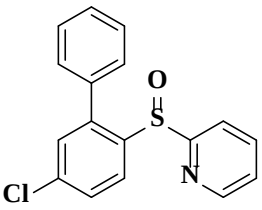
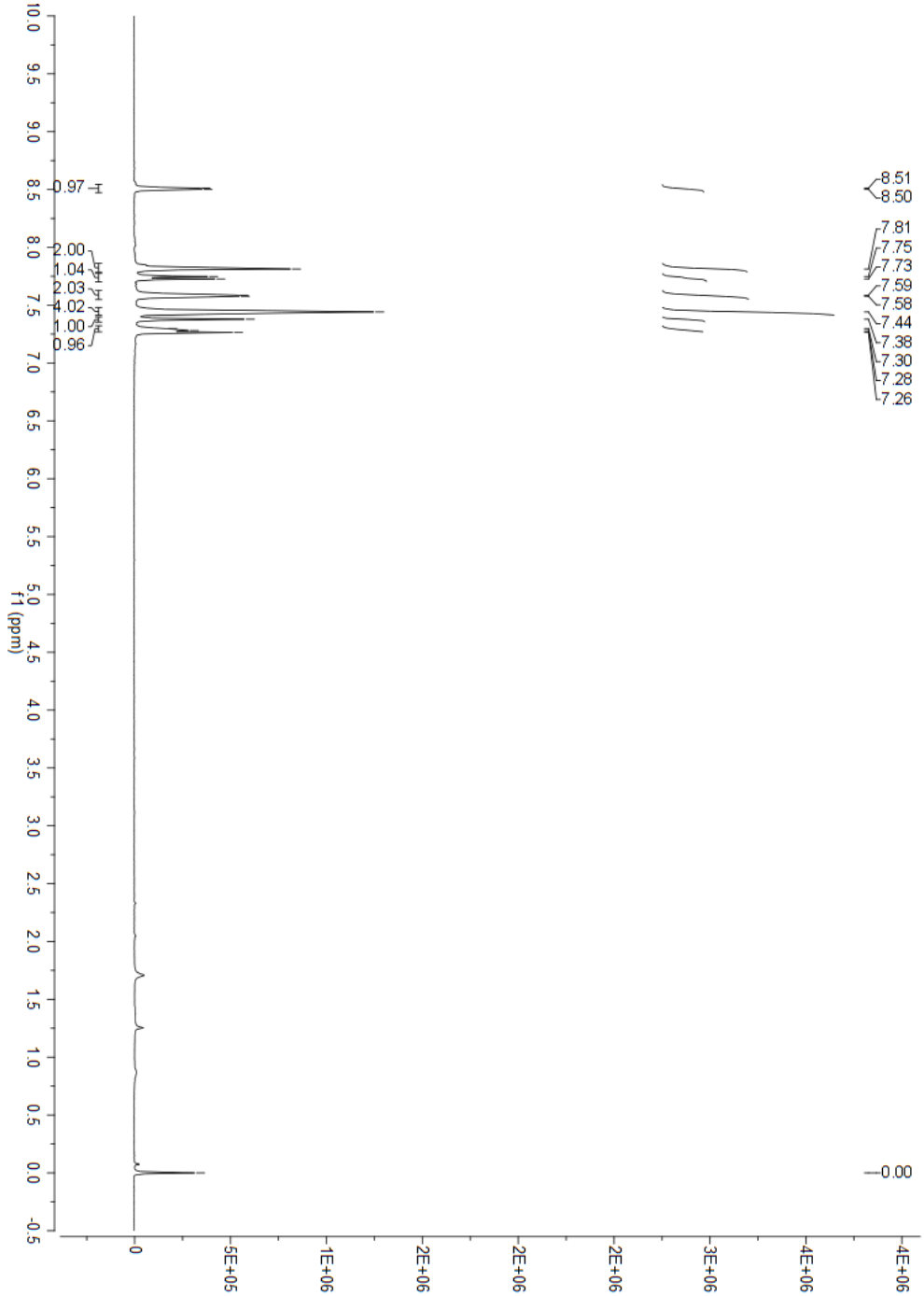
117.11
116.11
115.89
77.32
77.00
76.68
f1 (ppm)


O
S
N
Cl


8.51
8.50
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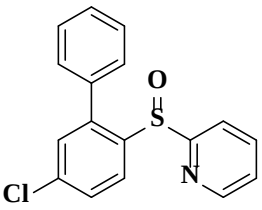
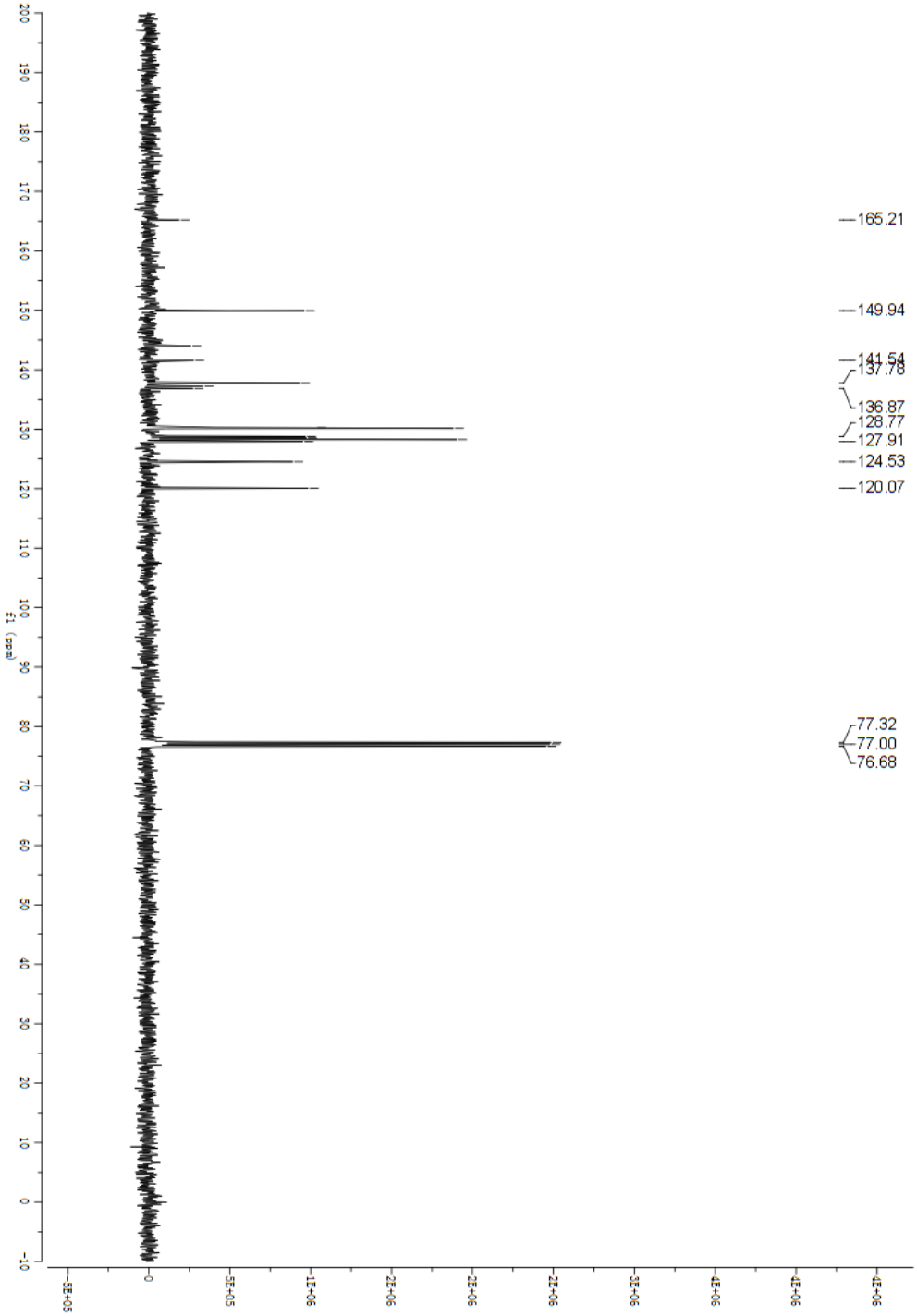
7.75
7.73
7.59
7.58
7.44
7.38
7.30
7.28
7.26
0.97
2.00
1.04
2.03
4.02
1.00
0.96
0.00
f1 (ppm)


O
S
N
Cl


165.21
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141.54
137.78
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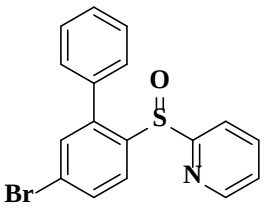
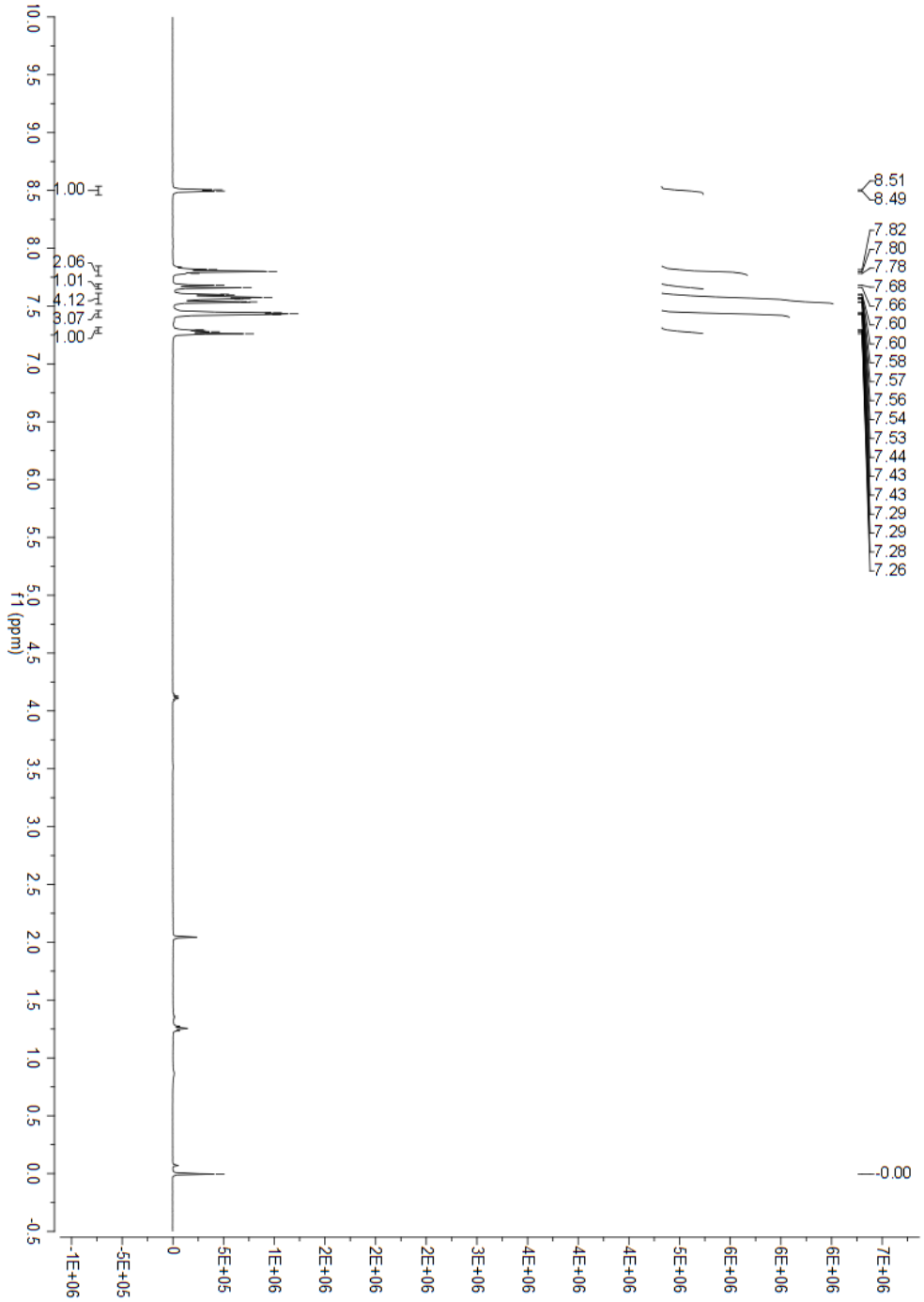
128.77
127.91
124.53
120.07
77.32
77.00
76.68
f1 (ppm)


O
S
N
Br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2.06
1.01
4.12
3.07
1.00
8.51
8.49
7.82
7.80
7.78
7.68
7.66
7.60
7.60
7.58
7.57
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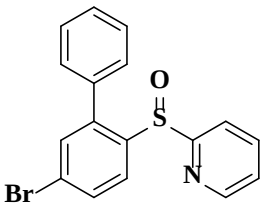
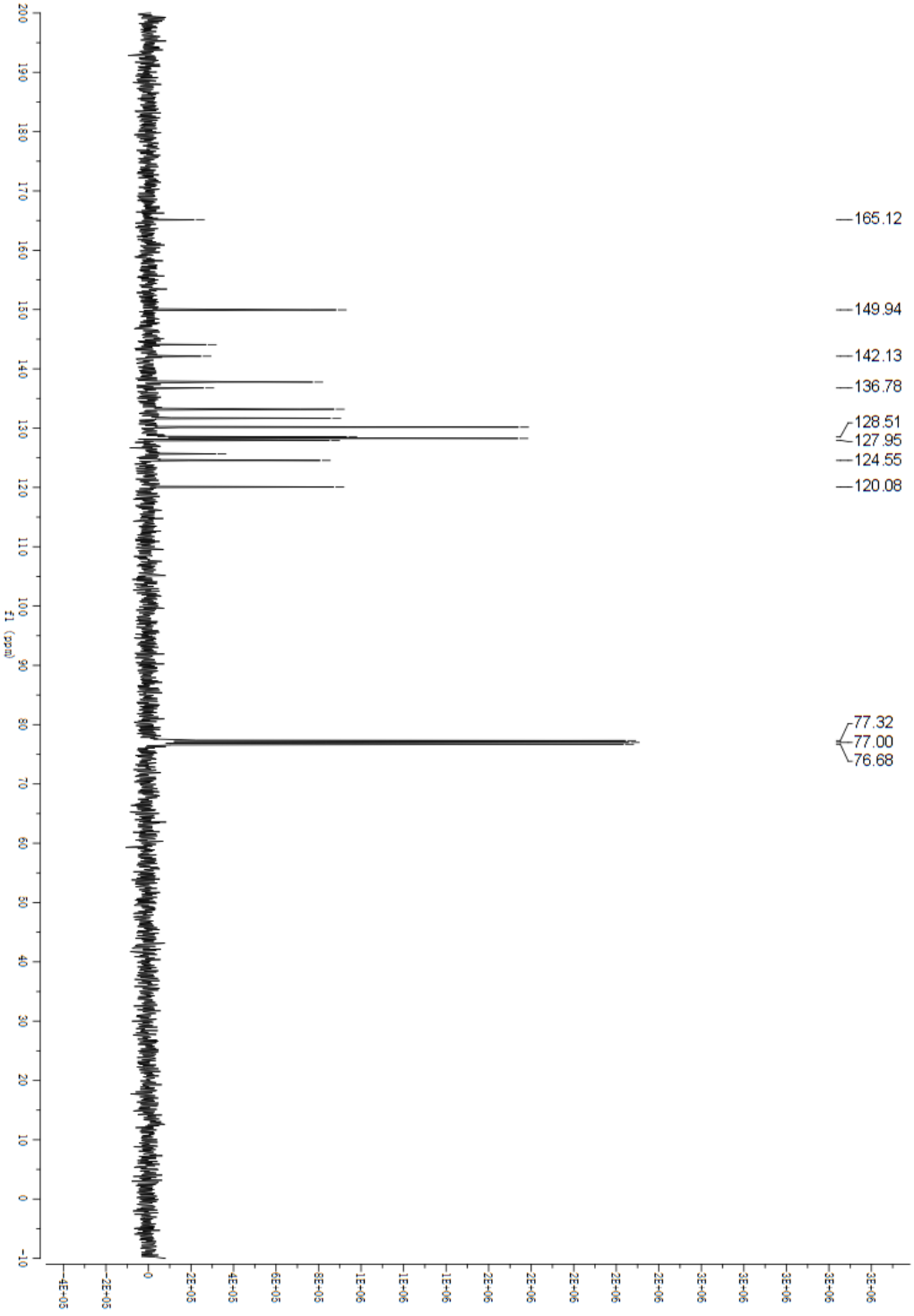
7.29
7.28
7.26
-0.00
f1 (ppm)


O
S
N
Br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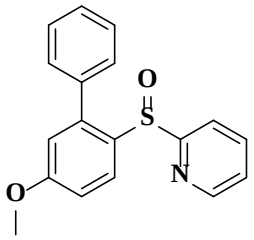
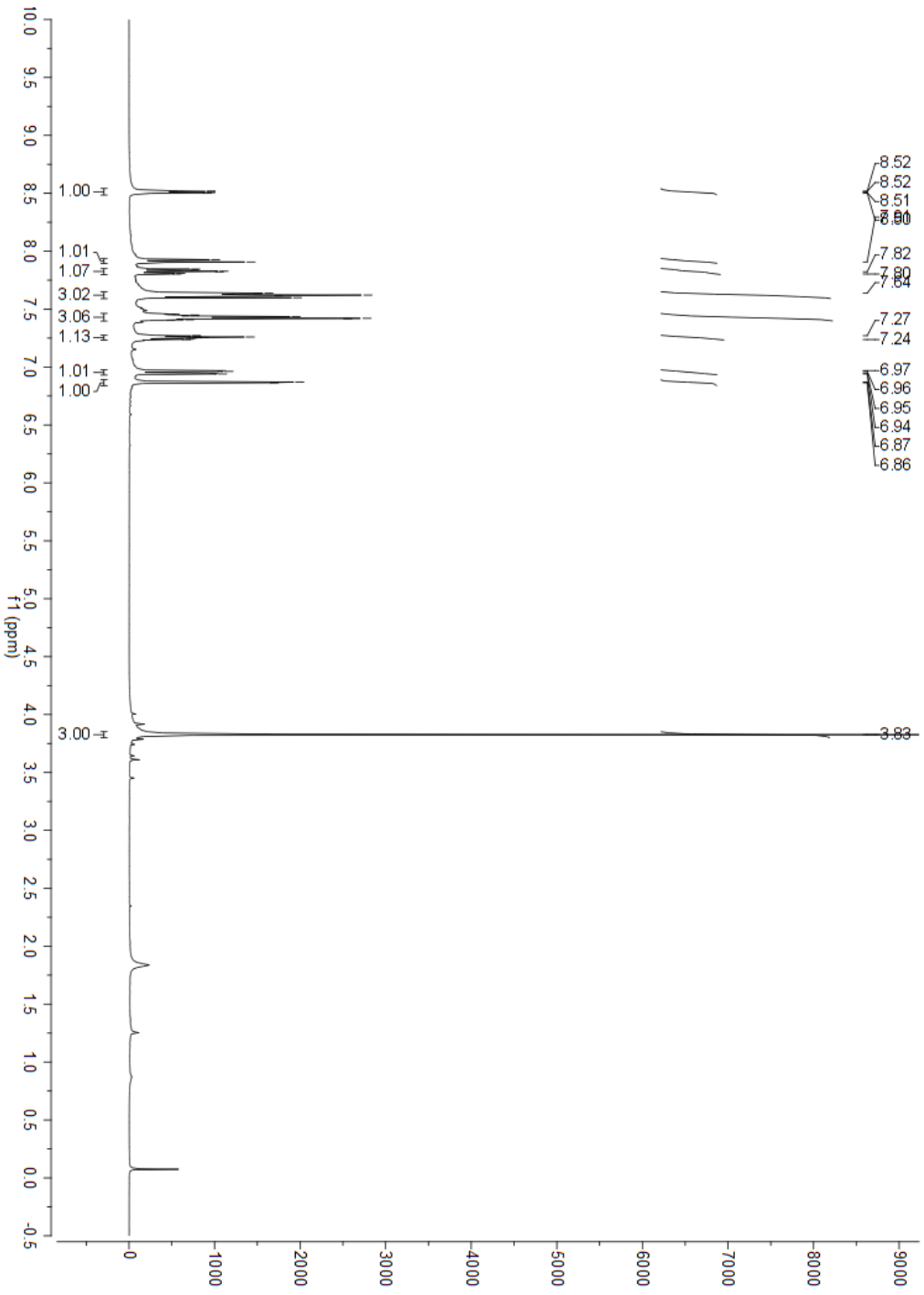
149.94
142.13
136.78
128.51
127.95
124.55
120.08
77.32
77.00
76.68
f1 (ppm)


O
S
N
O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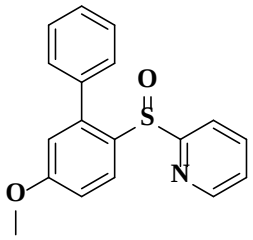
1.01
1.07
3.02
3.06
1.13
1.01
1.00
3.00
8.52
8.52
8.51
7.82
7.80
7.64
7.27
7.24
6.97
6.96
6.95
6.94
6.87
6.86
3.83
f1 (ppm)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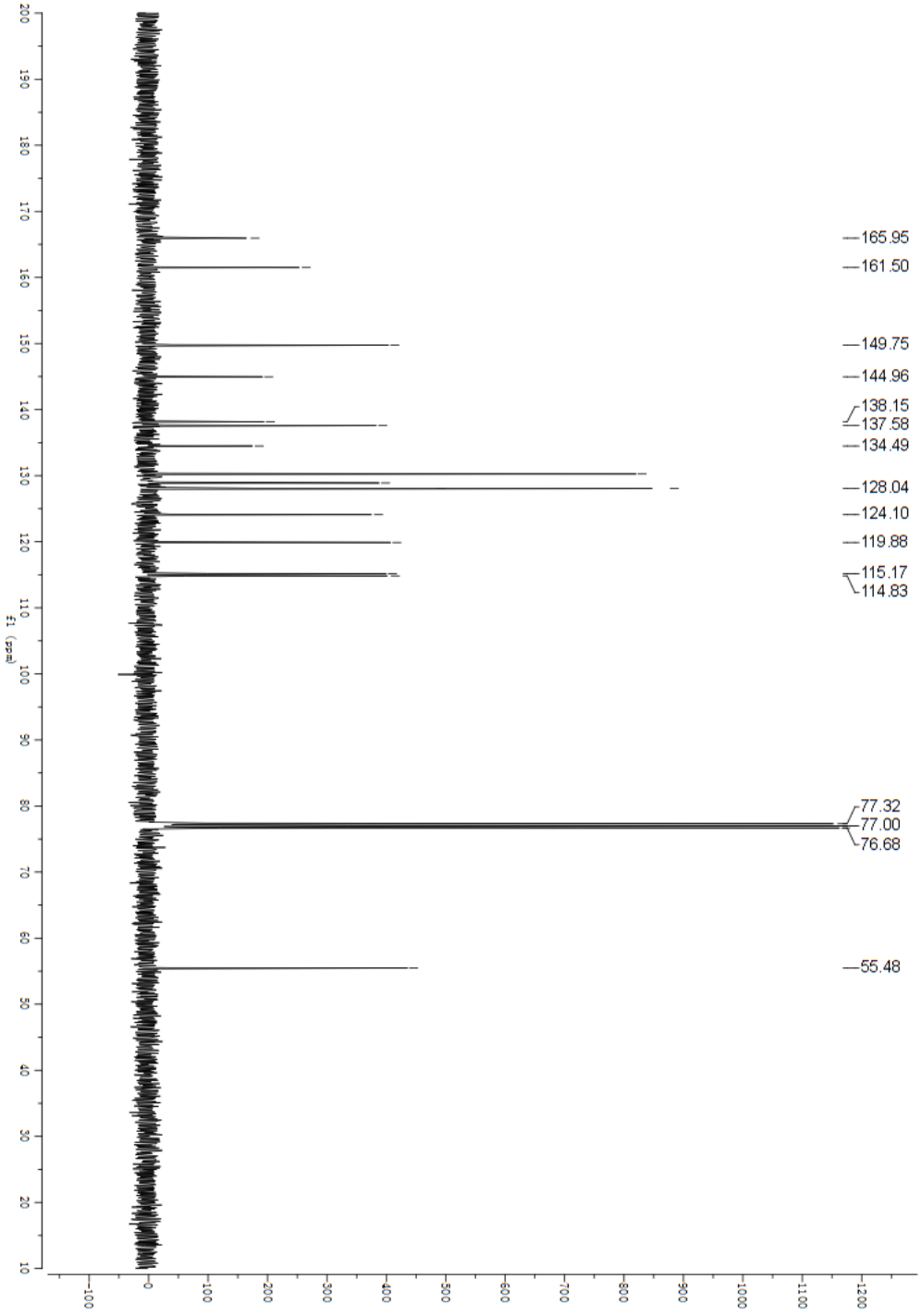
S
N
O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144.96
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134.49
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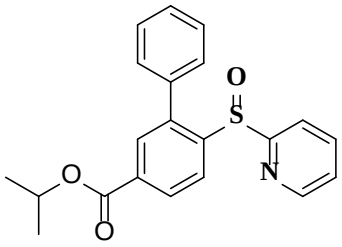
124.10
119.88
115.17
114.83
77.32
77.00
76.68
55.48
f1 (ppm)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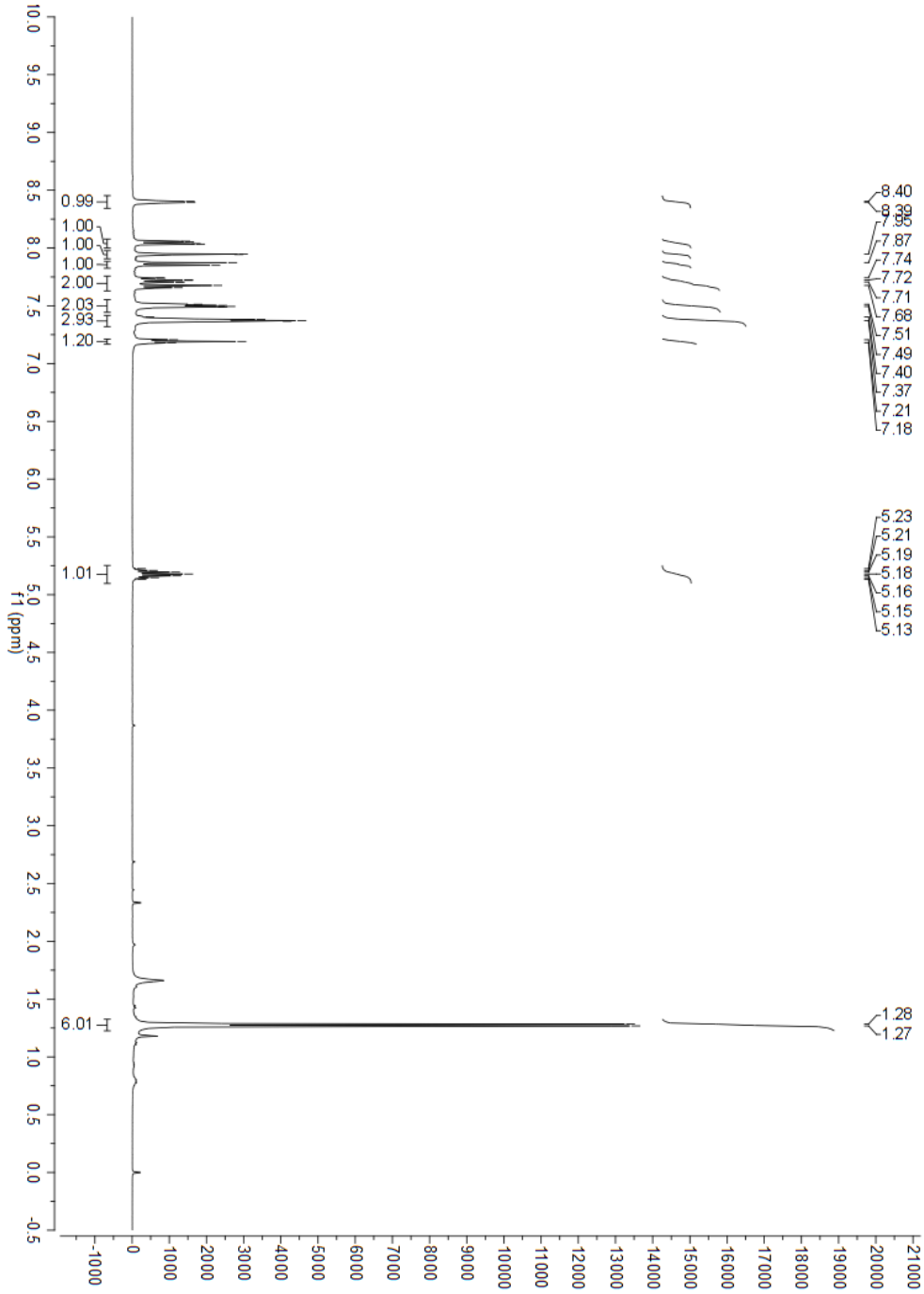
S
N
O
O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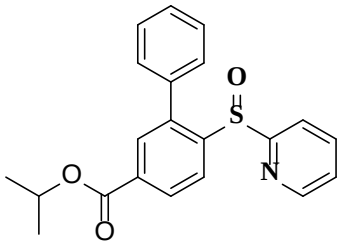
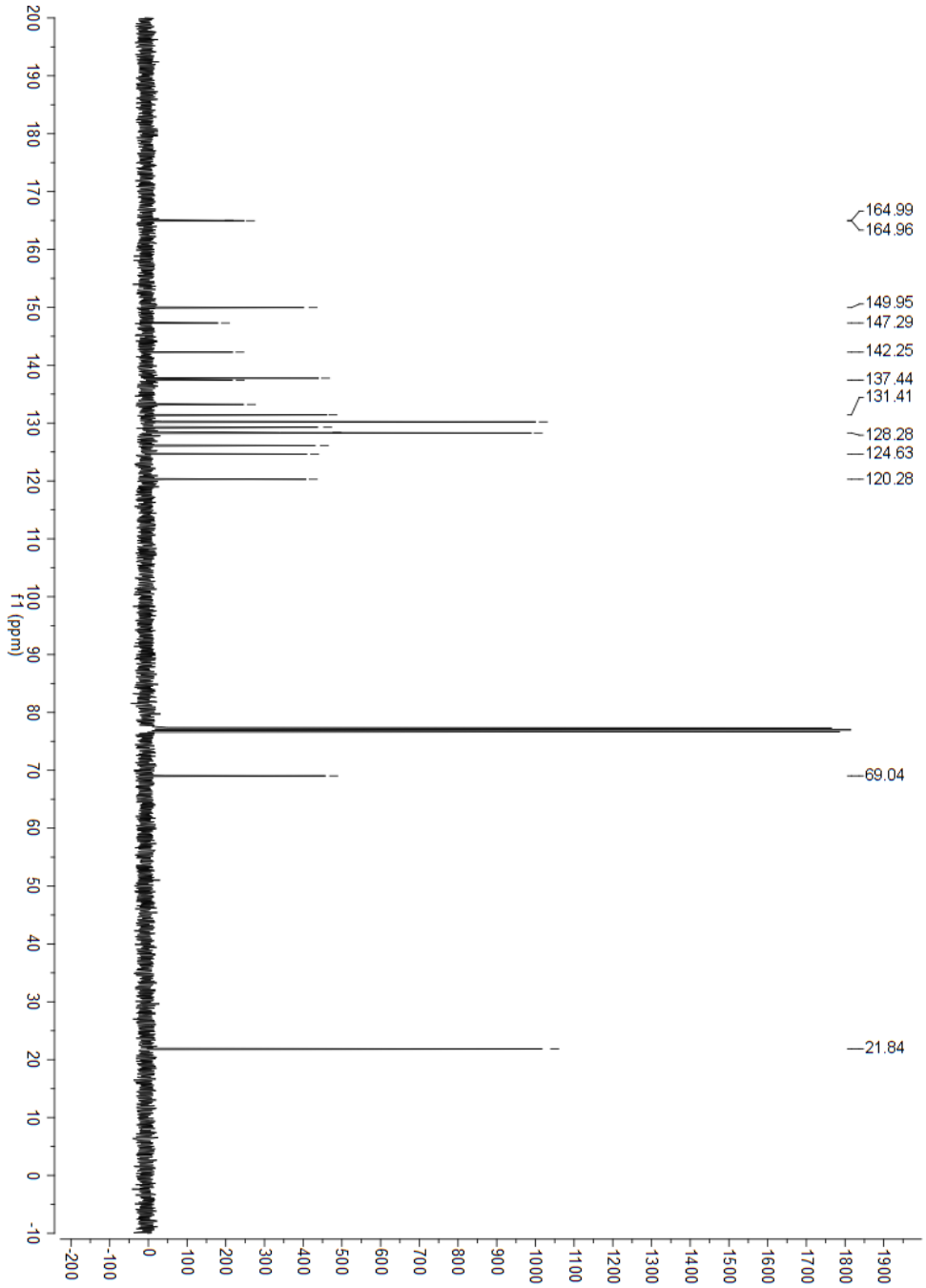
1.00
1.00
1.00
2.00
2.03
2.93
1.20
1.01
6.01
8.40
8.39
7.95
7.87
7.74
7.72
7.71
7.68
7.51
7.49
7.40
7.37
7.21
7.18
5.23
5.21
5.19
5.18
5.16
5.15
5.13
1.28
1.27
f1 (ppm)


O
S
N
O
O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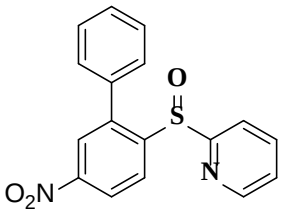
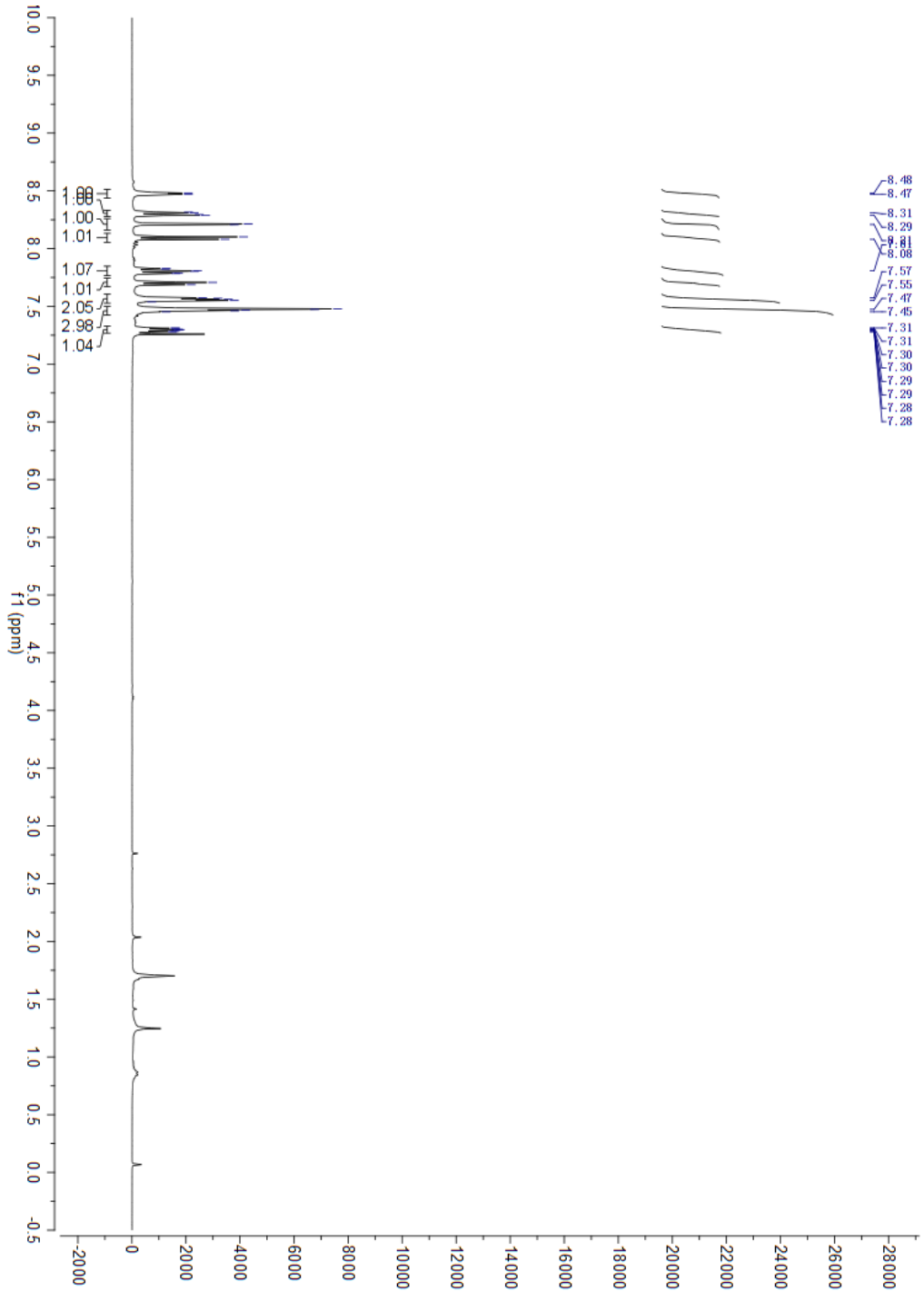
164.96
149.95
147.29
142.25
137.44
131.41
128.28
124.63
120.28
69.04
21.84
f1 (ppm)


O
S
N
O2N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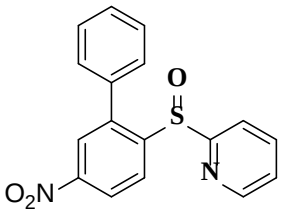
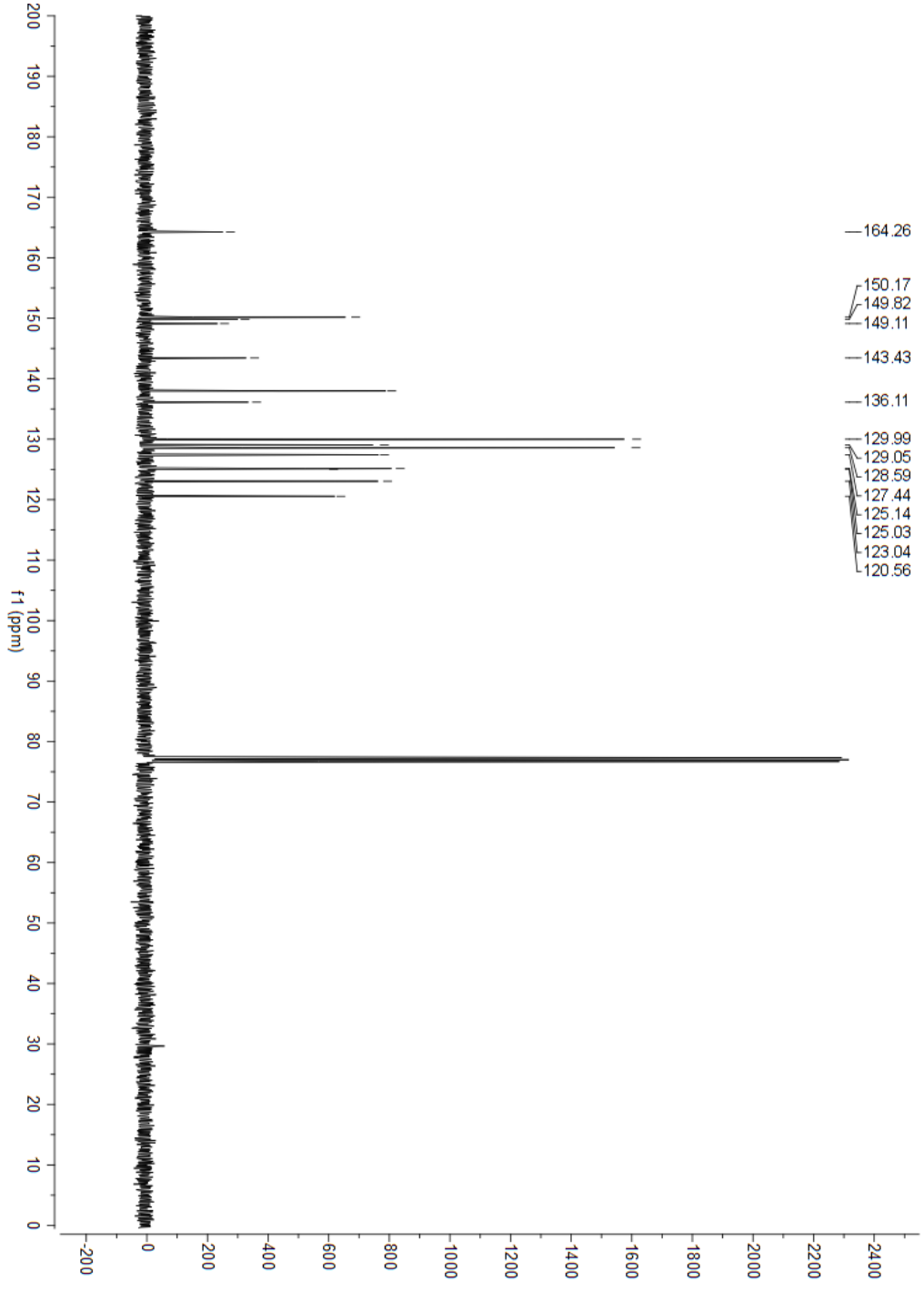
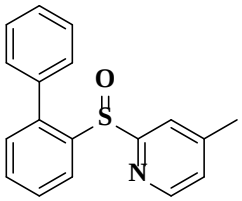
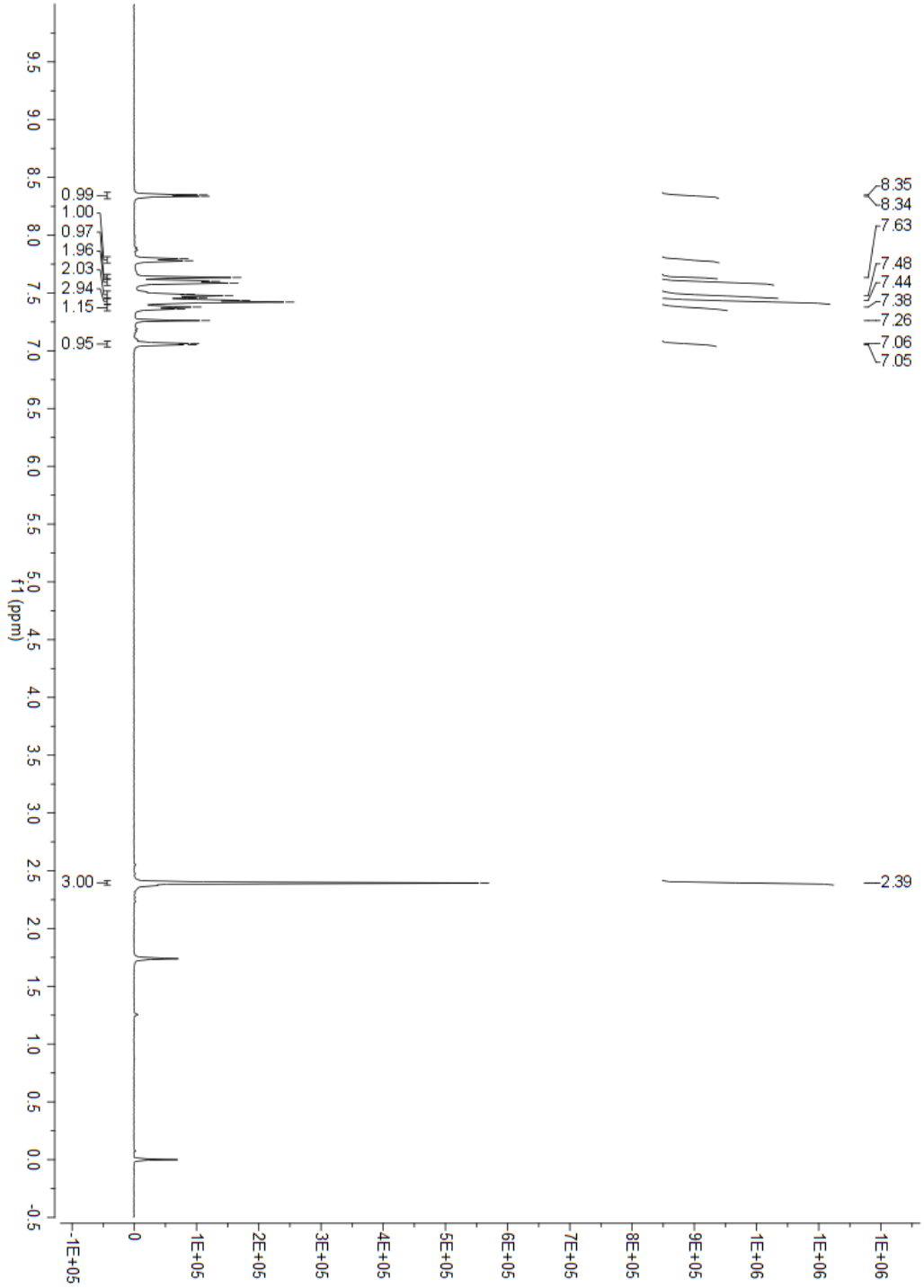
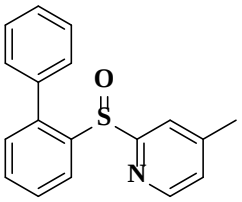
1.00
1.01
1.07
1.01
2.05
2.98
1.04
8.48
8.47
8.31
8.29
8.08
7.57
7.55
7.47
7.45
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.28
f1 (ppm)

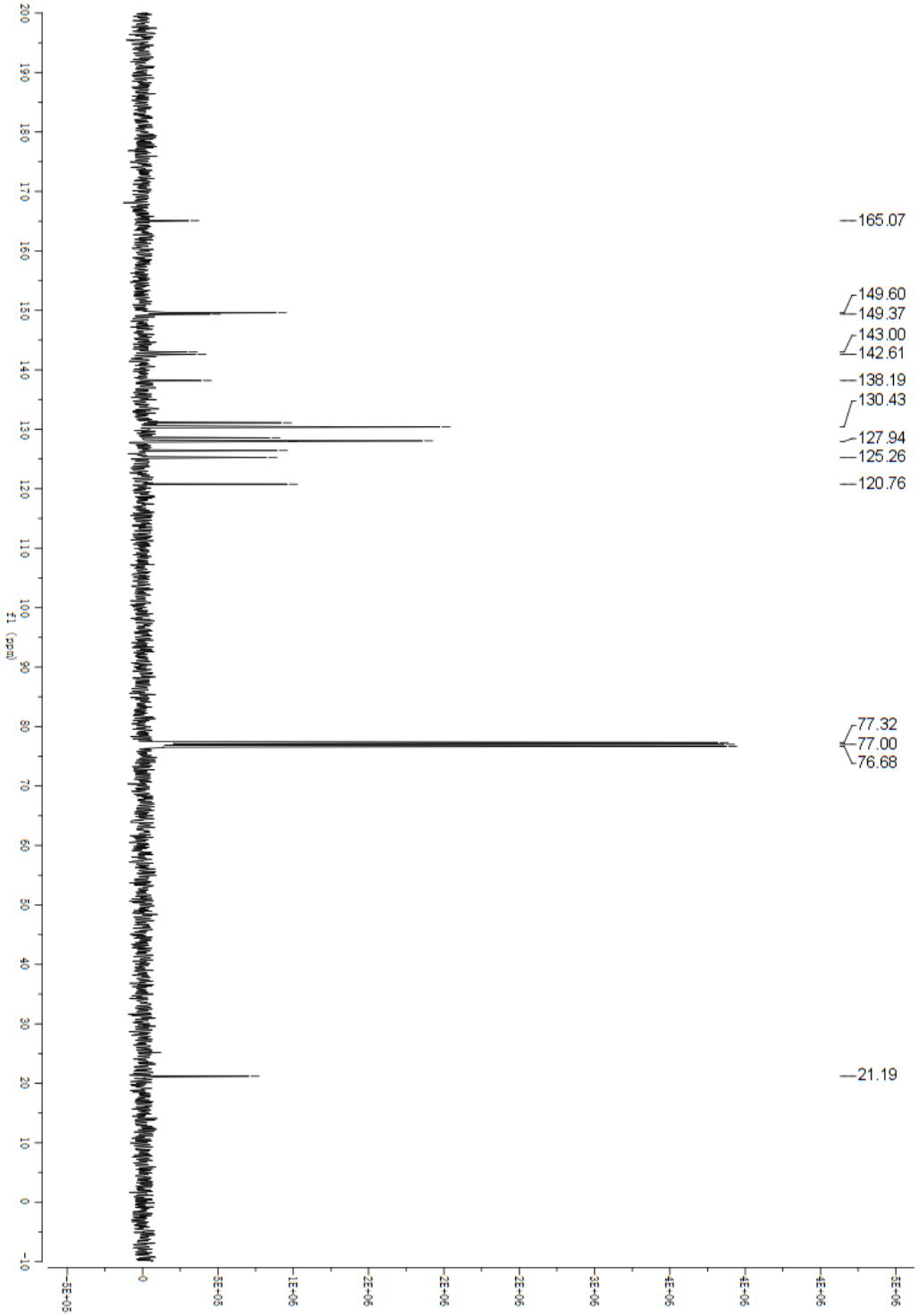

O
S
N
O2N

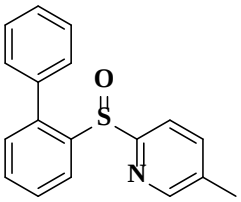

164.26
150.17
149.82
149.11
143.43
136.11
129.99
129.05
128.59
127.44
125.14
125.03
123.04
120.56
f1 (ppm)

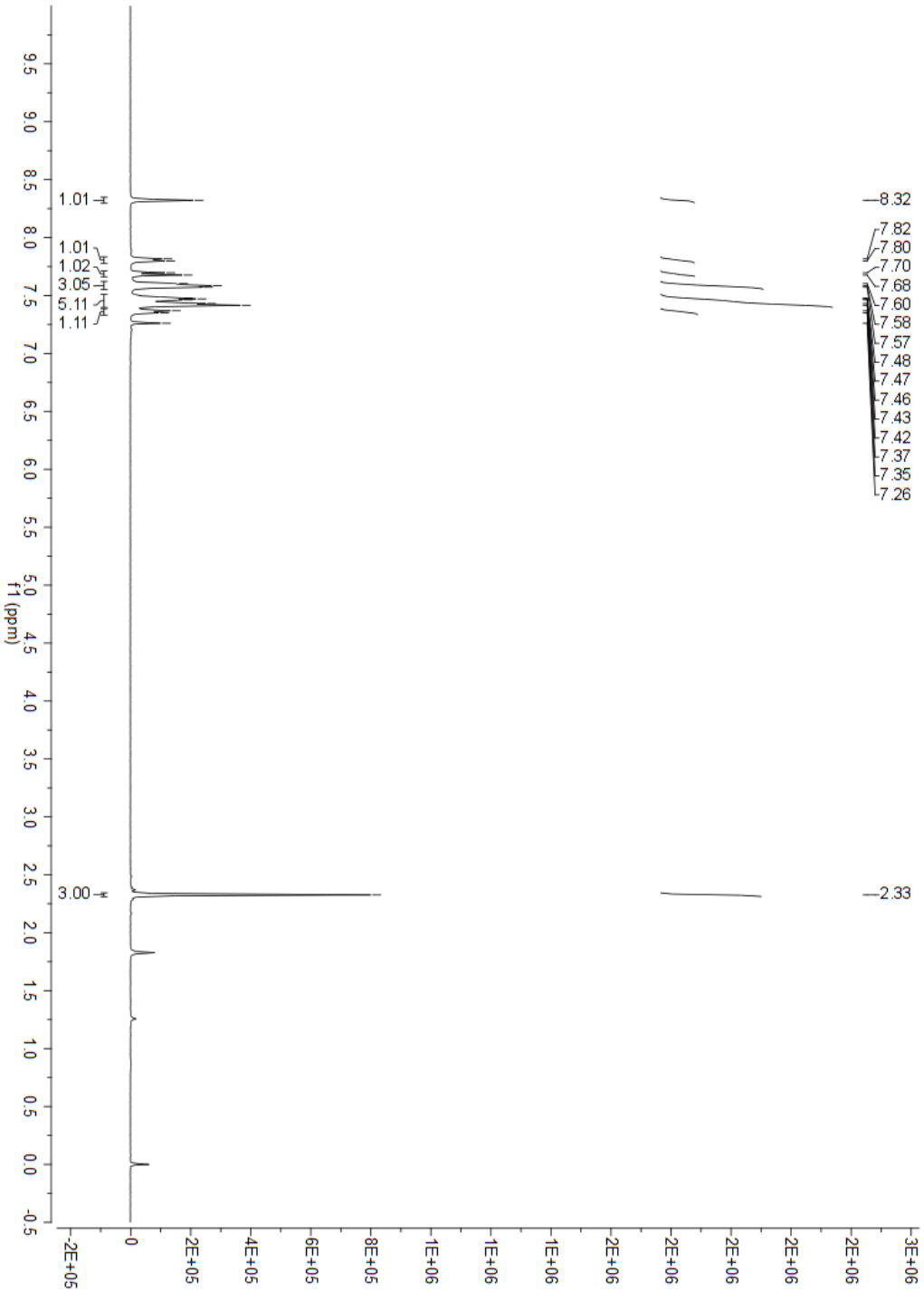

O
S
N

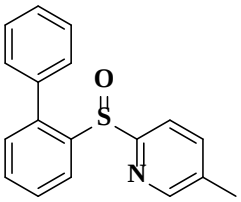

0.99
1.00
0.97
1.96
2.03
2.94
1.15
0.95
3.00
8.35
8.34
7.63
7.48
7.44
7.38
7.26
7.06
7.05
2.39
f1 (ppm)

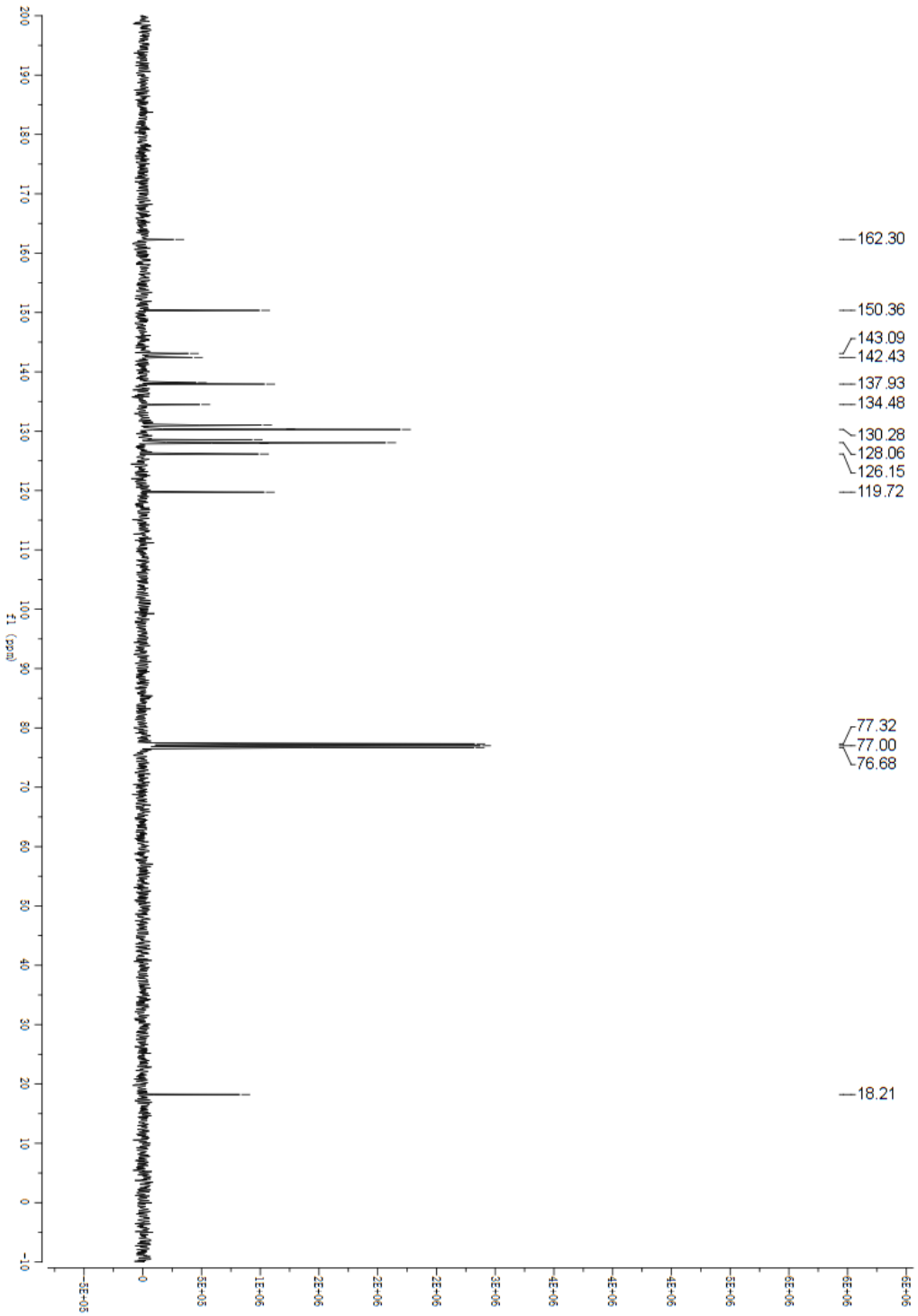

O
S
N


165.07
149.60
149.37
143.00
142.61
138.19
130.43
127.94
125.26
120.76
77.32
77.00
76.68
21.19
f1 (ppm)


O
S
N


1.01
1.01
1.02
3.05
5.11
1.11
3.00
8.32
7.82
7.80
7.70
7.68
7.60
7.58
7.57
7.48
7.47
7.46
7.43
7.42
7.37
7.35
7.26
2.33
f1 (ppm)


O
S
N


f1 (ppm)
162.30
150.36
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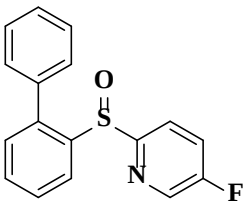
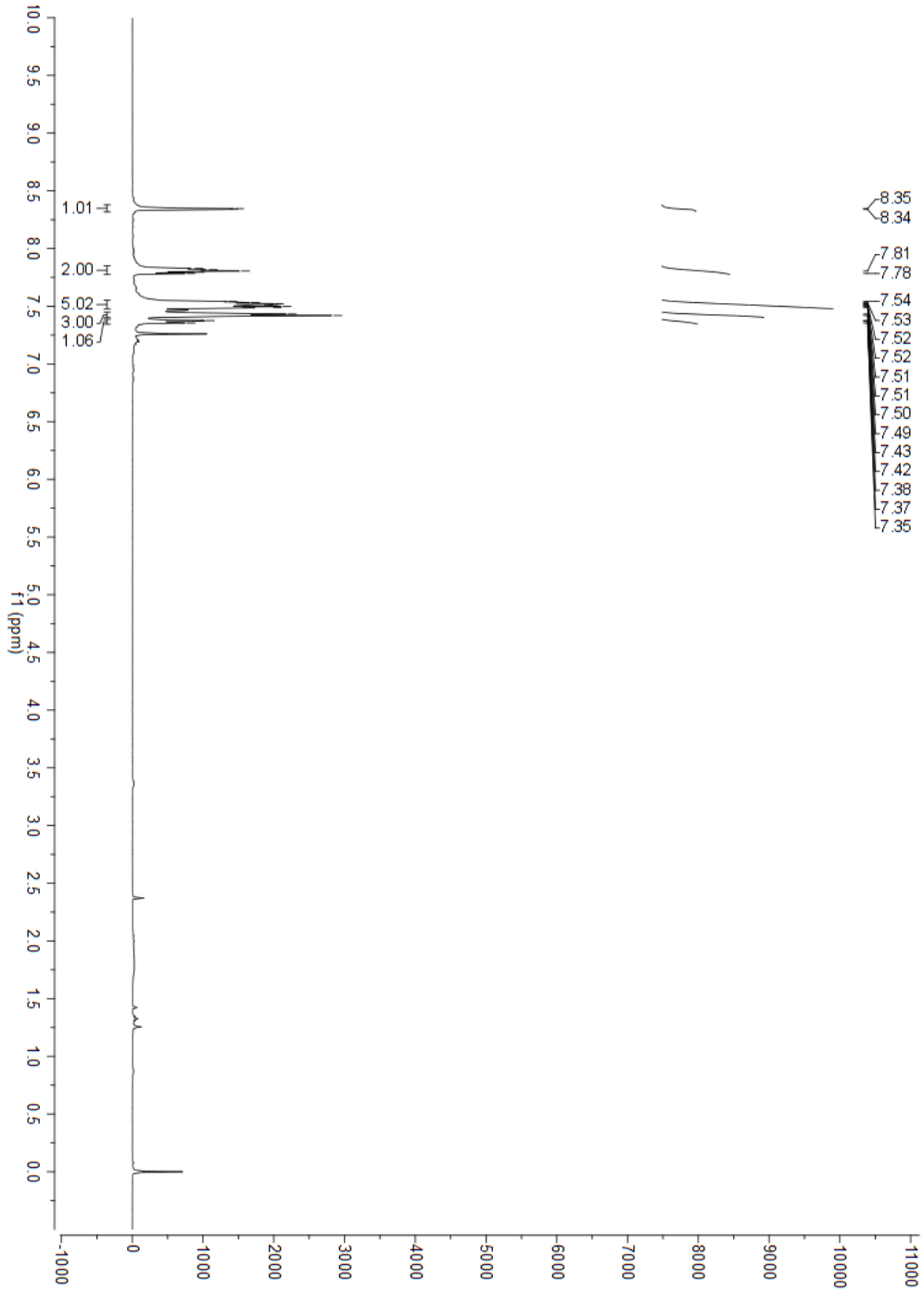
137.93
134.48
130.28
128.06
126.15
119.72
77.32
77.00
76.68
18.21


O
S
N
F


1.01
2.00
5.02
3.00
1.06
8.35
8.34
7.81
7.78
7.54
7.53
7.52
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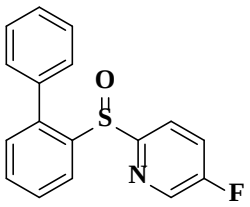
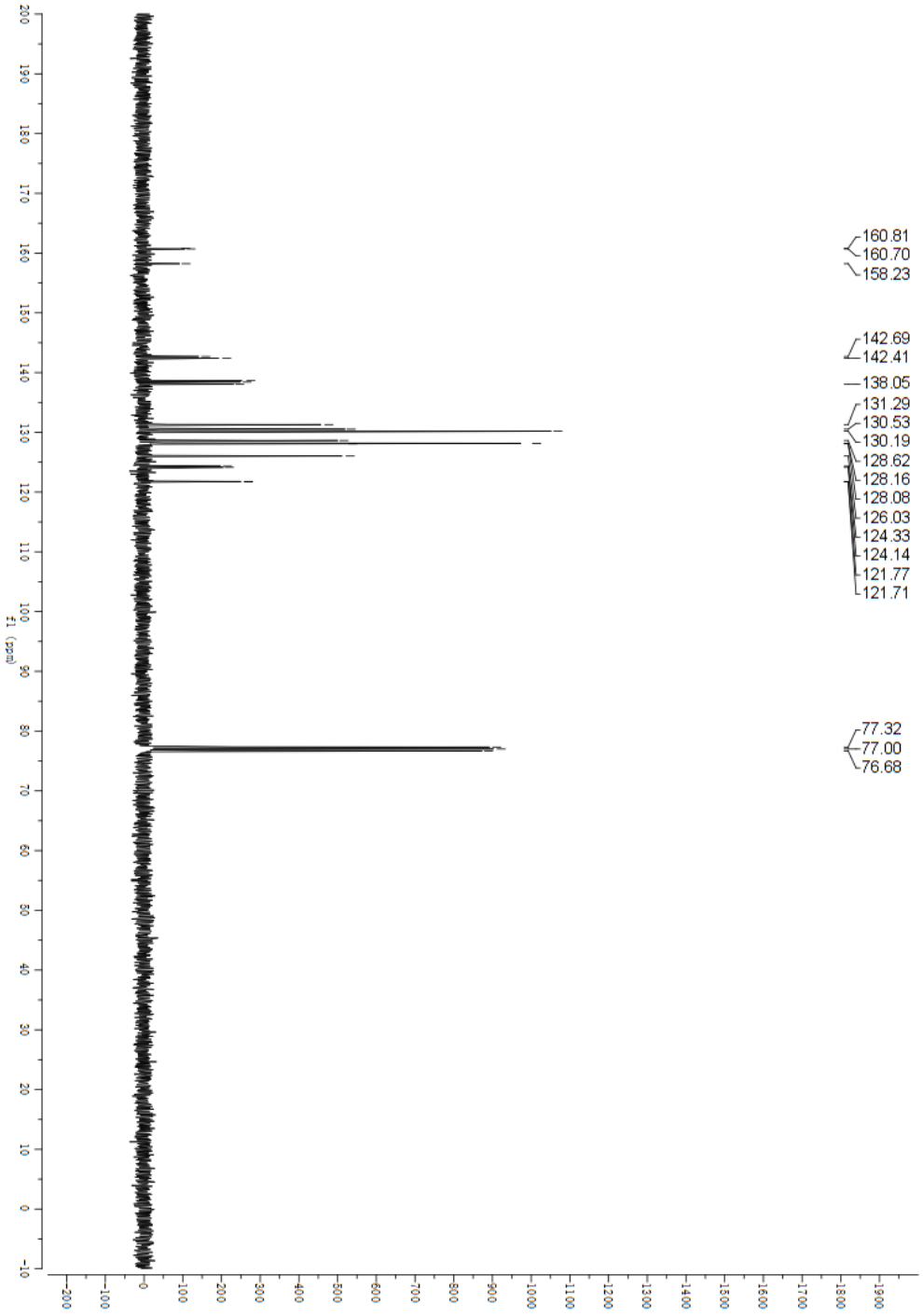
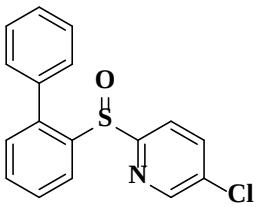
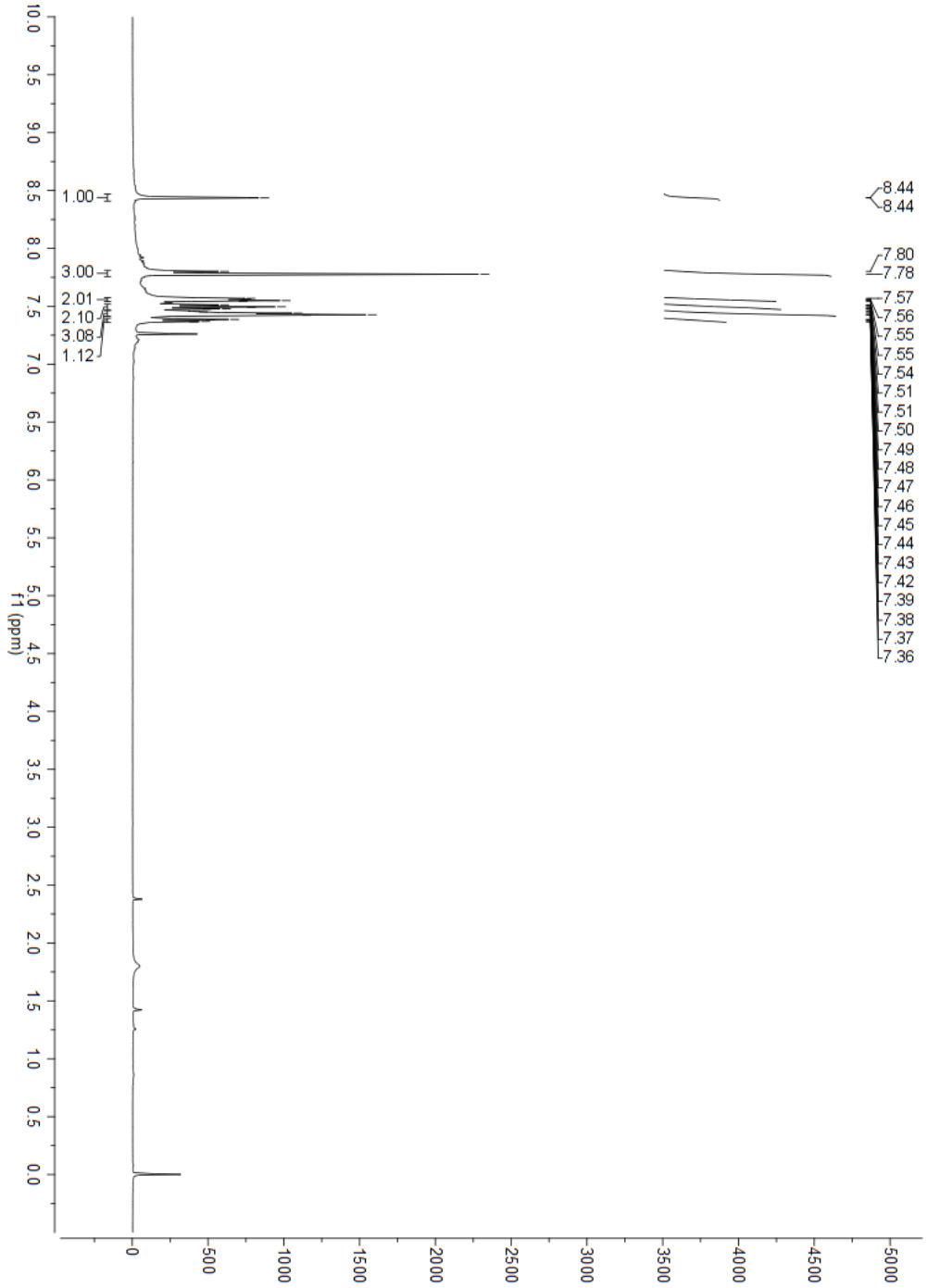
7.42
7.38
7.37
7.35
f1 (ppm)


O
S
N
F


160.81
160.70
158.23
142.69
142.41
138.05
131.29
130.53
130.19
128.62
128.16
128.08
126.03
124.33
124.14
121.77
121.71
77.32
77.00
76.68
f1 (ppm)


O
S
N
Cl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3.00
2.01
2.10
3.08
1.12
8.44
8.44
7.80
7.78
7.57
7.56
7.55
7.55
7.54
7.51
7.51
7.50
7.49
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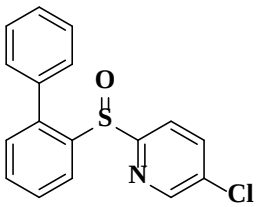
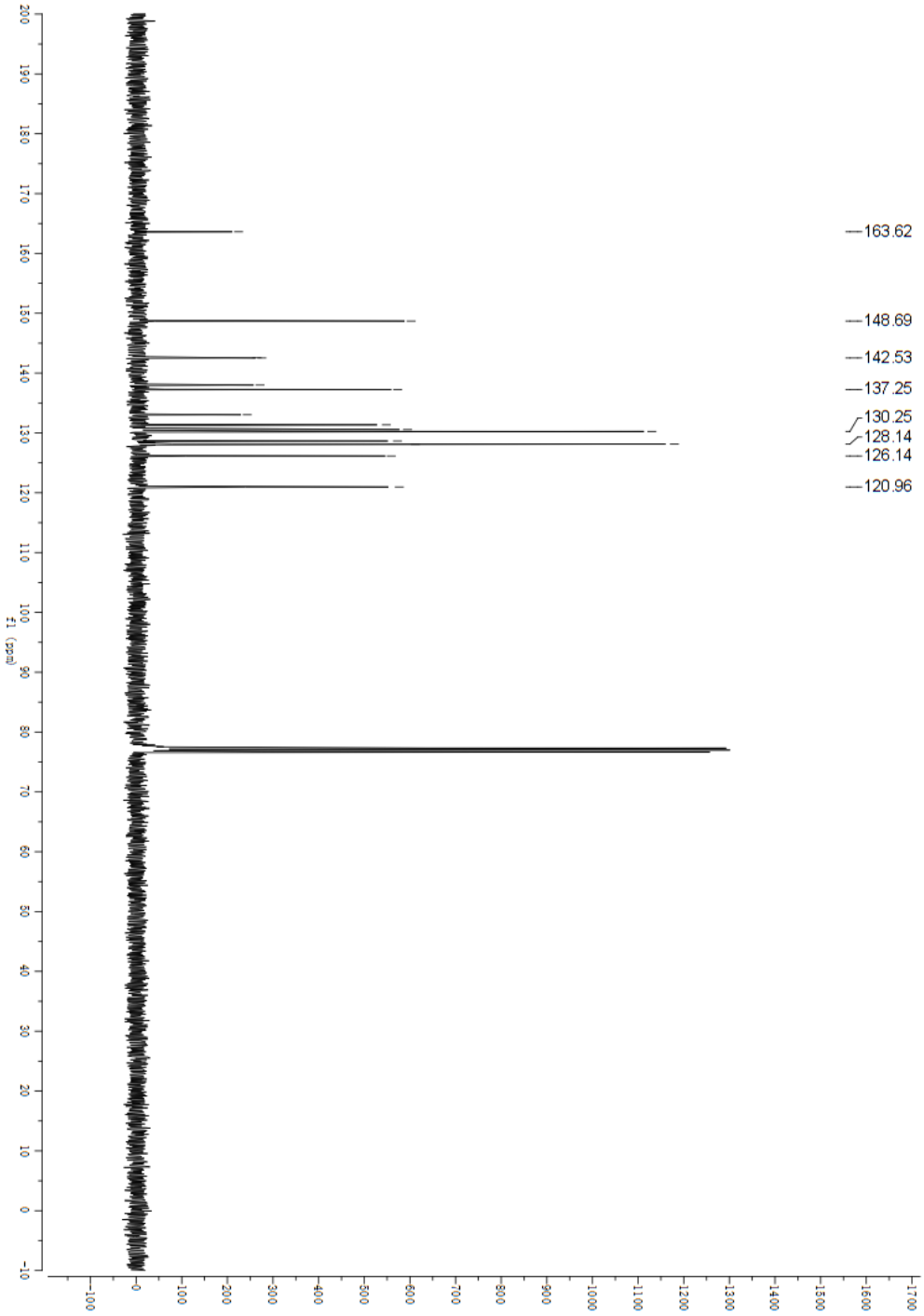
7.39
7.38
7.37
7.36
f1 (ppm)


O
S
N
Cl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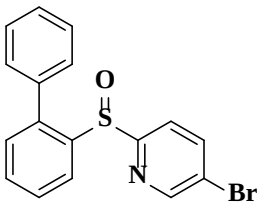
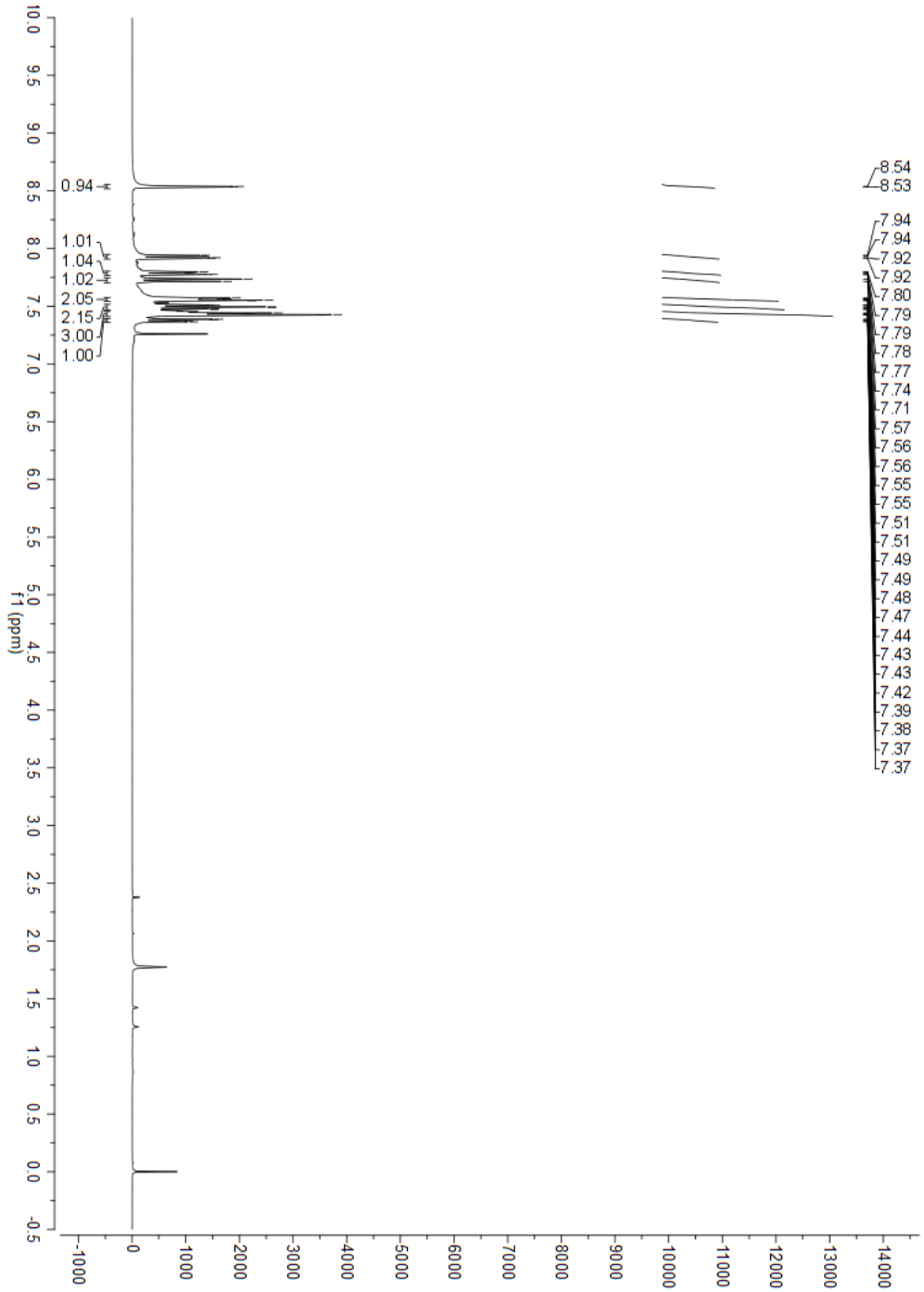
142.53
137.25
130.25
128.14
126.14
120.96
f1 (ppm)


O
S
N
Br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2.05
2.15
3.00
1.00
8.54
8.53
7.94
7.94
7.92
7.92
7.80
7.79
7.79
7.78
7.77
7.74
7.71
7.57
7.56
7.56
7.55
7.55
7.51
7.51
7.49
7.49
7.48
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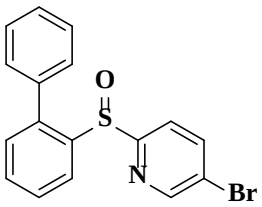
7.39
7.38
7.37
7.37
f1 (ppm)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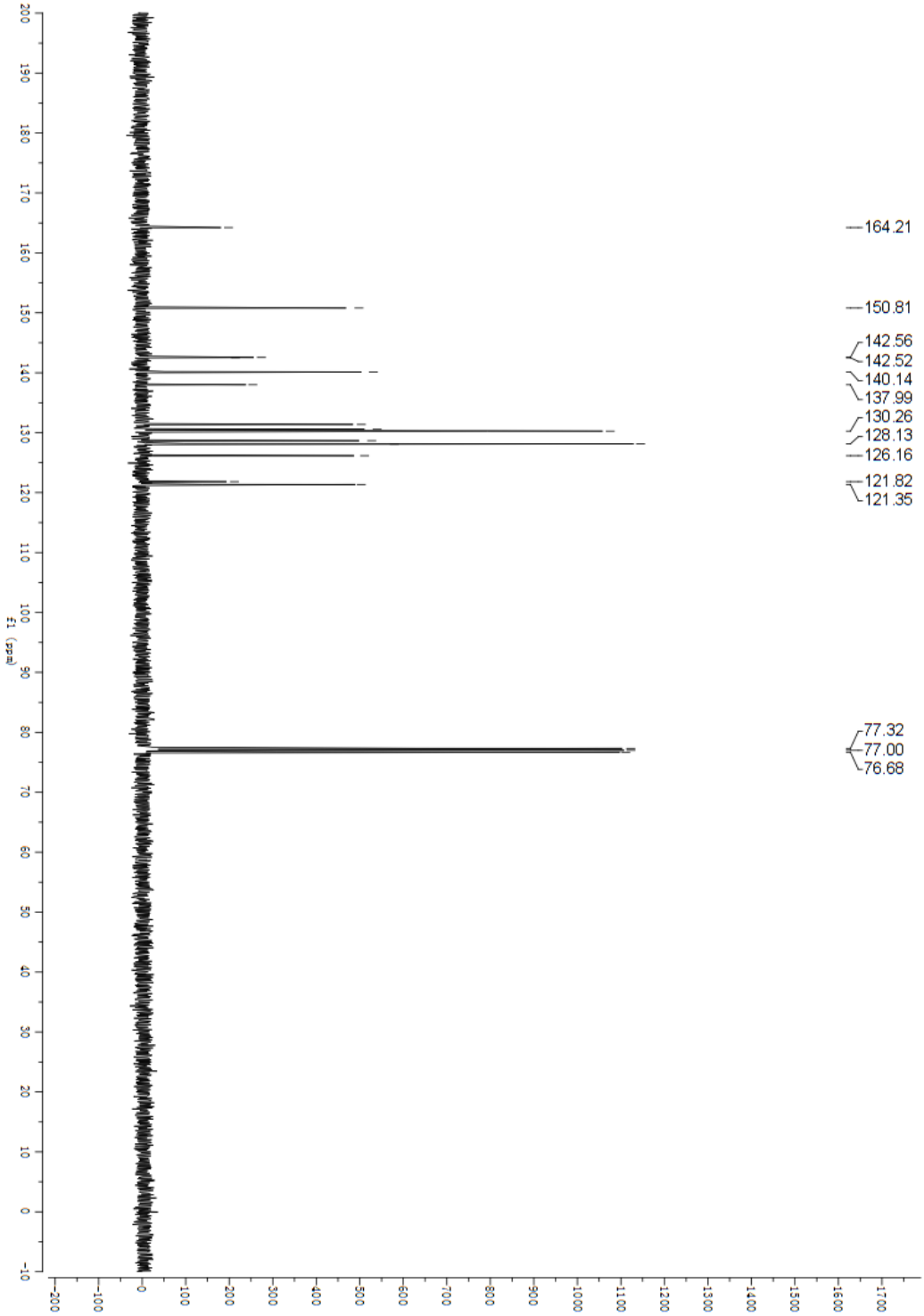
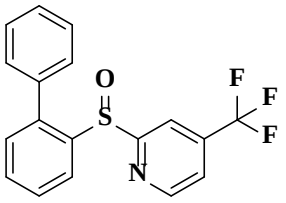
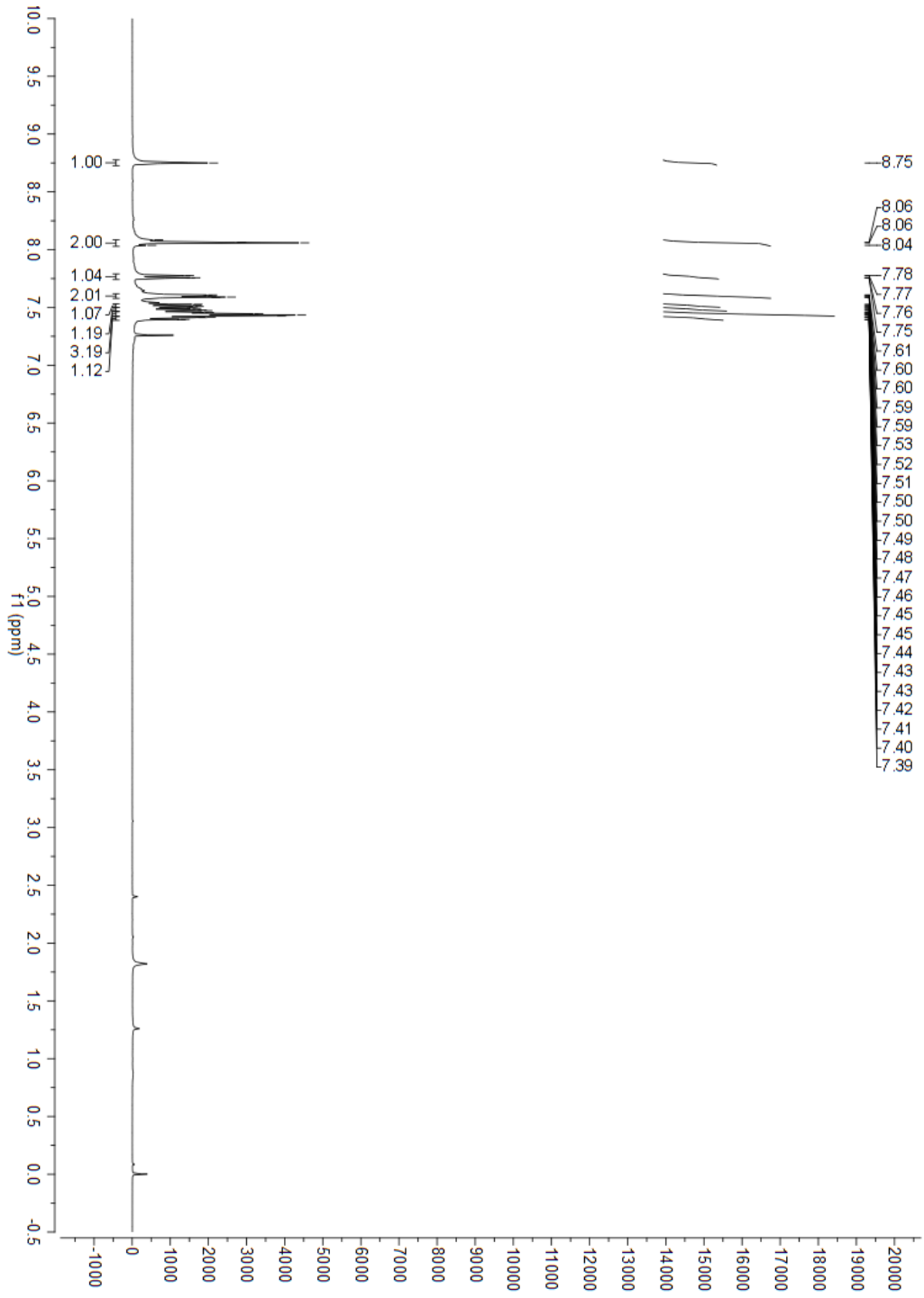
S
N
Br


164.21
150.81
142.56
142.52
140.14
137.99
130.26
128.13
126.16
121.82
121.35
77.32
77.00
76.68
f1 (ppm)


O
S
N
F
F
F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2.00
1.04
2.01
1.07
1.19
3.19
1.12
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8.06
8.06
8.04
7.78
7.77
7.76
7.75
7.61
7.60
7.60
7.59
7.59
7.53
7.52
7.51
7.50
7.50
7.49
7.48
7.47
7.46
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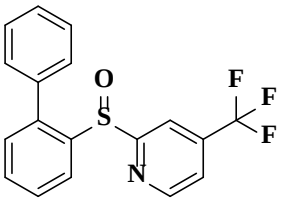
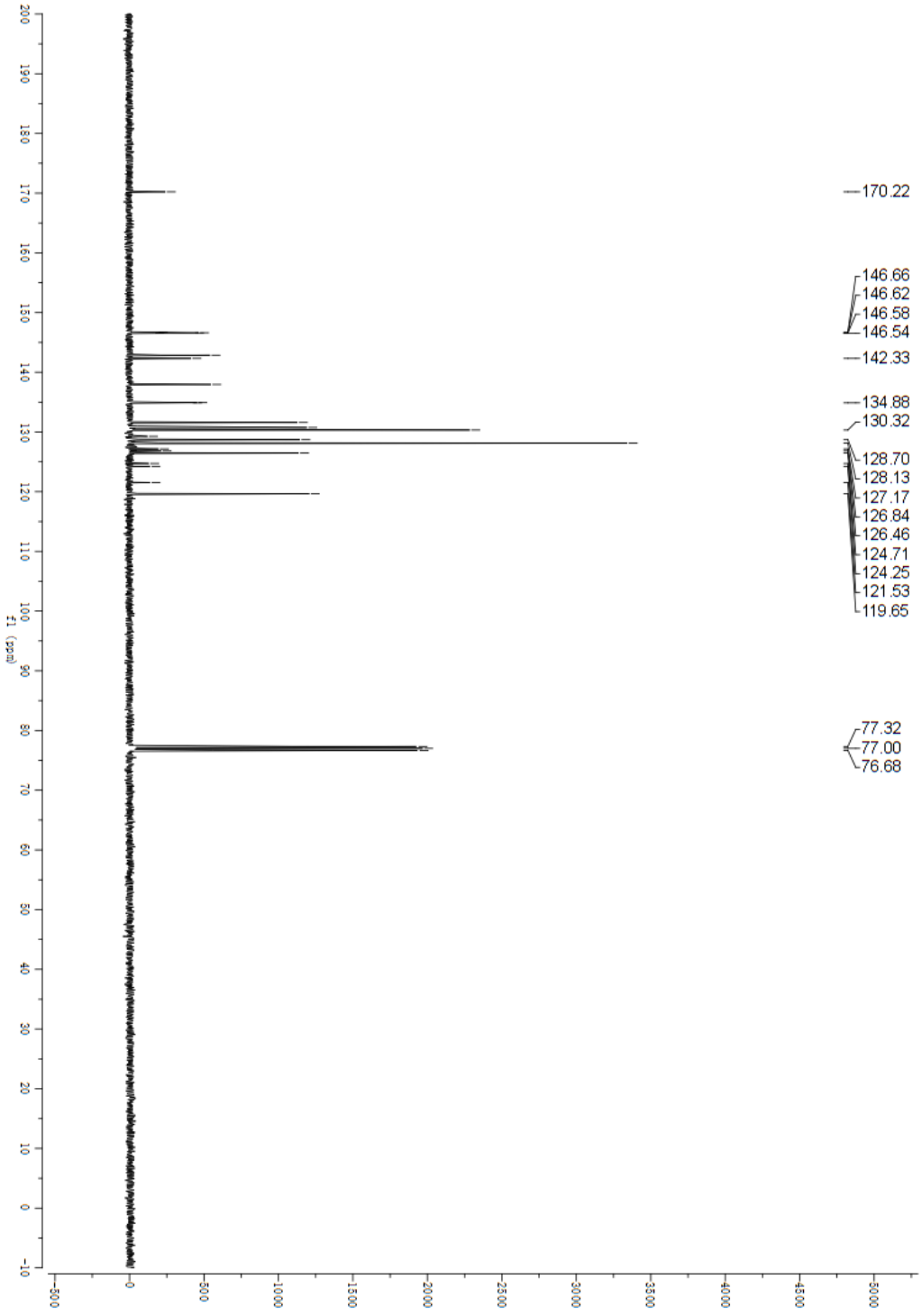
7.45
7.44
7.43
7.43
7.42
7.41
7.40
7.39
f1 (ppm)


O
S
N
F
F
F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130.32
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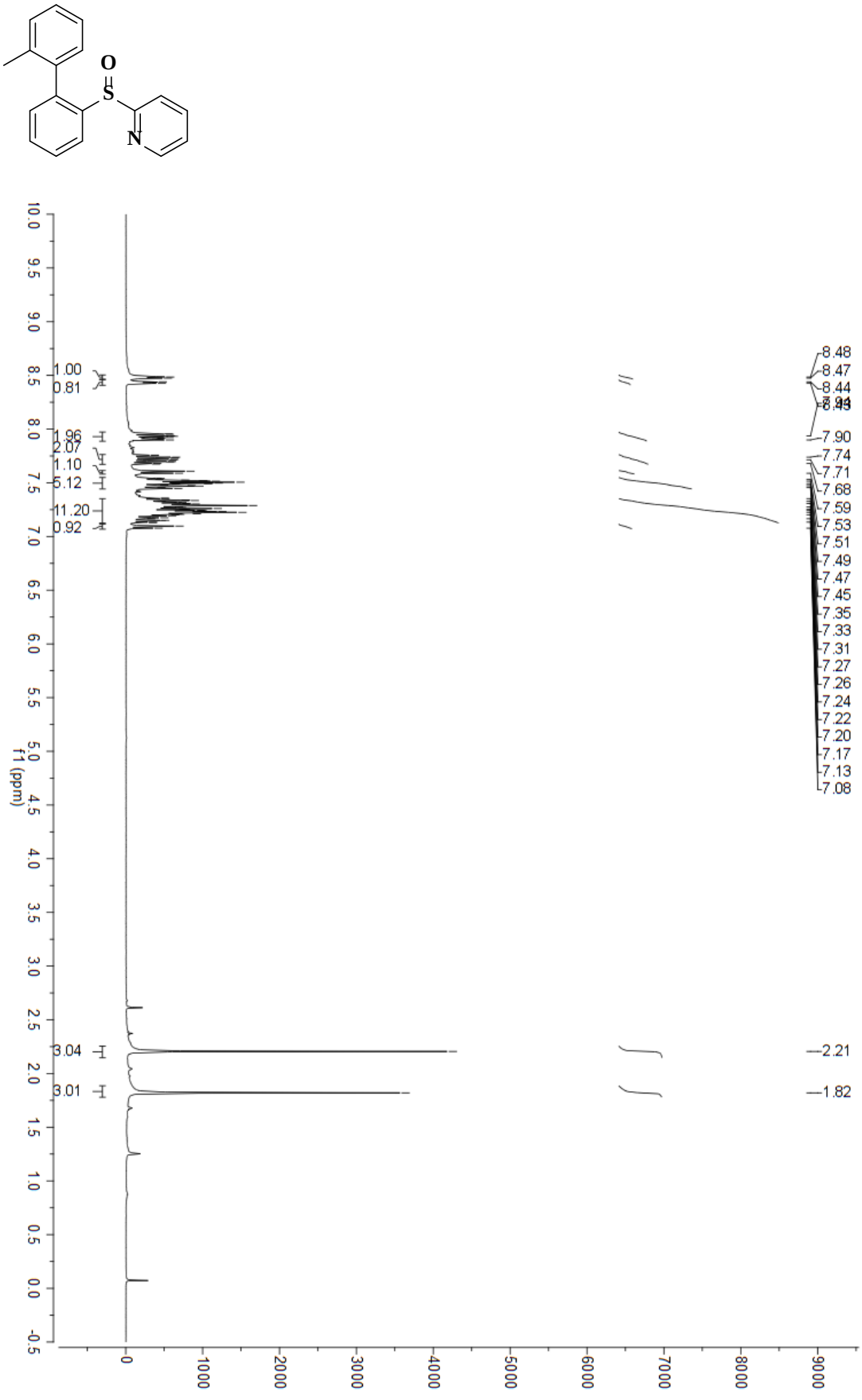
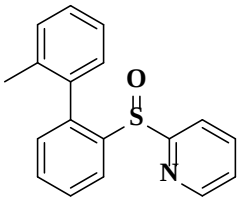
127.17
126.84
126.46
124.71
124.25
121.53
119.65
77.32
77.00
76.68
f1 (ppm)


O
S
N
f1 (ppm)
1.00
0.81
1.96
2.07
1.10
5.12
11.20
0.92
3.04
3.01
8.48
8.47
8.44
7.90
7.74
7.71
7.68
7.59
7.53
7.51
7.49
7.47
7.45
7.35
7.33
7.31
7.27
7.26
7.24
7.22
7.20
7.17
7.13
7.08
2.21
1.82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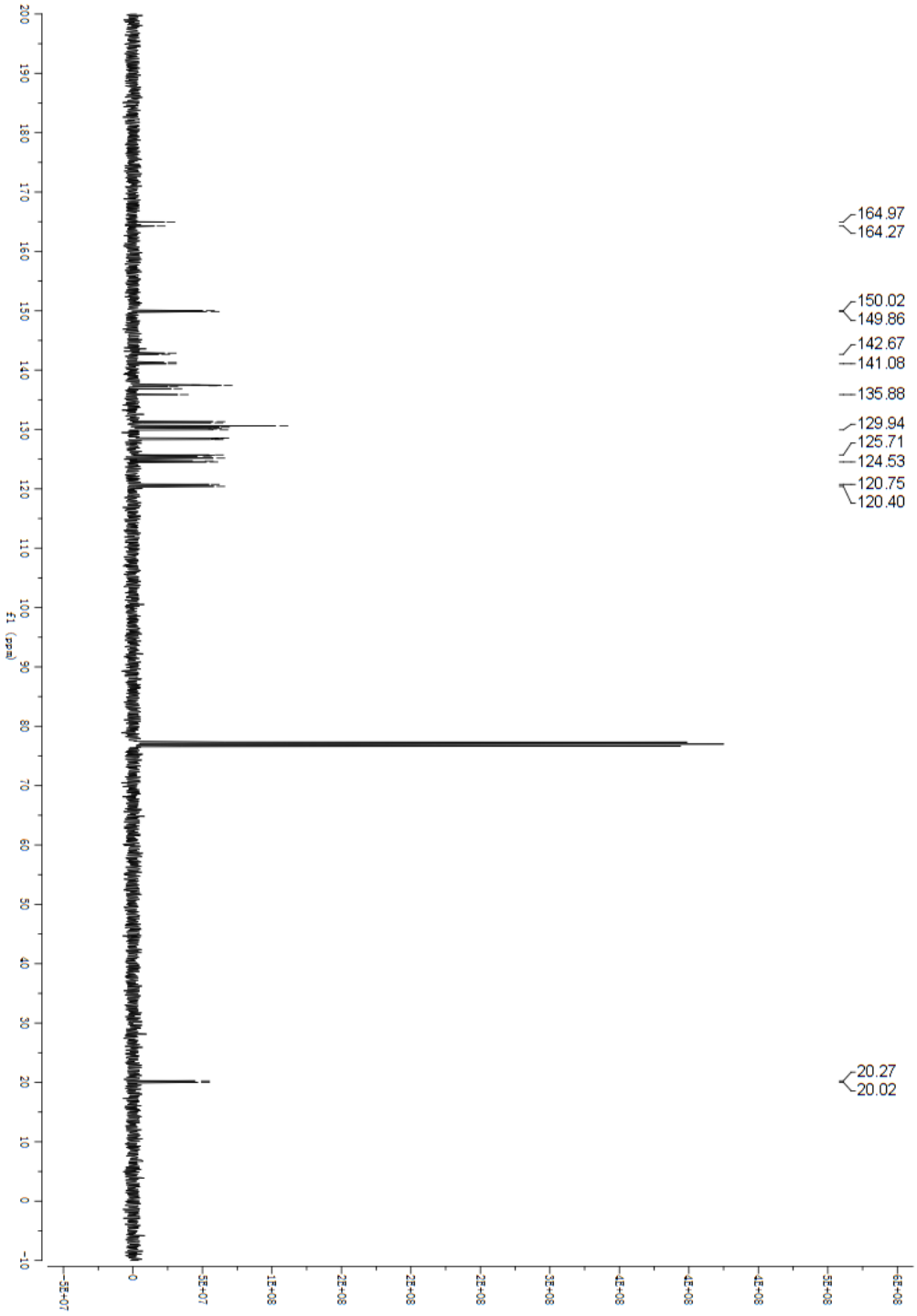
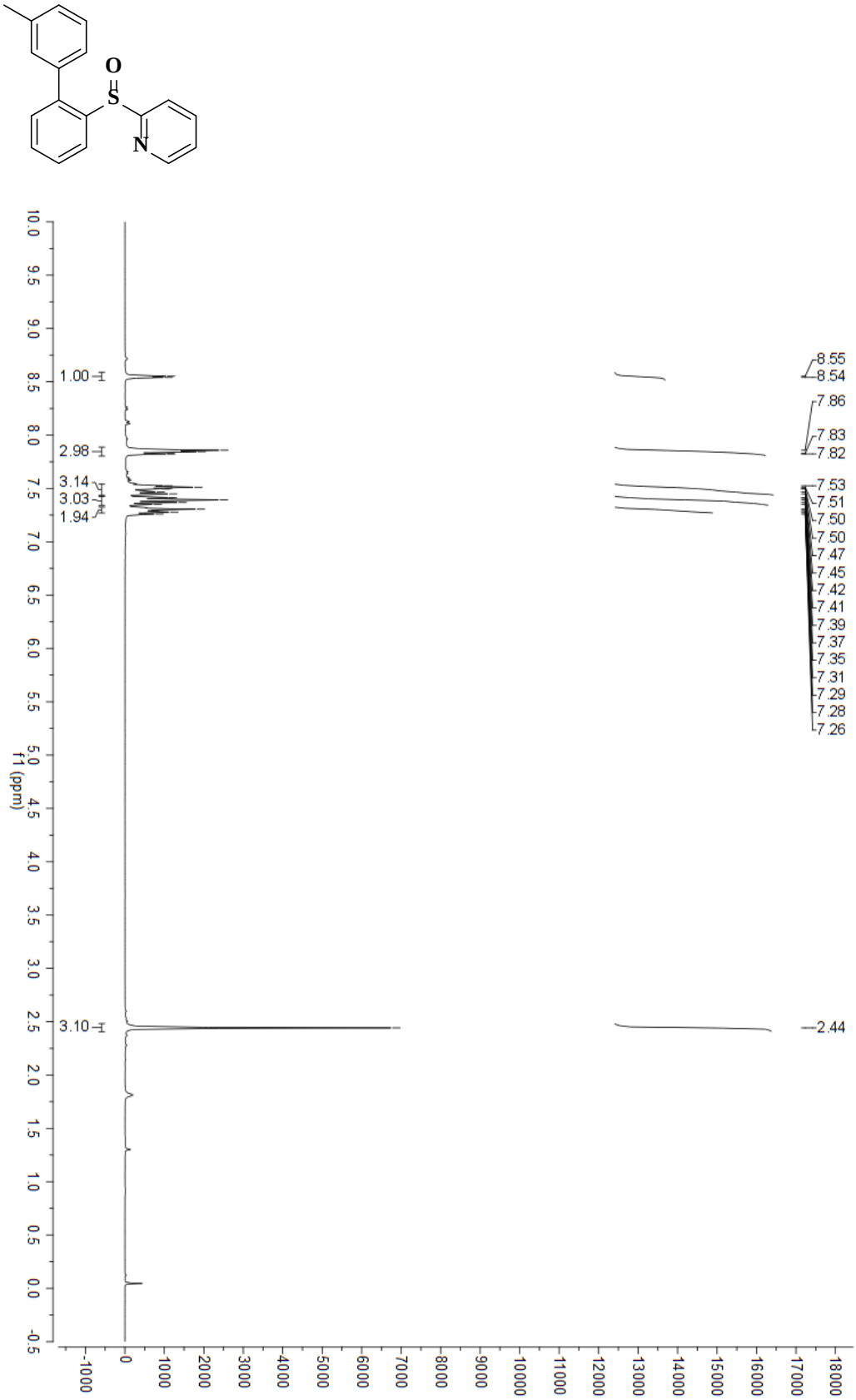
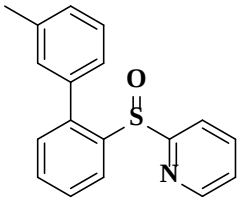
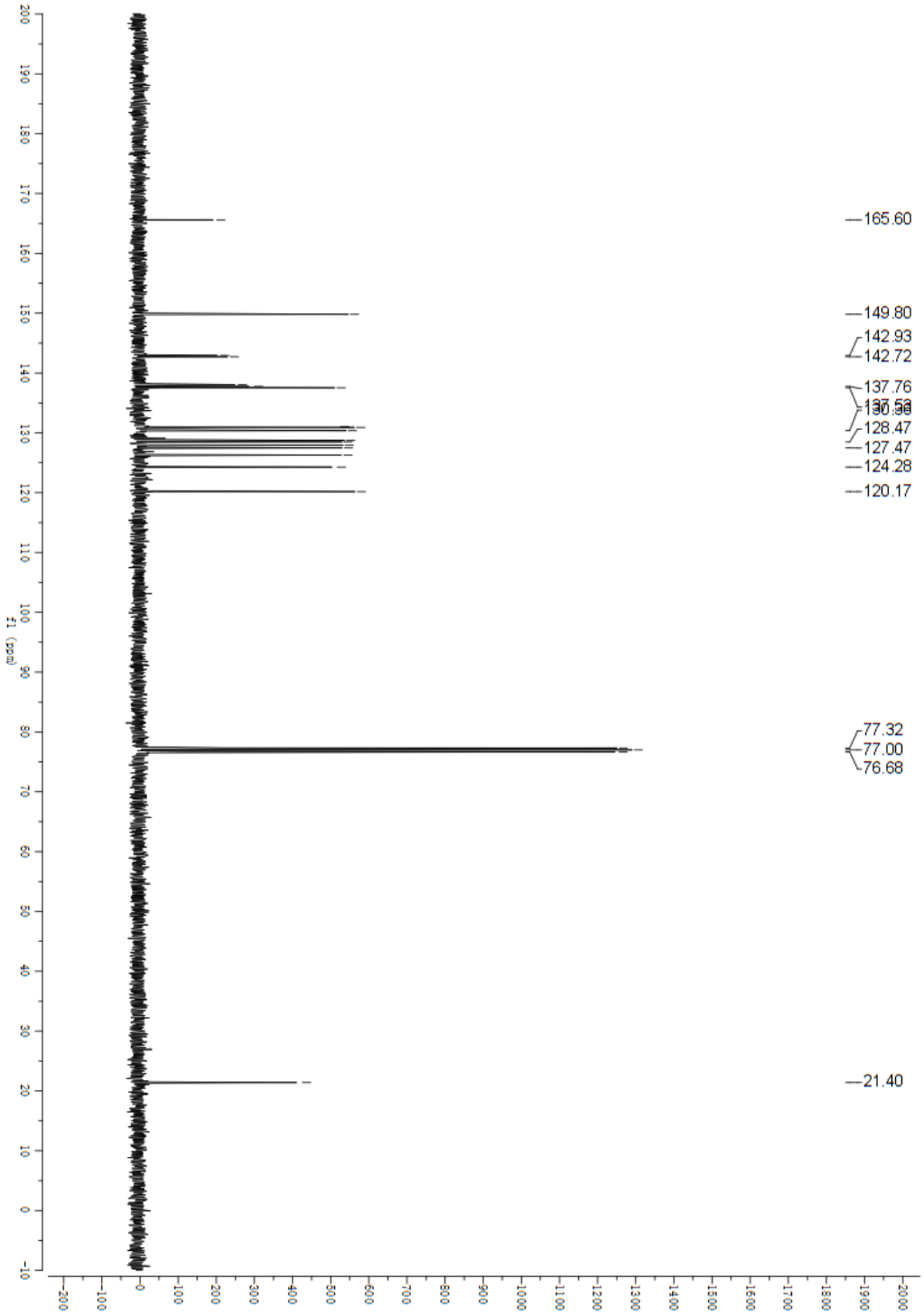
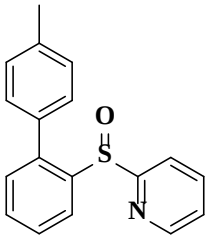
S
N

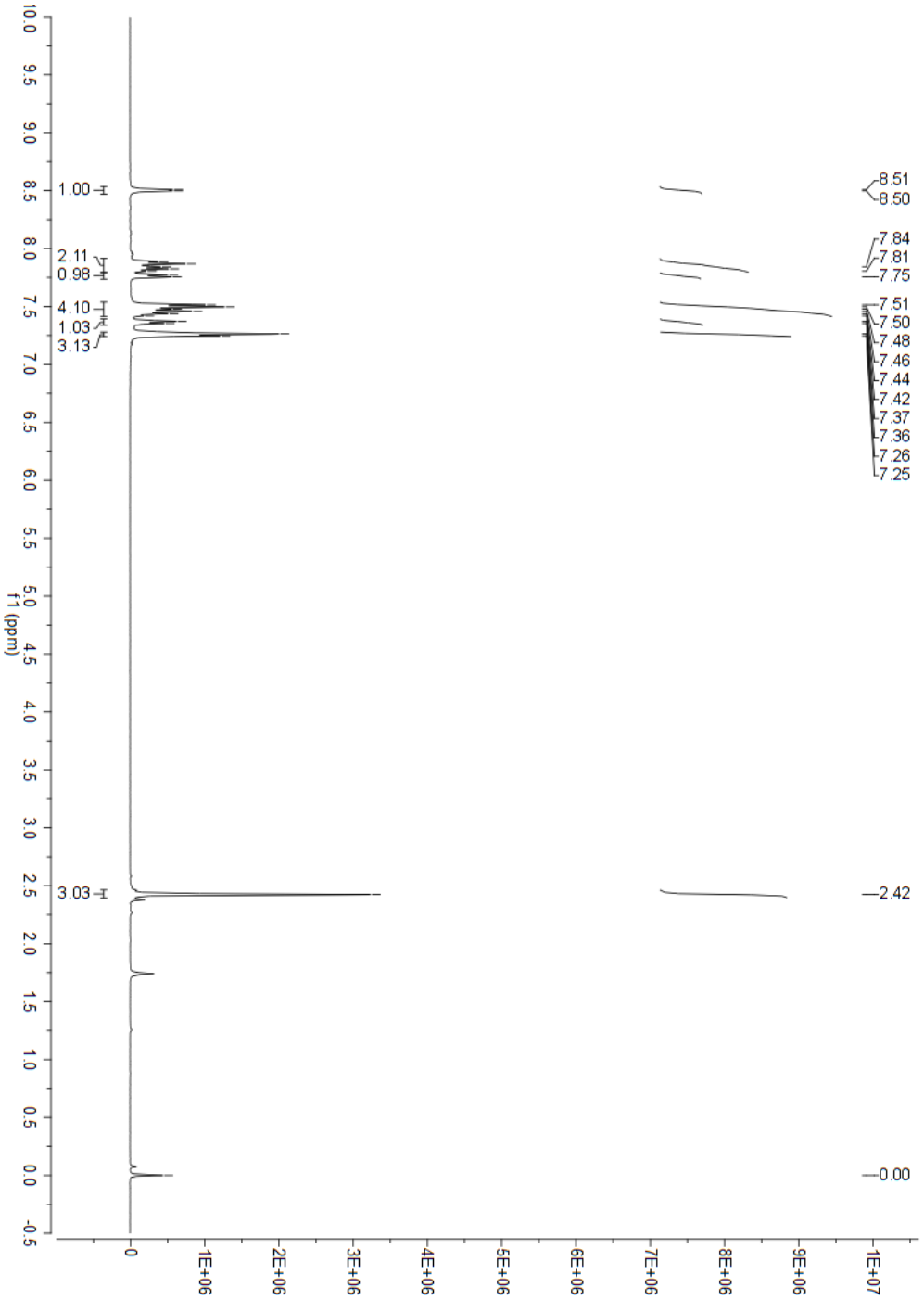

164.97
164.27
150.02
149.86
142.67
141.08
135.88
129.94
125.71
124.53
120.75
120.40
20.27
20.02
f1 (ppm)

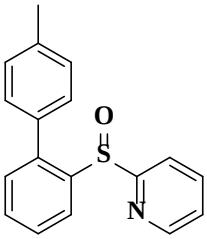

O
S
N
1.00
2.98
3.14
3.03
1.94
3.10
2.44
8.55
8.54
7.86
7.83
7.82
7.53
7.51
7.50
7.50
7.47
7.45
7.42
7.41
7.39
7.37
7.35
7.31
7.29
7.28
7.26
f1 (ppm)

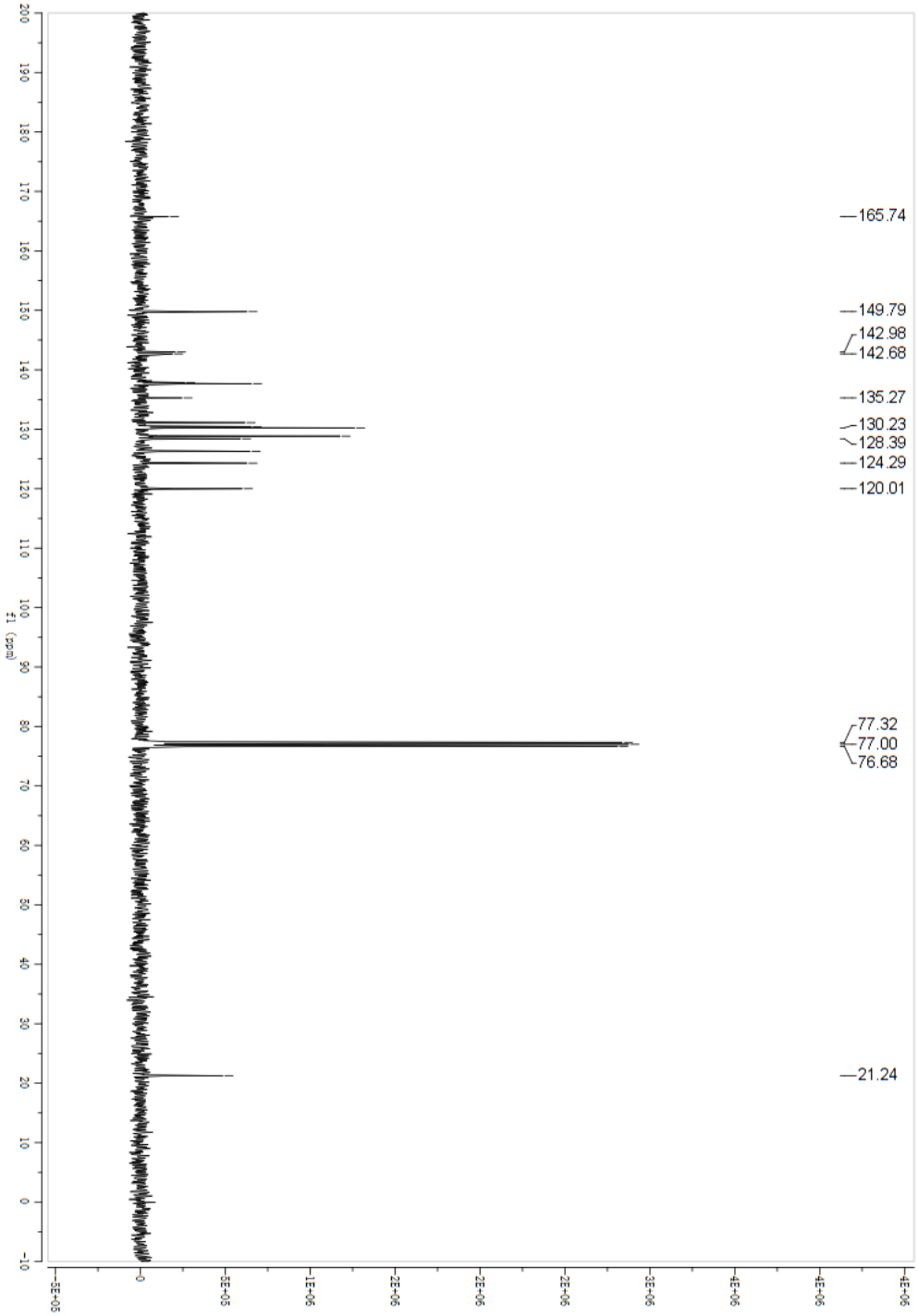

O
S
N

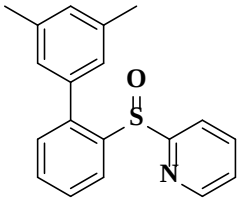

165.60
149.80
142.93
142.72
137.76
128.47
127.47
124.28
120.17
77.32
77.00
76.68
21.40
f1 (ppm)

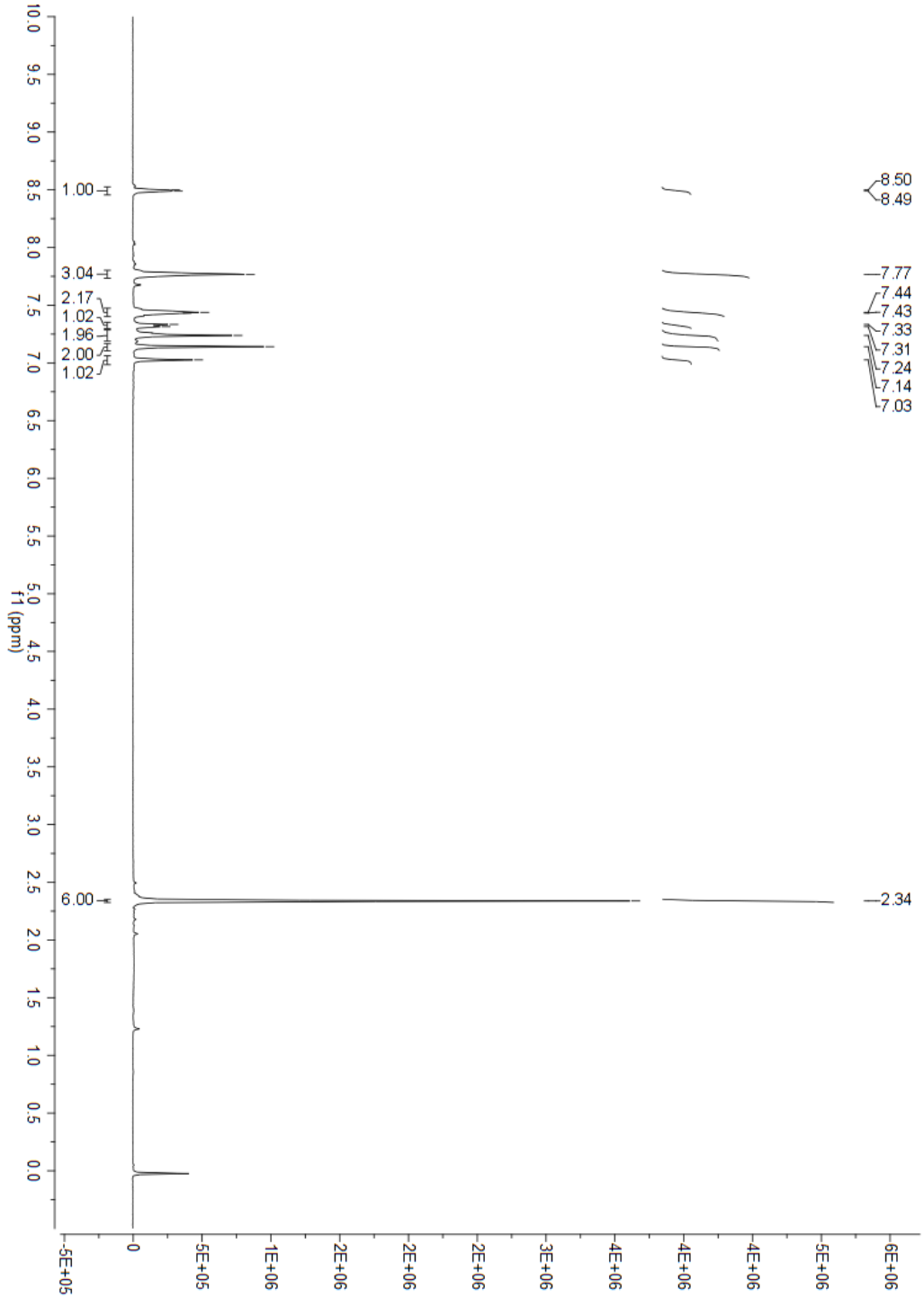

O
S
N

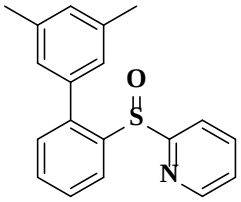

1.00
2.11
0.98
4.10
1.03
3.13
3.03
8.51
8.50
7.84
7.81
7.75
7.51
7.50
7.48
7.46
7.44
7.42
7.37
7.36
7.26
7.25
2.42
0.00
f1 (ppm)

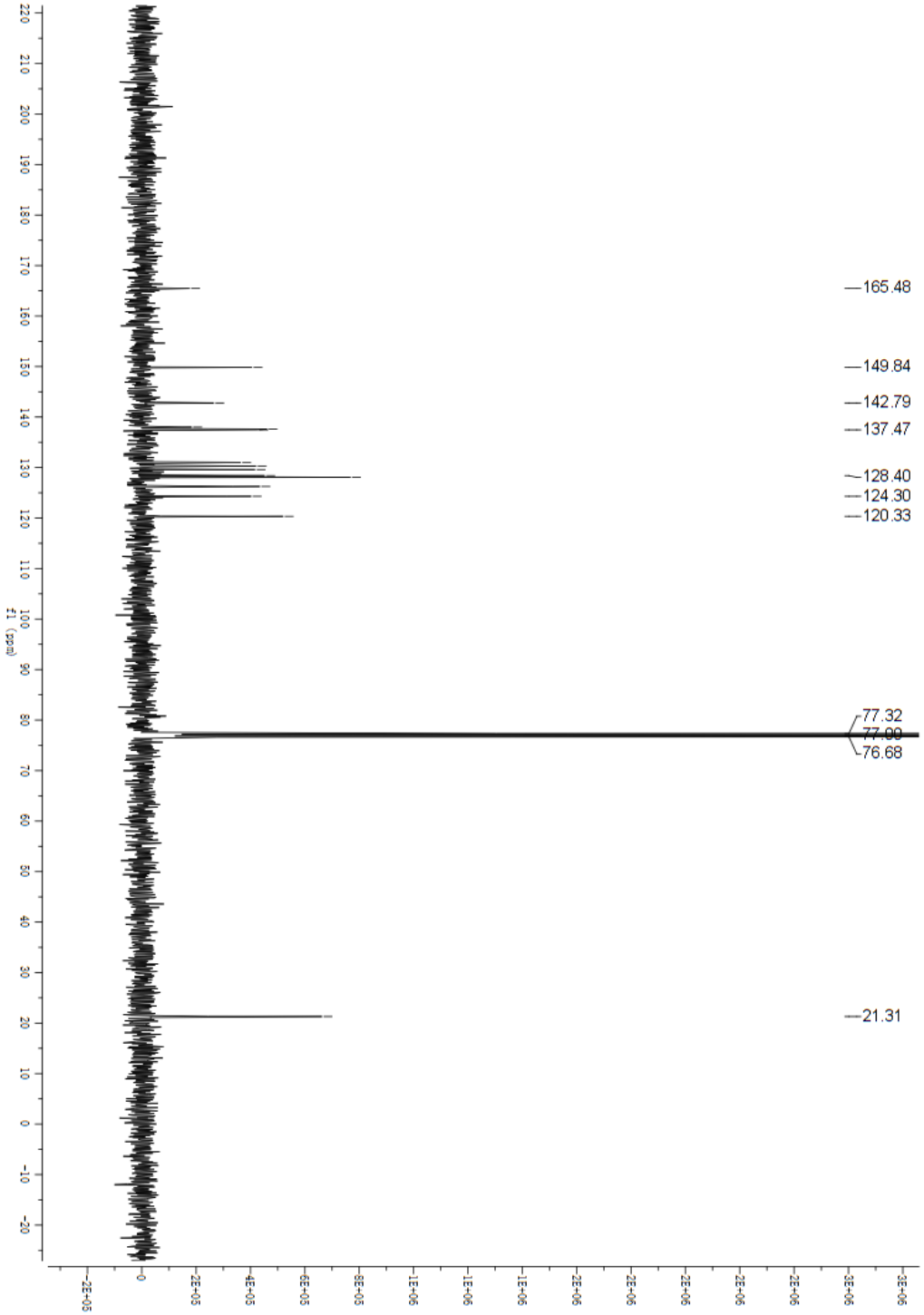

O
S
N

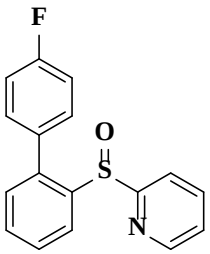

165.74
149.79
142.98
142.68
135.27
130.23
128.39
124.29
120.01
77.32
77.00
76.68
21.24
f1 (ppm)

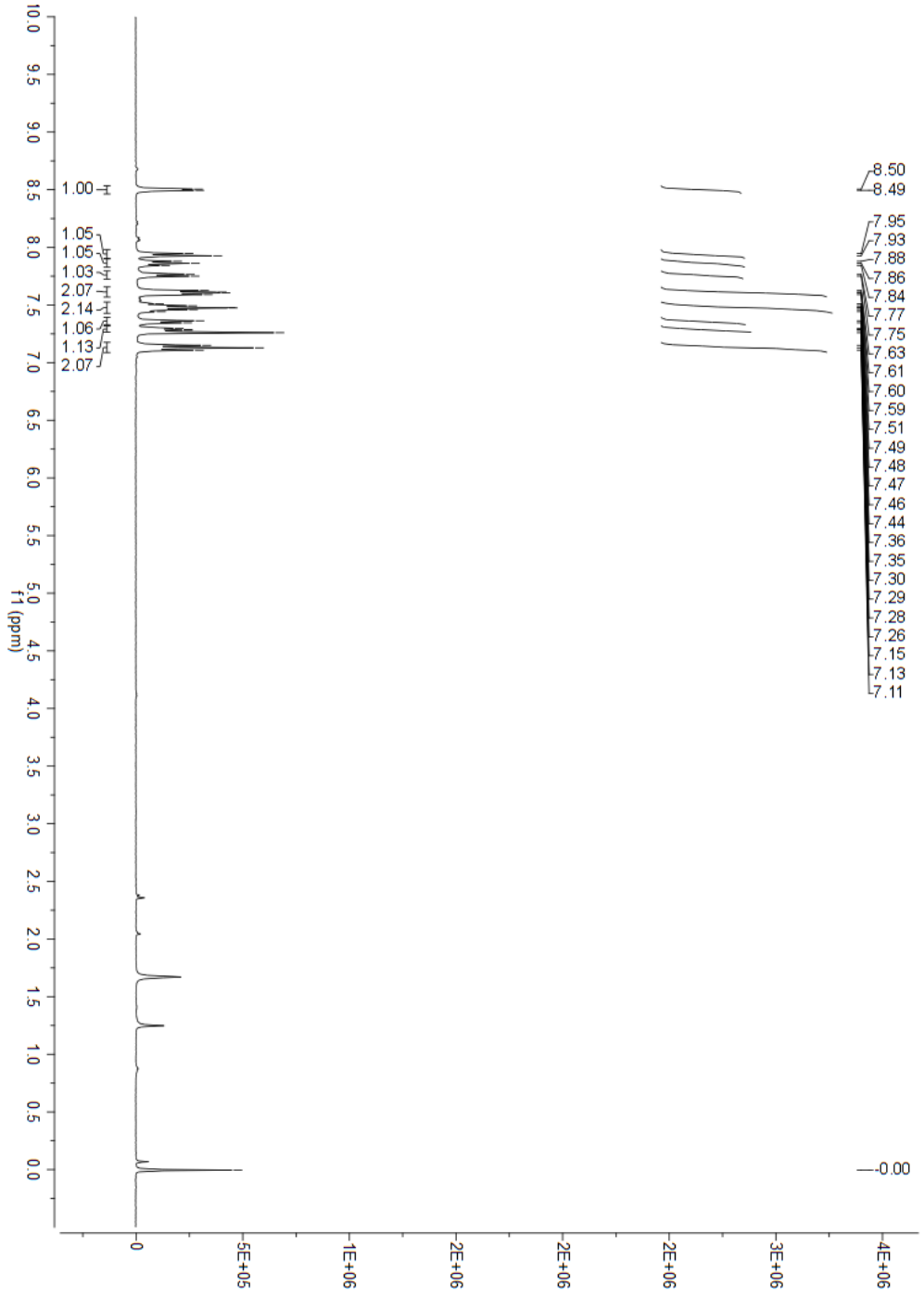

O
S
N


1.00
3.04
2.17
1.02
1.96
2.00
1.02
6.00
8.50
8.49
7.77
7.44
7.43
7.33
7.31
7.24
7.14
7.03
2.34
f1 (ppm)


O
S
N


165.48
149.84
142.79
137.47
128.40
124.30
120.33
77.32
77.09
76.68
21.31
f1 (ppm)


F
O
S
N


1.00
1.05
1.05
1.03
2.07
2.14
1.06
1.13
2.07
8.50
8.49
7.95
7.93
7.88
7.86
7.84
7.77
7.75
7.63
7.61
7.60
7.59
7.51
7.49
7.48
7.47
7.46
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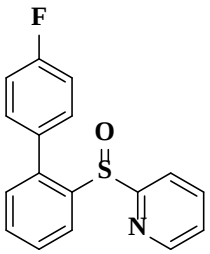
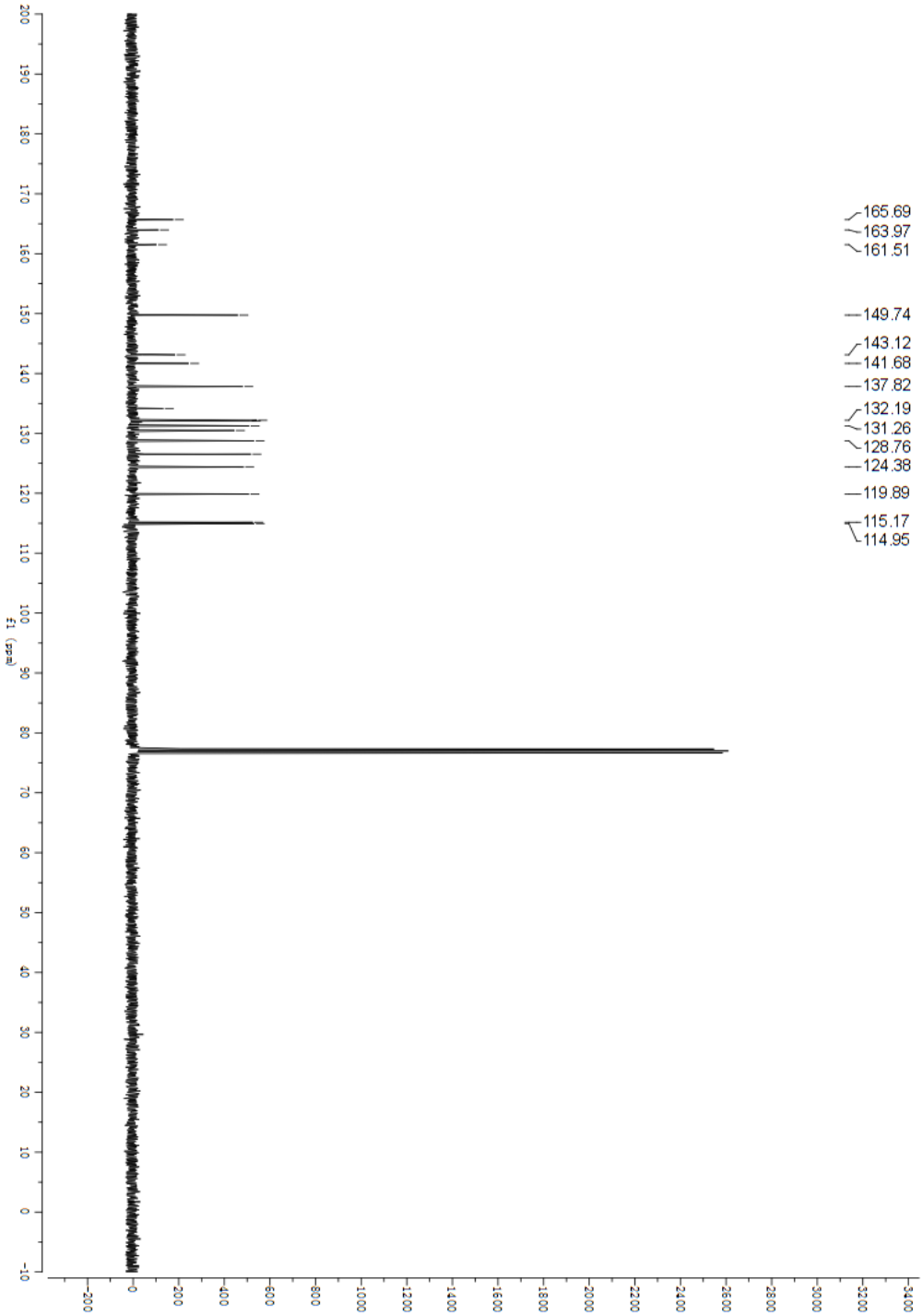
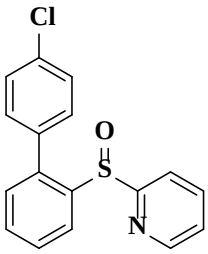
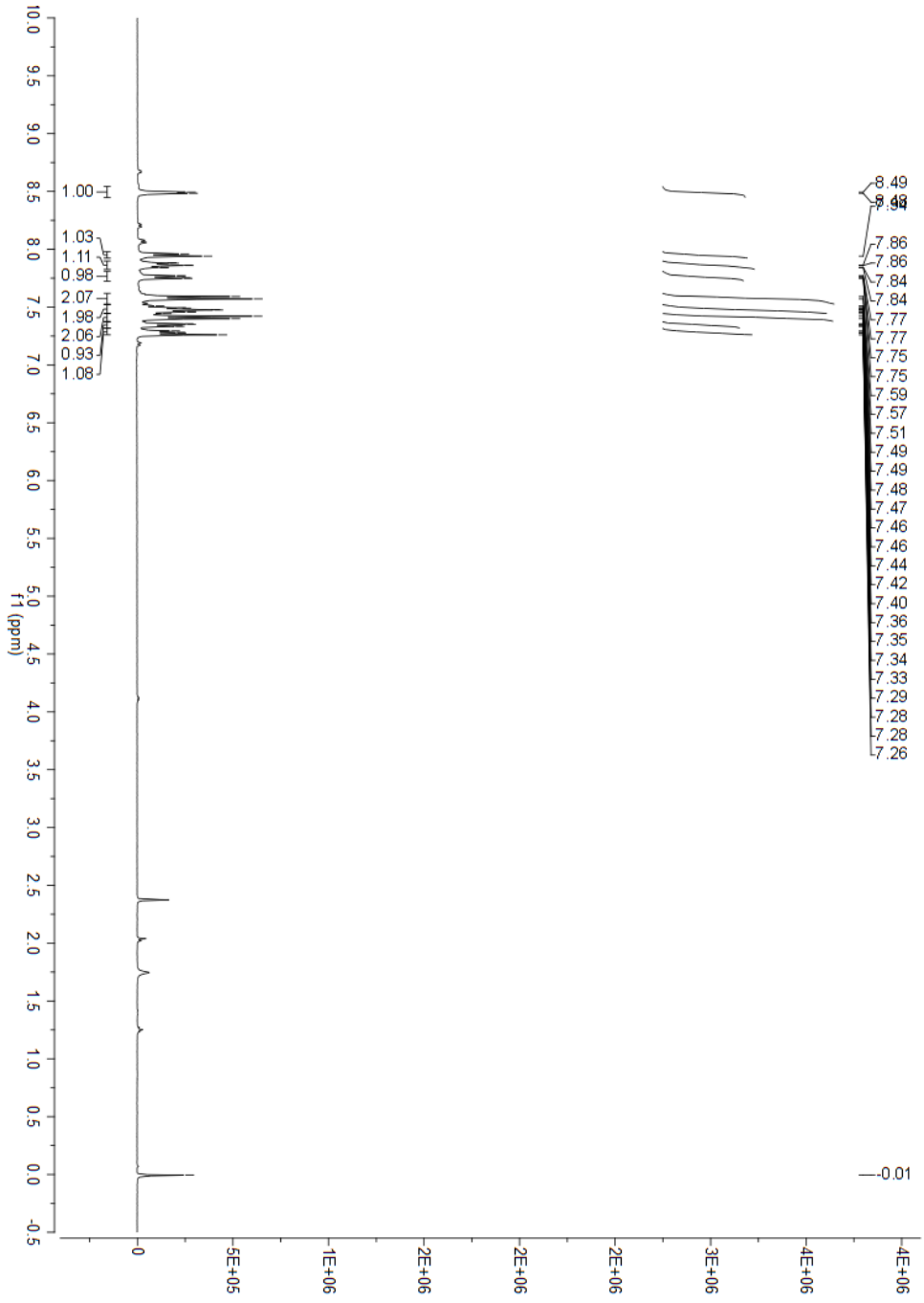
7.15
7.13
7.11
0.00
f1 (ppm)


F
O
S
N


165.69
163.97
161.51
149.74
143.12
141.68
137.82
132.19
131.26
128.76
124.38
119.89
115.17
114.95
f1 (ppm)


Cl
O
S
N


1.00
1.03
1.11
0.98
2.07
1.98
2.06
0.93
1.08
8.49
7.86
7.86
7.84
7.84
7.77
7.77
7.75
7.75
7.59
7.57
7.51
7.49
7.49
7.48
7.47
7.46
7.46
7.44
7.42
7.40
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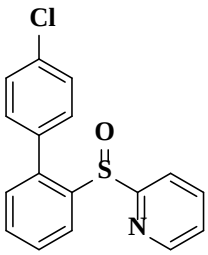
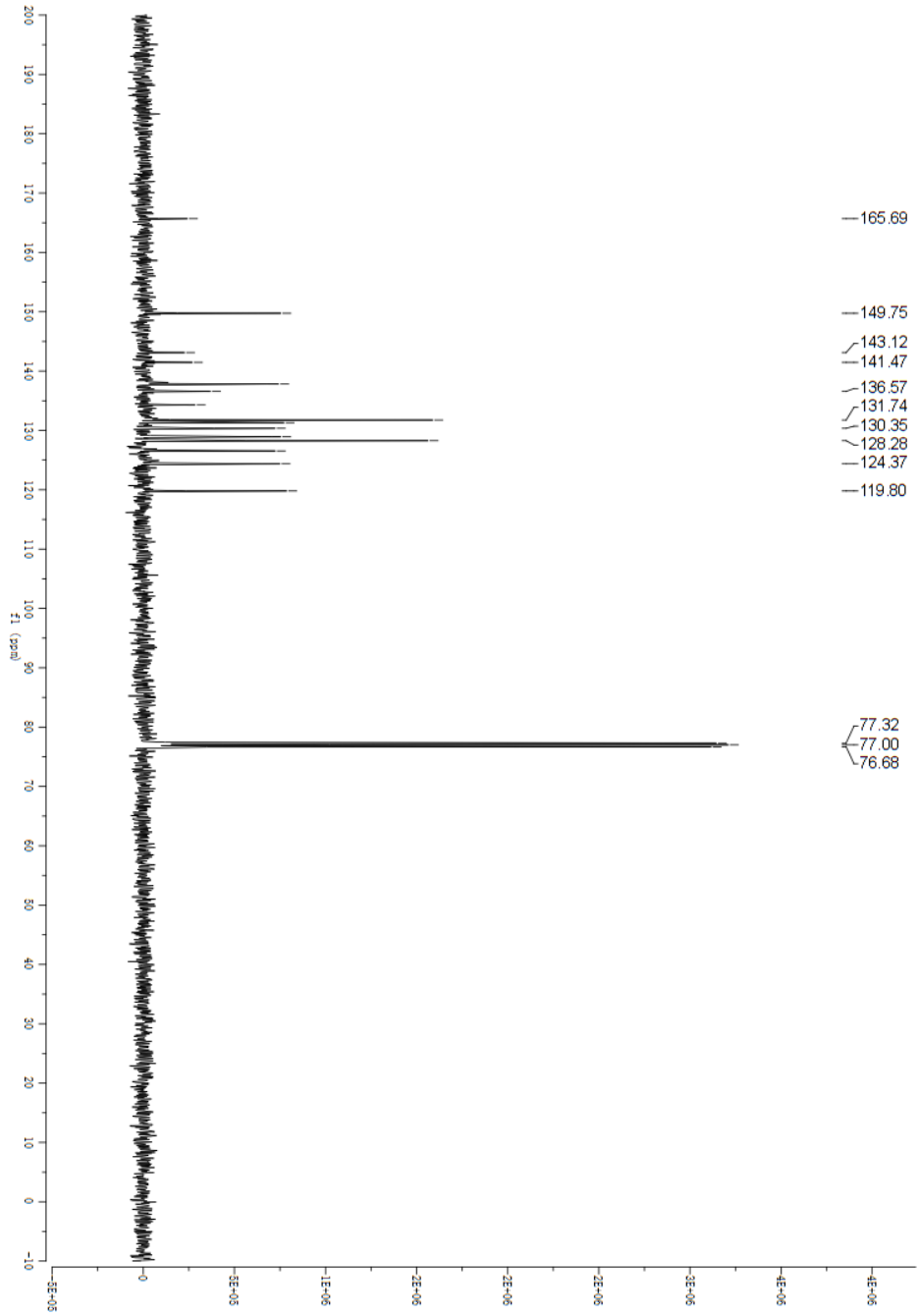
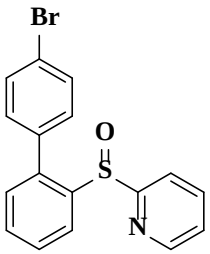
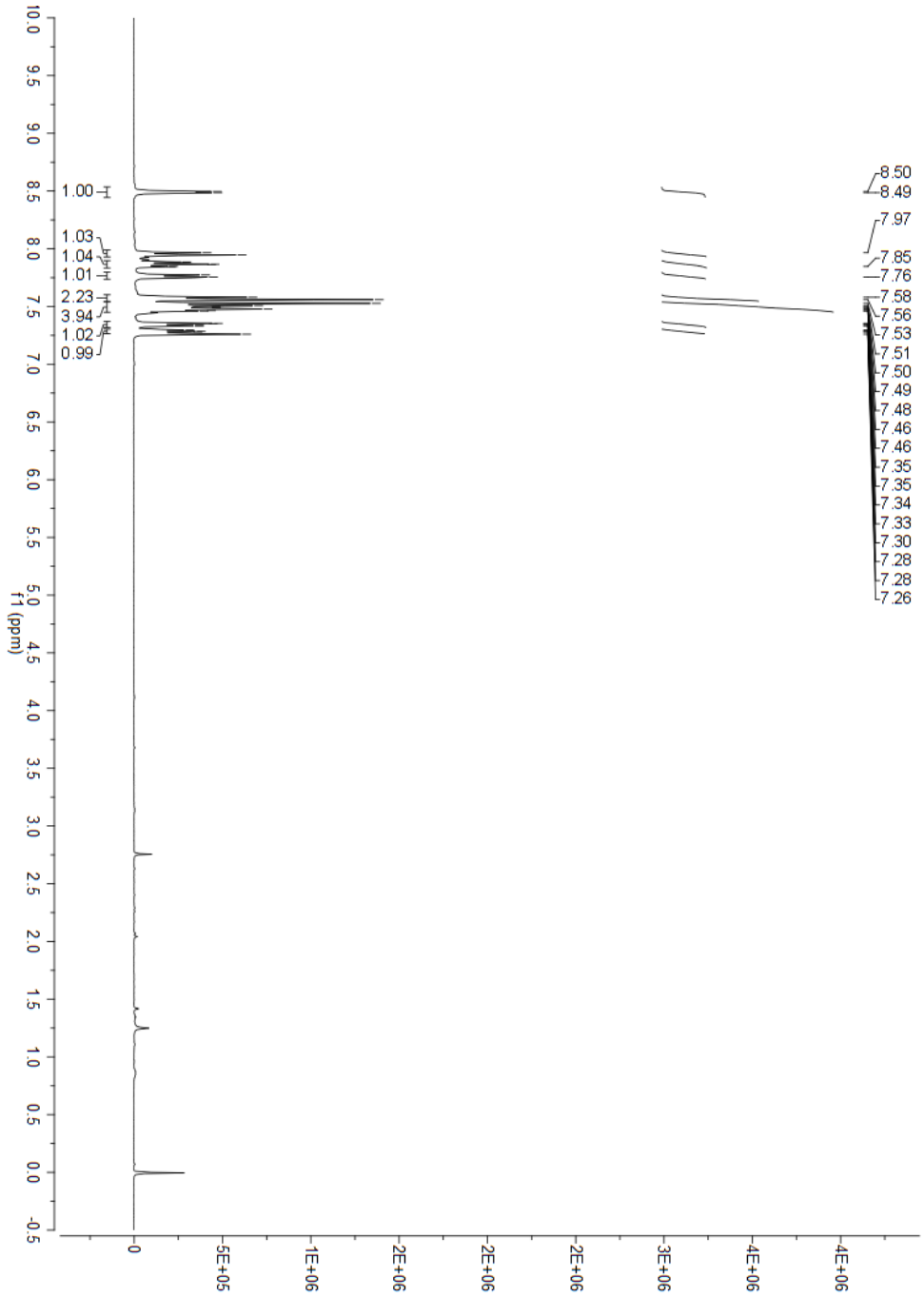
7.29
7.28
7.28
7.26
-0.01
f1 (ppm)


Cl
O
S
N


165.69
149.75
143.12
141.47
136.57
131.74
130.35
128.28
124.37
119.80
77.32
77.00
76.68
f1 (ppm)


Br
O
S
N


1.00
1.03
1.04
1.01
2.23
3.94
1.02
0.99
8.50
8.49
7.97
7.85
7.76
7.58
7.56
7.53
7.51
7.50
7.49
7.48
7.46
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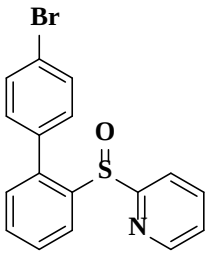
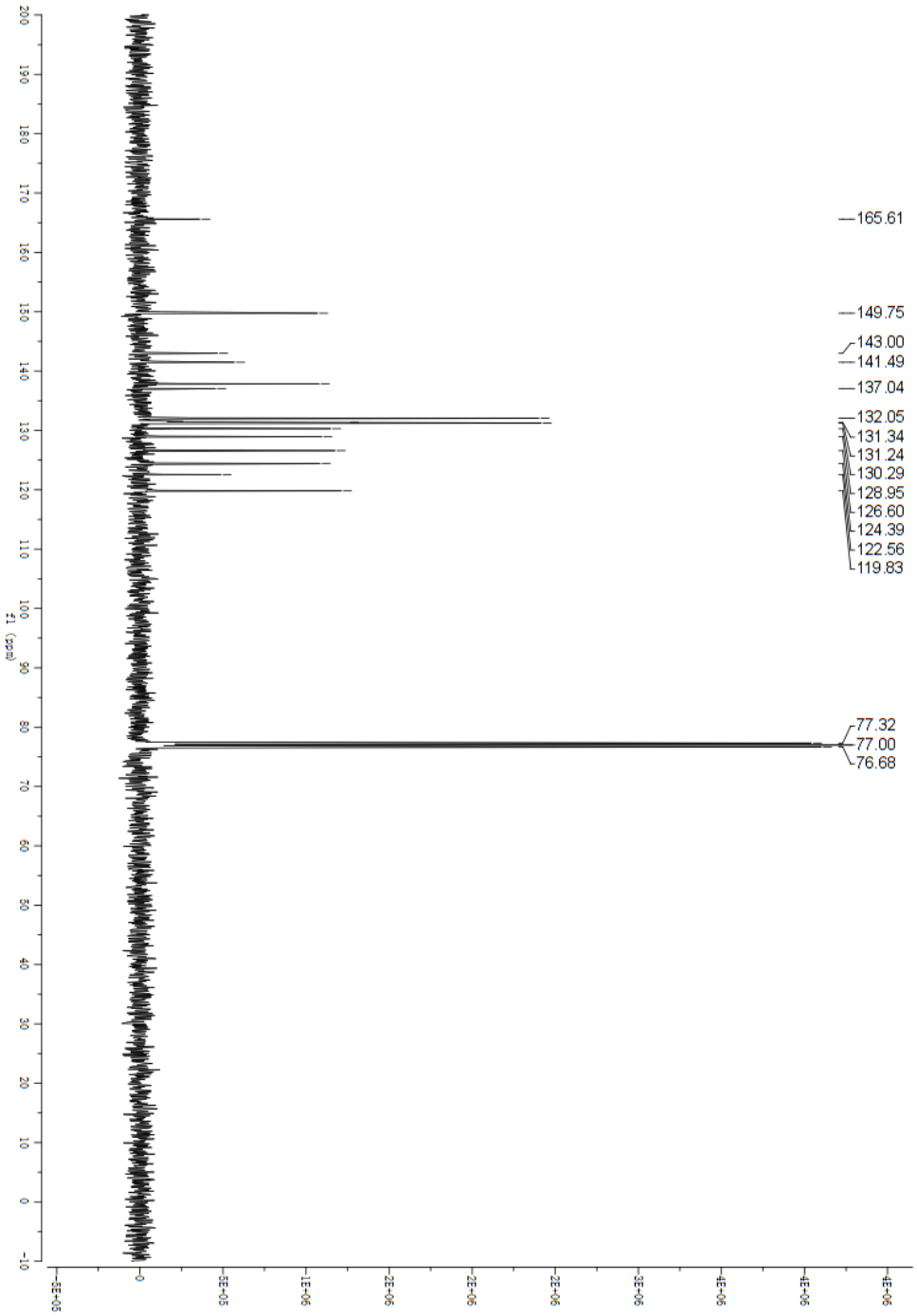
7.35
7.34
7.33
7.30
7.28
7.28
7.26
f1 (ppm)


Br
O
S
N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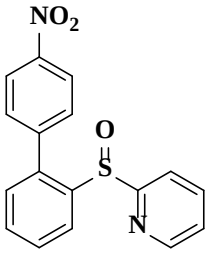
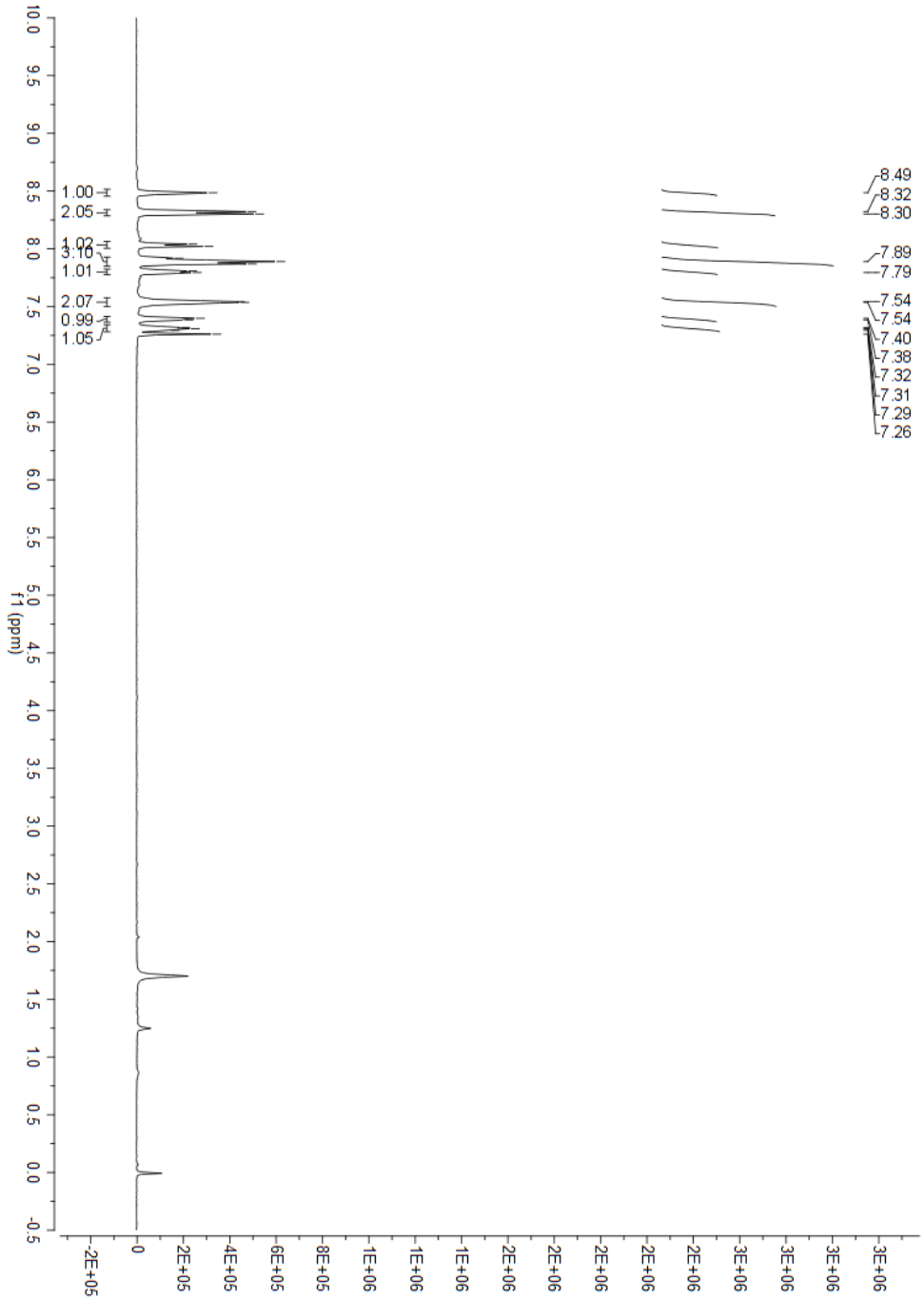
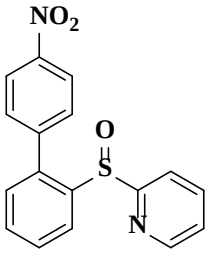
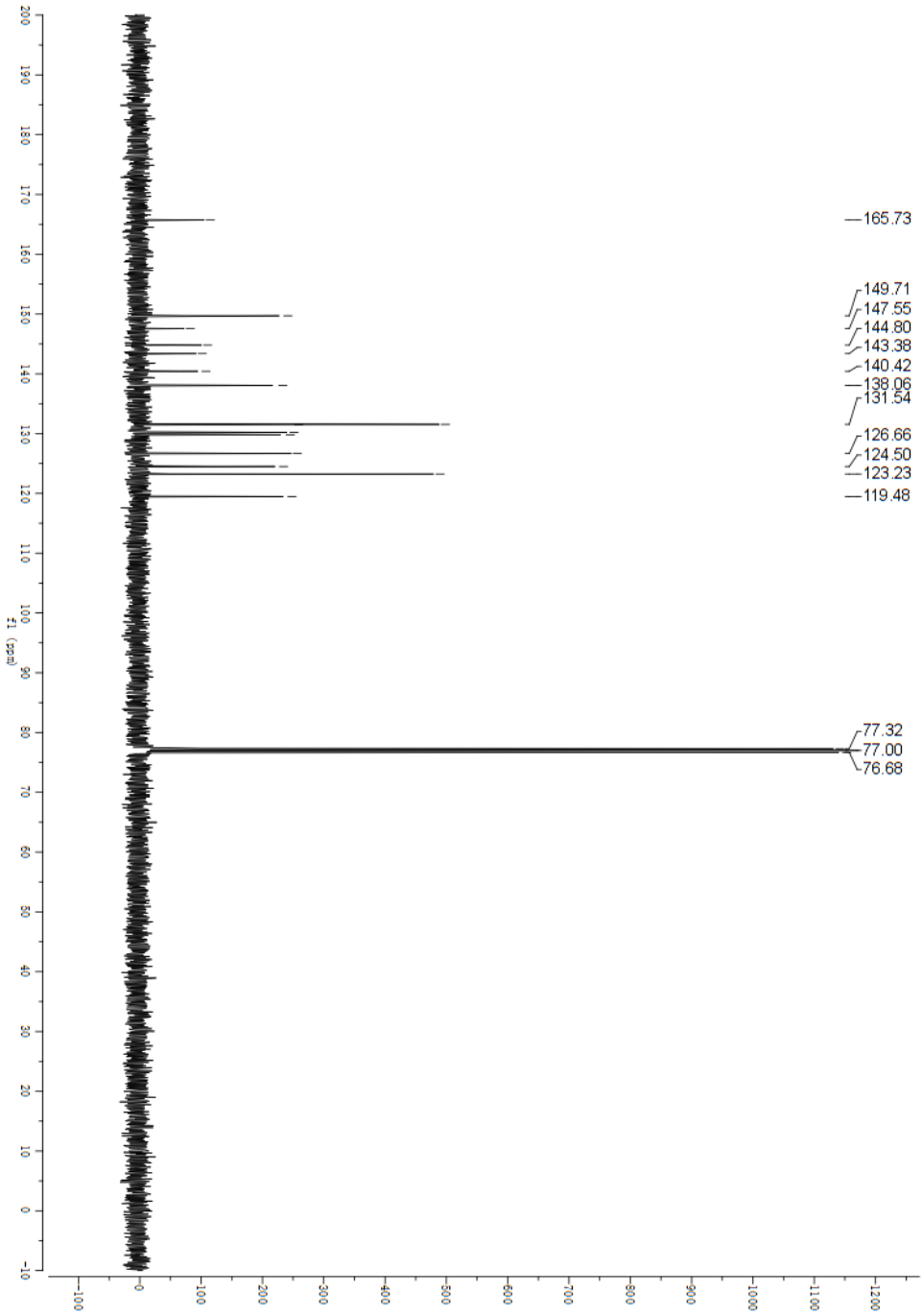
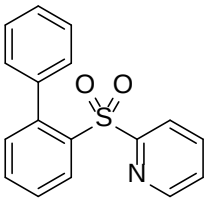
149.75
143.00
141.49
137.04
132.05
131.34
131.24
130.29
128.95
126.60
124.39
122.56
119.83
77.32
77.00
76.68
f1 (ppm)

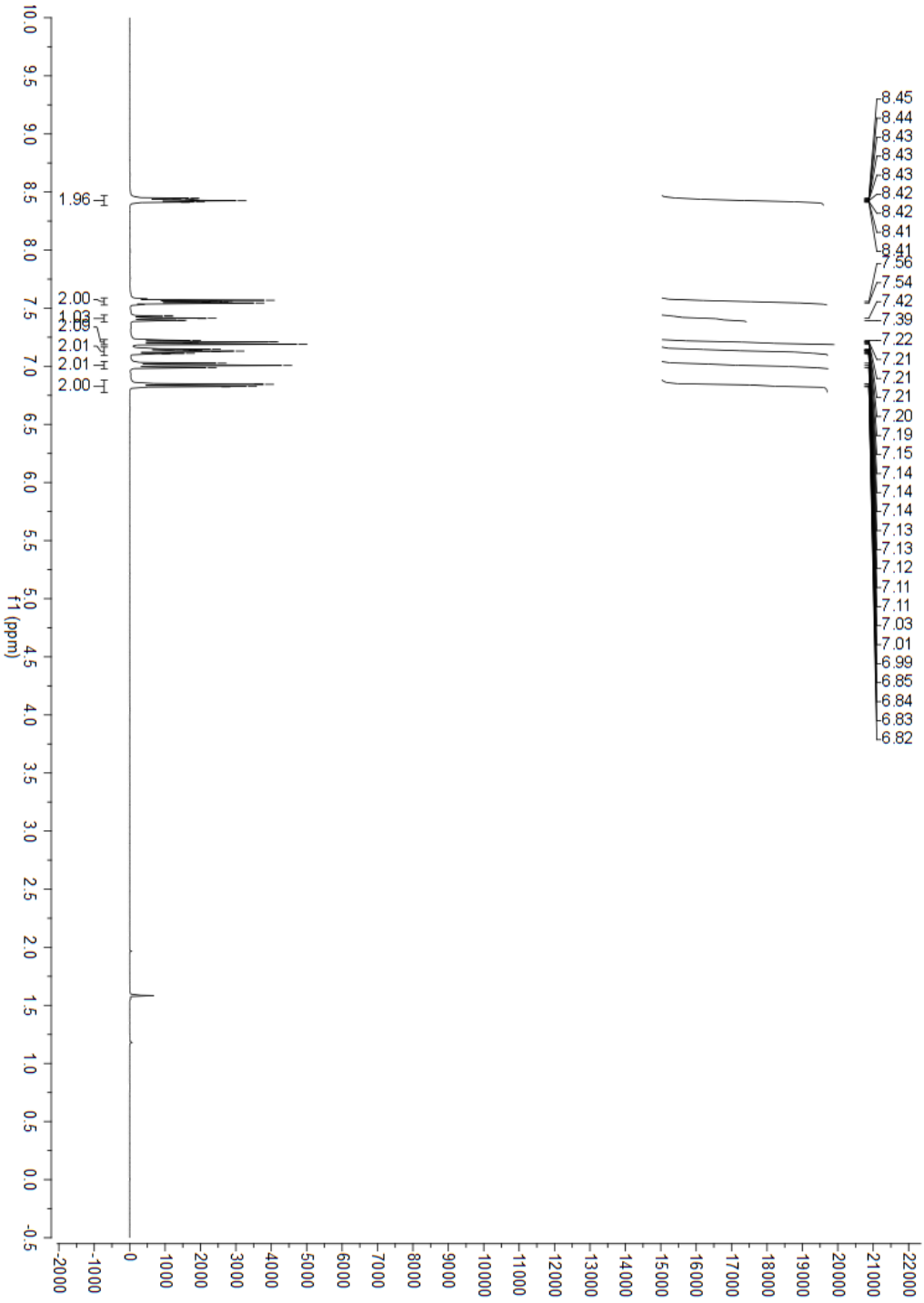

NO2
O
S
N

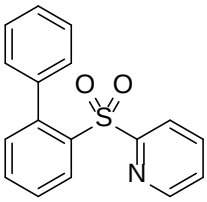

1.00
2.05
1.02
3.10
1.01
2.07
0.99
1.05
8.49
8.32
8.30
7.89
7.79
7.54
7.54
7.40
7.38
7.32
7.31
7.29
7.26
f1 (ppm)

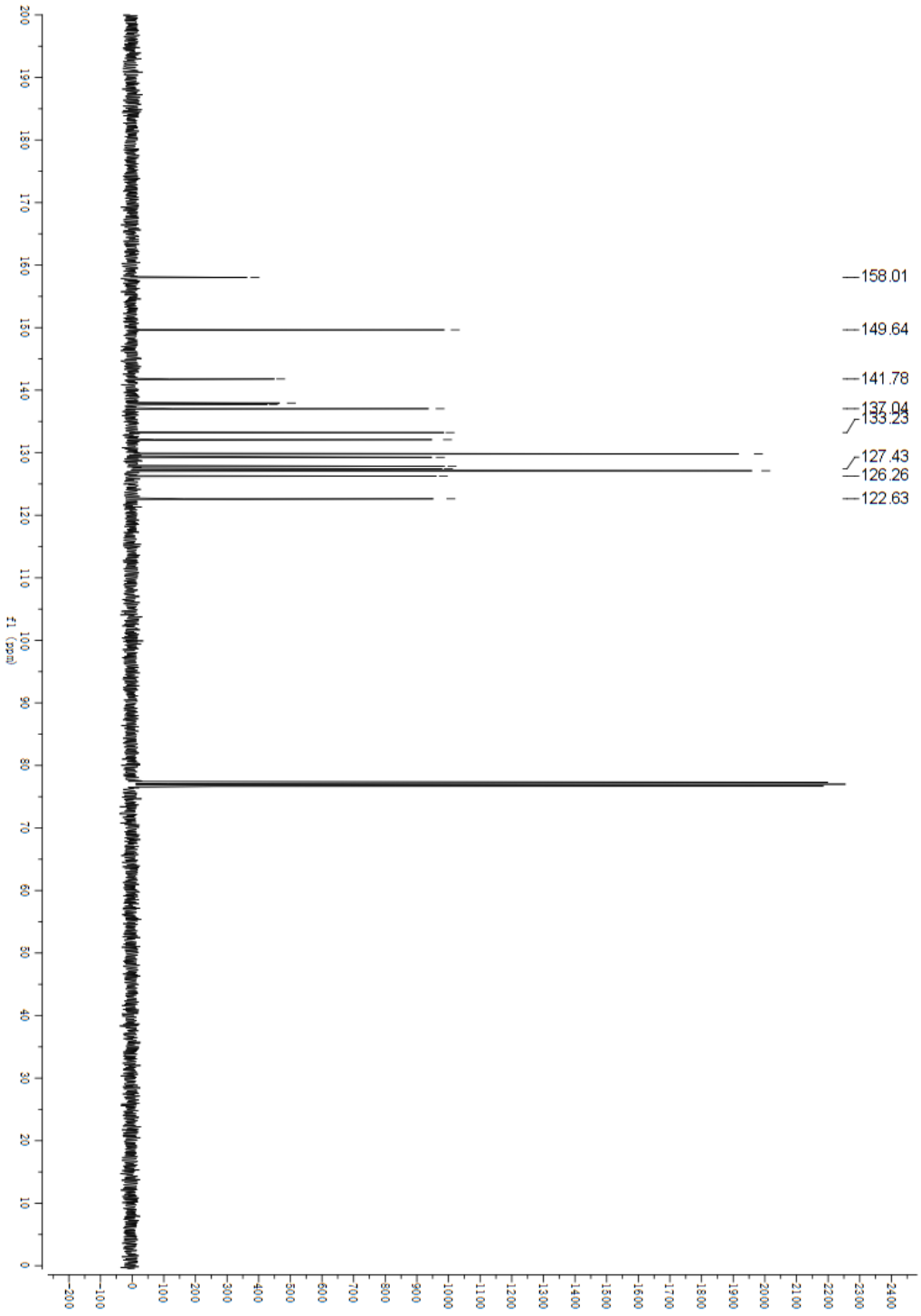

NO2
O
S
N

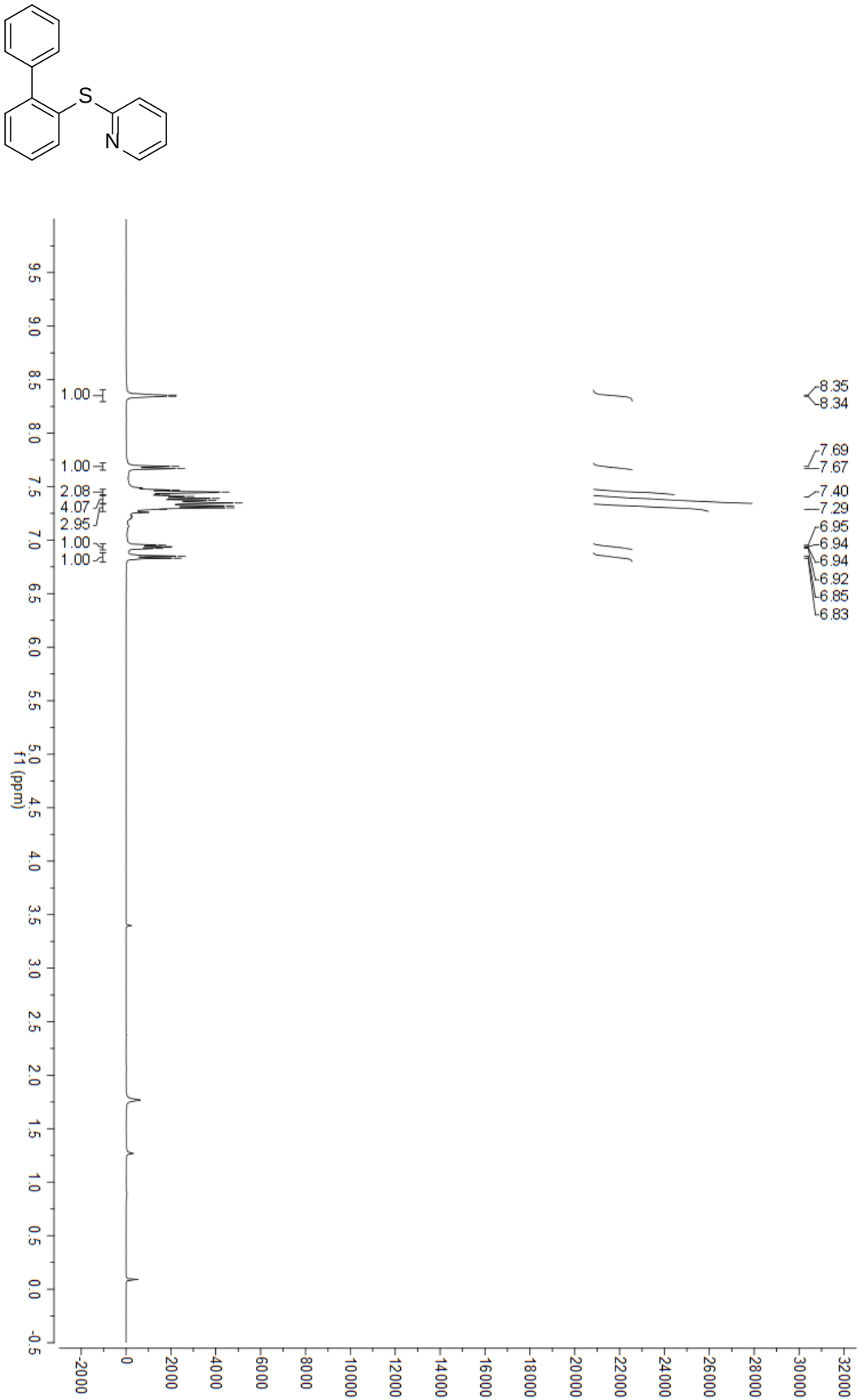

165.73
149.71
147.55
144.80
143.38
140.42
138.06
131.54
126.66
124.50
123.23
119.48
77.32
77.00
76.68
f1 (ppm)


O
O
S
N


1.96
2.00
1.03
2.09
2.01
2.01
2.00
8.45
8.44
8.43
8.43
8.43
8.42
8.42
8.41
8.41
7.56
7.54
7.42
7.39
7.22
7.21
7.21
7.21
7.20
7.19
7.15
7.14
7.14
7.14
7.13
7.13
7.12
7.11
7.11
7.03
7.01
6.99
6.85
6.84
6.83
6.82
f1 (ppm)


O
O
S
N


158.01
149.64
141.78
137.04
133.23
127.43
126.26
122.63
f1 (ppm)


S
N
1.00
1.00
2.08
4.07
2.95
1.00
1.00
8.35
8.34
7.69
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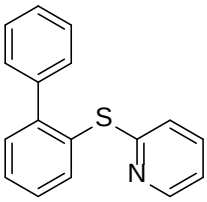
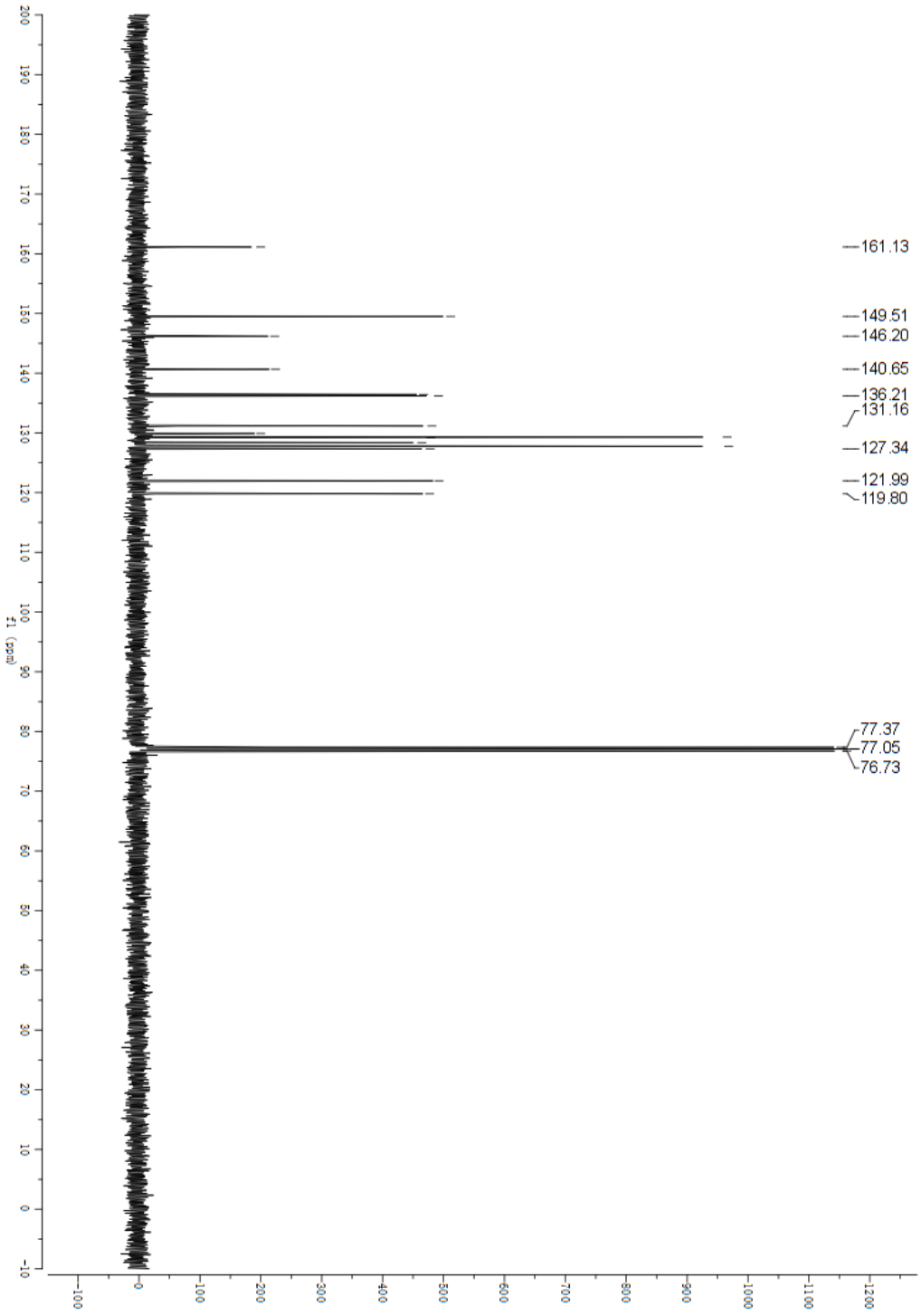
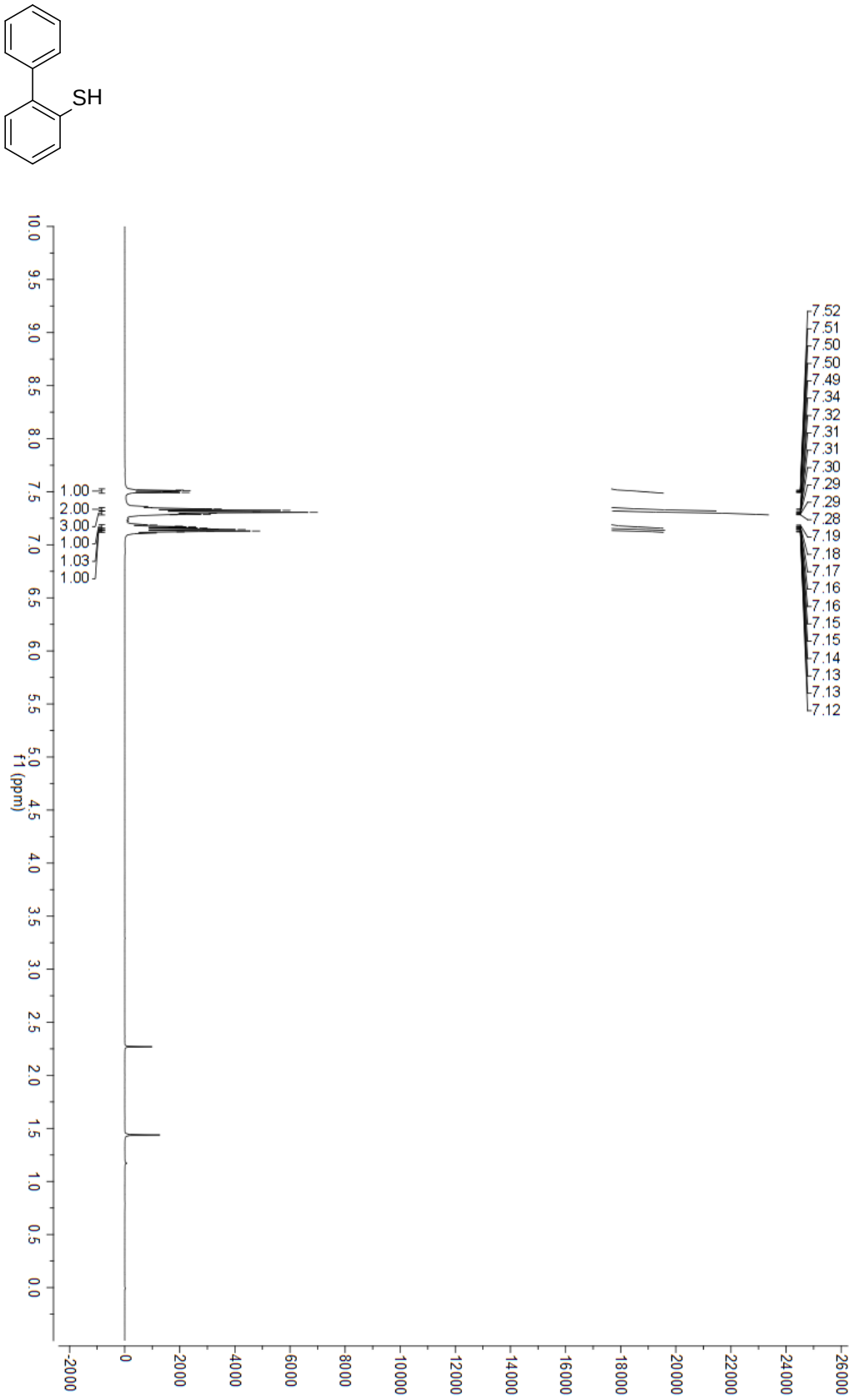
7.40
7.29
6.95
6.94
6.94
6.92
6.85
6.83
f1 (ppm)


S
N


161.13
149.51
146.20
140.65
136.21
131.16
127.34
121.99
119.80
77.37
77.05
76.73
f1 (ppm)


SH
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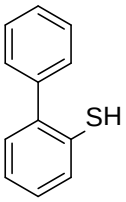
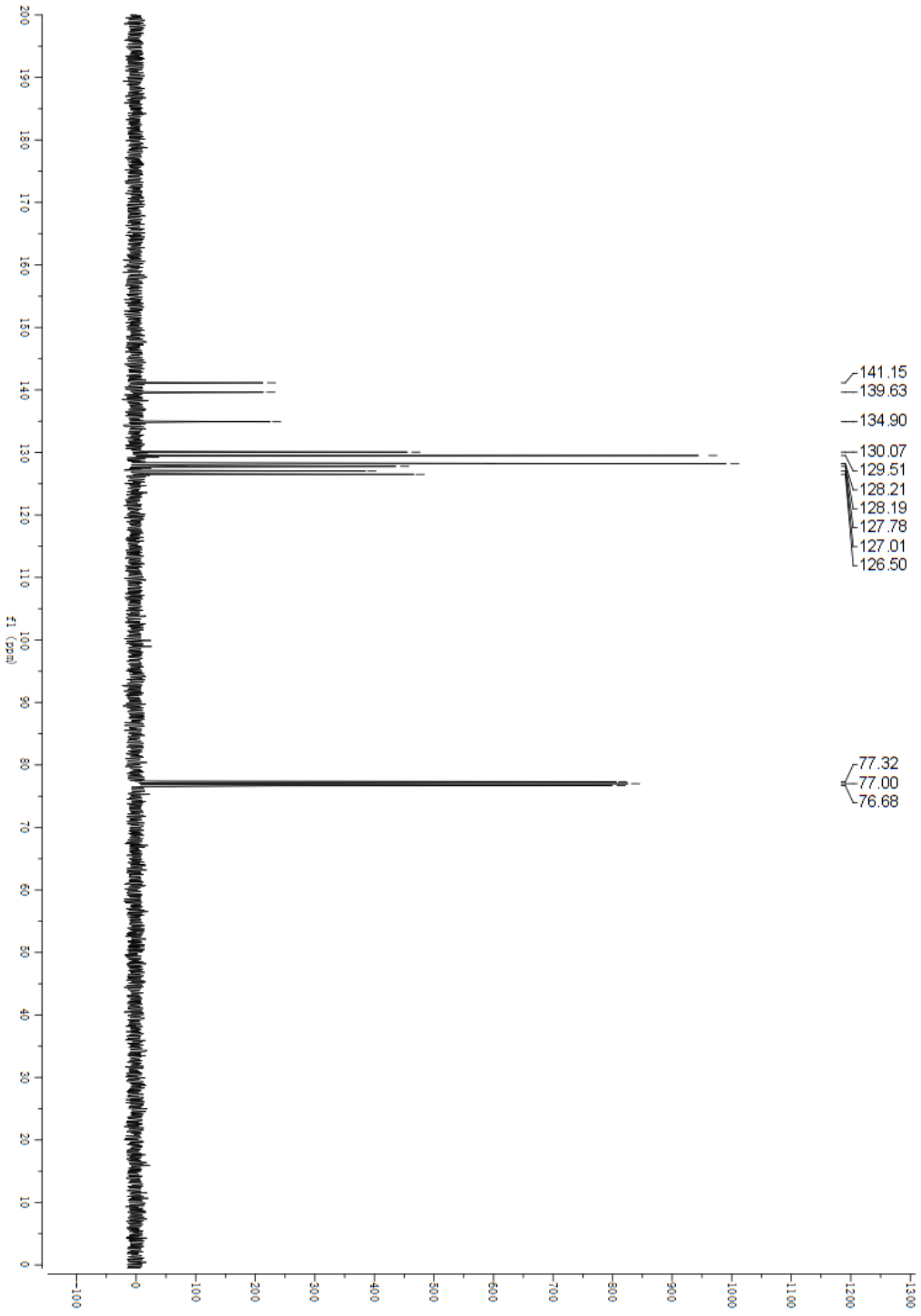
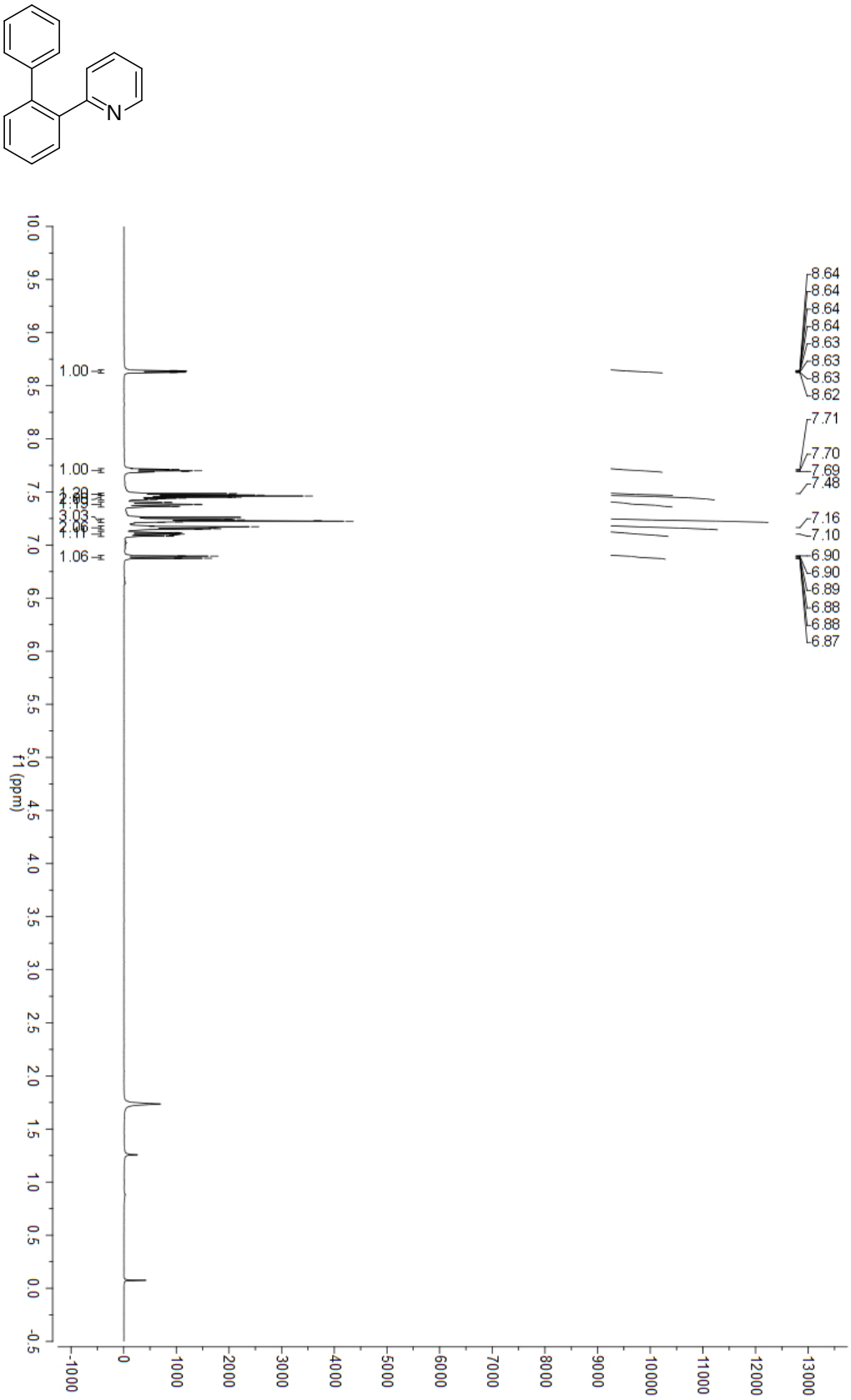
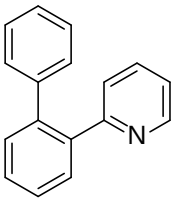
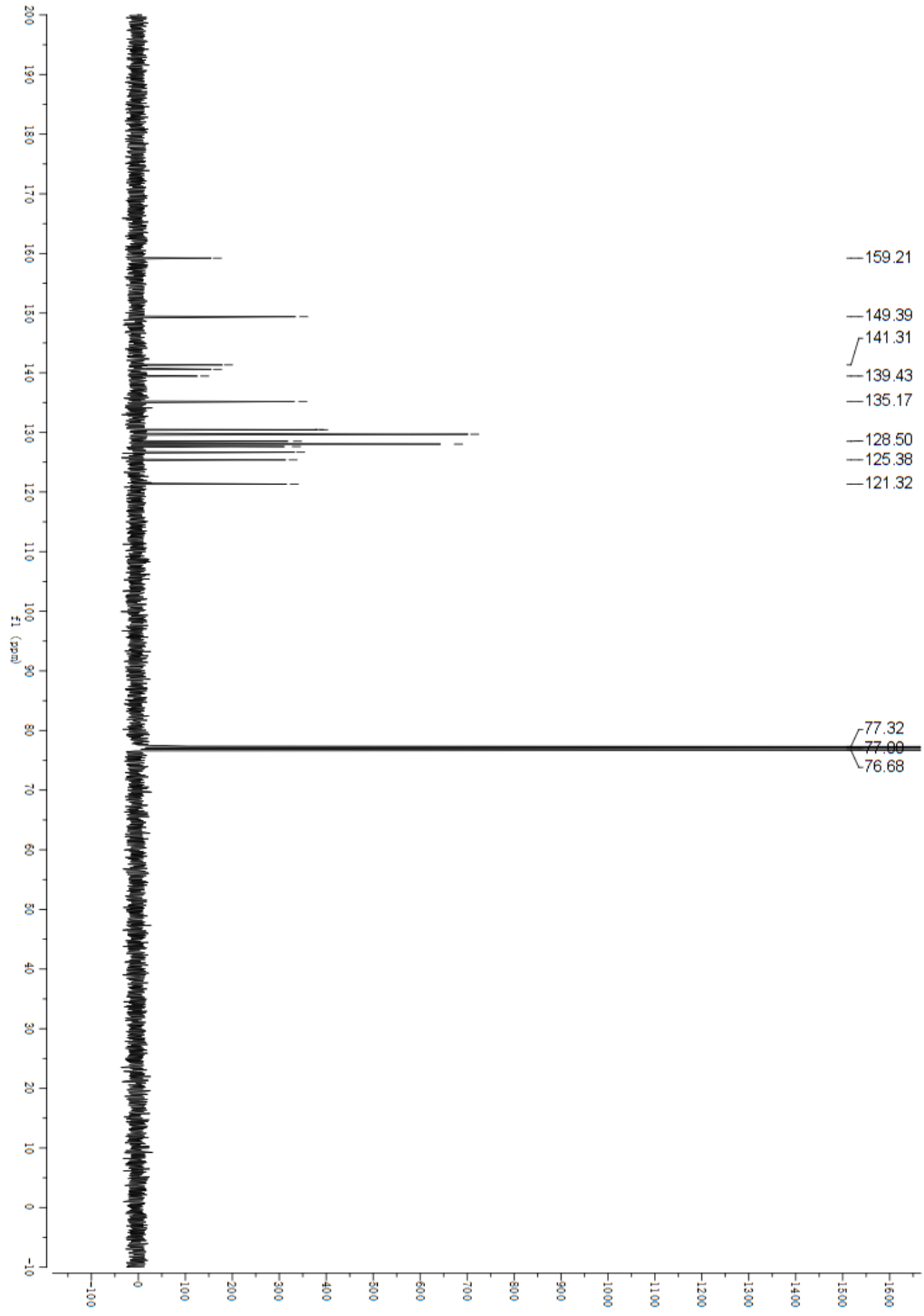
2.00
3.00
1.00
1.03
1.00
7.52
7.51
7.50
7.50
7.49
7.34
7.32
7.31
7.31
7.30
7.29
7.29
7.28
7.19
7.18
7.17
7.16
7.16
7.15
7.15
7.14
7.13
7.13
7.12
f1 (ppm)


SH


141.15
139.63
134.90
130.07
129.51
128.21
128.19
127.78
127.01
126.50
77.32
77.00
76.68
f1 (ppm)


N
8.64
8.64
8.64
8.64
8.63
8.63
8.63
8.62
7.71
7.70
7.69
7.48
7.16
7.10
6.90
6.90
6.89
6.88
6.88
6.87
1.00
1.00
1.06
f1 (ppm)


N


159.21
149.39
141.31
139.43
135.17
128.50
125.38
121.32
77.32
77.00
76.68
f1 (ppm)

4. References

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