Electronic Supplementary Material (ESI) for New Journal of Chemistry.

$CuMoO_4$ nano catalyst for *Csp2-O* cross-couplings; Easy access to nitrofen derivatives.

1. Table of Content

2. Materials:

All Solvents such as acetonitrile (99.8%), DMF (99.8%), 1,4-dioxane (99.8%), DMSO (99.9%), *t*-BuOH (99.5%), ethanol (99.8%) and toluene (99.8%) Are of analytical grade and were purchased from Merck and distilled before its use for reaction. Deuteriated NMR solvents $CDCl_3$ (99.8%) is purchased from Sigma-Aldrich. $Cu(OAc)_2.2H_2O$ (purchased from Sigma-Aldrich), $(NH_4)_6Mo_7O_{24}.4H_2O$ (99.98%) were purchased from Sigma-Aldrich. All other solvents are purchased from Merck of high purity grade. DMF was sparged with nitrogen (N_2 gas) for 5 min at room temperature and stored under nitrogen atmosphere. K_2CO_3 (99%), KO^tBu (99%), Cs_2CO_3 (*Reagent Plus*®, 99%) and KOH (99%) were purchased from Sigma-Aldrich. Iodobenzene (98%), 4-methoxyiodobenzene (98%), 4-methyliodobenzene (99%), bromobenzene (98%), chlorobenzene (99.8%), 4-nitroiodobenzene (98%), 4-bromoacetophenone (99%) and all Phenols such as 4-chlorophenol (98%), 4-Bromophenol (98%), 4-methoxyphenol (99%) were purchased from Sigma-Aldrich and stored carefully.

3. Instrumentation:

NMR spectra were recorded on Bruker Avance III, 400 MHz (IISER Berhampur) and 500 MHz (University of Hyderabad) spectrometers in appropriate solvents $CDCl_3$ using TMS as internal standard or the solvent signals as secondary standards and the chemical shifts are shown in δ scales. The ^1H and ^{13}C NMR spectra were recorded at 400 MHz for ^1H and 100 MHz for ^{13}C NMR respectively. Deuterated solvents were purchased from Sigma-Aldrich and used as received. All ^1H NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for residual chloroform (7.26 ppm) in the deuterated solvents. Data for ^1H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets…etc, br = broad), coupling constant (Hz) and integration. All ^{13}C NMR spectra are reported in ppm relative to $CDCl_3$ (77.0 ppm). 1,4-di iodobenzene was used as an internal standard for NMR yields from proton analysis. Elemental analysis was performed in 2400 Series II CHNS/O analyzer in CHNS mode. Flash column chromatography was performed by using a 90-120 times weight excess of flash silica gel 60-120 μm from Aldrich. Fractions were analyzed by TLC using TLC silica gel F254 250 μm pre-coated-plates from Merck and stains (permanganate, 2,4-dnp and CAM) was

used for UV-inactive compounds. Melting point is determined in Digital melting point apparatus, Electronics India (EI)-2935 model; Visualized through LCD Screen and is uncorrected by ±5 °C. XPS is performed with Al-Kα line at IIT Roorkee. HRMS is done at IISER Berhampur ESI mode.

4. General Procedure for *Csp²-O* cross-coupling:

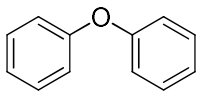
In N_2 atmosphere, $CuMoO_4$ (3 mol%, 6.7 mg), KOH (2 equiv., 112 mg), DMF (1 mL), aryl halide (1 mmol, 204 mg) and phenol (1.2 mmol, 112 mg) was taken in 5 mL vial and stirred for appropriate time at 100 °C. Reaction progress was monitored in TLC. After the completion of the reaction, it was worked-up with 5 mL cold water and 10 mL of dichloromethane (2 × 10 mL). The organic layer was collected and concentrated. The crude product was subjected to flash chromatography. The isolated product was characterised by proton and carbon NMR.

4.1. Catalytic Performance:

Sl No.	Catalyst amount in (mol%)	Yield (%)
1	3	90 (20h)
2	5	90 (20h)
3	10	90 (20h) and 86(16h)

On increasing the catalyst dosage from the 3 mol% to 5 mol%, the resulted yield still constant. The reaction time is approximately same. However, in case of 10 mole % two consecutive reaction simultaneously putted one workup at 16 hr and the other workup at 20hr the resulted yield 86% and 90%.

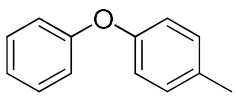
5. Characterization of diarylether products:



1-phenoxybenzene (3a)[20]: Colourless liquid, yield: 90% (77 mg).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.03-7.00 (m, 4 H), 7.12-7.07 (m, 2 H), 7.36-7.30 (m, 4 H).

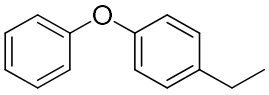
^{13}C NMR (100 MHz, $CDCl_3$): 118.8, 123.2, 129.7, 157.2.



1-methyl-4-phenoxybenzene(3b) [20]: White solid, yield: 88% (80 mg), Mp: 102-106 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 2.25 (s, 3 H), 6.85 (t, J= 8 Hz, 2H), 6.91 (d, J=8 Hz, 2H), 6.98 (t, J=6 Hz, 1H), 7.07 (d, J=8 Hz, 2H), 7.23 (t, J=8 Hz, 2H).

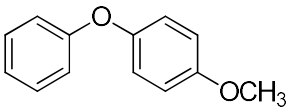
^{13}C NMR (100 MHz, $CDCl_3$): 120.6, 118.3, 119.1, 122.7, 129.6, 130.2, 132.8, 154.7, 157.8,



1-ethyl-4-phenoxybenzene (3c) [27]: Colourless liquid**,** yield: 90% (89mg)

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.24(t, J = 8 Hz, 3H), 2.65 (q, J = 8 Hz, 2H), 6.95 (d, J = 8 Hz, 2H), 7.0(d, J = 8 Hz, 2H), 7.07 (t, J = 6 Hz, 1H), 7.17 (d, J = 8 Hz, 2H), 7.32(t, J = 8 Hz, 2H),

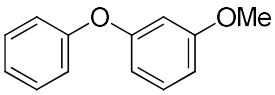
^{13}C NMR (100 MHz, $CDCl_3$):δ 15.7, 28.1, 118.4, 119.0, 122.8, 129.0, 129.6, 139.2, 154.8, 157.7.



1-(4-methoxyphenoxy) benzene(3d) [20]: Yellow liquid, yield: 83% (83 mg).

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.73 (s, 3 H), 6.79 (d, J=8 Hz, 2H), 6.89-6.86(m, 4H), 6.92 (t, J=6 Hz, 2H), 7.22 (t, J=8 Hz, 2H).

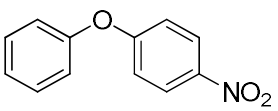
^{13}C NMR (100 MHz, $CDCl_3$): δ 55.6. 114.8, 117.5, 120.8, 122.4, 129.5, 150.1, 155.8, 158.5,



1-methoxy-3-phenoxybenzene (3e) [25]: Yellow oil, yield: 82% (82 mg)

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.84(s, 3H), 6.66(d, J = 8 Hz, 2H), 6.70(d, J = 8 Hz, 1H), 7.10(d, J = 8 Hz, 2H), 7.17 (t, J = 8 Hz, 1H), 7.30(t, J = 8 Hz, 1H), 7.40(t, J = 8 Hz, 2H).

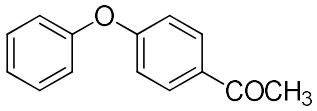
^{13}C NMR (100 MHz, $CDCl_3$):δ 55.3, 104.8, 108.4, 110.9, 119.0, 123.3, 129.7, 130.1, 158.4, 160.9,



1-nitro-4-phenoxybenzene (3f) [21]: Yellow solid, yield: 95% (102 mg), Mp: 57-59 ^oC

1H NMR (400 MHz, CDCl3): 6.94(d, J=8 Hz, 2H), 7.02 (d, J=8 Hz, 2H), 7.18(d, J=8 Hz, 1H), 7.36 (d, J=8 Hz, 2H), 8.13 (d, J=8 Hz, 2H).

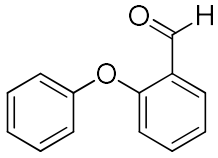
^{13}C NMR (100 MHz, $CDCl_3$): 117.0, 120.5, 125.3, 125.9, 130.2, 142.6, 154.6, 163.3,



1-(4-phenoxyphenyl)ethanone (3g) [21]: Yellow solid, yield: 92% (98 mg), 47-52 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 2.57 (s, 3H), 7.01 (d, J=8 Hz, 2H), 7.08, (d, J=8 Hz, 2H), 7.20 (t, J=8 Hz, 2H), 7.40 (t, J=8 Hz, 2H), 7.95 (d, J=8 Hz, 2H),

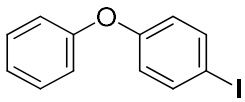
^{13}C NMR (100 MHz, $CDCl_3$): δ 26.4, 117.3, 120.2, 124.6, 130.0, 130.6, 131.9, 155.5, 161.9, 196.7,



2-phenoxybenzaldehyde (3h) [23]: Colourless oil, yield: 82% (81mg)

^{1}H NMR (400 MHz, $CDCl_3$): δ 6.91 (d, J = 8 Hz, 2H), 7.08 (d, J = 8 Hz, 2H), 7.19(t, J = 8 Hz, 2H), 7.40 (t, J = 8 Hz, 2H), 7.51 (t, J = 8 Hz, 1H), 7.73(d, J = 8 Hz, 1H), 10.52(s, 1H),

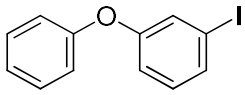
^{13}C NMR (100 MHz, $CDCl_3$):δ 118.4, 119.4, 123.3, 124.3, 128.4, 130.0, 135.7, 156.01, 159.7, 189.4.



1-iodo-4-phenoxybenzene (3i)[25]: Yellow solid, yield: 85% (125 mg), Mp 129-134 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 6.78 (d, J = 8 Hz, 2H), 7.02 (d, J = 8 Hz, 2H), 7.13 (t, J = 8 Hz, 1H), 7.35 (t, J = 8 Hz, 2H), 7.62(d, J = 8 Hz, 2H),

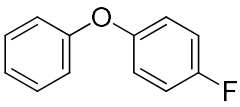
^{13}C NMR (100 MHz, $CDCl_3$):δ 85.8, 119.1, 120.8, 123.7, 129.8, 138.6, 156.5, 157.4,



1-iodo-3-phenoxybenzene (3j) [32]: Colourless oil, yield: 79% (116 mg)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.07-6.96(m, 4H), 7.15 (t, J = 8 Hz, 1H), 7.38-7.34(m, 3H), 7.44(d, J = 8 Hz, 2H).

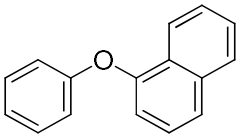
^{13}C NMR (100 MHz, $CDCl_3$):δ 94.1, 117.9, 119.2, 123.9, 127.5, 129.9, 131.0, 132.1, 156.3, 158.0.



1-fluoro-4-phenoxybenzene (3k)[22] : Colourless oil, yield: 50% (46 mg)

^{1}H NMR (400 MHz, $CDCl_3$): δ 6.99 (d, J = 8 Hz, 2H), 7.12-7.06(m, 4H), 7.26-7.16(m, 1H), 7.35-7.31 (m, 2H).

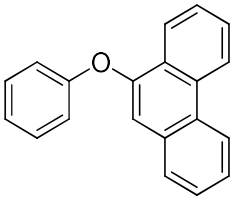
^{13}C NMR (100 MHz, $CDCl_3$):δ 117.0, 117.3, 121.8, 123.1, 124.7, 129.6.



1-phenoxynaphthalene (3l) [20] : Yellow liquid, yield: 92% (101 mg)

^{1}H NMR (400 MHz, $CDCl_3$): δ 6.95(d, J = 8.0 Hz, 1H), 7.04(d, J = 8.0 Hz, 2H), 7.11 (t, J = 8 Hz, 1H), 7.40-7.33(m, 3H), 7.55-7.47(m, 2H), 7.63(d, J = 8.0 Hz, 1H), 7.89 (d, J = 8 Hz, 1H), 7.22 (d, J = 8.0 Hz, 1H),

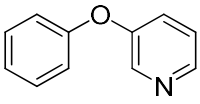
^{13}C NMR (100 MHz, $CDCl_3$):δ 113.4, 118.5, 122.1, 123.1, 123.3, 125.7, 125.9, 126.5, 127.7, 129.7, 134.9, 153.1, 157.8.



9-phenoxyphenanthrene (3m) [26]: White solid, yield: 78% (105 mg), Mp: 165-170 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.20-7.13(m, 4H), 7.40 (t, J = 8 Hz, 2H), 7.61-7.55(m, 2H), 7.75-7.63(m, 3H), 8.33 (d, J = 8 Hz, 1H), 8.67(d, J = 8 Hz, 1H), 8.74(d, J = 8 Hz, 1H),

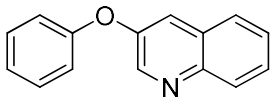
^{13}C NMR (100 MHz, $CDCl_3$):δ 111.4, 119.1, 122.5, 122.7, 123.5, 125.3, 126.9, 127.3, 127.6, 127.8, 129.8, 131.7, 132.2, 151.6, 157.3,



3-phenoxypyridine (3n) [25]: White solid, yield: 90% (76mg)**,** Mp – 262 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$): δ6.77(d, J = 8 Hz, 4H),6.85 (t, J = 8 Hz, 2H),7.17(t, J = 8 Hz, 4H).

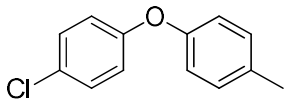
^{13}C NMR (100 MHz, $CDCl_3$):δ 119.2, 120.1, 124.3, 127.0, 127.2, 127.8, 128.5, 129.1, 130.0, 144.6, 145.1, 151.0, 156.2.



3-phenoxyquinoline (3o) [24]: White solid, yield: 86% (95mg)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.01 (d, J = 8 Hz, 2H), 7.10(t, J = 8 Hz, 1H), 7.31 (t, J = 6 Hz, 2H), 7.42-7.39(m, 2H), 7.57-7.50(m, 2H), 8.02(d, J = 8 Hz, 1H), 8.72 (s, 1H).

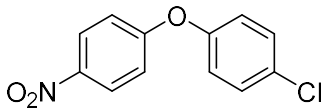
^{13}C NMR (100 MHz, $CDCl_3$):δ 119.2, 120.1, 124.3, 127.0, 127.2, 127.8, 128.5, 129.1, 130.0, 144.6, 145.1, 151.0, 156.2.



1-(4-chlorophenoxy)-4-methylbenzene(3p) [30]: White solid, yield: 82% (90 mg).

^{1}H NMR (400 MHz, $CDCl_3$): δ 2.27 (s,3H), 6.84(d, J = 8.0 Hz, 4H), 7.09 (d, J = 12 Hz, 2H), 7.19 (t, J = 6.0 Hz, 3H),

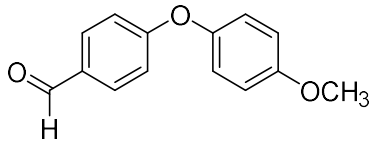
^{13}CNMR (100 MHz, $CDCl_3$):δ 20.7, 119.1, 119.1, 119.4, 127.7, 129.5, 130.3, 133.3, 154.3, 156.5,



1-chloro-4-(4-nitrophenoxy)benzene (3r) [31]: Yellow solid, yield: 91% (113mg), Mp :79-84 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.05-7.00(m, 4H), 7.43(d, J = 12 Hz, 2H), 8.22(d, J = 8 Hz, 2H).

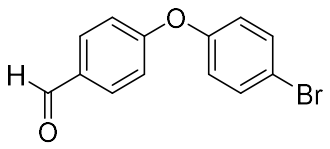
^{13}C NMR (100 MHz, $CDCl_3$):δ 117.1, 121.7, 126.0, 130.3, 142.9, 153.3, 162.8.



4-(4-methoxyphenoxy)benzaldehyde (3s) [23]: Solid, Yield: 90% (102 mg), Mp – 62 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.83(s, 3H), 6.95(d, J = 8 Hz, 2H), 7.04-6.99 (m, 4H), 7.83(d, J = 8 Hz, 2H), 9.90(s, 1H).

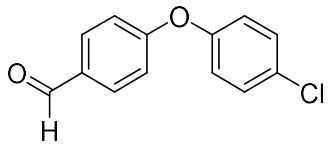
^{13}C NMR (100 MHz, $CDCl_3$):δ 156.6, 115.1, 116.7, 121.8, 130.8, 131.9, 148.1, 156.8, 164.1, 190.7.



4-(4-bromophenoxy)benzaldehyde (3t) [23]: Light yellow Solid, Yield: 88%(121 mg), Mp 68-73 ^{o}C

^{1}H NMR (400 MHz, CDCl$_3$): δ 6.91(d, J = 8 Hz, 2H), 7.00(d, J = 8 Hz, 2H), 7.45(d, J = 8 Hz, 2H), 7.80(d, J = 8 Hz, 2H), 9.86(s, 1H).

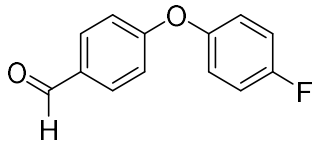
^{13}C NMR (100 MHz, CDCl$_3$):δ 117.6, 117.7, 122.0, 131.6, 131.9, 133.1, 154.3, 162.5, 190.6.



4-(4-chlorophenoxy)benzaldehyde (3u) [23]: Yellow solid, yield: 82% (96 mg), Mp 56-60 ^{o}C

^{1}H NMR (400 MHz, CDCl$_3$): δ 7.13-7.01 (m, 6H), 7.85(d, J = 8 Hz, 2H), 9.92(s, 1H),

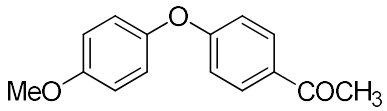
^{13}C NMR (100 MHz, CDCl$_3$):δ 116.6, 116.9, 117.1, , 121.9, 122.0, 131.3, 131.9, 150.8, 158.4, 160.9, 163.3, 190.69.



4-(4-fluorophenoxy)benzaldehyde (3v) [23] : White Solid,Yield: 72% (78 mg), Mp: 74-78 ^{o}C

^{1}H NMR (400 MHz, CDCl$_3$): δ 7.11-7.02 (m, 6H), 7.86(d, J = 8 Hz, 2H), 9.92(s, 1H).

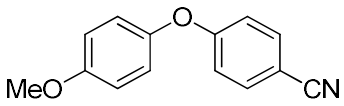
^{13}C NMR (100 MHz, CDCl$_3$):δ 116.6, 117.1, 121.9, 122.0, 131.3, 131.9, 150.8, 158.4, 160.9, 190.69.



1-(4-(4-methoxyphenoxy)phenyl)ethanone (3w) [29]: White Solid , yield: 87% (105 mg), Mp: 56- 59 ^{o}C

^{1}H NMR (400 MHz, CDCl$_3$): δ 2.55 (s, 3H), 3.81 (s, 3H), 6.95-6.91 (m, 4H), 7.0(d, J = 9.0 Hz, 2H), 7.92 (d, J = 9.0 Hz, 2H),

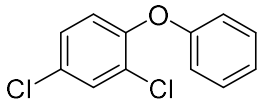
^{13}C NMR (100 MHz, $CDCl_3$): 26.3, 55.5, 115.3, 116.2, 121.6, 130.5, 131.3, 148.4, 156.6, 162.8, 196.6,



4-(4-methoxyphenoxy)benzonitrile (3x) [28]: Yellow solid, yield: 20% (23 mg), Mp: 142-146 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.82 (s, 3H), 6.94 (dd, J = 8.0, 7.2 Hz, 4H), 7.01 (d, J = 8 Hz, 2H), 7.57 (d, J = 8.0 Hz, 2H),

^{13}C NMR (100 MHz, $CDCl_3$): δ 55.5, 105.1, 115.1,117.0, 118.8, 121.7, 134.0, 147.7, 156.9, 162.4,

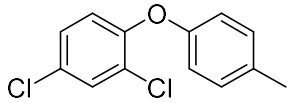


2,4-dichloro-1-phenoxybenzene (5a) [33] : Liquid , Yield 82 % (97 mg)

^{1}H NMR (400 MHz, $CDCl_3$) : δ 6.84 (d, J = 8.7 Hz, 1H), 6.84 (d, J = 8.7 Hz, 1H), 6.89 (d, J = 8.1 Hz, 2H), 7.05 (t, J = 7.4 Hz, 1H), 7.11 (d, J = 8.7 Hz, 1H), 7.27 (t, J = 7.5 Hz, 2H), 7.40 (s, 1H),

^{13}C NMR (100 MHz, $CDCl_3$): ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.6, 151.5, 130.5, 129.91, 129.2, 128.1, 126.6, 123.7, 121.4, 118.1, 29.7.

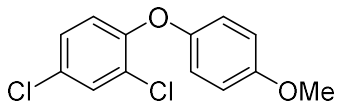
(Org. Lett. 2004, 6, 6, 913–916)



2,4-dichloro-1-(p-tolyloxy)benzene (5b): Yellow Liquid, Yield 76% (96 mg)

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 3H), 6.78 (dd, *J* = 8.5, 5.2 Hz, 3H), 7.07 (dd, *J* = 8.4, 4.6 Hz, 3H), 7.37 (d, *J* = 2.4 Hz, 1H).

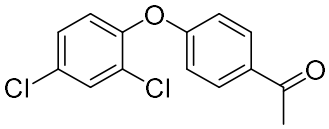
^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 148.9, 143.1, 131.7, 131.0, 128.7, 127.9, 126.1, 123.7, 116.3, 29.7.



2,4-dichloro-1-(4-methoxyphenoxy)benzene (5c) [34]**:** Yellow Liquid, Yield 88% (118 mg)

^{1}H NMR (400 MHz, $CDCl_3$) : δ 7.37 (d, *J* = 2.4 Hz, 1H), 7.19 (s, 1H), 7.06 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.90 – 6.84 (m, 2H), 6.84 – 6.79 (m, 2H), 6.71 (d, *J* = 8.8 Hz, 1H), 3.73 (s, 3H).

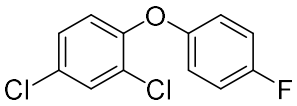
^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2 , 151.7, 148.6, 129.3, 126.8, 124.4, 119.1, 118.5, 113.9, 54.6, 28.7.



1-(4-(2,4-dichlorophenoxy) phenyl)ethan-1-one (5d) : Viscos Liquid, Yield 88% (124mg)

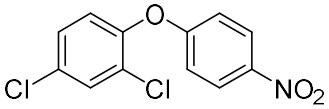
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.7 Hz, 2H), 7.44 (d, J = 2.4 Hz, 1H), 7.24 – 7.19 (m, 1H), 6.98 (d, J = 8.7 Hz, 1H), 6.87 (d, J = 8.7 Hz, 2H), 2.50 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.6, 160.9, 149.7, 132.4, 130.8, 128.5, 127.7 , 123.2, 116.4, 29.7, 26.5.



2,4-dichloro-1-(4-fluorophenoxy)benzene (5e) : Yellow Liquid, Yield 80% (102mg)

^{1}H NMR (400 MHz, $CDCl_3$) : δ 7.39 (d, *J* = 2.5 Hz, 1H), 7.11 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.97 (t, *J* = 8.5 Hz, 2H), 6.90 – 6.82 (m, 2H), 6.78 (d, *J* = 8.8 Hz, 1H).



2,4-dichloro-1-(4-nitrophenoxy)benzene (5f) : Yellow Liquid, Yield 90% (128mg)

^{1}H NMR (400 MHz, $CDCl_3$) : δ 8.13 (d, *J* = 9.2 Hz, 2H), 7.44 (d, *J* = 2.3 Hz, 1H), 7.24 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.03 (d, *J* = 8.7 Hz, 1H), 6.88 (d, *J* = 9.2 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ ^{13}C NMR (101 MHz, $CDCl_3$) : δ 162.1, 148.9, 143.1, 131.7, 131.0, 128.7, 127.9, 126.0, 123.7, 116.4, 29.7.

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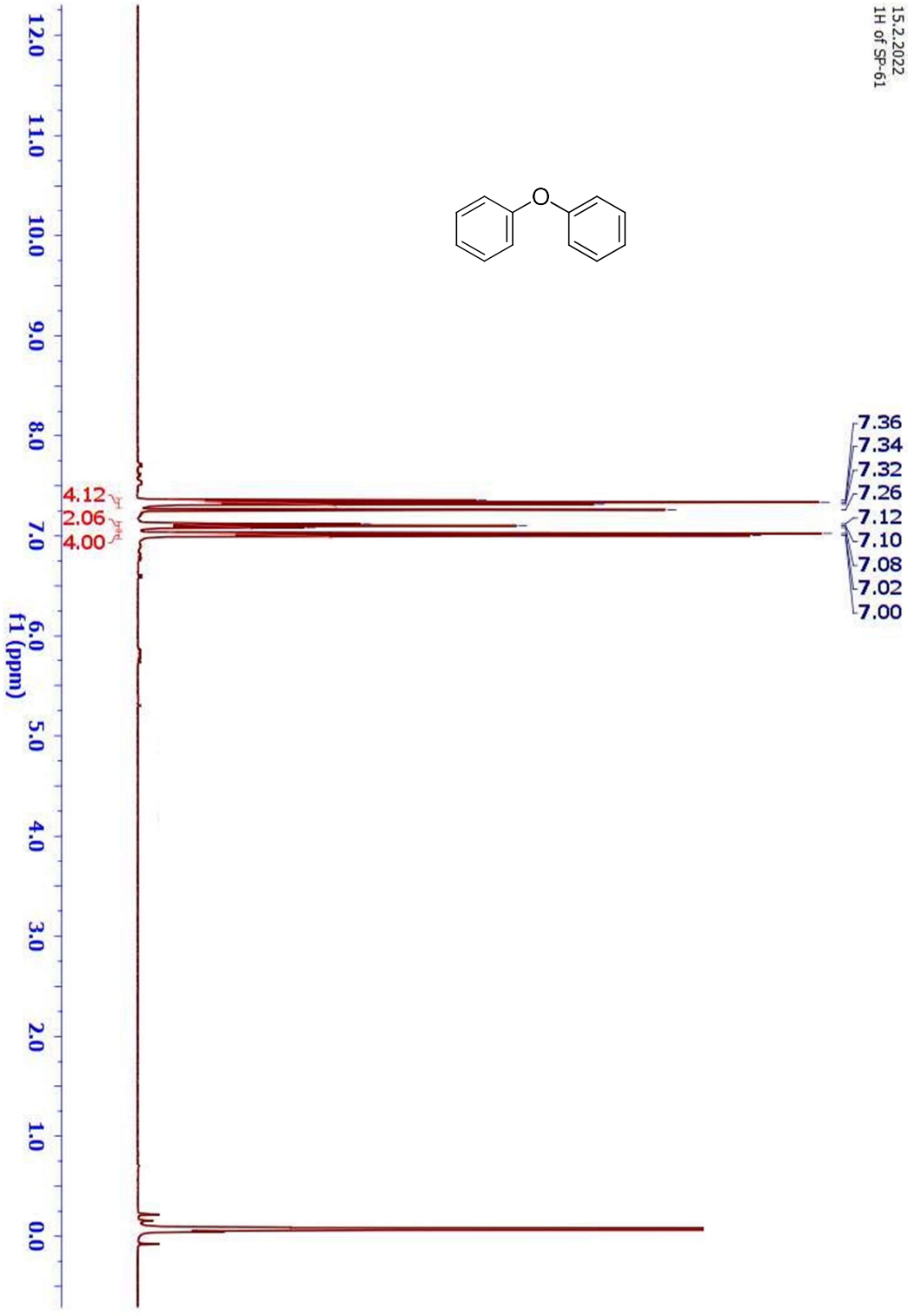
Selected Proton (400 MHz)
and
Carbon NMR (100 MHz) Spectra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O
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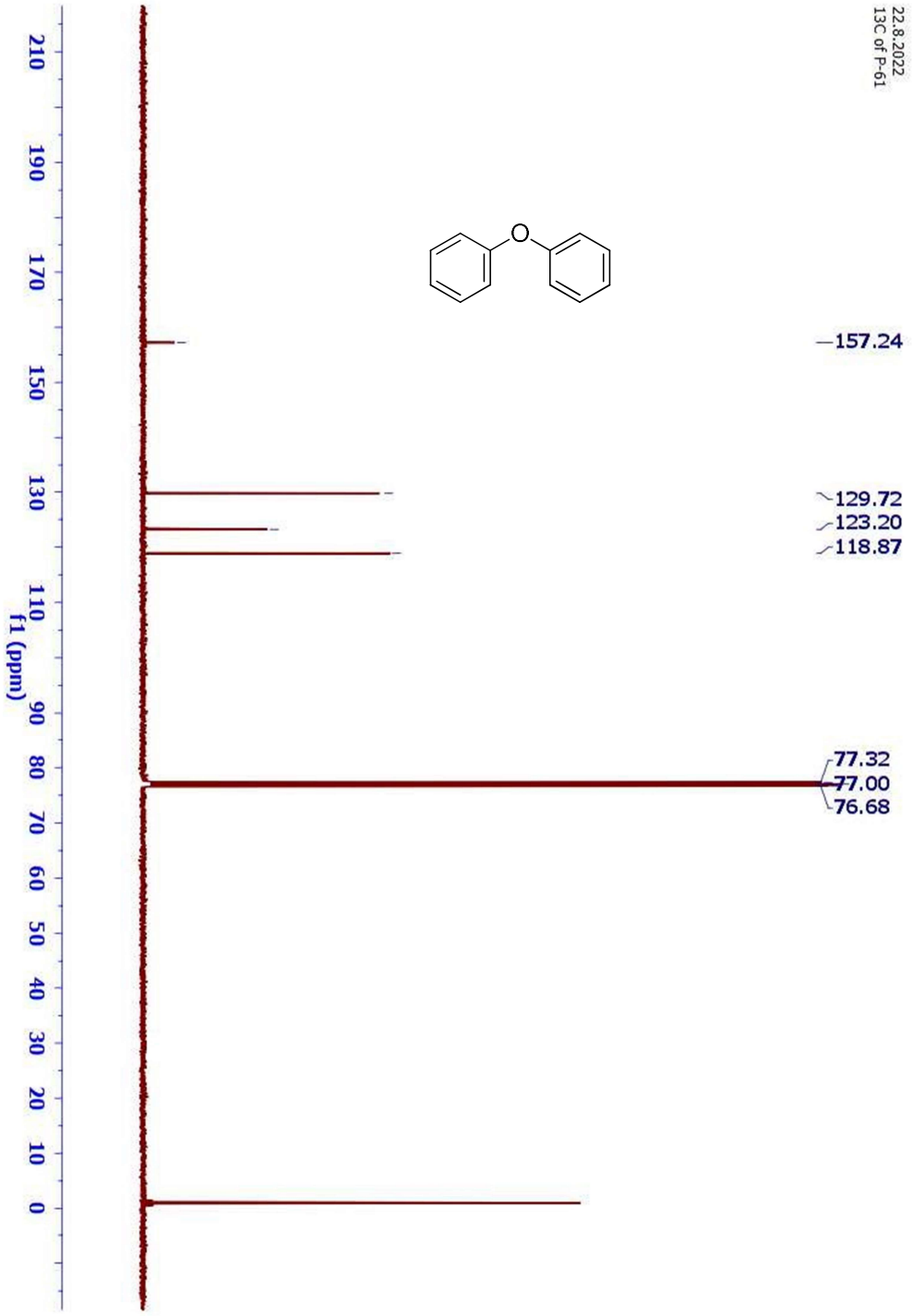
7.34
7.32
7.26
7.12
7.10
7.08
7.02
7.00
4.12
2.06
4.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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123.20
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77.32
77.00
76.68
f1 (ppm)
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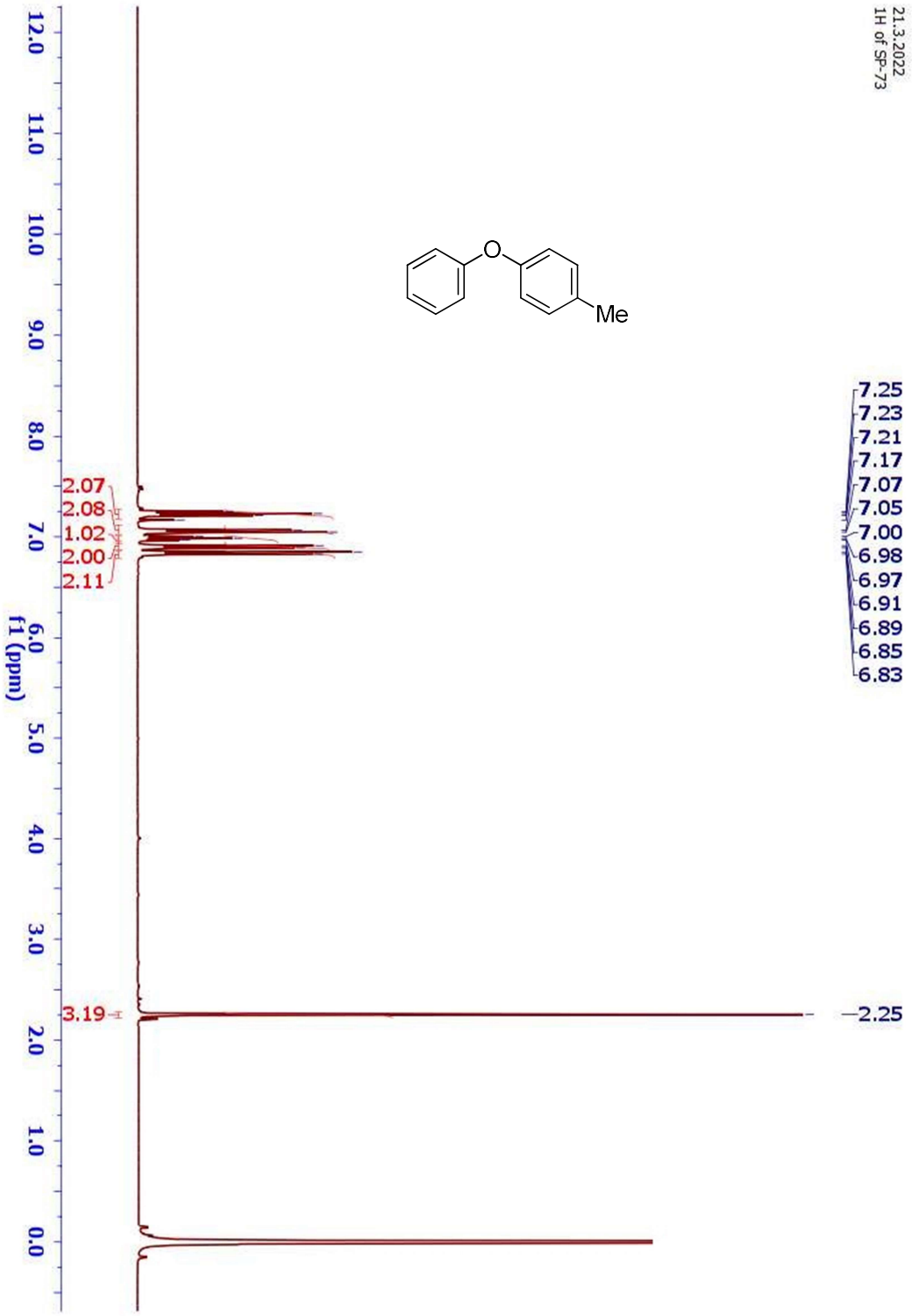
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0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Me
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7.23
7.21
7.17
7.07
7.05
7.00
6.98
6.97
6.91
6.89
6.85
6.83
2.07
2.08
1.02
2.00
2.11
3.19
2.25
f1 (ppm)
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7.0
6.0
5.0
4.0
3.0
2.0
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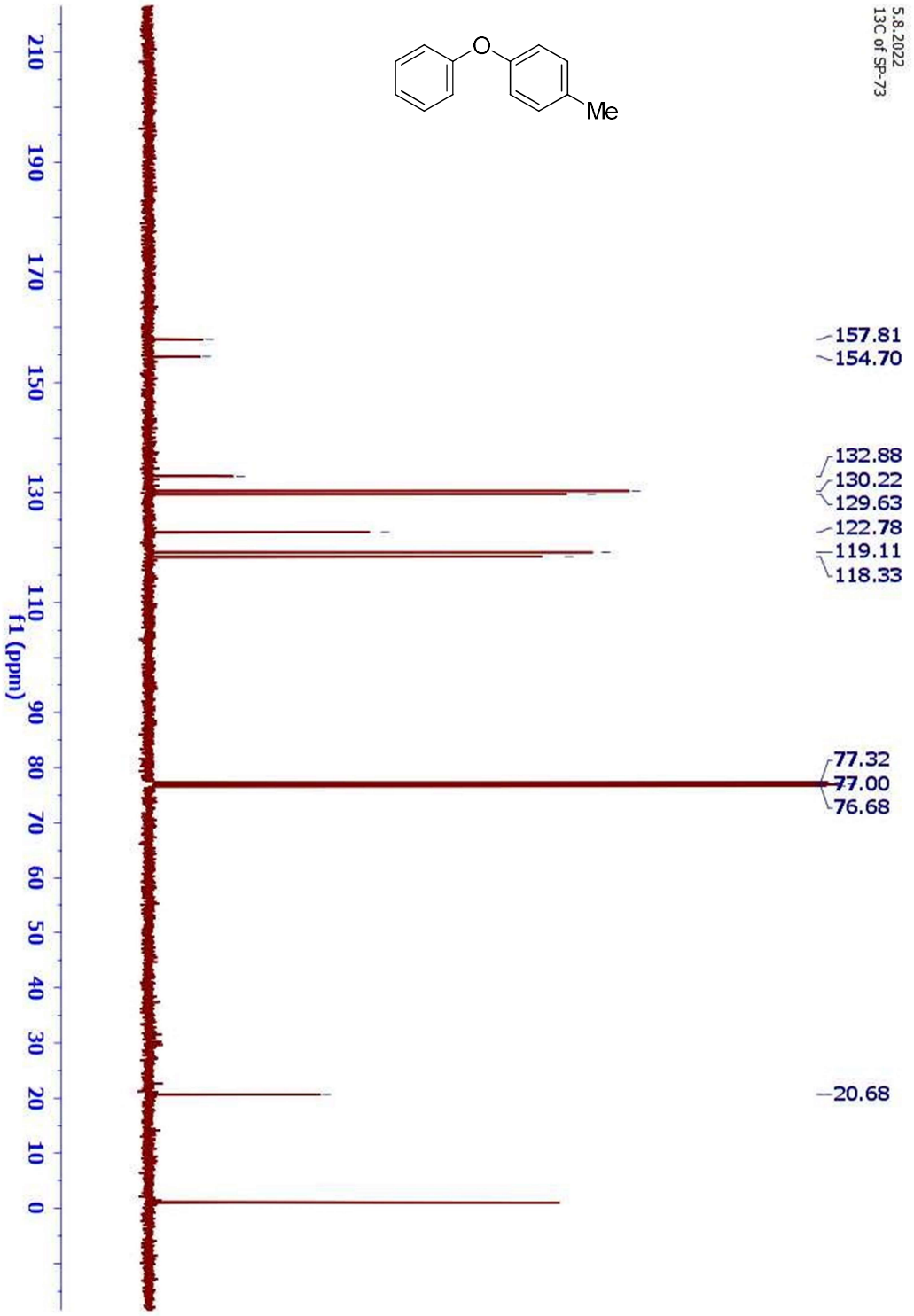
0.0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122.78
119.11
118.33
77.32
77.00
76.68
20.68
f1 (ppm)
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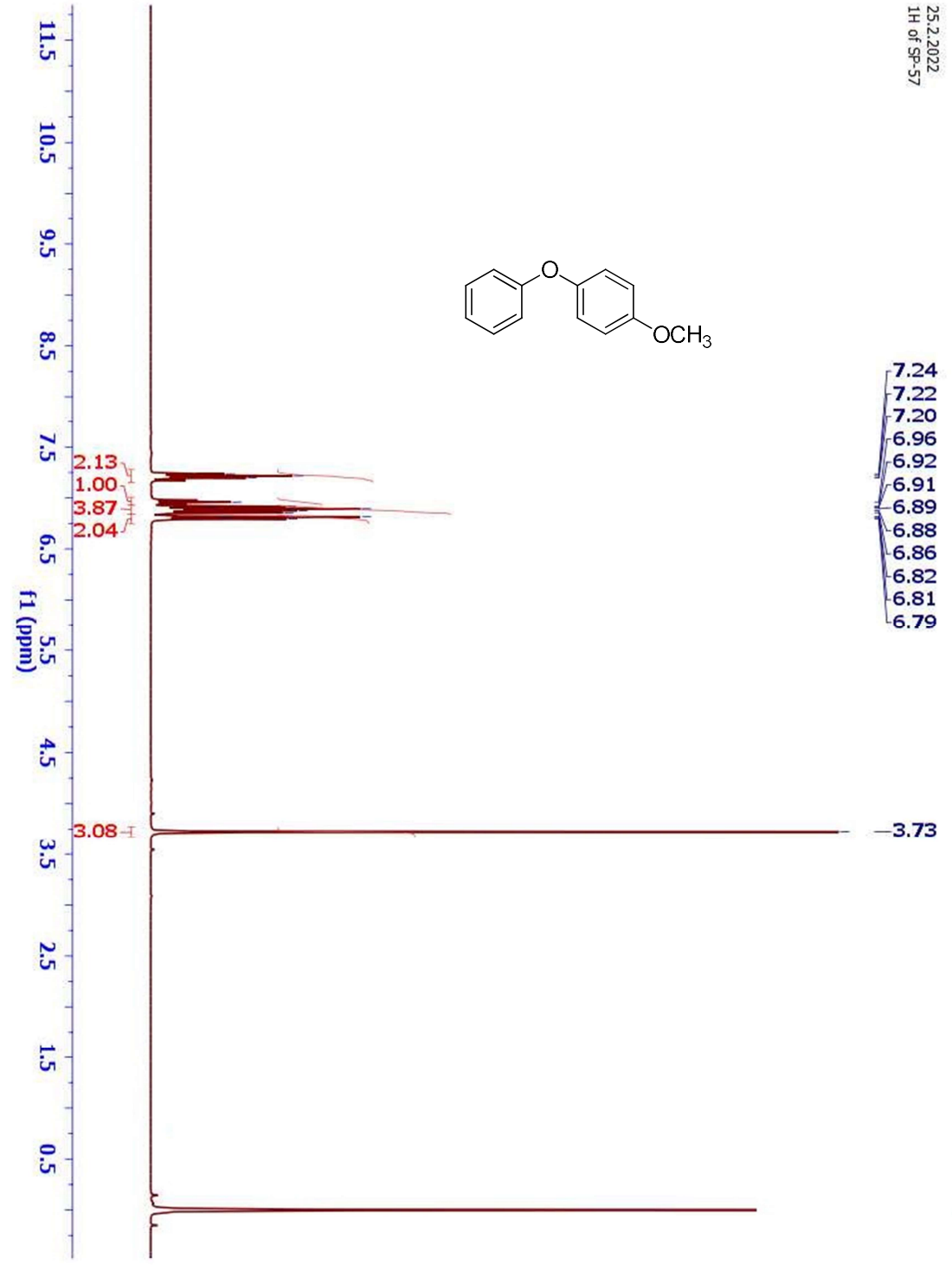
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0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6.92
6.91
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6.88
6.86
6.82
6.81
6.79
3.73
2.13
1.00
3.87
2.04
3.08
f1 (ppm)
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4.5
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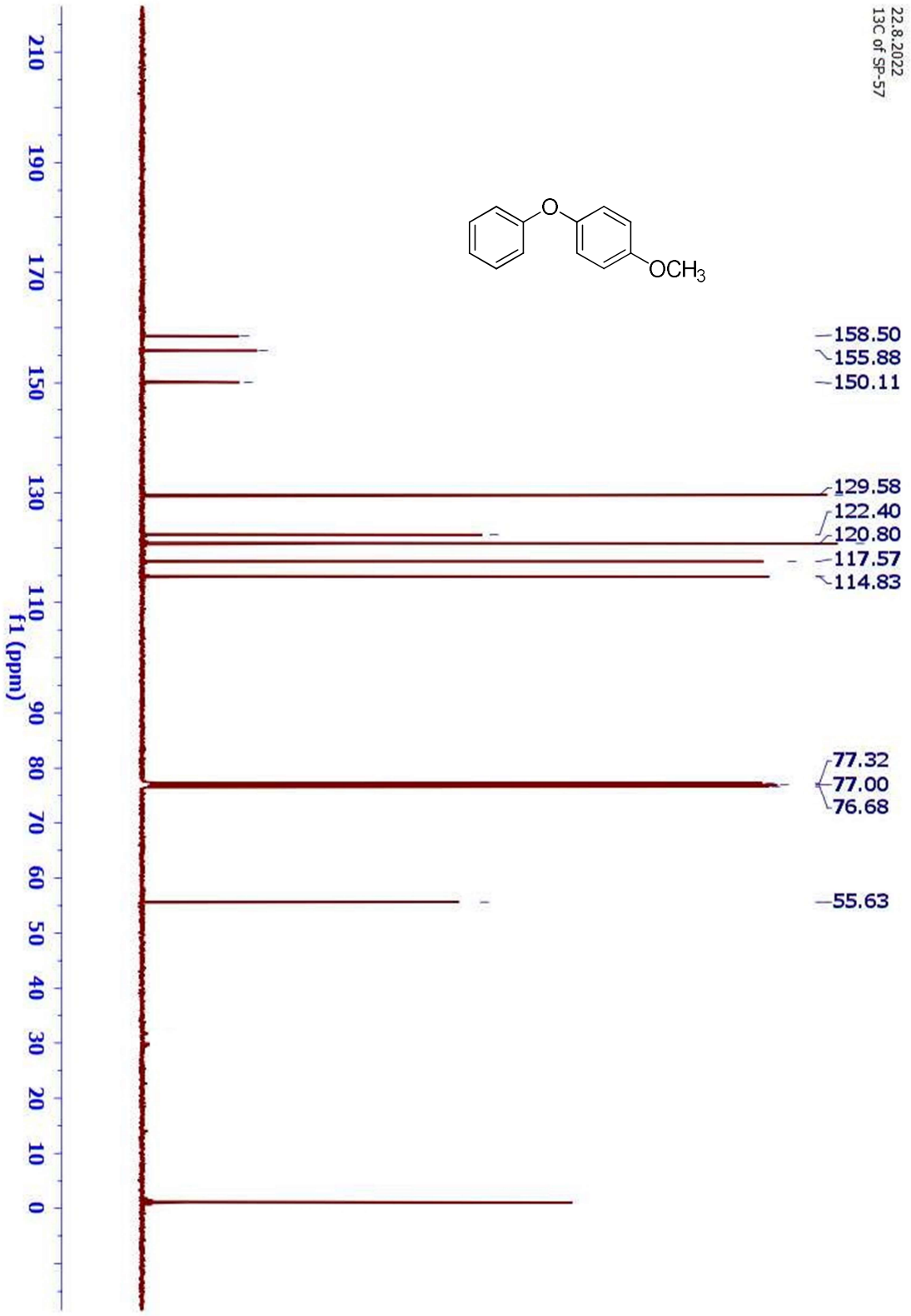
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OCH3
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122.40
120.80
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77.00
76.68
55.63
f1 (ppm)
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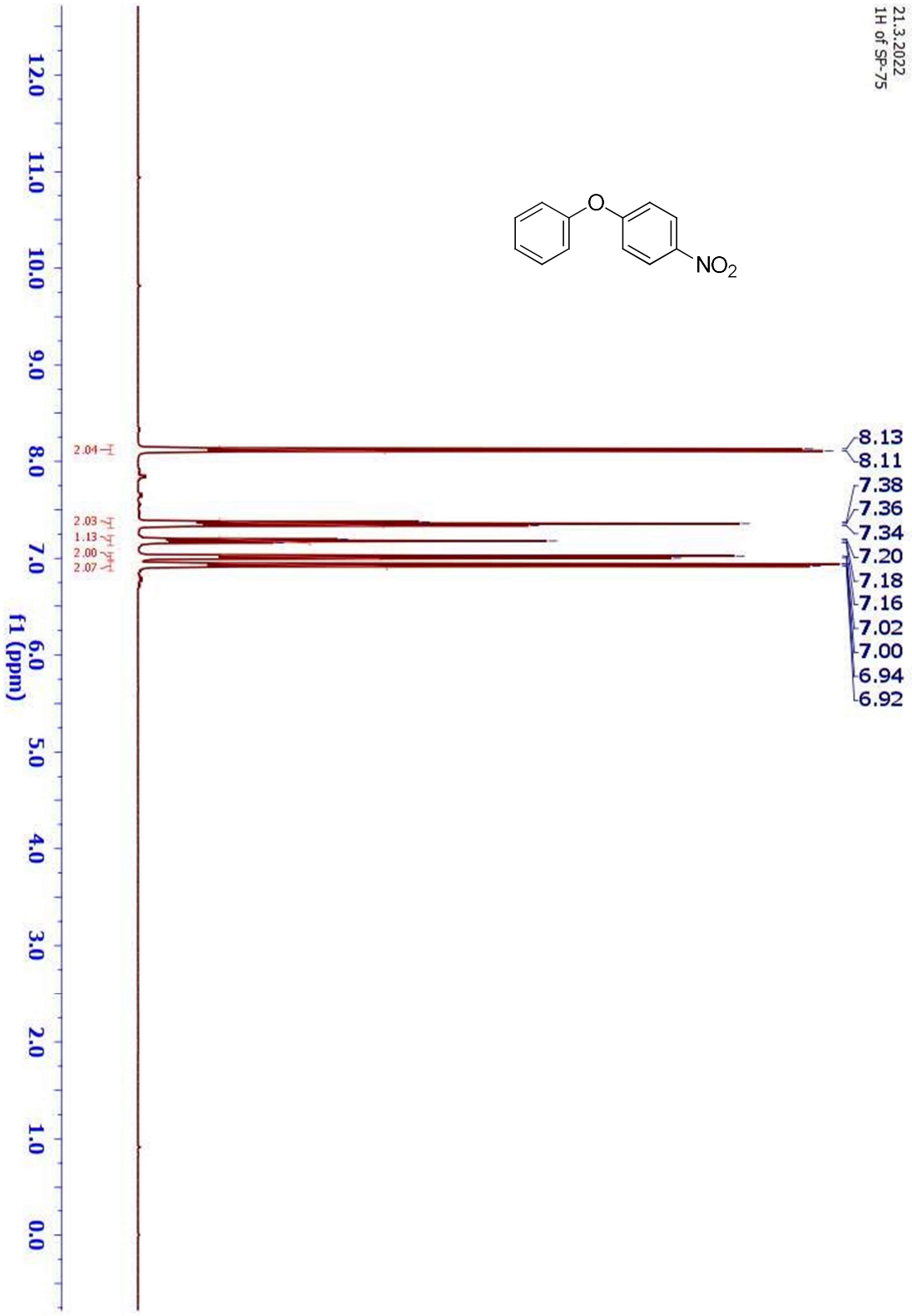
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0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7.16
7.02
7.00
6.94
6.92
2.04
2.03
1.13
2.00
2.07
f1 (ppm)
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4.0
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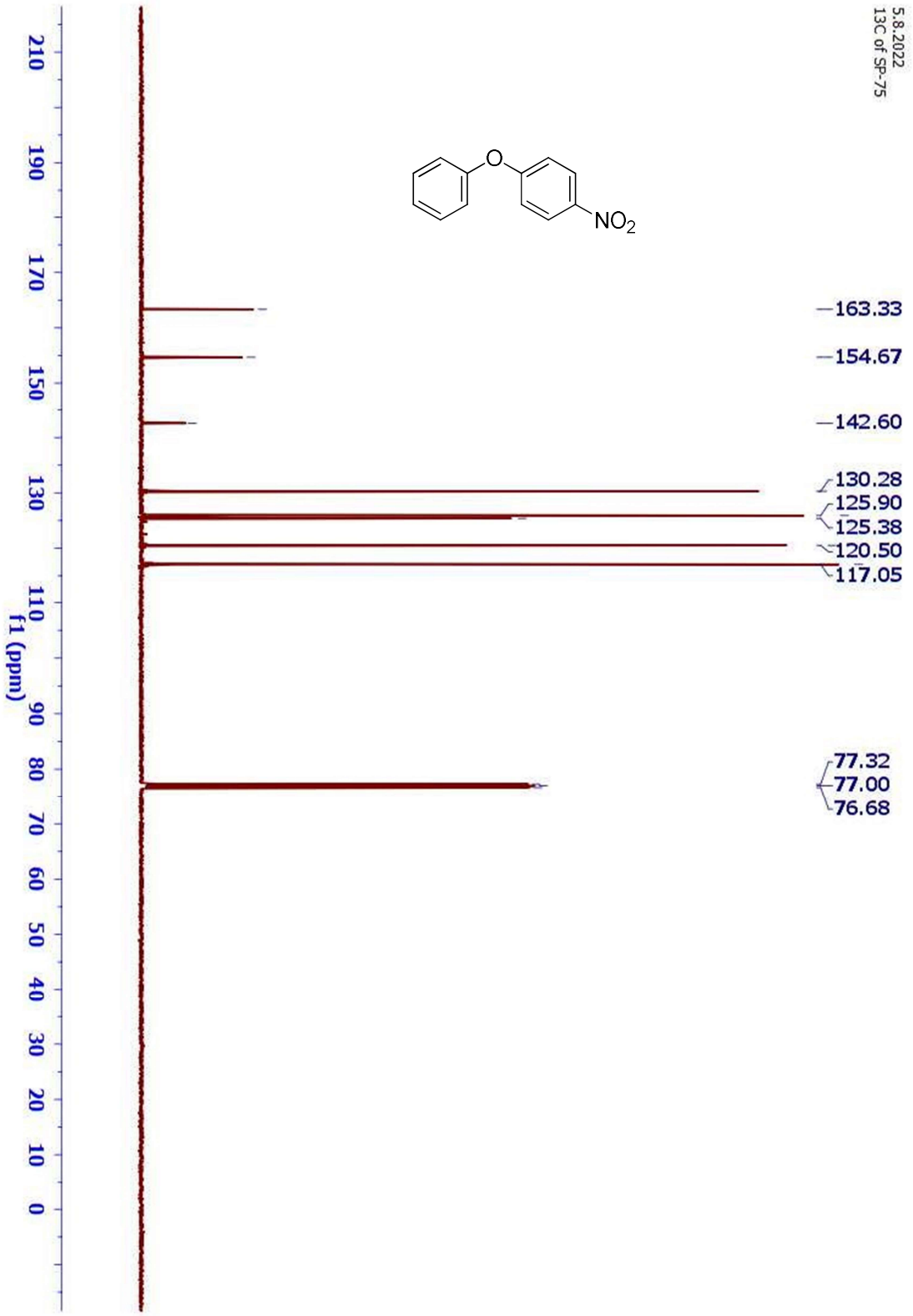
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77.32
77.00
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170
150
130
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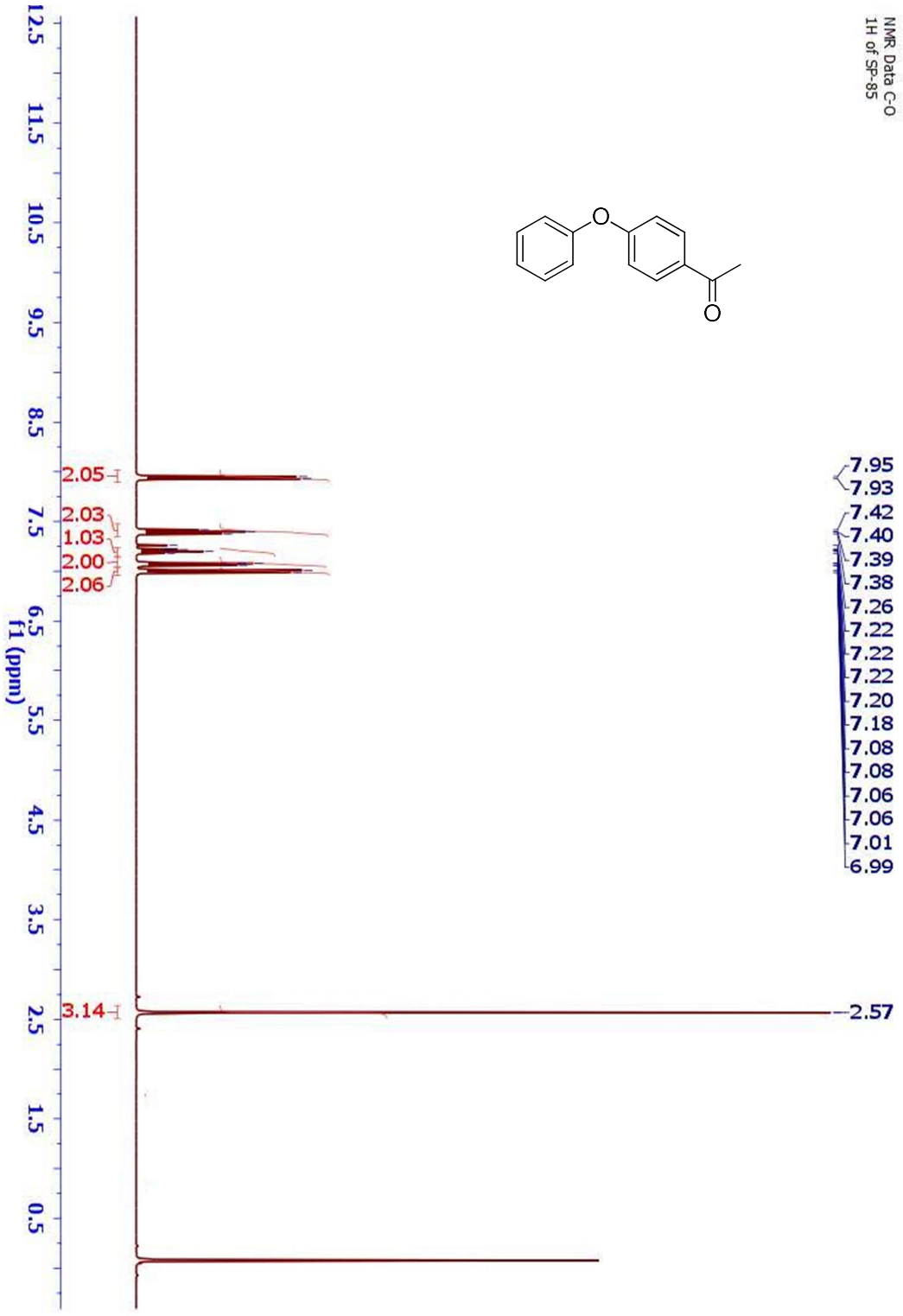
90
80
70
60
50
40
30
20
10
0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10.5
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7.5
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5.5
4.5
3.5
2.5
1.5
0.5
2.05
2.03
1.03
2.00
2.06
3.14
7.95
7.93
7.42
7.40
7.39
7.38
7.26
7.22
7.22
7.22
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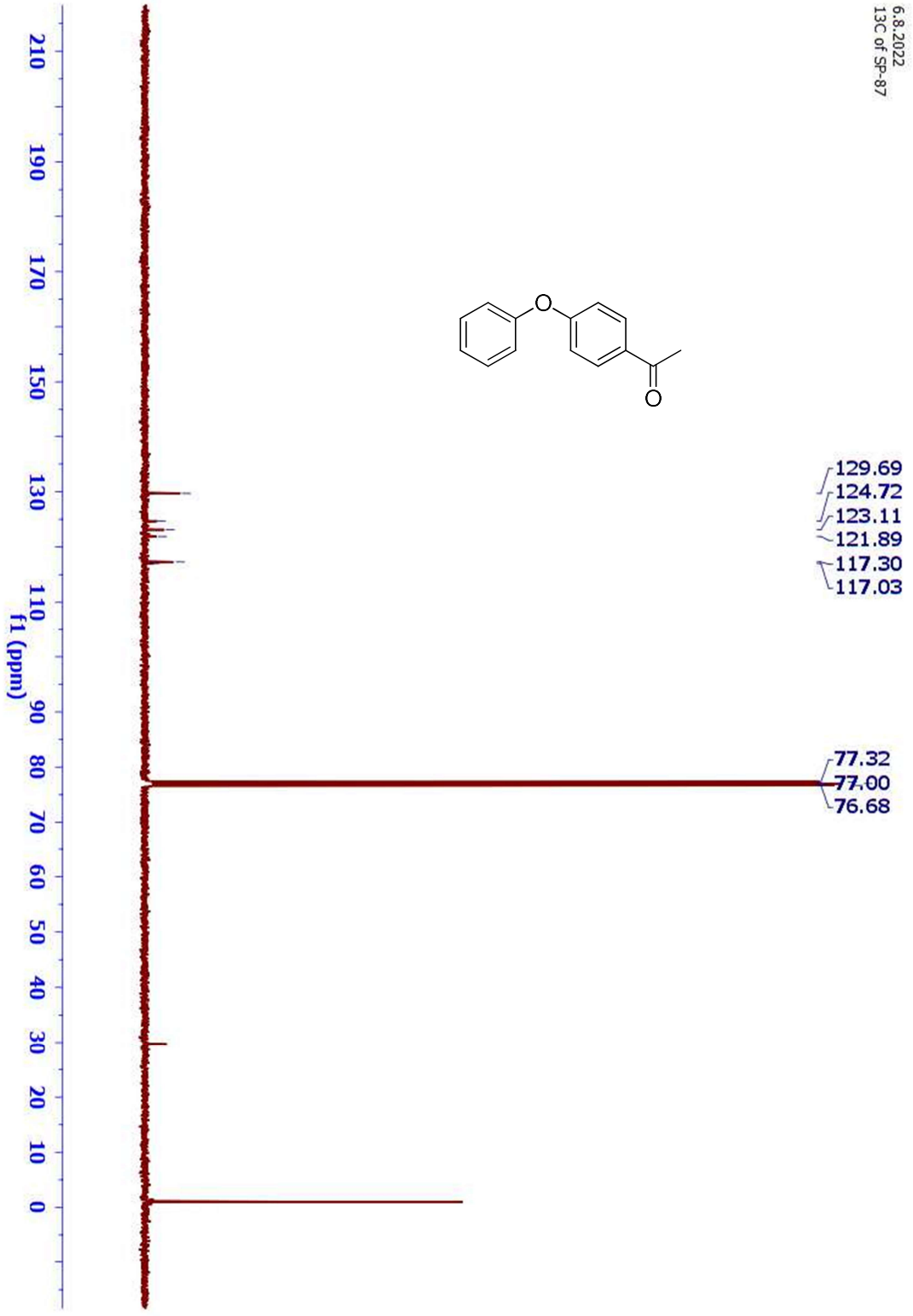
7.18
7.08
7.08
7.06
7.06
7.01
6.99
2.57
O
O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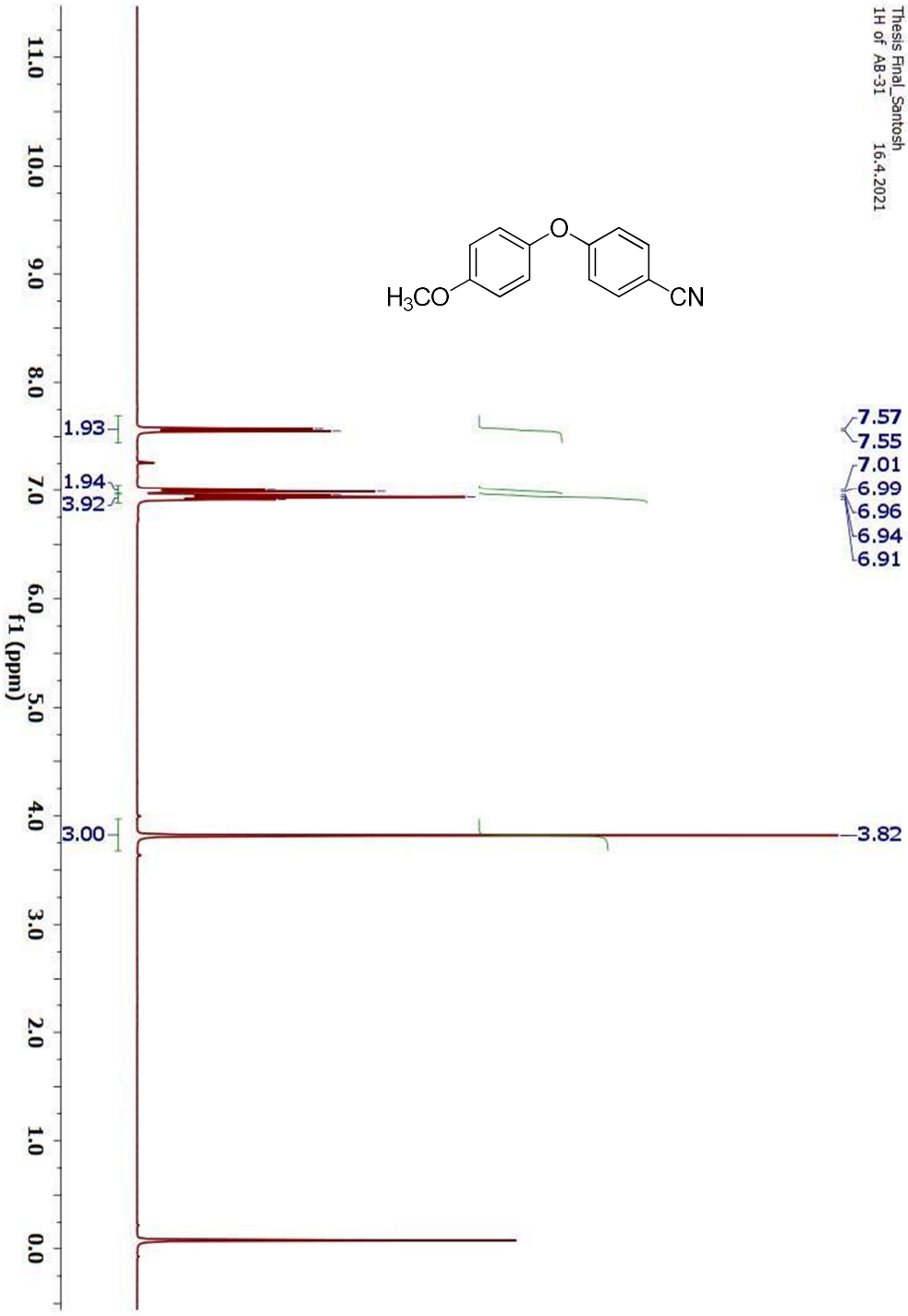
170
150
130
110
90
80
70
60
50
40
30
20
10
0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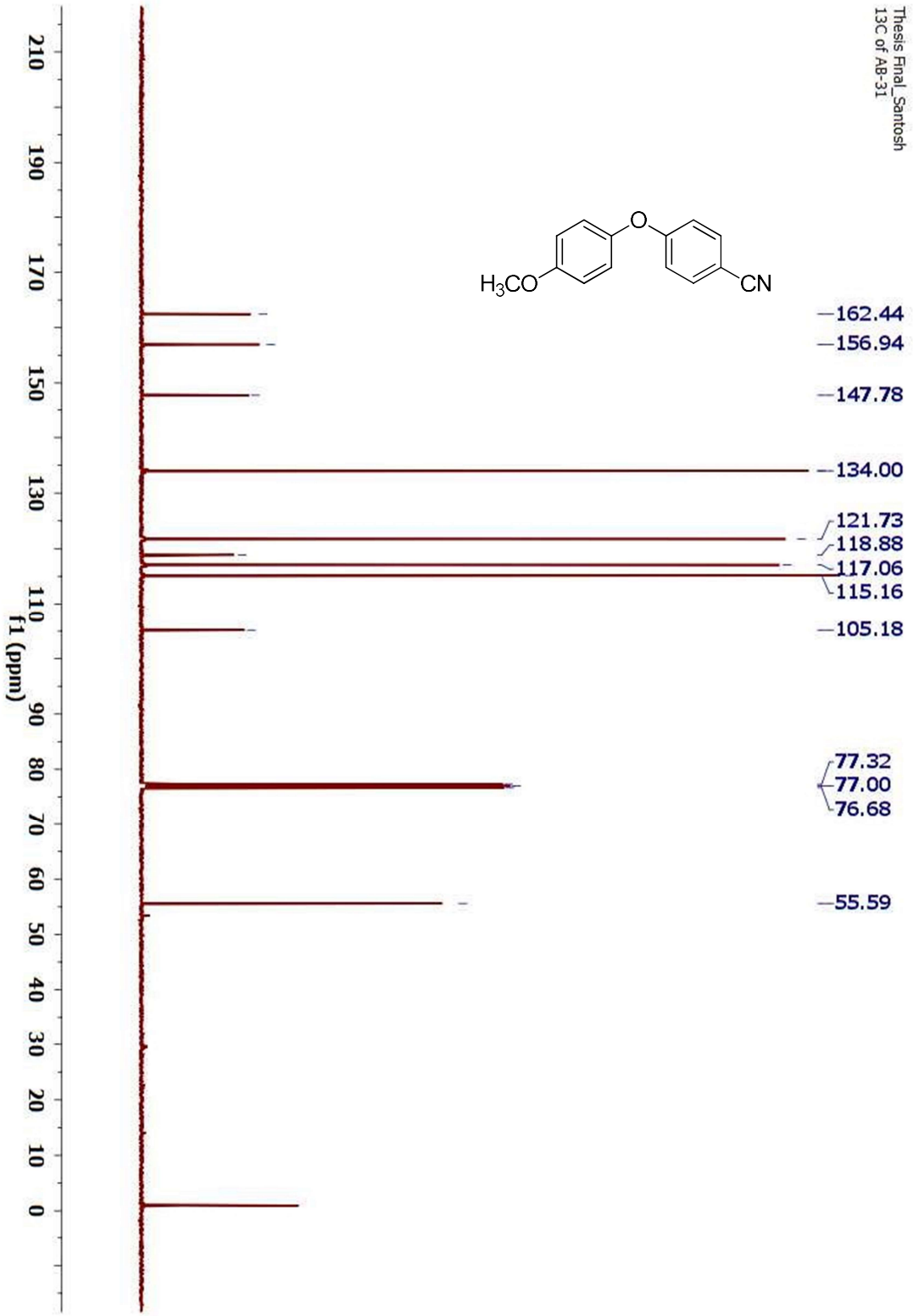
1.94
3.92
3.00
f1 (ppm)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117.06
115.16
105.18
77.32
77.00
76.68
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190
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150
130
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80
70
60
50
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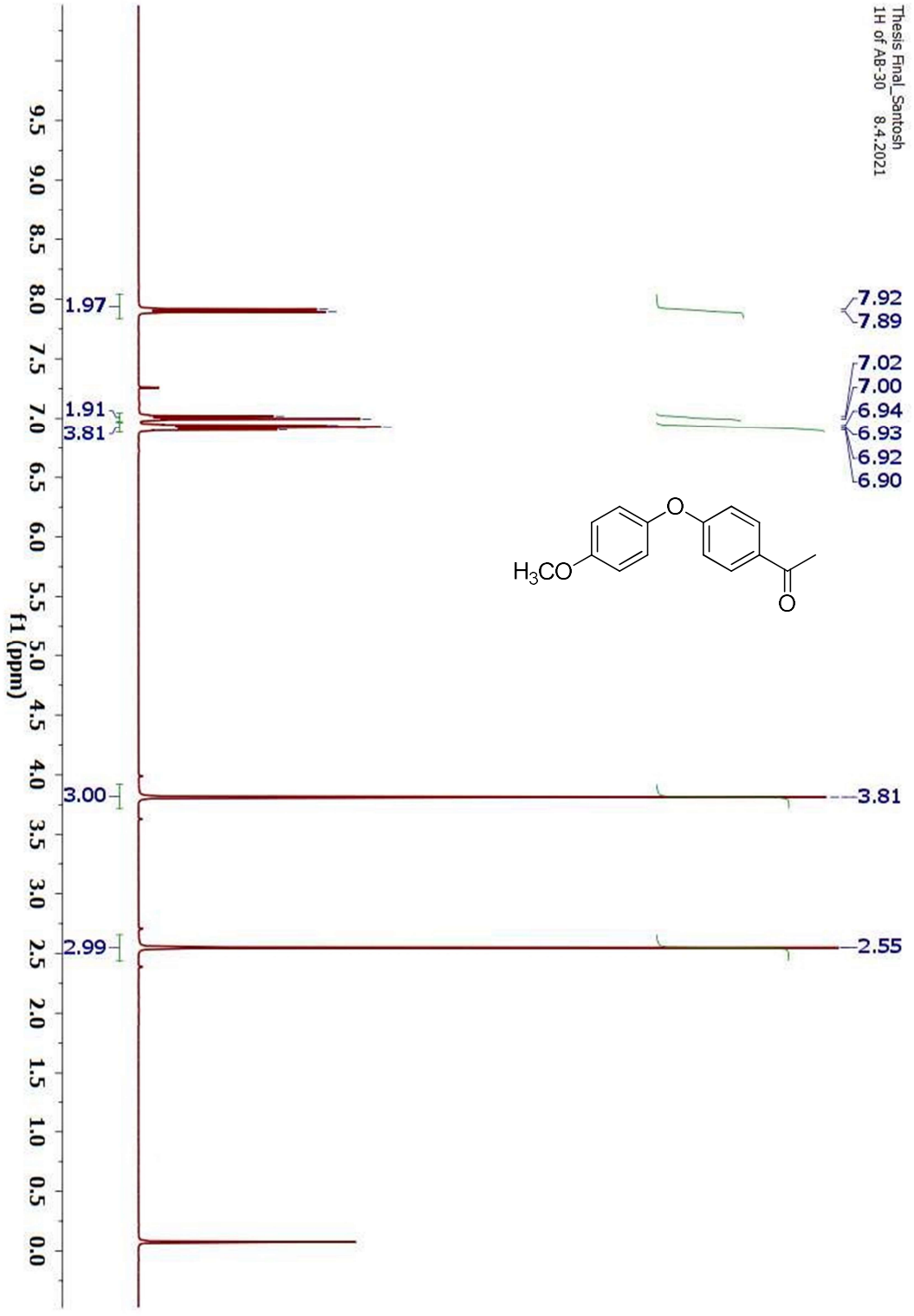
30
20
10
0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1.91
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3.00
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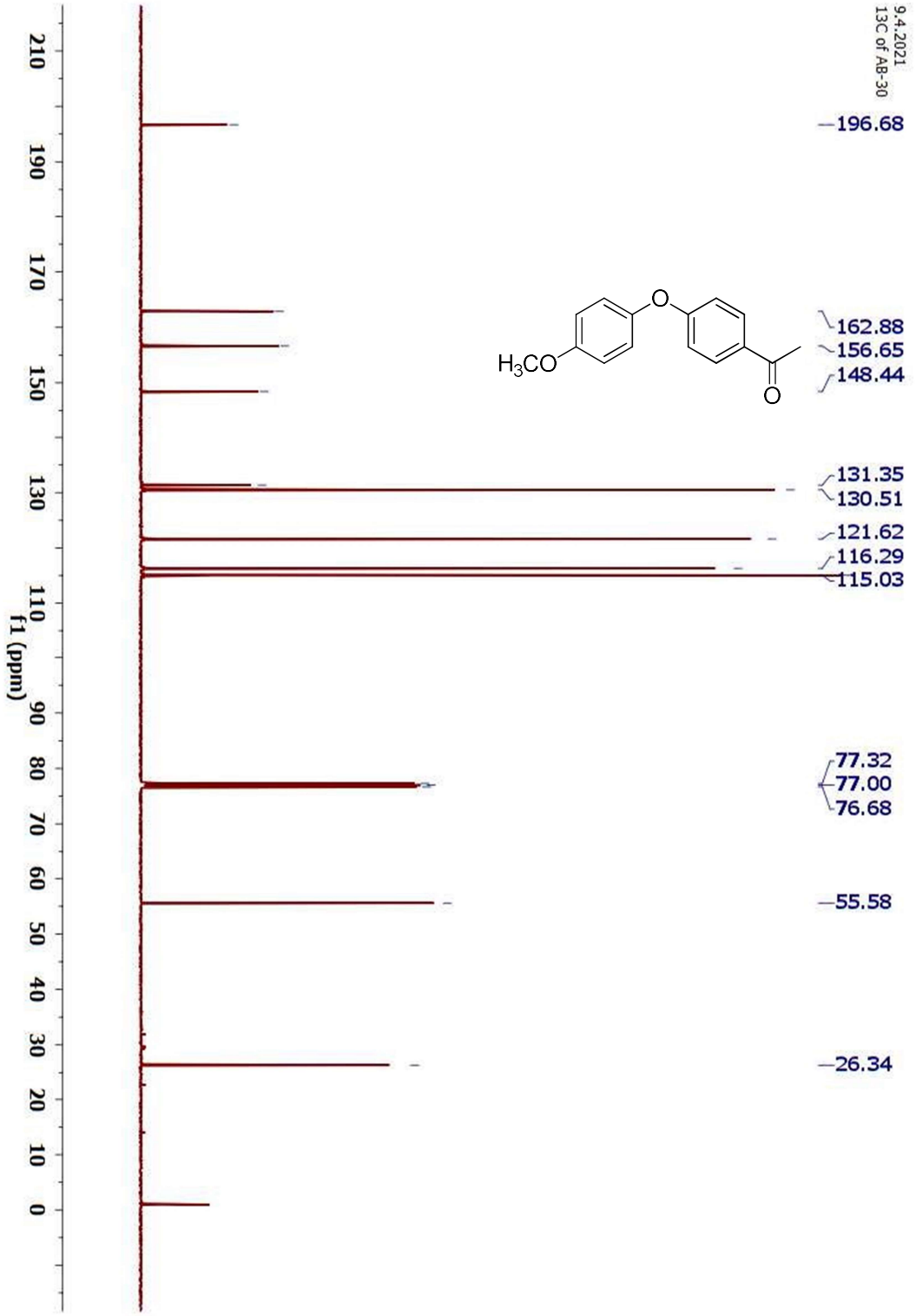
3.81
2.55
H3CO
O
O
f1 (ppm)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26.34
H3CO
O
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170
150
130
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90
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70
60
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30
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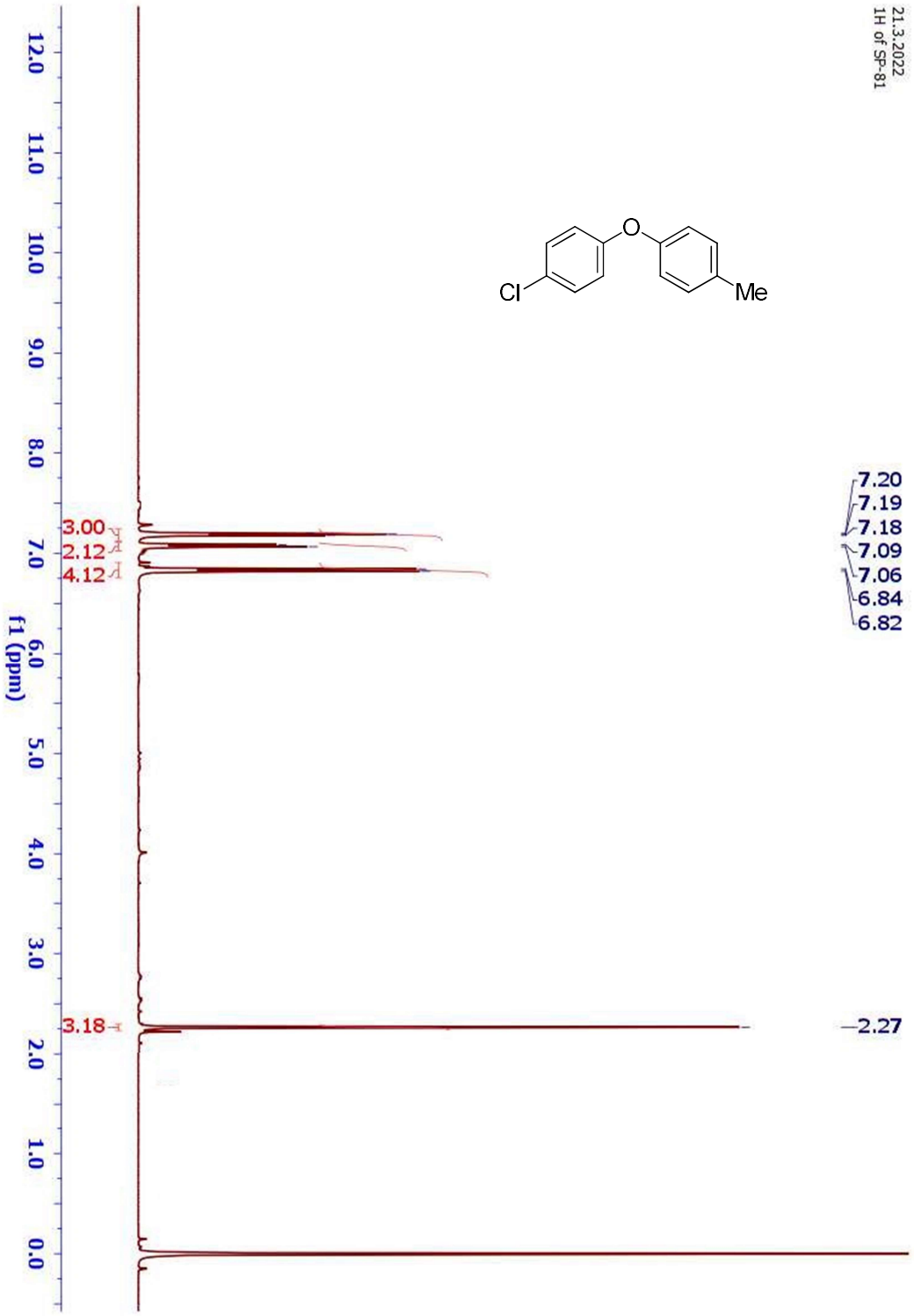
10
0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7.06
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6.82
3.00
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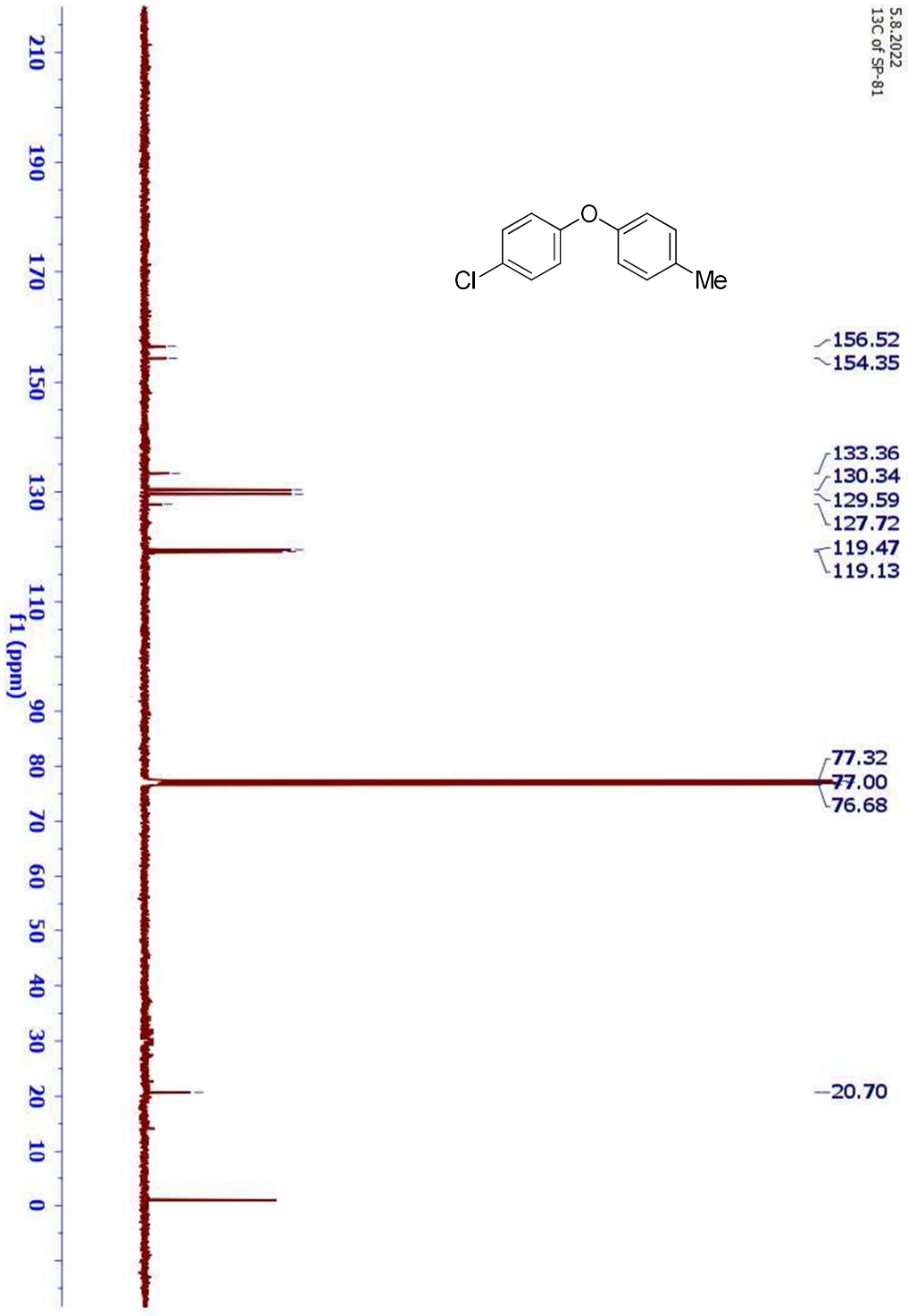
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Me
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77.00
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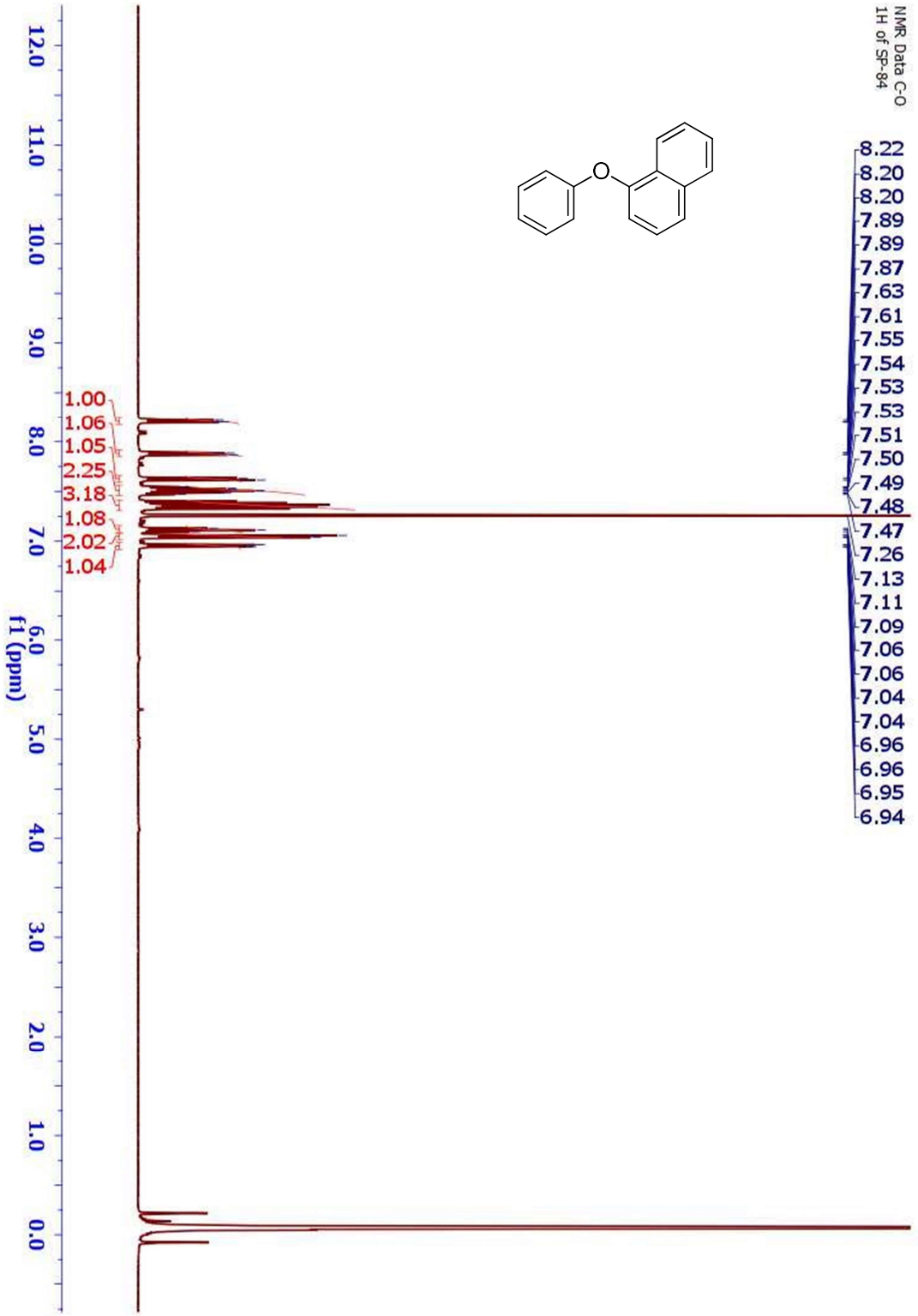
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12.0
11.0
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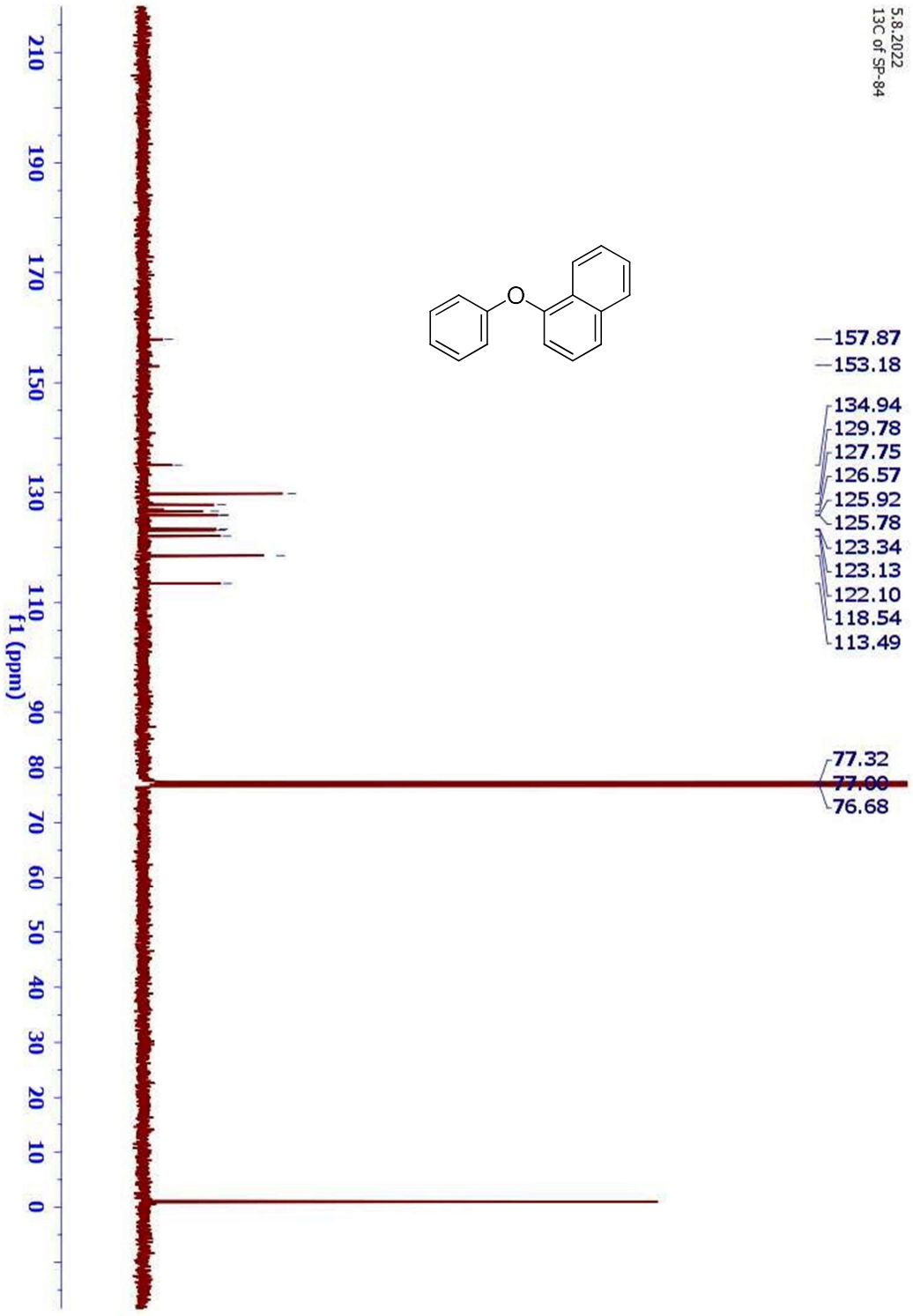
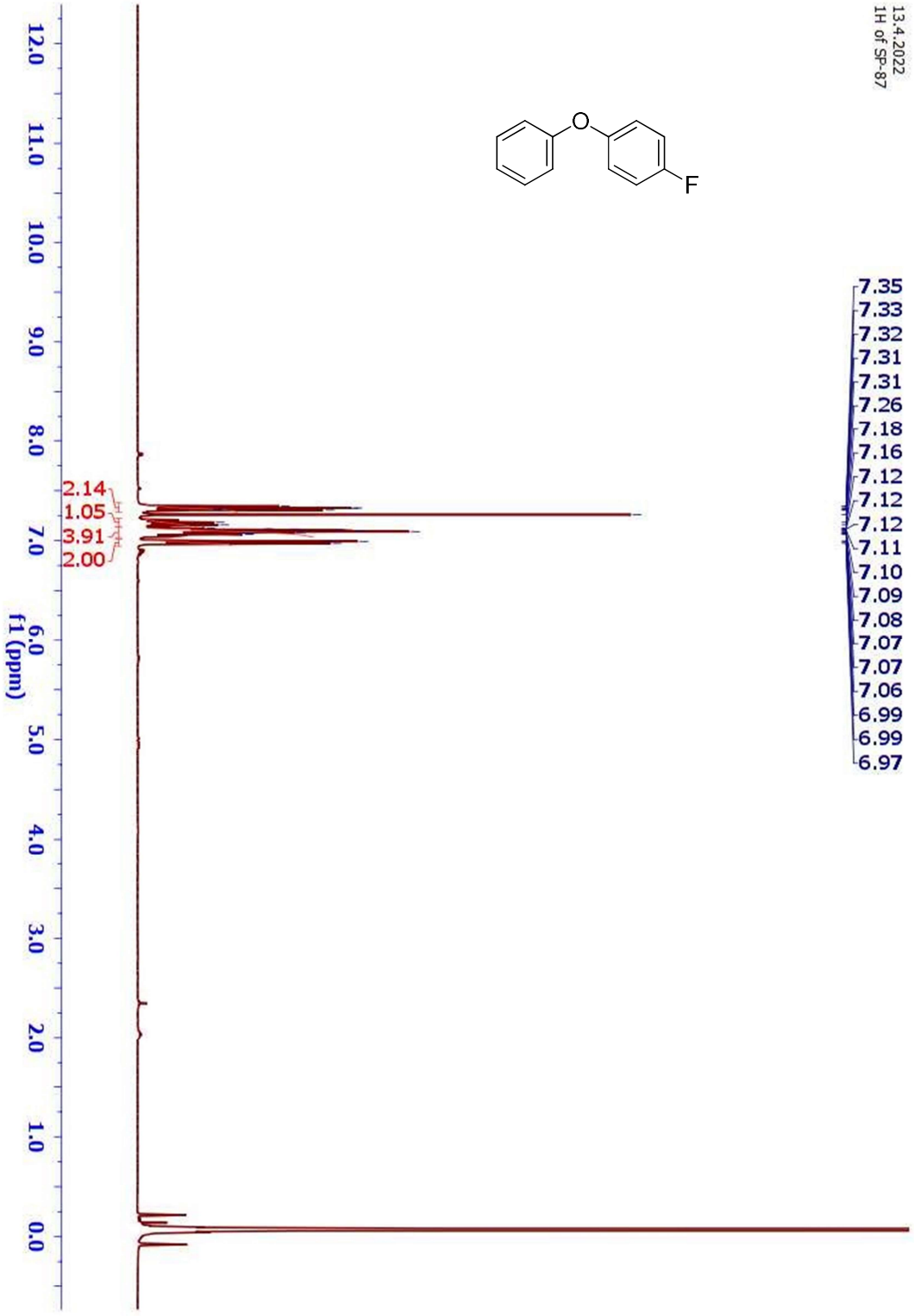
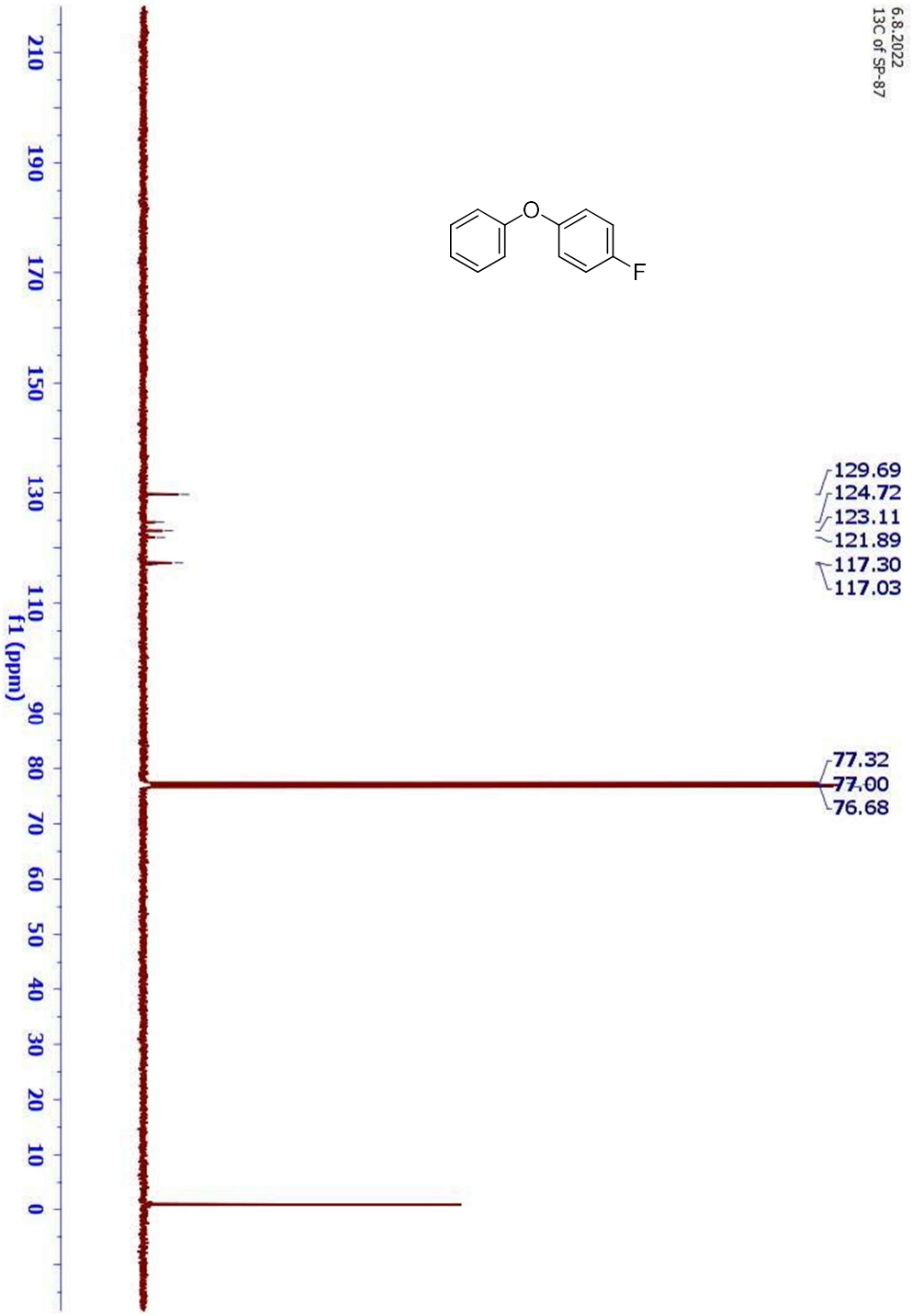
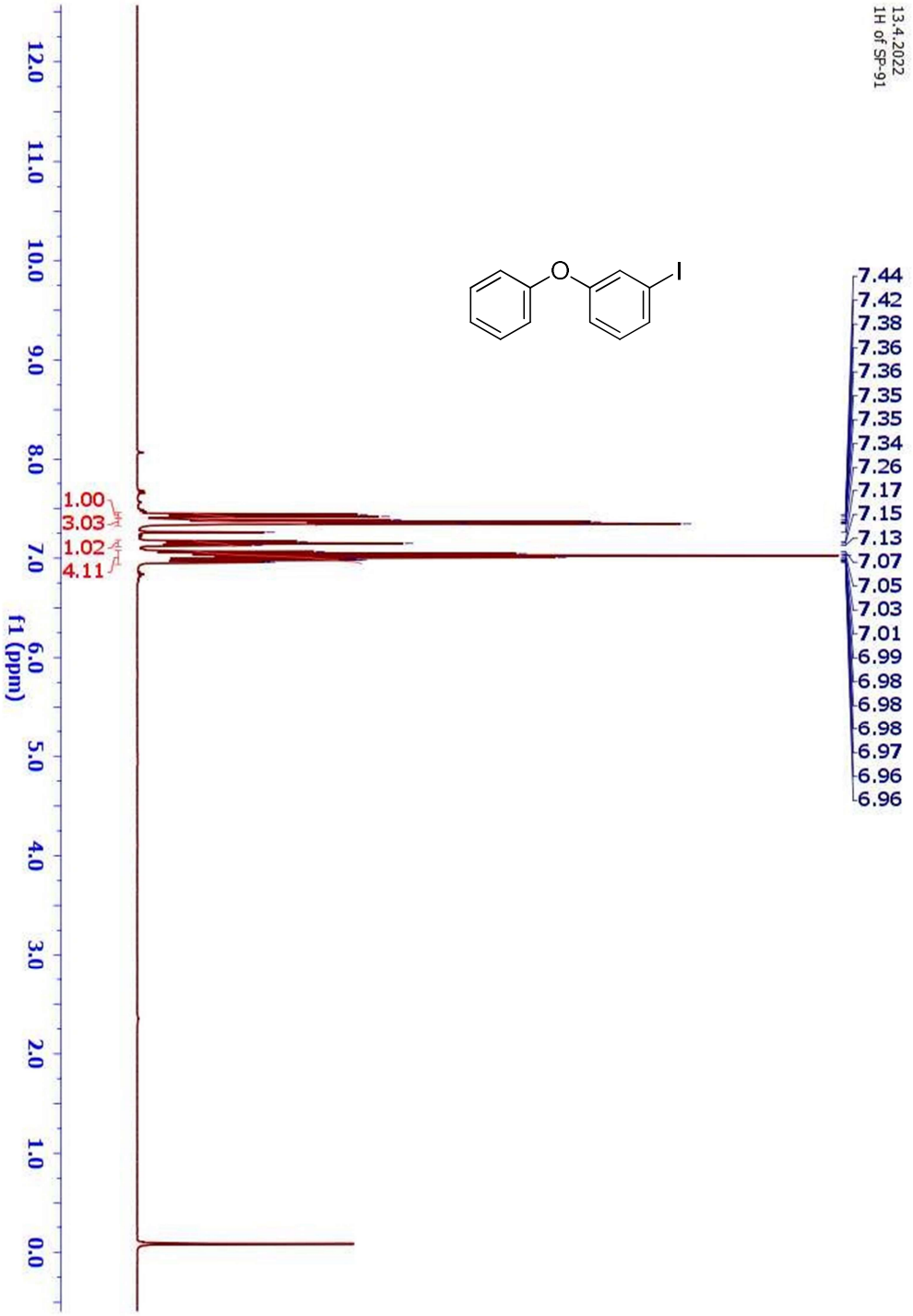
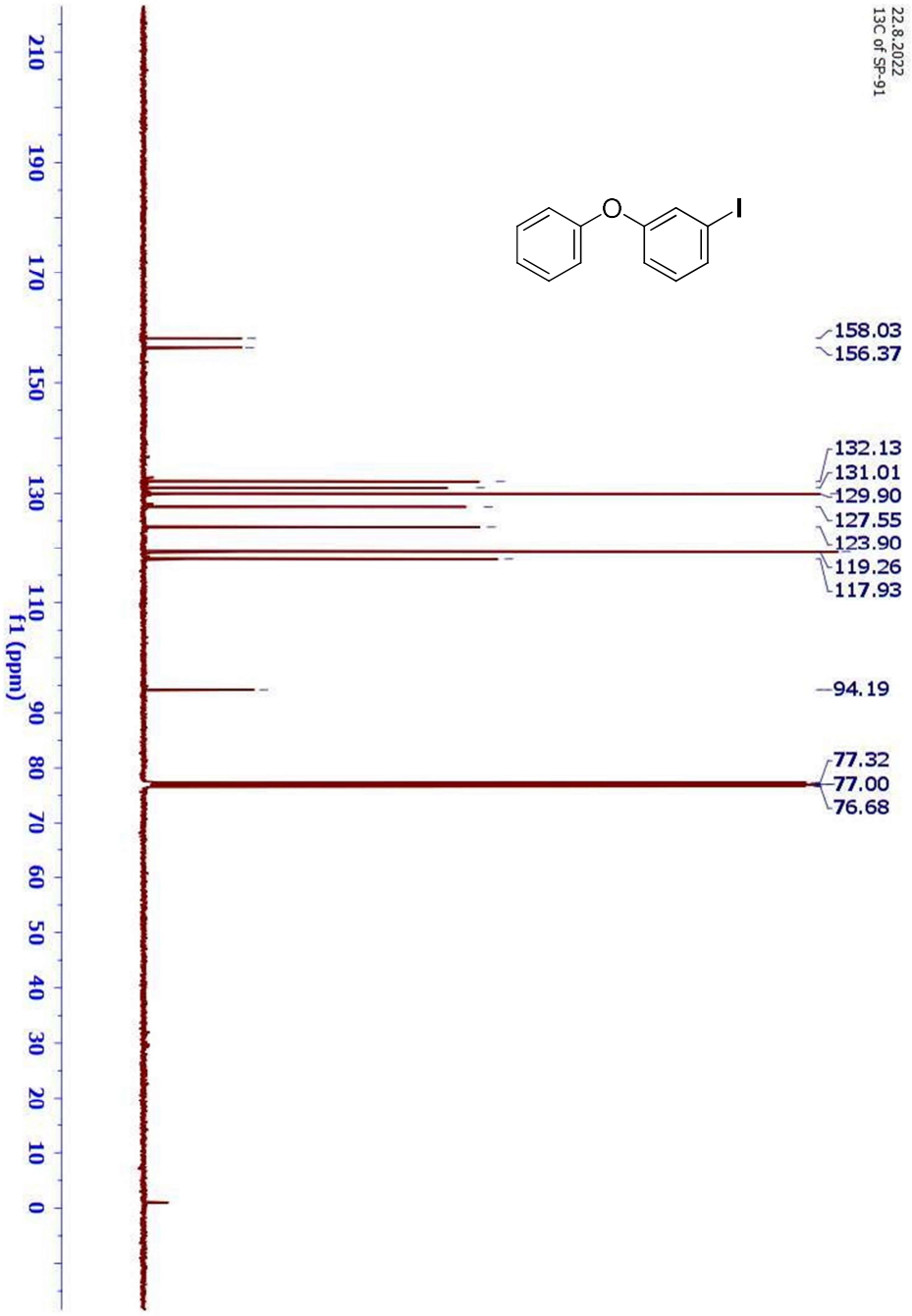
f1 (ppm)

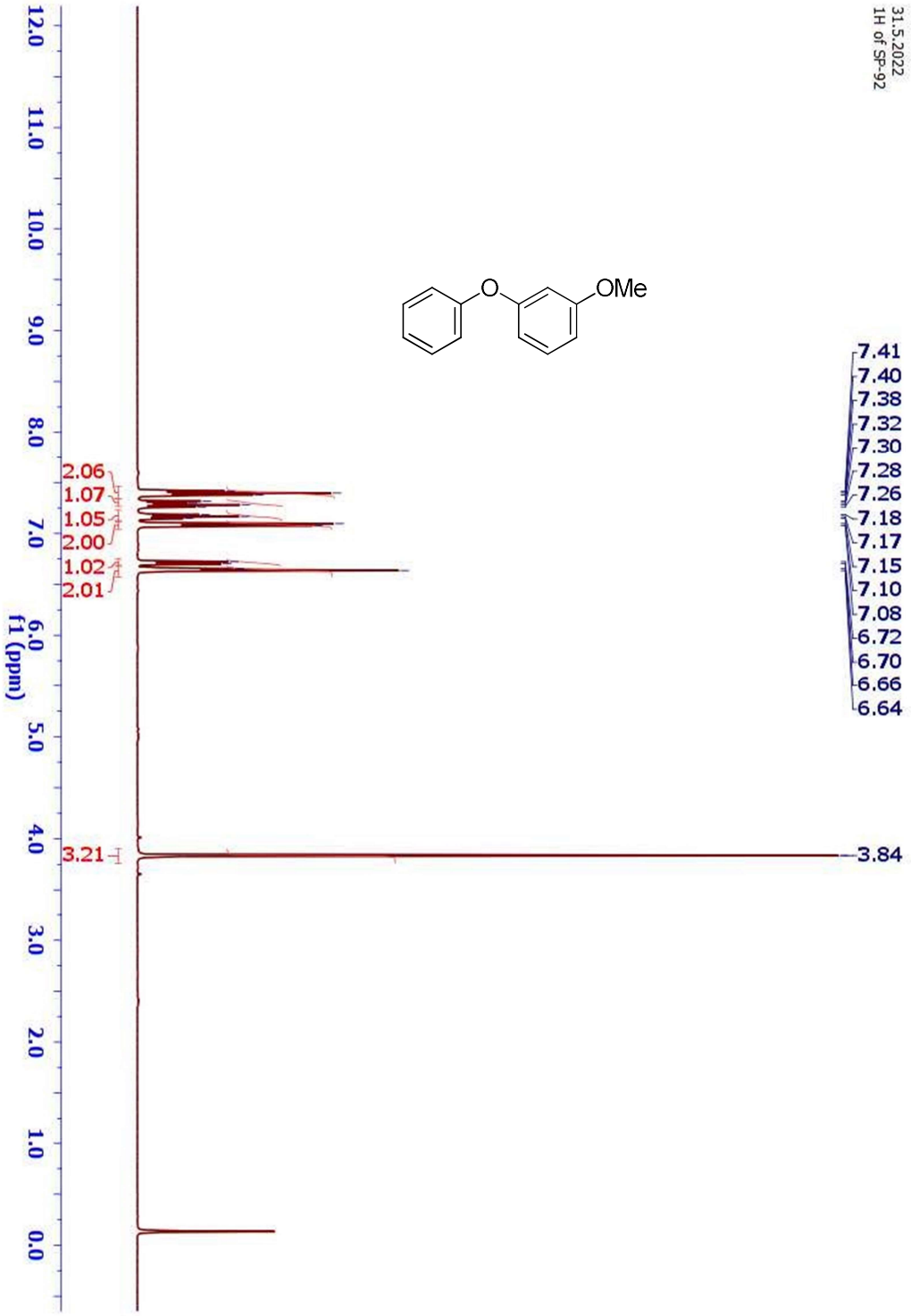

5.8.2022
13C of SP-84
157.87
153.18
134.94
129.78
127.75
126.57
125.92
125.78
123.34
123.13
122.10
118.54
113.49
77.32
77.00
76.68
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
O

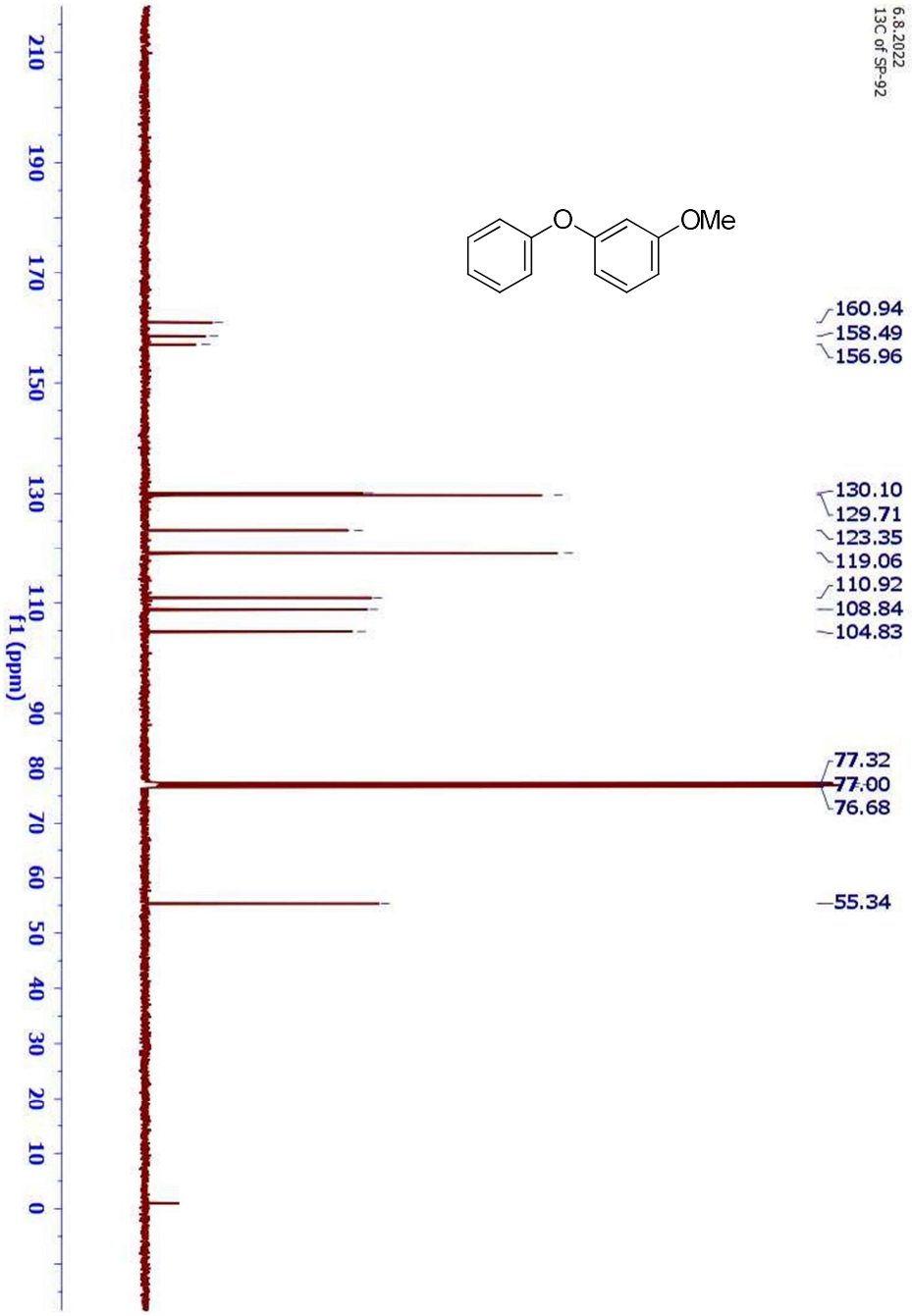

13.4.2022
1H of SP-87
O
F
7.35
7.33
7.32
7.31
7.31
7.26
7.18
7.16
7.12
7.12
7.12
7.11
7.10
7.09
7.08
7.07
7.07
7.06
6.99
6.99
6.97
2.14
1.05
3.91
2.00
f1 (ppm)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

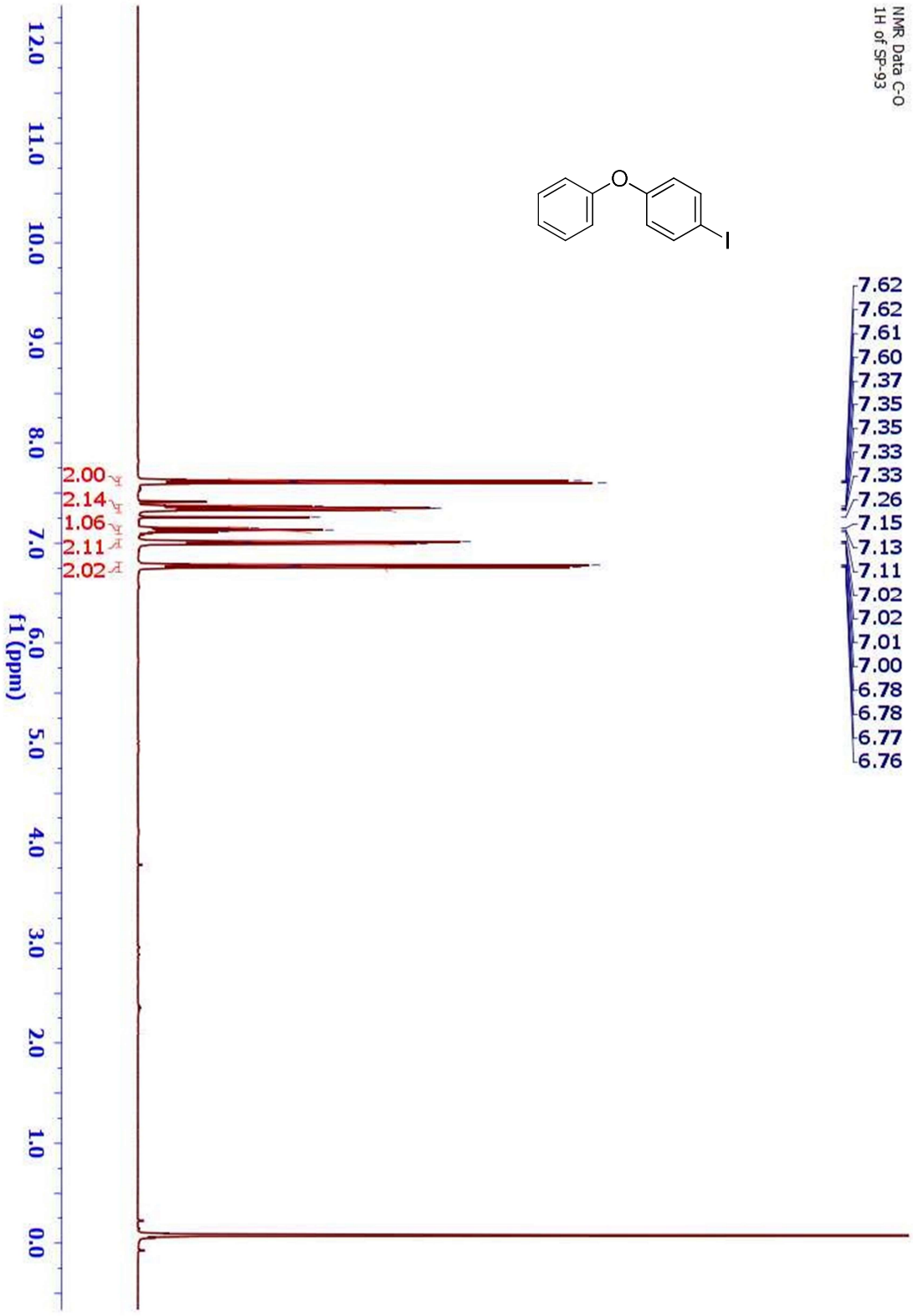

6.8.2022
13C of SP-87
O
F
129.69
124.72
123.11
121.89
117.30
117.03
77.32
77.00
76.68
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

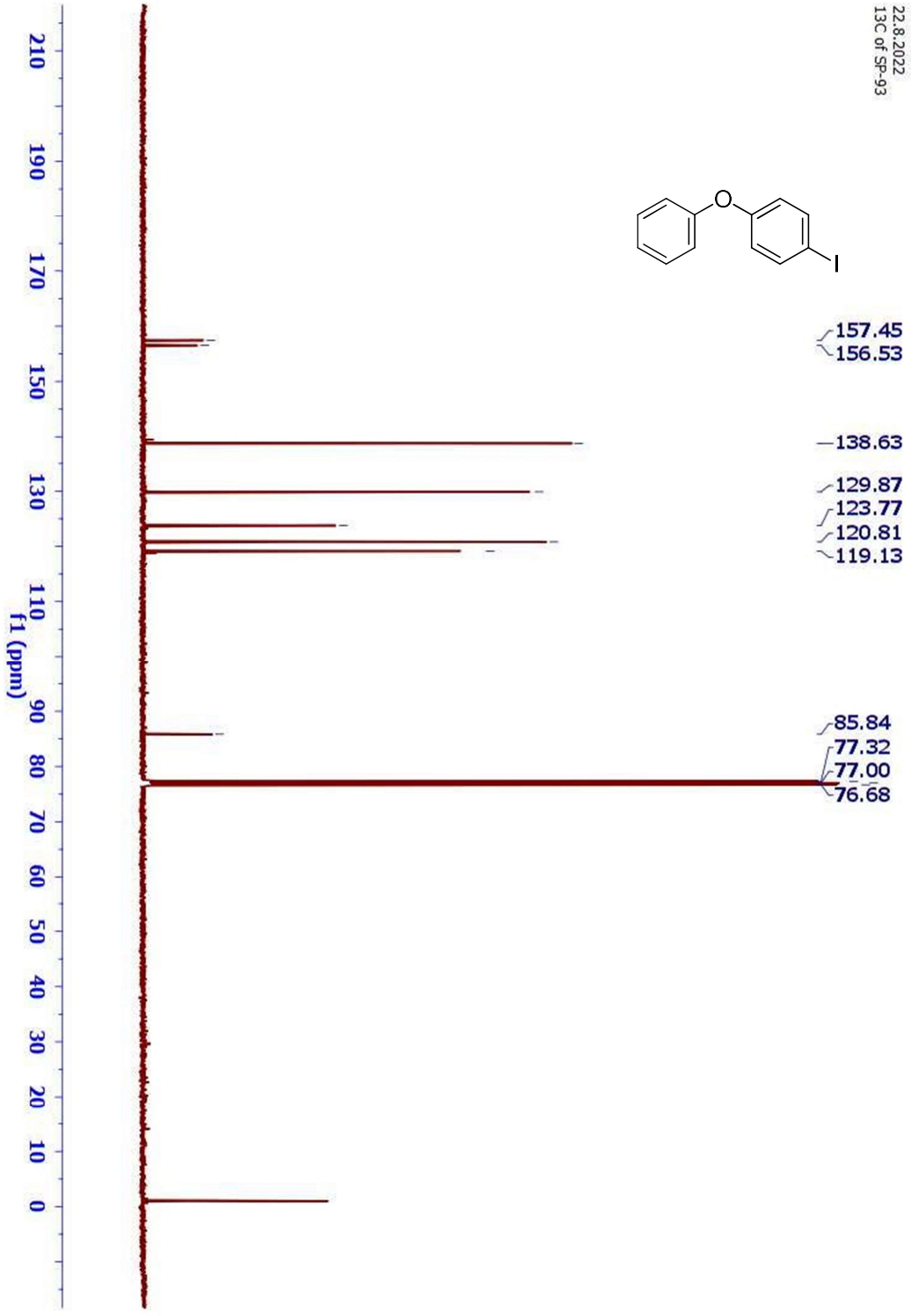

13.4.2022
1H of SP-91
7.44
7.42
7.38
7.36
7.36
7.35
7.35
7.34
7.26
7.17
7.15
7.13
7.07
7.05
7.03
7.01
6.99
6.98
6.98
6.98
6.97
6.96
6.96
1.00
3.03
1.02
4.11
f1 (ppm)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
O
I

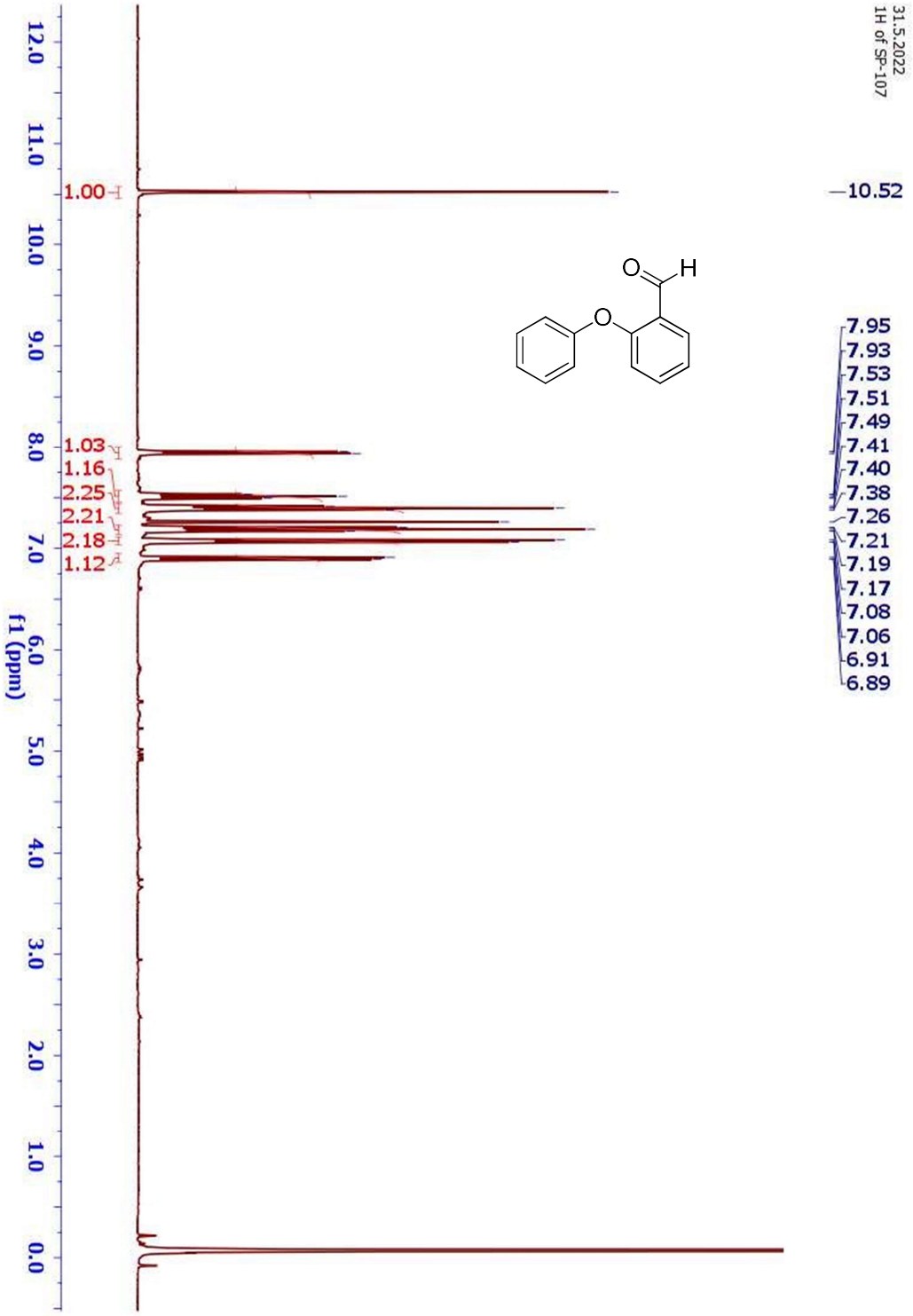

22.8.2022
13C of SP-91
O
I
158.03
156.37
132.13
131.01
129.90
127.55
123.90
119.26
117.93
94.19
77.32
77.00
76.68
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

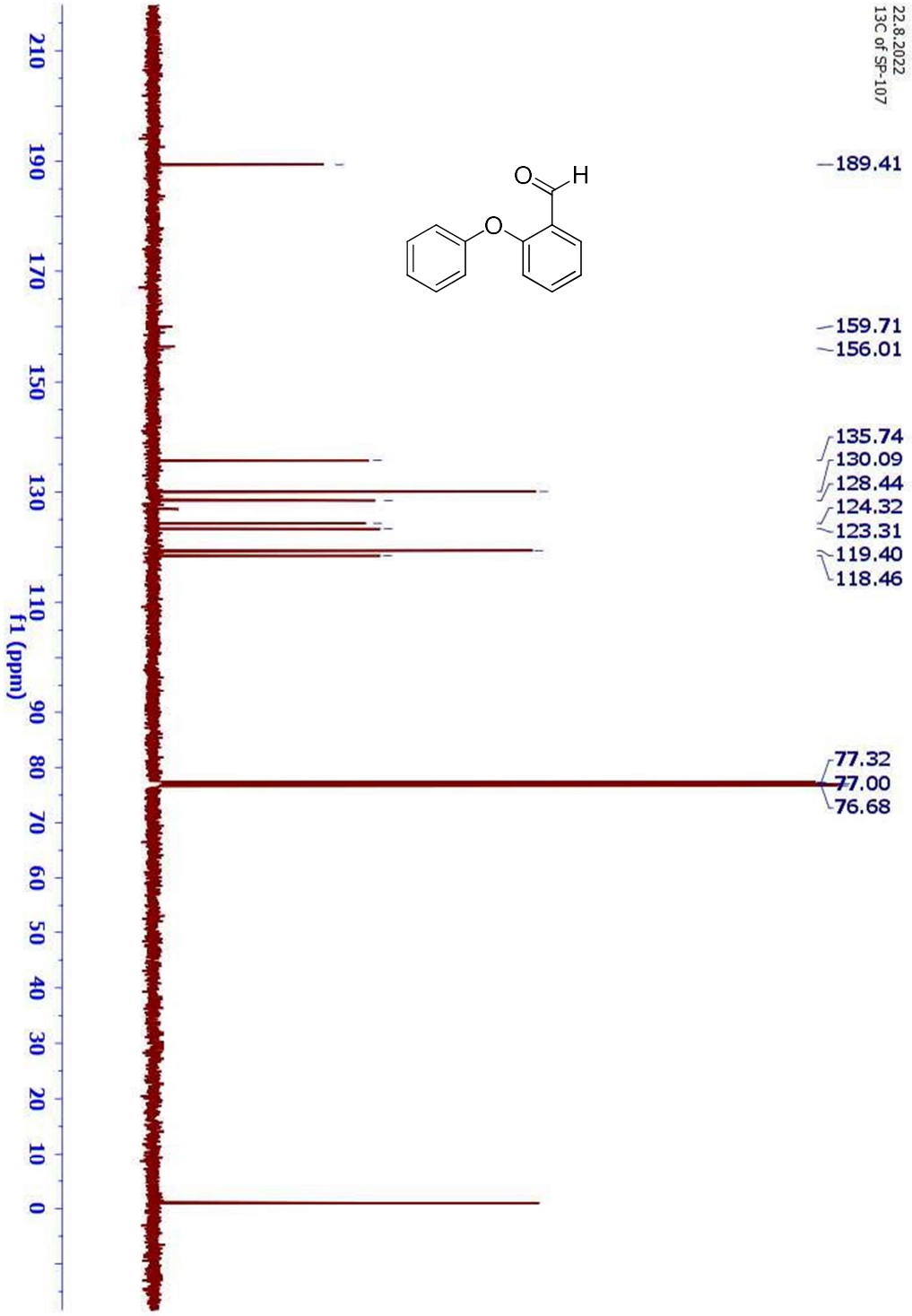

31.5.2022
1H of SP-92
O
OMe
7.41
7.40
7.38
7.32
7.30
7.28
7.26
7.18
7.17
7.15
7.10
7.08
6.72
6.70
6.66
6.64
3.84
2.06
1.07
1.05
2.00
1.02
2.01
3.21
f1 (ppm)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

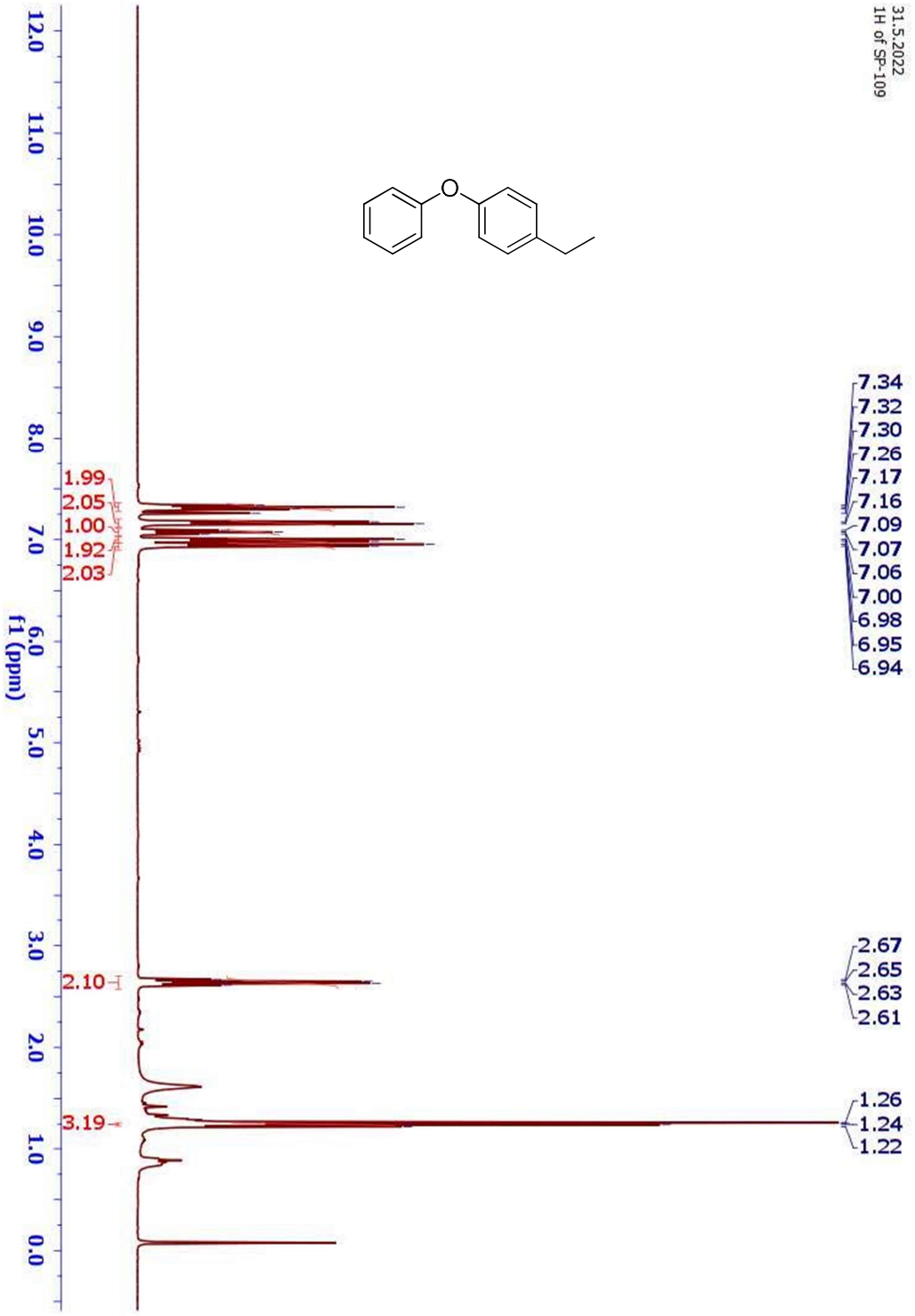

6.8.2022
13C of SP-92
O
OMe
160.94
158.49
156.96
130.10
129.71
123.35
119.06
110.92
108.84
104.83
77.32
77.00
76.68
55.34
f1 (ppm)

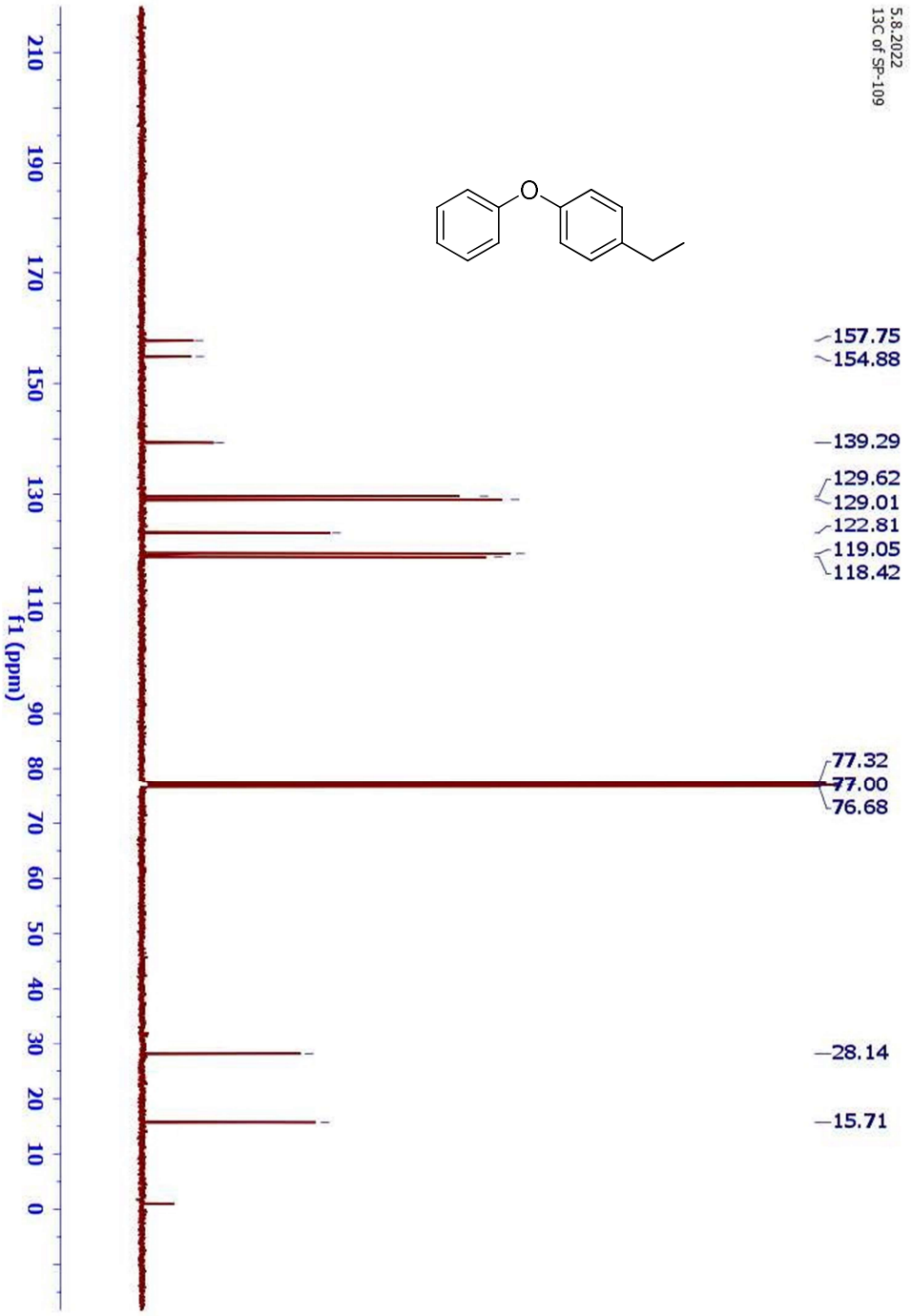

NMR Data C-O
1H of SP-93
O
I
7.62
7.62
7.61
7.60
7.37
7.35
7.35
7.33
7.33
7.26
7.15
7.13
7.11
7.02
7.02
7.01
7.00
6.78
6.78
6.77
6.76
2.00
2.14
1.06
2.11
2.02
f1 (ppm)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

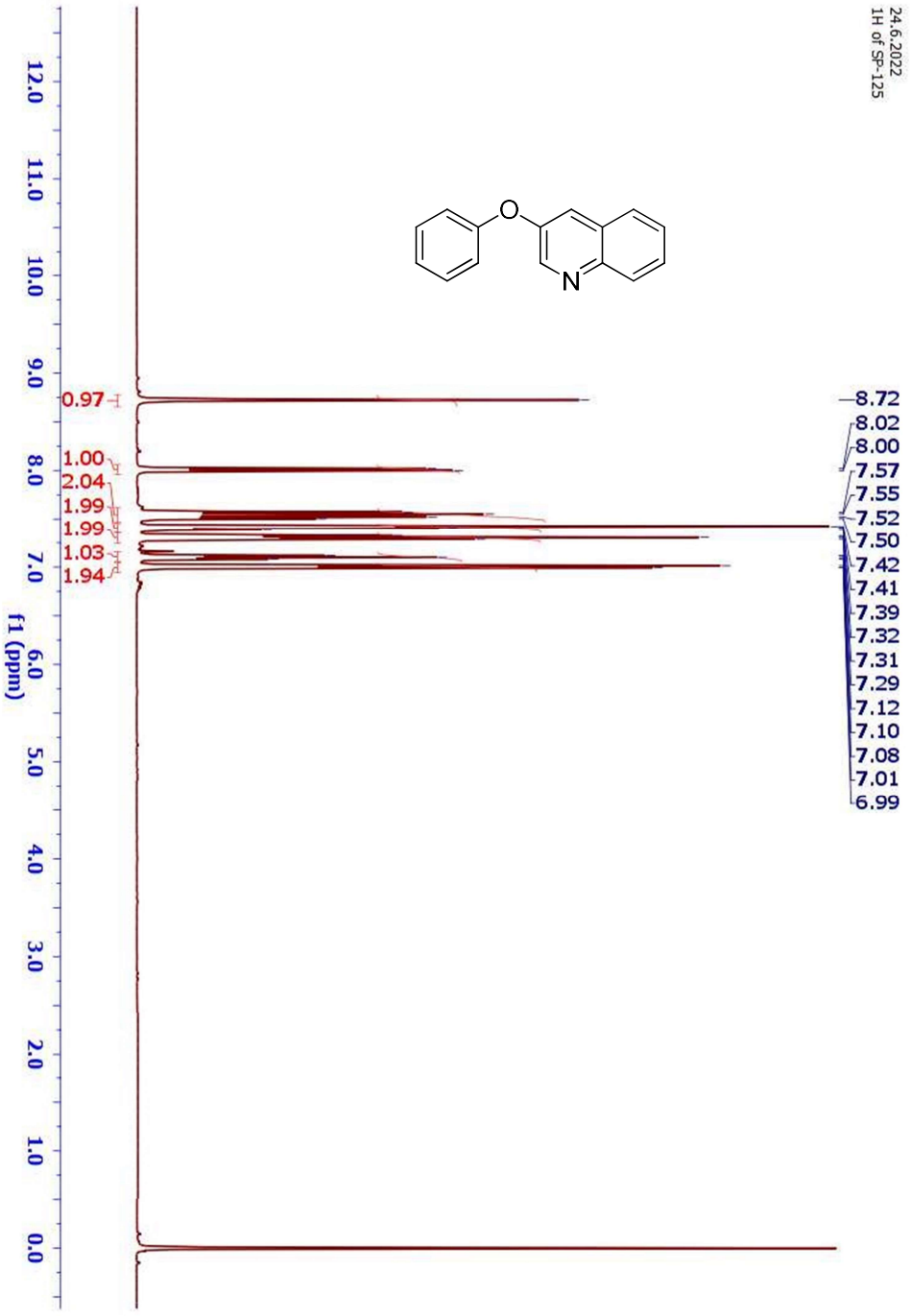

22.8.2022
13C of SP-93
157.45
156.53
138.63
129.87
123.77
120.81
119.13
85.84
77.32
77.00
76.68
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
O
I

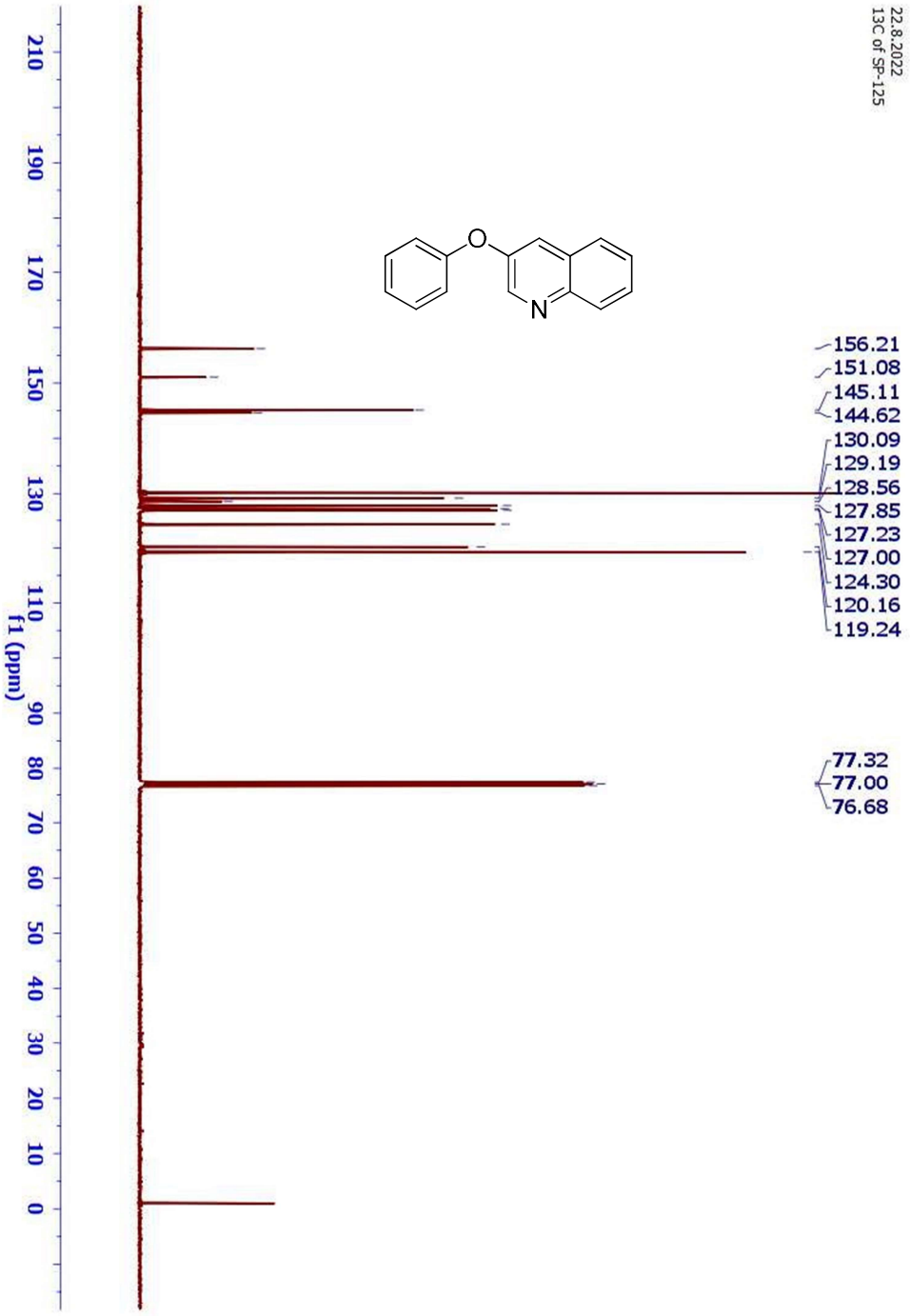

31.5.2022
1H of SP-107
10.52
7.95
7.93
7.53
7.51
7.49
7.41
7.40
7.38
7.26
7.21
7.19
7.17
7.08
7.06
6.91
6.89
1.00
1.03
1.16
2.25
2.21
2.18
1.12
O
H
O
f1 (ppm)

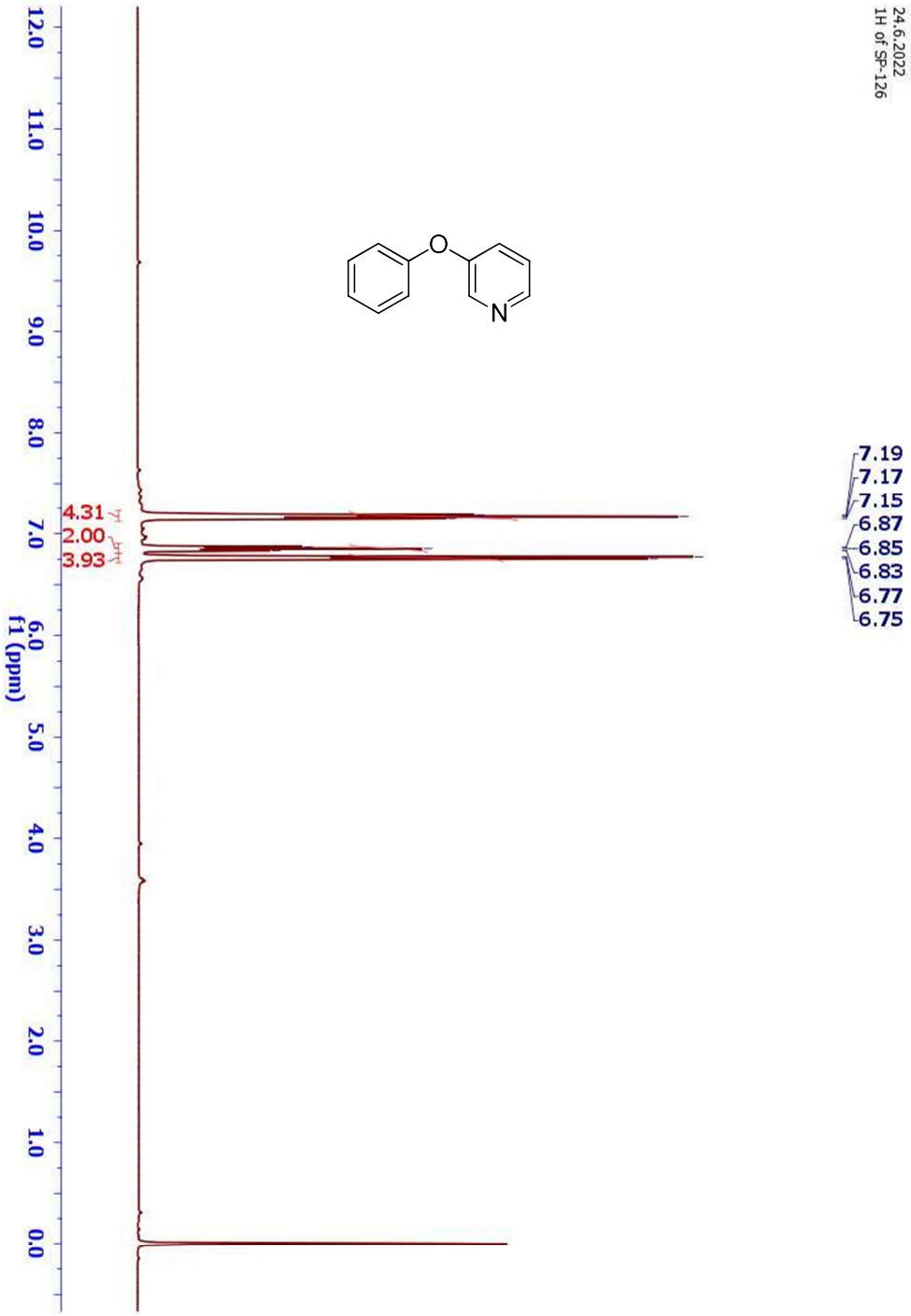

22.8.2022
13C of SP-107
189.41
159.71
156.01
135.74
130.09
128.44
124.32
123.31
119.40
118.46
77.32
77.00
76.68
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
O
H
O

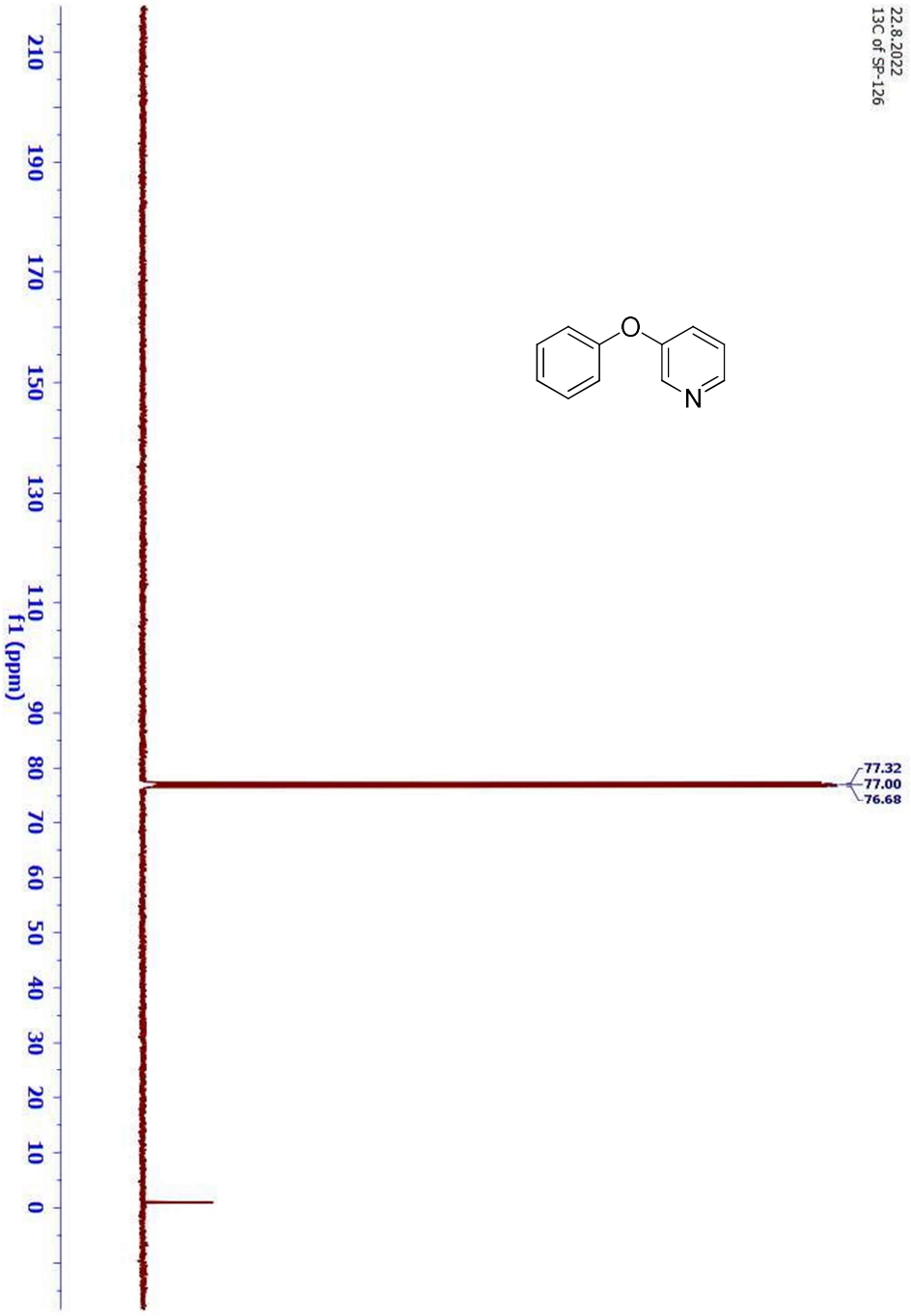

31.5.2022
1H of SP-109
7.34
7.32
7.30
7.26
7.17
7.16
7.09
7.07
7.06
7.00
6.98
6.95
6.94
2.67
2.65
2.63
2.61
1.26
1.24
1.22
1.99
2.05
1.00
1.92
2.03
2.10
3.19
f1 (ppm)

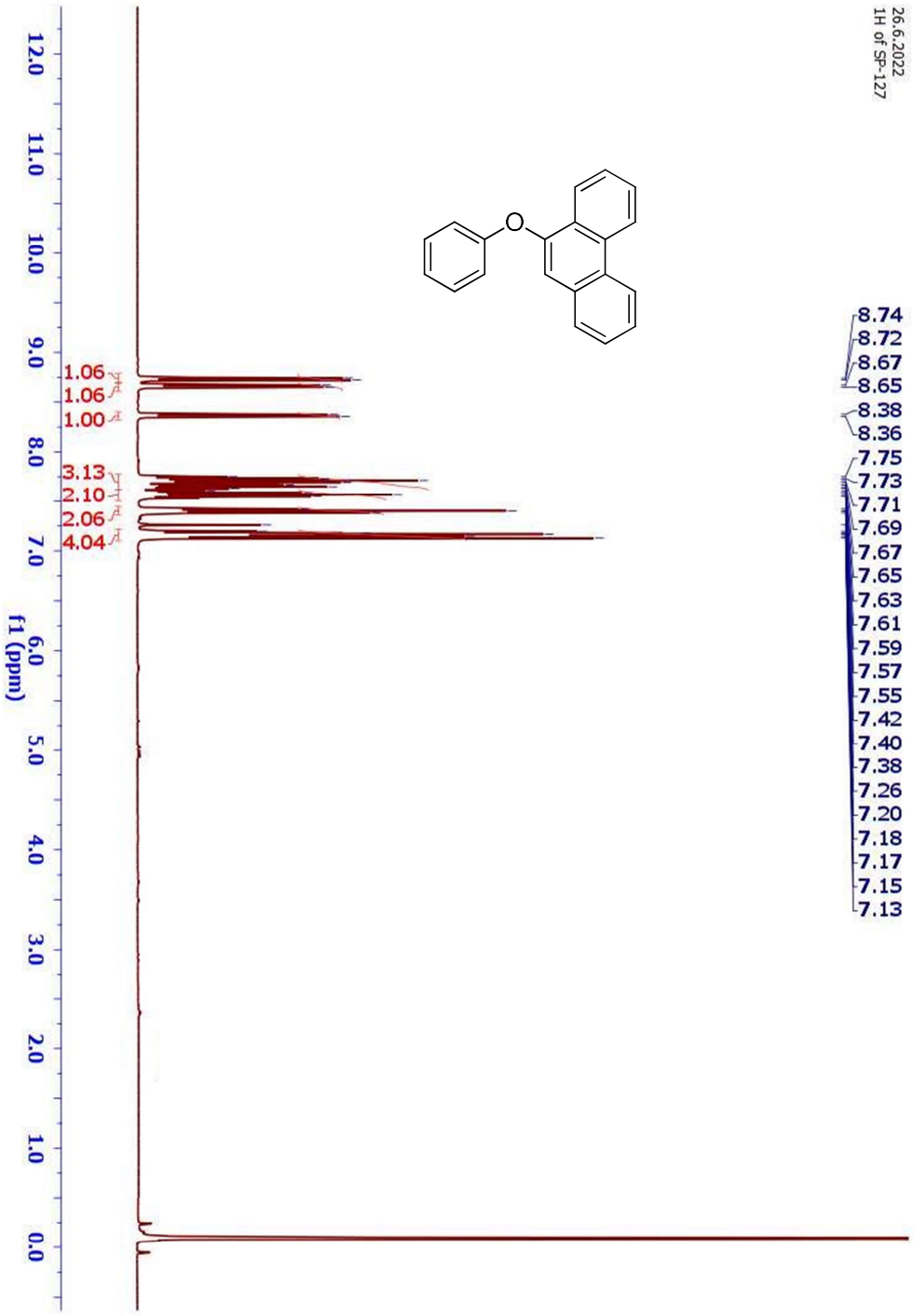

5.8.2022
13C of SP-109
157.75
154.88
139.29
129.62
129.01
122.81
119.05
118.42
77.32
77.00
76.68
28.14
15.71
f1 (ppm)

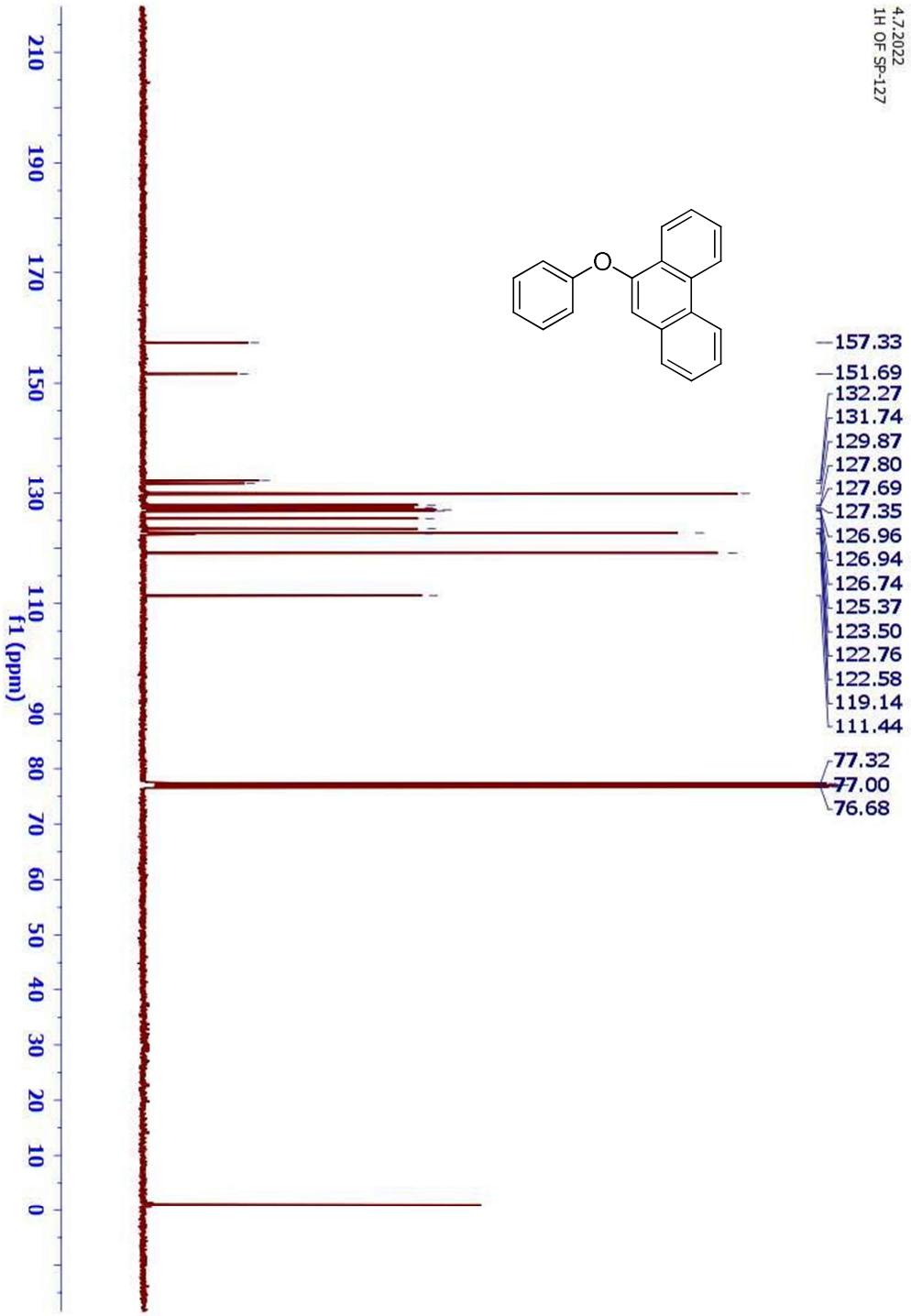

24.6.2022
1H of SP-125
O
N
0.97
1.00
2.04
1.99
1.99
1.03
1.94
8.72
8.02
8.00
7.57
7.55
7.52
7.50
7.42
7.41
7.39
7.32
7.31
7.29
7.12
7.10
7.08
7.01
6.99
f1 (ppm)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

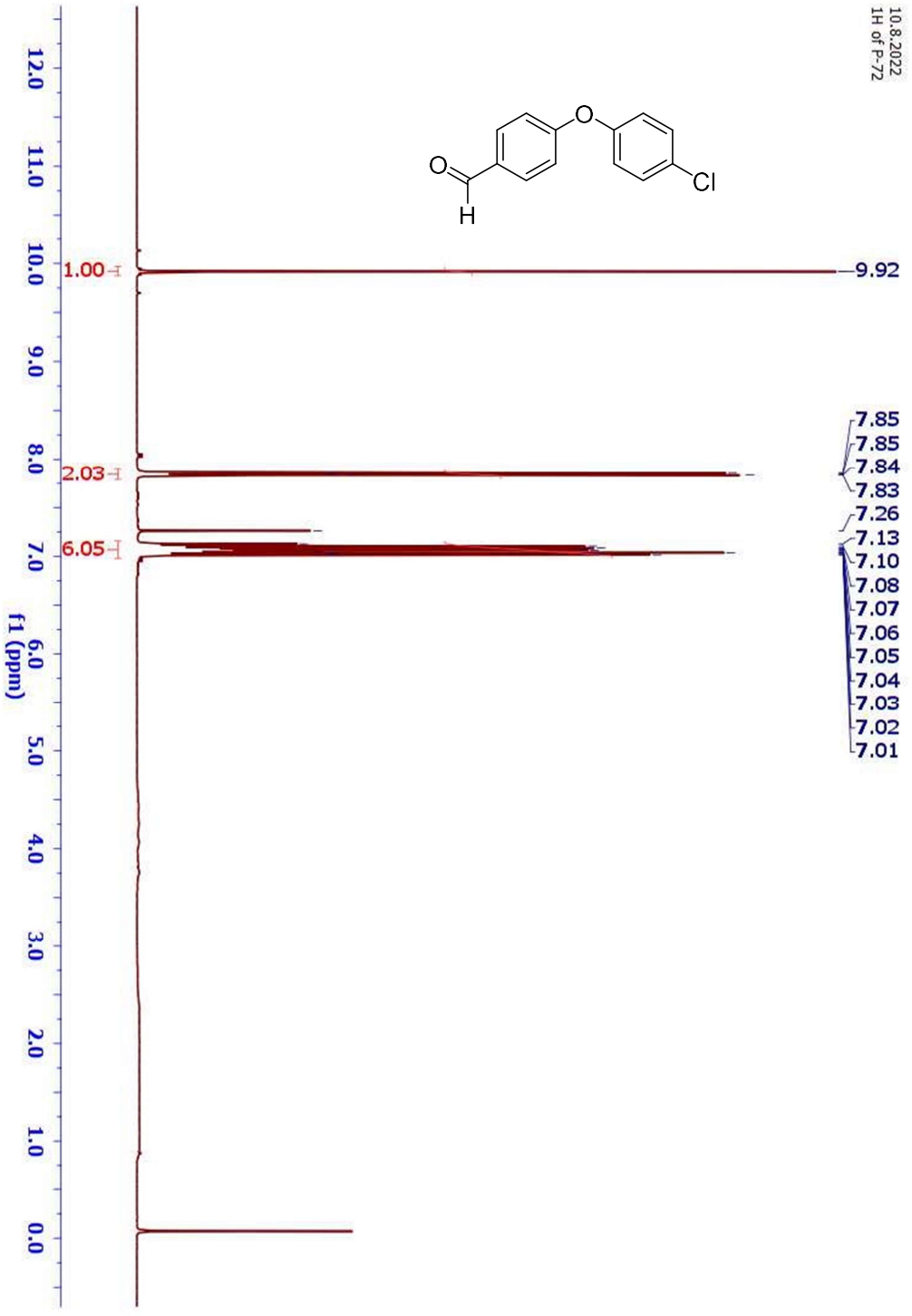

22.8.2022
13C of SP-125
O
N
156.21
151.08
145.11
144.62
130.09
129.19
128.56
127.85
127.23
127.00
124.30
120.16
119.24
77.32
77.00
76.68
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

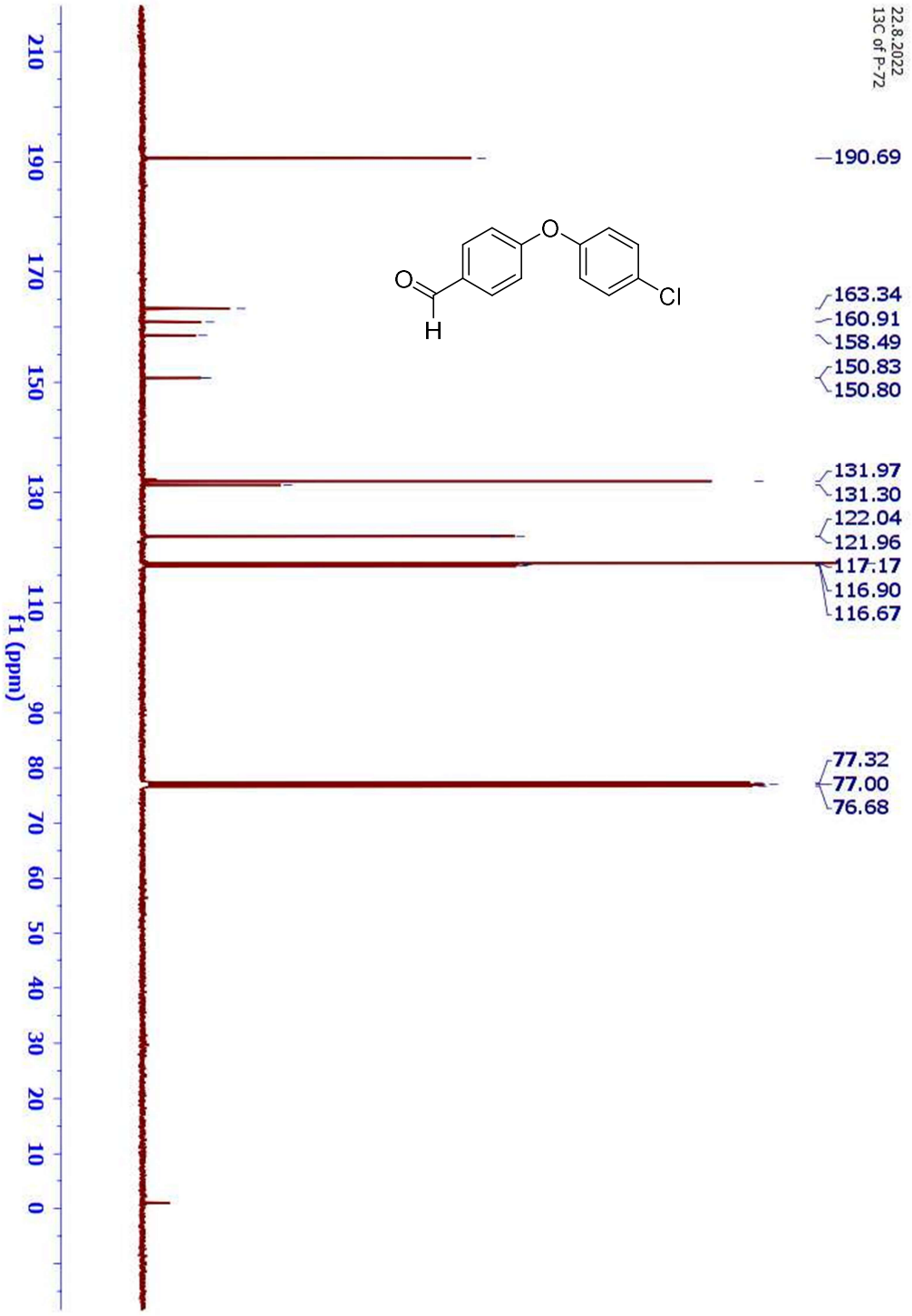

24.6.2022
1H of SP-126
7.19
7.17
7.15
6.87
6.85
6.83
6.77
6.75
4.31
2.00
3.93
f1 (ppm)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
O
N

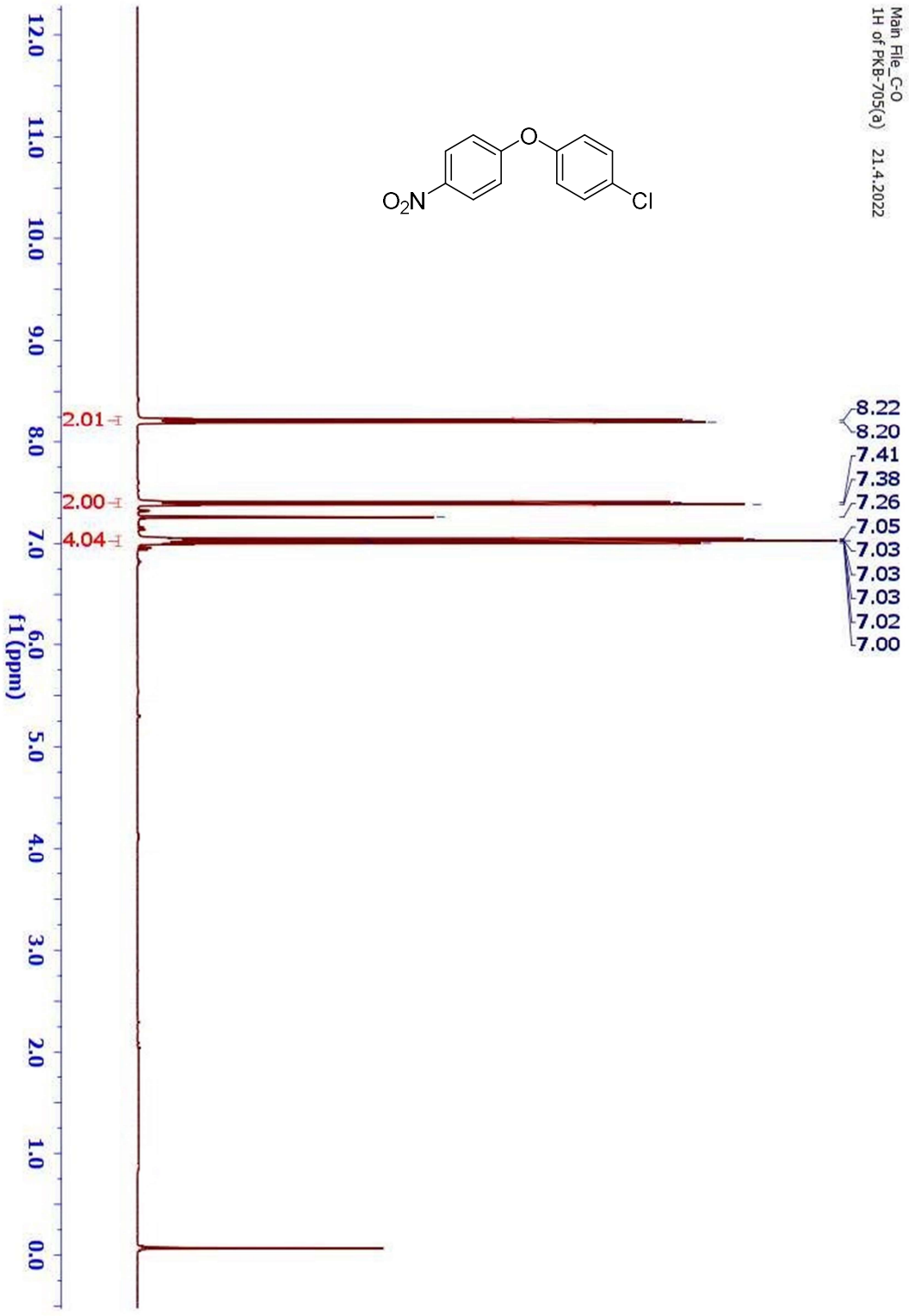

22.8.2022
13C of SP-126
O
N
77.32
77.00
76.68
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

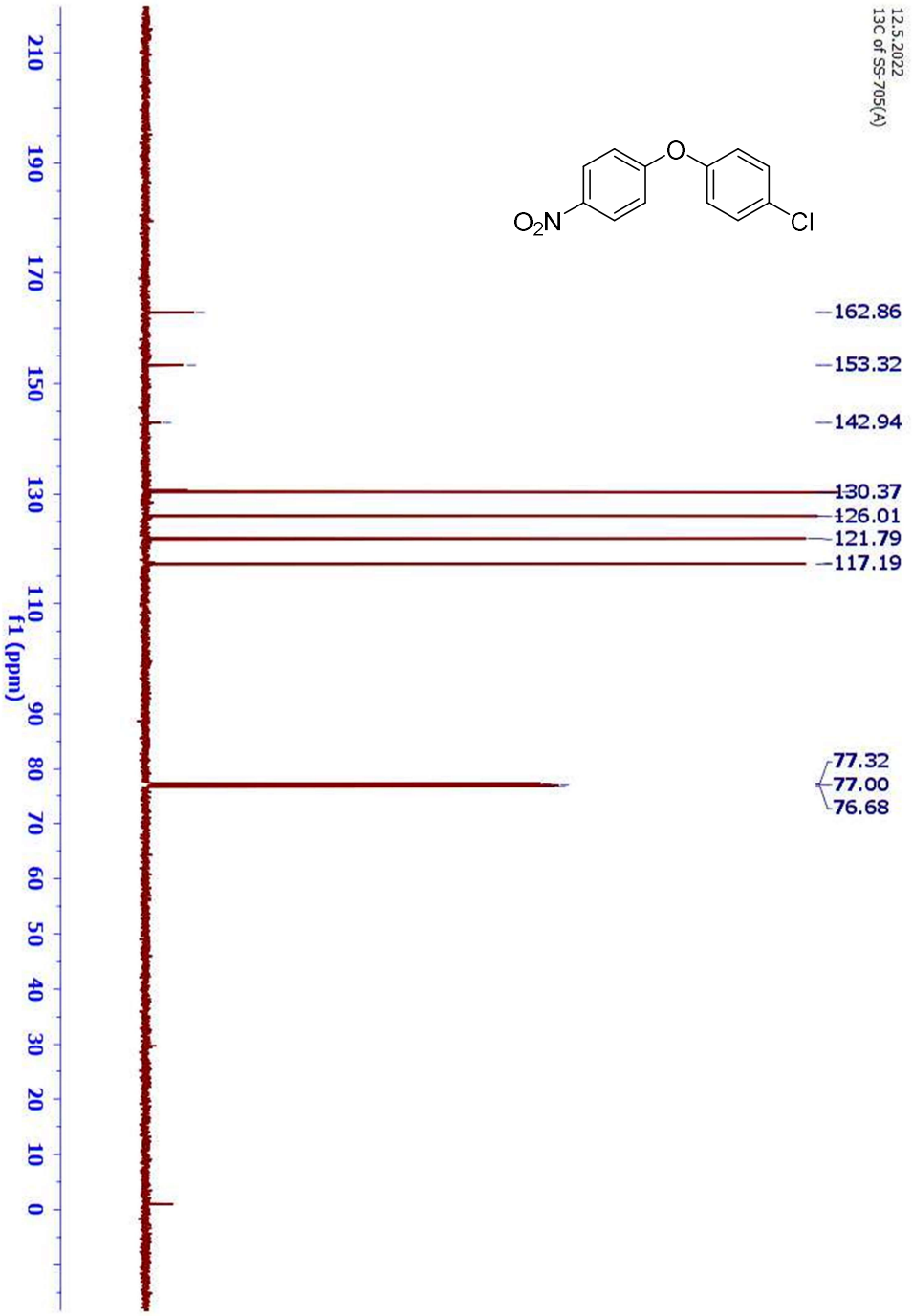

26.6.2022
1H of SP-127
8.74
8.72
8.67
8.65
8.38
8.36
7.75
7.73
7.71
7.69
7.67
7.65
7.63
7.61
7.59
7.57
7.55
7.42
7.40
7.38
7.26
7.20
7.18
7.17
7.15
7.13
1.06
1.06
1.00
3.13
2.10
2.06
4.04
O
f1 (ppm)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

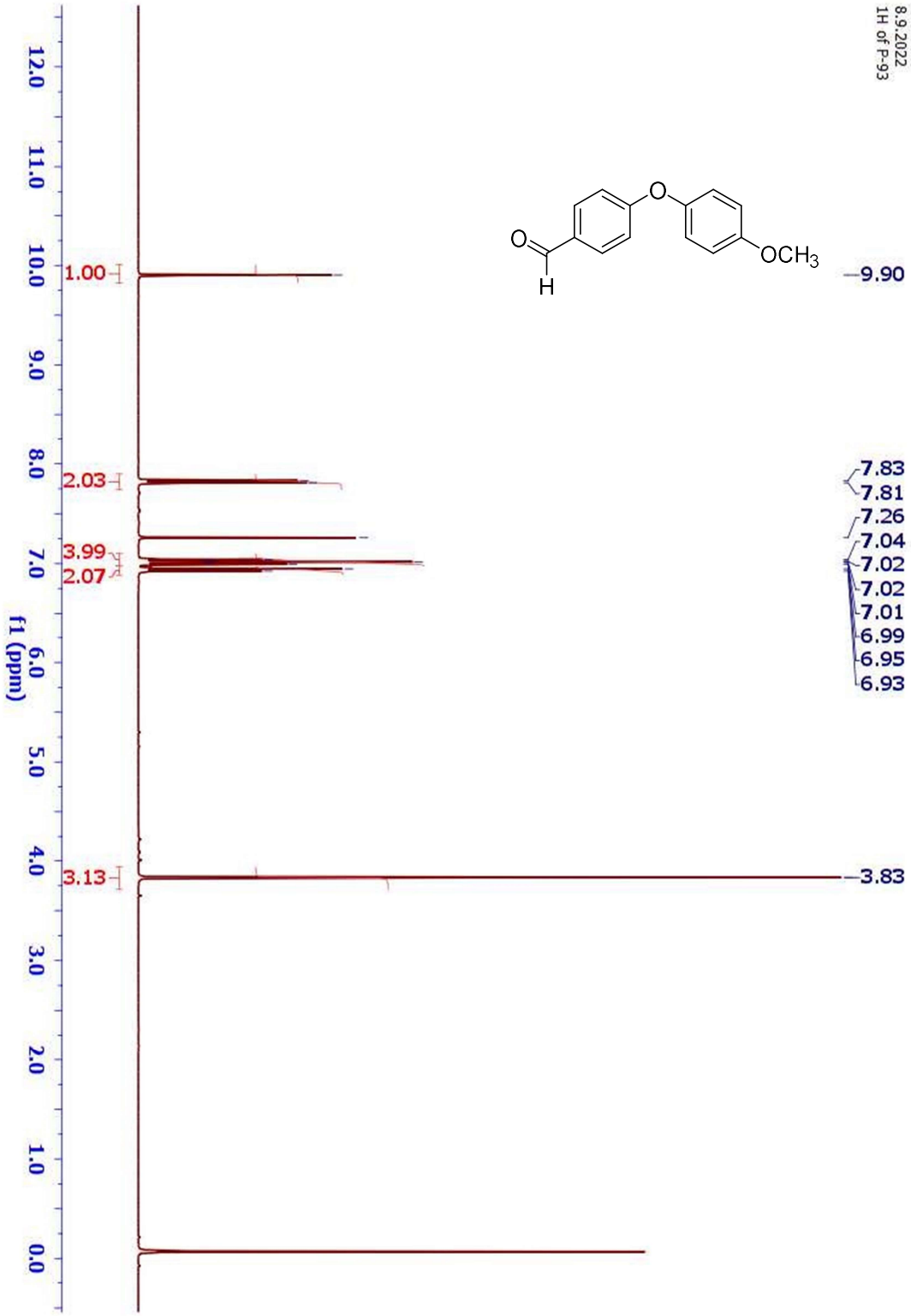

4.7.2022
1H OF SP-127
157.33
151.69
132.27
131.74
129.87
127.80
127.69
127.35
126.96
126.94
126.74
125.37
123.50
122.76
122.58
119.14
111.44
77.32
77.00
76.68
f1 (ppm)

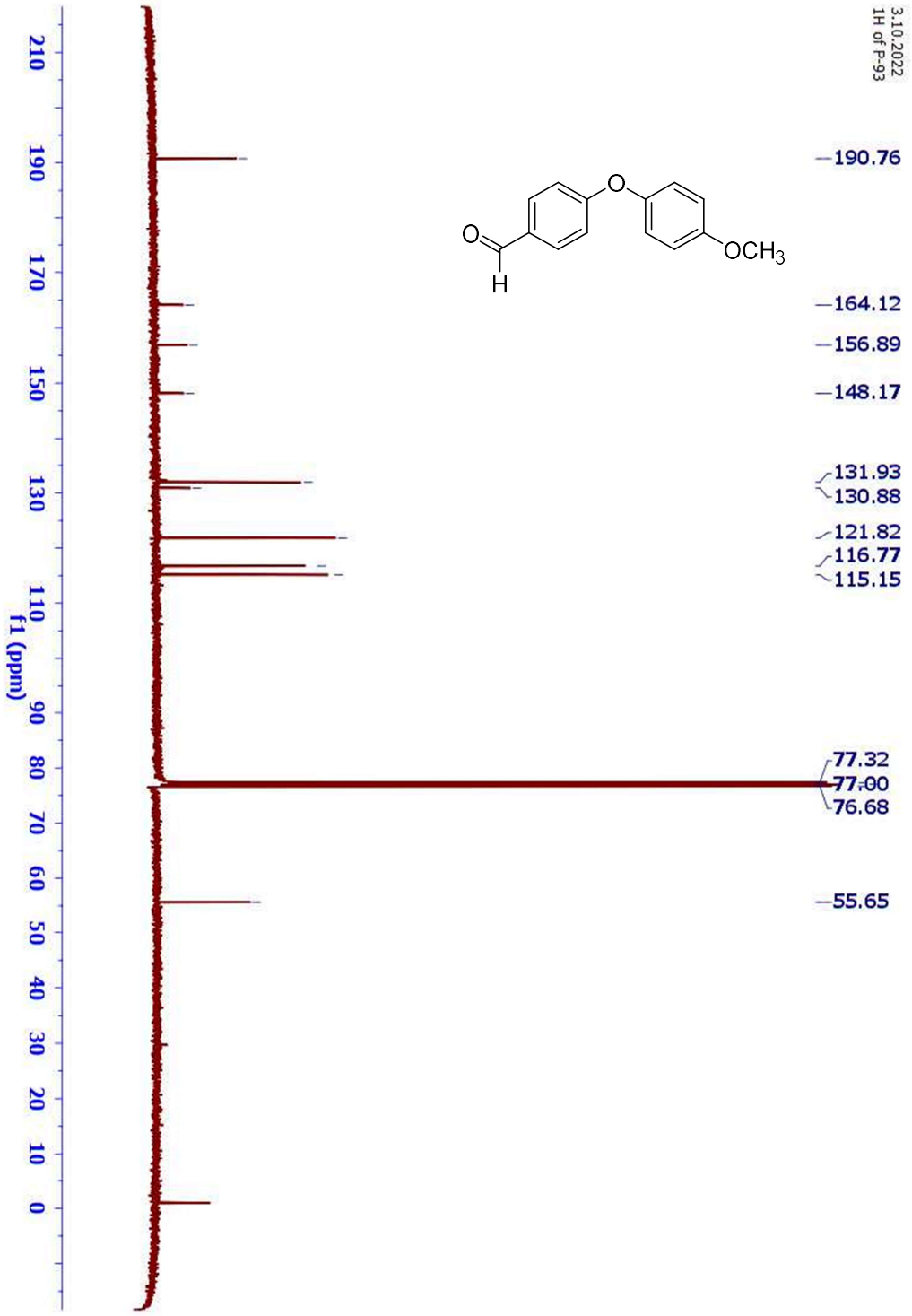

10.8.2022
1H of P-72
O
O
H
Cl
1.00
2.03
6.05
9.92
7.85
7.85
7.84
7.83
7.26
7.13
7.10
7.08
7.07
7.06
7.05
7.04
7.03
7.02
7.01
f1 (ppm)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

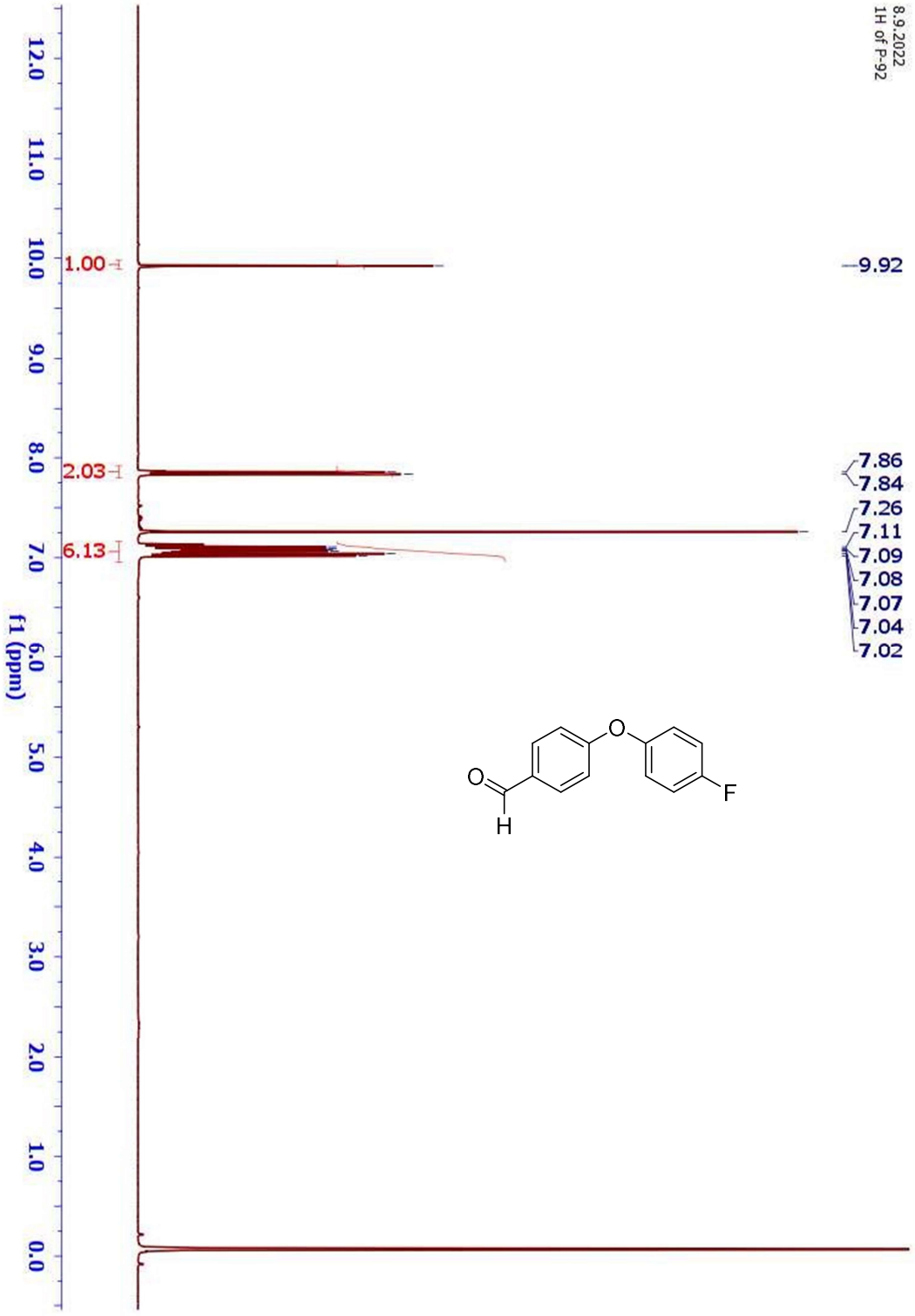

22.8.2022
13C of P-72
190.69
163.34
160.91
158.49
150.83
150.80
131.97
131.30
122.04
121.96
117.17
116.90
116.67
77.32
77.00
76.68
O
O
H
Cl
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

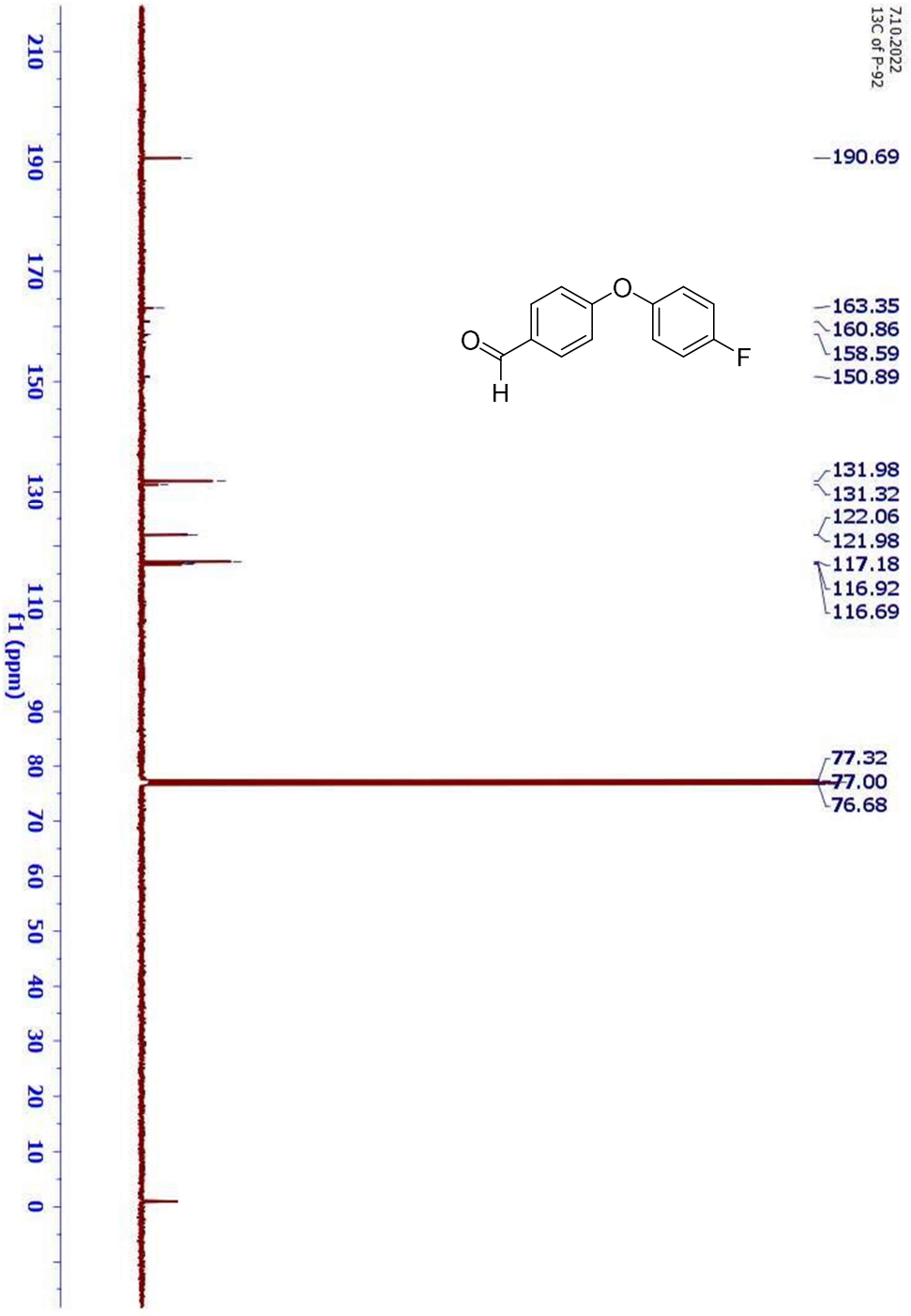

Main File_C-O
1H of PKB-705(a) 21.4.2022
O
O2N
Cl
2.01
2.00
4.04
8.22
8.20
7.41
7.38
7.26
7.05
7.03
7.03
7.03
7.02
7.00
f1 (ppm)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

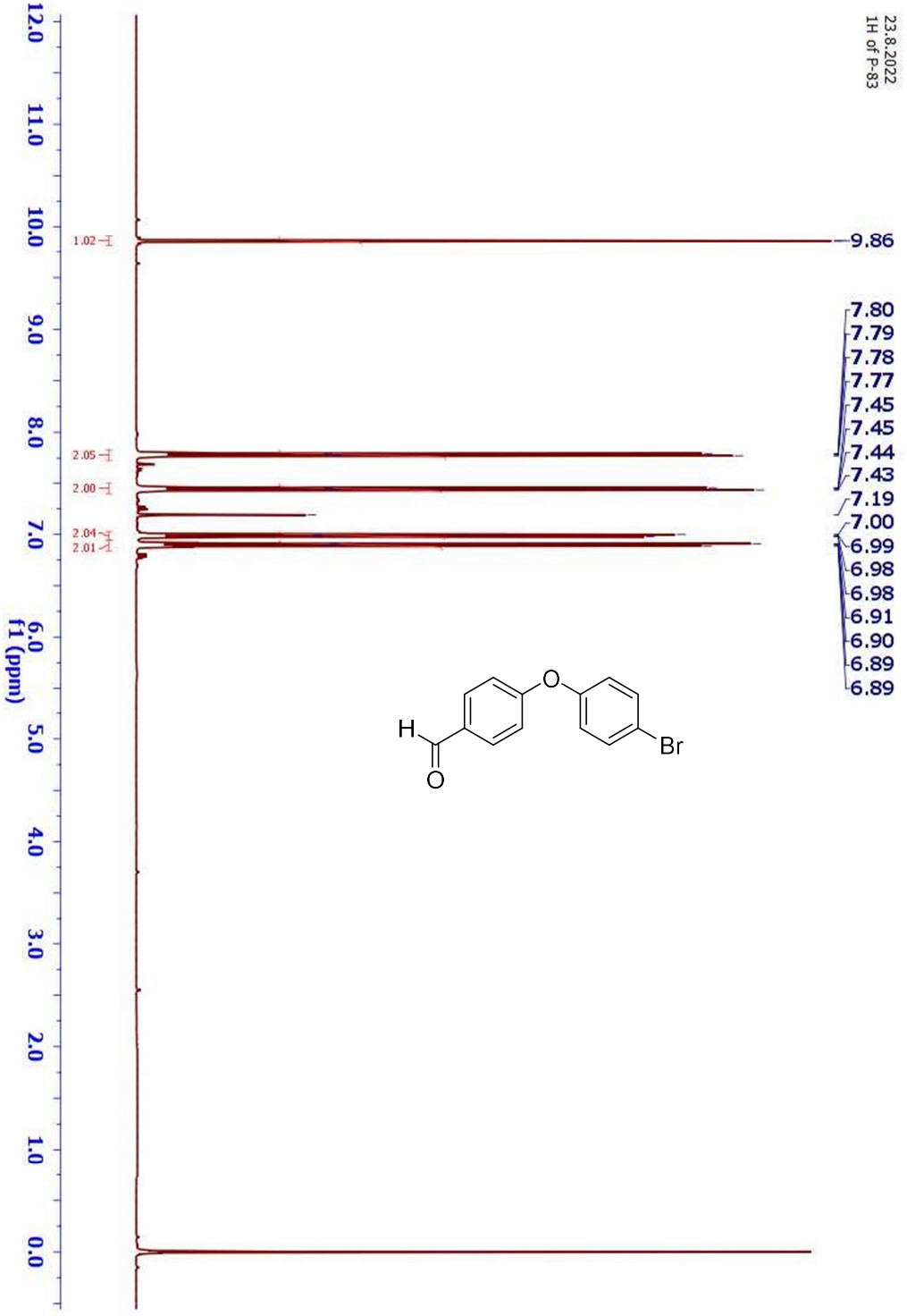

12.5.2022
13C of SS-705(A)
O
O2N
Cl
162.86
153.32
142.94
130.37
126.01
121.79
117.19
77.32
77.00
76.68
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

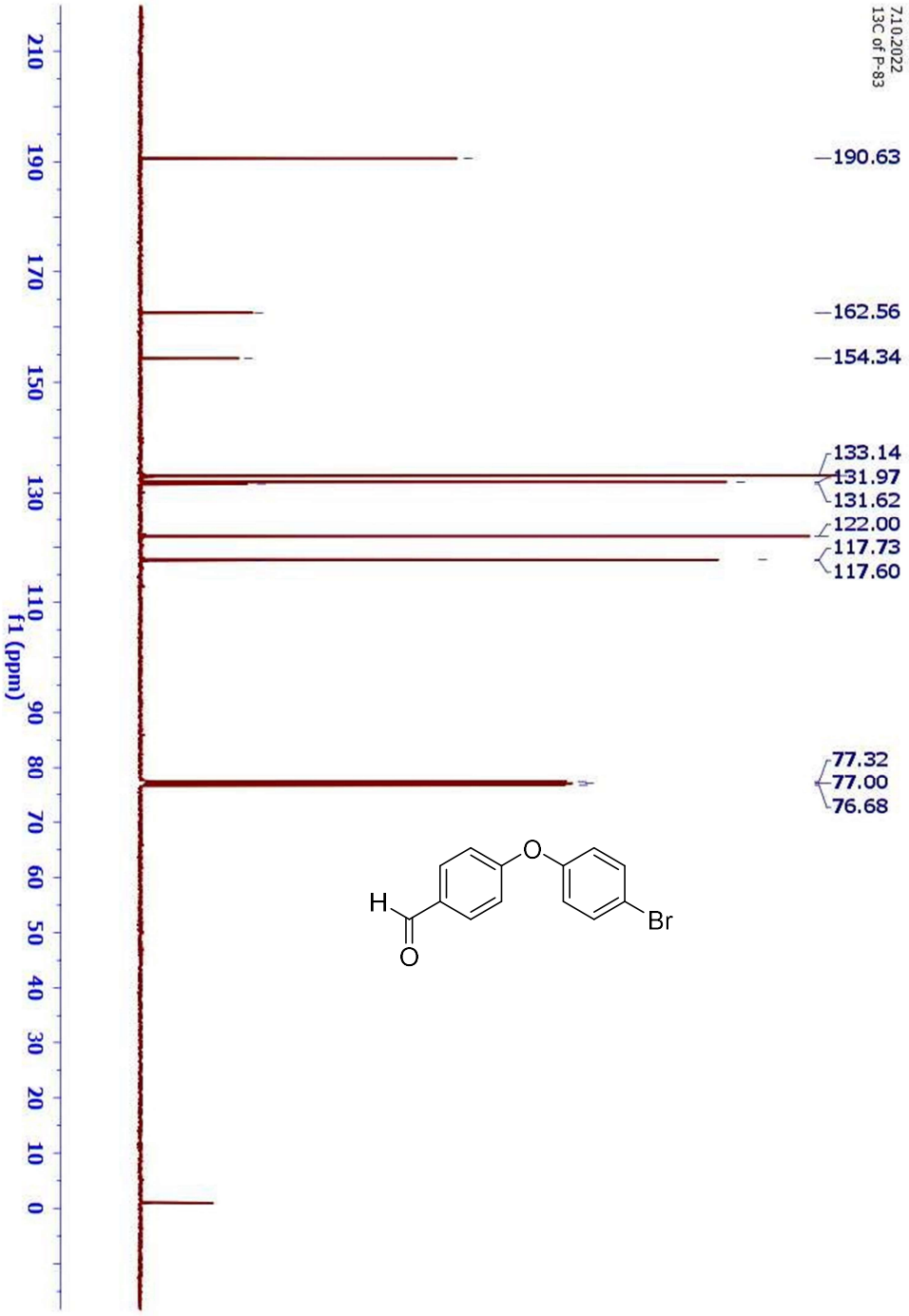

8.9.2022
1H of P-93
O
O
H
OCH3
9.90
7.83
7.81
7.26
7.04
7.02
7.02
7.01
6.99
6.95
6.93
3.83
1.00
2.03
3.99
2.07
3.13
f1 (ppm)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

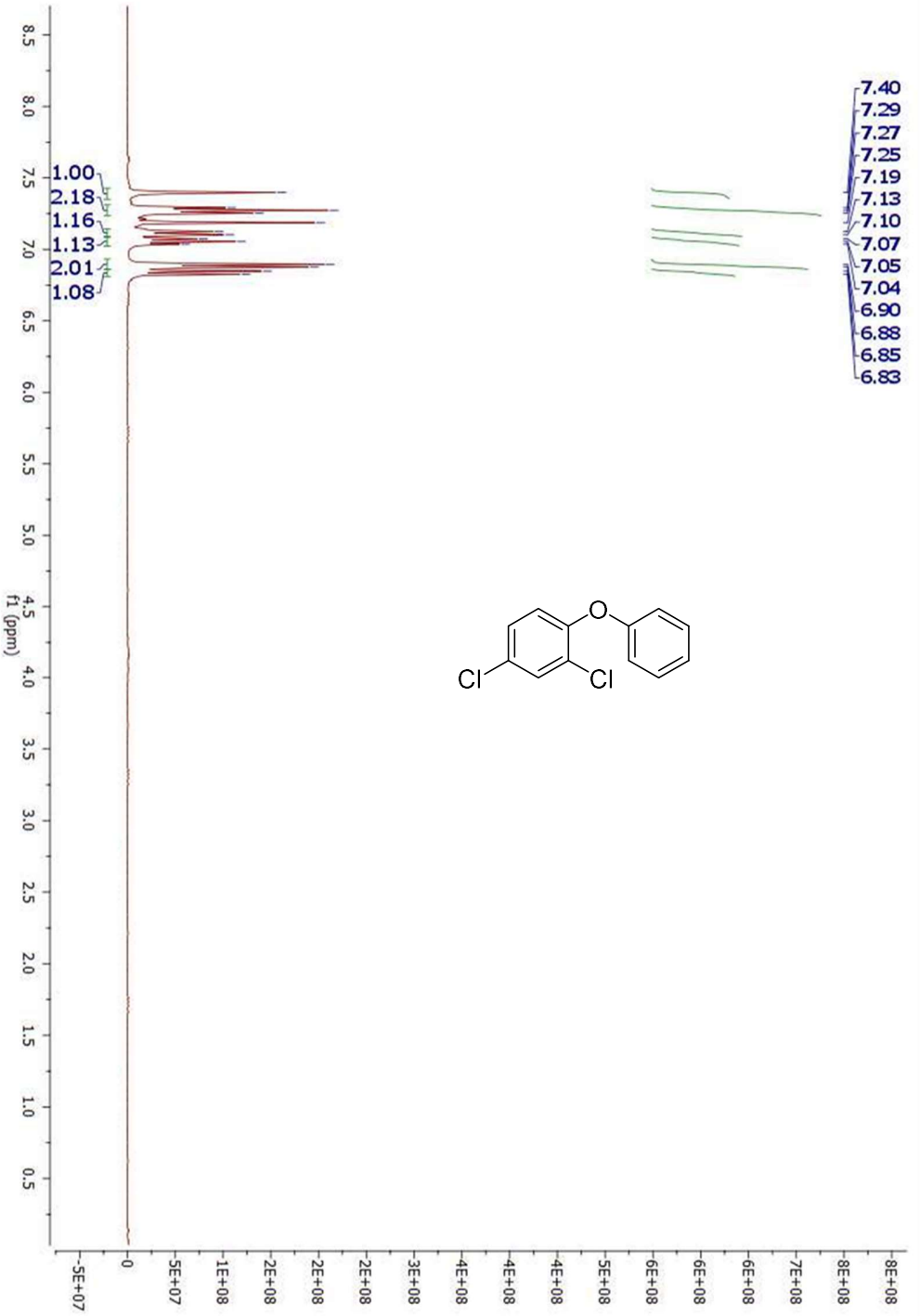

3.10.2022
1H of P-93
190.76
164.12
156.89
148.17
131.93
130.88
121.82
116.77
115.15
77.32
77.00
76.68
55.65
O
O
H
OCH3
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

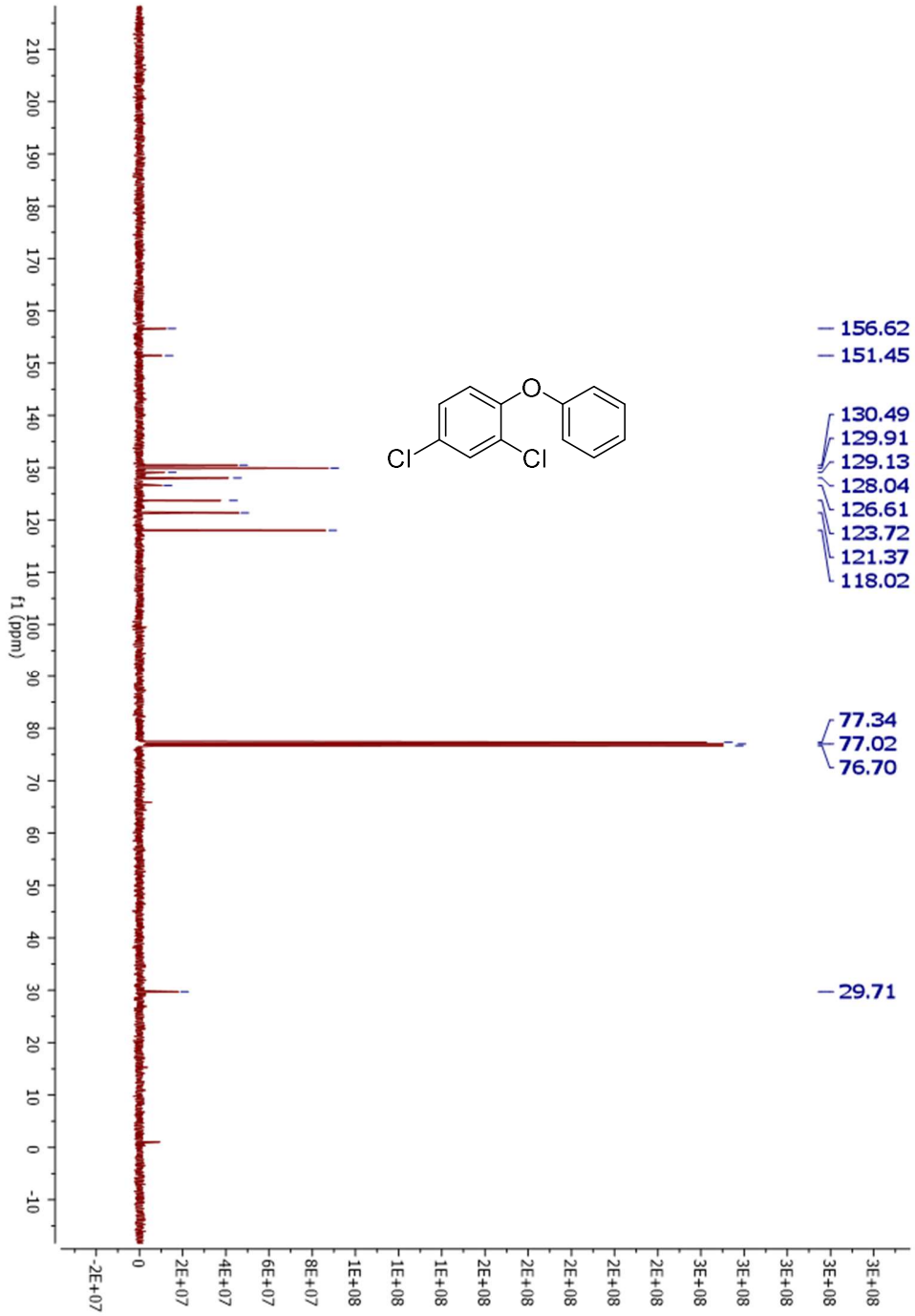

8.9.2022
1H of P-92
9.92
7.86
7.84
7.26
7.11
7.09
7.08
7.07
7.04
7.02
1.00
2.03
6.13
f1 (ppm)
O
O
H
F

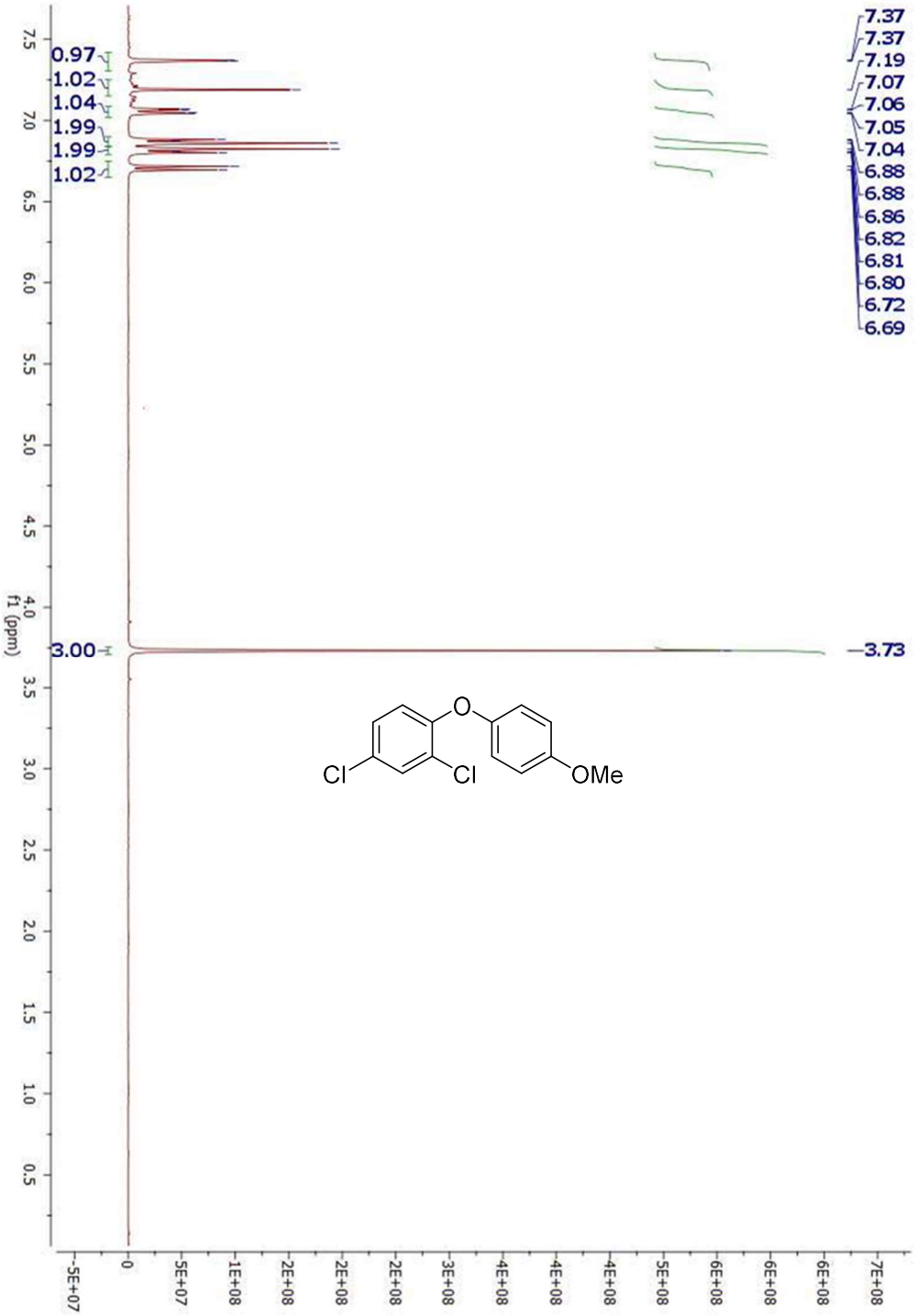

7.10.2022
13C of P-92
190.69
163.35
160.86
158.59
150.89
131.98
131.32
122.06
121.98
117.18
116.92
116.69
77.32
77.00
76.68
O
O
H
F
f1 (ppm)

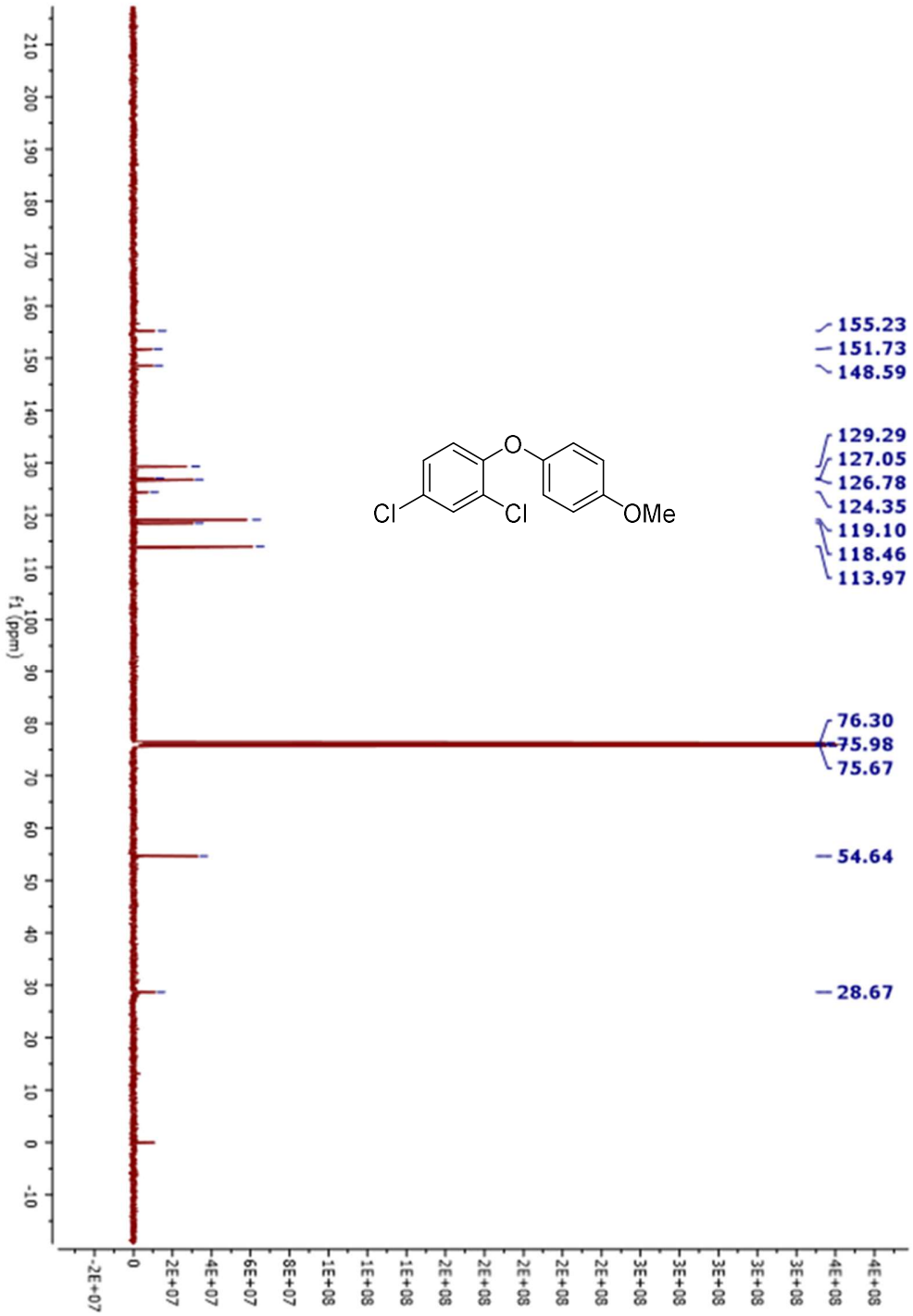

23.8.2022
1H of P-83
9.86
7.80
7.79
7.78
7.77
7.45
7.45
7.44
7.43
7.19
7.00
6.99
6.98
6.98
6.91
6.90
6.89
6.89
1.02
2.05
2.00
2.04
2.01
f1 (ppm)
H
O
O
Br

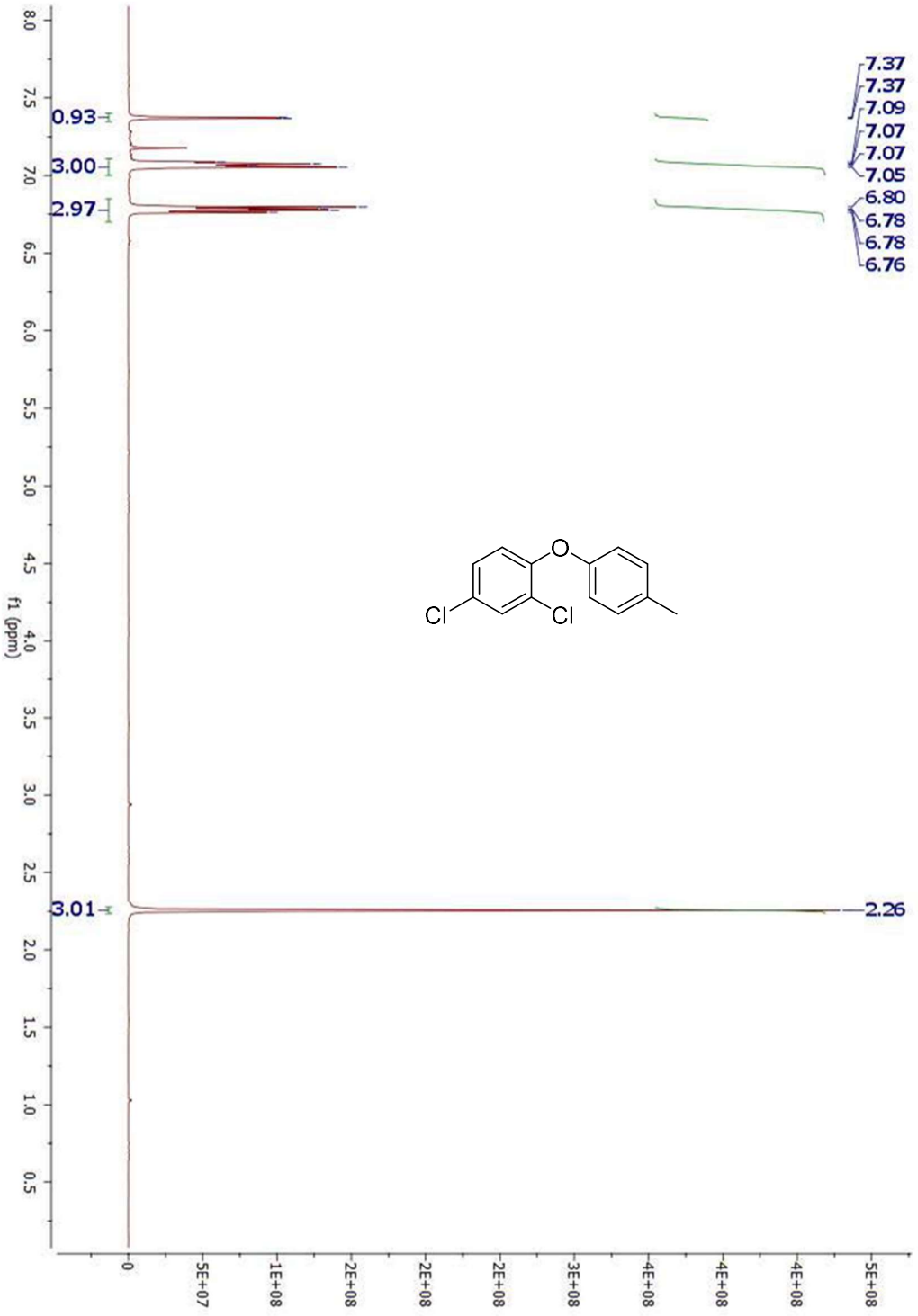

7.10.2022
13C of P-83
190.63
162.56
154.34
133.14
131.97
131.62
122.00
117.73
117.60
77.32
77.00
76.68
f1 (ppm)
O
H
O
Br

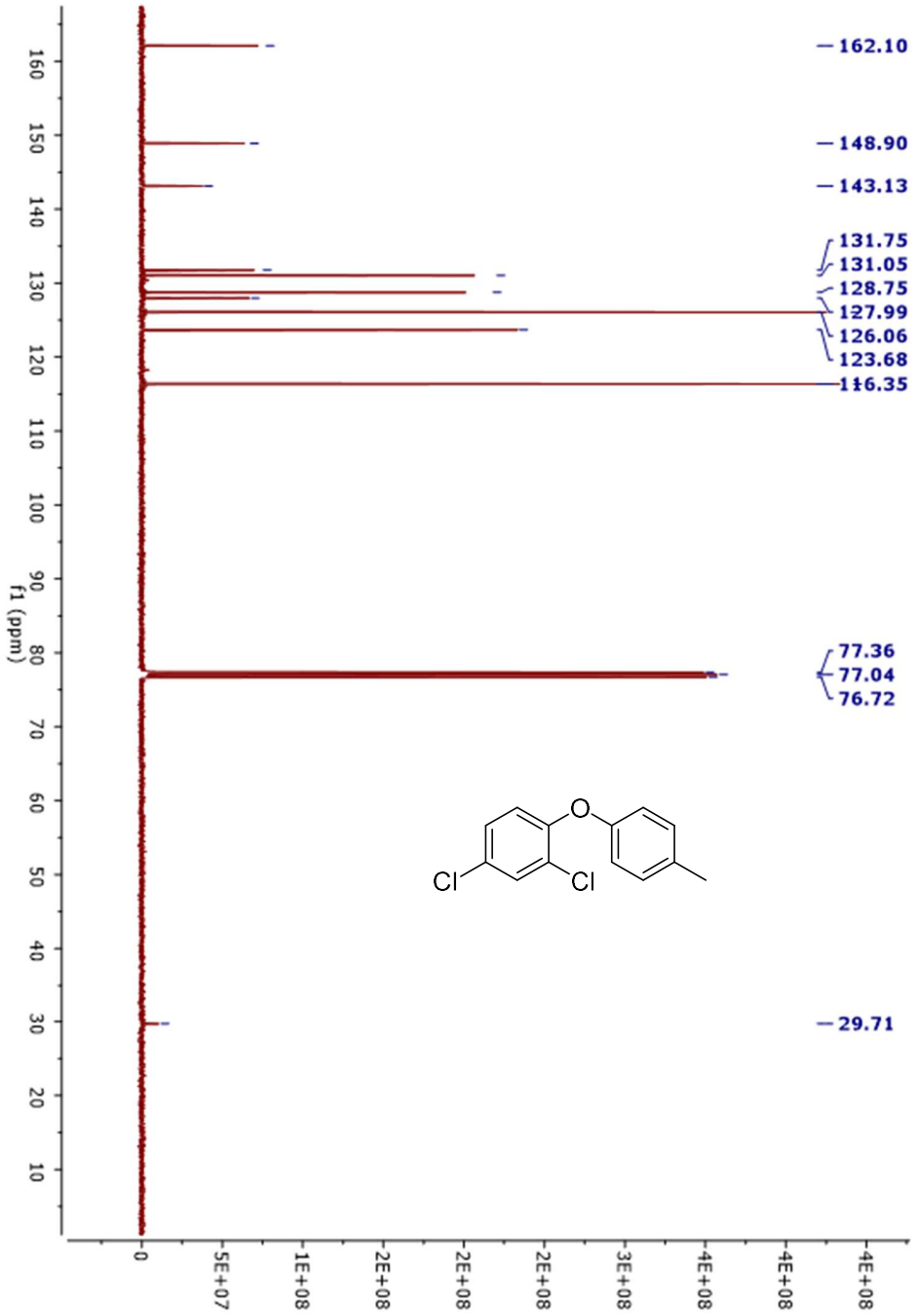

1.00
2.18
1.16
1.13
2.01
1.08
7.40
7.29
7.27
7.25
7.19
7.13
7.10
7.07
7.05
7.04
6.90
6.88
6.85
6.83
f1 (ppm)
O
Cl
Cl

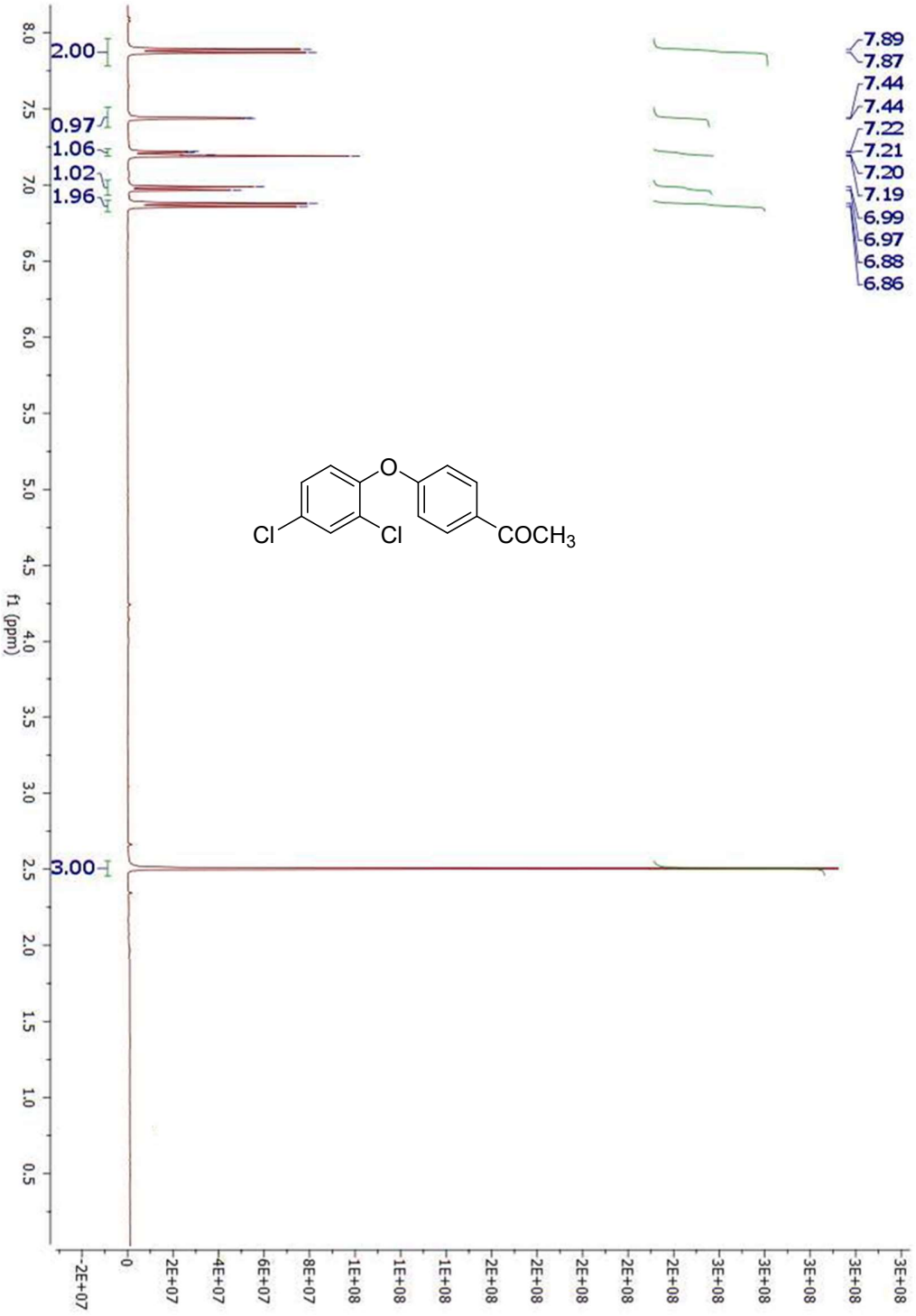

156.62
151.45
130.49
129.91
129.13
128.04
126.61
123.72
121.37
118.02
77.34
77.02
76.70
29.71
Cl
Cl
O
f1 (ppm)

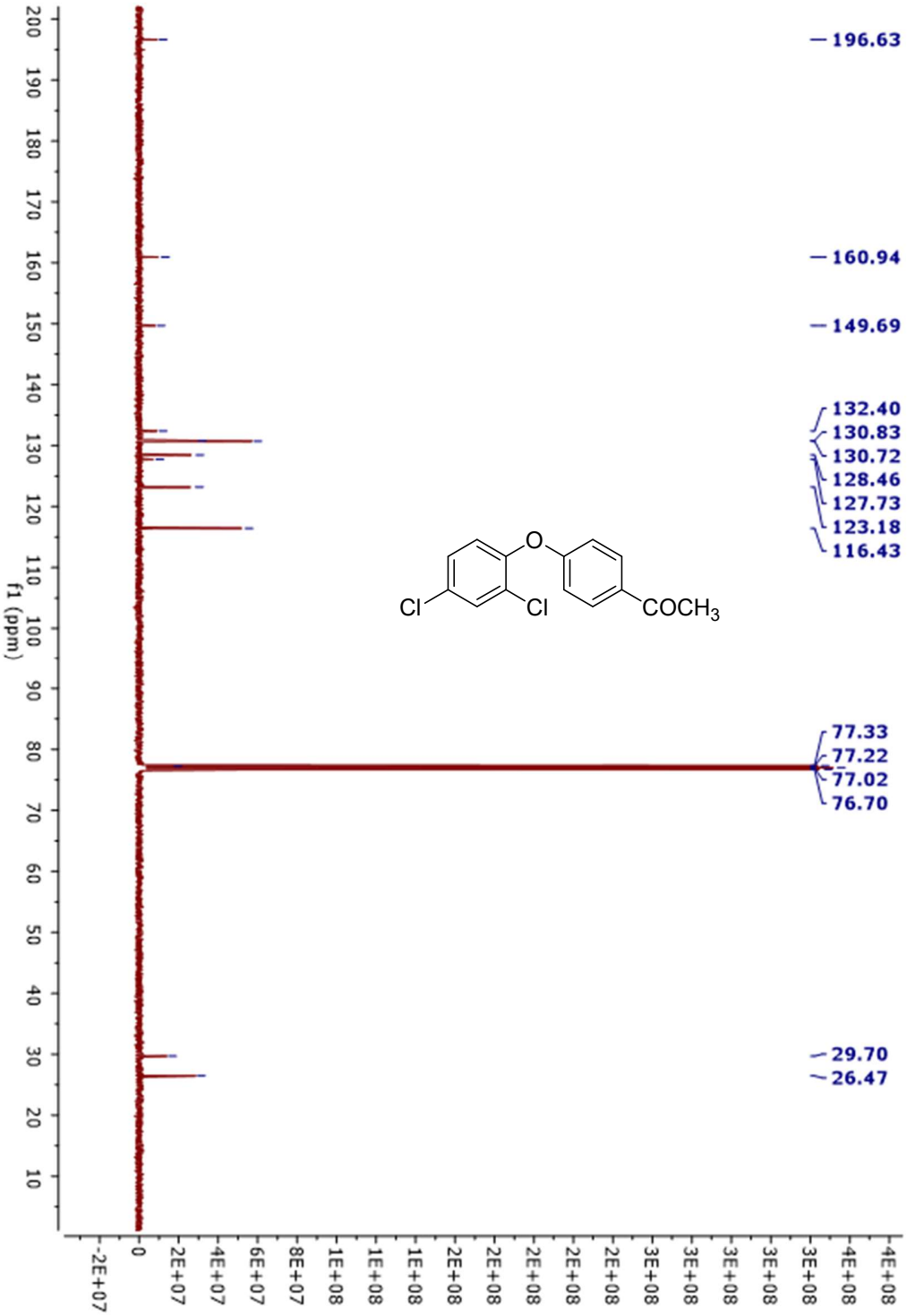

7.37
7.37
7.19
7.07
7.06
7.05
7.04
6.88
6.88
6.86
6.82
6.81
6.80
6.72
6.69
0.97
1.02
1.04
1.99
1.99
1.02
3.00
3.73
f1 (ppm)
Cl
Cl
O
OMe

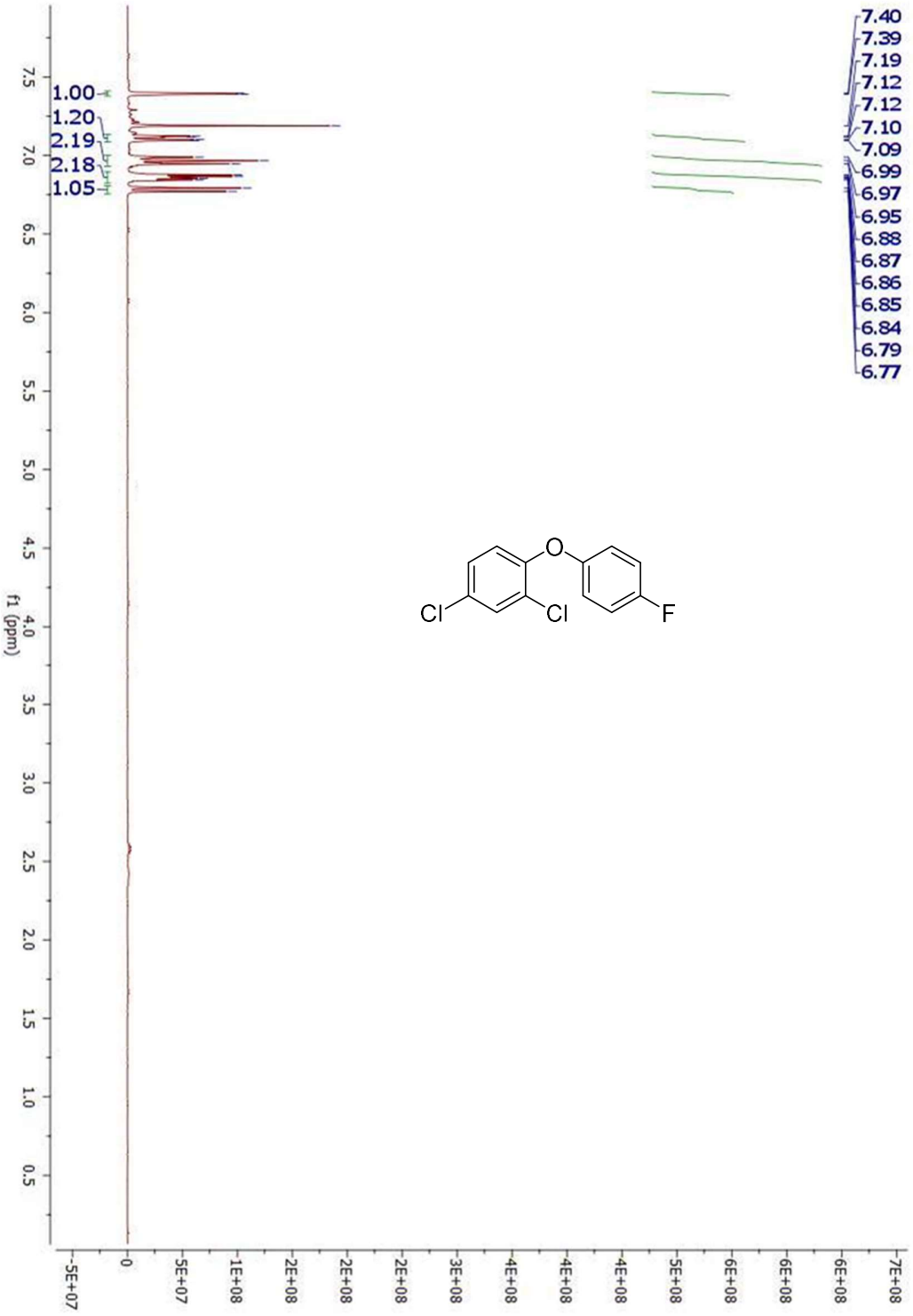

155.23
151.73
148.59
129.29
127.05
126.78
124.35
119.10
118.46
113.97
76.30
75.98
75.67
54.64
28.67
Cl
Cl
O
OMe
f1 (ppm)

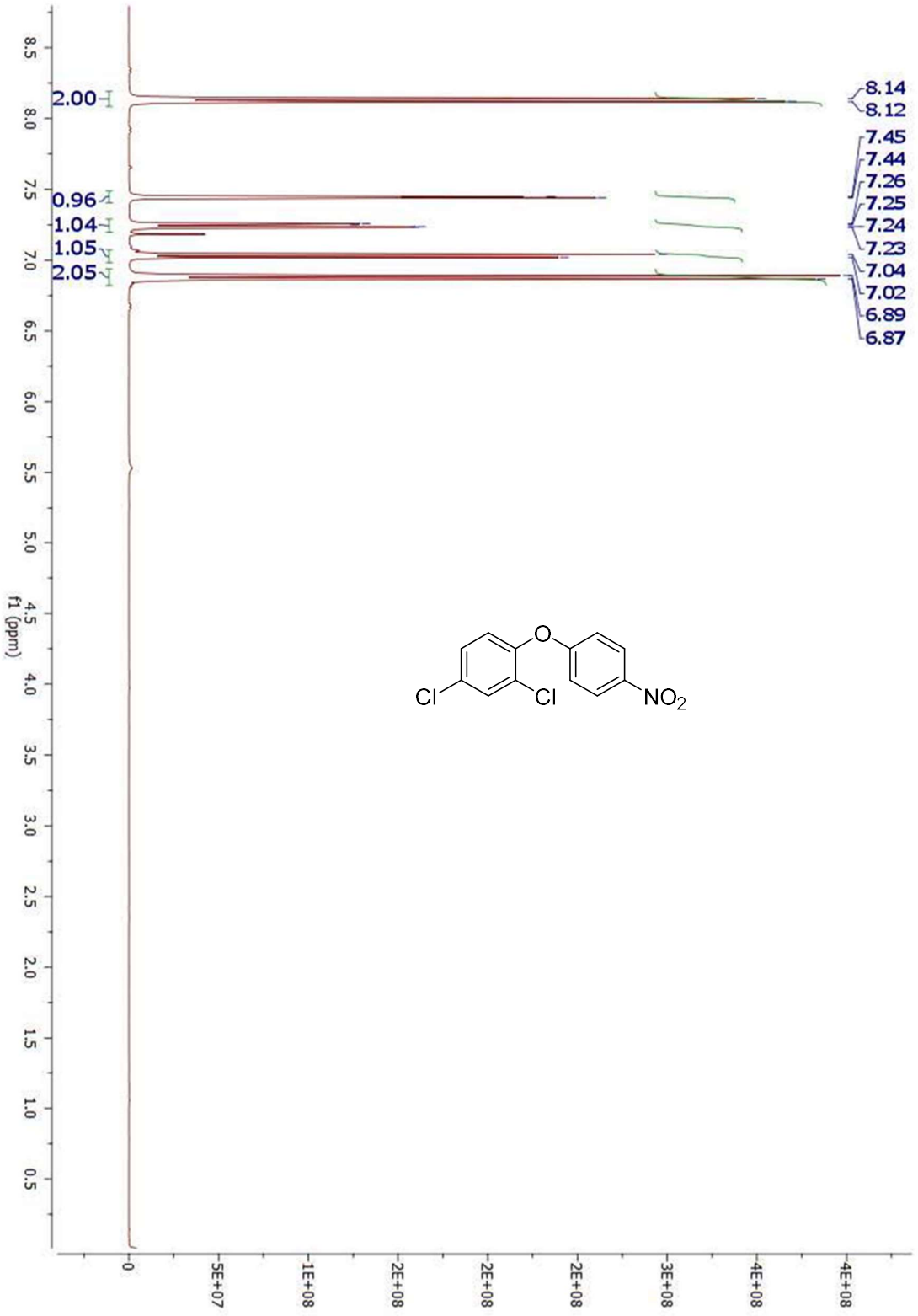

7.37
7.37
7.09
7.07
7.07
7.05
6.80
6.78
6.78
6.76
0.93
3.00
2.97
3.01
2.26
Cl
Cl
O
f1 (ppm)

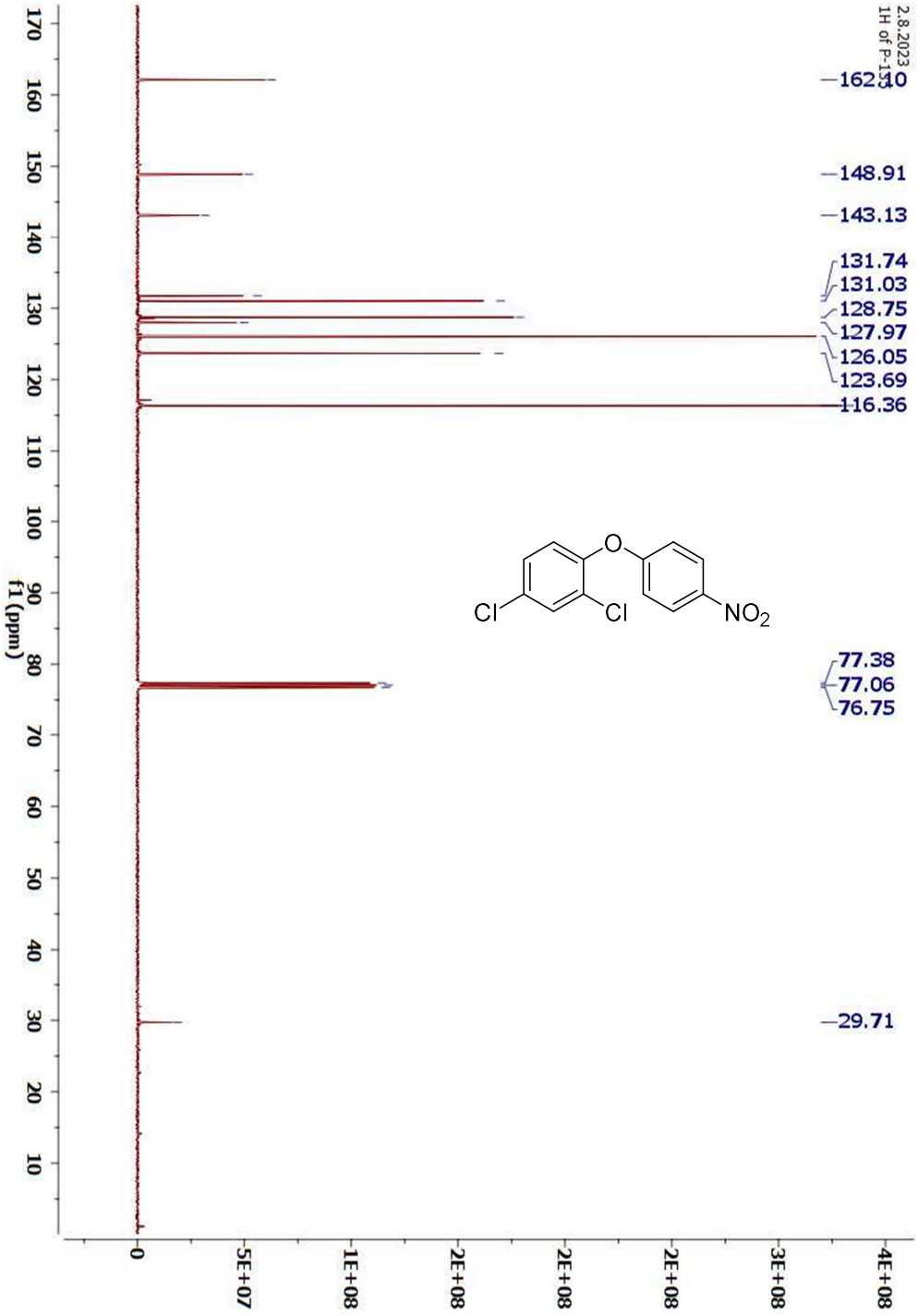

162.10
148.90
143.13
131.75
131.05
128.75
127.99
126.06
123.68
116.35
77.36
77.04
76.72
29.71
f1 (ppm)
Cl
Cl
O


7.89
7.87
7.44
7.44
7.22
7.21
7.20
7.19
6.99
6.97
6.88
6.86
2.00
0.97
1.06
1.02
1.96
3.00
O
Cl
Cl
COCH3
f1 (ppm)

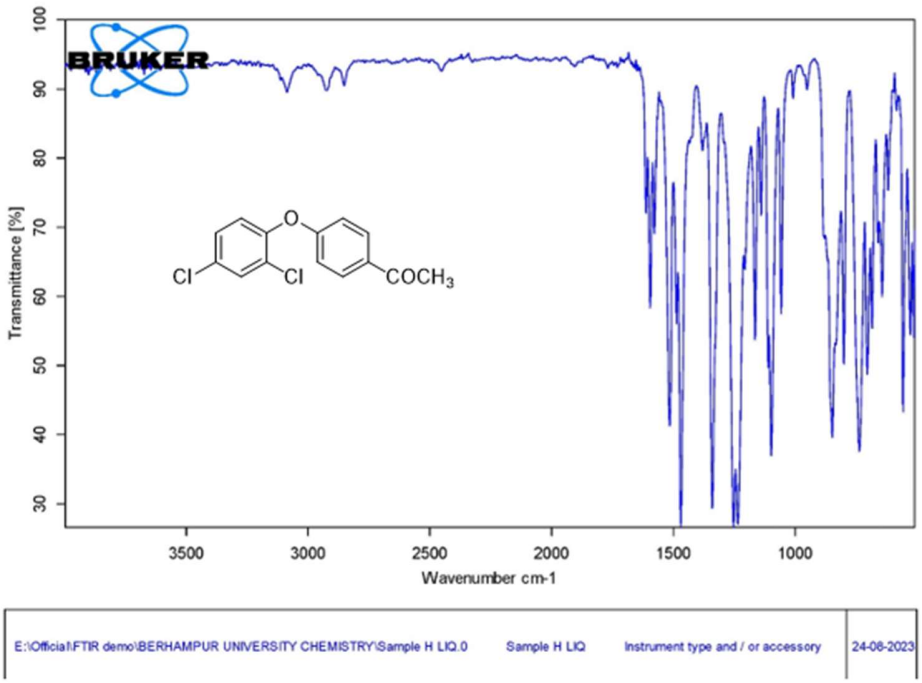

196.63
160.94
149.69
132.40
130.83
130.72
128.46
127.73
123.18
116.43
77.33
77.22
77.02
76.70
29.70
26.47
Cl
Cl
O
COCH3
f1 (ppm)

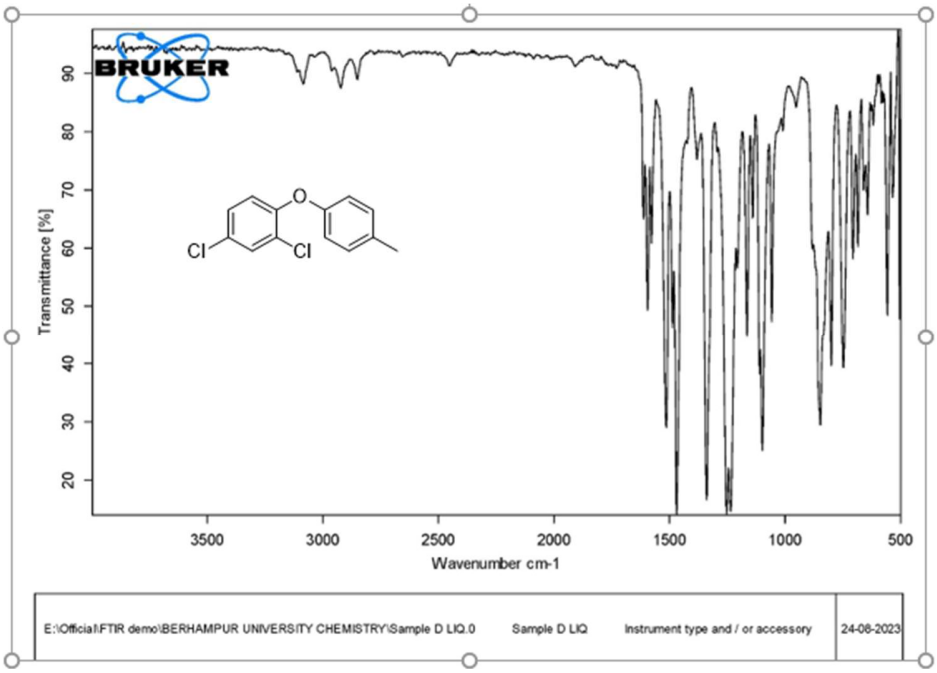

7.40
7.39
7.19
7.12
7.12
7.10
7.09
6.99
6.97
6.95
6.88
6.87
6.86
6.85
6.84
6.79
6.77
1.00
1.20
2.19
2.18
1.05
f1 (ppm)
Cl
Cl
O
F

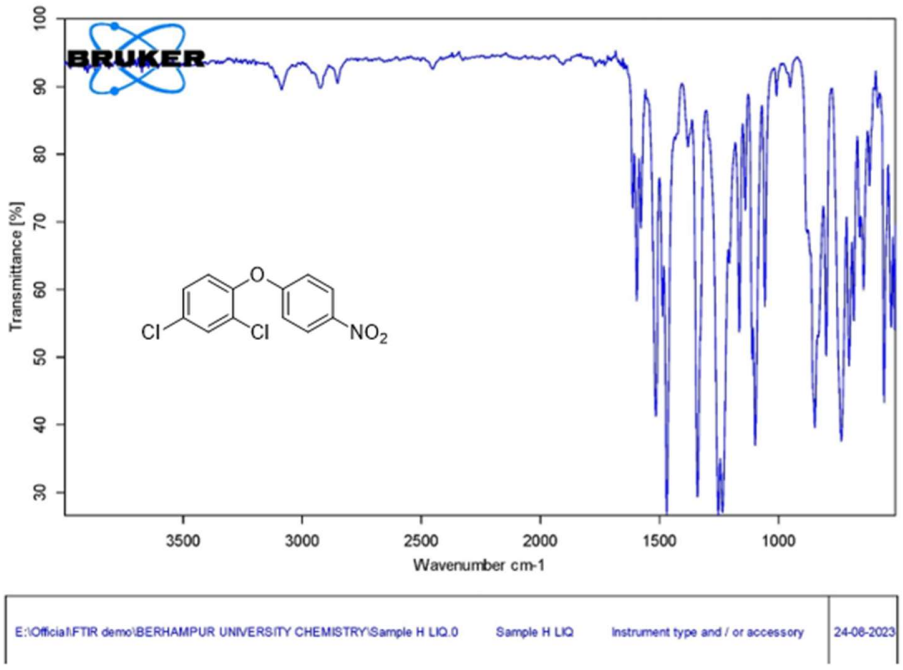

8.14
8.12
7.45
7.44
7.26
7.25
7.24
7.23
7.04
7.02
6.89
6.87
2.00
0.96
1.04
1.05
2.05
f1 (ppm)
O
Cl
Cl
NO2


2.8.2023
1H of P-15
162.10
148.91
143.13
131.74
131.03
128.75
127.97
126.05
123.69
116.36
77.38
77.06
76.75
29.71
Cl
Cl
O
NO2
f1 (ppm)

IR Spectra of New Compounds




BRUKER
Transmittance [%]
90
80
70
60
50
40
30
20
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
O
Cl
Cl
E:\Official\FTIR demo\BERHAMPUR UNIVERSITY CHEMISTRY\Sample D LIQ.0
Sample D LIQ
Instrument type and / or accessory
24-08-2023


BRUKER
Transmittance [%]
100
90
80
70
60
50
40
30
3500
3000
2500
2000
1500
1000
Wavenumber cm-1
O
Cl
Cl
NO2
E:\Official\FTIR demo\BERHAMPUR UNIVERSITY CHEMISTRY\Sample H LIQ.0
Sample H LIQ
Instrument type and / or accessory
24-08-2023

IR Data: The Recycle procedure follow as per the reported journal; *Chem. Eur. J.* 2020, **24**, 620-624.

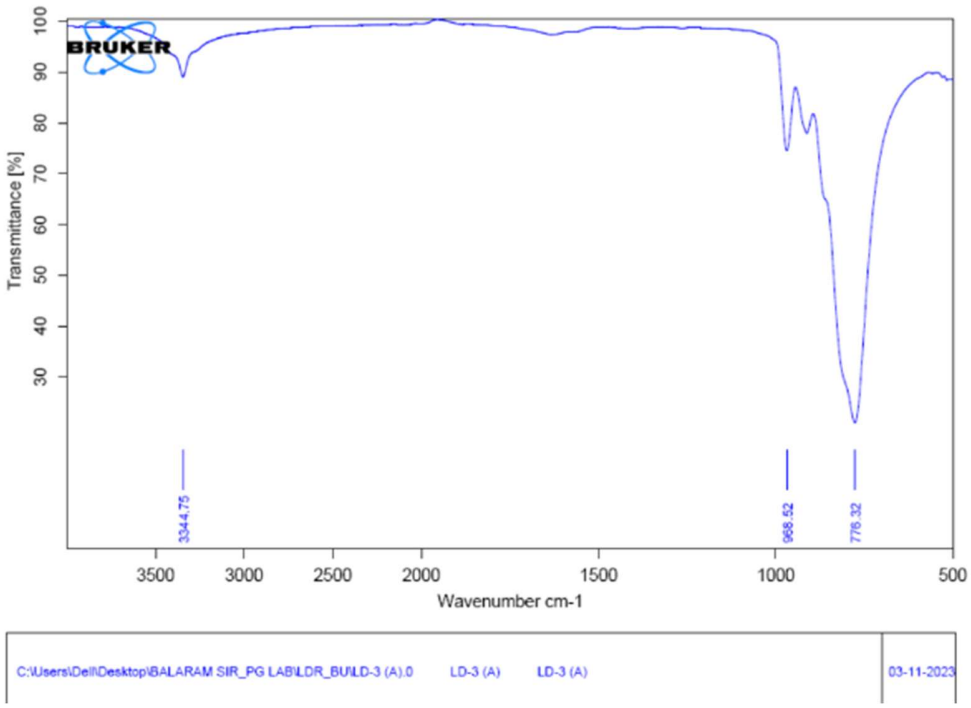


Figure – 1 : *IR Data of Original $CuMoO_4$ Catalyst*

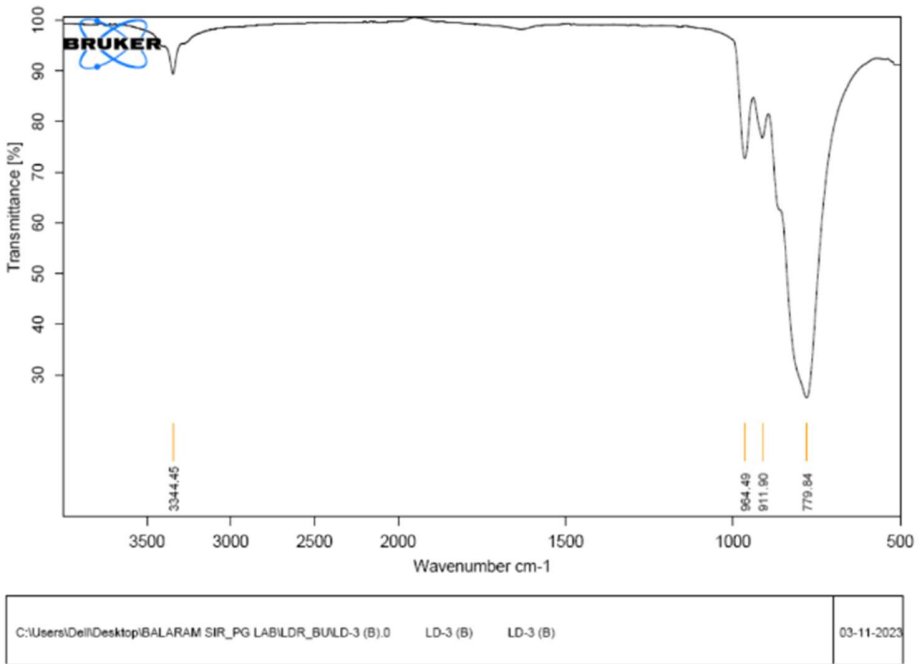


Figure – 1 : *IR Data of Recovered $CuMoO_4$ Catalyst*