Suzuki-Miyaura Cross-Coupling of Unprotected, Nitrogen-Rich Heterocycles: Substrate Scope and Mechanistic Investigation

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Supporting Information

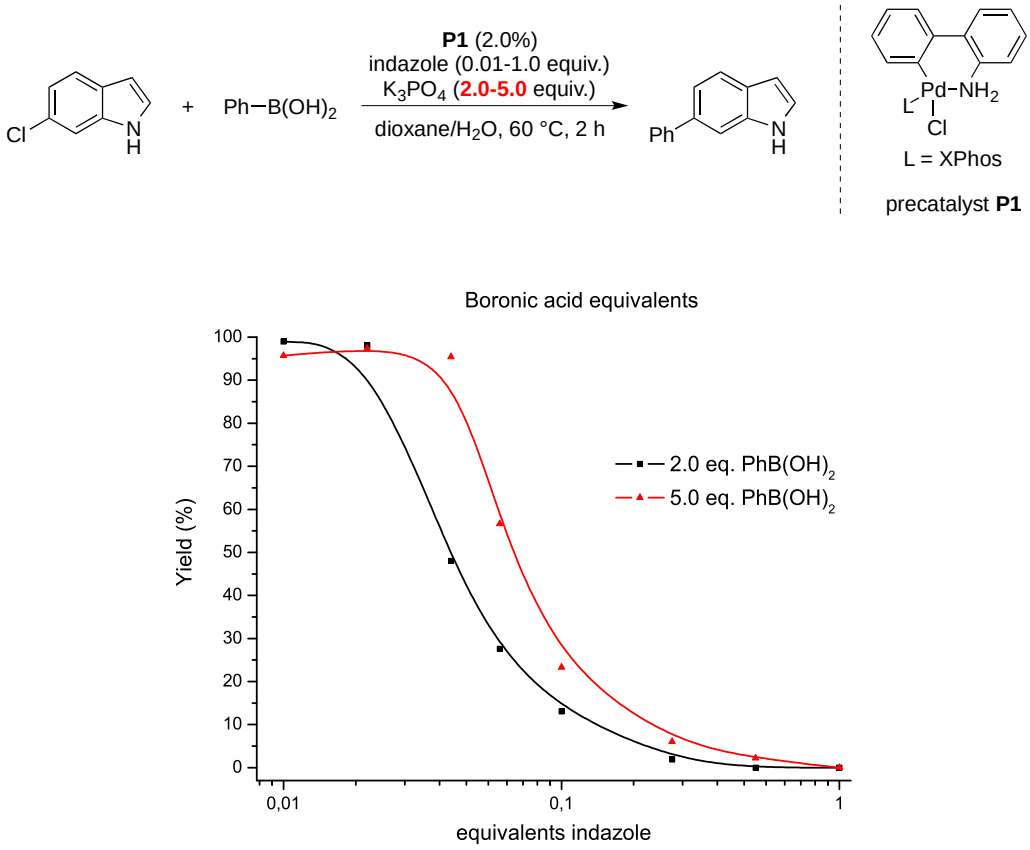


Figure S1. Influence of the amount of boronic acid on the Suzuki-Miyaura cross-coupling.

Kinetics Data Figure S1

	Yield 6-phenylindole [%]	
Indazole equiv.	**2.0 eq. $PhB(OH)_2$**	**5.0 eq. $PhB(OH)_2$**
1.00	0	0
0.50	0	2.2
0.25	1.9	6.0
0.10	13.1	23.3
0.06	27.6	56.6
0.04	48.0	95.4
0.02	98.1	97.4
0.01	99.0	95.7

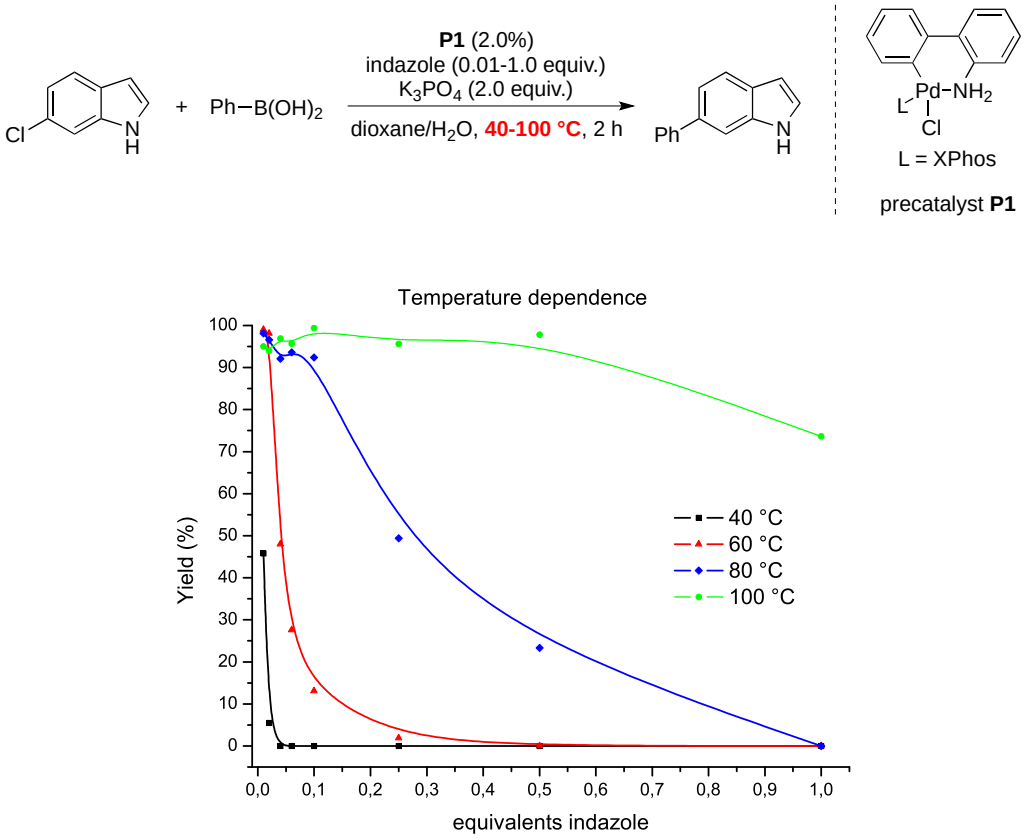


Figure S2. Influence of the reaction temperature on the Suzuki-Miyaura cross-coupling.

Kinetics Data Figure S2

	Yield 6-phenylindole [%]			
Indazole equiv.	**40 °C**	**60 °C**	**80 °C**	**100 °C**
1.00	0	0	0	73.6
0.50	0	0	23.3	97.8
0.25	0	1.9	49.4	95.6
0.10	0	13.1	92.4	99.4
0.06	0	27.6	93.6	95.7
0.04	0	48.0	92.1	96.9
0.02	5.5	98.1	96.6	94.0
0.01	45.8	99.0	98.1	95.0

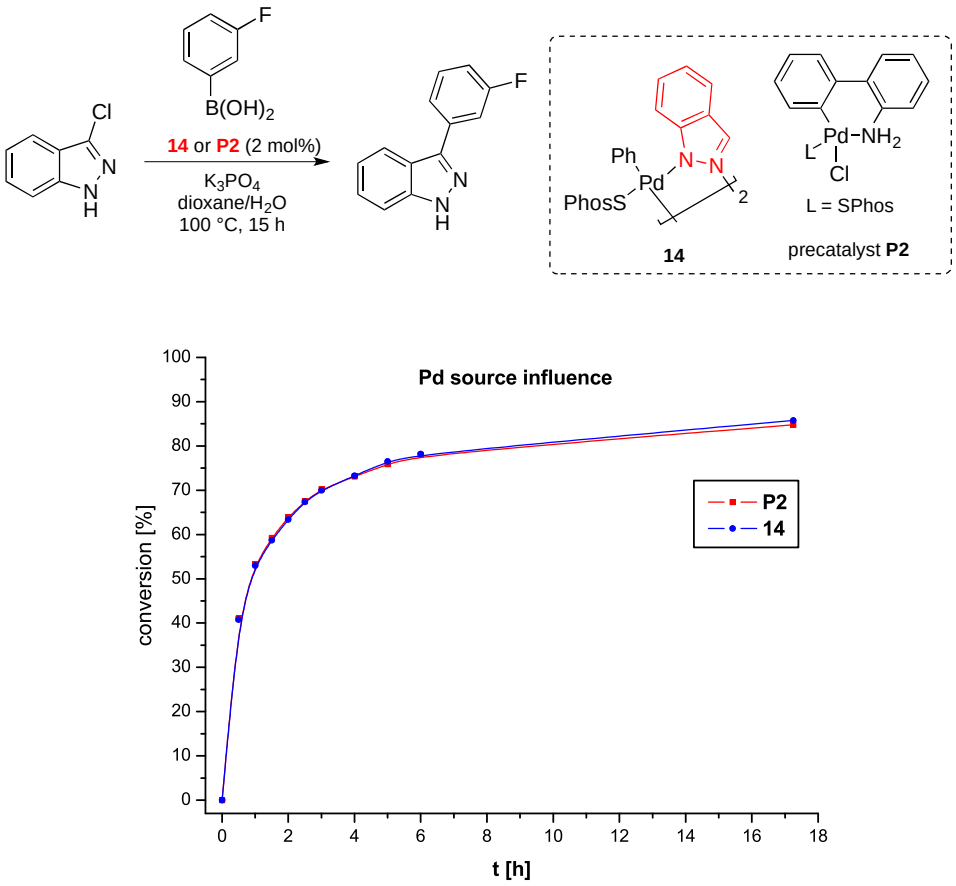


Figure S3. Effect of Pd sources on the cross-coupling of 3-chloroindazole.

Kinetics Data Figure S3

	conversion of 3-chloroindazole [%]	
t [h]	**P2**	**5**
0	0	0
0.5	41.0	40.8
1	53.3	53.0
1.5	59.2	58.7
2	63.9	63.4
2.5	67.5	67.4
3	70.2	70.0
4	73.1	73.3
5	75.9	76.5
6	78.0	78.2
17.25	84.8	85.8

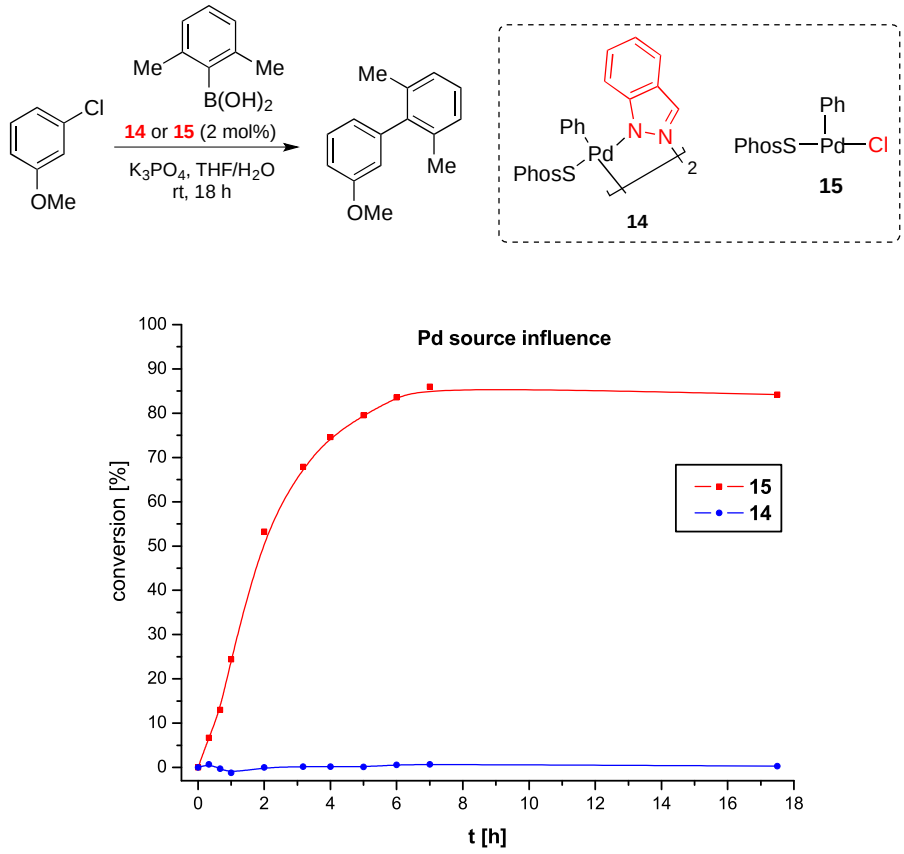
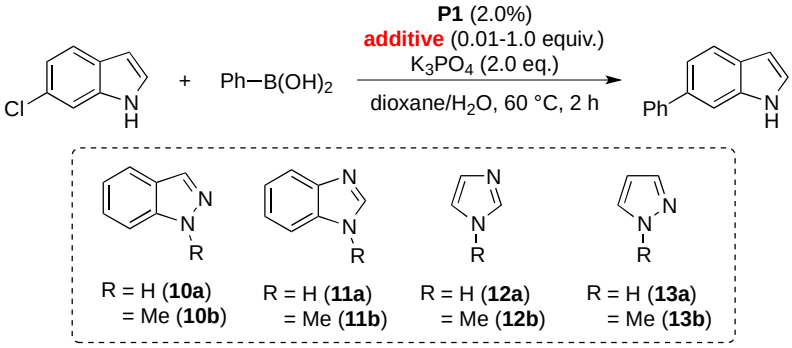


Figure S4. Effect of Pd sources on the cross-coupling of 3-chloroanisole.

Kinetics Data Figure S4

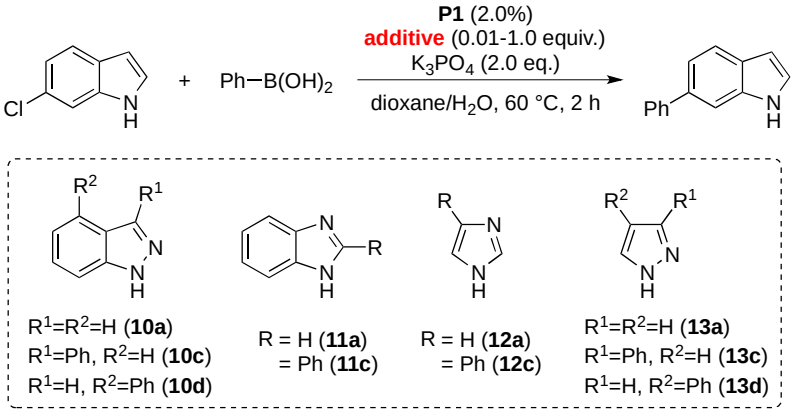
	conversion of 3-chloroindazole [%]	
t [h]	**6**	**5**
0	0.0	0.0
0.5	6.7	0.7
1	13.0	-0.3
1.5	24.4	-1.2
2	53.3	0.0
2.5	67.9	0.2
3	74.6	0.2
4	79.5	0.1
5	83.6	0.6
6	86.0	0.7
17.25	84.2	0.3

Kinetics Data Figure 3



	Yield 6-phenylindole [%]							
Additive equiv.	**10a**	**10b**	**11a**	**11b**	**12a**	**12b**	**13a**	**13b**
1.00	0	61.0	0	33.5	0	2.4	0	94.7
0.50	0	77.3	0	96.4	0	13.1	0	93.1
0.25	1.9	86.6	0	95.6	0	39.8	1.2	95.9
0.10	13.1	92.7	0	88.2	0	82.7	5.3	97.5
0.06	27.6	94.1	0	97.5	0	95.7	15.6	93.6
0.04	48.0	97.4	0	96.8	2.9	96.6	27.4	97.9
0.02	98.1	98.0	5.6	95.9	40.7	98.0	83.6	95.2
0.01	99.0	95.6	47.5	98.0	98.0	95.6	96.7	93.5

Kinetics Data Figure 5



	Yield 6-phenylindole [%]									
Additive equiv.	**10a**	**10c**	**10d**	**11a**	**11c**	**12a**	**12c**	**13a**	**13c**	**13d**
1.00	0	25.6	0	0	0	0	0	0	0	0
0.50	0	60.9	4.5	0	4.6	0	0	0	9.3	0
0.25	1.9	94.2	7.9	0	94.5	0	0	1.2	29.9	0
0.10	13.1	99.1	28.9	0	99.9	0	7.0	5.3	94.1	0
0.06	27.6	98.6	48.4	0	94.5	0	19.3	15.6	94.9	7.1
0.04	48.0	97.9	95.8	0	97.3	2.9	47.0	27.4	94.3	22.4
0.02	98.1	99.2	97.0	5.6	96.3	40.7	91.6	83.6	94.7	60.4
0.01	99.0	98.0	96.4	47.5	94.1	98.0	95.3	96.7	96.7	97.6

General reagent information

Reactions were set-up open to the air. All reactions were performed in oven-dried test-tubes fitted with screw-caps with Teflon seals under an atmosphere of argon. Dioxane was purchased from Aldrich in a Sure-Seal bottle and was used as received. THF and toluene were purchased from J.T. Baker in CYCLE-TAINER® solvent-delivery kegs and vigorously purged with argon for 2 h. The solvents were further purified by passing them under argon pressure through two packed columns of neutral alumina (for THF) or through neutral alumina and copper (II) oxide (for toluene). Unless stated otherwise, solvents were not further degassed. Aryl chlorides, boronic acids, heterocyclic additives, phenylmagnesium bromide and phenyltributylstannane were purchased from Aldrich, Frontier Scientific, Combi-Blocks, Alfa Aesar or TCI America and were used as received without further purification. Anhydrous K_3PO_4 was purchased from Aldrich and stored on the benchtop under air. Precatalysts **P1** and **P3** were a gift from Merck and are commercially available from Aldrich or Strem. Precatalyst **P2** was synthesized according to a published procedure.[1,2] SPhos was purchased from Strem. BrettPhos was a gift from Aldrich. Column chromatography was performed using Silicycle SiliaFlash® F60 silica gel (40-63 μm particle size, 230-400 mesh). Vanillin/sulphuric acid stain or Ninhydrin stain was used for staining TLC plates.

General analytical information

All compounds were characterized by ^{1}H-NMR, ^{13}C-NMR, IR spectroscopy, as well as, in most instances, elemental analysis and ^{19}F-NMR spectroscopy where applicable. Copies of the ^{1}H-, ^{13}C- and ^{19}F-NMR spectra can be found at the end of the Supporting Information. NMR spectra were recorded on Varian 300 or 500 MHz instruments. All ^{1}H-/^{13}C-NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for residual deuterated solvents (CD_3OD, DMSO-d_6, CD_2Cl_2 or THF-d_8). All ^{31}P-NMR spectra are reported in ppm relative to 85% aq. phosphoric acid (0.00 ppm). The following abbreviations are used singularly or in combination to indicate the multiplicity of signals: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). NMR spectra were acquired at 298 K. All IR spectra were taken on a Thermo-Fischer Nicolet iS5 FT-ATR spectrometer. Selected absorption maxima ($\tilde{\nu}$) are reported in wavenumbers (cm^{-1}). Melting points were obtained on a Stanford Research Systems EZ-Melt melting point apparatus.

Elemental analyses were performed by Atlantic Microlabs Inc., Norcross, GA. The yields reported in tables 2–5 refer to isolated yields and represent an average of at least two independent runs. The pure compounds are estimated to be ≥ 95% pure as determined by ^{1}H-NMR, ^{19}F-NMR, ^{31}P-NMR spectroscopy (where applicable) and HPLC analysis. All GC analyses were performed on an Agilent 6890A gas chromatograph with an FID detector using a J & W DB-1 column. HPLC analyses were performed on an Agilent 1100 Series instrument using an Agilent Eclipse XDB-C18 column (5 μm, 4.6 x 150 mm).

Experimental details

General Procedure 1 (indazoles, benzimidazoles – tables 2 & 3):

An oven-dried test tube was charged with the aryl halide (1.00 mmol, 1.00 eq.),[3] boronic acid (2.00 mmol, 2.00 eq.), precatalyst **P2** (0.02-0.035 mmol, 0.02-0.035 eq.), and K_3PO_4 (2.00 mmol, 2.00 eq.). The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). Dioxane (4 mL) and H_2O (0.8 mL) were then added via syringe, and the test tube was placed in a preheated oil bath and stirred at 100 °C for 15-20 h. The reaction mixture was then cooled to room temperature and was subsequently filtered through a short plug of Celite, the filter cake washed with EtOAc (25 mL), and the solvent removed in vacuo. The crude product was purified by column chromatography (SiO_2, Hexane/EtOAc 15:1→1:1).

General procedure 2 (pyrazoles – table 4):

An oven-dried test tube was charged with the aryl halide (1.00 mmol, 1.00 eq.), boronic acid (2.00 mmol, 2.00 eq.), precatalyst **P1** (0.06-0.07 mmol, 0.06-0.07 eq.), XPhos (0.06-0.10 mmol, 0.06-0.10 eq.) and K_3PO_4 (2.00 mmol, 2.00 eq.). The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). Degassed dioxane (4 mL) and thoroughly degassed H_2O (0.8 mL) were then added via syringe, and the test tube placed in a preheated oil bath and stirred at 100 °C for 24-26 h. The reaction mixture was then cooled to room temperature and was subsequently filtered through a short plug of silica gel, the filter cake was washed with Et_2O (50 mL) and the solvent removed by rotary evaporation and high vacuum.[4,5] The residue was taken up in Et_2O (70-80 mL) and HCl (4.0 mL, 2M in Et_2O) was added,[6] stirred for 5-10 min and filtered. The precipitate was washed with Et_2O (50 mL). Afterwards, it was dispersed in EtOAc (25 mL) and 1M aq. NaOH (15 mL), and the biphasic mixture was vigorously stirred for 5-10 min until complete dissolution of all solids. After separation of the phases the aqueous phase was extracted with EtOAc (2x25 mL), the combined organic phases dried over $MgSO_4$ and the solvent removed in vacuo to give the desired product.

General Procedure 3 (indoles, azaindoles, oxindoles – table 5):

An oven-dried test tube was charged with the aryl halide (1.00 mmol, 1.00 eq.), boronic acid (1.50 mmol, 1.50 eq.), precatalyst **P1** (0.01-0.015 mmol, 0.01-0.015 eq.), and K_3PO_4 (2.00

mmol, 2.00 eq.). The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). Dioxane (4 mL) and H_2O (0.8 mL) were then added via syringe, and the test tube placed in a preheated oil bath and stirred at 60 °C for 5-8 h. The reaction mixture was then cooled to room temperature and was subsequently filtered through a short plug of Celite, the filter cake washed with EtOAc (25 mL), and the solvent removed in vacuo. The product was purified by column chromatography (SiO_2, Hexane/EtOAc 15:1→1:1).

Compounds **3c**, **4c**, **5d** and **5f** were reacted according to the General Procedures 1-3 but with different work up or purification procedures. See pages S18, S20, S23, S24 for details.

General procedure 4 for the Suzuki-Miyaura cross-coupling in the presence of heterocyclic additives (Figures 3, 5):

For every data point in Figure 3 or 5, a separate reaction was set up, differing only in the amount of heterocyclic additive (**10**-**13**) used (1.00, 0.50, 0.25, 0.10, 0.06, 0.04, 0.02, 0.01 equiv.):

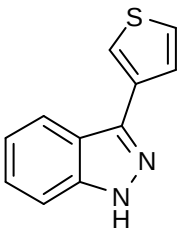
An oven-dried test tube was charged with 6-chloroindole (37.9 mg, 0.250 mmol, 1.00 equiv.), phenylboronic acid (61.0 mg, 0.500 mmol, 2.00 equiv.), precatalyst **P1** (3.9 mg, 0.005 mmol, 0.02 equiv.), and K_3PO_4 (106.0 mg, 0.500 mmol, 2.00 equiv.). If the corresponding heterocyclic additive was a solid, it was added at this time. The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). Liquid heterocyclic additives (if applicable), dioxane (1 mL) and H_2O (0.2 mL) were then added via syringe, and the test tube was placed in a preheated oil bath and stirred at 60 °C for 120 min. The reaction mixture was cooled to room temperature, a sat. aq. solution of NH_4Cl (2 mL), EtOAc (1 mL) and dodecane (250 μL, 0.250 mmol, 1.00 equiv., 1M in EtOAc) were added. GC samples could then be directly prepared by taking an aliquot from the organic layer, filtering it through a short silica plug and flushing it with EtOAc.

For investigating the effect of added boronic acid (**Figure S1**), General Procedure 4 was followed with indazole (**10a**) as additive but using 5.00 equivalents of phenylboronic acid (152.4 mg, 1.250 mmol) instead of 2.00 equivalents.

For investigating the effect of the temperature (**Figure S2**), General Procedure 4 was followed with indazole (**10a**) as additive but the reaction temperature was varied (40, 60, 80, 100 °C).

Preparation of compounds in table 2

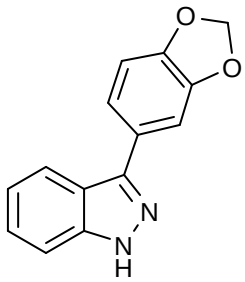
3-(thiophen-3-yl)-1*H*-indazole (**2a**): 3-Chloroindazole (153 mg, 1.00 mmol, 1.00 eq.), 3-thienyl boronic acid (256 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (14.4 mg, 0.02 mmol, 0.02 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was purified via column chromatography (SiO_2, Hexane/EtOAc 15:1→2:1) to provide the product as a light yellow solid (185 mg, 0.92 mmol) in 92% yield.



2a

Mp. = 119-120 °C. $\mathbf{R_f}$ = 0.24 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 3110 cm^{-1}, 2922, 1620, 1472, 1324, 1253, 1015, 857, 734, 668. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.05 (dt, *J* = 8.2, 1.0 Hz, 1H), 7.93 (dd, *J* = 2.9, 1.3 Hz, 1H), 7.70 (dd, *J* = 5.1, 1.3 Hz, 1H), 7.51–7.57 (m, 2H), 7.41 (ddd, *J* = 8.2, 6.9, 1.0 Hz, 1H), 7.22 (ddd, *J* = 8.2, 6.9, 1.0 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 142.0, 140.6, 135.5, 127.3, 127.2, 126.9, 122.3, 121.6, 121.3, 120.7, 111.6. Anal. Calcd. for $C_{11}H_8N_2S$: C, 65.97; H, 4.03. Found: C, 65.77; H, 4.20.

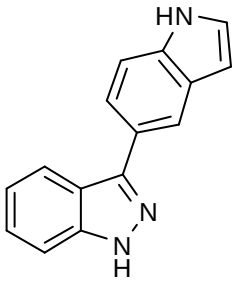
3-(benzo[*d*][1,3]dioxol-5-yl)-1*H*-indazole (**2b**): 3-Chloroindazole (152.6 mg, 1.00 mmol, 1.00 eq.), benzo[*d*][1,3]dioxol-5-ylboronic acid (331.9 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (18.0 mg, 0.025 mmol, 0.025 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 15:1→2:1) to provide the product as a colorless, crystalline solid (220 mg, 0.92 mmol) in 92% yield.



2b

Mp. = 171 °C. $\mathbf{R_f}$ = 0.20 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 3283 cm^{-1}, 1459, 1254, 1232, 1039, 806, 747, 689. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 7.95 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.53 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.34–7.46 (m, 3H), 7.19 (ddd, *J* = 8.4, 6.8, 1.0 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 6.01 (s, 2H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 148.5, 147.6, 143.7, 142.3, 128.6, 126.8, 121.6, 121.3, 121.2, 120.5, 111.2, 109.4, 107.7, 101.8. Anal. Calcd. for $C_{14}H_{10}N_2O_2$: C, 70.58; H, 4.08. Found: C, 70.36; H, 4.08.

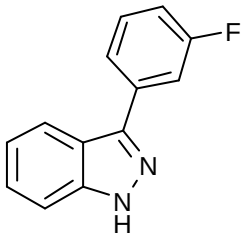
3-(1*H*-indol-5-yl)-1*H*-indazole (**2c**): 3-Chloroindazole (153 mg, 1.00 mmol, 1.00 eq.), indol-5-ylboronic acid (322 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (21.6 mg, 0.03 mmol, 0.03 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 10:1→1:1) to provide the product as a light yellow solid (197 mg, 0.84 mmol) in 84%.



2c

Mp. = 223-224 °C. $\mathbf{R_f}$ = 0.10 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 3407 cm^{-1}, 3237, 1456, 1340, 1314, 885, 754, 728, 689, 578. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.10 (d, *J* = 1.0 Hz, 1H), 8.04 (dt, *J* = 8.3, 1.0 Hz, 1H), 7.68 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.52 (dt, *J* = 8.4, 0.8 Hz, 2H), 7.40 (ddd , *J* = 8.4, 6.8, 1.0 Hz, 1H), 7.29 (d, *J* = 3.2 Hz, 1H), 7.19 (ddd , *J* = 8.4, 6.8, 1.0 Hz, 1H), 6.55 (dd, *J* = 3.2, 0.9 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d6): δ [ppm] = 145.5, 142.3, 136.3, 128.7, 126.6, 126.5, 125.5, 121.6, 121.4, 121.2, 120.9, 119.3, 112.5, 111.1, 102.4. Anal. Calcd. for $C_{14}H_{10}N_2O_2$: C, 70.58; H, 4.08. Found: C, 70.36; H, 4.08.

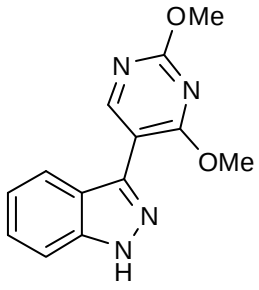
3-(3-fluorophenyl)-1*H*-indazole (**2d**): 3-Chloroindazole (153 mg, 1.00 mmol, 1.00 eq.), 3-fluorophenylboronic acid (280 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (18.0 mg, 0.025 mmol, 0.025 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 20:1→1:1) to provide the product as a light yellow solid (197 mg, 0.93 mmol) in 93% yield.



2d

Mp. = 106-107 °C. $\mathbf{R_f}$ = 0.46 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 2305 cm^{-1}, 1612, 1449, 1338, 1265, 855, 739, 694. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.01 (dt, *J* = 8.3, 1.0 Hz, 1H), 7.78 (ddd, *J* = 7.8, 1.5, 1.0 Hz, 1H), 7.66 (ddd, *J* = 10.3, 2.6, 1.5 Hz, 1H), 7.57 (dt, *J* = 8.5, 0.9 Hz, 1H), 7.47–7.54 (m, 1H), 7.42 (ddd, *J* = 8.5, 6.8, 1.0 Hz, 1H), 7.23 (ddd, *J* = 8.2, 6.8, 1.0 Hz, 1H), 7.13 (ddd, *J* = 8.3, 2.6, 1.0 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 163.3 (d, *J* = 243.2 Hz), 142.6, 142.1, 136.8 (d, *J* = 8 Hz), 131.6 (d, *J* = 9 Hz), 126.96, 123.4 (d, *J* = 3 Hz), 122.1, 121.2, 120.6, 115.1 (d, *J* = 21 Hz), 113.7 (d, *J* = 22 Hz), 111.4. **^{19}F-NMR** (273 MHz, DMSO-d_6): δ [ppm] = -112.97 (td, *J* = 10.6, 6.5 Hz). Anal. Calcd. for $C_{13}H_9FN_2$: C, 73.57; H, 4.27. Found: C, 73.53; H, 4.43.

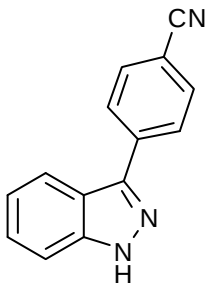
3-(2,4-dimethoxypyrimidin-5-yl)-1*H*-indazole (**2e**): 3-Chloroindazole (153 mg, 1.00 mmol, 1.00 eq.), 2,4-dimethoxypyrimidin-5-ylboronic acid (368 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (18.0 mg, 0.025 mmol, 0.025 eq.) for 20 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 15:1→1:2) to provide the product as a white, puffy solid (226 mg, 0.88 mmol) in 88% yield.



2e

Mp. = 190 °C. $\mathbf{R_f}$ = 0.08 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 3199 cm^{-1}, 1610, 1558, 1501, 1386, 1285, 1073, 1009, 939, 713. **^{1}H-NMR** (300 MHz, DMSO-d_6): δ [ppm] = 13.27 (s, 1H), 8.52 (s, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.54 (d, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 7.2 Hz, 1H), 7.11 (t, *J* = 6.9 Hz, 1H), 3.95 (s, 6H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 168.7, 165.3, 159.1, 141.7, 138.2, 126.8, 122.2, 122.0, 121.1, 111.0, 109.6, 55.38, 54.55. Anal. Calcd. for $C_{13}H_{12}N_4O_2$: C, 60.93; H, 4.72. Found: C, 60.86; H, 4.77.

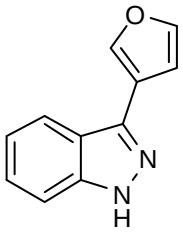
4-(1*H*-indazol-3-yl)benzonitrile (**2f**): 3-Chloroindazole (153 mg, 1.00 mmol, 1.00 eq.), 4-cyanophenylboronic acid (294 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (18.0 mg, 0.025 mmol, 0.025 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 15:1→1:1) to provide the product as a white crystalline solid (199 mg, 0.91 mmol) in 91% yield.



2f

Mp. = 162-164 °C. $\mathbf{R_f}$ = 0.23 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 3294 cm^{-1}, 2227, 1608, 1339, 1104, 987, 847, 726, 699. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.17 (d, *J* = 8.6 Hz, 2H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 8.6 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.45 (ddd, *J* = 8.3, 6.8, 0.7 Hz, 1H), 7.27 (ddd, *J* = 8.3, 6.8, 0.7 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 142.4, 142.0, 139.0, 133.5, 127.8, 127.1, 122.5, 121.1, 120.7, 119.7, 111.6, 110.5. Anal. Calcd. for $C_{14}H_9N_3$: C, 76.70; H, 4.14. Found: C, 76.61; H, 4.26.

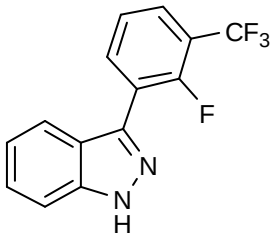
3-(furan-3-yl)-1*H*-indazole (**2g**): 3-Chloroindazole (153 mg, 1.00 mmol, 1.00 eq.), furan-3-ylboronic acid (224 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (18.0 mg, 0.025 mmol, 0.025 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 10:1→3:1) to provide the product as a white solid (176 mg, 0.96 mmol) in 96% yield.



2g

Mp. = 117-120 °C. $\mathbf{R_f}$ = 0.17 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 2286 cm^{-1}, 1330, 1157, 870, 782, 747, 677, 590. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.19 (dd, *J* = 1.5, 0.9 Hz, 1H), 7.93 (dt, *J* = 8.2, 1.0 Hz, 1H), 7.65 (dd, *J* = 1.9, 1.5 Hz, 1H), 7.52 (dt, *J* = 8.4, 0.9 Hz, 1H), 7.41 (ddd, *J* = 8.5, 6.8, 1.0 Hz, 1H), 7.20 (ddd, *J* = 8.2, 6.8, 1.0 Hz, 1H), 7.01 (dd, *J* = 1.9, 0.9 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 144.5, 141.6, 140.6, 137.6, 127.0, 121.3, 121.2, 120.7, 120.1, 111.0, 109.7. Anal. Calcd. for $C_{11}H_8N_2O$: C, 71.73; H, 4.38. Found: C, 71.45; H, 4.38.

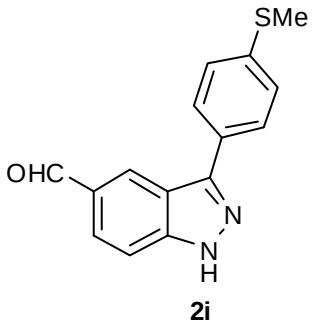
3-(2-fluoro-3-(trifluoromethyl)phenyl)-1*H*-indazole (**2h**): 3-Chloroindazole (153 mg, 1.00 mmol, 1.00 eq.), 2-fluoro-3-(trifluoromethyl)phenylboronic acid (416 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (25.2 mg, 0.035 mmol, 0.035 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 15:1→3:1) to provide the product as a light yellow oil (249 mg, 0.89 mmol, 89%) that slowly solidified over the course of days.



2h

Mp. = 106-107 °C. $\mathbf{R_f}$ = 0.20 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 3286 cm^{-1}, 2450, 1496, 1319, 1165, 1108, 772, 737, 701. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.00–8.09 (m, 1H), 7.70–7.82 (m, 2H), 7.59 (dt, *J* = 8.5, 0.8 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.44 (ddd, *J* = 8.5, 6.9, 1.0 Hz, 1H), 7.22 (dddd, *J* = 8.2, 6.9, 1.0, 0.3 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 156.8 (d, *J* = 257 Hz), 141.6, 138.3, 136.3 (d, *J* = 4 Hz), 127.5 (q, *J* = 4 Hz), 127.1, 125.9 (d, *J* = 4 Hz), 123.5 (d, *J* = 14 Hz), 123.5 (q, *J* = 272 Hz), 122.0, 121.6, 121.1 (d, *J* = 7 Hz), 118.3 (dq, *J* = 32, 12 Hz), 111.3. **^{19}F-NMR** (273 MHz, CD_3OD): δ [ppm] = -63.19, -118.69. Anal. Calcd. for $C_{14}H_8F_4N_2$: C, 60.01; H, 2.88. Found: C, 60.01; H, 2.84.

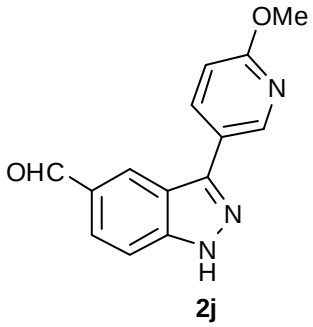
3-(4-(methylthio)phenyl)-1*H*-indazole-5-carbaldehyde (**2i**): 3-Chloro-1*H*-indazole-5-carbaldehyde (181 mg, 1.00 mmol, 1.00 eq.), 4-(methylthio)phenylboronic acid (336 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (18.0 mg, 0.025 mmol, 0.025 eq.) for 16 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 5:1→1:1) to provide the product as an off-white solid (247 mg, 0.92 mmol) in 92% yield.



2i

Mp. = 179-180 °C. $\mathbf{R_f}$ = 0.15 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 3178 cm^{-1}, 1658, 1604, 1469, 1210, 828, 780, 689. **^{1}H-NMR** (300 MHz, CD_3OD): δ = 10.04 (s, 1H), 8.62 (dd, *J* = 1.4, 0.8 Hz, 1H), 7.89 – 8.04 (m, 3H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.44 (d, *J* = 8.7 Hz, 2H), 2.55 (s, 3H). **^{13}C-NMR** (125 MHz, DMSO-d6): δ [ppm] = 193.1, 145.8, 144.6, 139.3, 131.2, 130.0, 128.8, 128.1, 126.9, 125.0, 120.5, 112.2, 15.22. Anal. Calcd. for $C_{15}H_{12}N_2OS$: C, 67.14; H, 4.51. Found: C, 67.35; H, 4.44.

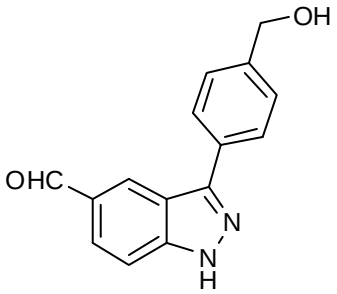
3-(6-methoxypyridin-3-yl)-1*H*-indazole-5-carbaldehyde (**2j**): 3-Chloro-1*H*-indazole-5-carbaldehyde (181 mg, 1.00 mmol, 1.00 eq.), 6-methoxypyridin-3-ylboronic acid (306 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (21.6 mg, 0.03 mmol, 0.03 eq.) for 16 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 3:1→1:1) to provide the product as a white solid (238 mg, 0.94 mmol) in 94% yield.



2j

Mp. = 212-213 °C. $\mathbf{R_f}$ = 0.11 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 1679 cm^{-1}, 1606, 1318, 1283, 1255, 1014, 822, 781. **^{1}H-NMR** (300 MHz, DMSO-d_6): δ [ppm] = 13.69 (s, 1H), 10.05 (s, 1H), 8.84 (d, *J* = 2.3 Hz, 1H), 8.72 (s, 1H), 8.30 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.85 (d, *J* = 8.7 Hz, 1H), 7.68 (d, *J* = 8.7 Hz, 1H), 6.98 (d, *J* = 8.6 Hz, 1H), 3.92 (s, 3H). **^{13}C-NMR** (125 MHz, DMSO-d6): δ [ppm] = 193.1, 164.1, 145.6, 144.4, 143.7, 138.3, 131.3, 129.2, 124.8, 123.2, 120.4, 112.2, 111.7, 54.1. Anal. Calcd. for $C_{14}H_{11}N_3O_2$: C, 66.40; H, 4.38. Found: C, 66.36; H, 4.42.

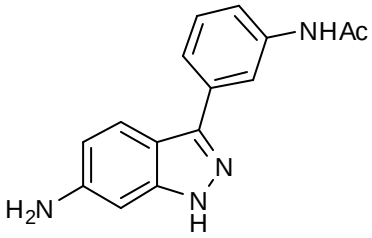
3-(4-(hydroxymethyl)phenyl)-1*H*-indazole-5-carbaldehyde (**2k**): 3-Chloro-1*H*-indazole-5-carbaldehyde (181 mg, 1.00 mmol, 1.00 eq.), 4-(hydroxymethyl)phenylboronic acid (304 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (25.2 mg, 0.035 mmol, 0.035 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 3:1→1:2) to provide the product as an off-white solid (218 mg, 0.87 mmol) in 87% yield.



2k

Mp. = 170 °C. $\mathbf{R_f}$ = 0.21 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 3175 cm^{-1}, 1655, 1607, 1209, 989, 801, 779, 705. **^{1}H-NMR** (300 MHz, $CDCl_3$): δ [ppm] = 10.04 (d, *J* = 0.6 Hz, 1H), 8.62 (dd, *J* = 1.4, 0.8 Hz, 1H), 7.92 – 8.08 (m, 3H), 7.63 – 7.77 (m, 1H), 7.55 (dd, *J* = 8.0, 0.6 Hz, 2H), 4.70 (s, 2H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 193.1, 146.3, 144.6, 143.5, 131.9, 131.3, 128.9, 127.7, 127.5, 125.0, 120.6, 112.2, 63.38.

***N*-(3-(6-amino-1*H*-indazol-3-yl)phenyl)acetamide** (**2l**): 3-chloro-1*H*-indazol-6-amine (168 mg, 1.00 mmol, 1.00 eq.), 3-acetamidophenylboronic acid (358 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (14.4 mg, 0.02 mmol, 0.02 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 3:1→pure EtOAc) to provide the product as an off-white, foamy resin (241 mg, 0.90 mmol) in 90% yield.

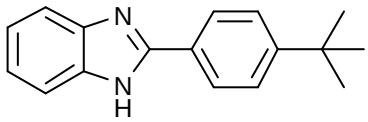


2l

Mp. = 117 °C. $\mathbf{R_f}$ = 0.05 (hexane/EtOAc 1:1). **IR**: $\tilde{\nu}$ = 2366 cm^{-1}, 1660, 1627, 1452, 1427, 1401, 965, 792, 698. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.15 (t, *J* = 1.7 Hz, 1H), 7.76 (d, *J* = 9.3 Hz, 1H), 7.61 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.56 (ddd, *J* = 8.1, 2.1, 1.1 Hz, 1H), 7.41 (t, *J* = 7.9 Hz, 1H), 6.68 – 6.74 (m, 2H), 2.15 (d, *J* = 5.2 Hz, 3H). **^{13}C-NMR** (125 MHz, DMSO-d6): δ [ppm] = 169.0, 148.3, 144.4, 143.3, 140.2, 135.4, 129.7, 121.7, 121.5, 118.3, 117.6, 113.6, 113.4, 91.26, 24.75.

Preparation of compounds in table 3

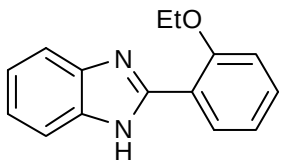
2-(4-*tert*-butylphenyl)-1*H*-benzo[*d*]imidazole (**3a**): 2-Chlorobenzimidazole (153 mg, 1.00 mmol, 1.00 eq.), 4-*tert*-butylphenylboronic acid (356 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (18.0 mg, 0.025 mmol, 0.025 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 10:1→1:1) to provide the product as a white, flaky solid (246 mg, 0.98 mmol) in 98% yield.



3a

Mp. = 249-250 °C. $\mathbf{R_f}$ = 0.29 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 2965 cm^{-1}, 1428, 1276, 741. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.02 (d, *J* = 8.8 Hz, 2H), 7.59 (d, *J* = 8.8 Hz, 4H), 7.24 (dd, *J* = 6.1, 3.2 Hz, 2H), 1.38 (s, 9H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 153.2, 152.0, 128.2, 126.9, 126.4, 35.27, 31.66. Anal. Calcd. for $C_{17}H_{18}N_2$: C, 81.56; H, 7.25. Found: C, 81.26; H, 7.27.

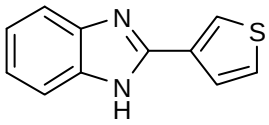
2-(2-ethoxyphenyl)-1*H*-benzo[*d*]imidazole (**3b**): 2-Chlorobenzimidazole (152.6 mg, 1.00 mmol, 1.00 eq.), 2-ethoxyphenylboronic acid (332.0 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (18.0 mg, 0.025 mmol, 0.025 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 10:1→1:1) to provide the product as a white, crystalline solid (225 mg, 0.94 mmol) in 94% yield.



3b

Mp. = 138-143 °C. $\mathbf{R_f}$ = 0.24 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 1441 cm^{-1}, 1276, 1231, 740. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.16 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.63 (dd, *J* = 5.7, 3.1 Hz, 2H), 7.46 (ddd, *J* = 8.7, 7.3, 1.5 Hz, 1H), 7.25 (dd, *J* = 6.1, 0.3 Hz, 1H), 7.24 (dd, *J* = 6.1, 0.3 Hz, 1H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.10 (ddd, *J* = 7.3, 1.0, 0.3 Hz, 1H), 4.33 (q, *J* = 7.0 Hz, 2H), 1.51 (t, *J* = 7.0 Hz, 3H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 156.5, 149.8, 143.5, 135.2, 131.9, 130.9, 122.7, 122.2, 121. 5, 119.3, 119.2, 113.7, 112.6, 64.6, 15.0. Anal. Calcd. for $C_{15}H_{14}N_2O$: C, 75.61; H, 5.92. Found: C, 75.21; H, 6.01.

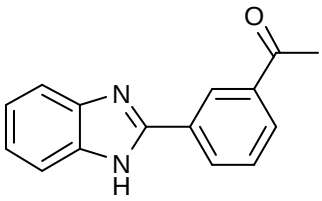
2-(thiophen-3-yl)-1*H*-benzo[*d*]imidazole (**3c**): 2-Chlorobenzimidazole (153 mg, 1.00 mmol, 1.00 eq.), 3-thienylboronic acid (256 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (18.0 mg, 0.025 mmol, 0.025 eq.) for 15 h at 100 °C according to General Procedure 1 with a modified work-up procedure. After cooling to room temperature MeOH (10 mL) was added, and the reaction mixture was filtered through a plug of Celite and $MgSO_4$, washing with EtOAc (25 mL). Afterwards, all volatiles were removed in vacuo. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 10:1→1:2) to provide the product as an off-white crystalline solid (185 mg, 0.92 mmol) in 92% yield.



3c

Mp. = 347 °C (decomposition). $\mathbf{R_f}$ = 0.17 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 1427 cm^{-1}, 1342, 987, 739. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.12 (dd, *J* = 2.9, 1.3 Hz, 1H), 7.76 (dd, *J* = 5.1, 1.3 Hz, 1H), 7.60 (dd, *J* = 5.1, 2.9 Hz, 1H), 7.52–7.60 (m, 2H), 7.20–7.29 (m, 2H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 148.7, 133.2, 128.3, 127.0, 125.7, 122.7. Anal. Calcd. for $C_{11}H_8N_2S$: C, 65.97; H, 4.03. Found: C, 65.76; H, 4.26.

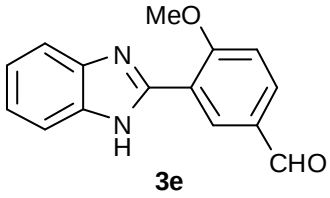
1-(3-(1*H*-benzo[*d*]imidazol-2-yl)phenyl)ethanone (**3d**): 2-Chlorobenzimidazole (153 mg, 1.00 mmol, 1.00 eq.), 3-acetylphenylboronic acid (328 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (21.6 mg, 0.03 mmol, 0.03 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 10:1→1:2) to provide the product as a white solid (212 mg, 0.90 mmol) in 90% yield.



3d

Mp. = 196 °C. $\mathbf{R_f}$ = 0.09 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 1682 cm^{-1}, 1355, 1250, 740, 684. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.73 (d, *J* = 1.8 Hz, 1H), 8.31 (dd, *J* = 7.8, 1.1 Hz, 1H), 8.11 (d, *J* = 7.8 Hz, 1H), 7.67 (dd, *J* = 8.1, 7.5 Hz, 2H), 7.55–7.68 (m, 2H), 7.23–7.33 (m, 2H), 2.69 (s, 3H). **^{13}C-NMR** (125 MHz, DMSO-d6): δ [ppm] = 198.3, 151.1, 144.4, 138.1, 135.7, 131.5, 131.3, 130.1, 126.6, 123.5, 122.6, 119.7, 112.2, 27.58. Anal. Calcd. for $C_{15}H_{12}N_2O$: C, 76.25; H, 5.12. Found: C, 75.96; H, 5.39.

3-(1*H*-benzo[*d*]imidazol-2-yl)-4-methoxybenzaldehyde (**3e**): 2-Chlorobenzimidazole (153 mg, 1.00 mmol, 1.00 eq.), 5-formyl-2-methoxyphenylboronic acid (360 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (25.2 mg, 0.035 mmol, 0.035 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 10:1→1:4) to provide the product as a white solid (239 mg, 0.95 mmol) in 95% yield.

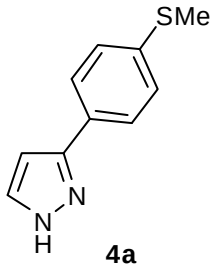


3e

Mp. = 195 °C. $\mathbf{R_f}$ = 0.22 (hexane/EtOAc 1:1). **IR**: $\tilde{\nu}$ = 2517 cm^{-1}, 1678, 1593, 1267, 1250, 1023, 804, 760. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 9.96 (s, 1H), 8.76 (d, *J* = 2.2 Hz, 1H), 8.03 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.58–7.70 (m, 2H), 7.39 (d, *J* = 8.7 Hz, 1H), 7.22–7.33 (m, 2H), 4.15 (s, 3H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 192.2, 161.7, 148.3, 143.3, 135.3, 133.0, 132.6, 130.4, 123.2, 122.5, 119.4, 119.3, 113.5, 112.7, 57.3. Anal. Calcd. for $C_{15}H_{12}N_2O$: C, 71.42; H, 4.79. Found: C, 71.54; H, 4.90.

Preparation of compounds in table 4

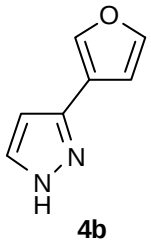
3-(4-(Methylthio)phenyl)-1*H*-pyrazole (4a): 3-Bromopyrazole (147 mg, 1.00 mmol, 1.00 eq.), 4-(methylthio)phenylboronic acid (336 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (47.2 mg, 0.06 mmol, 0.06 eq.) and XPhos (28.6 mg, 0.06 mmol, 0.06 eq.) for 24 h at 100 °C according to General Procedure 2. The crude product was purified by precipitation of the pyrazole hydrochloride from Et_2O and its subsequent liberation with 1M aq. NaOH to give the desired product as a light orange solid (160 mg, 0.84 mmol) in 84% yield.



4a

Mp. = 105-107 °C. **IR** (neat): $\tilde{\nu}$ = 2915 cm^{-1}, 1447, 1083, 1048, 956, 827, 764. **^{1}H-NMR** (300 MHz, $CDCl_3$): δ [ppm] = 7.68 (d, *J* = 8.7 Hz, 2H), 7.61 (d, *J* = 2.3 Hz, 1H), 7.29 (d, *J* = 8.7 Hz, 2H), 6.59 (d, *J* = 2.3 Hz, 1H), 2.51 (d, *J* = 1.0 Hz, 3H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 138.1, 135.8, 131.0, 127.3, 126.8, 102.8, 100.5, 15.9. Anal. Calcd. for $C_{10}H_{10}N_2S$: C, 63.13; H, 5.30. Found: C, 62.93; H, 5.17.

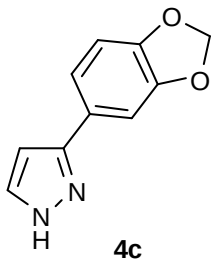
3-(furan-3-yl)-1*H*-pyrazole (4b): 3-Bromopyrazole (147 mg, 1.00 mmol, 1.00 eq.), 3-furanylboronic acid (224 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (51.1 mg, 0.065 mmol, 0.065 eq.) and XPhos (31.0 mg, 0.065 mmol, 0.065 eq.) for 24 h at 100 °C according to General Procedure 2. The crude product was purified by precipitation of the pyrazole hydrochloride from Et_2O and its subsequent liberation with 1M aq. NaOH to give the desired product as a light yellow solid (116 mg, 0.86 mmol) in 86% yield.



4b

Mp. = 101-103 °C. **IR** (neat): $\tilde{\nu}$ = 3138 cm^{-1}, 1520, 1348, 1192, 1154, 1047, 873, 757, 593. **^{1}H-NMR** (300 MHz, $CDCl_3$): δ [ppm] = 7.78 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.59 (d, *J* = 2.3 Hz, 1H), 7.47 (td, *J* = 1.8, 0.8 Hz, 1H), 6.73 (dd, *J* = 1.7, 0.8 Hz, 1H), 6.43 (d, *J* = 2.3 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 144.9, 140.2, 130.5, 126.0, 110.0, 103.3.

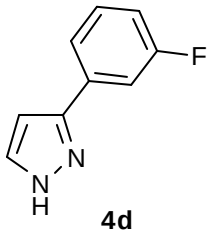
3-(3,4-(methylendioxy)phenyl)-1*H*-pyrazole (4c): 3-Bromopyrazole (147 mg, 1.00 mmol, 1.00 eq.), 3,4-(methylenedioxy)phenylboronic acid (332 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (47.2 mg, 0.06 mmol, 0.06 eq.) and XPhos (28.6 mg, 0.06 mmol, 0.06 eq.) for 24 h at 100 °C according to General Procedure 2. The crude product was first purified by precipitation of the pyrazole hydrochloride from Et_2O and its subsequent liberation with 1M aq. NaOH to give the product. It was redissolved in Et_2O (50 mL) and filtered through a cotton plug. HCl (1.5 mL, 2M in Et_2O) was added, the mixture stirred for 10 min and filtered. The precipitate was washed with Et_2O (50 mL). Afterwards, it was suspended in Et_2O (25 mL) and 1M aq. NaOH (15 mL) and the biphasic mixture was vigorously stirred until complete dissolution (15-20 min). After separation of the phases the aqueous phase was extracted with Et_2O (2x25 mL), the combined organic phases dried over $MgSO_4$ and the solvent removed in vacuo to give the desired product as an off-white solid (157 mg, 0.83 mmol) in 83% yield.



4c

Mp. = 119-128 °C. **IR** (neat): $\tilde{\nu}$ = 2871 cm^{-1}, 1458, 1226, 1040, 935, 812, 753. **^{1}H-NMR** (300 MHz, $CDCl_3$): δ [ppm] = 7.59 (d, *J* = 2.3 Hz, 1H), 7.25 (s, 1H), 7.23 (dd, *J* = 7.2, 1.6 Hz, 1H), 6.80–6.89 (m, 1H), 6.51 (d, *J* = 2.3 Hz, 1H), 5.99 (s, 2H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 151.0, 148.8, 147.7, 141.1, 130.9, 119.9, 109.6, 106.8, 102.6, 102.1.

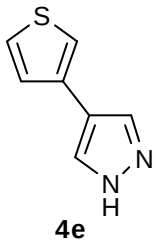
3-(3-fluorophenyl)-1*H*-pyrazole (4d): 3-Bromopyrazole (147 mg, 1.00 mmol, 1.00 eq.), 3-fluorophenylboronic acid (280 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (55.0 mg, 0.07 mmol, 0.07 eq.) and XPhos (47.7 mg, 0.10 mmol, 0.10 eq.) for 26 h at 100 °C according to General Procedure 2. The crude product was purified by precipitation of the pyrazole hydrochloride from Et_2O and its subsequent liberation with 1M aq. NaOH to give the desired product as a white solid (100 mg, 0.61 mmol) in 61% yield.[7]



4d

Mp. = 70-72 °C. **IR** (neat): $\tilde{\nu}$ = 3151 cm^{-1}, 2907, 1584, 1473, 1161, 1054, 850, 770, 676. **^{1}H-NMR** (300 MHz, $CDCl_3$): δ [ppm] = 7.63 (d, *J* = 2.3 Hz, 1H), 7.56 (d, *J* = 7,7. 1.3, 0.8 Hz, 1H), 7.49 (ddd, *J* = 10.1, 2.6, 1.6 Hz, 1H), 7.37 (td, *J* = 8.0, 6.0 Hz, 1H), 7.02 (tdd, *J* = 8.6, 2.6, 1.0 Hz, 1H), 6.63 (d, *J* = 2.3 Hz, 1H). **^{19}F-NMR** (273 MHz, $CDCl_3$): δ [ppm] = -113.40 (dd, *J* = 15.1, 9.2 Hz). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 163.8 (d, *J* = 242 Hz), 131.8 (d, *J* = 6 Hz), 131.2, 122.3 (d, *J* = 3 Hz), 115.0 (d, *J* = 13 Hz), 112.8 (d, *J* = 23 Hz), 103.5. Anal. Calcd. for $C_9H_7FN_2$: C, 66.66; H, 4.35. Found: C, 66.44; H, 4.72.

4-(thiophen-3-yl)-1*H*-pyrazole (4e): 4-Bromopyrazole (147 mg, 1.00 mmol, 1.00 eq.), 3-thienylboronic acid (256 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (47.2 mg, 0.06 mmol, 0.06 eq.) and XPhos (28.6 mg, 0.06 mmol, 0.06 eq.) for 24 h at 100 °C according to General Procedure 2. The crude product was purified by precipitation of the pyrazole hydrochloride from Et_2O and its subsequent liberation with 1M aq. NaOH to give the desired product as a white solid (107 mg, 0.71 mmol) in 71% yield.

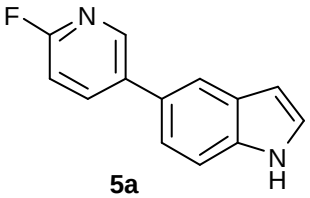


4e

Mp. = 214-216 °C. **IR** (neat): $\tilde{\nu}$ = 3109 cm^{-1}, 2883, 1143, 1086, 1036, 816, 773, 606. **^{1}H-NMR** (300 MHz, $CDCl_3$): δ [ppm] = 7.79 (s, 2H), 7.36 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.29 (dd, *J* = 3.0, 1.3 Hz, 1H), 7.23 (dd, *J* = 5.0, 1.3 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 137.7, 135.0, 127.5, 127.5, 126.6, 118.9, 118.1.

Preparation of compounds in table 5

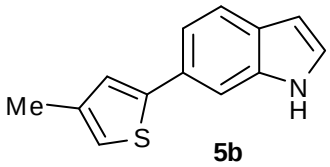
5-(6-fluoropyridin-3-yl)-1*H*-indole (**5a**): 5-Chloroindole (152 mg, 1.00 mmol, 1.00 eq.), 6-fluoropyridin-3-ylboronic acid (211 mg, 1.50 mmol, 1.50 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (7.9 mg, 0.01 mmol, 0.01 eq.) for 5 h at 60 °C according to General Procedure 3. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 10:1→2:1) to provide the product as a white solid (210 mg, 0.99 mmol) in 99% yield.



5a

Mp. = 155-156 °C. $\mathbf{R_f}$ = 0.38 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 3220 cm^{-1}, 1589, 1455, 1240, 877, 837, 811. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.42 (dd, *J* = 1.8, 0.9 Hz, 1H), 8.18 (ddd, *J* = 8.5, 7.7, 2.6 Hz, 1H), 7.79 (dd, *J* = 1.8, 0.7 Hz, 1H), 7.48 (dt, *J* = 8.5, 0.8 Hz, 1H), 7.35 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.29 (d, *J* = 3.2 Hz, 1H), 7.11 (ddd, *J* = 8.6, 2.6, 0.7 Hz, 1H), 6.52 (dd, *J* = 3.2, 0.9 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 163.1 (d, *J* = 235 Hz), 146.1 (d, *J* = 15 Hz), 141.2 (d, *J* = 8 Hz), 137.0 (d, *J* = 4 Hz), 136.9, 129.5, 128.0, 127.6, 121.4, 119.7, 113.3, 110.5 (d, *J* = 38 Hz), 102.8. **^{19}F-NMR** (273 MHz, DMSO-d_6): δ [ppm] = -76.46 (d, *J* = 7.3 Hz). Anal. Calcd. for $C_{13}H_9FN_2$: C, 73.57; H, 4.27. Found: C, 73.29; H, 4.46.

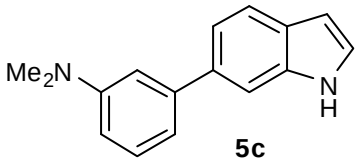
6-(4-methylthiophen-2-yl)-1*H*-indole (**5b**): 6-Chloroindole (152 mg, 1.00 mmol, 1.00 eq.), 4-methylthiophen-2-ylboronic acid (211 mg, 1.50 mmol, 1.50 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (7.9 mg, 0.01 mmol, 0.01 eq.) for 7.5 h at 60 °C according to General Procedure 3. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 25:1→3:1) to provide the product as off-white, flaky crystals (195 mg, 0.91 mmol) in 91% yield.



5b

Mp. = 130 °C. $\mathbf{R_f}$ = 0.44 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 3381 cm^{-1}, 1455, 1317, 859, 811, 718, 617, 588. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 7.59 (t, *J* = 0.8 Hz, 1H), 7.51 (dd, *J* = 8.3, 0.6 Hz, 1H), 7.28 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.23 (d, *J* = 3.1 Hz, 1H), 7.13 (d, *J* = 1.4 Hz, 1H), 6.83 (t, *J* = 1.2 Hz, 1H), 6.42 (dd, *J* = 3.1, 0.9 Hz, 1H), 2.26 (d, *J* = 1.1 Hz, 3H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 145.6, 138.9, 136.9, 128.0, 127.8, 127.1, 125.2, 121.2, 119.9, 117.9, 108.6, 102.0, 16.35. Anal. Calcd. for $C_{13}H_{11}NS$: C, 73.20; H, 5.20. Found: C, 73.17; H, 5.35.

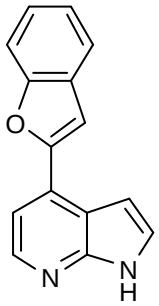
3-(1*H*-indol-6-yl)-*N*,*N*-dimethylaniline (**5c**): 6-Chloroindole (152 mg, 1.00 mmol, 1.00 eq.), 3-(dimethylamino)phenylboronic acid (248 mg, 1.50 mmol, 1.50 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (7.9 mg, 0.01 mmol, 0.01 eq.) for 5 h at 60 °C according to General Procedure 3. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 15:1→3:1) to provide the product as a light brown oil that slowly solidified over the course of days (233 mg, 0.99 mmol) in 99% yield.



5c

Mp. = 87-88 °C. $\mathbf{R_f}$ = 0.33 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 2513 cm^{-1}, 1595, 1445, 1308, 1225, 1126, 991, 818, 766, 721, 687. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 7.55–7.59 (m, 2H), 7.27 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.24 (ddd, *J* = 8.0, 7.6, 0.3 Hz, 1H), 7.23 (d, *J* = 3.1 Hz, 1H), 7.03 (dd, *J* = 2.5, 1.8 Hz, 1H), 6.99 (ddd, *J* = 7.6, 1.6, 1.0 Hz, 1H), 6.74 (ddd, *J* = 8.3, 2.6, 0.9 Hz, 1H), 6.43 (dd, *J* = 3.1, 0.9 Hz, 1H), 2.97 (s, 6H) **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 151.5, 143.2, 137.0, 135.2, 130.0, 127.7, 126.5, 120.9, 119.2, 115.8, 111.6, 110.1, 101.6, 40.97.

4-(benzofuran-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine (**5d**): 4-chloro-7-azaindole (153 mg, 1.00 mmol, 1.00 eq.), benzofuran-2-ylboronic acid (243 mg, 1.50 mmol, 1.50 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (11.8 mg, 0.015 mmol, 0.015 eq.) for 5.5 h at 60 °C according to a slightly modified General Procedure 3.



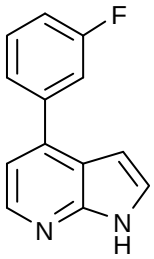
5d

The reaction was set up as usual. After 15 min of reaction time with very vigorous stirring, more dioxane (1.5 mL) was added to dissolve precipitated solids. Once the reaction was done it was cooled to room temperature and subsequently filtered through a plug of Celite, washing with EtOAc (25 mL) and DMF (15 mL). After removal of all volatiles in vacuo the residue was dried on high vacuum for at least one hour. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 3:1→pure EtOAc) to provide the product as a light yellow solid (223 mg, 0.95 mmol) in 95% yield.

Mp. = 268 °C (decomposition). $\mathbf{R_f}$ = 0.10 (hexane/EtOAc 1:1). **IR**: $\tilde{\nu}$ = 1603 cm^{-1}, 1338, 1184, 1111, 838, 798, 729, 598. **^{1}H-NMR** (300 MHz, DMSO-d_6): δ [ppm] = 11.92 (s, 1H), 8.31 (d, *J* = 5.1 Hz, 1H), 7.76 (s, 1H), 7.75 – 7.68 (m, 2H), 7.68 – 7.62 (m, 1H), 7.59 (d, *J* = 5.0 Hz, 1H), 7.43 – 7.34 (m, 1H), 7.34 – 7.26 (m, 1H), 7.04 (dd, *J* = 3.4, 1.8 Hz, 1H).

^{13}C-NMR (125 MHz, DMSO-d_6): δ [ppm] = 155.0, 154.4, 150.3, 143.4, 129.3, 128.8, 128.2, 126.1, 124.1, 122.3, 115.4, 112.1, 111.9, 107.0, 100.8. Anal. Calcd. for $C_{15}H_{10}N_2O$: C, 76.91; H, 4.30. Found: C, 76.44; H, 4.43.

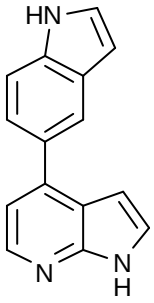
4-(3-fluorophenyl)-1*H*-pyrrolo[2,3-*b*]pyridine (**5e**): 4-chloro-7-azaindole (153 mg, 1.00 mmol, 1.00 eq.), 3-fluorophenylboronic acid (210 mg, 1.50 mmol, 1.50 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (11.8 mg, 0.015 mmol, 0.015 eq.) for 7.5 h at 60 °C according to General Procedure 3. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 5:1→1:2) to provide the product as a white solid (207 mg, 0.97 mmol) in 97% yield.



5e

Mp. = 177 °C. **R_f** = 0.10 (hexane/EtOAc 3:1). **IR**: $\tilde{\nu}$ = 1569 cm^{-1}, 1395, 1340, 1275, 1203, 876, 794, 733, 696. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.24 (d, *J* = 5.1 Hz, 1H), 7.44–7.62 (m, 4H), 7.14–7.24 (m, 2H), 6.65 (d, *J* = 3.6 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 162.8 (d, *J* = 235 Hz), 145.8 (d, *J* = 15 Hz), 140.9 (d, *J* = 8 Hz), 137.1, 136.4 (d, *J* = 4 Hz), 129.5, 128.3, 127.4, 121.4, 118.9, 110.5, 110.1 (d, *J* = 38 Hz), 101.7. **^{19}F-NMR** (273 MHz, CD_3OD): δ [ppm] = -115.17 (td, *J* = 9.3, 5.3 Hz). Anal. Calcd. for $C_{13}H_9NF_2$: C, 73.57; H, 4.27. Found: C, 73.45; H, 4.25.

4-(1*H*-indol-5-yl)-1*H*-pyrrolo[2,3-*b*]pyridine (**5f**): 4-chloro-7-azaindole (153 mg, 1.00 mmol, 1.00 eq.), indol-5-ylboronic acid (242 mg, 1.50 mmol, 1.50 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (11.8 mg, 0.015 mmol, 0.015 eq.) for 7.5 h at 60 °C according to General Procedure 3 with a modified work-up procedure: After cooling to room temperature MeOH (10 mL) was added, and the reaction was filtered through a plug of Celite and $MgSO_4$, washing with EtOAc (25 mL). Afterwards, all volatiles were removed in vacuo. The crude product was purified via column chromatography (SiO_2, Hexane/EtOAc 3:1→1:4) to provide the product as a light brown solid (208 mg, 0.98 mmol) in 98% yield.

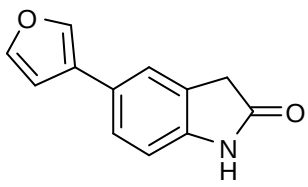


5f

Mp. = 217-219 °C. **R_f** = 0.13 (hexane/EtOAc 1:1). **IR**: $\tilde{\nu}$ = 1580 cm^{-1}, 1347, 1313, 801, 733, 715. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 8.19 (d, *J* = 5.1 Hz, 1H), 7.95–8.00 (m, 1H), 7.53 (d, *J* = 1.3 Hz, 2H), 7.40 (d, *J* = 3.4 Hz, 1H), 7.30 (d, *J* = 3.4 Hz, 1H), 7.23 (d, *J* = 5.1 Hz, 1H), 6.74 (d, *J* = 3.6 Hz, 1H), 6.55 (d, *J* = 3.2 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d_6):

δ [ppm] = 149.9, 143.6, 142.9, 136.6, 130.1, 128.8, 127.0, 126.6, 122.3, 120.7, 118.2, 115.0, 112.5, 102.5, 102.4, 100.1, 100.1. Anal. Calcd. for $C_{15}H_{11}N_3$: C, 77.23; H, 4.75. Found: C, 76.77; H, 4.88.

5-(furan-3-yl)indolin-2-one (**5g**): 6-chlorooxindole (168 mg, 1.00 mmol, 1.00 eq.), furan-3-ylboronic acid (168 mg, 1.50 mmol, 1.50 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P1** (11.8 mg, 0.015 mmol, 0.015 eq.) for 8.5 h at 60 °C according to General Procedure 3. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 3:1→1:4) to provide the product as a light yellow solid (189 mg, 0.94 mmol) in 94% yield.

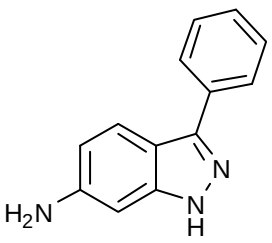


5g

Mp. = 209-210 °C. $\mathbf{R_f}$ = 0.40 (hexane/EtOAc 1:1). **IR**: $\tilde{\nu}$ = 3113 cm^{-1}, 1694, 1306, 1238, 1159, 1020, 830, 786, 720, 589. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 7.80 (dd, *J* = 1.5, 1.0 Hz, 1H), 7.51 (t, *J* = 1.7 Hz, 1H), 7.44 (d, *J* = 1.1 Hz, 1H), 7.39 (dt, *J* = 8.1, 0.8 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 6.74 (dd, *J* = 1.9, 0.9 Hz, 1H), 3.54 (s, 2H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 177.0, 144.7, 143.3, 138.8, 127.2, 126.7, 125.9, 125.4, 122.5, 110.0, 109.3, 36.46. Anal. Calcd. for $C_{12}H_9NO_2$: C, 72.35; H, 4.55. Found: C, 72.13; H, 4.53.

Synthesis of JNK3-inhibitor 8

3-phenyl-1*H*-indazol-6-amine (**7**): 3-chloro-1*H*-indazol-6-amine (168 mg, 1.00 mmol, 1.00 eq.), phenylboronic acid (244 mg, 2.00 mmol, 2.00 eq.) and K_3PO_4 (425 mg, 2.00 mmol, 2.00 eq.) in dioxane (4 mL) and H_2O (0.8 mL) were reacted in the presence of precatalyst **P2** (14.4 mg, 0.02 mmol, 0.02 eq.) for 15 h at 100 °C according to General Procedure 1. The crude product was then purified via column chromatography (SiO_2, Hexane/EtOAc 5:1→1:2) to provide the product as an off-white solid (199 mg, 0.95 mmol) in 95% yield.

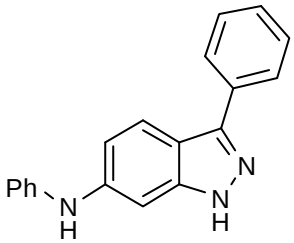


7

Mp. = 211-212 °C. $\mathbf{R_f}$ = 0.54 (hexane/EtOAc 1:1). **IR**: $\tilde{\nu}$ = 2356 cm^{-1}, 1621, 1257, 814, 678, 596. **^{1}H-NMR** (300 MHz, DMSO-d_6): δ [ppm] = 7.86 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.71 (d, *J* = 9.2 Hz, 1H), 7.44 – 7.53 (m, 2H), 7.33 – 7.41 (m, 1H), 6.68 – 6.74 (m, 2H). **^{13}C-NMR**

(125 MHz, DMSO-d_6): δ [ppm] = 148.4, 144.6, 143.5, 135.1, 129.4, 127.9, 127.2, 121.5, 113.6, 113.4, 91.3.

***N*,3-diphenyl-1*H*-indazol-6-amine** (**8**): An oven-dried test tube was charged with the amine



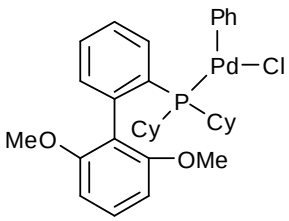
8

7 (30.0 mg, 0.143 mmol, 1.20 eq.), bromobenzene (18.8 mg, 12.5 µL, 0.119 mmol, 2.00 eq.), precatalyst **P3** (1.4 mg, 0.015 mmol, 0.015 eq.), BrettPhos (1.0 mg, 0.015 mmol, 0.015 eq.) and NaO*t*Bu (33.1 mg, 0.344 mmol, 2.40 eq.). The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). Dioxane (0.5 mL) was then added via syringe, and the test tube was placed in a preheated oil bath and stirred at 100 °C for 15 h. After cooling to room temperature EtOAc (10 mL) was added and the reaction mixture was filtered through Celite, and the filter cake washed with EtOAc (15 mL). The solvent was then removed in vacuo. The crude product was purified via column chromatography (SiO_2, Hexane/EtOAc 20:1→3:1) to yield the title compound as an off-white solid (29.2 mg, 0.102 mmol, 86%).

Mp. = 245 °C. $\mathbf{R_f}$ = 0.51 (hexane/EtOAc 1:1). **IR**: $\tilde{\nu}$ = 3360 cm^{-1}, 3209, 1630, 1433, 1344, 1313, 989, 806, 749, 698. **^{1}H-NMR** (300 MHz, CD_3OD): δ [ppm] = 7.90 (dd, *J* = 8.5 Hz, 1H), 7.89 (dd, *J* = 8.3 Hz, 1H), 7.82 (dd, *J* = 8.9, 0.7 Hz, 1H), 7.45–7.54 (m, 2H), 7.39 (ddd, *J* = 8.9, 6.6, 1.4 Hz, 1H), 7.47–7.31 (m, 2H), 7.16–7.22 (m, 3H), 6.96 (dd, *J* = 8.8, 1.9 Hz, 1H), 6.91 (ddd, *J* = 8.7, 7.3, 1.4 Hz, 1H). **^{13}C-NMR** (125 MHz, DMSO-d_6): δ [ppm] = 143.9, 143.8, 143.7, 143.1, 134.7, 129.9, 129.5, 128.2, 127.2, 122.0, 121.0, 118.3, 115.3, 94.09.

Mechanistic studies

Formation of complex 15:

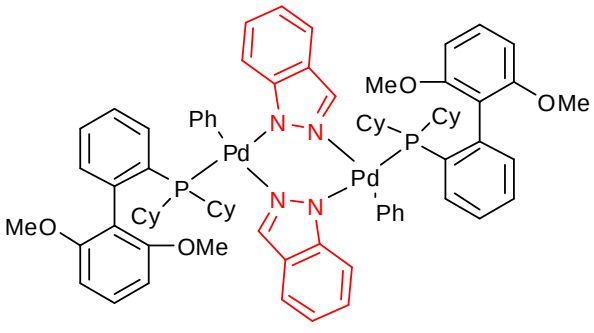


15

The reaction was set up and worked up outside of the glovebox:
An oven-dried test-tube was charged with (COD)Pd($CH_2TMS)_2$ (200 mg, 0.514 mmol, 1.00 equiv.) and SPhos (211 mg, 0.514 mmol, 1.00 equiv.). The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). After addition of cyclohexane (4 mL) and chlorobenzene (231 mg, 209 µL, 2.056 mmol, 4.00 equiv.) the reaction mixture was stirred at room temperature for 10 h during which time a precipitate had formed. After filtration, the solid was washed with hexane (2 x 10 mL) and the resulting solid dried under high vacuum to give the product as an off-white, air-stable solid (278 mg, 0.442 mmol, 86%).[8]

^{1}H-NMR (500 MHz, $CDCl_3$): δ [ppm] = 7.77 (t, *J* = 8.4 Hz, 1H), 7.61 (t, *J* = 6.9 Hz, 1H), 7.35-7.50 (m, 2H), 7.07 (d, *J* = 6.6 Hz, 2H), 6.80-6.95 (m, 4H), 6.63 (d, *J* = 8.4 Hz, 2H), 3.76 (s, 6H), 2.04-2.29 (m, 2H), 1.56-1.93 (m, 12H), 0.96-1.36 (m, 7H), 0.57 (d, *J* = 12.5 Hz, 1H). **^{13}C NMR** (125 MHz, THF-d_8): δ [ppm] = 161.1, 158.3, 138.9, 137.4, 136.4, 134.5, 133.6, 132.2, 131.8, 129.9, 129.3, 127.7, 127.4, 126.7, 126.3, 124.0, 122.9, 106.3, 104.5, 56.4, 38.5, 34.8, 34.5, 33.0, 31.0, 29.0, 28.9, 28.6, 28.3, 28.2, 28.1, 28.0, 27.7, 27.6, 27.3, 26.5 (observed complexity due to P-C splitting and monomer/dimer equilibrium). **^{31}P-NMR** (162 MHz, THF-d_8): δ [ppm] = 40.0, 35.5 (monomer/dimer equilibrium). **HRMS** for $C_{32}H_{40}ClO_2PPd$: calcd. 593.1801 $[M-Cl]^+$, found 593.1840 [ESI-HRMS]. Anal. Calcd. for $C_{32}H_{40}ClO_2PPd$: C, 61.05; H, 6.40. Found: C, 61.48; H, 6.73.

Formation of indazole-bridged Pd complex 14:



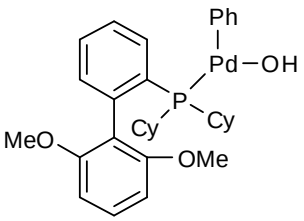
14

In a glovebox, an oven-dried vial was charged with indazole (8.3 mg, 0.070 mmol, 2.20 equiv.), KH (2.8 mg, 0.070 mmol, 2.20 equiv.) and THF (1 mL). After stirring at room temperature for 10 min, the solution was added to a solution of **15** (40.0 mg, 0.064 mmol, 2.00 equiv.) in THF (1 mL) and stirred for 15 min at room temperature. The pure product was obtained by slow vapour diffusion of pentane into the reaction mixture over

several days to give **14** as a colorless, crystalline solid (30.0 mg, 0.018 mmol, 56%) containing two molecules of THF and one molecule of pentane per molecule of **14**. These crystals were suitable for X-ray crystallography and are stable to ambient air and moisture over weeks.

^{1}H-NMR (500 MHz, CD_2Cl_2): δ [ppm] = 7.86-8.39 (m, 3H), 7.60 (s, 1H), 7.31-7.48 (m, 2H), 6.82-7.28 (m, 9H), 6.78 (d, *J* = 8.3 Hz, 1H), 6.43-6.75 (m, 8H), 5.12 (s, 2H), 3.86 (s, 5H), 3.71 (s, 3H), 3.64 (s, 4H), 3.09-3.59 (m, 4H), 0.63-2.65 (m, 40H) **^{31}P-NMR** (162 MHz, CD_2Cl_2): δ [ppm] = 49.8, 48.0, 46.0. **HRMS** for $C_{78}H_{90}N_4O_4P_2Pd_2$: calcd. 1445.4435 $[M+Na]^+$, 593.1801 $[Sphos\text{-}Pd\text{-}Ph]^+$, found 1445.4453, 593.1646 [ESI-HRMS].

Formation of complex 16:

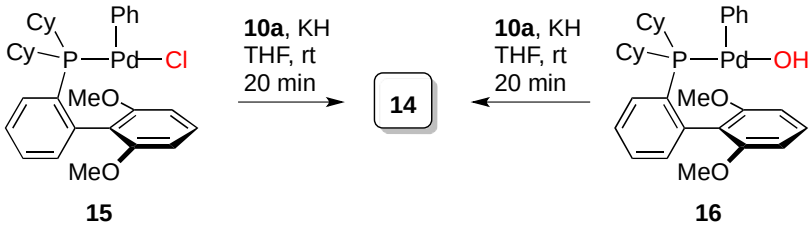


16

The Pd complex **15** (40.0 mg, 0.063 mmol, 1.00 equiv.) was added to an oven-dried test tube. The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). CH_2Cl_2 (0.4 mL, freshly degassed) was added and stirred until a clear solution was obtained. MeOH (1.6 mL, freshly degassed) was added quickly, directly follwed by dropwise addition of 4 M aq. K_3PO_4 solution (640 µL, 2.056 mmol, 40.00 equiv., freshly degassed) over 2 minutes under rapid and very efficient stirring. After 2 h at room temperature during which time a precipitate had formed, MeOH (0.5 mL) and H_2O (1 mL) were added and the reaction mixture stirred for an additional 5 minutes. The solid was filtered and washed successively with MeOH (1 mL), H_2O (1 mL) and MeOH (1 mL) and dried on high vacuum to give **16** as as an off-white to light-grey solid (31 mg, 0.047 mmol, 75%) containing 5% CH_2Cl_2. Crystals suitable for X-ray analysis were obtained by recrystallization from CH_2Cl_2/pentane.

^{1}H-NMR (500 MHz, CD_2Cl_2): δ [ppm] = 8.53 (dd, *J* = 13.7, 9.2 Hz, 1H), 7.32-7.40 (m, 2H), 7.21-7.30 (m, 3H), 6.84 (dd, *J* = 9.1, 2.6 Hz, 1H), 6.65-6.78 (m, 3H), 6.52 (d, *J* = 8.4 Hz, 2H), 3.34 (s, 6H), 1.34-1.78 (m, 12H), 1.12 (dt, *J* = 13.1, 10.0 Hz, 4H), 0.64-0.82 (m, 4H), -2.26 (d, *J* = 2.8 Hz, 1H). **^{13}C NMR** (125 MHz, THF-d_8): δ [ppm] = 159.0, 158.7, 151.5, 139.6, 137.6, 137.3, 137.2, 136.9, 134.3, 134.3, 133.9, 133.9, 130.2, 130.0, 129.8, 129.1, 128.8, 125.9, 125.8, 122.0, 121.9, 119.8, 104.0, 103.9, 100.5, 55.8, 55.3, 37.1, 36.4, 36.2, 32.5, 32.0, 30.9, 30.3, 29.0, 28.9, 28.4, 28.3, 28.2, 27.3, 27.1 (observed complexity due to P-C splitting). **^{31}P-NMR** (121 MHz, THF-d_8): δ [ppm] = 51.6. **HRMS** for $C_{32}H_{41}O_3PPd$: calcd. 1223.3769 $[2M+H]^+$, 593.1801 $[M\text{-}OH]^+$, found 1223.3809, 593.1895 [ESI-HRMS]. Anal. Calcd. for $C_{98}H_{127}Cl_4O_9P_3Pd$: C, 58.76; H, 6.39. Found: C, 58.74; H, 6.40.

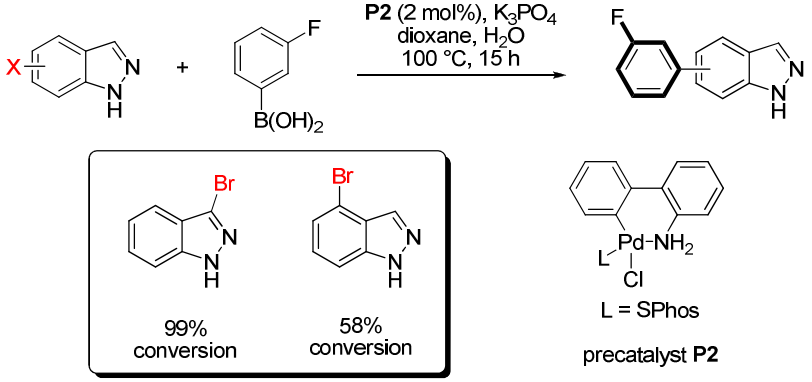
Conversion of 15 or 16 to 14:



15 **16**

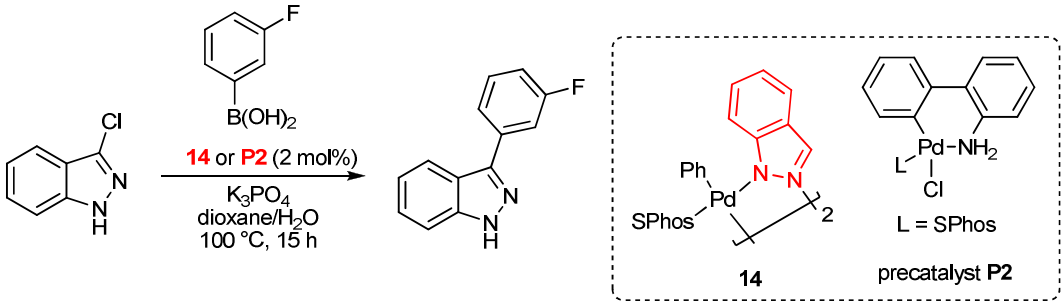
In a glovebox, an oven-dried vial was charged with **15** (10.0 mg, 0.016 mmol, 1.00 equiv.) or **16** (9.7 mg, 0.016 mmol, 1.00 equiv.), indazole (9.4 mg, 0.079 mmol, 5.00 equiv.), KH (3.2 mg, 0.079 mmol, 5.00 equiv.) and THF (1 mL). After stirring at room temperature for 20 min, a ^{31}P-NMR spectrum was taken to determine the ratio of starting material to **14**.

Comparison of indazole halides in the Suzuki-Miyaura cross-coupling (Scheme 5):



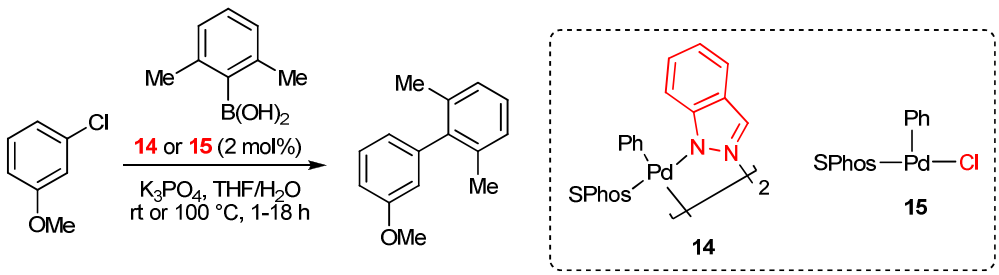
An oven-dried test tube was charged with the indazole halide (0.150 mmol, 1.00 equiv.), 3-fluorophenylboronic acid (31.5 mg, 0.225 mmol, 1.50 equiv.), **P2** (2.3 mg, 0.003 mmol, 0.02 equiv.) and K_3PO_4 (63.7 mg, 0.300 mmol, 2.00 equiv.). The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). Dioxane (1 mL) and H_2O (0.2 mL) were then added via syringe, and the test tube was placed in a preheated oil bath and stirred at 100 °C for 15 h. The reaction mixture was cooled to room temperature, a sat. aq. solution of NH_4Cl (2 mL), EtOAc (1 mL) and naphthalene (600 µL, 0.150 mmol, 1.00 equiv., 1 M in EtOAc) were added. HPLC samples could then be directly prepared by taking an aliquot from the organic layer, filtering it through a short silica plug and flushing it with EtOAc.

Comparison of 14 vs. P2 as Pd source in the cross-coupling of 3-chloroindazole (Figure S3):



An oven-dried test tube was charged with 3-chloroindazole (38.1 mg, 0.250 mmol, 1.00 equiv.), 3-fluorophenylboronic acid (52.5 mg, 0.375 mmol, 1.50 equiv.), **P2** (3.8 mg, 0.005 mmol, 0.02 equiv.) or **14** (3.6 mg, 0.003 mmol, 0.01 equiv.), K_3PO_4 (106.0 mg, 0.500 mmol, 2.00 equiv.) and naphthalene (32.0 mg, 0.250 mmol, 1.00 equiv.). The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). Dioxane (1 mL) and H_2O (0.2 mL) were then added via syringe, and the test tube was placed in a preheated oil bath and stirred at 100 °C for 15 h. At defined intervals (0.5, 1, 1.5, 2, 2.5, 3, 4, 5, 6, 17.25 h), aliquots (50 µL) were taken from the reaction mixture and analyzed by HPLC using the added naphthalene as internal standard.

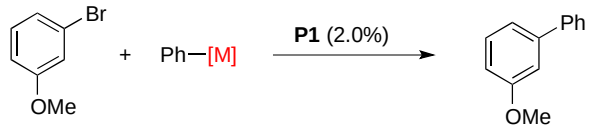
Comparison of 14 vs. 15 as Pd source in the cross-coupling of 3-chloroindazole (Figure S4):



An oven-dried test tube was charged with **14** (7.2 mg, 0.005 mmol, 0.01 equiv.) or **15** (6.3 mg, 0.010 mmol, 0.02 equiv.). The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). Dodecane (85.2 mg, 114 µL, 0.500 mmol, 1.00 equiv.) and THF (1 mL) were added via syringe and an aliquot (50 µL) withdrawn for t = 0 min. After addition of a degassed 1.5 M aq. K_3PO_4 solution (1 mL, 1.500 mmol, 3.00 equiv.)

and a solution of 2,6-dimethylphenylboronic acid (112 mg, 0.750 mmol, 1.50 equiv.) in THF (1 mL) the reaction mixture was stirred at room temperature for 18 h. At defined intervals (20, 40 min, 1, 2, 3.17, 4, 5, 6, 7, 17.5 h), aliquots (50 µL) were taken from the reaction mixture and analyzed by GC using the added dodecane as internal standard. The reaction was also conducted at 100 °C; under these conditions, samples were taken after 5, 10, 20, 30 min.

Comparison of cross-coupling methods in the presence of indazole



		no indazole	1.0 eq. indazole
[M] =	$SnBu_3$	91%	0%
	$B(OH)_2$	99%	2%
	ZnBr	96%	97%
	MgBr	97%	98%

The cross-coupling conditions for the Stille, Suzuki-Miyaura, Negishi and Kumada cross-coupling were chosen from published procedures and adapted so that the Pd species and the ligand were the same in all cases.[9-11] The remaining parameters (solvent, temperature, reaction time, additives) were followed according to the respective publication. The reactions in the absence of indazole were also run according to the following procedures but without addition of indazole.

Stille cross-coupling:

An oven-dried test tube was charged with precatalyst **P1** (3.9 mg, 0.005 mmol, 0.02 equiv.), CsF (122.0 mg, 0.800 mmol, 3.20 equiv.) and indazole (29.5 mg, 0.250 mmol, 1.00 equiv.). The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). 3-bromoanisole (46.8 mg, 31.7 µL, 0.250 mmol, 1.00 equiv.), tributylphenylstannane (101.0 mg, 89.8 µL, 0.275 mmol, 1.10 equiv.), and DME (1 mL) were then added via syringe, and the test tube was placed in a preheated oil bath and stirred at 80 °C for 4 h. The reaction mixture was cooled to room temperature, a sat. aq. solution of NH_4Cl (2 mL), EtOAc (1 mL) and dodecane (250 µL, 0.250 mmol, 1.00 equiv., 1M in EtOAc) were added. GC samples could then be directly prepared by taking an aliquot from the organic layer, filtering it through a short silica plug and flushing it with EtOAc.

Suzuki-Miyaura cross-coupling:

An oven-dried test tube was charged with precatalyst **P1** (3.9 mg, 0.005 mmol, 0.02 equiv.), phenylboronic acid (39.6 mg, 0.326 mmol, 1.30 equiv.), K_3PO_4 (106 mg, 0.500 mmol, 2.00 equiv.) and indazole (29.5 mg, 0.250 mmol, 1.00 equiv.). The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). 3-bromoanisole (46.8 mg, 31.7 µL, 0.250 mmol, 1.00 equiv.), dioxane (1 mL) and H_2O (0.2 mL) were then added via syringe, and the test tube was placed in a preheated oil bath and stirred at 60 °C for 2 h. The reaction mixture was cooled to room temperature, a sat. aq. solution of NH_4Cl (2 mL), EtOAc (1 mL) and dodecane (250 µL, 0.250 mmol, 1.00 equiv., 1M in EtOAc) were added. GC samples could then be directly prepared by taking an aliquot from the organic layer, filtering it through a short silica plug and flushing it with EtOAc.

Negishi cross-coupling:[12]

In a glovebox, an oven-dried test tube was charged with solid $ZnCl_2$ (83.5 mg, 0.613 mmol, 2.45 equiv.). After addition of a solution of phenylmagnesium bromide (588 µL, 0.588 mmol, 2.35 equiv., 1M in THF) and THF (0.5 mL) the reaction mixture was stirred at room temperature for 1.5 h. 3-bromoanisole (46.8 mg, 31.7 µL, 0.250 mmol, 1.00 equiv.) was added via syringe, followed by precatalyst **P1** (3.9 mg, 0.005 mmol, 0.02 equiv.), XPhos (2.4 mg, 0.005 mmol, 0.02 equiv.) and indazole (29.5 mg, 0.250 mmol, 1.00 equiv.) by quickly opening the reaction vessel and adding the solids under argon backpressure. The test tube was placed in a preheated oil bath and stirred at 60 °C for 2 h. The reaction mixture was cooled to room temperature, a sat. aq. solution of NH_4Cl (2 mL), EtOAc (1 mL) and dodecane (250 µL, 0.250 mmol, 1.00 equiv., 1M in EtOAc) were added. GC samples could then be directly prepared by taking an aliquot from the organic layer, filtering it through a short silica plug and flushing it with EtOAc.

Kumada cross-coupling:

An oven-dried test tube was charged with precatalyst **P1** (3.9 mg, 0.005 mmol, 0.02 equiv.), and indazole (29.5 mg, 0.250 mmol, 1.00 equiv.). The reaction vessel was evacuated and backfilled with argon (this process was repeated a total of three times). 3-bromoanisole (46.8 mg, 31.7 µL, 0.250 mmol, 1.00 equiv.), phenylmagnesium bromide (750 µL, 0.750 mmol, 3.00 equiv., 1M in THF), and toluene (0.75 mL) were then added via syringe, and the test tube was placed in a preheated oil bath and stirred at 60 °C for 2 h. The reaction

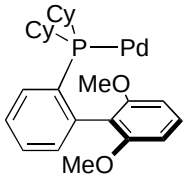
mixture was cooled to room temperature, a sat. aq. solution of NH_4Cl (2 mL), EtOAc (1 mL) and dodecane (250 μL, 0.250 mmol, 1.00 equiv., 1M in EtOAc) were added. GC samples could then be directly prepared by taking an aliquot from the organic layer, filtering it through a short silica plug and flushing it with EtOAc.

Computational details

All calculations were carried out with the Gaussian 03 software package.[13] All calculations were performed using the Becke three-parameter hybrid functional combined with Lee–Yang–Parr correlation functional.[14] C, H, N, O, P and Cl were computed at the 6-31+G(d,p) level of theory, and for the Pd center, LANL2DZ+ECP was used.[15,16] Frequency calculations were undertaken to confirm the nature of the stationary points, yielding one imaginary frequency (NImag = 1) for transition states (TS) with largest contributions from internal coordinates involved in the reaction and none (NImag = 0) for minima. All optimizations were performed without any constraints (*C*1 symmetry). Geometry optimizations were carried out in the gas phase. For the incorporation of solvent effects in the frequency calculations the self-consistent reaction field (SCRF) theory, using the PCM-united atom topological model (UAHF, radii of interlocking spheres),[17] was employed as implemented in Gaussian 03. The unscaled Gibbs free energies were calculated at 298.15 K and 1 atm and based upon ideal gas-phase conditions. For calculating the relative energies, the starting materials were chosen as reference.

Cartesian Coordinates of Computed Intermediates

Oxidative addition



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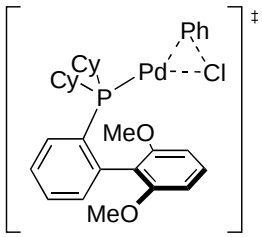

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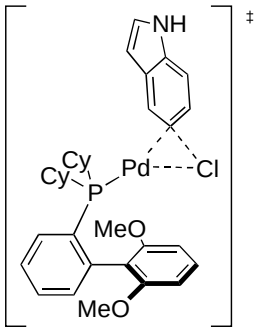

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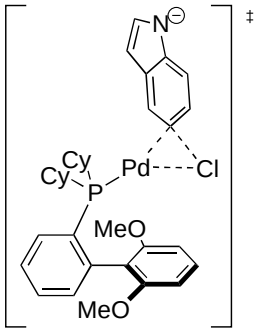

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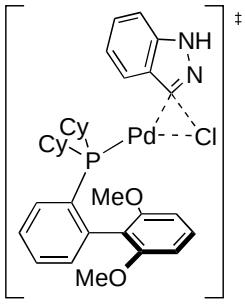

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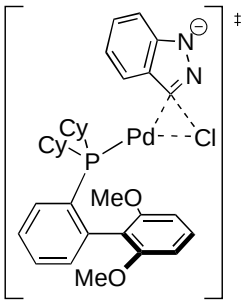

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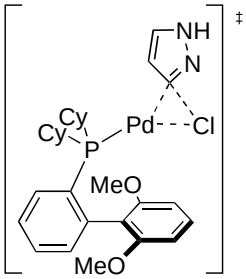

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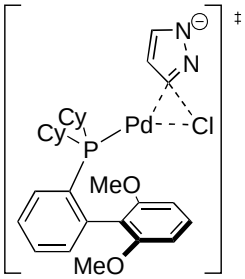

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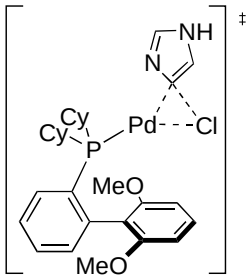

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H	3.15027835	5.86936352	2.55022948	C	5.74844843	4.90061774	-5.88194335
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C	-2.08025464	3.66891587	0.12419774	H	4.11890963	5.09092795	-7.3119026
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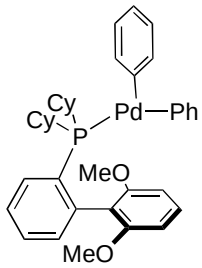
Reductive elimination



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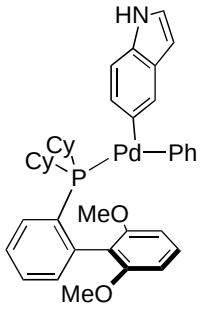

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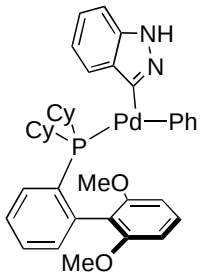

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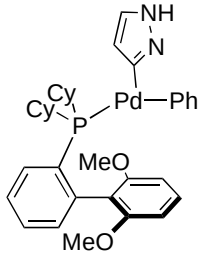

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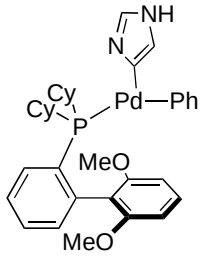

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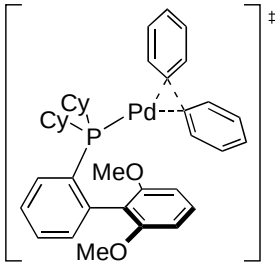

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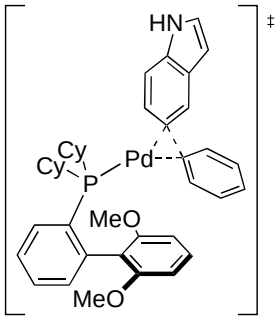

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C	0.67086858	-0.98714324	-3.7253342	H	-0.87023967	1.53519253	-8.56979914
C	2.96841599	-2.48423318	-3.21249384	H	0.62123865	1.66400122	-10.8192648
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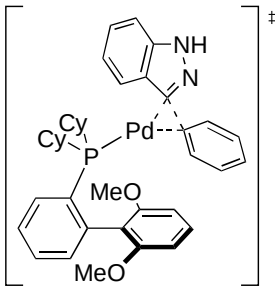

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C	-0.72912379	1.18930223	0.00286076	H	5.25574732	0.4846467	0.07800196
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C	2.5289418	4.55783503	-0.92495662	H	-0.0431911	4.95470623	-2.02297373
C	2.41077465	4.1395838	1.46338235	C	-0.58559534	7.4642967	-3.07961036
C	3.24113317	5.7343695	-0.63792232	H	1.3374507	6.93521581	-3.90881645
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H	-1.55306471	1.33167225	-9.24104087
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C	0.93226831	-1.10058183	-3.61113691
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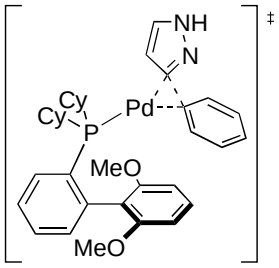

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C	3.19024502	5.76702717	-0.6219854
C	3.1334087	5.2965647	1.743113
H	2.14089196	3.46645189	2.28519241
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H	4.0057865	-0.46347089	0.93341793
H	4.04284564	-0.45393709	-0.85983792
H	5.25559485	0.4728665	0.0684109
C	0.42157751	5.20606633	-2.91188031
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C	4.76207197	4.32966932	-3.43597368	C	0.64182187	-0.96124154	-3.70233187
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C	5.58434428	4.95028255	-5.76084871	C	1.29624008	1.43196889	-7.46125065
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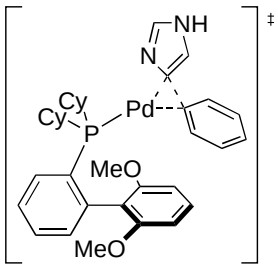

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H	1.93262162	-0.93653215	-0.03808659	H	-2.43185037	3.17888418	1.01153664
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C	2.26748996	4.27862774	1.38682148	H	5.25043913	0.47750722	0.13731802
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C	2.92411388	5.48783262	1.60684125	C	0.6747449	6.09814163	-3.37721454
H	1.86922984	3.71790007	2.22774898	C	-0.01832747	3.8660332	-4.37880721
C	3.42554292	6.19921417	0.51673007	H	0.10763379	4.33810055	-2.29008618
H	3.66190187	6.26274174	-1.60180595	C	-0.76095906	6.62580032	-3.56413518

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H	1.13806284	6.58654744	-2.51252087
C	-1.45134956	4.39700619	-4.56137896
H	0.543388	4.0343001	-5.30662204
H	-0.02868165	2.7840172	-4.21806632
C	-1.47726859	5.92464393	-4.72888138
H	-0.739026	7.71121725	-3.72573383
H	-1.32616854	6.45915355	-2.63586546
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H	-2.05218615	4.12016998	-3.68252504
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C	5.12831887	4.36518441	-3.34412101
C	3.53396112	4.56556665	-5.29606522
H	3.57534266	5.8607633	-3.58043071
C	6.21606356	5.09804931	-4.1479957
H	5.22804797	3.2812366	-3.49957894
H	5.27406881	4.54017843	-2.27316956
C	4.62026724	5.29923439	-6.10372434
H	3.58239386	3.48786143	-5.50340217
H	2.54570162	4.90307184	-5.62439604
C	6.03396608	4.8965229	-5.65946297
H	7.20664261	4.74778587	-3.83166943
H	6.17740938	6.1732091	-3.91766053
H	4.48299336	5.09519577	-7.1731812
H	4.49614998	6.38481983	-5.9756272
H	6.78588846	5.47040462	-6.21555269
H	6.20207029	3.83765991	-5.90463669
O	3.43227407	1.33717759	0.02673647
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H	-0.52999937	-0.948354	-0.00815109
C	3.33787289	-0.50652211	-3.8122342
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Pd	2.7400757	1.36920848	-3.32835299
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H	0.44644805	-0.66628239	-3.02285628
C	0.49649575	0.26432373	-6.7869742
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C	-0.64122912	-0.33956973	-6.23935878
H	-1.52539646	-1.1438572	-4.44119976
H	0.52577183	0.51194598	-7.84575679
H	-1.49884228	-0.56618315	-6.86690867
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H	4.81536882	-0.2609519	-5.49714737
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H	5.61230325	-2.56058723	-4.71568413
C	4.08105061	-2.46295062	-3.24093971
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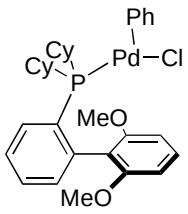
*Equilibrium between **15** and **17***



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H	-1.81475385	1.14758024	-0.00114294	C	3.12506078	5.98430775	-4.5794825
C	2.09857529	3.70224653	0.43322856	H	3.49747863	6.61973066	-2.56613293
C	2.47763967	4.75786486	-0.41546799	C	5.90320715	5.69132729	-3.57593025
C	2.42626935	3.78478159	1.79933182	H	4.65016339	3.92690904	-3.44296054
C	3.1861841	5.84694563	0.11924609	H	4.95258509	4.70268615	-1.89163322
C	3.121886	4.87198171	2.3218817	C	4.28872934	6.78130187	-5.19707842
H	2.13213047	2.96880299	2.45310746	H	2.98288062	5.0544304	-5.13759724
C	3.51142739	5.90987948	1.47353967	H	2.19775541	6.55783921	-4.6785239
H	3.5008868	6.66033265	-0.52509533	C	5.62677169	6.04161995	-5.04578794
H	3.36337988	4.90466559	3.38052392	H	6.83024256	5.11122695	-3.48878654
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P	1.98354634	4.72071581	-2.23585252	H	4.07637803	6.97295948	-6.25586868
C	-2.09803012	3.64685542	0.19984157	H	4.35942439	7.76448532	-4.7077631
H	-2.36767702	4.70043865	0.28665485	H	6.44520293	6.64912435	-5.4516843
H	-2.55194127	3.22537678	-0.70486608	H	5.59482081	5.11725716	-5.6388491
H	-2.46151429	3.10529621	1.0812835	O	3.42863349	1.3320846	0.0211008
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H	4.04863263	-0.51505896	0.77853856	H	-0.52799857	-0.94757301	-0.03581747
H	3.993825	-0.39225644	-1.01059038	Pd	1.43796928	2.44254839	-2.82767723
H	5.25071643	0.48123382	-0.08634541	Cl	0.75834338	0.23995904	-3.34000753
C	0.44944018	5.90346513	-2.22142282	C	1.84997864	2.63077732	-4.77357899
C	0.79165744	7.39045065	-2.02539687	C	3.10728973	2.22504179	-5.23442466
C	-0.47679039	5.68882123	-3.43079958	C	0.88933817	3.08058565	-5.68356521
H	-0.07850753	5.54956162	-1.32743856	H	3.84430197	1.8257732	-4.54478033
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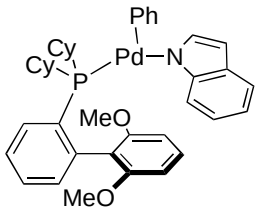

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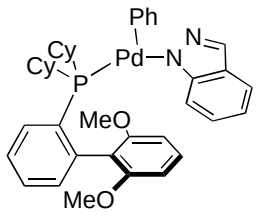

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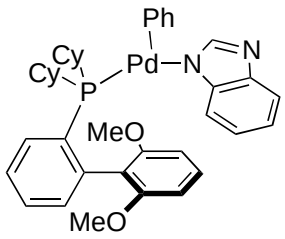

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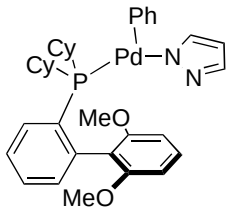

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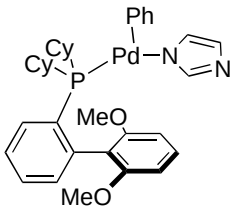
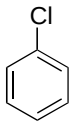
H	-2.6198605	3.17474003	0.65749017	C	1.55506252	2.38482787	-4.74752194
C	4.21935	0.15219205	0.04930547	C	0.66105634	2.81133314	-5.73511242
H	4.00631012	-0.45875841	0.93527205	C	2.77488354	1.80814148	-5.12364342
H	4.05569848	-0.44575053	-0.85557537	C	1.00557061	2.70027196	-7.0883572
H	5.2569487	0.48752885	0.08103304	H	-0.31207399	3.20489218	-5.46139484
C	0.72436605	5.94861035	-2.42067743	C	3.11122731	1.69113158	-6.47943886
C	1.21669427	7.40335532	-2.33992547	H	3.46780302	1.44290133	-4.37113352
C	-0.2108994	5.73572985	-3.62521898	C	2.23226944	2.14564478	-7.46631564
H	0.1549999	5.72493378	-1.50880909	H	0.30224494	3.03524559	-7.84698102
C	0.02992228	8.38636368	-2.31099579	H	4.06075051	1.24010788	-6.75844794
H	1.84545147	7.63457319	-3.21002082	H	2.49294181	2.05447708	-8.51714784
H	1.83158131	7.55384871	-1.44694812	C	-0.00231877	-0.40657454	-3.52400202
C	-1.38790125	6.72668425	-3.59272443	C	-1.2556611	-0.98885433	-3.70721472
H	0.34512714	5.86668137	-4.56272554	C	-2.15383483	0.06855279	-3.46418852
H	-0.58560336	4.70727041	-3.62449823	H	-3.23668181	0.0641645	-3.50084062
C	-0.9077754	8.18279492	-3.51017018	N	-0.17830485	0.89164628	-3.18105015
H	0.40722633	9.41644743	-2.28817758	N	-1.49893767	1.20110878	-3.15447306
H	-0.53453514	8.23870913	-1.37908645	H	0.98847589	-0.82792391	-3.62517209
H	-2.016447	6.57865353	-4.47925236	H	-1.47754705	-2.01011974	-3.9840112
H	-2.02152599	6.50482743	-2.72166631				
H	-1.76442808	8.86464373	-3.44173177				

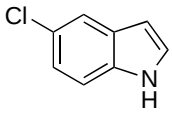


C	0	0	0	H	-1.03137345	8.23483312	-4.17659252
C	1.39156511	0	0	C	3.39408988	5.6315998	-3.15804597
C	2.07316867	1.22335465	0	C	4.73996481	4.90141141	-2.98426859
C	1.37065554	2.45909928	0	C	3.09394583	5.90067178	-4.64512811
C	-0.04924008	2.40750281	0.03419237	H	3.45798187	6.60237394	-2.64998706
C	-0.73249323	1.1881713	0.01920379	C	5.88479635	5.68287157	-3.65448548
H	1.92613497	-0.93884081	-0.04465411	H	4.66570654	3.90485309	-3.43578959
H	-1.81397066	1.15075042	0.01410788	H	4.96127029	4.75240531	-1.9219233
C	2.0959277	3.71379956	0.40757283	C	4.24411246	6.68553522	-5.30279917
C	2.4647216	4.76234061	-0.45537928	H	2.95331176	4.95163525	-5.17134865
C	2.41963979	3.81887018	1.77269915	H	2.16047813	6.46275228	-4.75277717
C	3.15611584	5.86892863	0.06488017	C	5.59052344	5.96636999	-5.1347961
C	3.10085756	4.92233376	2.28066344	H	6.8210635	5.12069937	-3.55041474
H	2.13313164	3.00952822	2.43803505	H	6.03311805	6.63549014	-3.12436445
C	3.4768738	5.95454984	1.41923638	H	4.02050901	6.83377618	-6.36620072
H	3.46060688	6.67812573	-0.59016198	H	4.30870004	7.68797984	-4.8532756
H	3.34097862	4.97238347	3.33890942	H	6.39837205	6.56412089	-5.57469868
H	4.01586058	6.81984667	1.79449849	H	5.56231466	5.01709541	-5.68732746
P	1.98575558	4.67768123	-2.27734348	O	3.42966271	1.33111935	0.03651687
C	-2.09216082	3.64774488	0.26226899	O	-0.67359353	3.6195172	0.12900882
H	-2.35772292	4.70049869	0.36842249	H	-0.52766889	-0.94721007	-0.03965991
H	-2.58617158	3.23361466	-0.6247649	Pd	1.49908684	2.35914511	-2.79583846
H	-2.41721997	3.09850134	1.15365081	C	1.89579452	2.48057296	-4.75535766
C	4.21332198	0.13910156	0.04253298	C	0.91791231	2.85075429	-5.68451365
H	4.00645302	-0.46647793	0.93319555	C	3.17048147	2.11728501	-5.20625977
H	4.03487728	-0.45762215	-0.85861375	C	1.22692067	2.89616552	-7.05060033
H	5.25152538	0.47297495	0.06372716	H	-0.08798808	3.09577499	-5.36083491
C	0.42055093	5.81430736	-2.30500419	C	3.47507785	2.16317355	-6.57281761
C	0.71142875	7.31662805	-2.14814474	H	3.93046513	1.78790739	-4.50390472
C	-0.49118251	5.53719622	-3.51358001	C	2.50686498	2.55971495	-7.4996143
H	-0.10184399	5.46963549	-1.40419529	H	0.45745332	3.1851595	-7.76238074
C	-0.59813513	8.12441646	-2.0594791	H	4.46880961	1.87731351	-6.90931036
H	1.29200279	7.68085487	-3.00608113	H	2.74198319	2.58948759	-8.55984782
H	1.3109376	7.50030666	-1.25030082	C	1.84029077	-0.67688107	-3.3563823
C	-1.79240913	6.35492203	-3.42187985	C	1.04366162	-1.79916874	-3.493536
H	0.02689961	5.78831705	-4.44774888	N	0.99875299	0.40001557	-3.18327522
H	-0.72089639	4.46787188	-3.56320577	H	2.91513262	-0.56579271	-3.38808581
C	-1.5134074	7.85681437	-3.26309516	H	1.3469834	-2.82719973	-3.64663392
H	-0.36551188	9.1939412	-1.98422091	N	-0.28193378	-1.44353011	-3.42054421
H	-1.12534882	7.8533066	-1.13344104	C	-0.25675044	-0.12350084	-3.24548022
H	-2.40640308	6.17115962	-4.31208884	H	-1.14299332	0.49148764	-3.16000345
H	-2.37916477	6.00380858	-2.56028341				
H	-2.45447647	8.41000356	-3.15544045				

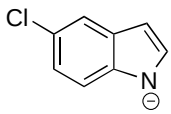
Halide starting materials



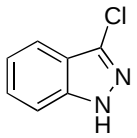
C	0	0	0	H	1.944668	-0.952513	0.001315
C	1.39516	0	0	H	1.945244	3.368403	-0.001258
C	2.092698	1.207751	0	H	-0.549903	3.36846301	-0.00262292
C	1.395044	2.41626	-0.001199	H	-1.796986	1.208159	-0.000862
C	0.000219	2.416182	-0.001678	Cl	3.8526977	1.20787903	0.00101469
C	-0.697382	1.207976	-0.000682				
H	-0.549759	-0.952317	0.00045				



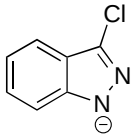
C	0	0	0	H	2.55222438	2.1683917	0
C	2.25411995	0	0	C	-1.85004236	2.03925322	0
C	0.44503617	1.35214461	0	H	-0.20746693	3.43016889	0
C	-1.35784551	-0.33741695	0	H	-3.34823192	0.48294466	0
C	1.88177687	1.32090554	0	N	1.12612628	-0.80017949	0
H	3.23982746	-0.44287257	0	Cl	-3.0701674	3.31560298	0
C	-0.50799272	2.38802111	0	H	1.1280865	-1.80747328	0
C	-2.28581931	0.69861291	0				
H	-1.68856232	-1.37196226	0				



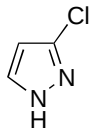
C	0	0	0	H	-1.66773257	-1.37860813	0
C	2.15299864	0	0	H	2.5064343	2.20847244	0
C	0.40179843	1.3967614	0	C	-1.9131641	2.02453452	0
C	-1.36603854	-0.33289588	0	H	-0.31440914	3.46423811	0
C	1.8229766	1.36651335	0	H	-3.38894359	0.44016223	0
H	3.15978581	-0.4138416	0	N	1.08244799	-0.83706997	0
C	-0.58098436	2.41039872	0	Cl	-3.18110466	3.29681503	0
C	-2.3296747	0.67689619	0				



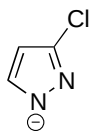
C	0	0	0	H	3.21003087	1.22363759	0
C	1.41772137	0	0	H	-0.5587785	3.32394831	0
C	-0.7421945	1.19340994	0	H	1.91225031	3.34910297	0
C	1.75156259	-1.38952777	0	N	-0.37460053	-1.31715662	-0.00020524
C	2.1247873	1.21604389	0	N	0.68998667	-2.16610594	0.00012113
C	-0.02241493	2.37967463	0	Cl	3.34595082	-2.06108438	0
H	-1.8277377	1.1900425	-0.00006858	H	-1.30202174	-1.71061551	-0.00026034
C	1.39494298	2.39485069	0				



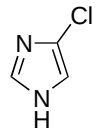
C	0	0	0	H	3.25007018	1.2096837	0
C	1.43963674	0	0	H	-0.49433336	3.36640303	-0.00004749
C	-0.69875137	1.22998306	0	H	1.98919137	3.35266185	0
C	1.70197708	-1.38434277	0	N	-0.48725414	-1.27072284	-0.00020107
C	2.16167394	1.21092842	0	N	0.58654264	-2.11287721	0.00034839
C	0.02856404	2.41151761	0	Cl	3.29463642	-2.14971856	0
H	-1.7868408	1.23590458	-0.00007029				
C	1.45333506	2.40546139	0				



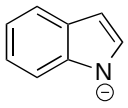
C	0	0	0	H	-0.701588	-0.833233	0.00009232
C	1.40175	0	0	H	2.046123	-0.872706	0
C	1.825748	1.370796	0	N	0.668691	2.16224899	-0.00008926
N	-0.439727	1.320508	0	Cl	3.48800081	1.94916925	0
H	-1.380055	1.611209	-0.00021502				



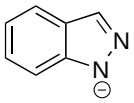
C	0	0	0	N	0.71739148	2.14944839	0.00015792
C	1.43487142	0	0	N	-0.41421076	1.33915365	0.00010399
C	1.84907631	1.33925841	0	Cl	-1.04372476	-1.41712336	-0.0001004
H	2.07819769	-0.87346848	-0.00009283				
H	2.85226558	1.76356612	-0.00011405				



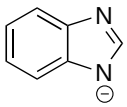
C	0	0	0	C	0.76936749	-1.99404043	0
C	1.51666014	0	0	N	-0.3464243	-1.23077368	0
H	-0.6460272	0.85296638	0	H	-1.28639745	-1.57201737	0.00003633
N	1.90156972	-1.23676088	0	H	0.76378498	-3.06402466	0
Cl	2.55999757	1.41740922	0				



C	0	0	0	H	-1.66247103	-1.38493145	0
C	2.15551433	0	0	H	2.50852146	2.20707617	0
C	0.40037481	1.39611468	0	C	-1.93767659	2.04236254	0
C	-1.36781518	-0.33646022	0	H	-0.30808112	3.45496138	0
C	1.82452532	1.36486607	0	H	-3.38414593	0.4235532	0
H	3.16247135	-0.41483788	0	H	-2.70407217	2.81646914	0
C	-0.58998828	2.40128042	0	N	1.08373542	-0.83805969	0
C	-2.32509828	0.67812477	0				

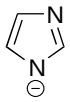


C	0	0	0	C	1.43336225	2.41635359	-0.00006204
C	1.44180252	0	0	H	3.23737624	1.2393546	0.00009412
C	-0.70749954	1.22430406	0	H	-0.5210423	3.36517403	-0.00007049
C	1.73954537	-1.38349181	0.0006876	H	1.96455715	3.36687175	-0.00001162
C	2.14730753	1.22309652	-0.00010247	N	-0.47775897	-1.27380088	-0.00083963
C	0.00943423	2.41398191	0	N	0.59934871	-2.10366782	-0.00026751
H	-1.79604306	1.22308984	-0.00023213				
H	2.70463086	-1.87988824	0.00133367				



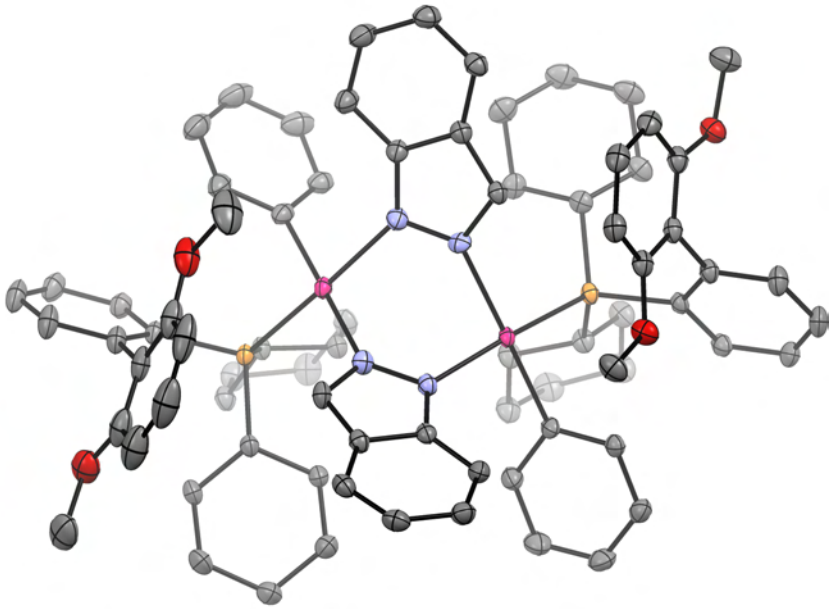
C	0	0	0	H	1.963939	3.34817	0.00013133
C	1.445779	0	0	H	-0.51799599	3.348136	0.00049396
C	2.144467	1.19044	0	H	-1.797303	1.207164	0.000454
C	1.417972	2.392928	0.00013	H	0.722722	-3.294794	-0.00051274
C	0.02800901	2.392927	0.00025616	N	-0.427004	-1.393719	-0.00023796
C	-0.698541	1.190462	0.000252	N	1.872756	-1.393559	-0.00013625
C	0.722621	-2.205199	-0.00032566				
H	3.243254	1.206973	-0.000147				

C	0	0	0	H	2.046123	-0.872706	0
C	1.40175	0	0	H	2.850311	1.727288	0
C	1.825748	1.370796	0	N	0.668691	2.16224899	-0.00008926
N	-0.439727	1.320508	0				
H	-0.701588	-0.833233	0.00009232				



C	0	0	0	N	1.825748	1.370796	0
C	1.40175	0	0	C	0.668691	2.16224899	-0.00008926
N	-0.439727	1.320508	0	H	0.64217233	3.23192032	-0.00021227
H	-0.701588	-0.833233	0.00009232				
H	2.046123	-0.872706	0				

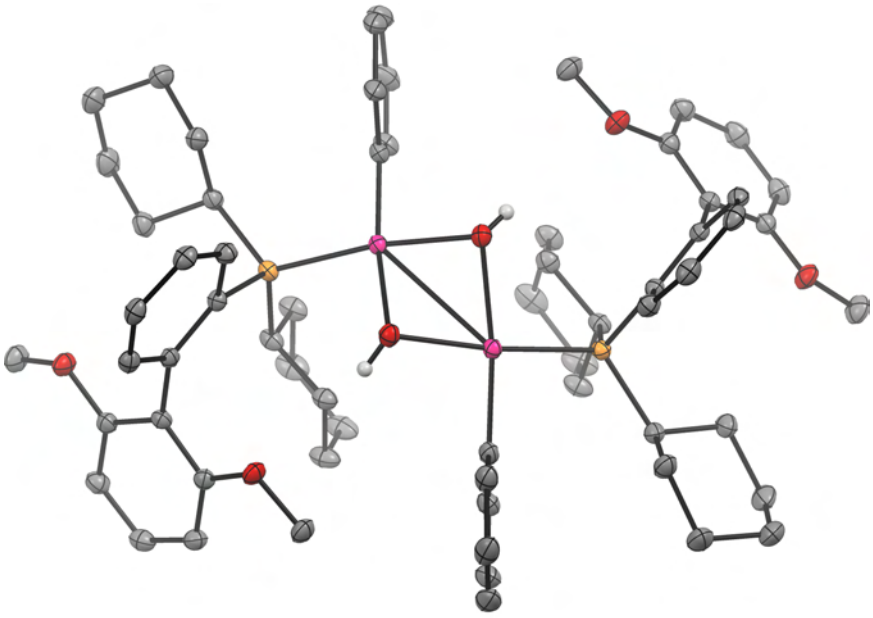
Table S1. Crystal data and structure refinement for Pd species **14**.



Empirical formula	C45.50 H59 N2 O3 P Pd	
Formula weight	819.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 16.574(2) Å	a= 109.424(2)°.
	b = 16.933(2) Å	b= 93.059(3)°.
	c = 17.319(2) Å	g = 116.144(2)°.
Volume	3998.4(9) $Å^3$	
Z	4	
Density (calculated)	1.361 Mg/m^3	
Absorption coefficient	0.547 mm^{-1}	
F(000)	1724	
Crystal size	0.13 x 0.13 x 0.02 mm^3	
Theta range for data collection	1.28 to 31.35°.	
Index ranges	-24<=h<=23, -24<=k<=24, -25<=l<=24	
Reflections collected	159045	
Independent reflections	26268 [R(int) = 0.0489]	

Completeness to theta = 31.35°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9891 and 0.9323
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	26268 / 443 / 1043
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0369, wR2 = 0.0809
R indices (all data)	R1 = 0.0563, wR2 = 0.0898
Largest diff. peak and hole	1.287 and -1.268 e.$Å^{-3}$

Table S2. Crystal data and structure refinement for **16**.



Empirical formula	C65 H84 Cl2 O6 P2 Pd2	
Formula weight	1306.96	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 21.2344(15) Å	a= 90°.
	b = 12.7861(9) Å	b= 94.0070(10)°.

	c = 22.3397(15) Å g = 90°.
Volume	6050.5(7) $Å^3$
Z	4
Density (calculated)	1.435 Mg/m^3
Absorption coefficient	0.786 mm^{-1}
F(000)	2712
Crystal size	0.25 x 0.20 x 0.12 mm^3
Theta range for data collection	1.28 to 31.61°.
Index ranges	-31<=h<=30, -18<=k<=18, -32<=l<=32
Reflections collected	455482
Independent reflections	20286 [R(int) = 0.0380]
Completeness to theta = 31.61°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9116 and 0.8277
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	20286 / 39 / 726
Goodness-of-fit on F^2	1.093
Final R indices [I>2sigma(I)]	R1 = 0.0225, wR2 = 0.0552
R indices (all data)	R1 = 0.0294, wR2 = 0.0608
Largest diff. peak and hole	0.517 and -0.543 $e.Å^{-3}$

References/Notes:

[1] Bruno, N.; Tudge, M. T.; Buchwald, S. L. Tudge, *Chem. Sci.* **2013**, *4*, 916-920. **P2** was synthesized from the corresponding μ-Cl-dimer in a solution of dichloromethane (rt, 4h).

[2] Commercially available **P1** normally contains one equivalent of acetone.

[3] Protective gloves should be worn when handling 3-chloroindazole.

[4] In order to ensure proper precipitation of the pyrazole hydrochloride adduct it is imperative that all residual dioxane be removed under high vacuum for up to 2 minutes.

[5] The crude mixture needs to be redissolved quickly in Et_2O after evaporation to prevent slow formation of insoluble compounds.

[6] The complete dissolution of the crude mixture in Et_2O is neccessary before addition of HCl in Et_2O.

[7] Sometimes insufficient precipitation of the hydrochloride adduct is observed, leading to lower yield. In this case, a second extraction was performed as follows:
The ethereal phase of the HCl-pyrazole precipitation was combined with the aqueous, basic phase of the subsequent liberation. Additional 1M aq. NaOH (5 mL) was added and the mixture was vigorously stirred for 10 min. After separation of the phases the aqueous phase was extracted with Et_2O (2x20 mL), the combined organic phases dried over $MgSO_4$ and the solvent removed by rotary evaporation and high vacuum. The residual product was then again precipitated as its HCl adduct according to General Procedure 2, albeit with slightly decreased amount of HCl (2.0 mL, 2M in Et_2O).

[8] Crystals suitable for X-ray crystallography could be obtained by dissolving solid **15** in CH_2Cl_2 and slowly letting pentane diffuse into the solution.

[9] The only adaptation used was replacing the Pd source by precatalyst **P1** to insure that the Pd species was uniform and different rates of catalyst activation could not influence the reaction.

[10] Naber, J. R.; Buchwald, S. L. *Adv. Syn. Cat.* **2008**, *350*, 957-961.

[11] Yang, Y.; Oldenhuis, N.; Buchwald, S. L.; *Angew. Chem. Int. Ed.* **2013**, *52*, 615-619.

[12] If the organozinc reagent was prepared by lithium/halide exchange from bromobenzene followed by transmetallation with $ZnCl_2$, the presence of the bromobutane byproduct led to formation of 3-(1'-butyl)-anisole as the main product. No formation of the desired cross-coupling product was observed. The necessity to use Grignard reagents as precursors in the reaction of unprotected 5-bromoindole was

previously reported: Manolikakes, G.; Hernandez, C. M.; Schade, M. A.; Metzger, A.; Knochel, P. *J. Org. Chem.* **2008**, *73*, 8422–8436.

[13] Gaussian 03, Revision E.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

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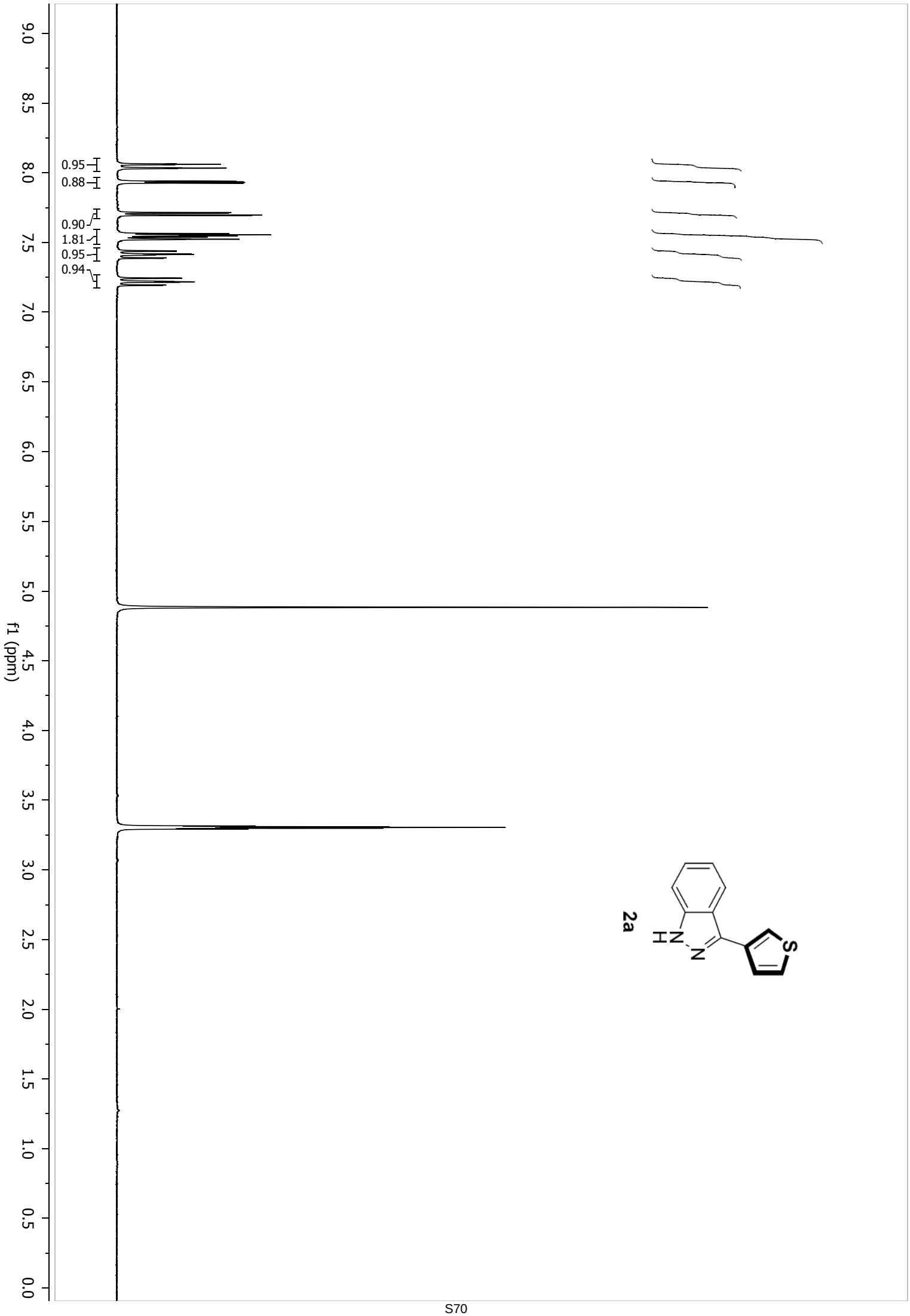
[15] (a) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. *J. Chem. Phys.* **1980**, *72*, 650–654. (b) McLean, A. D.; Chandler, G. S. *J. Chem. Phys.* **1980**, *72*, 5639–5648. (c) Curtiss, L. A.; McGrath, M. P.; Blaudeau, J.-P.; Davis, N. E.; Binning, R. C., Jr.; Radom, L. *J. Chem. Phys.* **1995**, *103*, 6104–6113. (d) Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. v. R. *J. Comput. Chem.* **1983**, *4*, 294–301.

[16] Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299-310.

[17] Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999–3093.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6.5
6.0
5.5
5.0
4.5
4.0
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2.5
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1.5
1.0
0.5
0.0
2a
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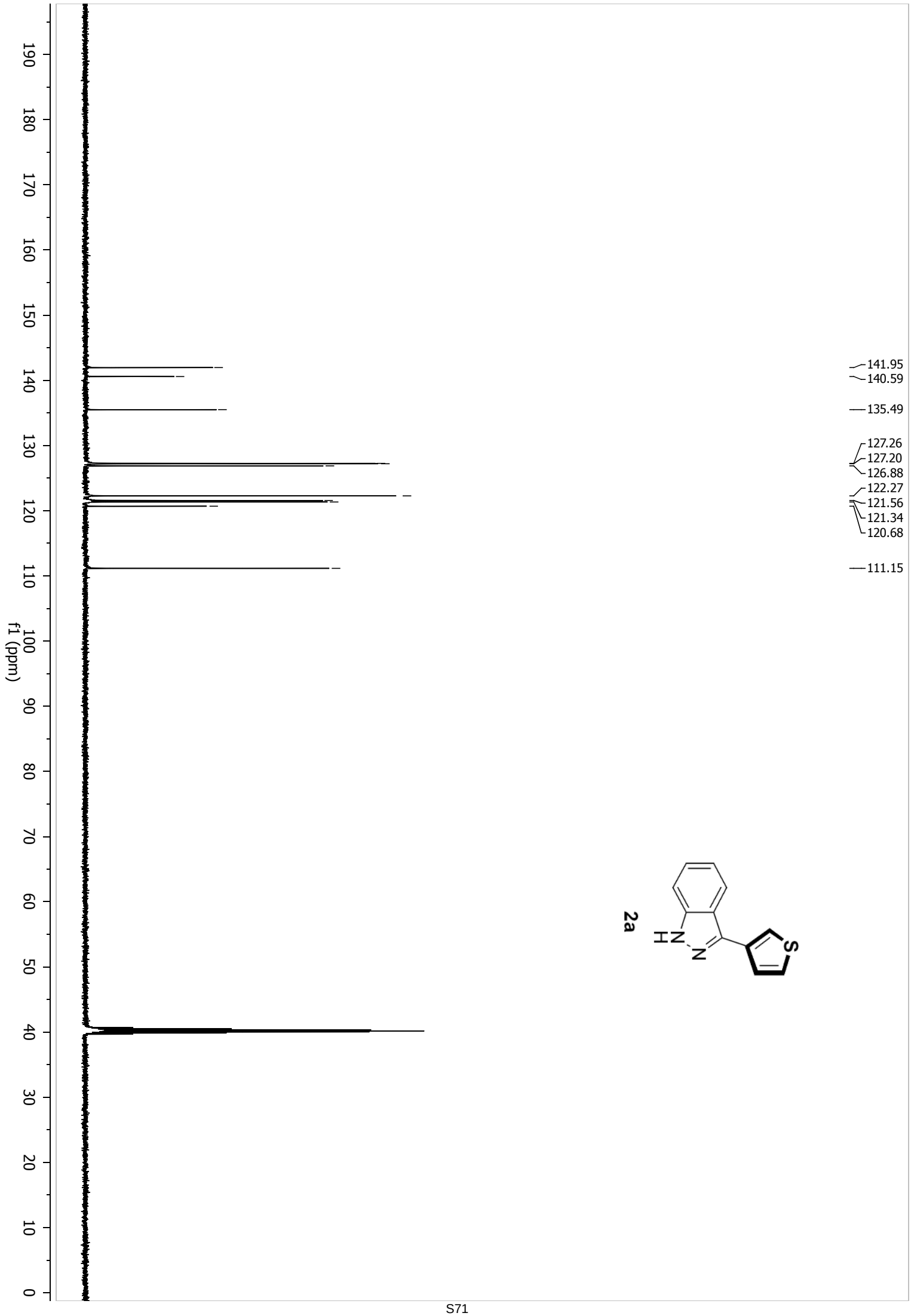
H
N
S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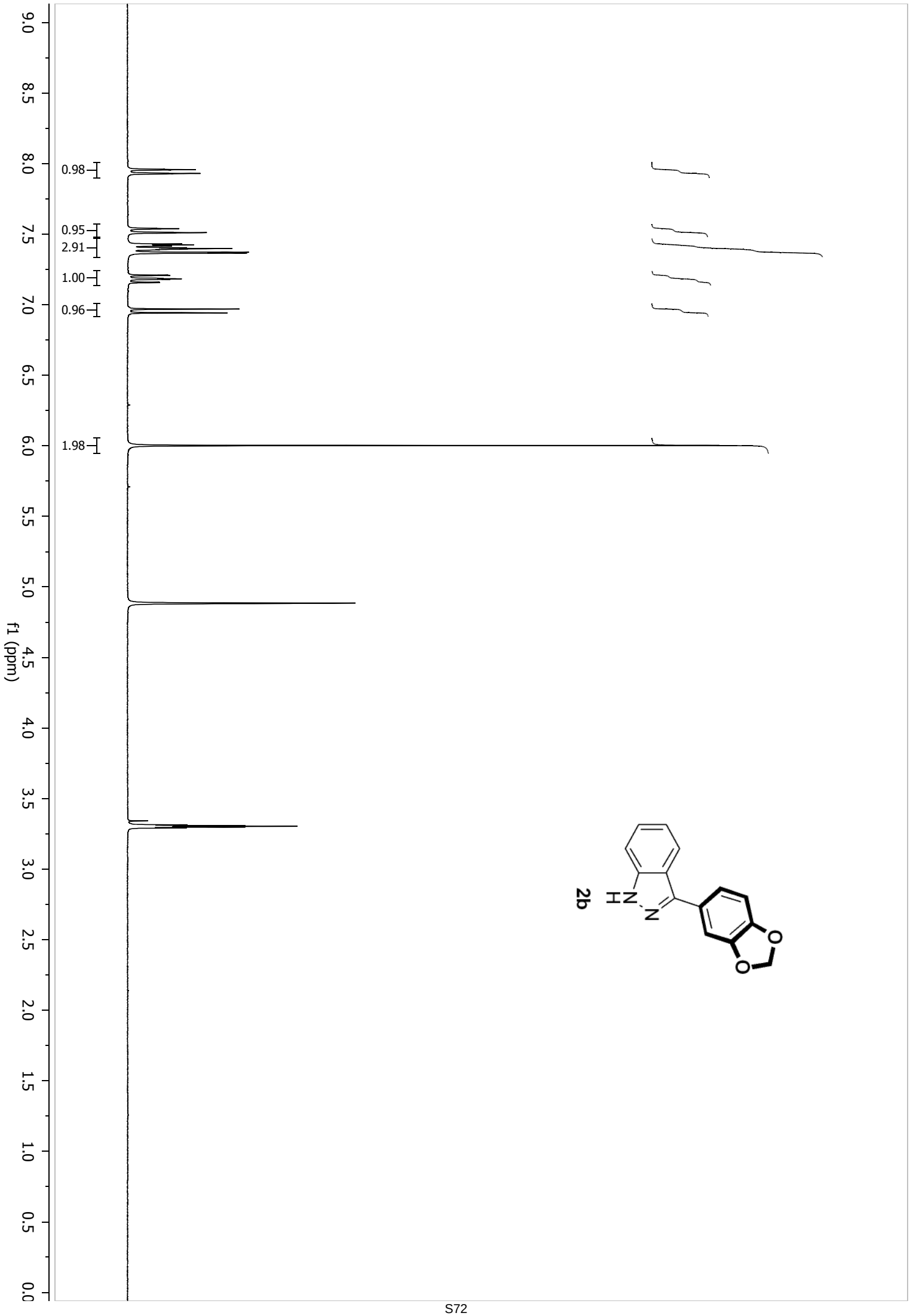
111.15
f1 (ppm)
2a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6.5
6.0
5.5
5.0
4.5
4.0
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2.0
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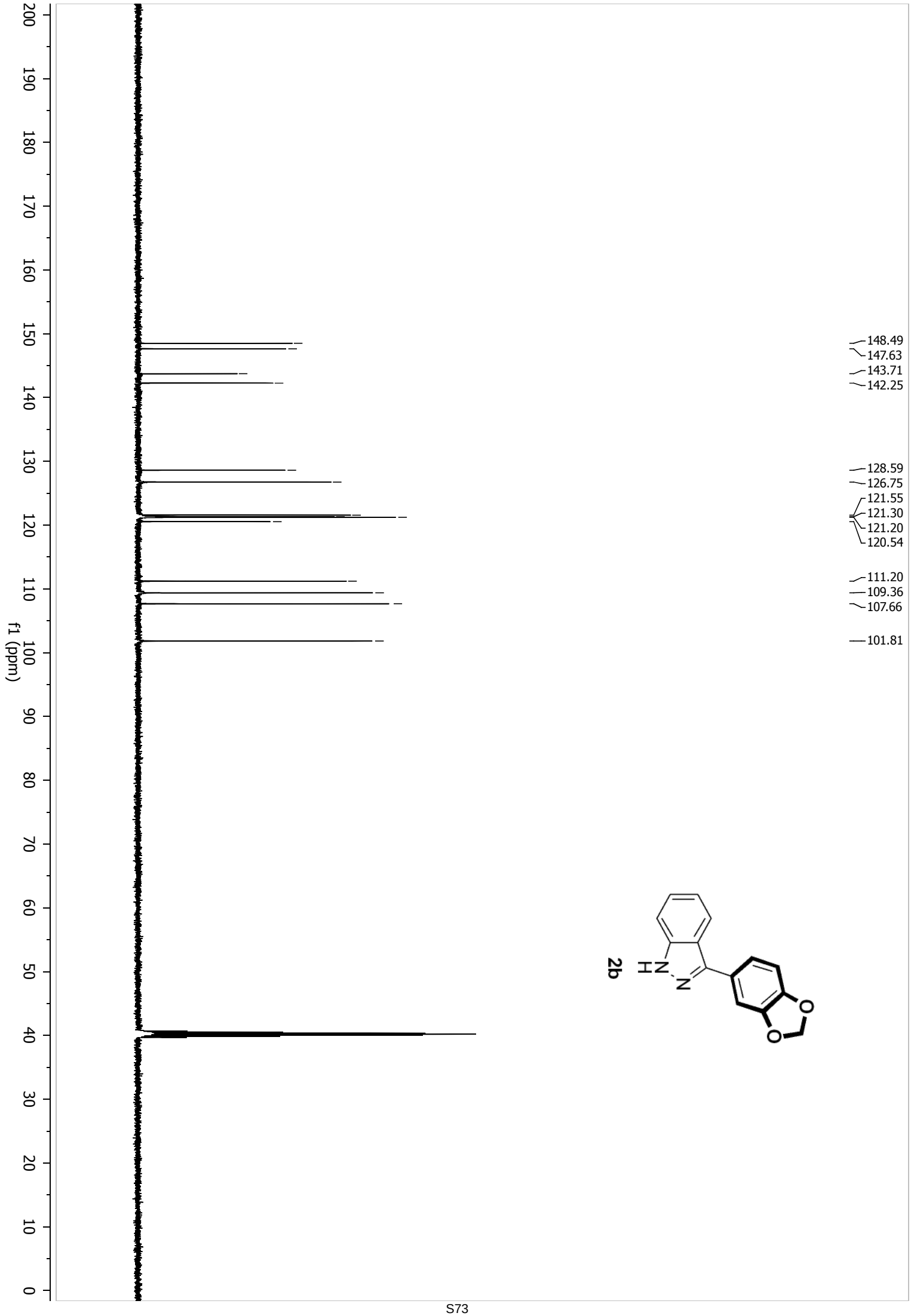
0.0
2b
H
N
N
O
O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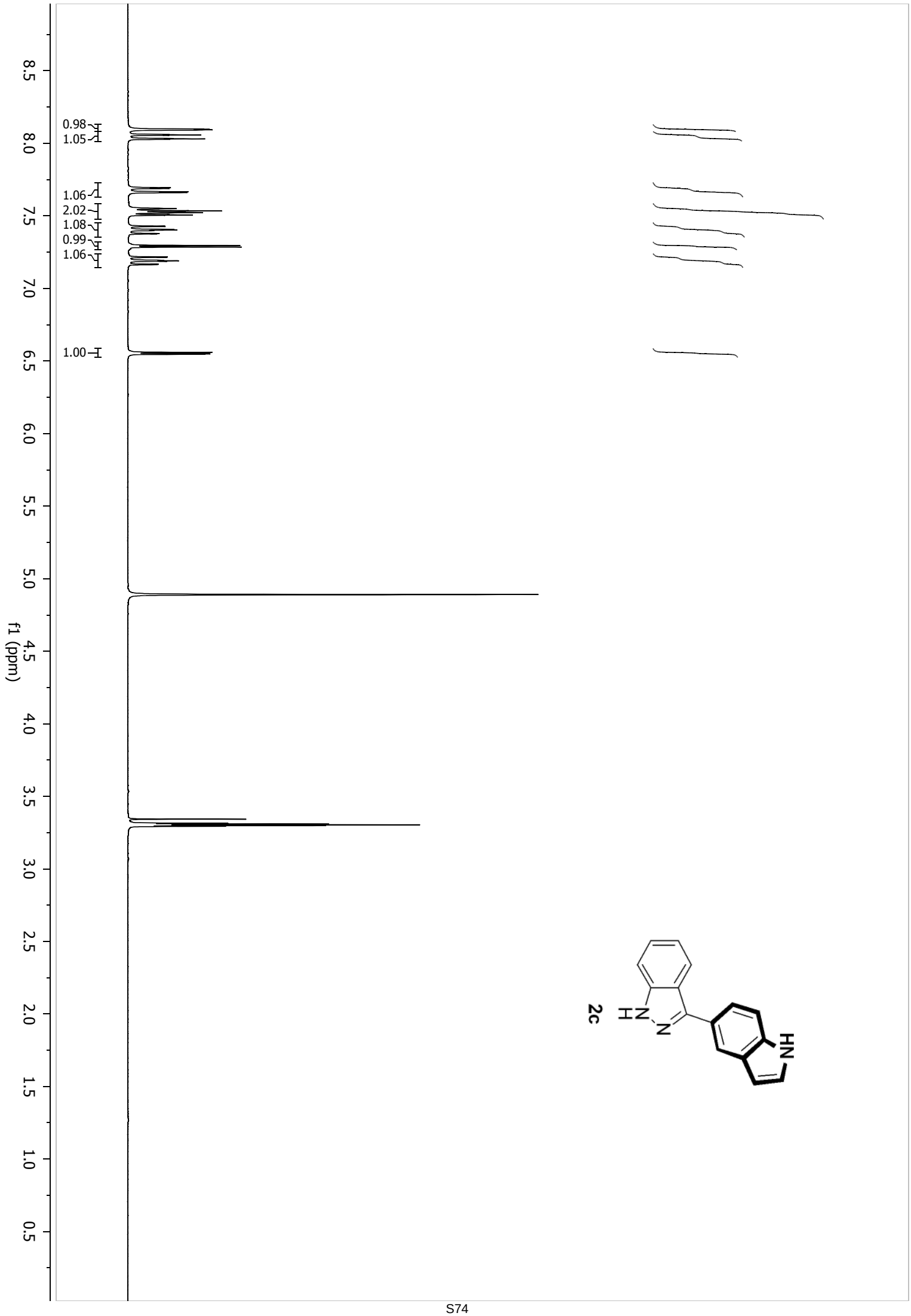
101.81
f1 (ppm)
2b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6.0
5.5
5.0
4.5
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f1 (ppm)
2c
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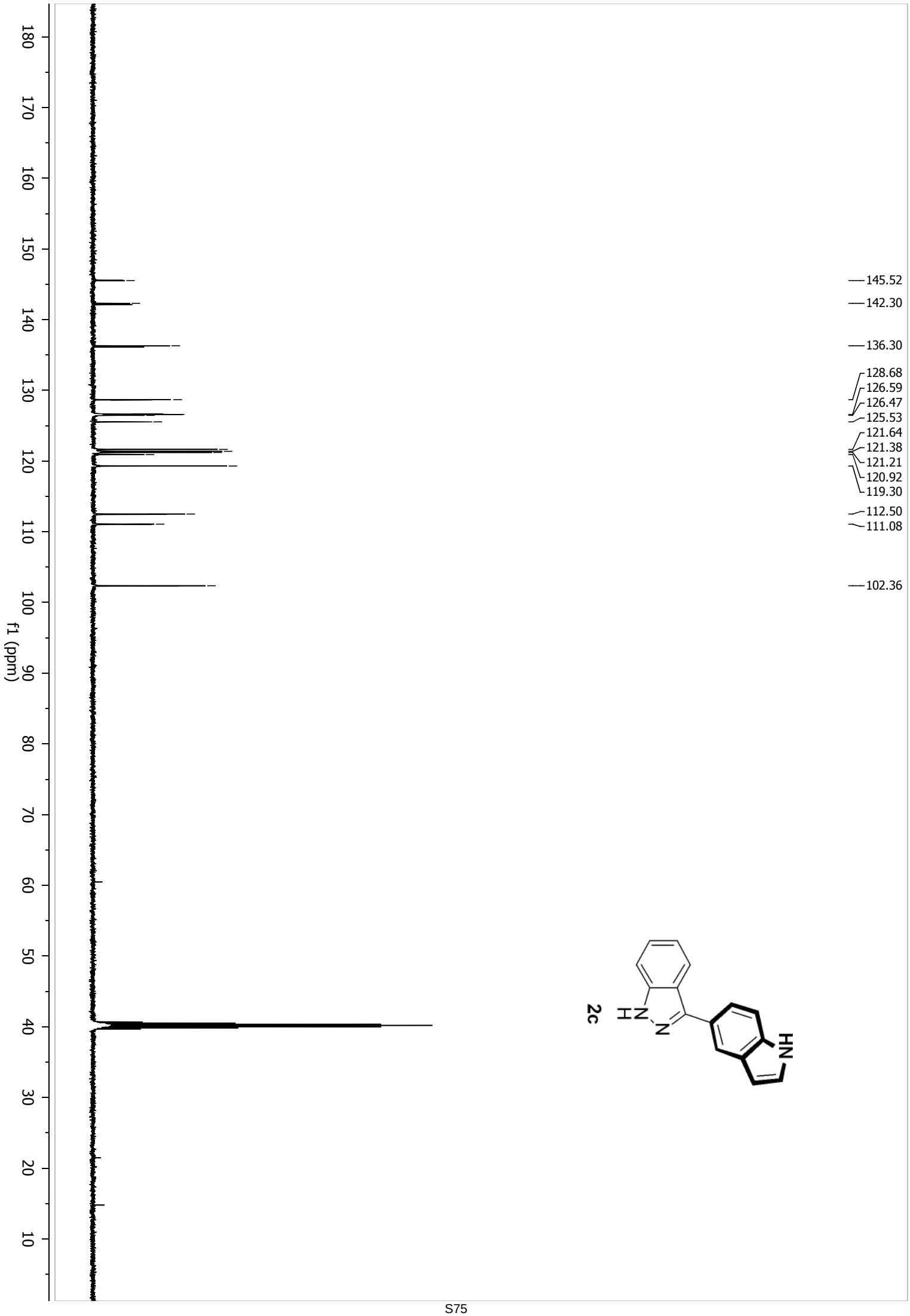
H
N
HN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112.50
111.08
102.36
f1 (ppm)
180
170
160
150
140
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110
100
90
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70
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50
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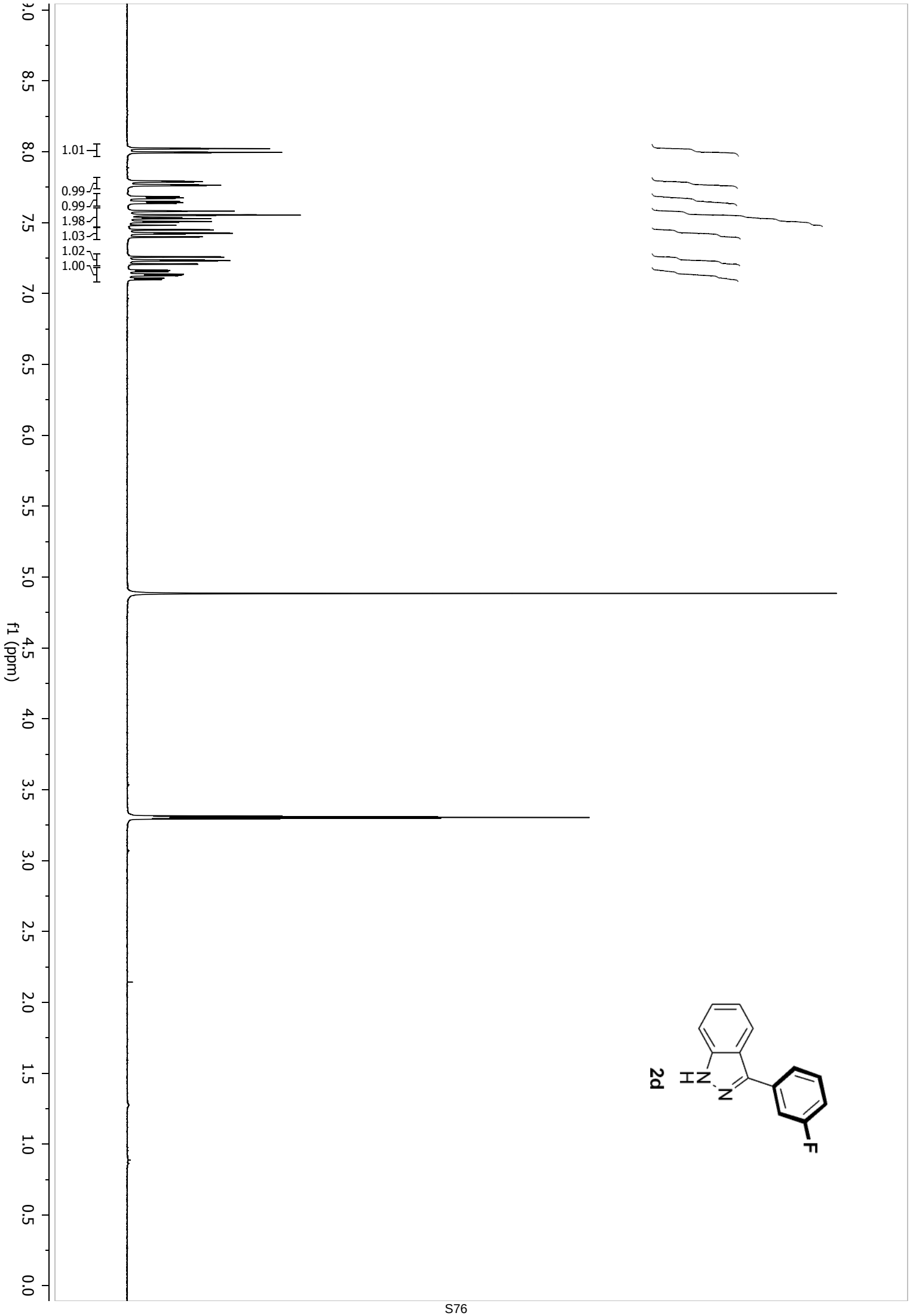
30
20
10
2c
N
H
N
HN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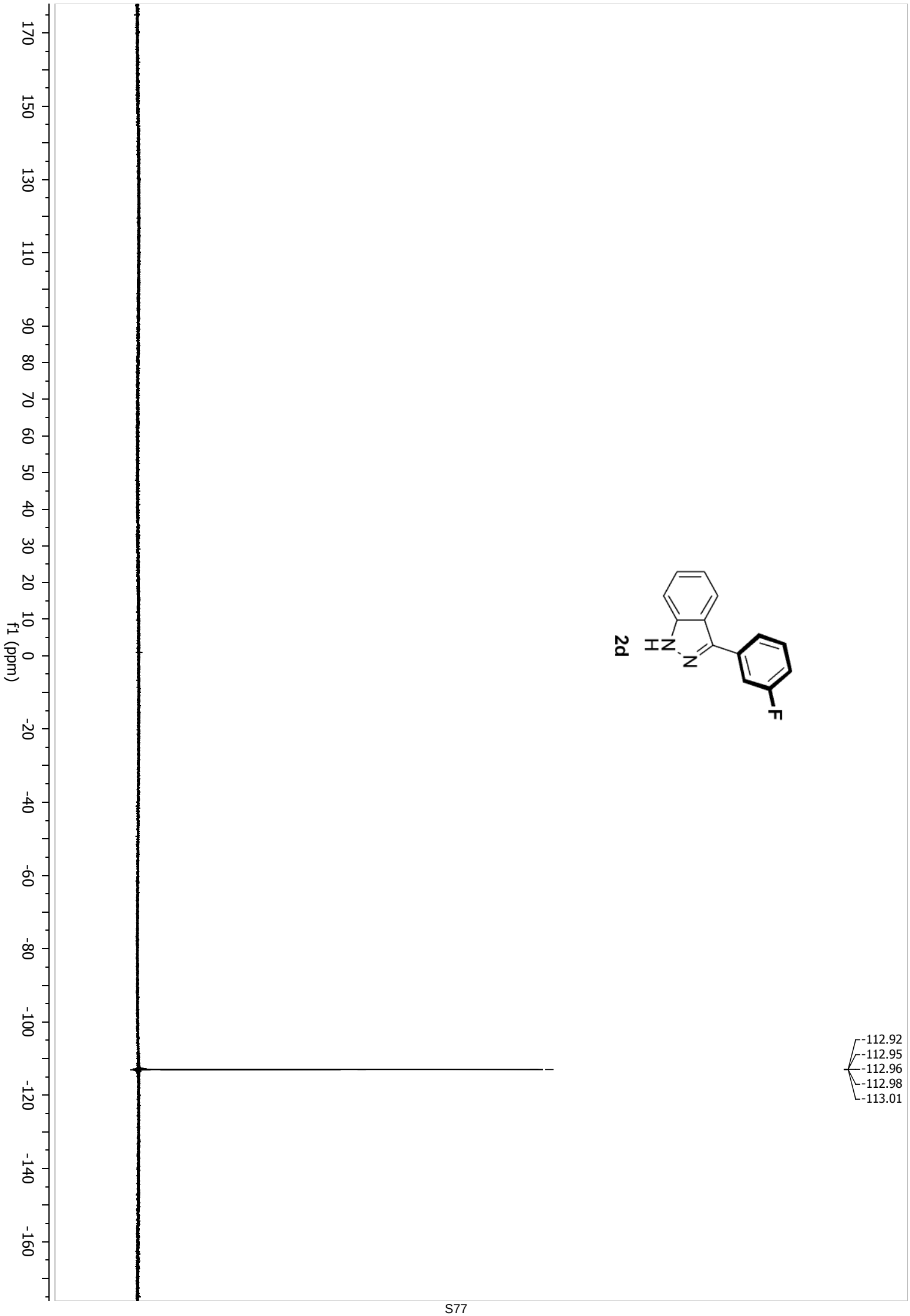
2d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20
10
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-40
-60
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-140
-160
f1 (ppm)
2d
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-112.95
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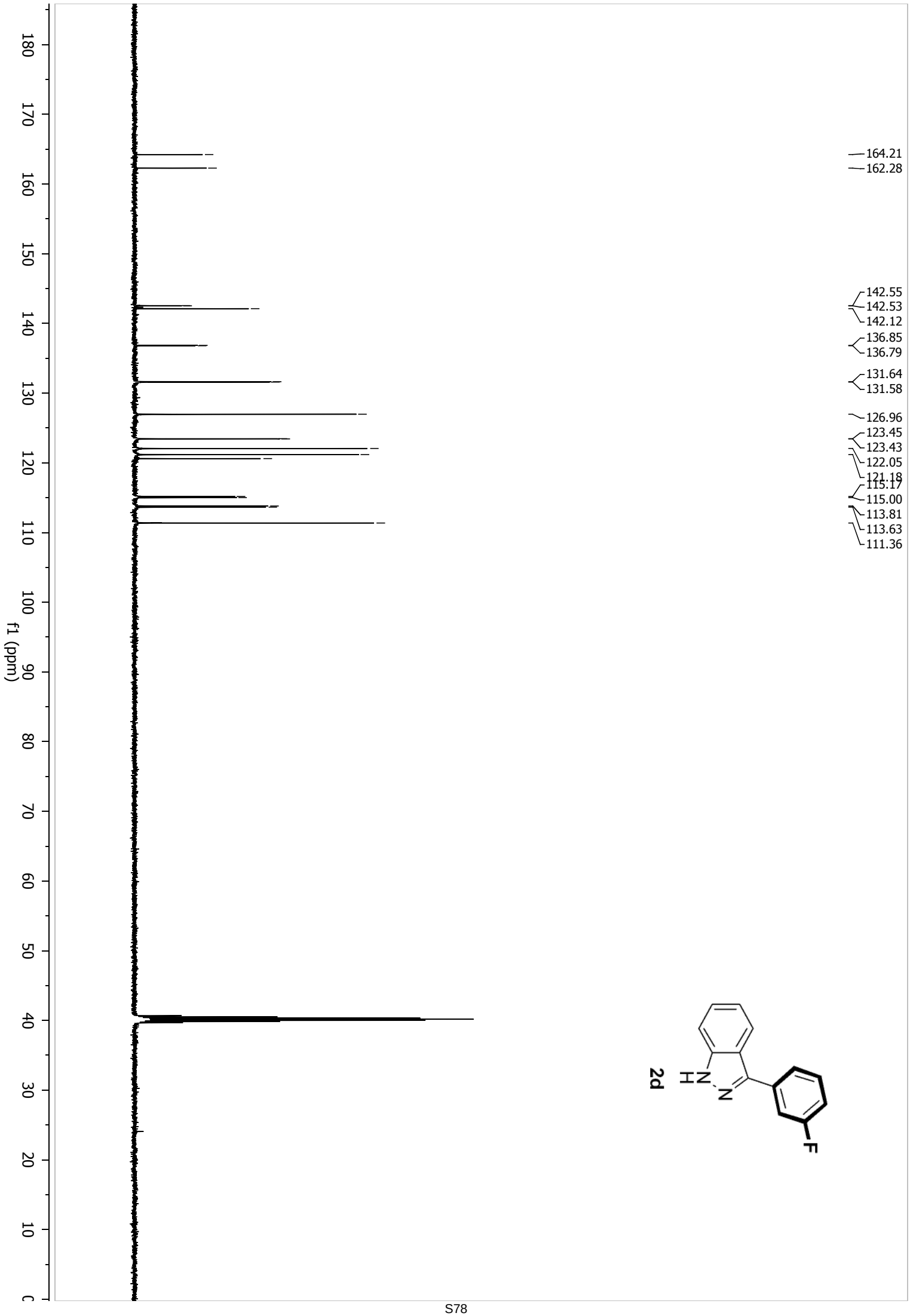
-112.98
-113.01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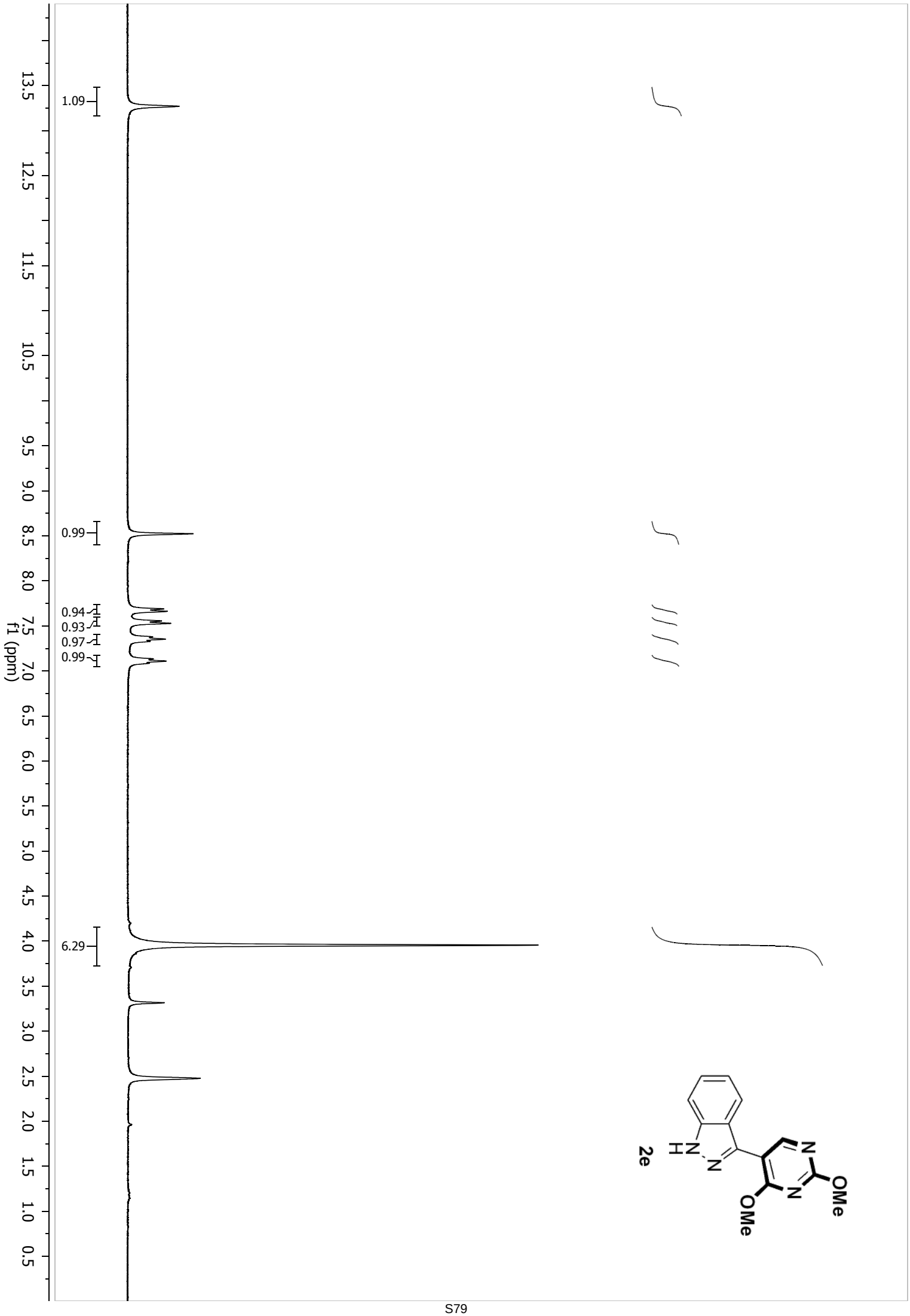
f1 (ppm)
2d
N
H
N
F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4.0
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H
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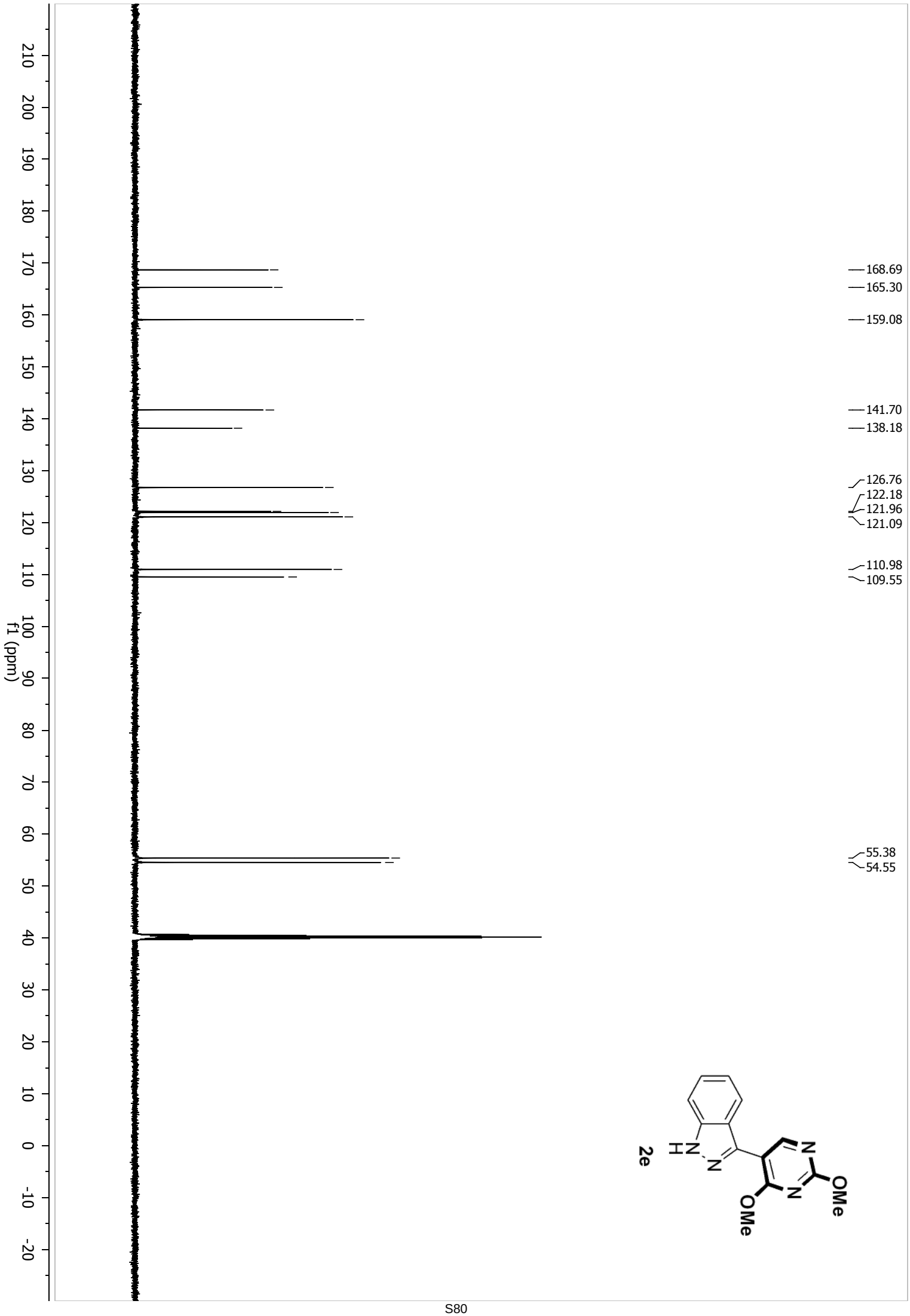
N
OMe
OMe

2e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f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
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30
20
10
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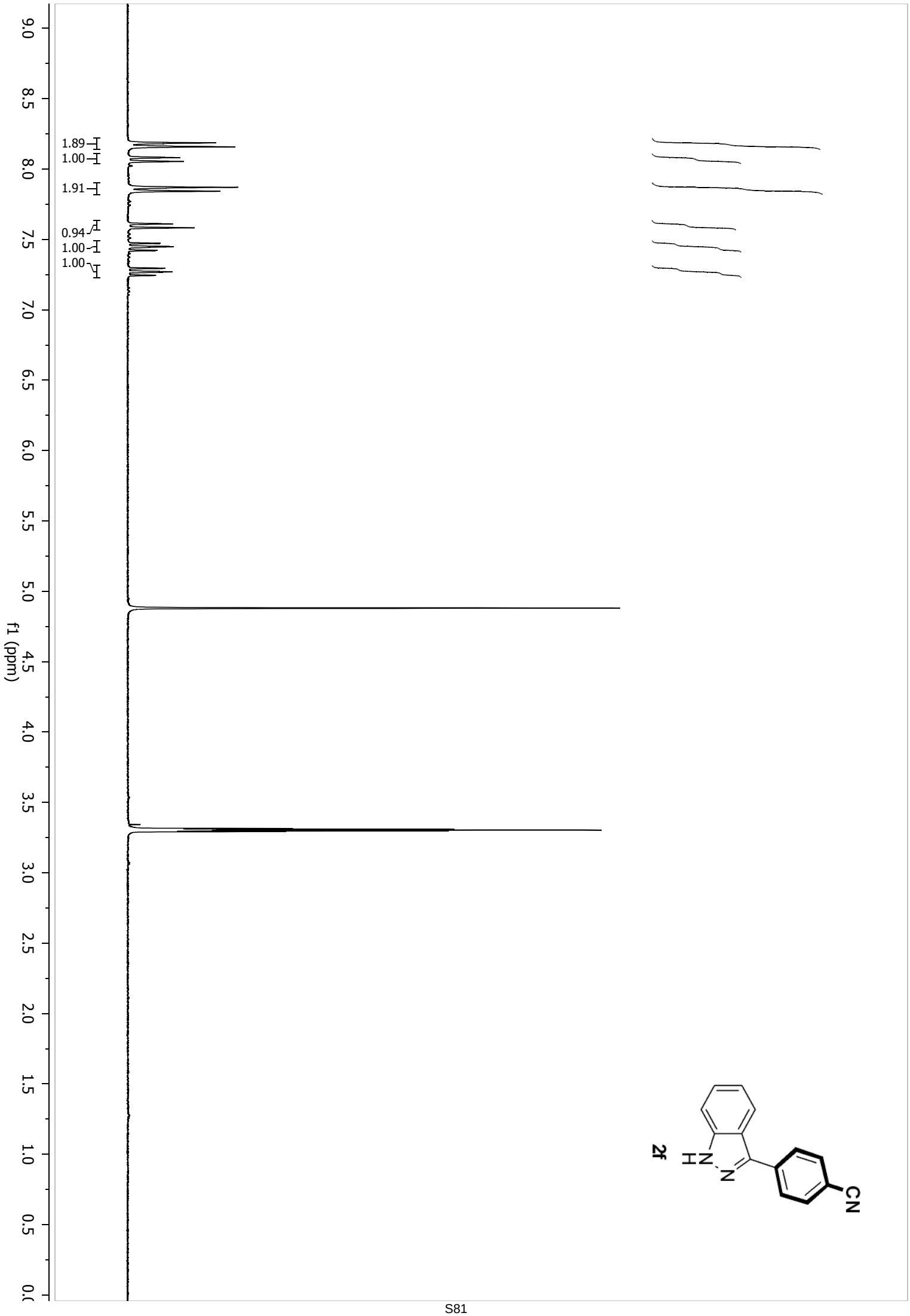
-10
-20
2e
N
H
N
N
N
OMe
OMe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4.5
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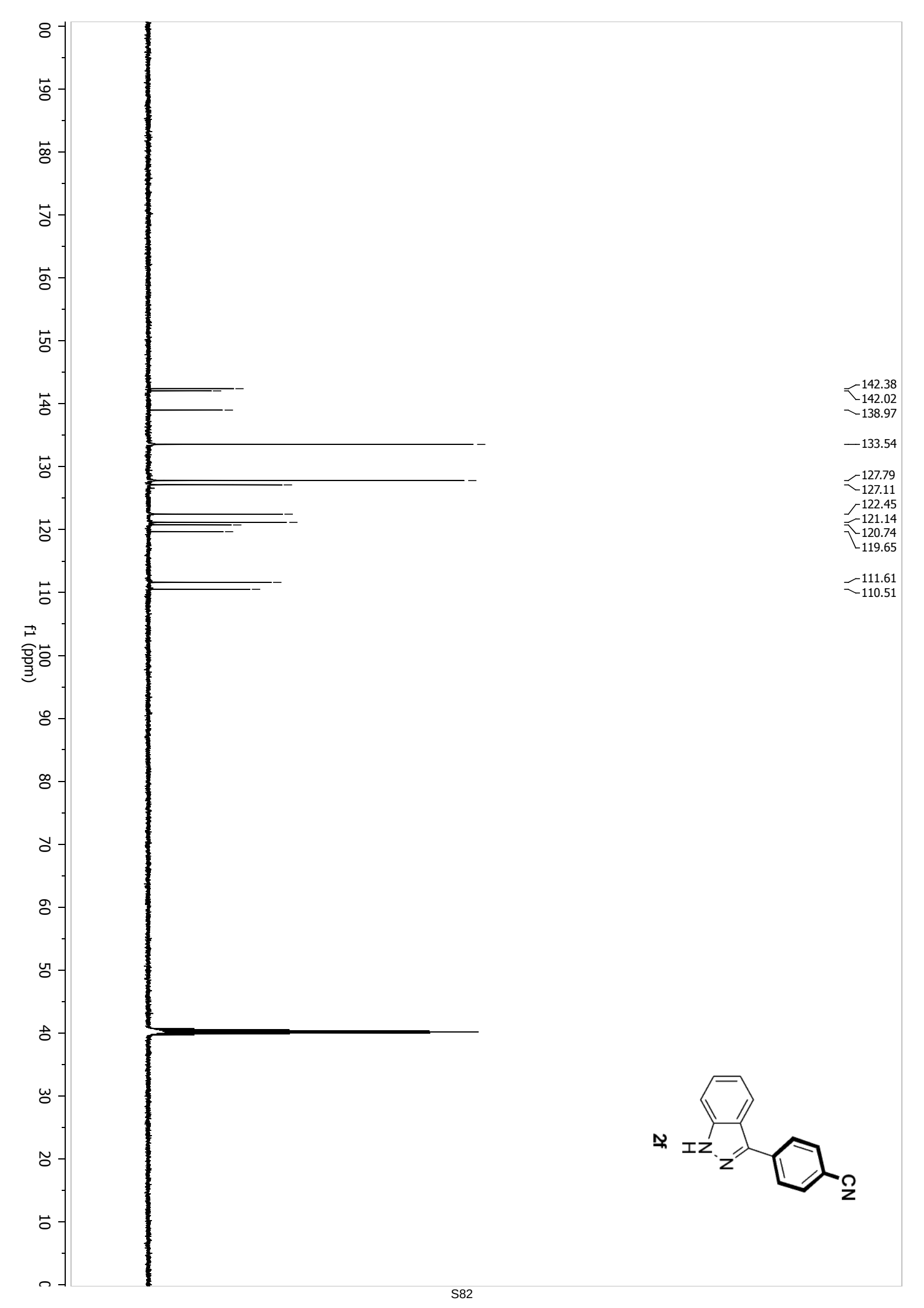
N
N
CN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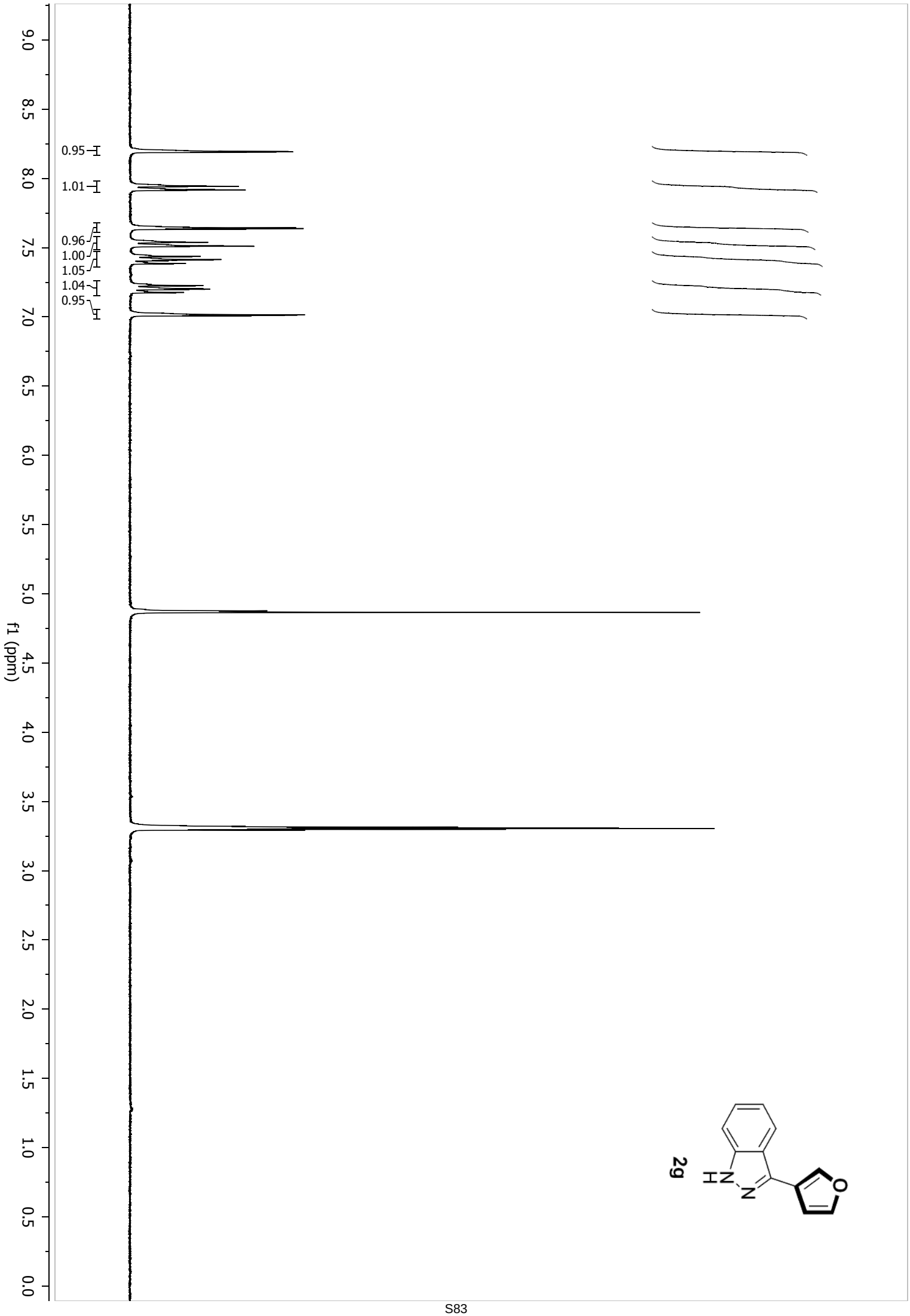
N
CN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6.5
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5.0
4.5
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0.0
2g
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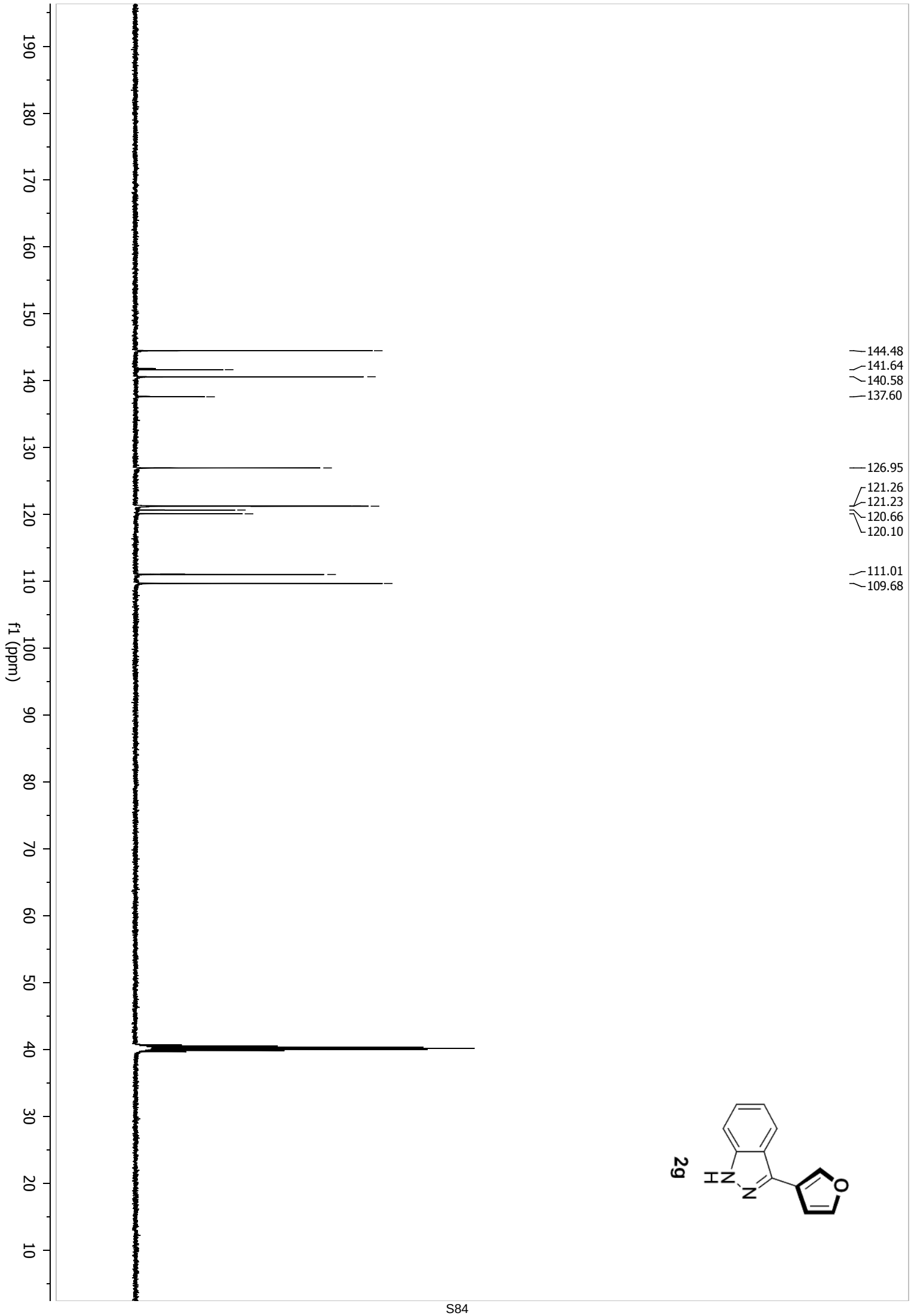
H
N
O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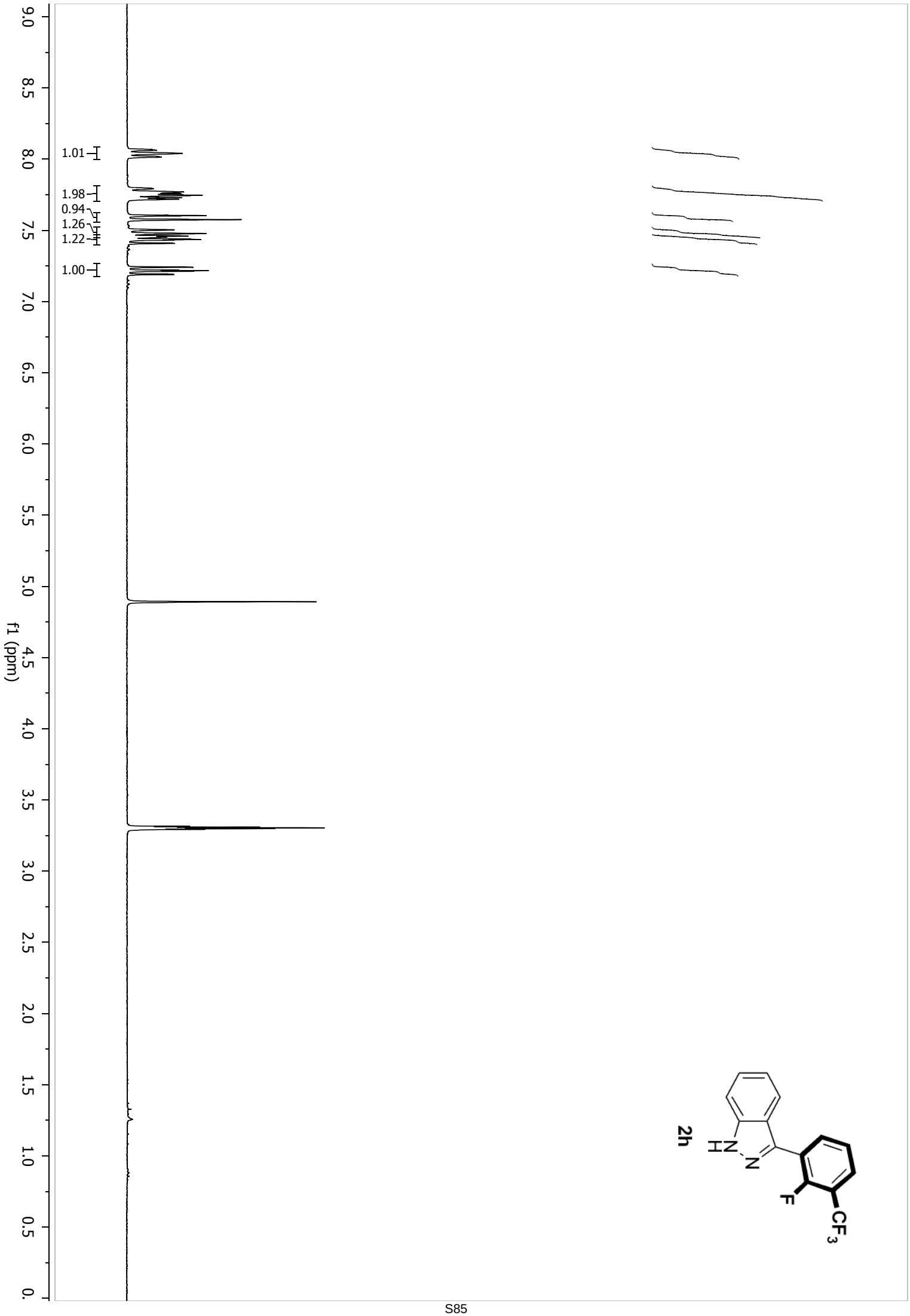
f1 (ppm)
2g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6.0
5.5
5.0
4.5
4.0
3.5
3.0
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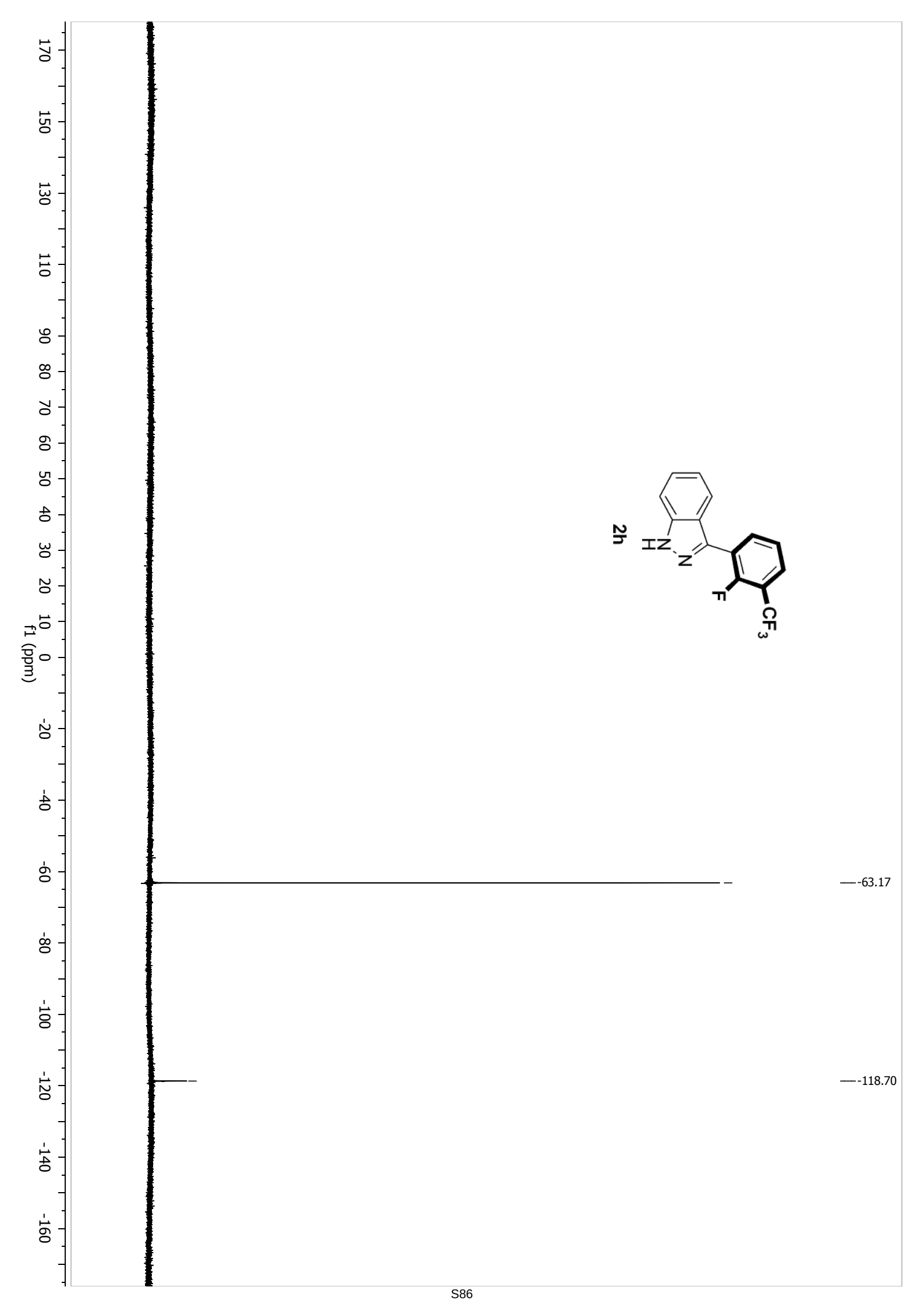
1.5
1.0
0.5
0.
f1 (ppm)
2h
N
H
N
F
CF3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130
110
90
80
70
60
50
40
30
20
10
0
-20
-40
-60
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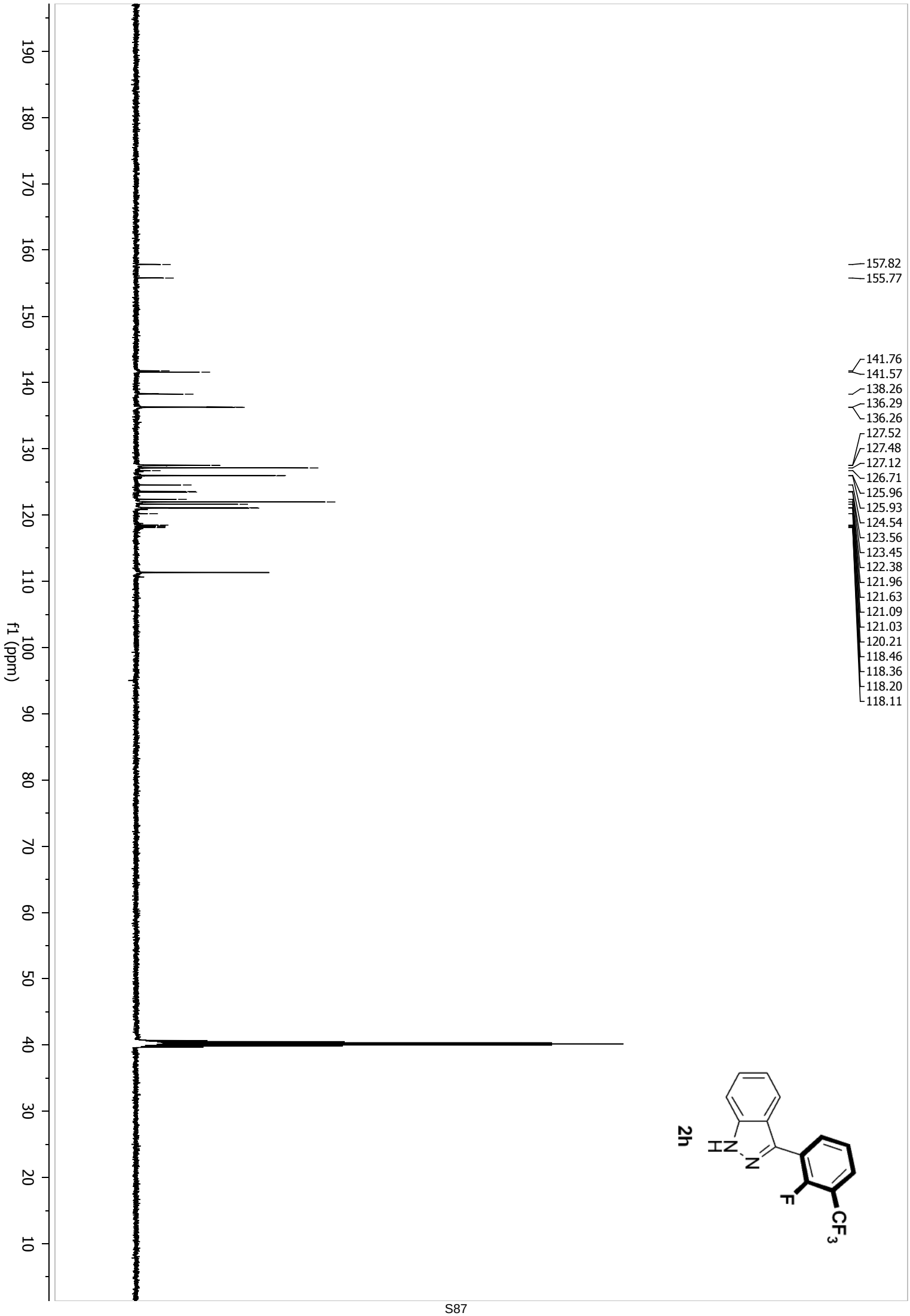
-100
-120
-140
-160
f1 (ppm)
2h
N
H
N
F
CF3
-63.17
-118.70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122.38
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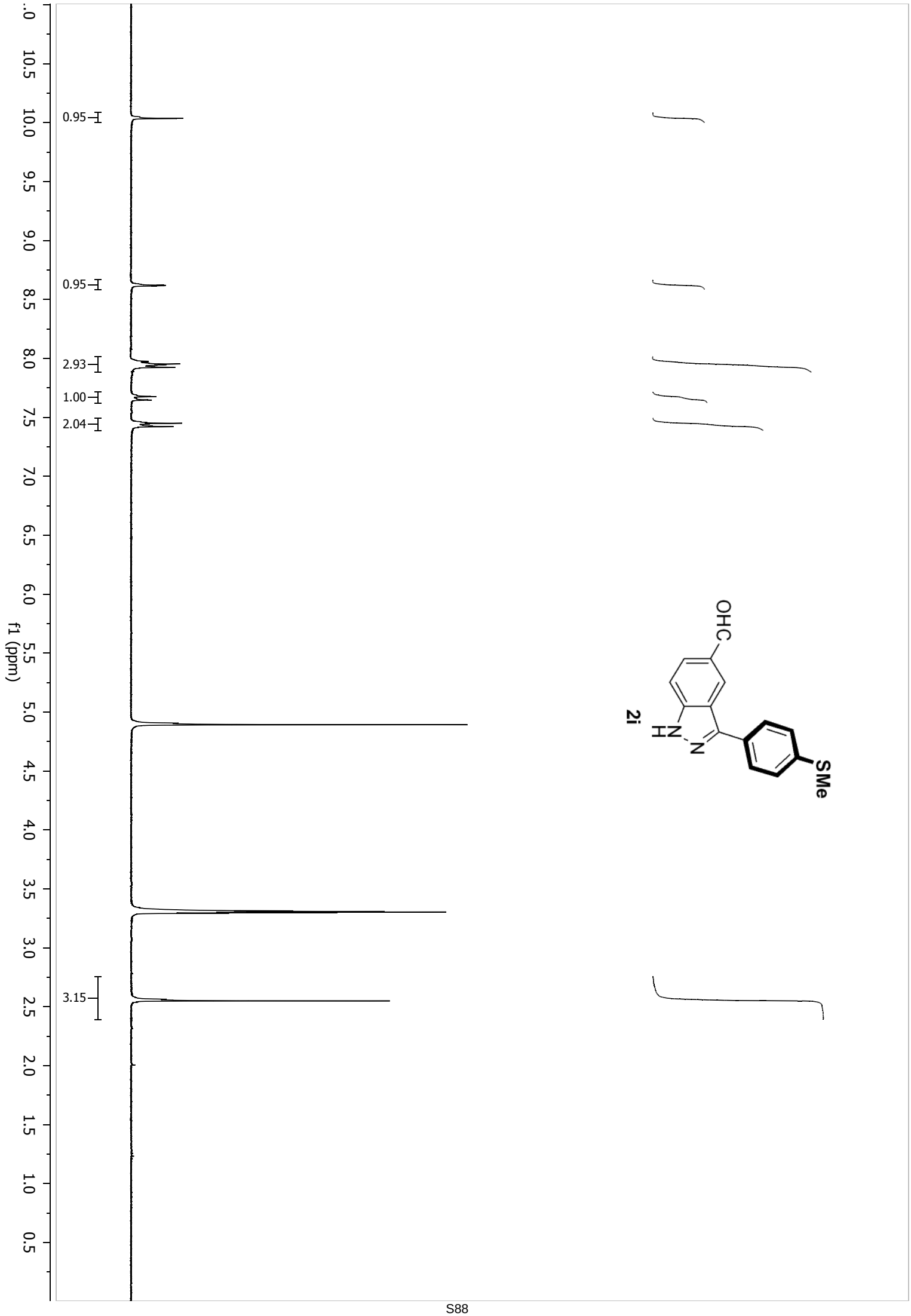
118.11
f1 (ppm)
2h
F
CF3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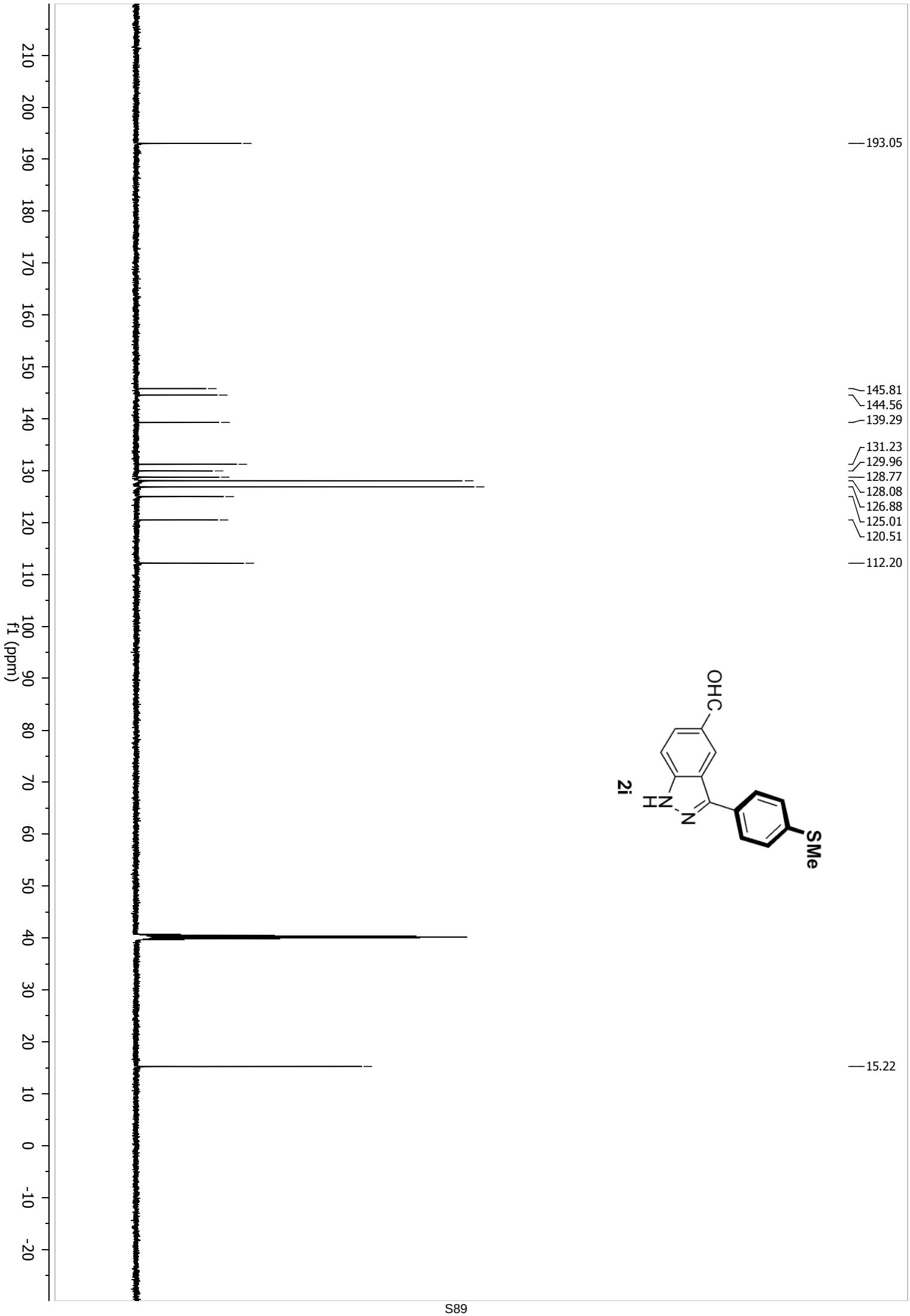
SMe
2i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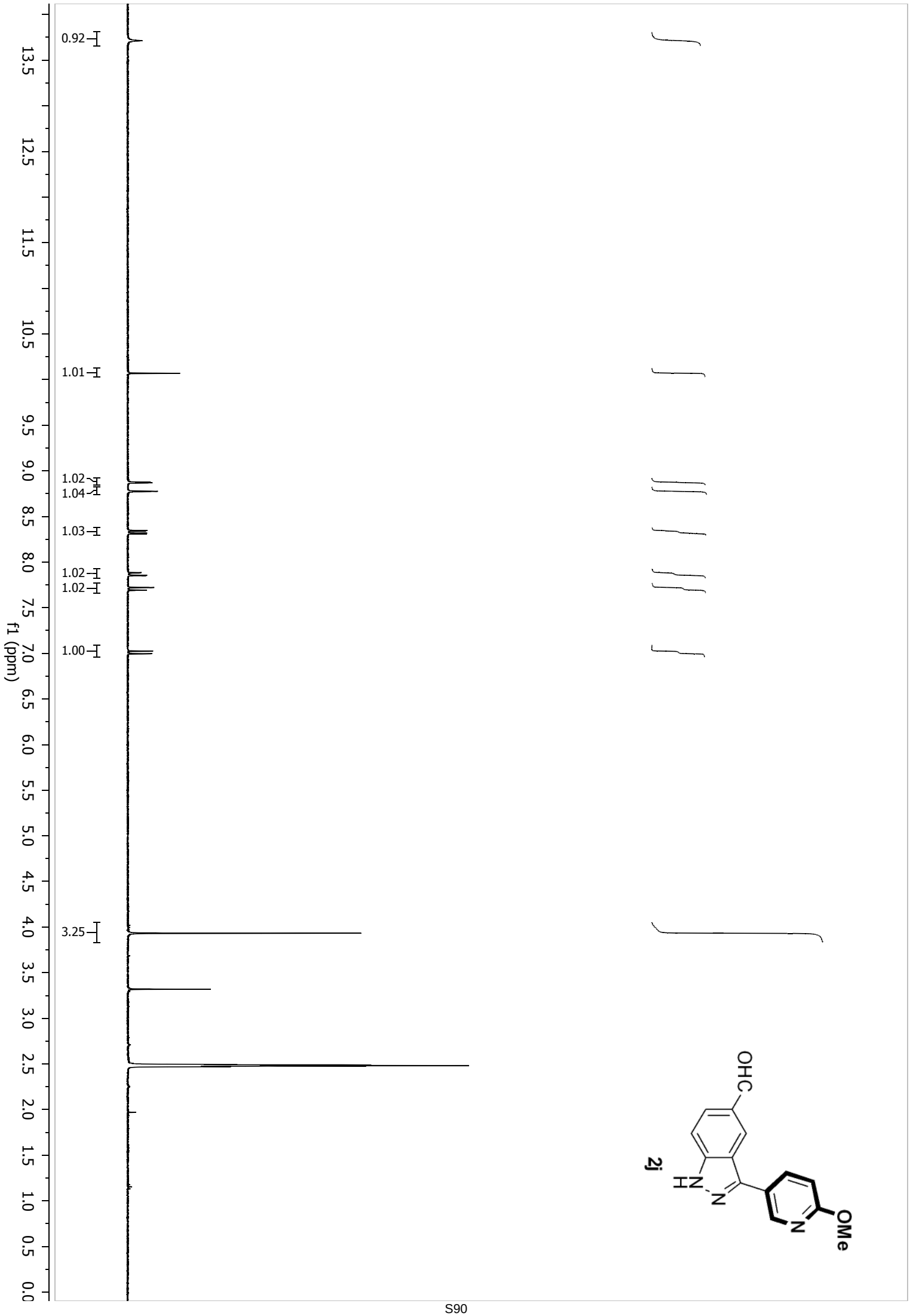
f1 (ppm)
OHC
N
H
N
SMe
2i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11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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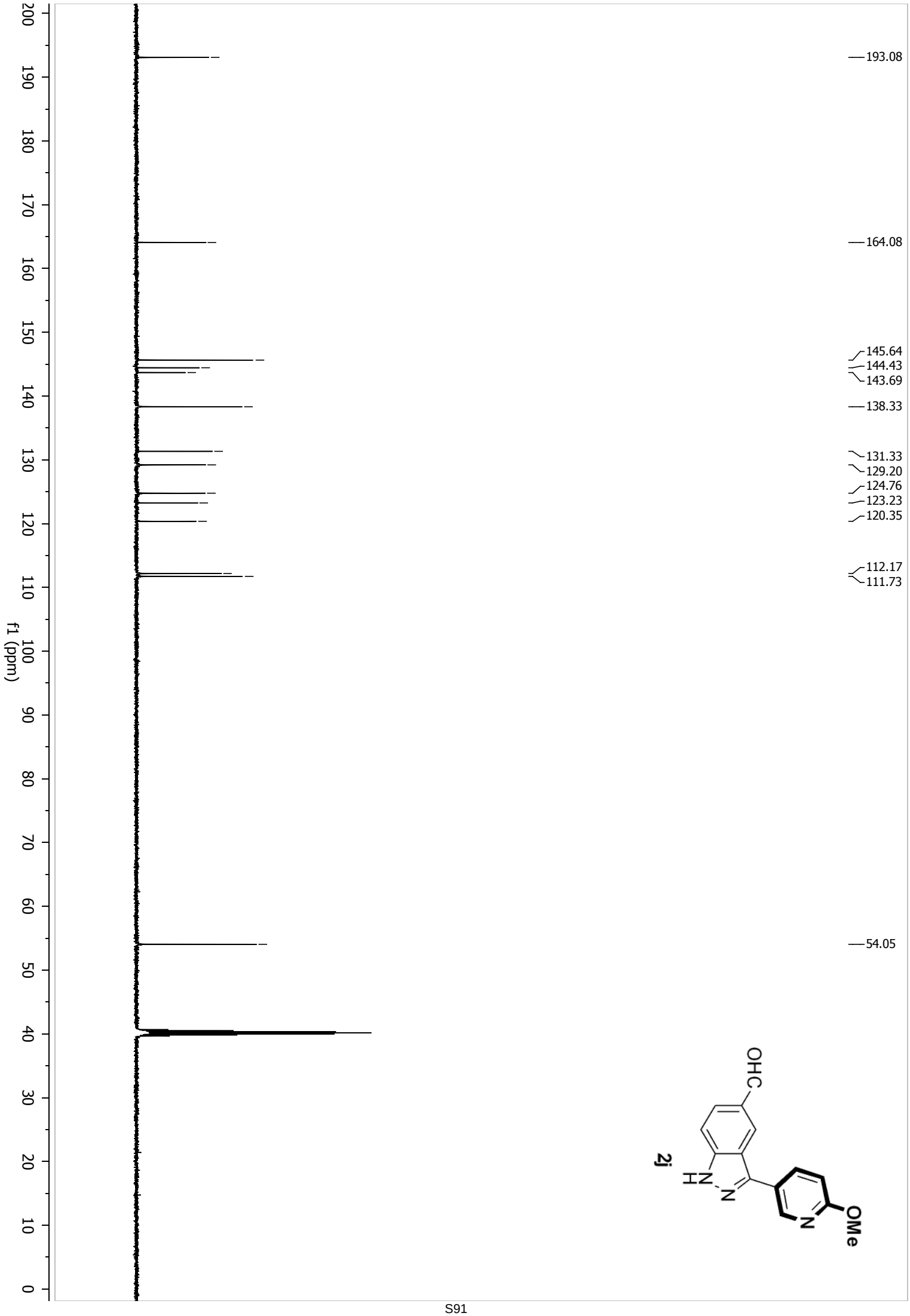
OHC
H
N
N
N
OMe
2j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OHC
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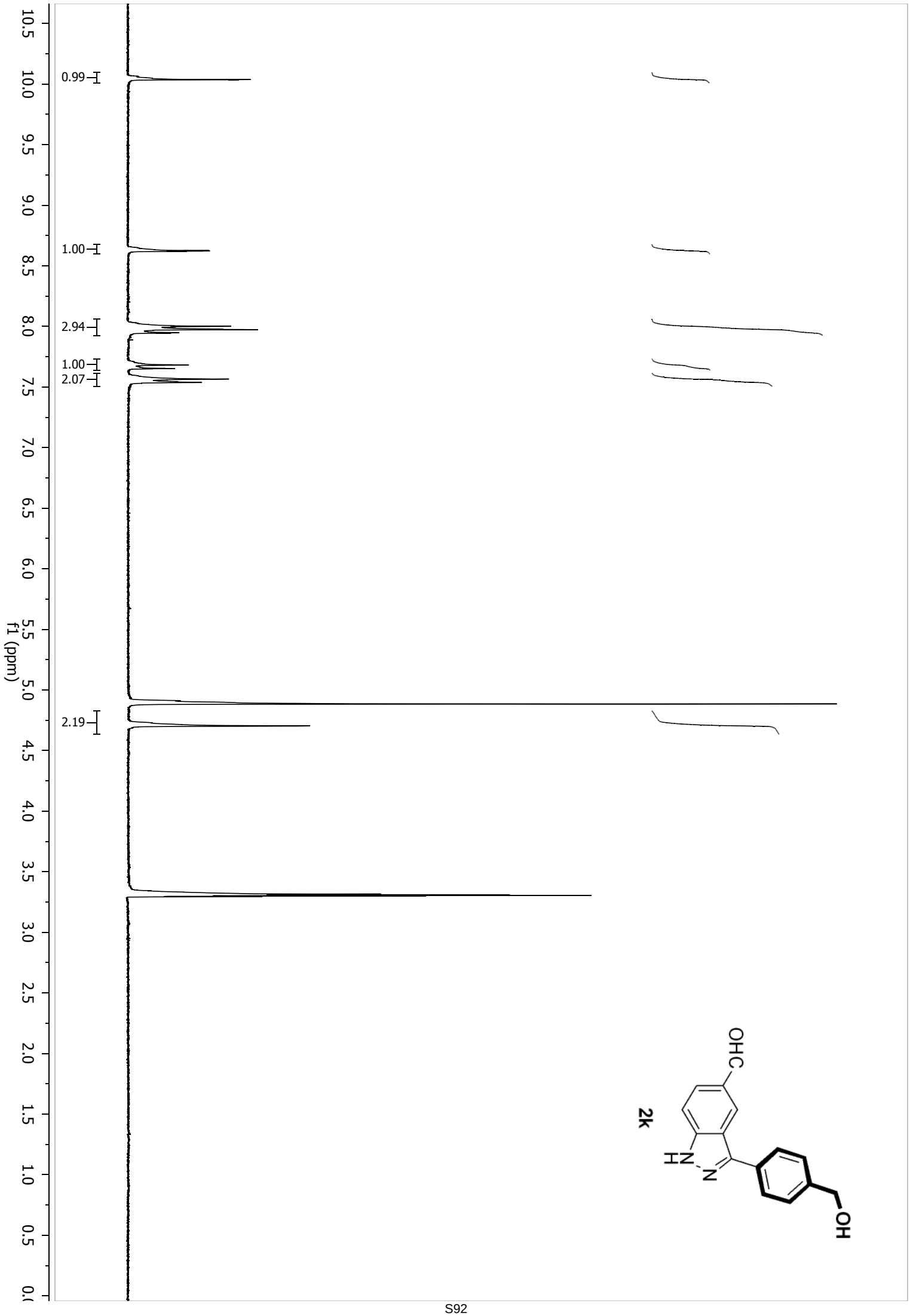
N
N
OMe
2j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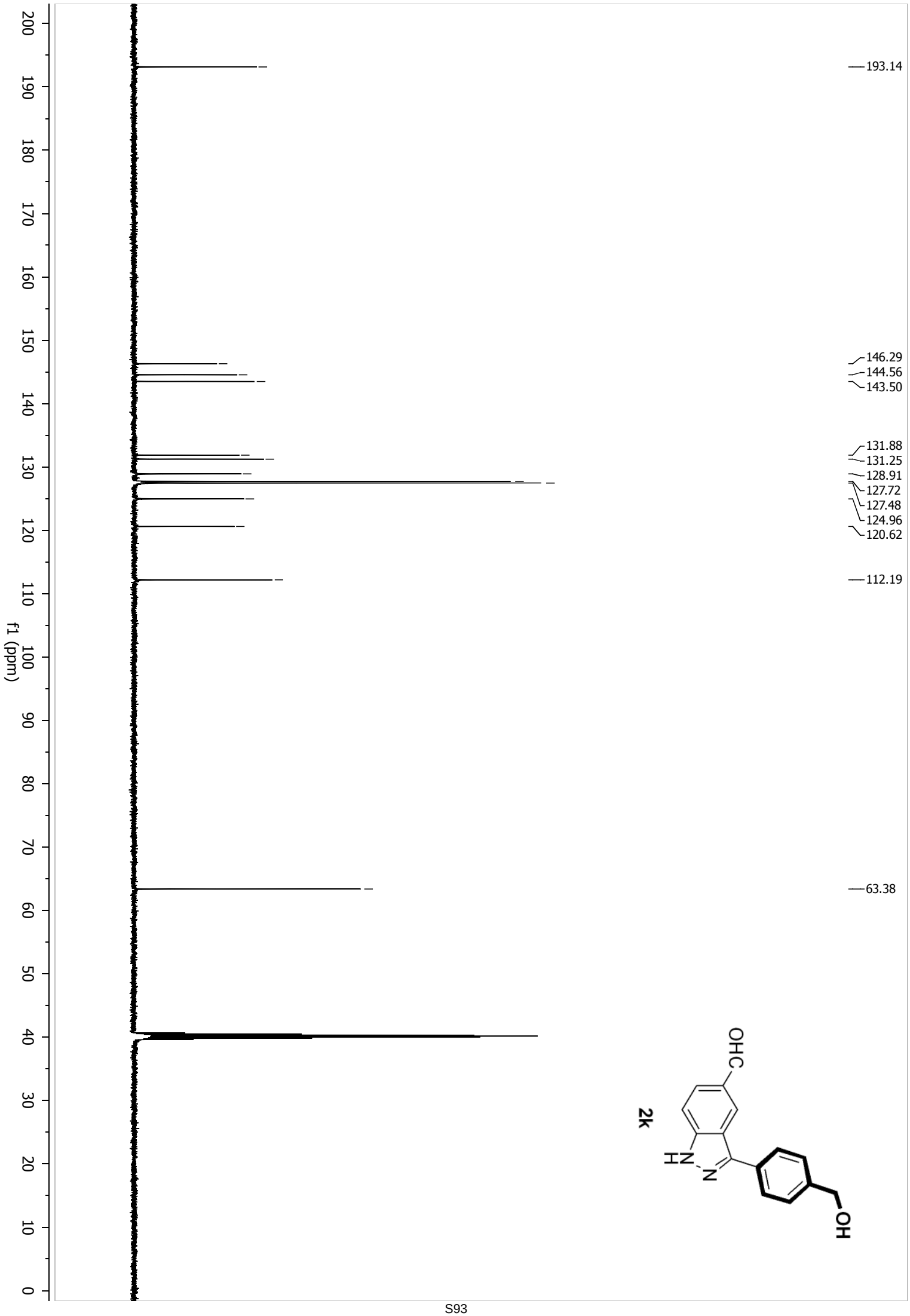
N
H
N
OH
2k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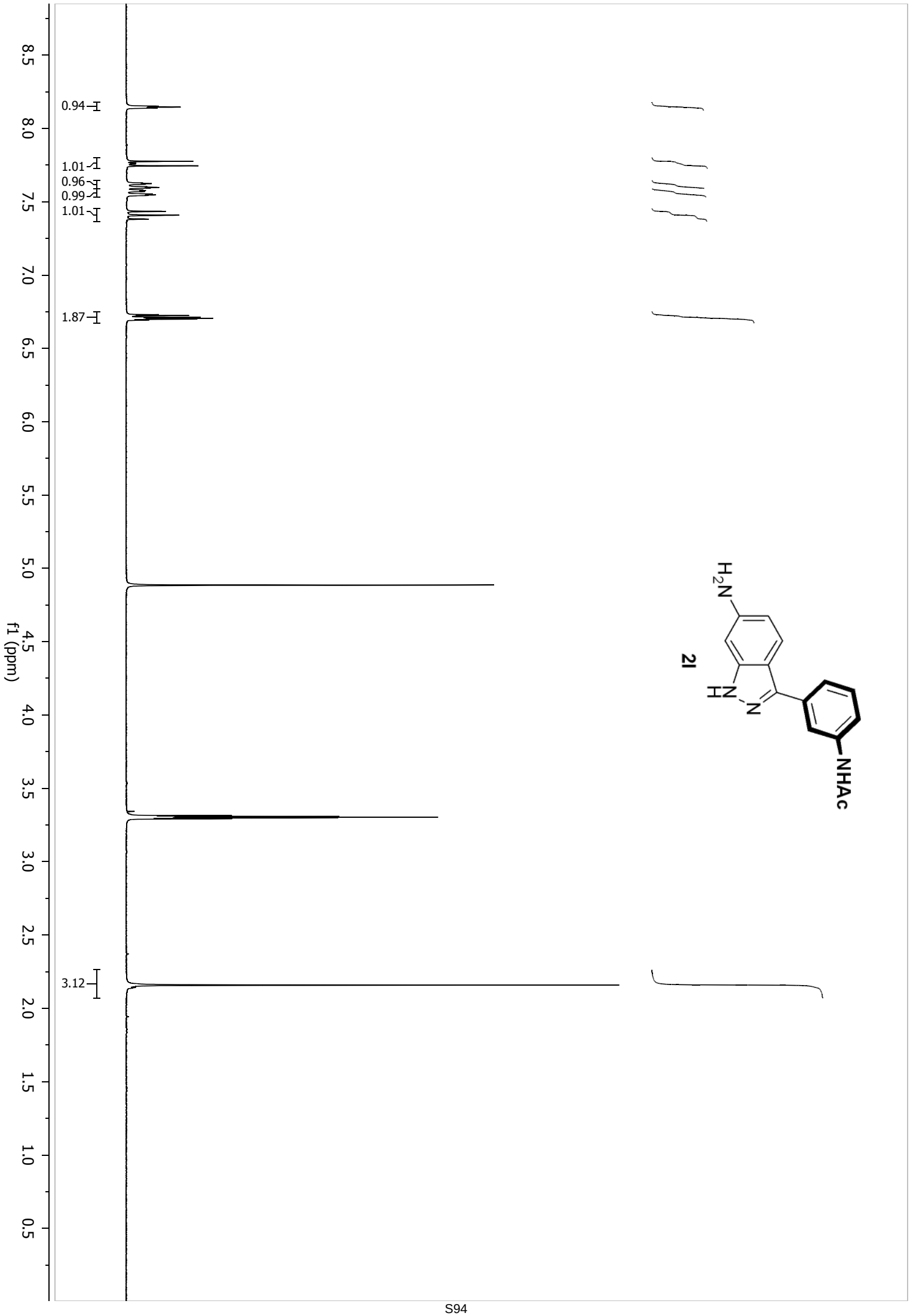
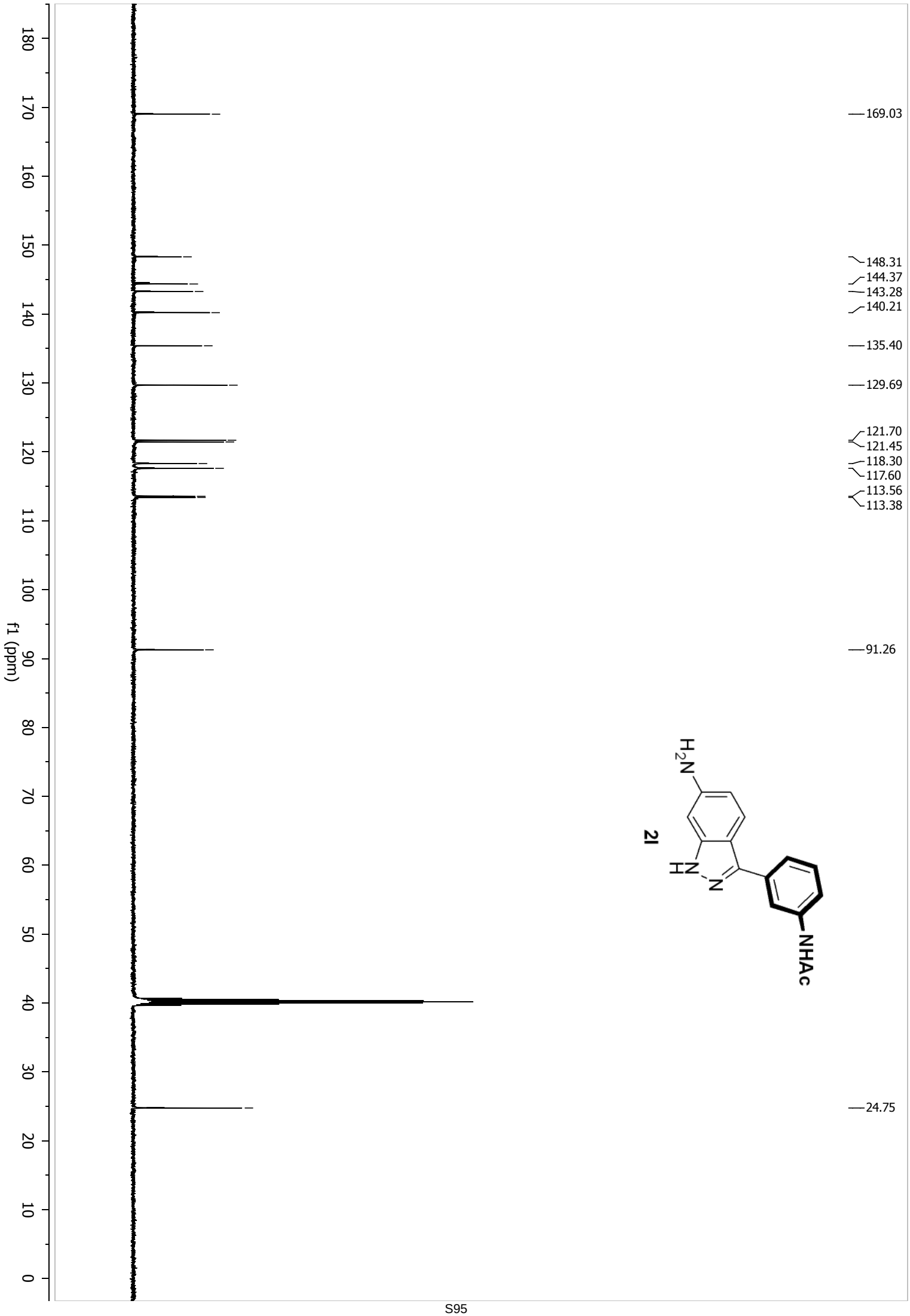
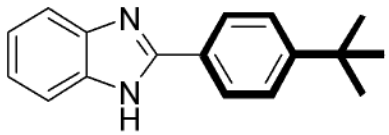
124.96
120.62
112.19
63.38
f1 (ppm)
OHC
OH
N
H
N

2k


0.94
1.01
0.96
0.99
1.01
1.87
3.12
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
H2N
N
H
N
NHAc
2l


169.03
148.31
144.37
143.28
140.21
135.40
129.69
121.70
121.45
118.30
117.60
113.56
113.38
91.26
24.75
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
H2N
N
H
N
NHAc
2l



3a

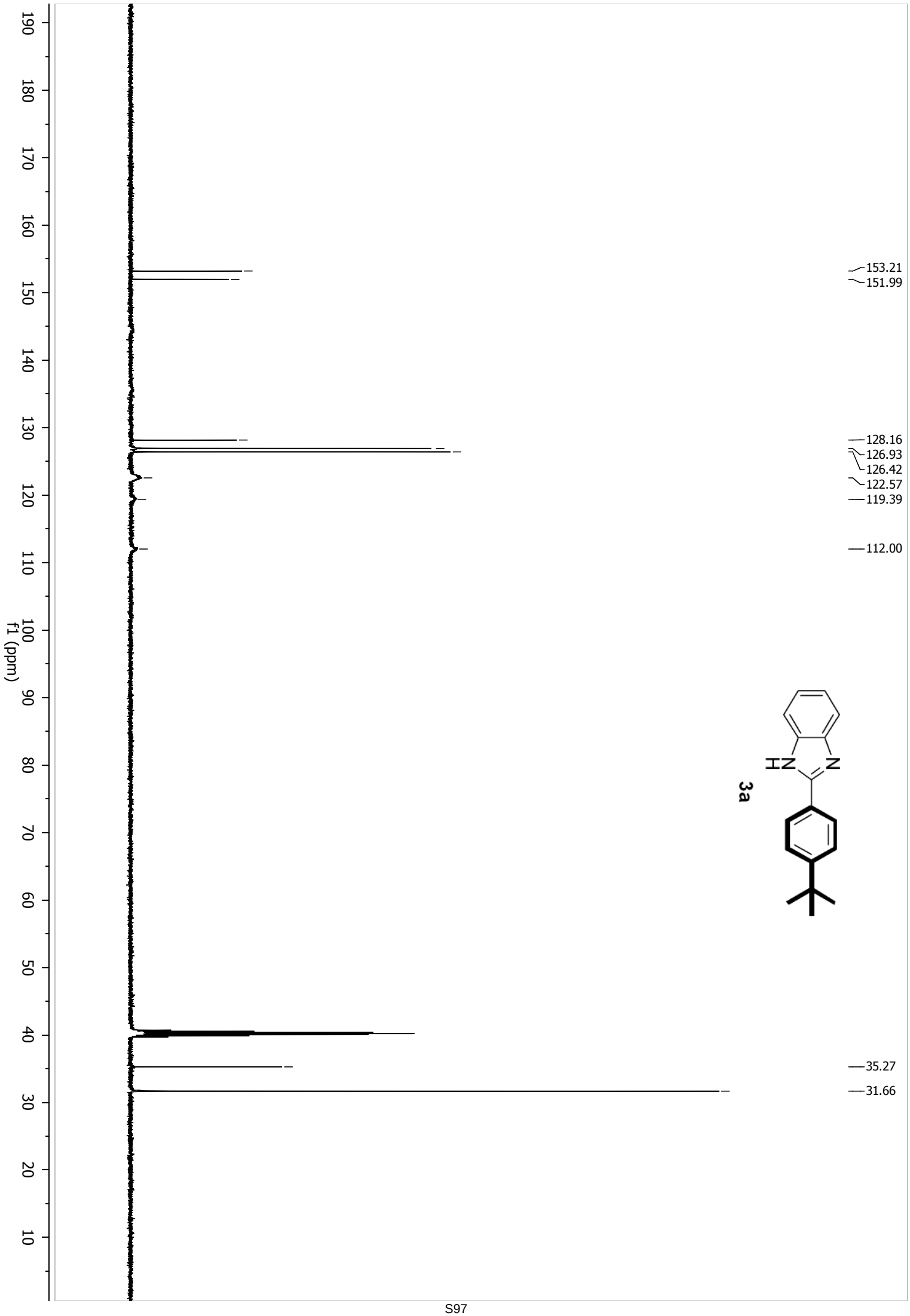
1.97

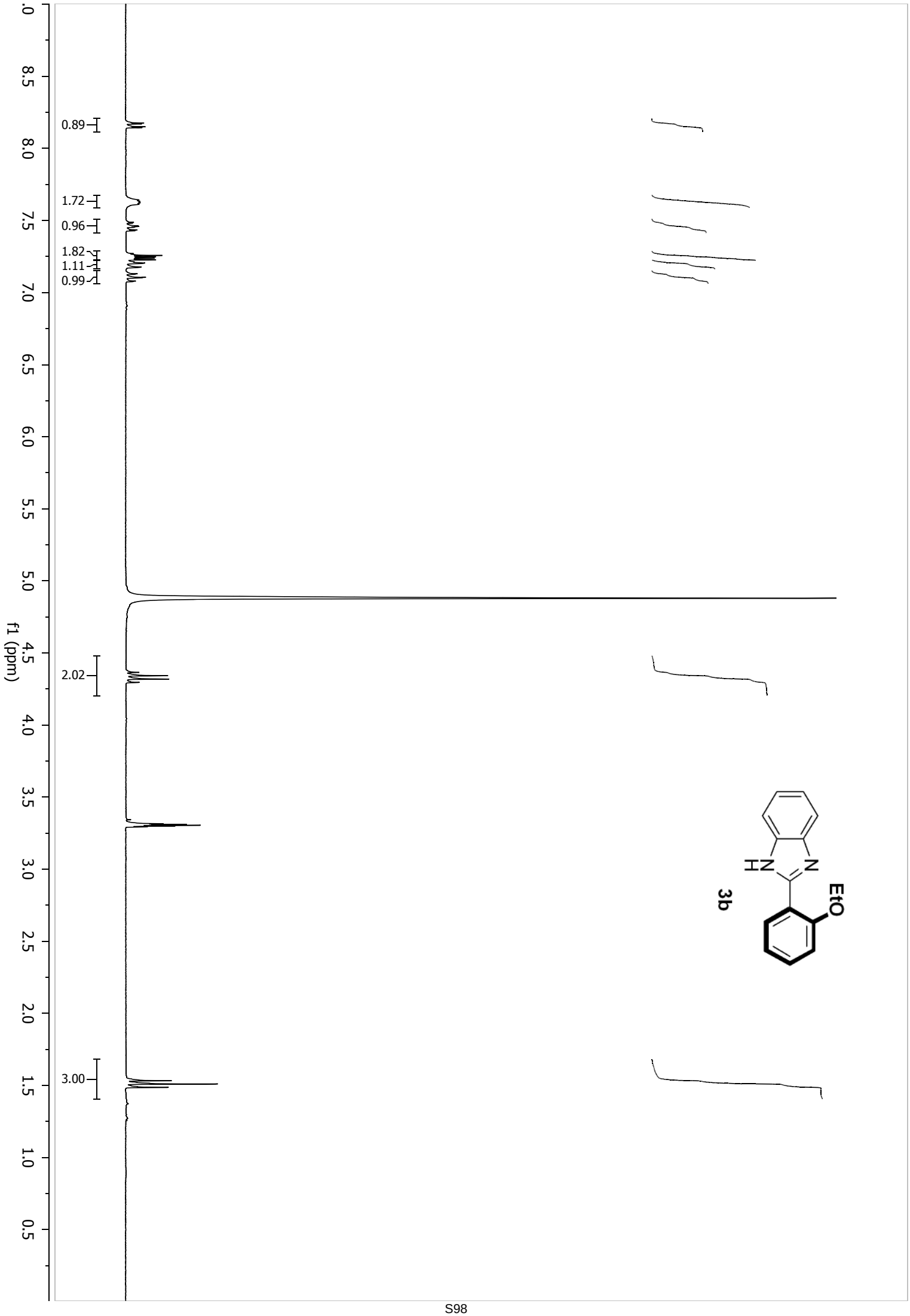
3.85

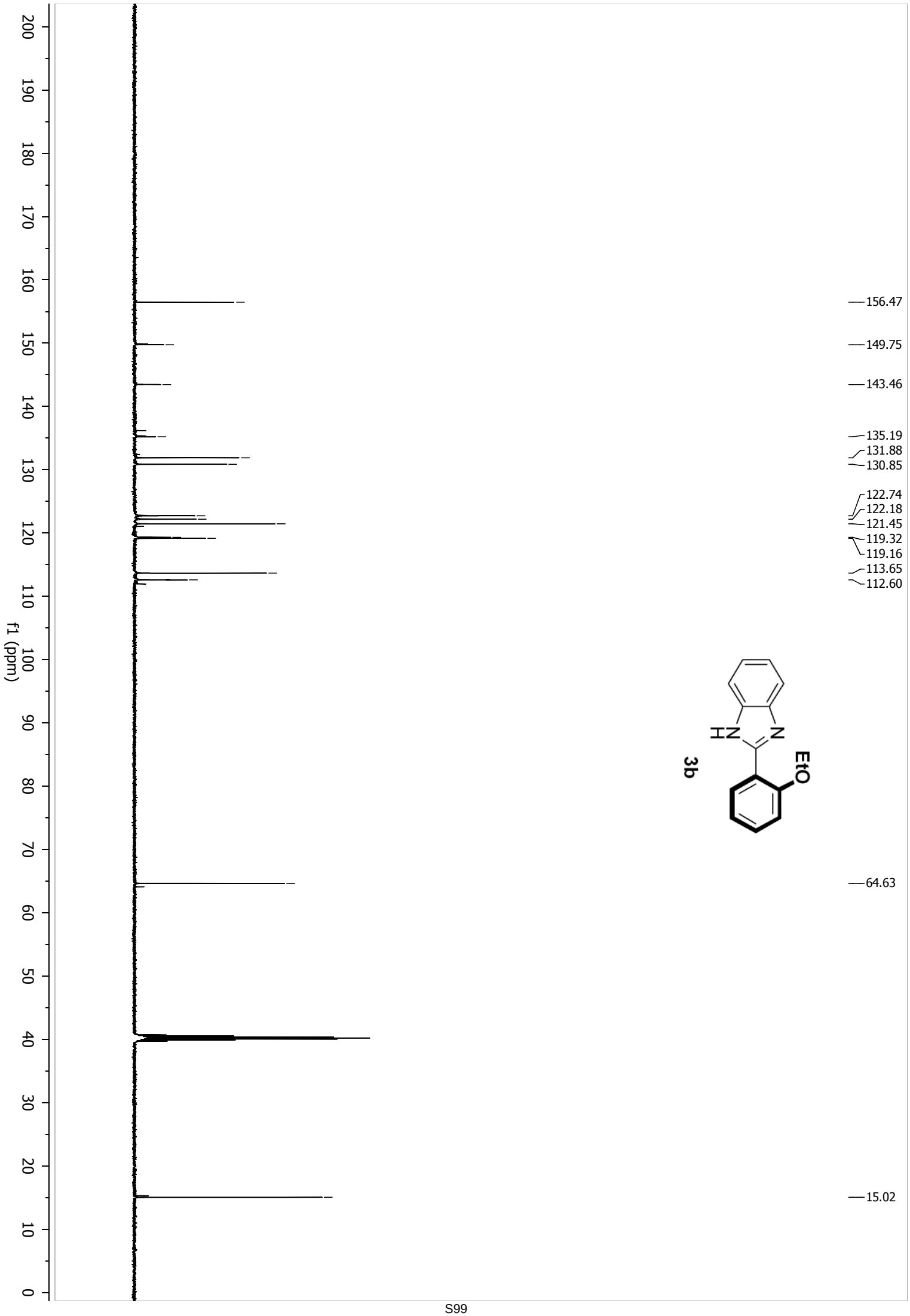
2.00

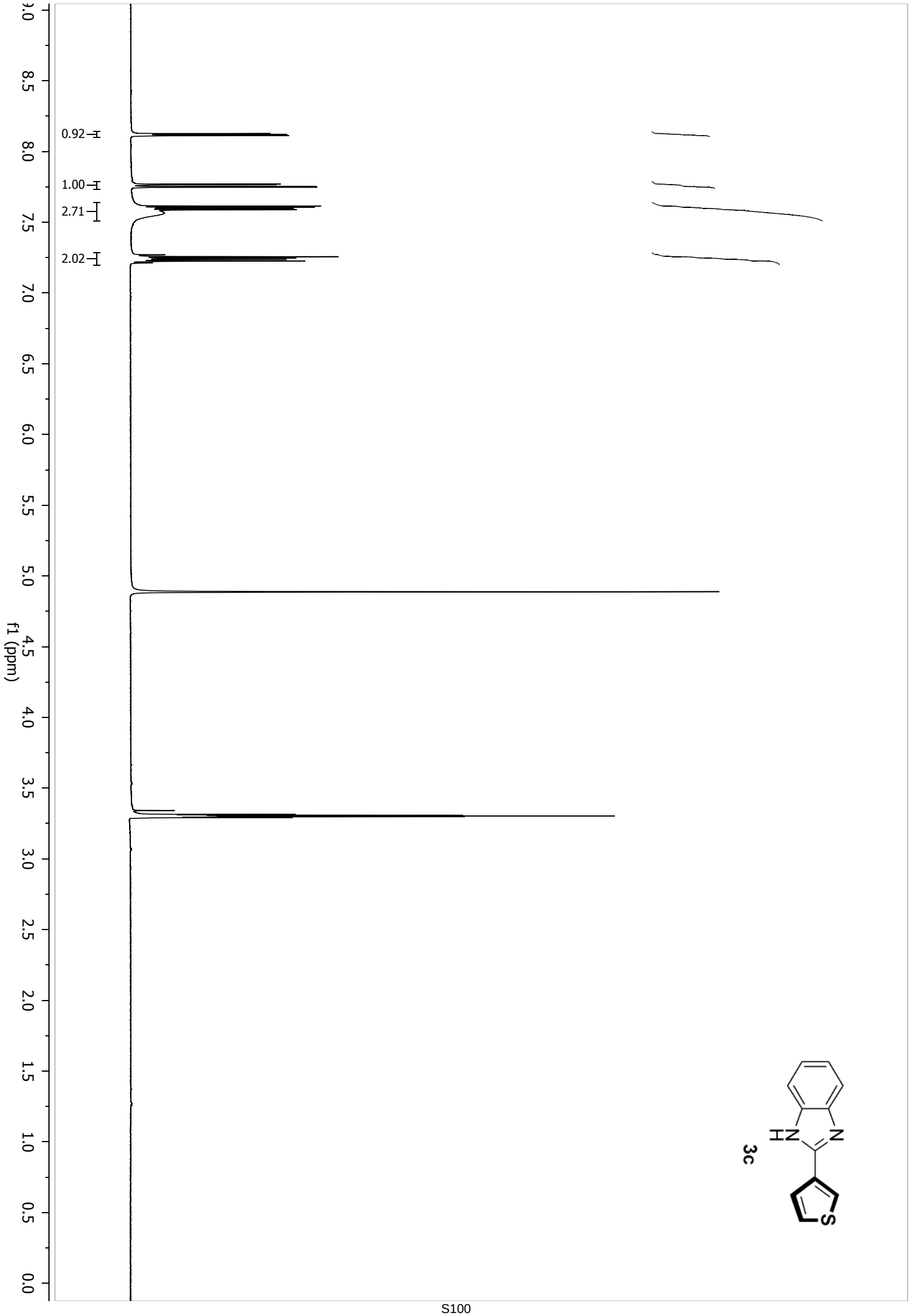
9.18

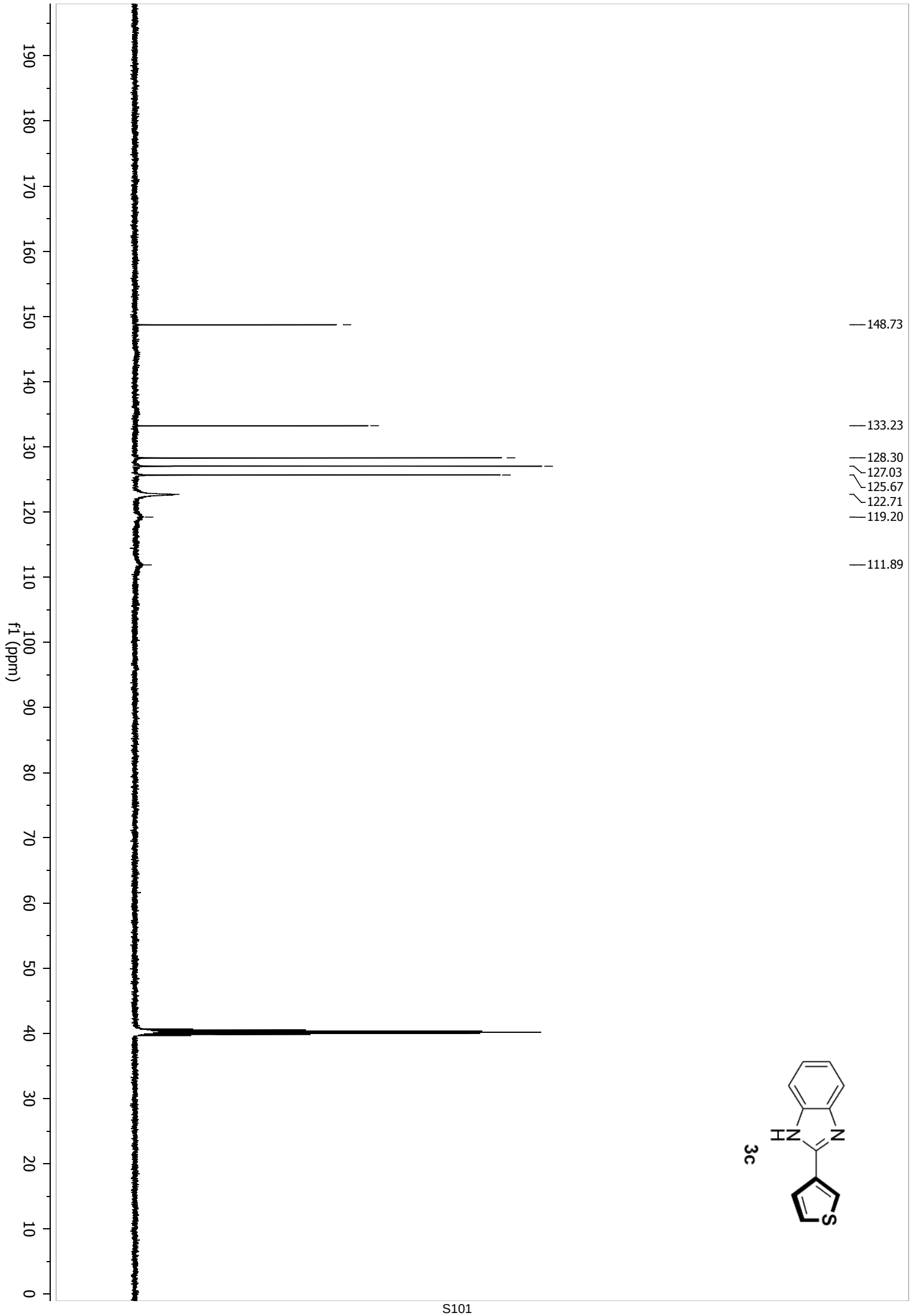
f1 (ppm)

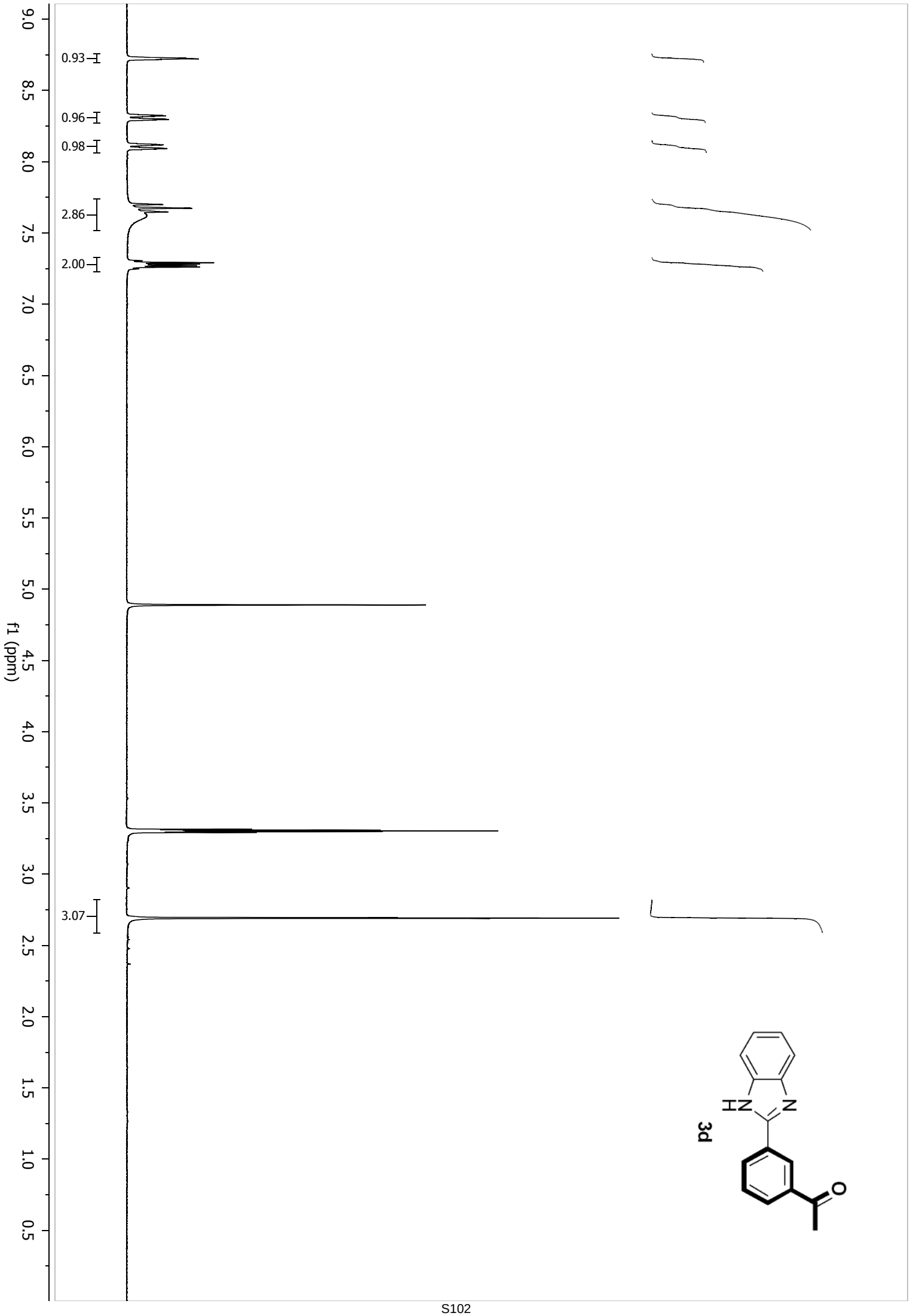

153.21
151.99
128.16
126.93
126.42
122.57
119.39
112.00
35.27
31.66
f1 (ppm)
3a

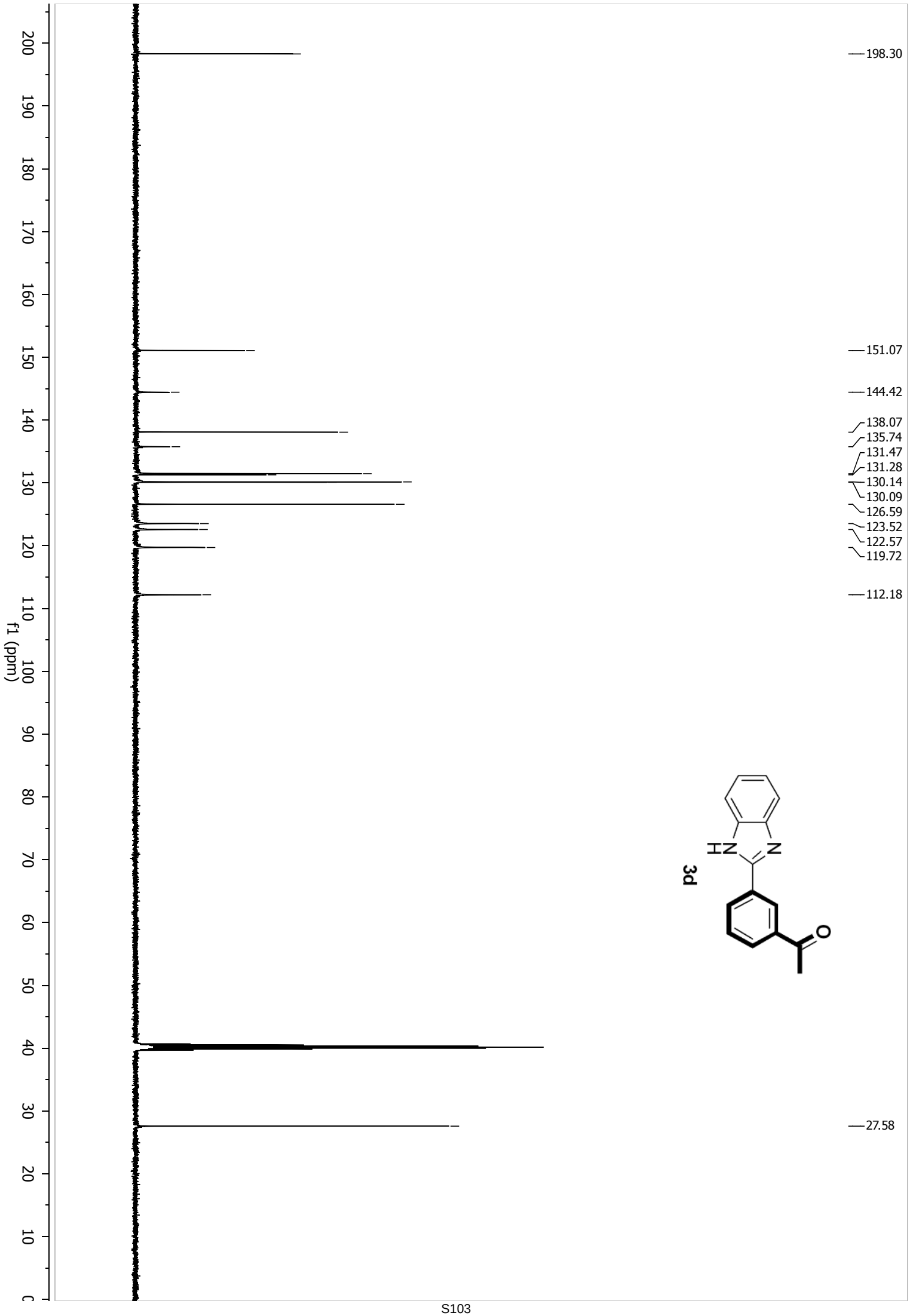

0.89
1.72
0.96
1.82
1.11
0.99
2.02
3.00
f1 (ppm)
3b
EtO

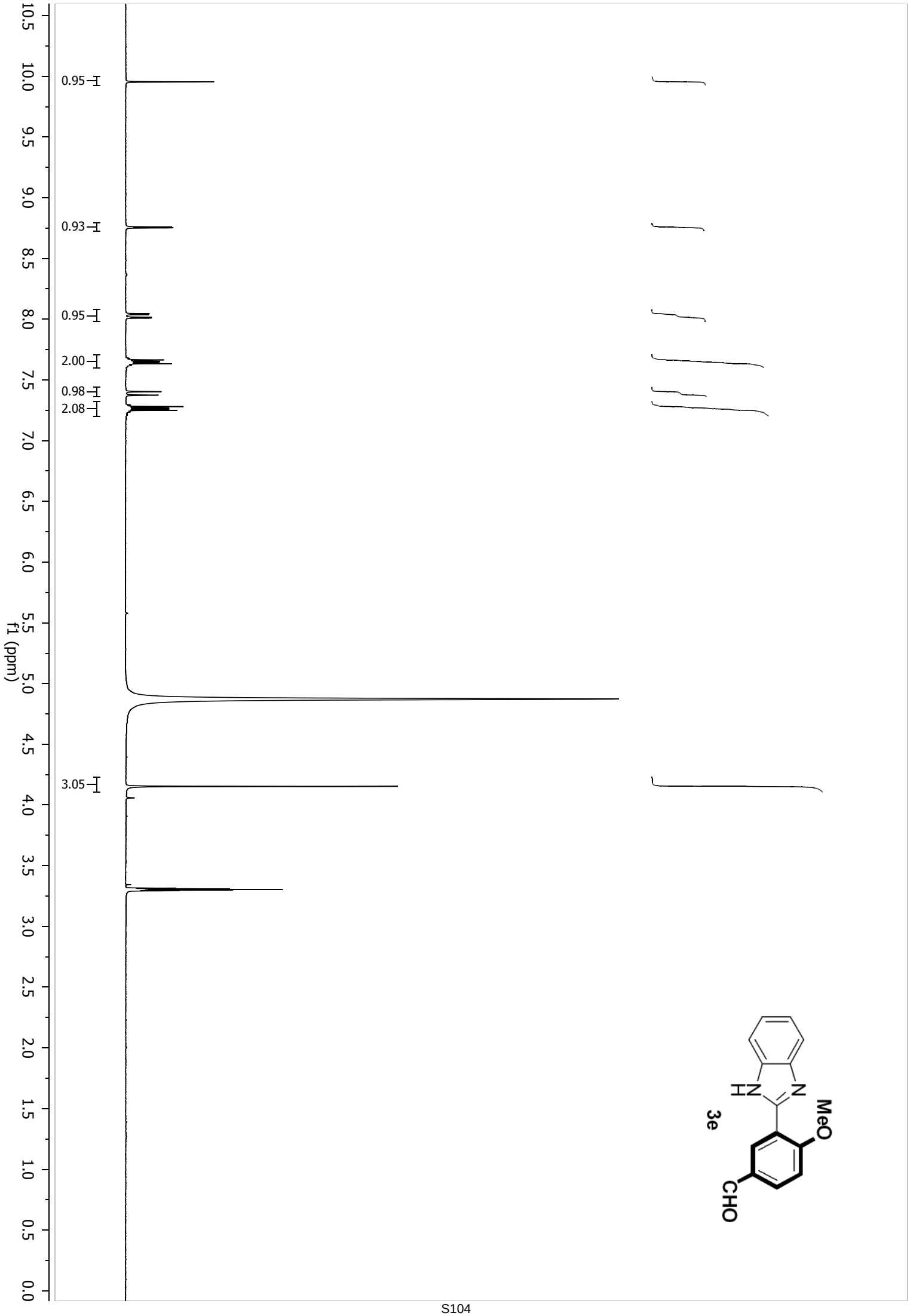

156.47
149.75
143.46
135.19
131.88
130.85
122.74
122.18
121.45
119.32
119.16
113.65
112.60
64.63
15.02
f1 (ppm)
3b
EtO
N
H
N

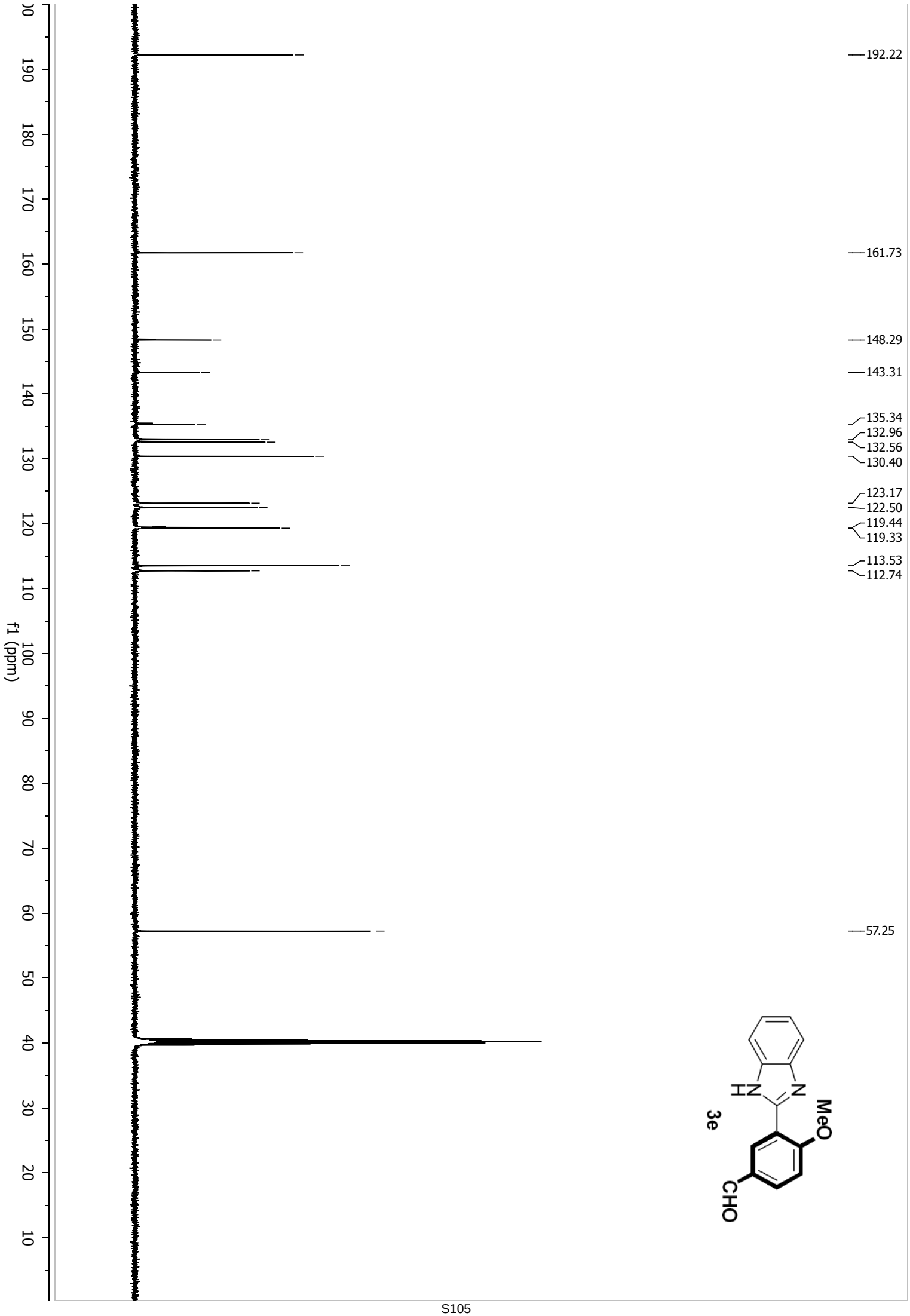

0.92
1.00
2.71
2.02
f1 (ppm)
3c

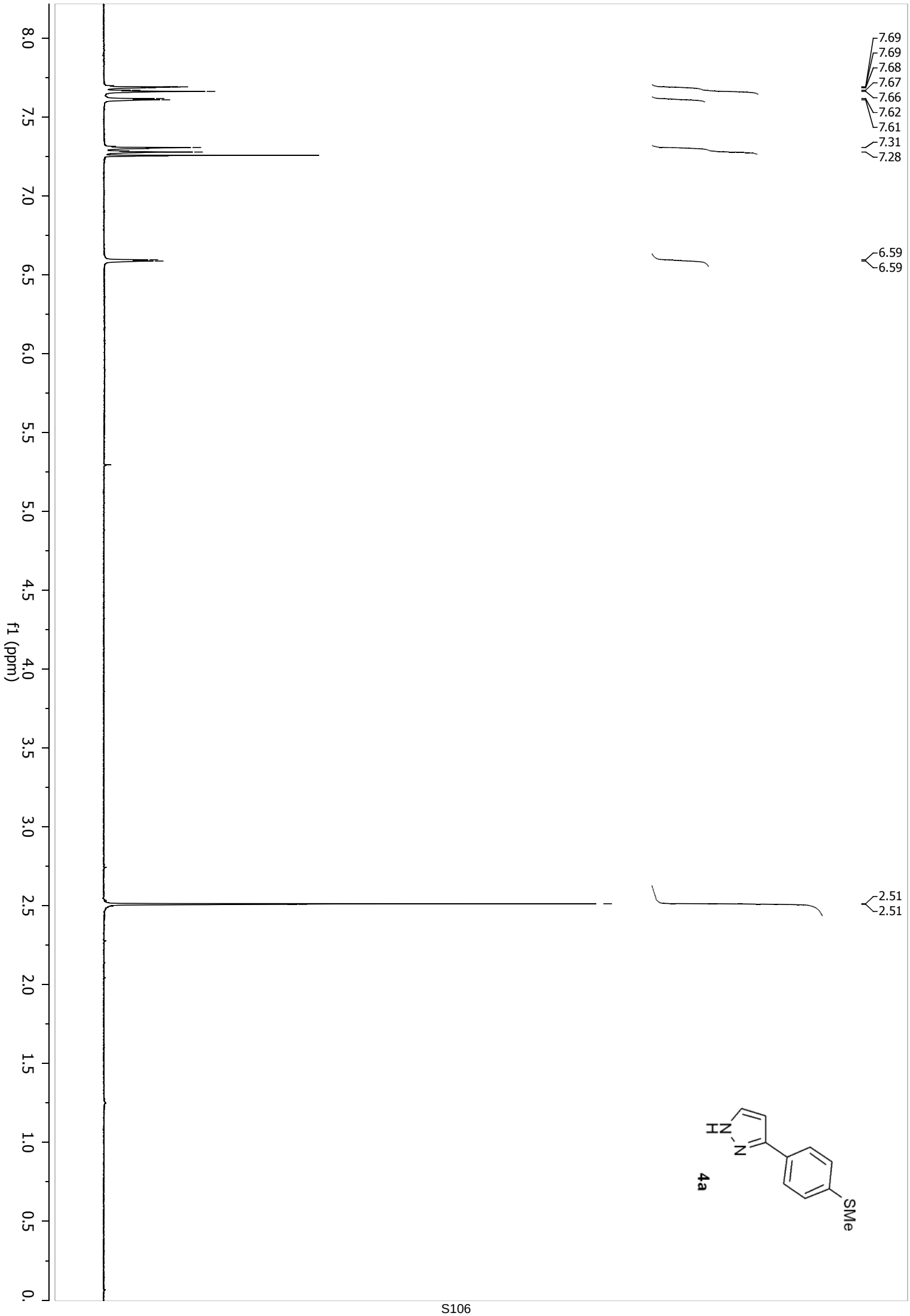

148.73
133.23
128.30
127.03
125.67
122.71
119.20
111.89
f1 (ppm)
3c

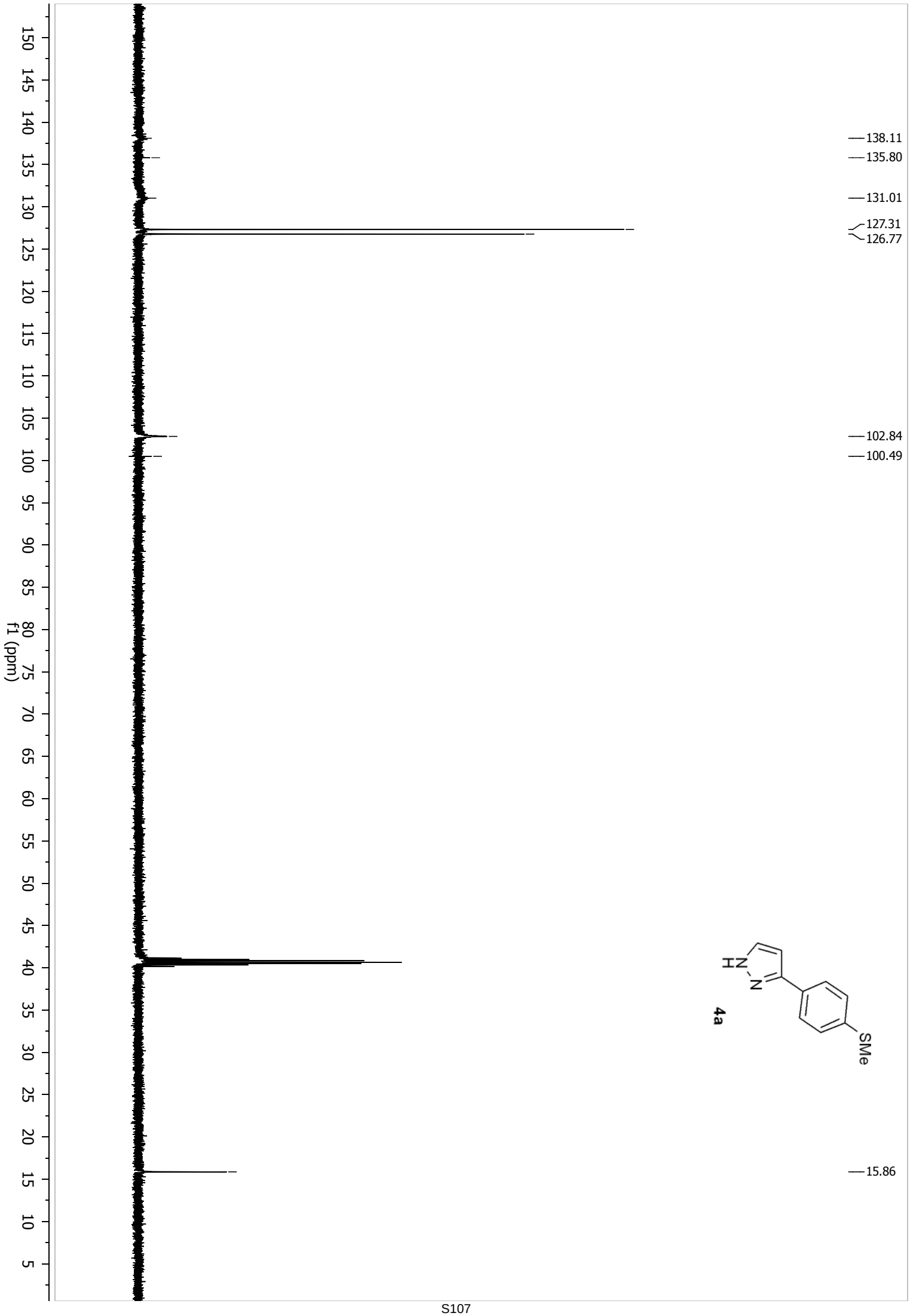

0.93
0.96
0.98
2.86
2.00
3.07
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
3d
HN
N
O

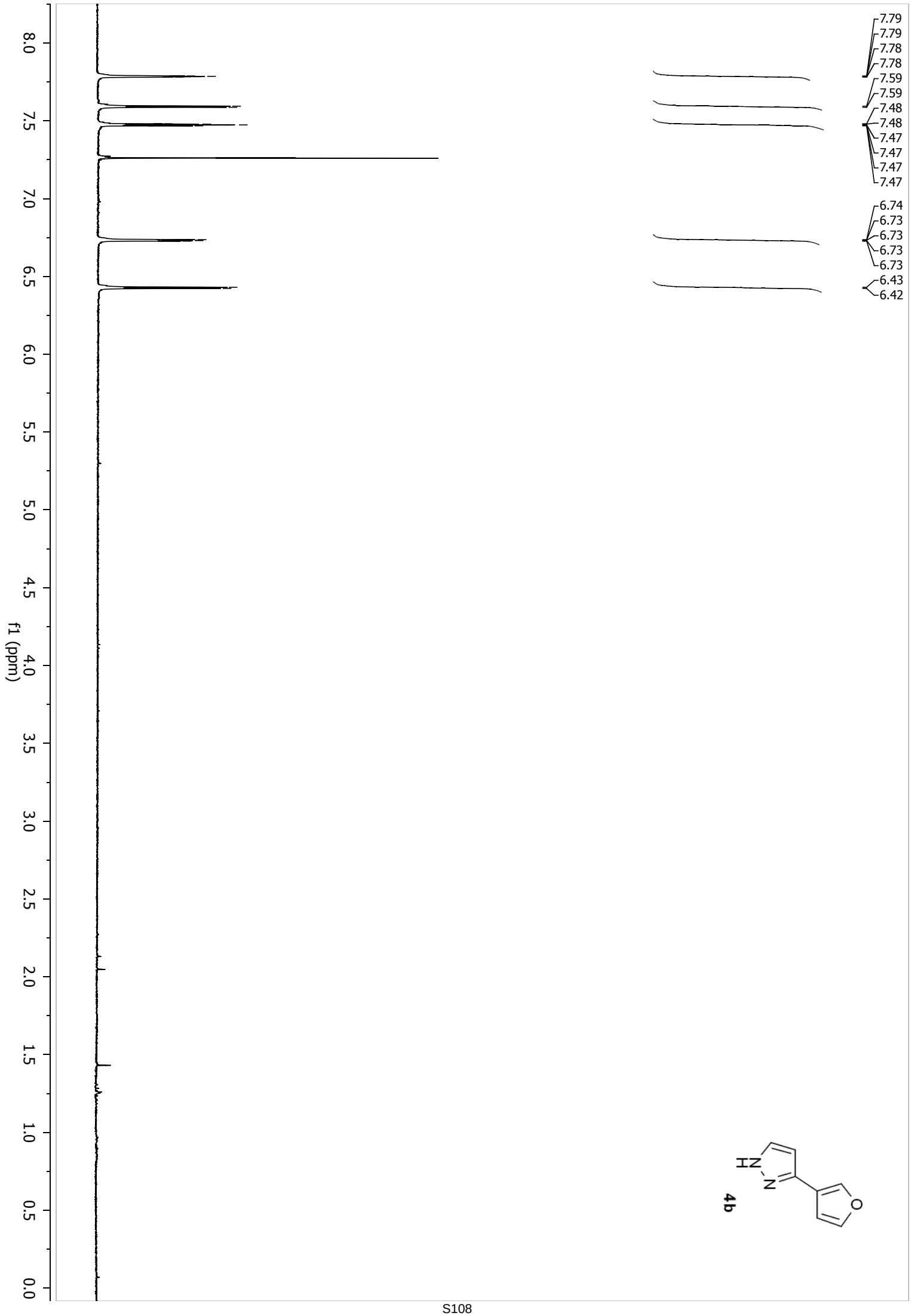

198.30
151.07
144.42
138.07
135.74
131.47
131.28
130.14
130.09
126.59
123.52
122.57
119.72
112.18
27.58
f1 (ppm)
3d

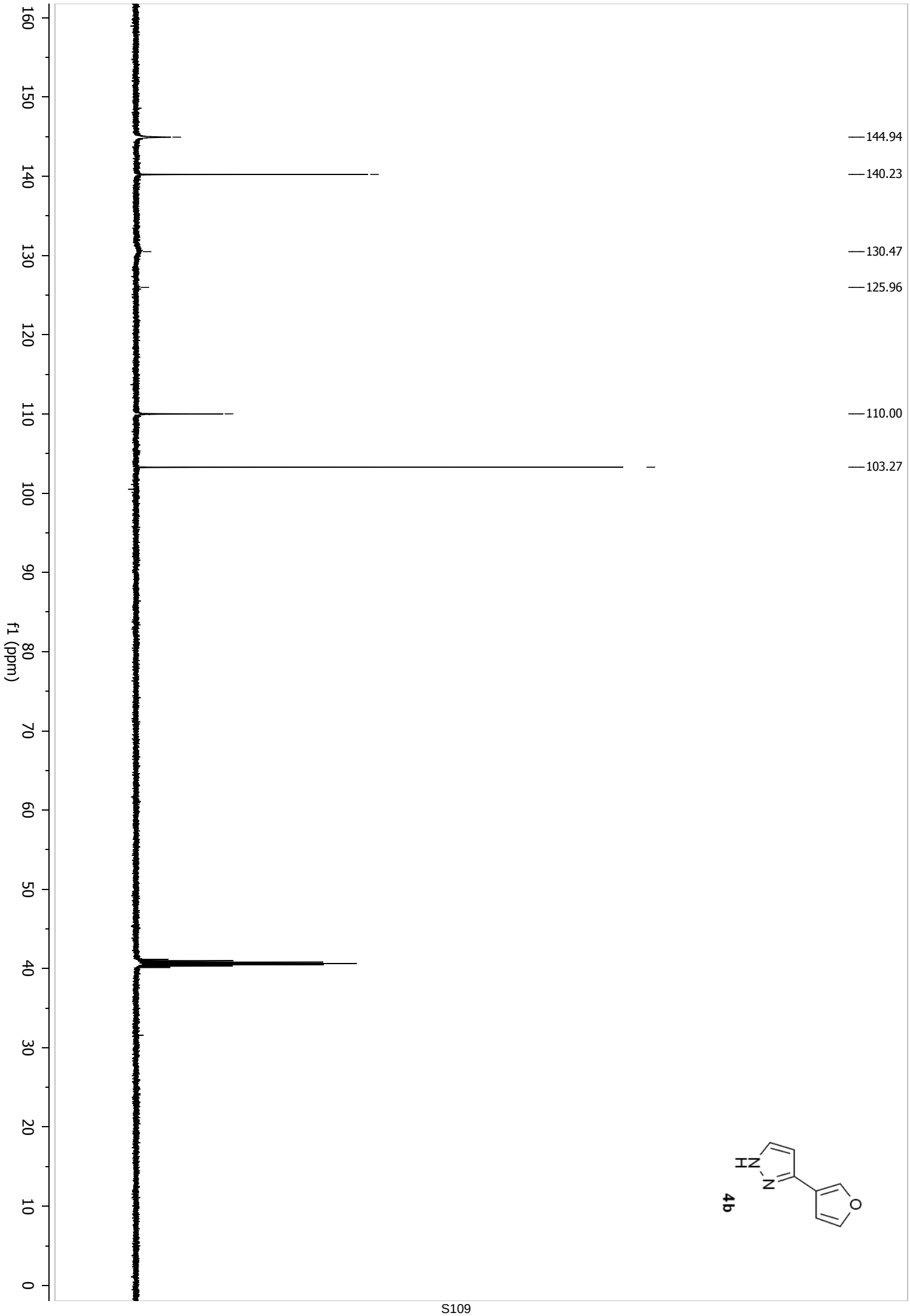

0.95
0.93
0.95
2.00
0.98
2.08
3.05
f1 (ppm)
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
HN
N
MeO
CHO
3e

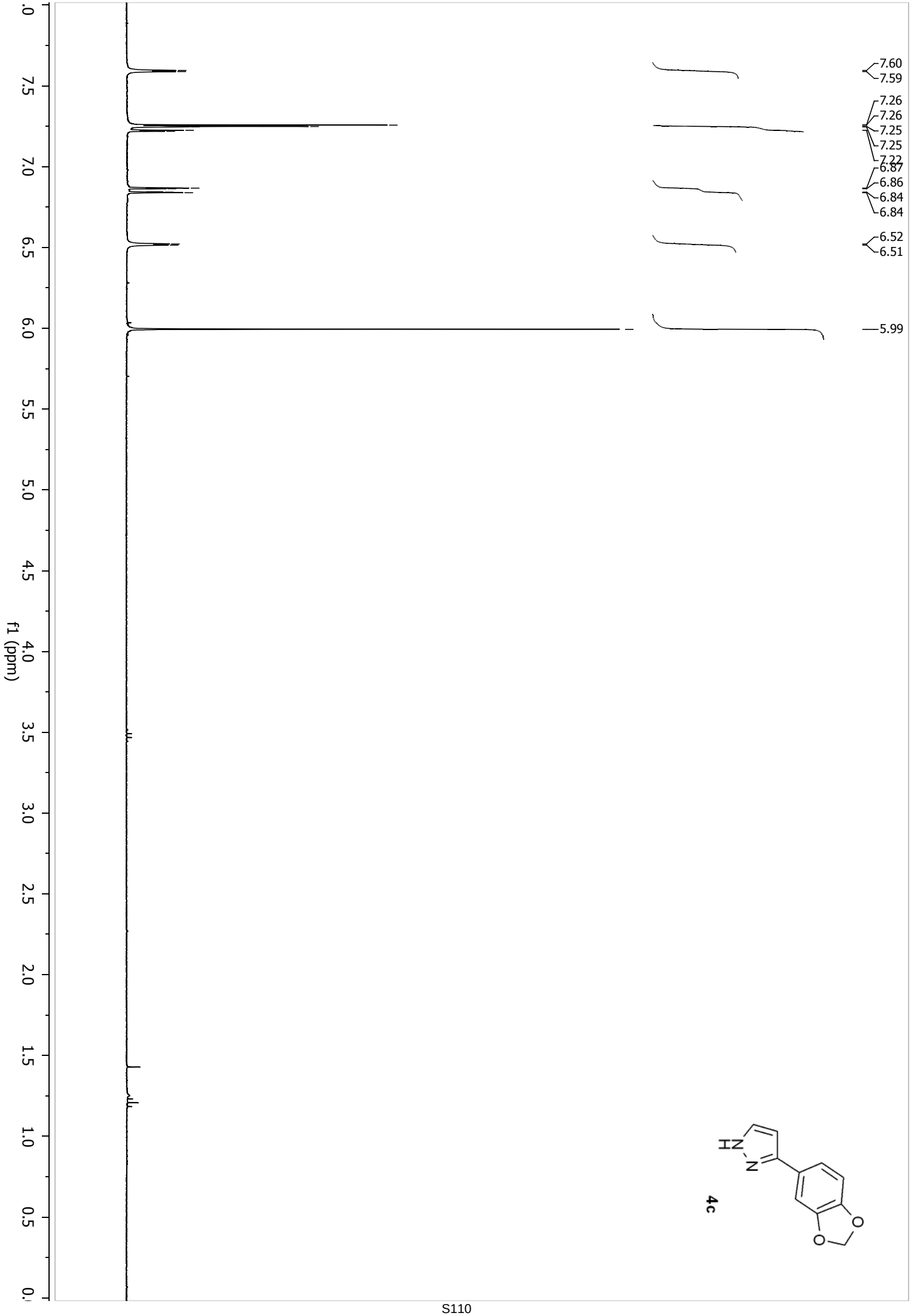

192.22
161.73
148.29
143.31
135.34
132.96
132.56
130.40
123.17
122.50
119.44
119.33
113.53
112.74
57.25
f1 (ppm)
3e
MeO
CHO
HN
N

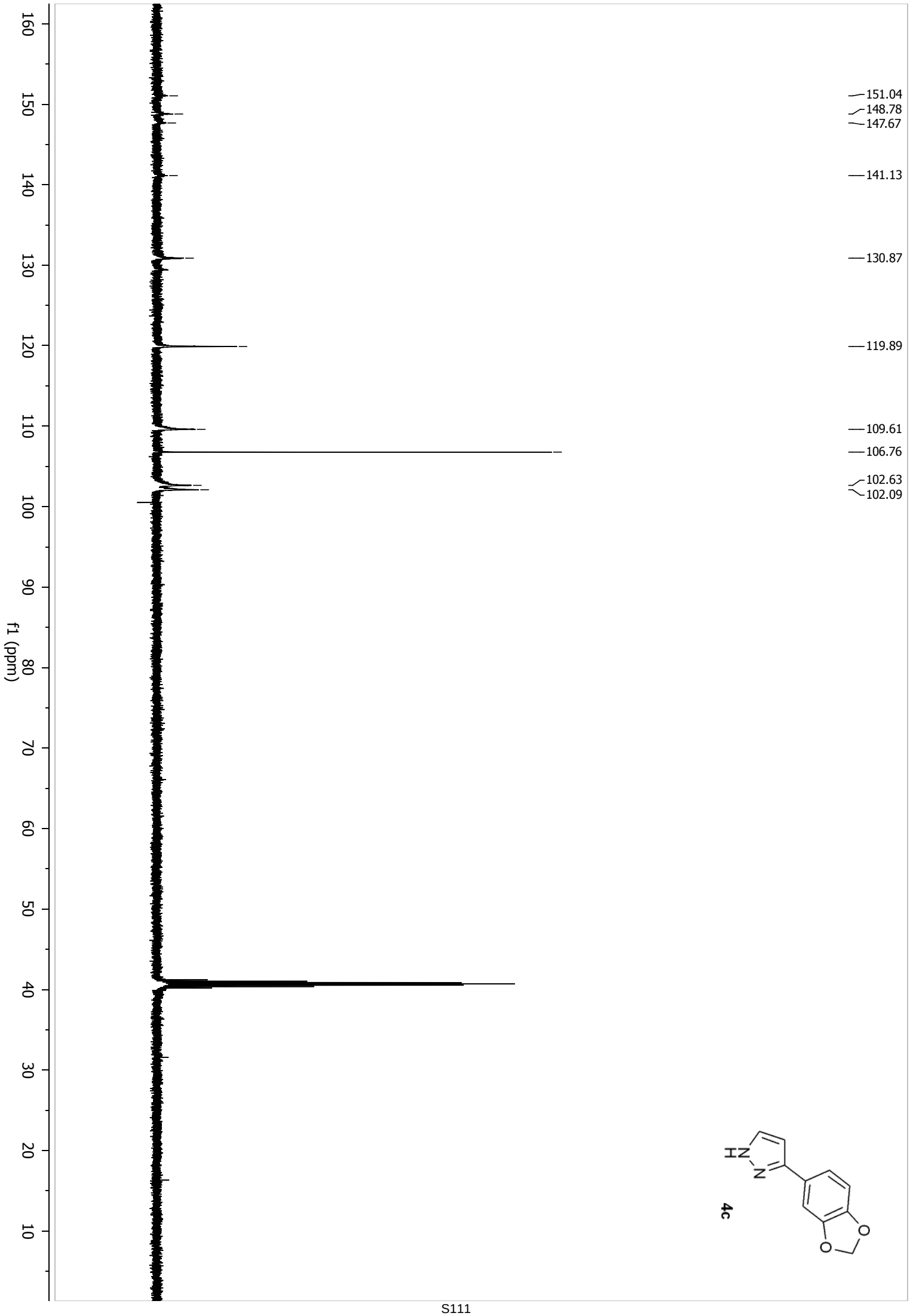

7.69
7.69
7.68
7.67
7.66
7.62
7.61
7.31
7.28
6.59
6.59
2.51
2.51
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
H
N
N
SMe
4a

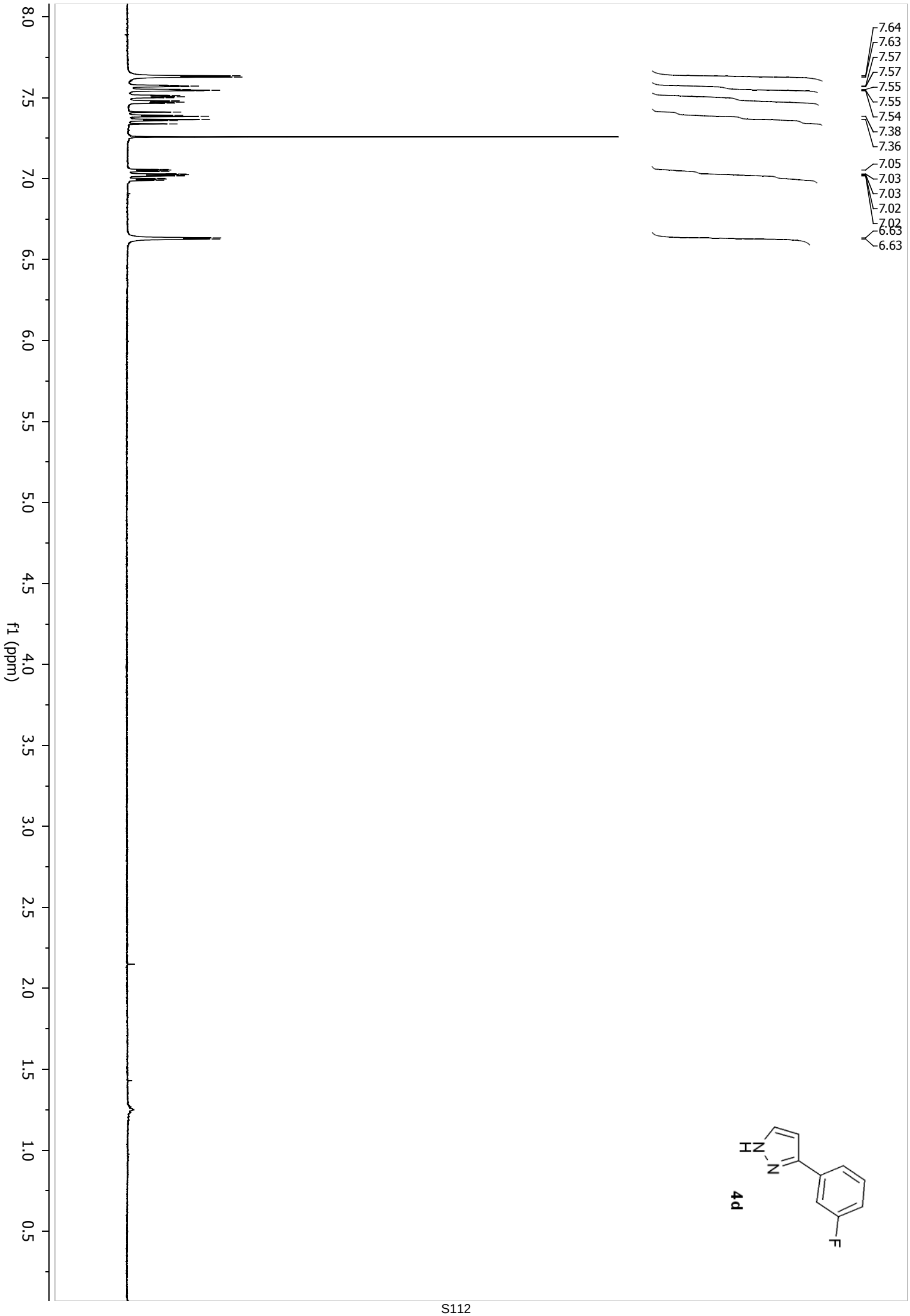

138.11
135.80
131.01
127.31
126.77
102.84
100.49
15.86
f1 (ppm)
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
H
N
N
SMe
4a

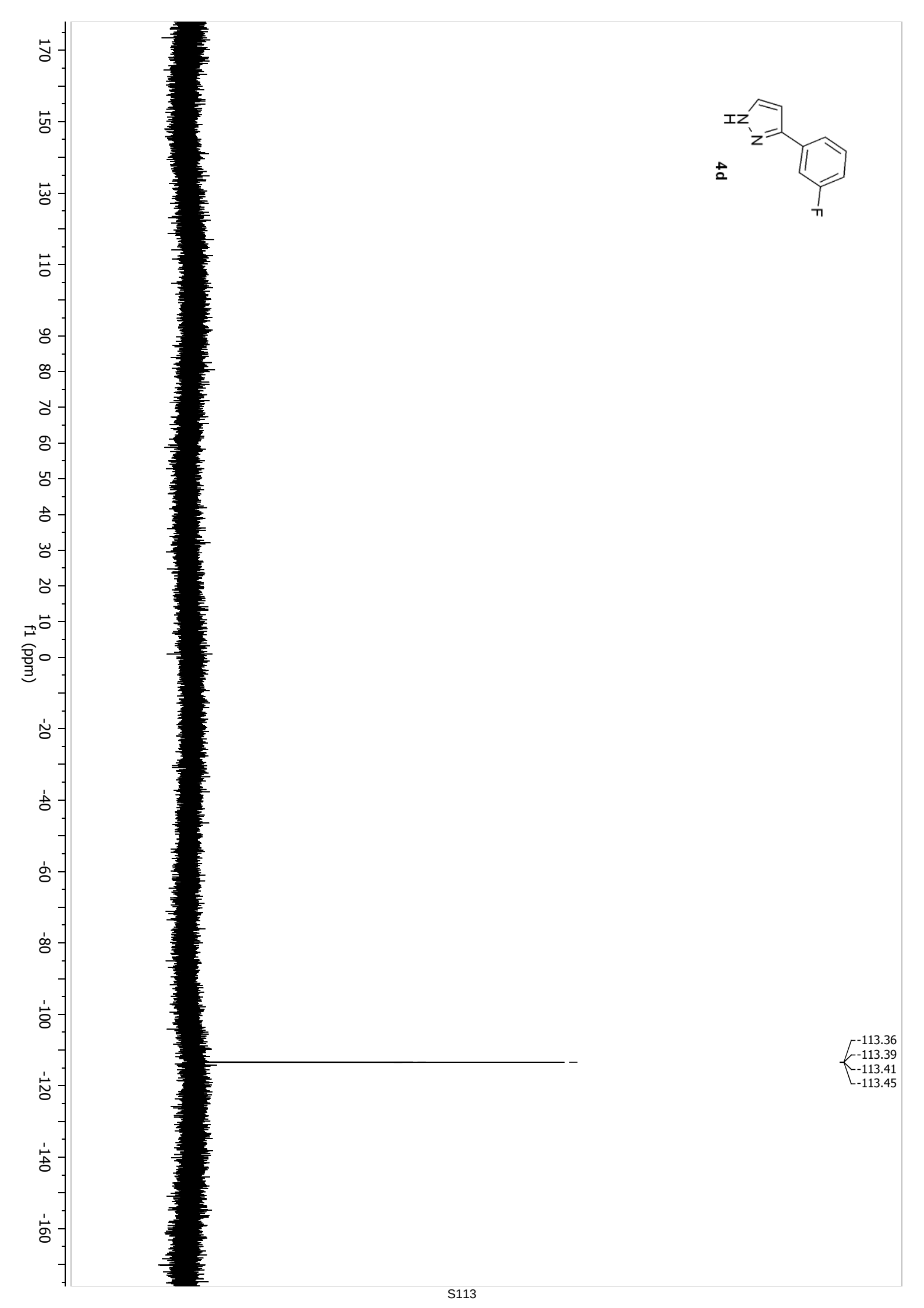

7.79
7.79
7.78
7.78
7.59
7.59
7.48
7.48
7.47
7.47
7.47
7.47
6.74
6.73
6.73
6.73
6.73
6.43
6.42
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
H
N
N
O
4b

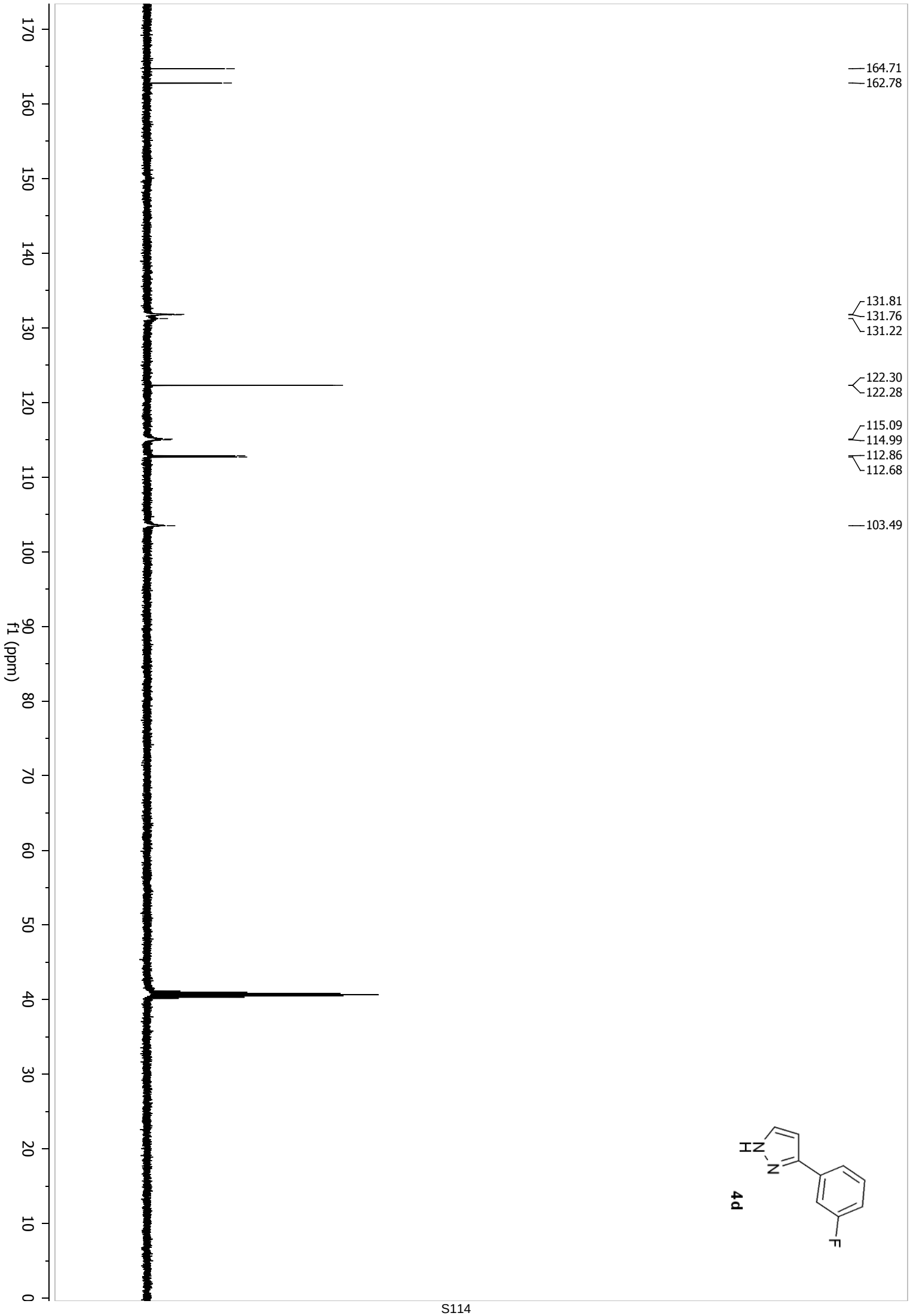

144.94
140.23
130.47
125.96
110.00
103.27
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
4b

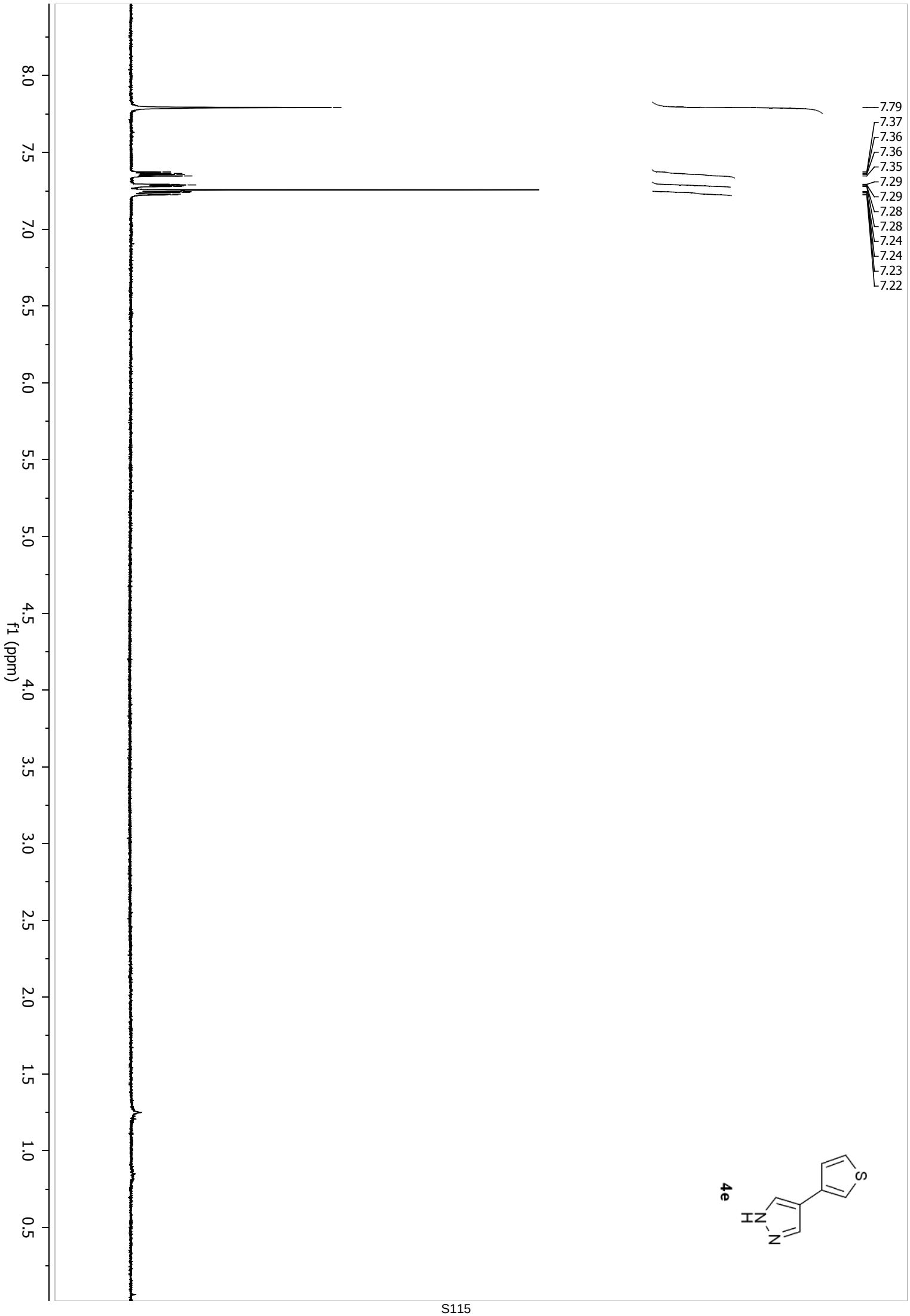

7.60
7.59
7.26
7.26
7.25
7.25
7.22
6.87
6.86
6.84
6.84
6.52
6.51
5.99
f1 (ppm)
4c

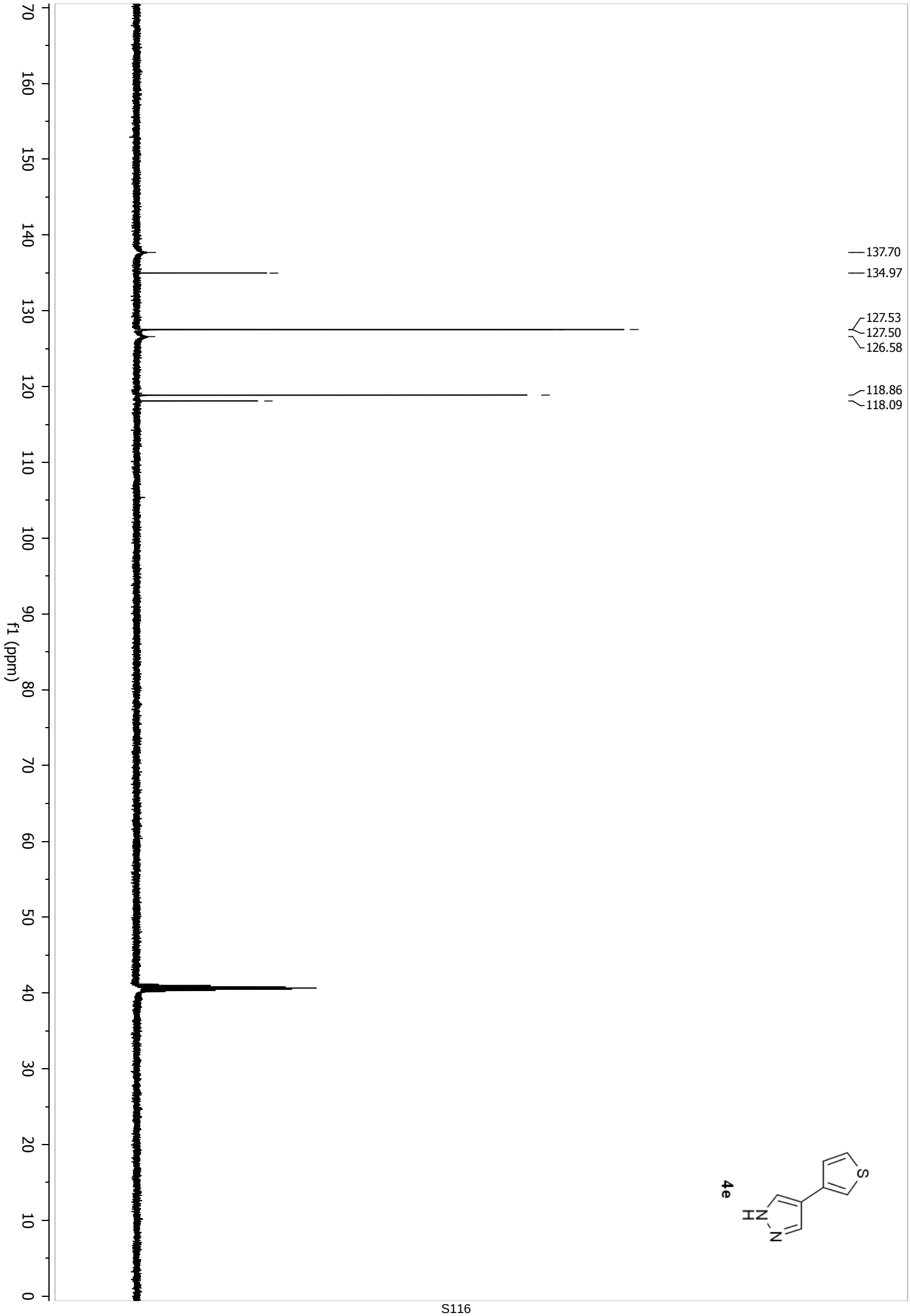

151.04
148.78
147.67
141.13
130.87
119.89
109.61
106.76
102.63
102.09
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
4c

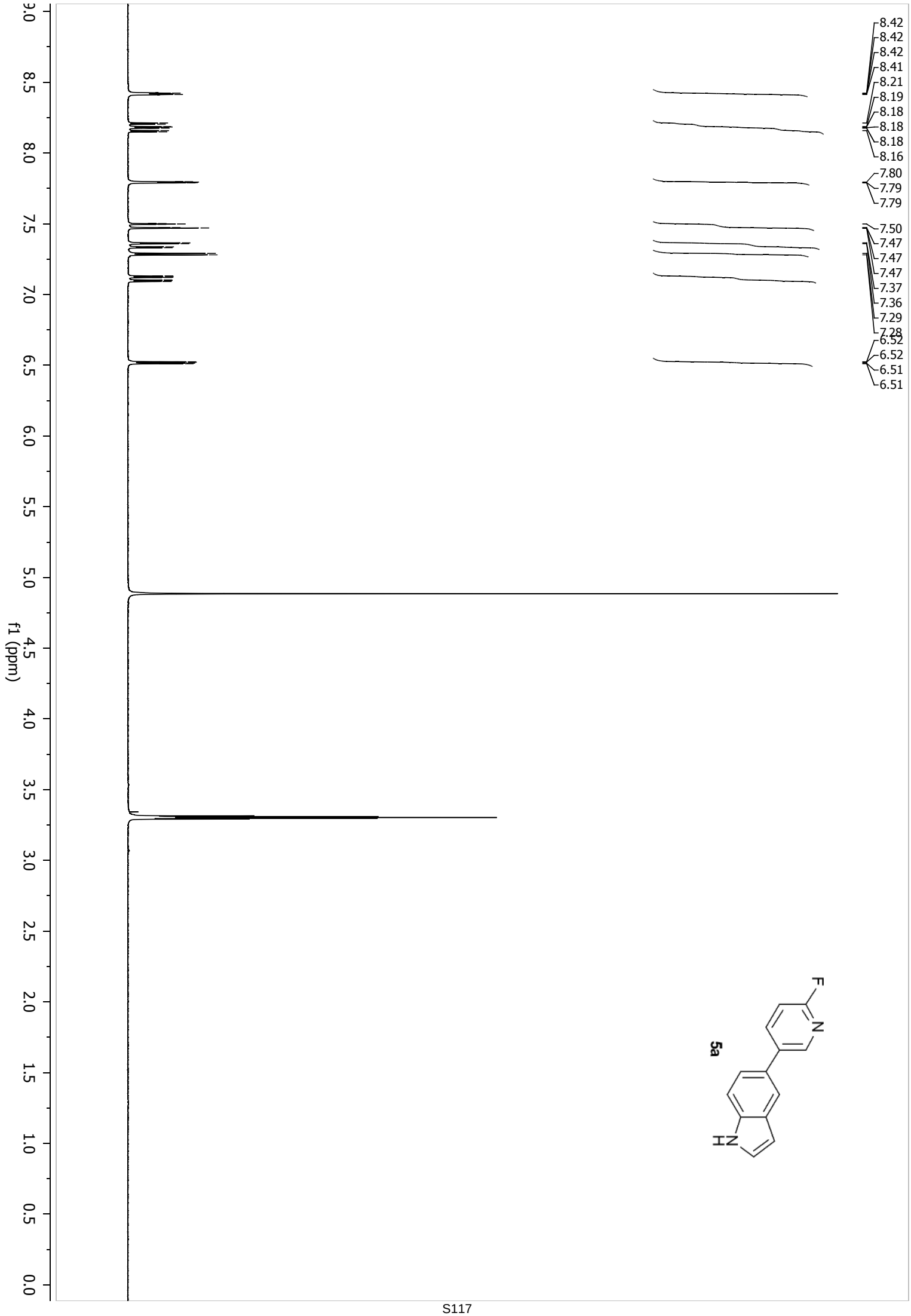

7.64
7.63
7.57
7.57
7.55
7.55
7.54
7.38
7.36
7.05
7.03
7.03
7.02
7.02
6.63
6.63
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
H
N
N
F
4d

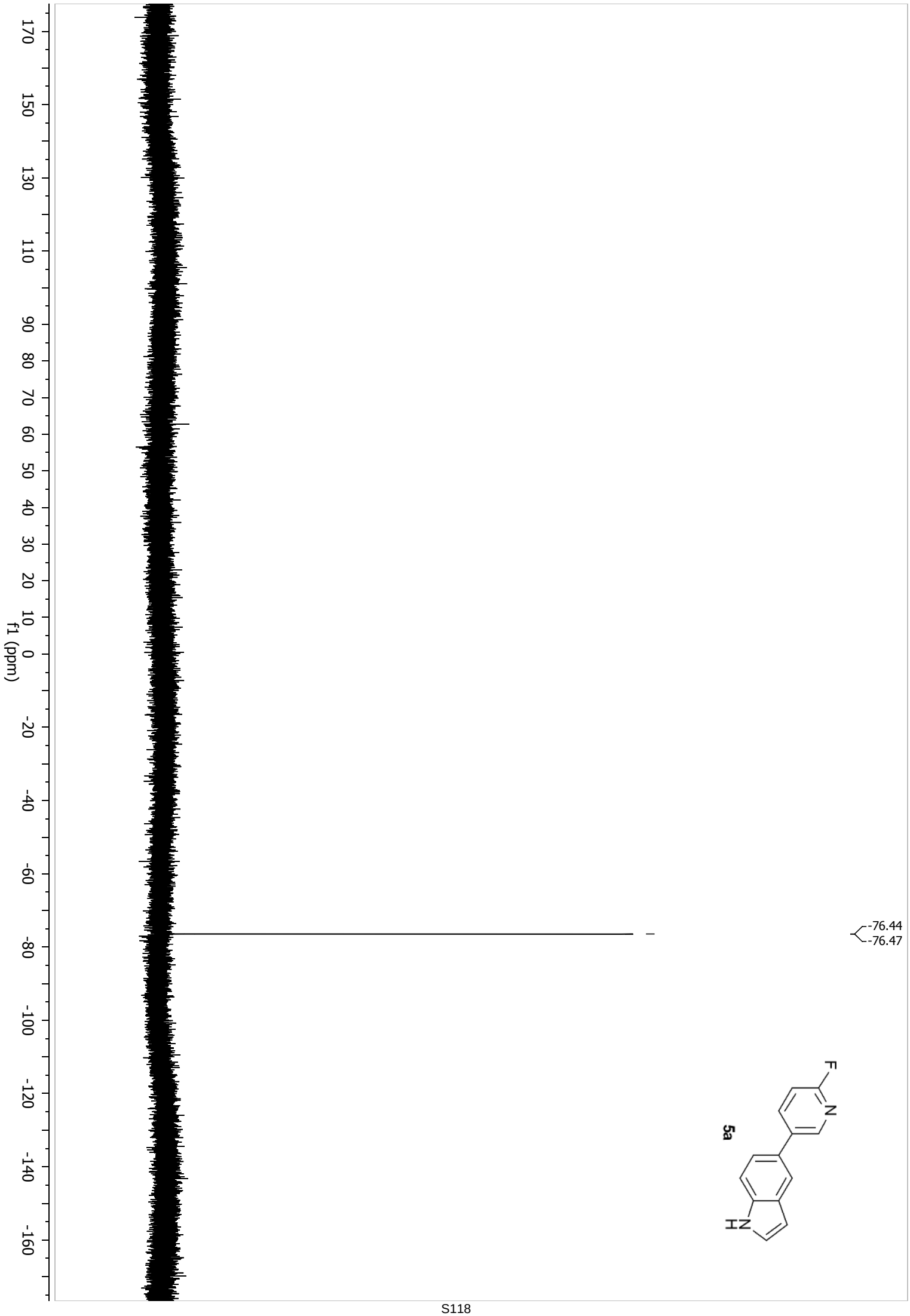

170
150
130
110
90
80
70
60
50
40
30
20
10
0
-20
-40
-60
-80
-100
-120
-140
-160
f1 (ppm)
4d
-113.36
-113.39
-113.41
-113.45

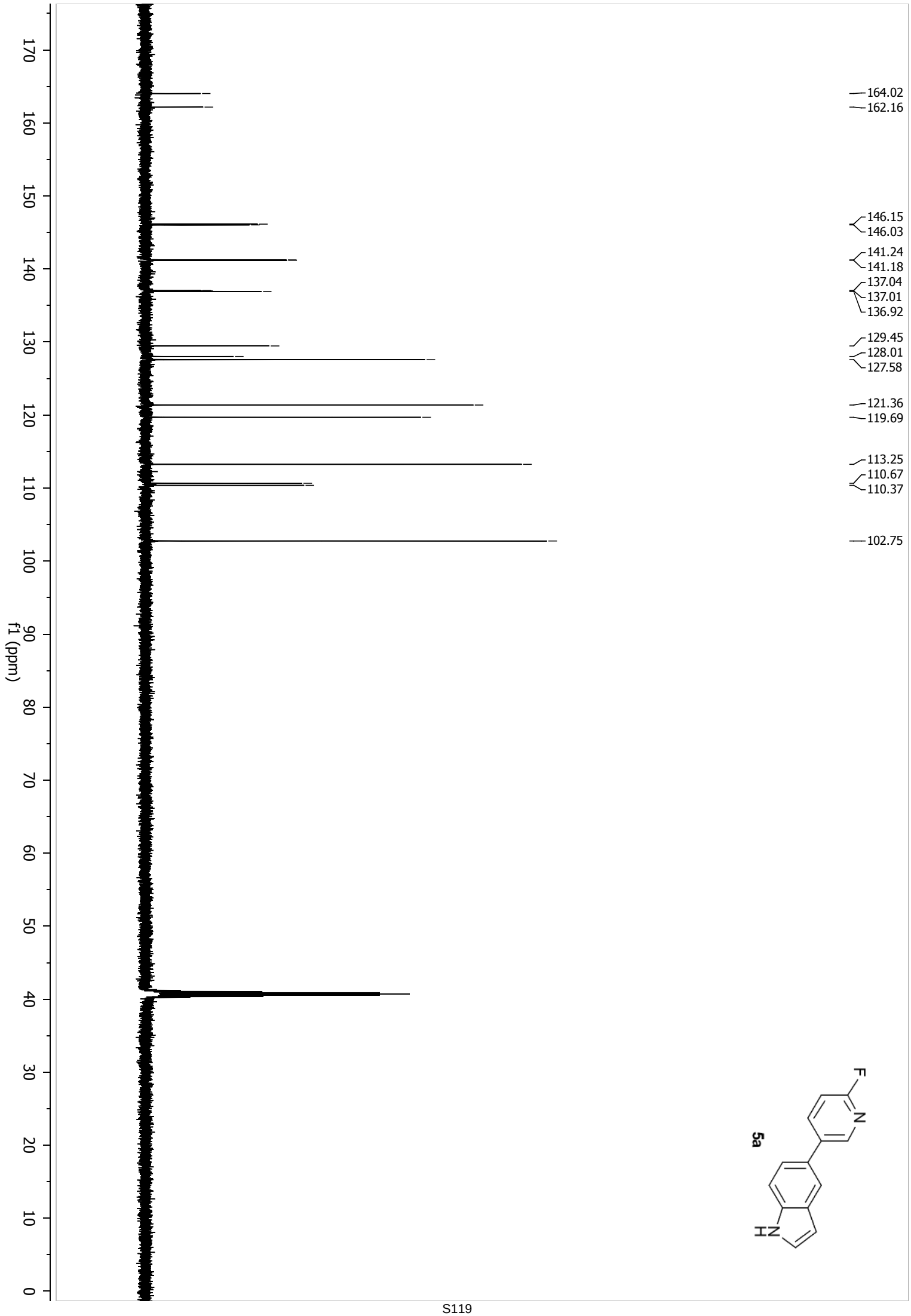

164.71
162.78
131.81
131.76
131.22
122.30
122.28
115.09
114.99
112.86
112.68
103.49
f1 (ppm)
4d

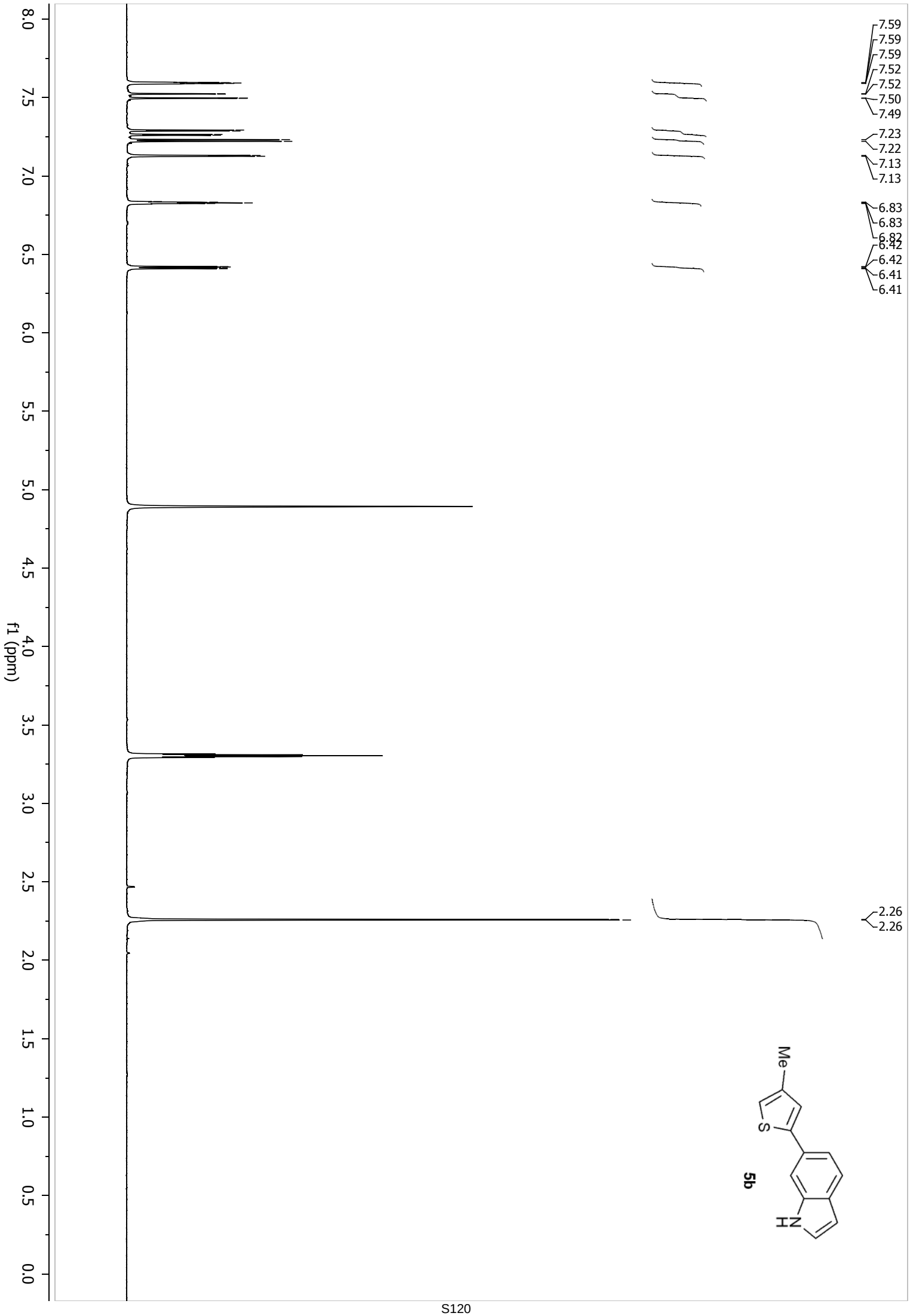

7.79
7.37
7.36
7.36
7.35
7.29
7.29
7.28
7.28
7.24
7.24
7.23
7.22
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
4e
S
N
H
N

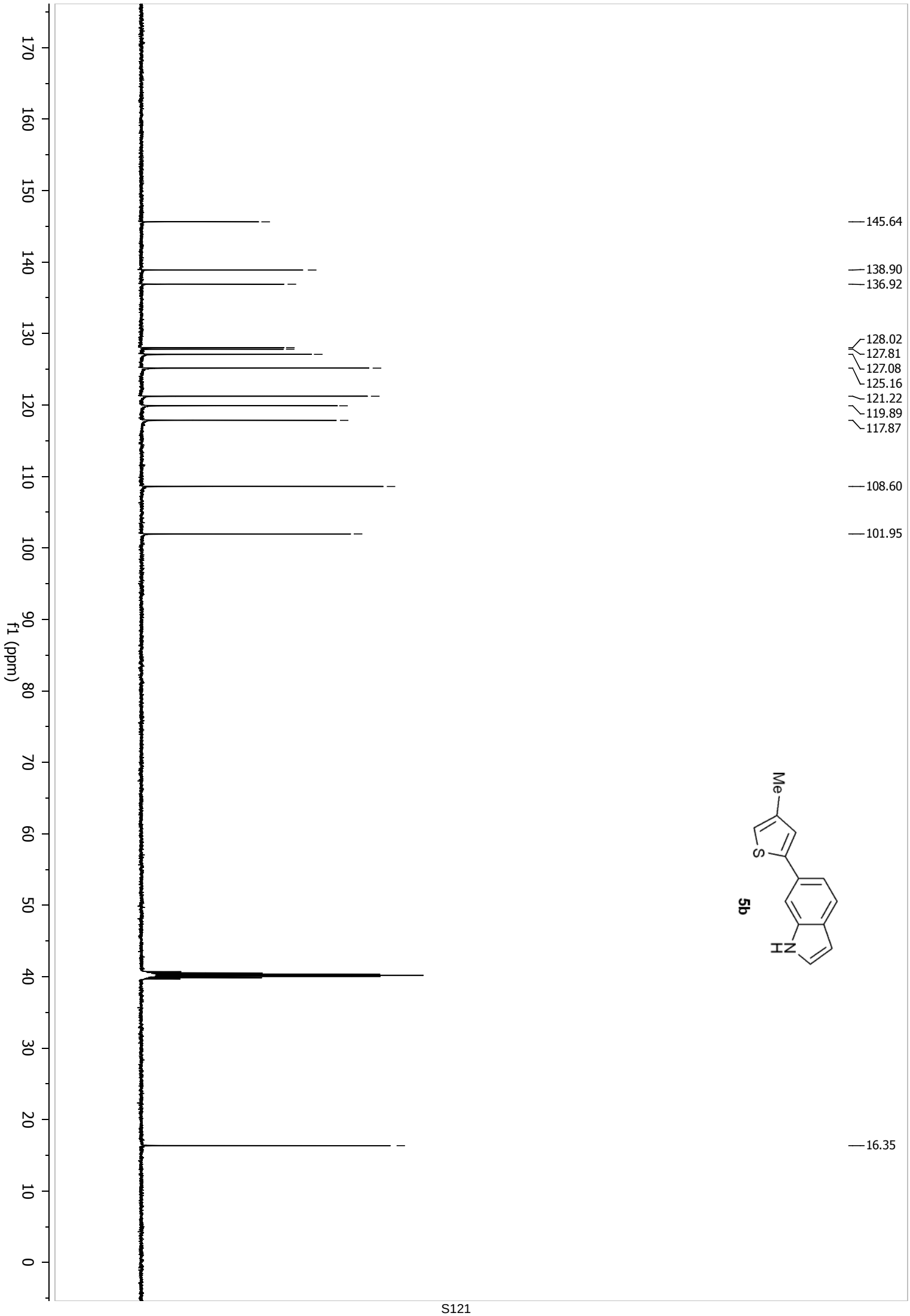

137.70
134.97
127.53
127.50
126.58
118.86
118.09
f1 (ppm)
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
4e
S
H
N
N

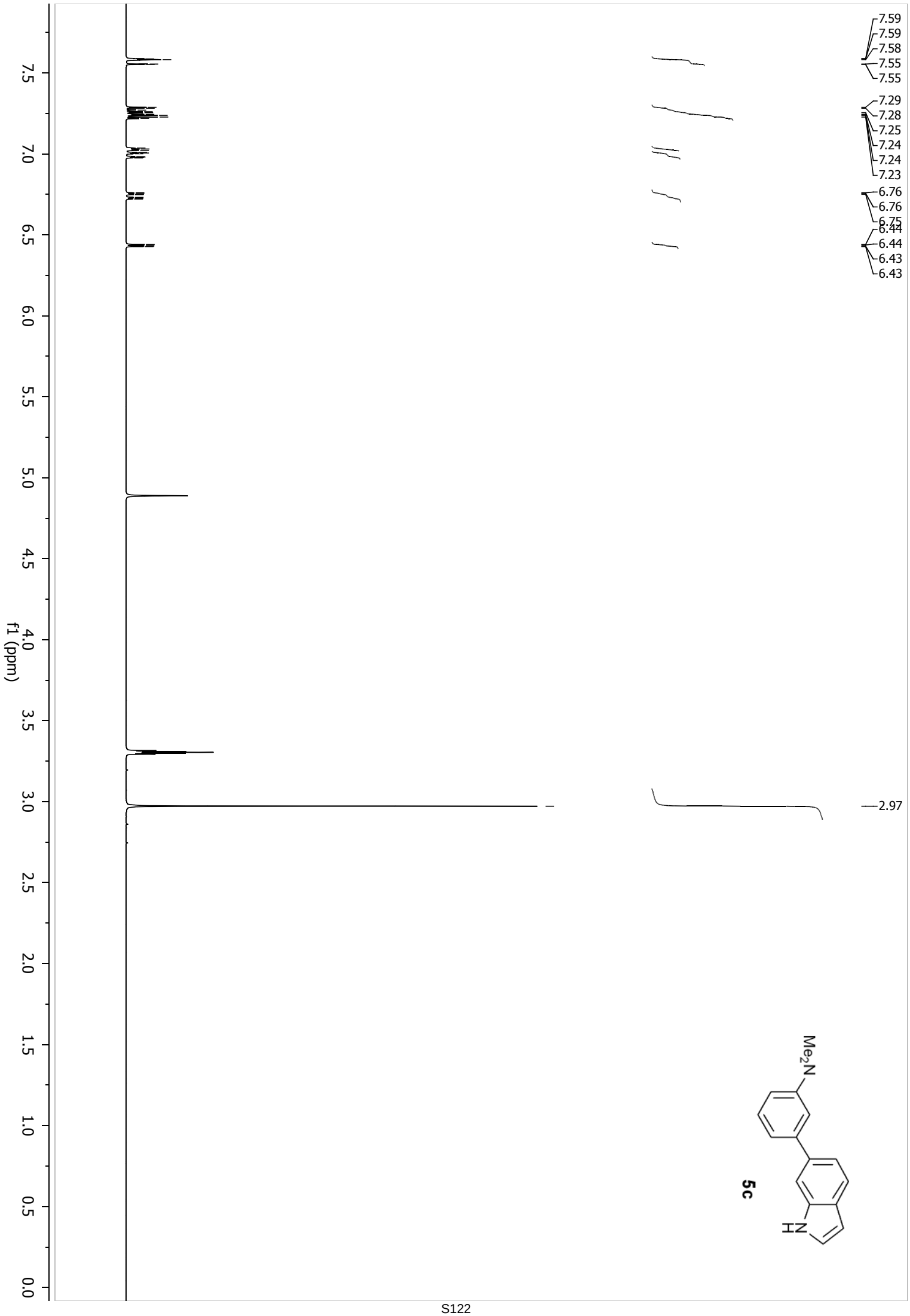

8.42
8.42
8.42
8.41
8.21
8.19
8.18
8.18
8.18
8.16
7.80
7.79
7.79
7.50
7.47
7.47
7.47
7.37
7.36
7.29
7.28
6.52
6.52
6.51
6.51
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
F
N
H
N
5a

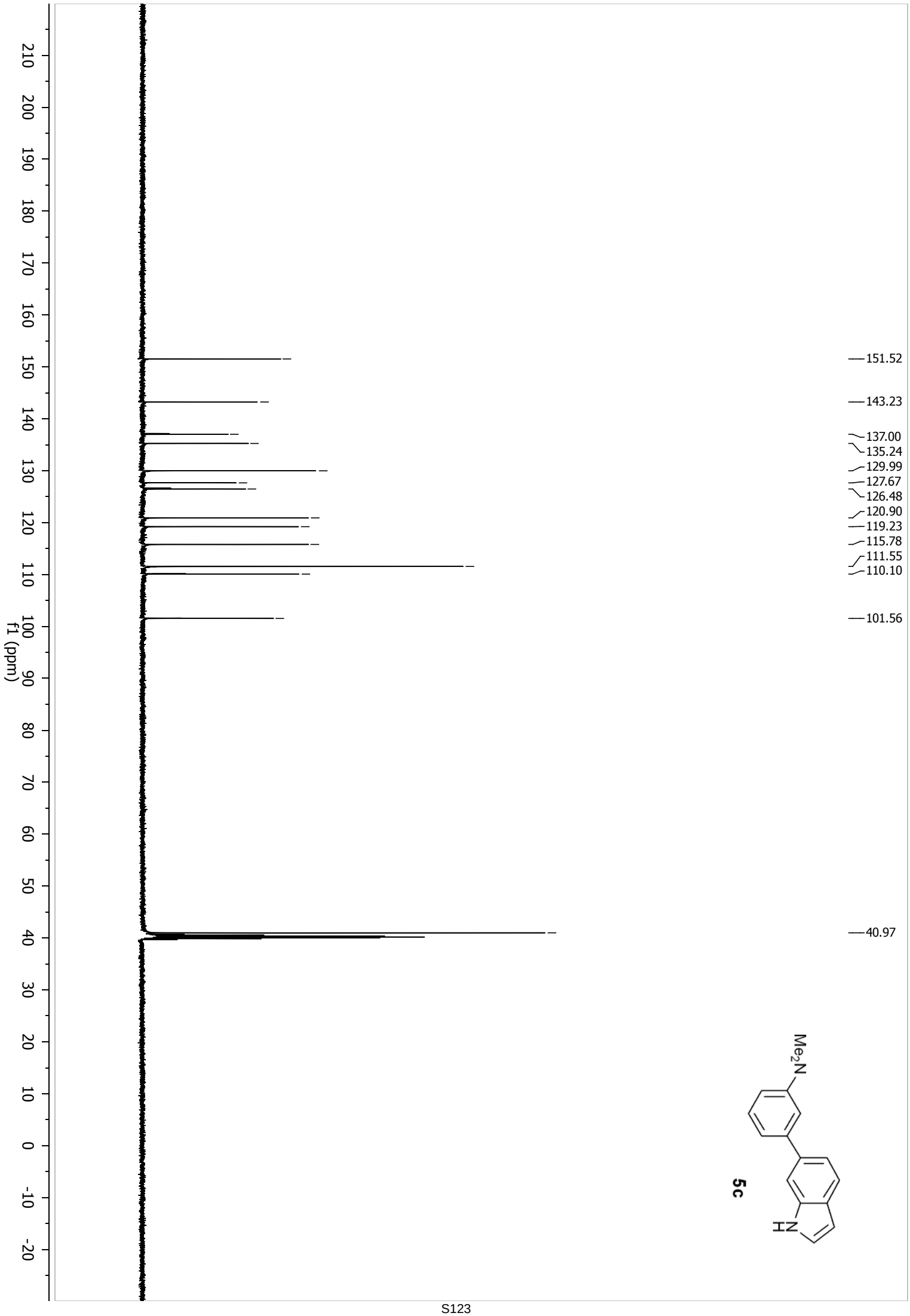

170
150
130
110
90
80
70
60
50
40
30
20
10
0
-20
-40
-60
-80
-100
-120
-140
-160
f1 (ppm)
-76.44
-76.47
F
N
N
H
5a

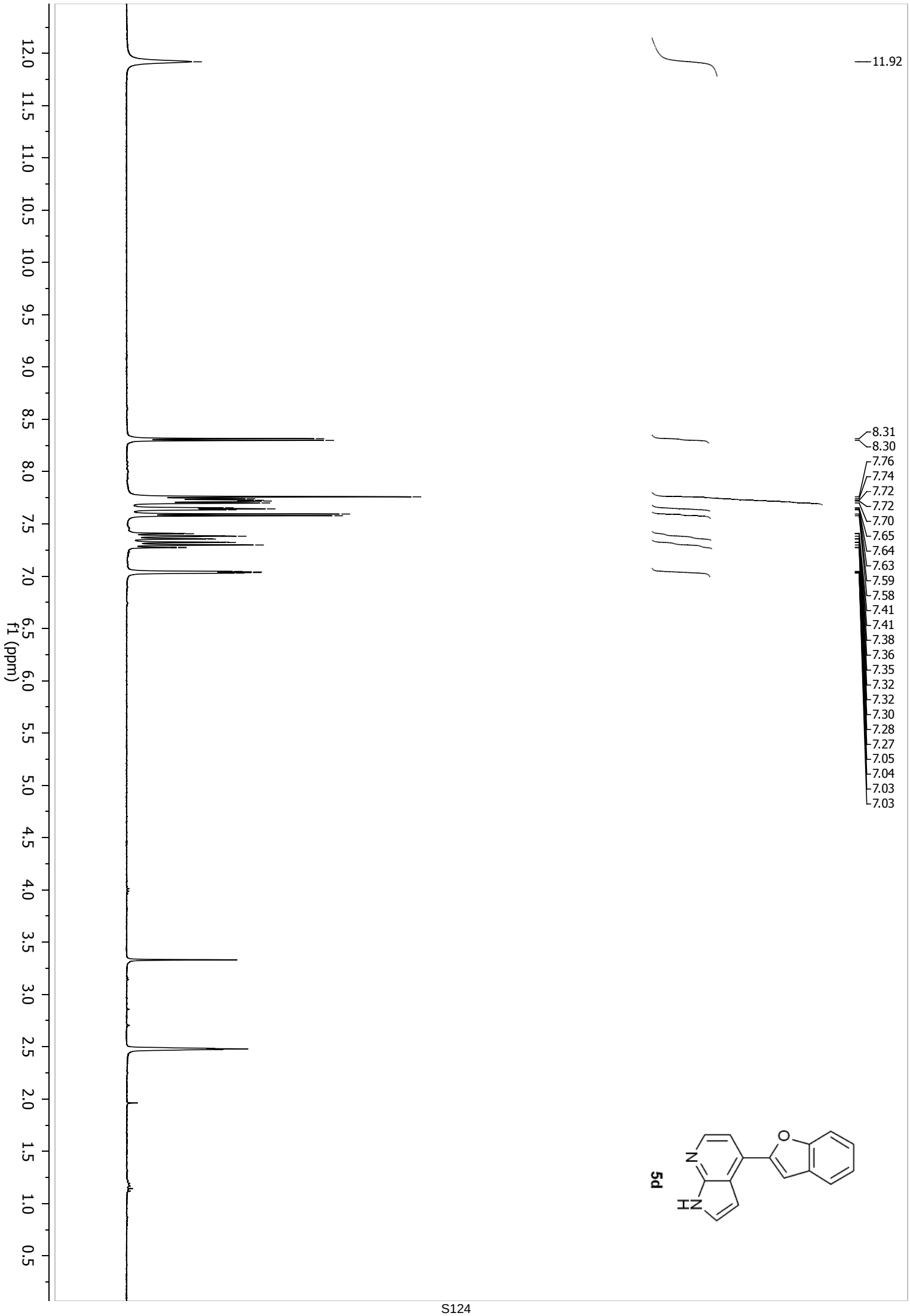

164.02
162.16
146.15
146.03
141.24
141.18
137.04
137.01
136.92
129.45
128.01
127.58
121.36
119.69
113.25
110.67
110.37
102.75
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
F
N
H
N
5a

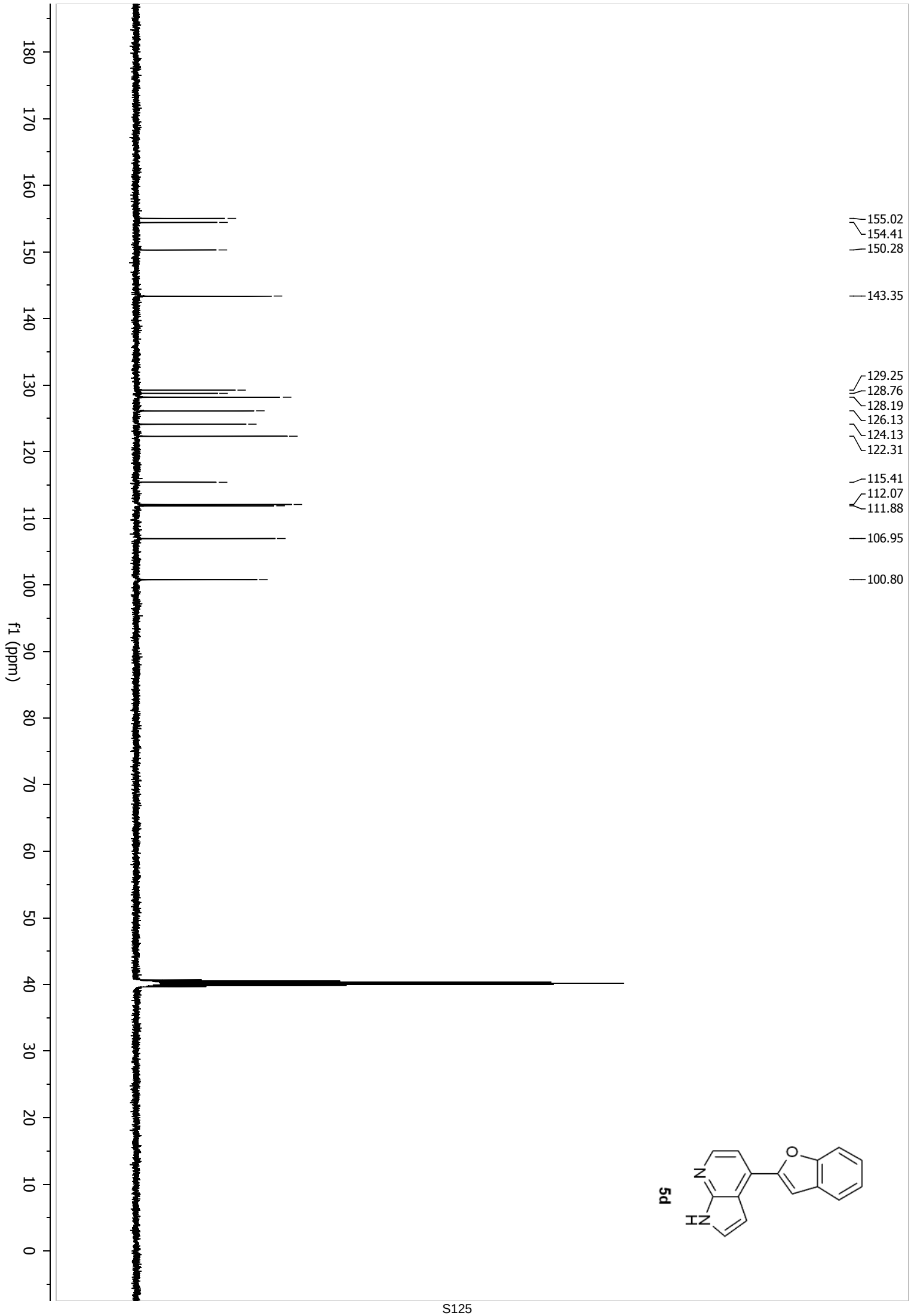

7.59
7.59
7.59
7.52
7.52
7.50
7.49
7.23
7.22
7.13
7.13
6.83
6.83
6.82
6.42
6.42
6.41
6.41
2.26
2.26
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Me
S
N
H
5b

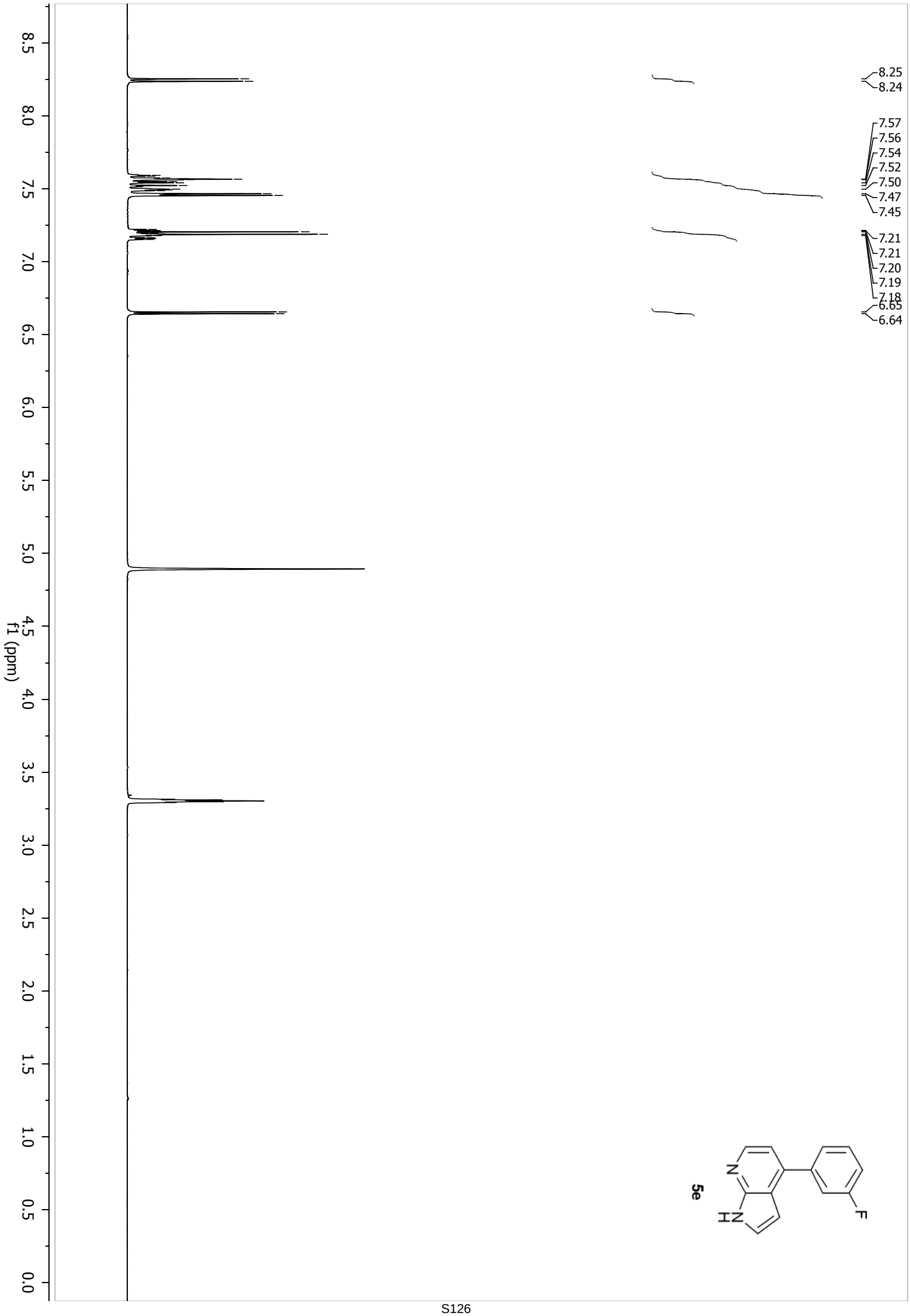

145.64
138.90
136.92
128.02
127.81
127.08
125.16
121.22
119.89
117.87
108.60
101.95
16.35
f1 (ppm)
Me
S
N
H
5b

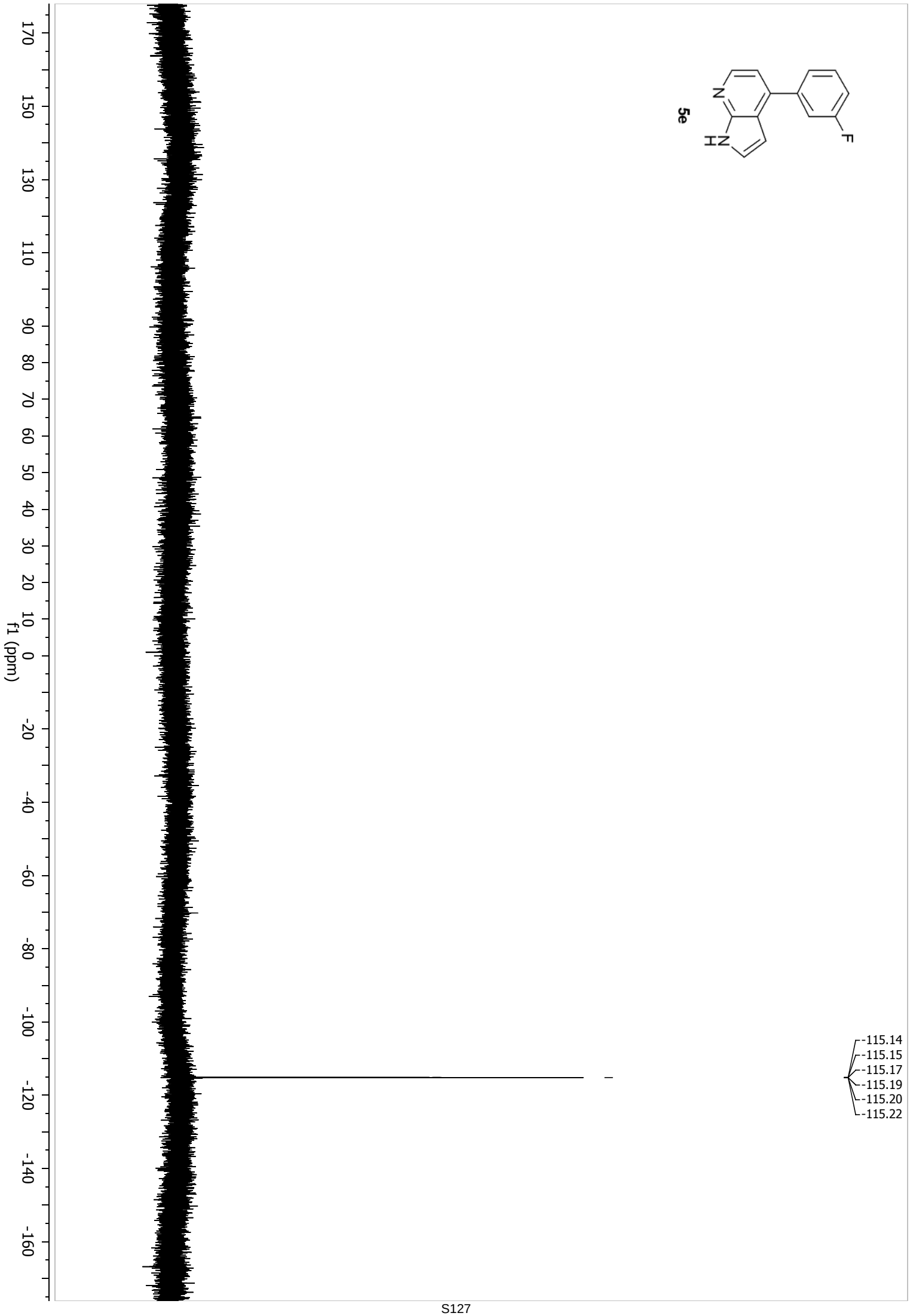

7.59
7.59
7.58
7.55
7.55
7.29
7.28
7.25
7.24
7.24
7.23
6.76
6.76
6.75
6.44
6.44
6.43
6.43
2.97
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Me2N
NH
5c

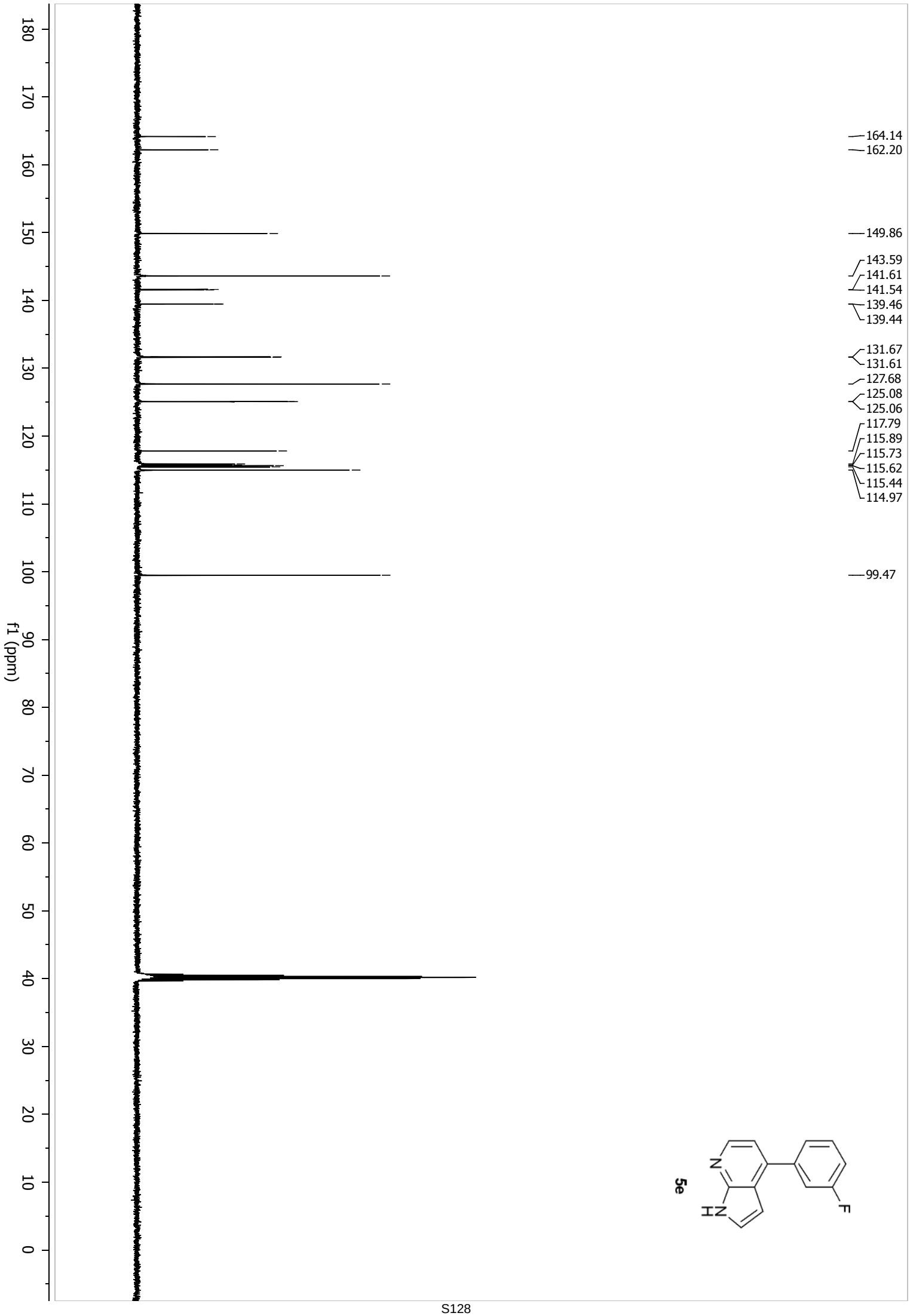

151.52
143.23
137.00
135.24
129.99
127.67
126.48
120.90
119.23
115.78
111.55
110.10
101.56
40.97
f1 (ppm)
Me2N
5c

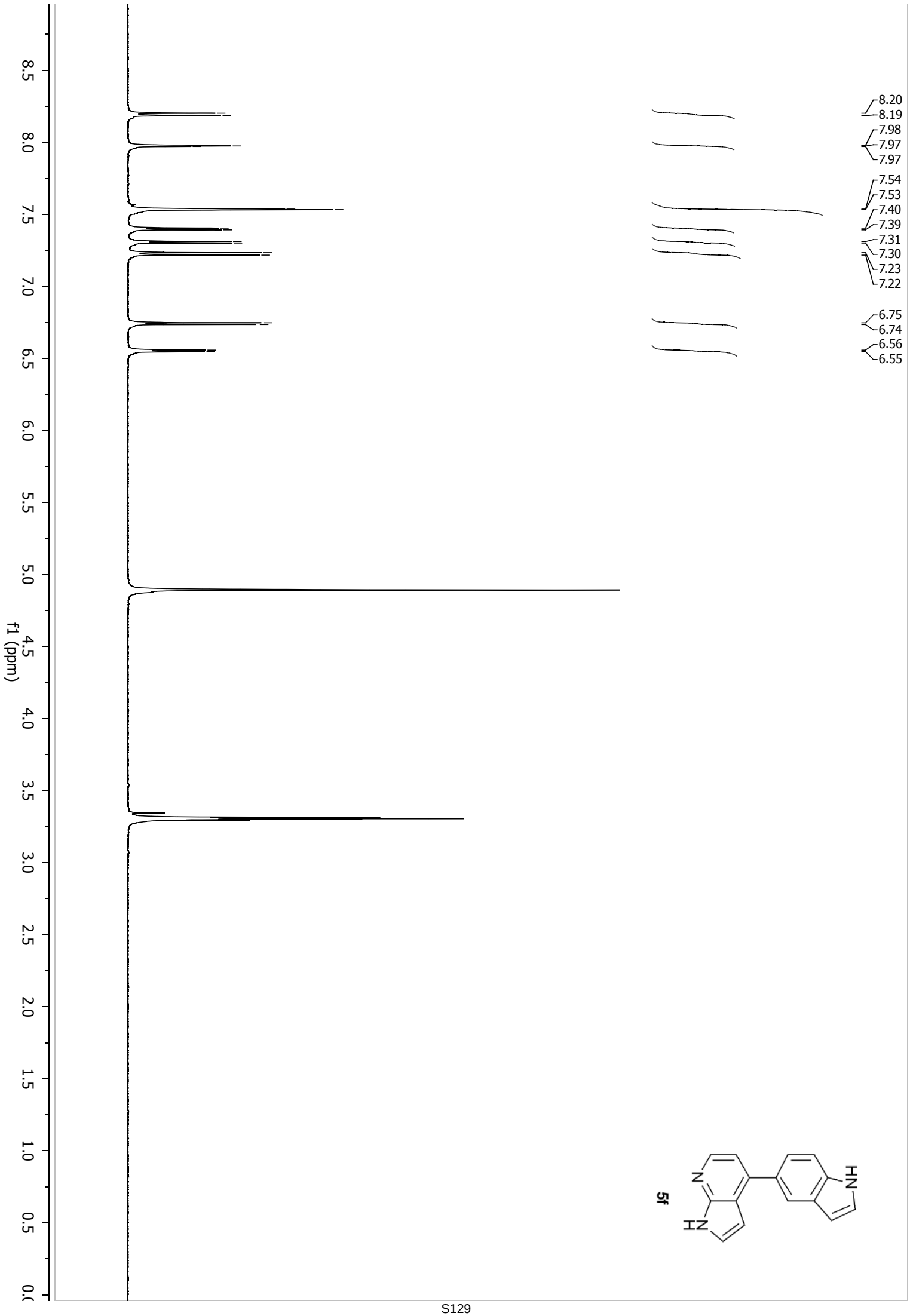

11.92
8.31
8.30
7.76
7.74
7.72
7.72
7.70
7.65
7.64
7.63
7.59
7.58
7.41
7.41
7.38
7.36
7.35
7.32
7.32
7.30
7.28
7.27
7.05
7.04
7.03
7.03
f1 (ppm)
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
5d
N
H
N
O

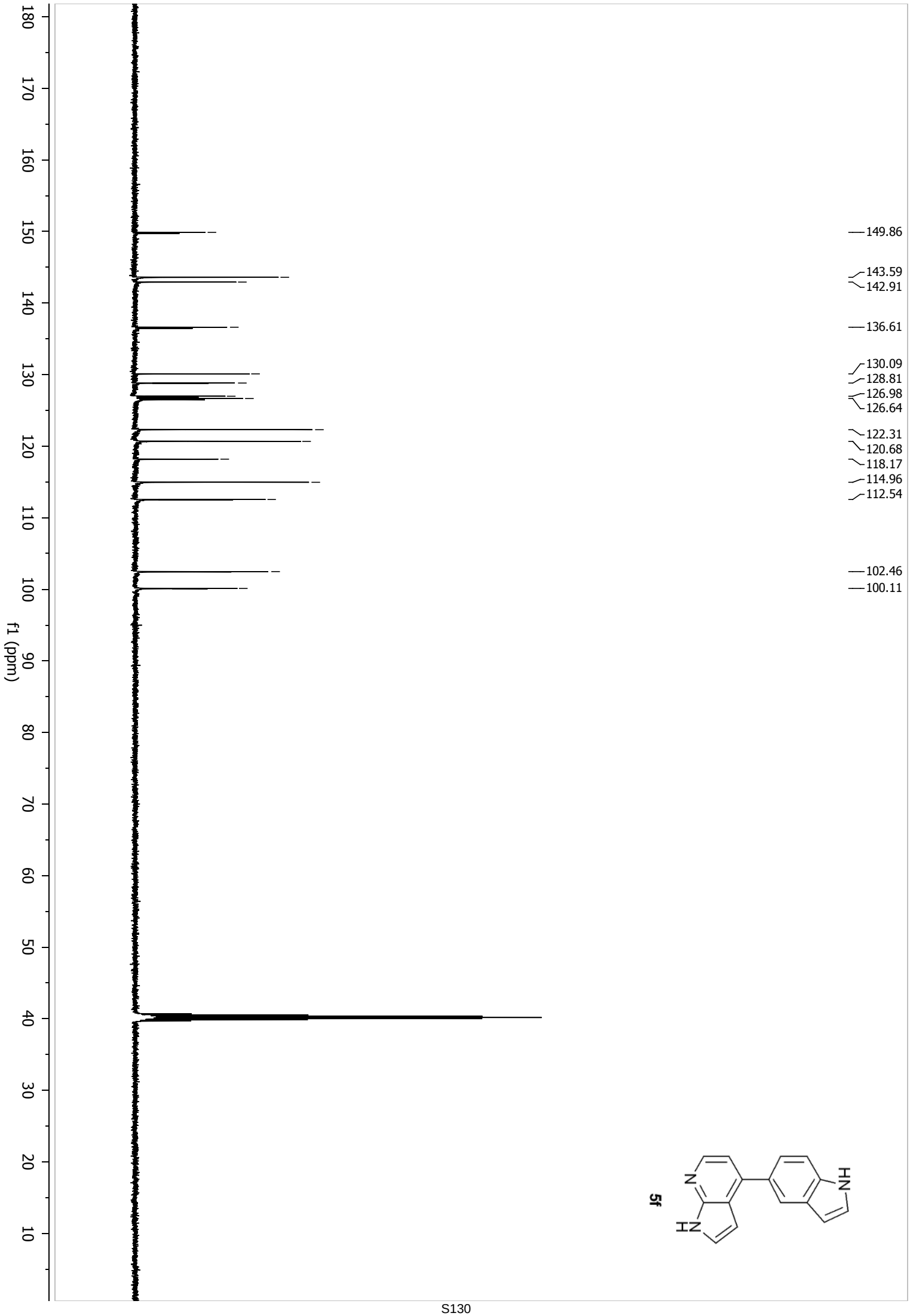

155.02
154.41
150.28
143.35
129.25
128.76
128.19
126.13
124.13
122.31
115.41
112.07
111.88
106.95
100.80
f1 (ppm)
5d

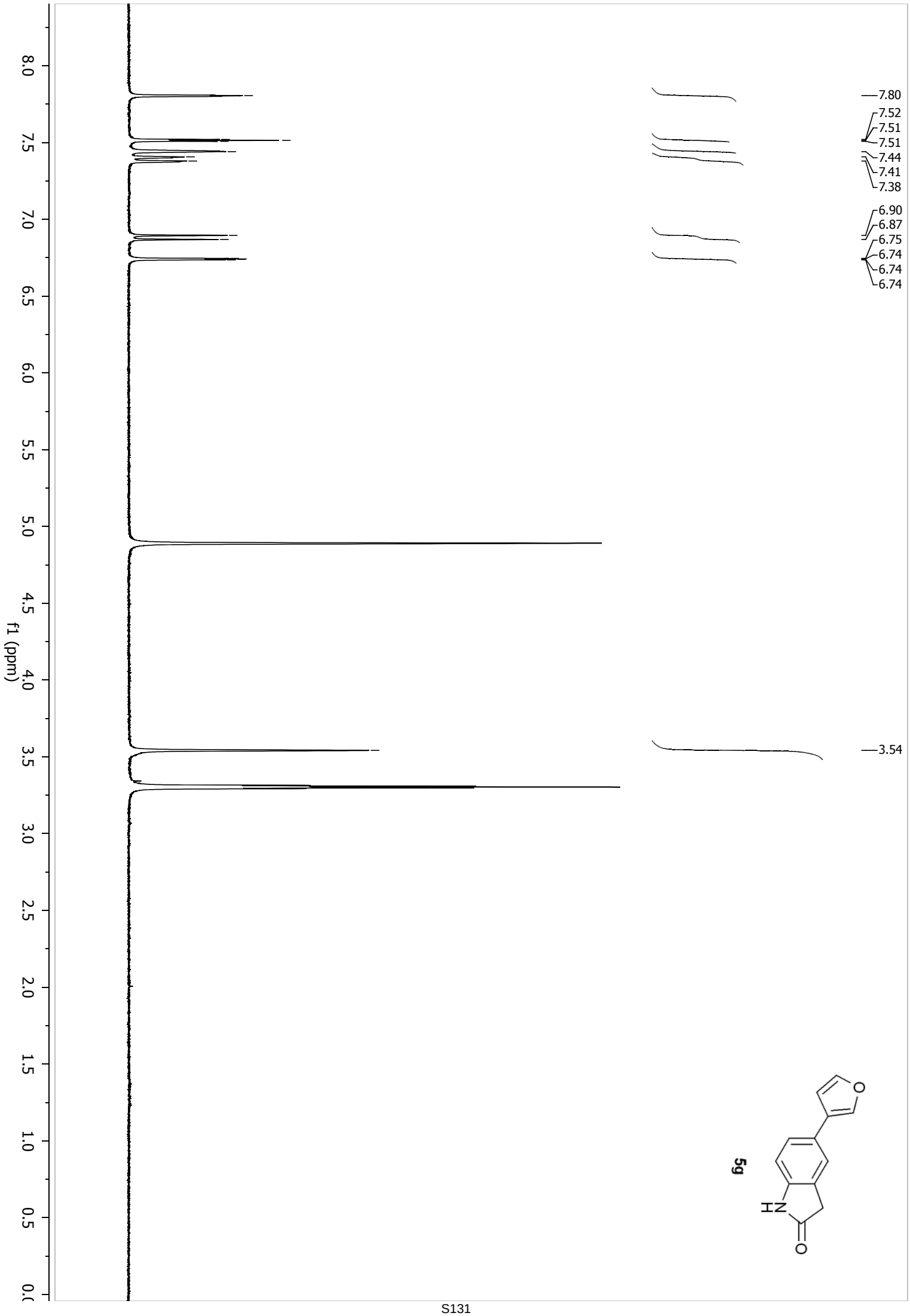

8.25
8.24
7.57
7.56
7.54
7.52
7.50
7.47
7.45
7.21
7.21
7.20
7.19
7.18
6.65
6.64
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
5e
N
HN
F

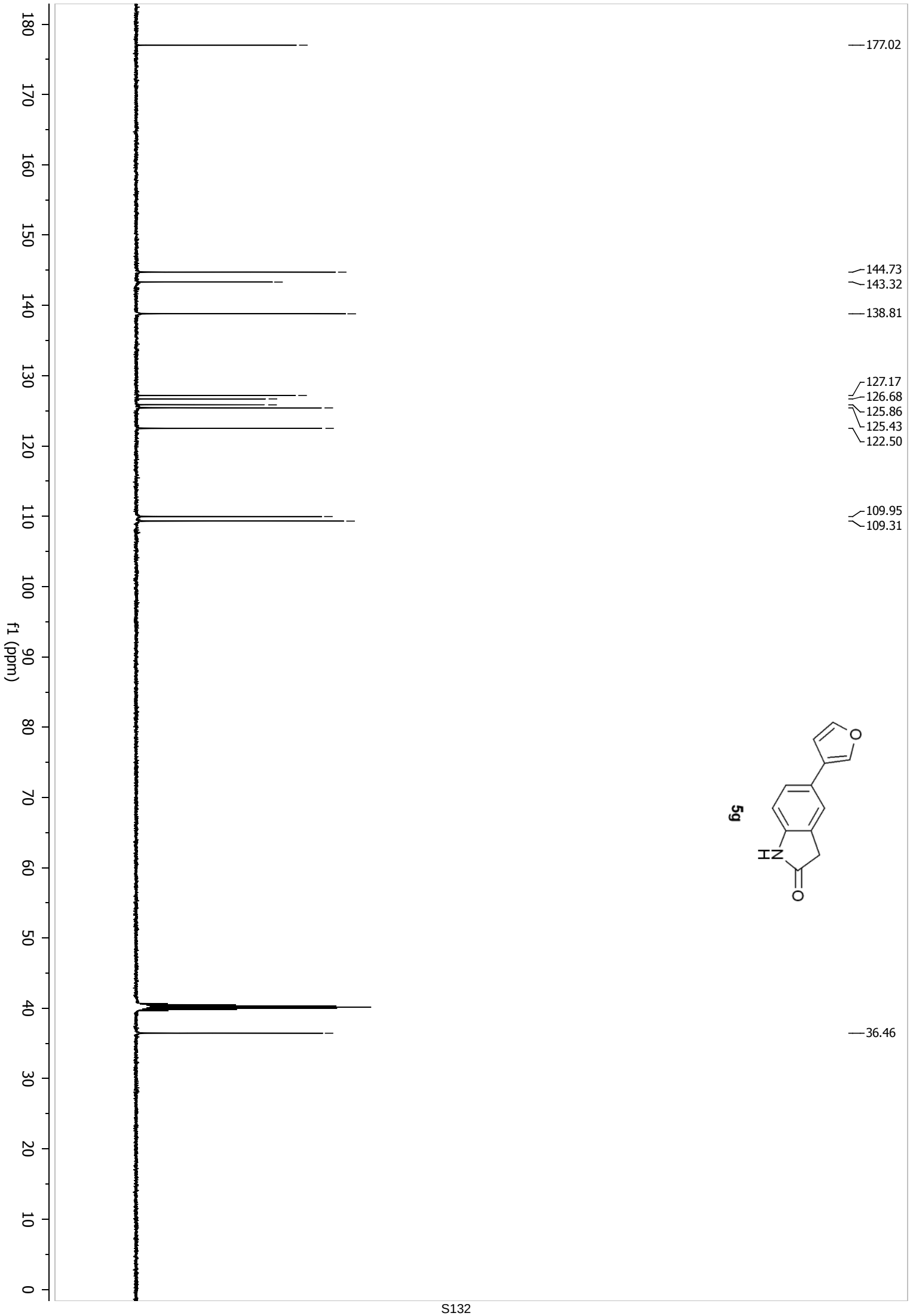

5e
N
H
N
F
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-20
-40
-60
-80
-100
-120
-140
-160
f1 (ppm)
-115.14
-115.15
-115.17
-115.19
-115.20
-115.22

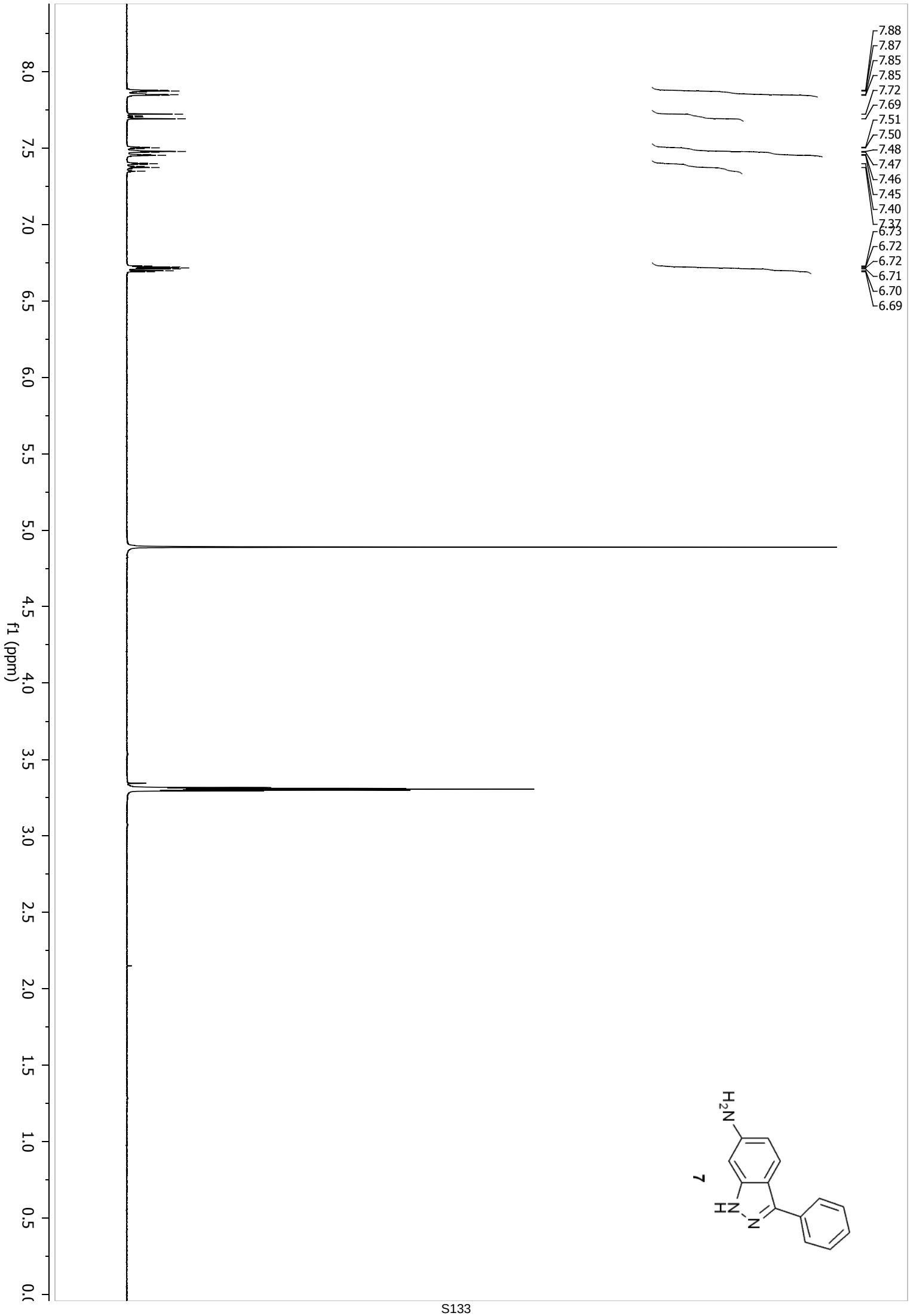

164.14
162.20
149.86
143.59
141.61
141.54
139.46
139.44
131.67
131.61
127.68
125.08
125.06
117.79
115.89
115.73
115.62
115.44
114.97
99.47
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
5e
N
H
N
F

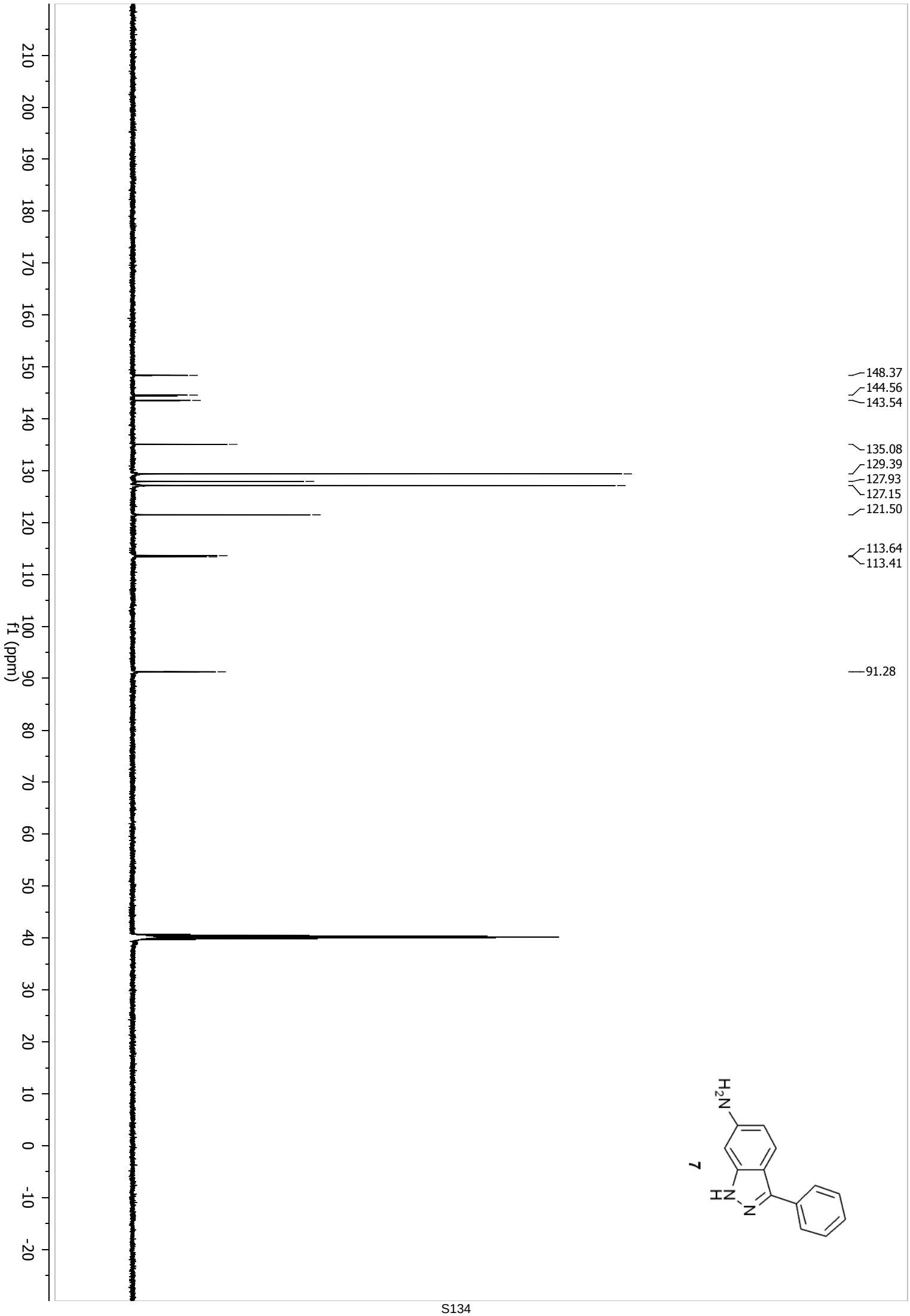

8.20
8.19
7.98
7.97
7.97
7.54
7.53
7.40
7.39
7.31
7.30
7.23
7.22
6.75
6.74
6.56
6.55
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
5f
N
H
N
H

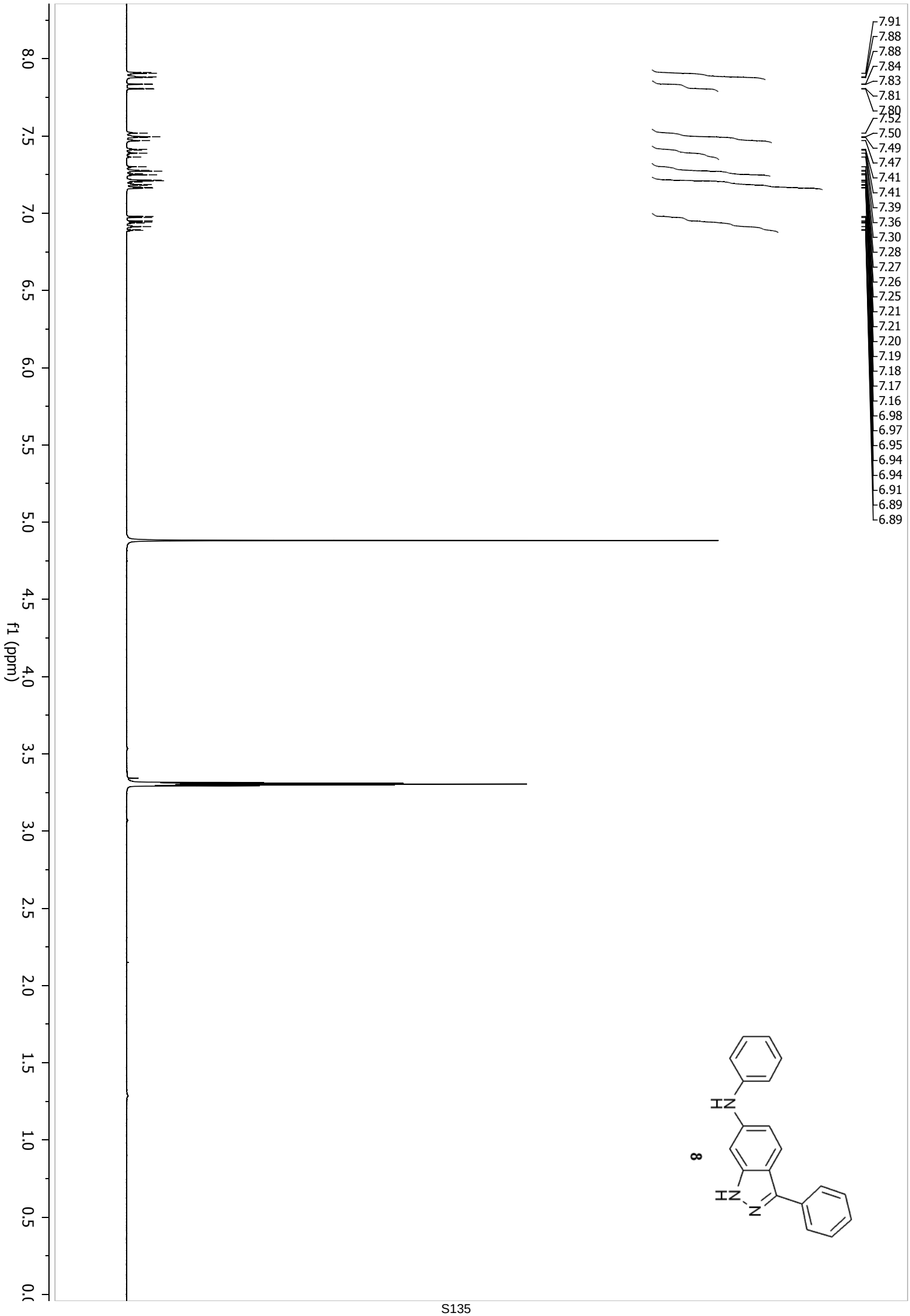

149.86
143.59
142.91
136.61
130.09
128.81
126.98
126.64
122.31
120.68
118.17
114.96
112.54
102.46
100.11
f1 (ppm)
5f

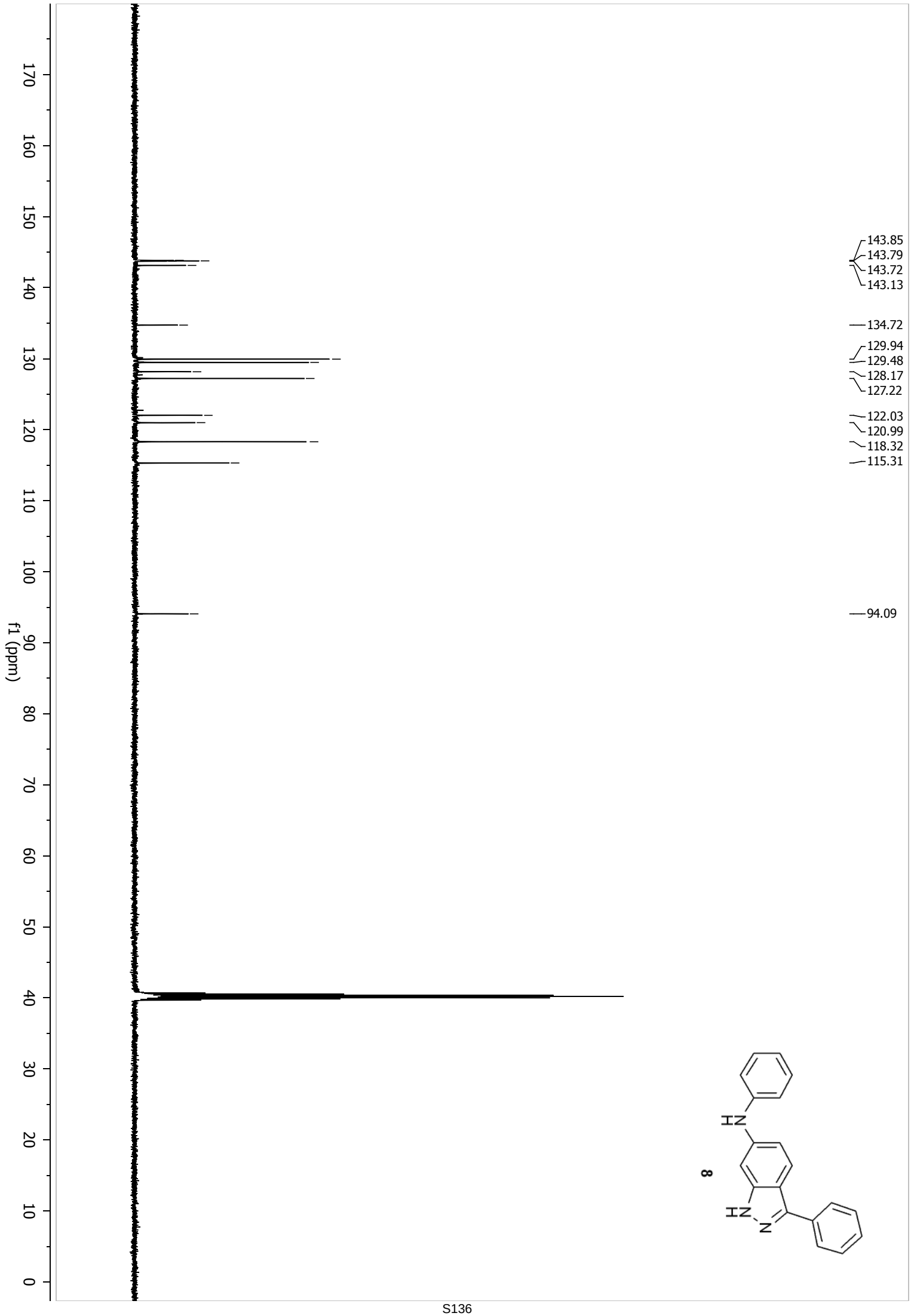

7.80
7.52
7.51
7.51
7.44
7.41
7.38
6.90
6.87
6.75
6.74
6.74
6.74
3.54
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
5g
O
HN
O

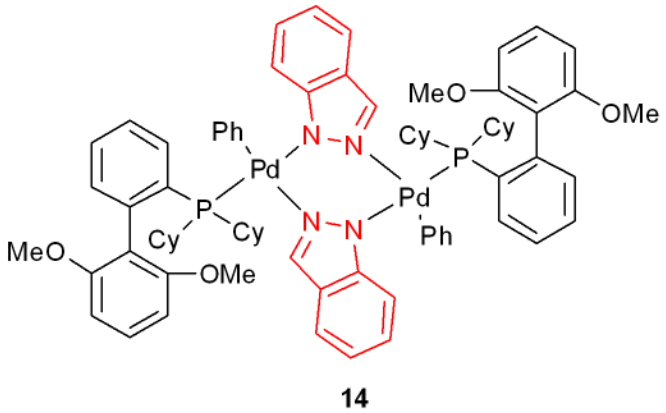

177.02
144.73
143.32
138.81
127.17
126.68
125.86
125.43
122.50
109.95
109.31
36.46
f1 (ppm)
5g


7.88
7.87
7.85
7.85
7.72
7.69
7.51
7.50
7.48
7.47
7.46
7.45
7.40
7.37
6.73
6.72
6.72
6.71
6.70
6.69
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
H2N
N
H
N
7


148.37
144.56
143.54
135.08
129.39
127.93
127.15
121.50
113.64
113.41
91.28
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
7
H2N
HN
N


7.91
7.88
7.88
7.84
7.83
7.81
7.80
7.52
7.50
7.49
7.47
7.41
7.41
7.39
7.36
7.30
7.28
7.27
7.26
7.25
7.21
7.21
7.20
7.19
7.18
7.17
7.16
6.98
6.97
6.95
6.94
6.94
6.91
6.89
6.89
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
HN
HN
N
8

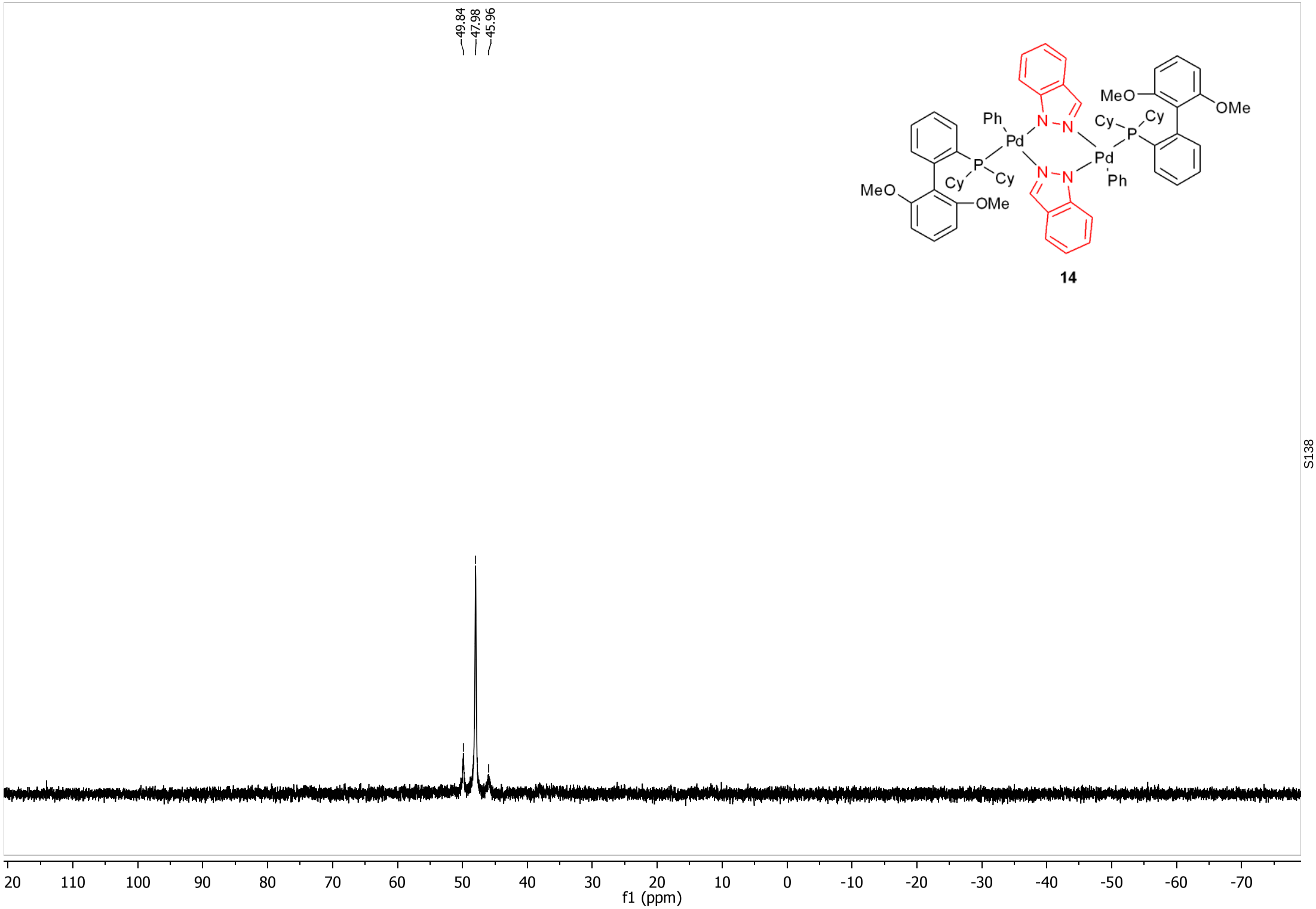

143.85
143.79
143.72
143.13
134.72
129.94
129.48
128.17
127.22
122.03
120.99
118.32
115.31
94.09
f1 (ppm)
8

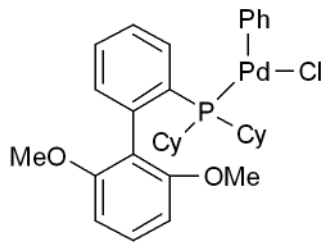


14

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

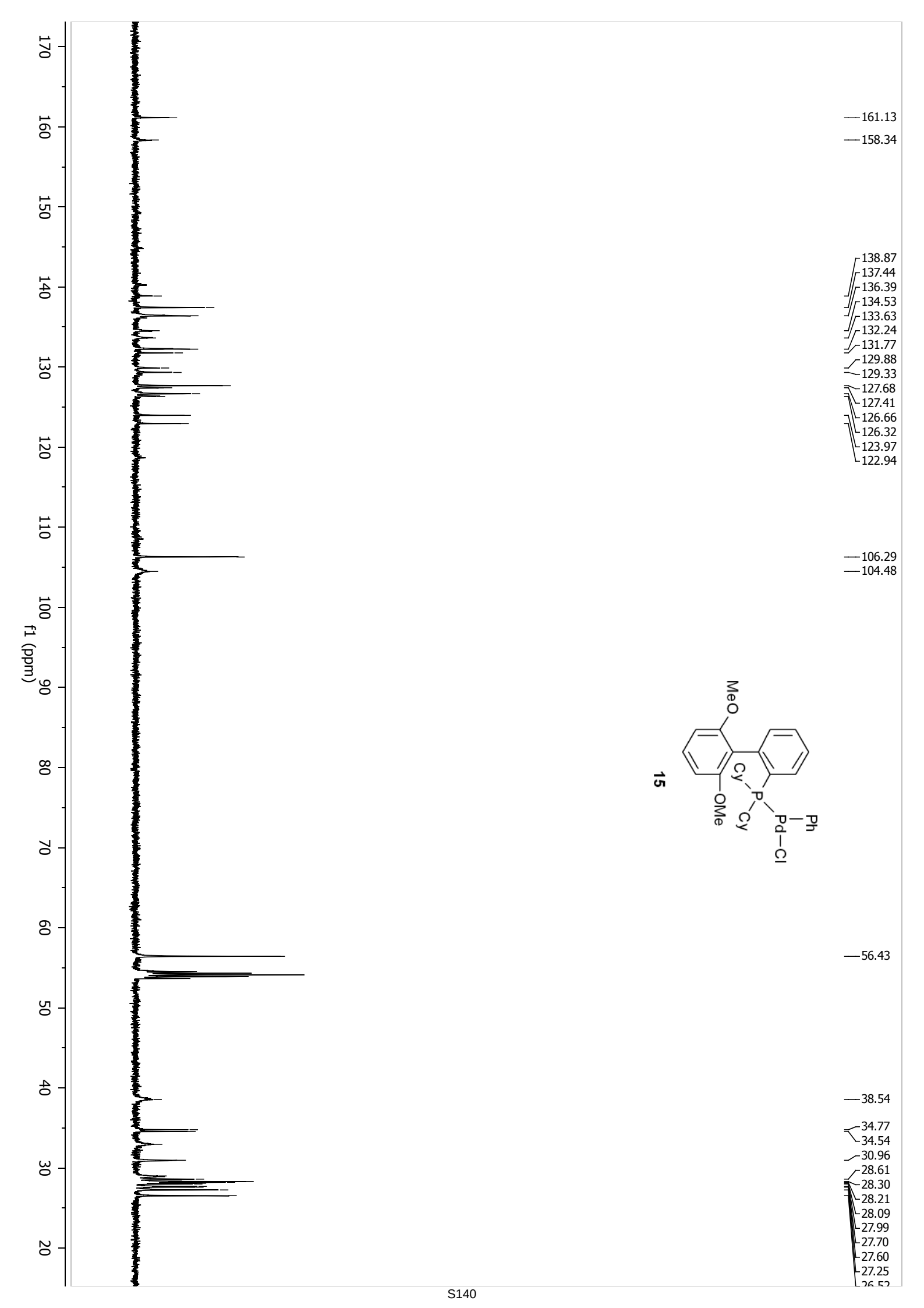
f1 (ppm)

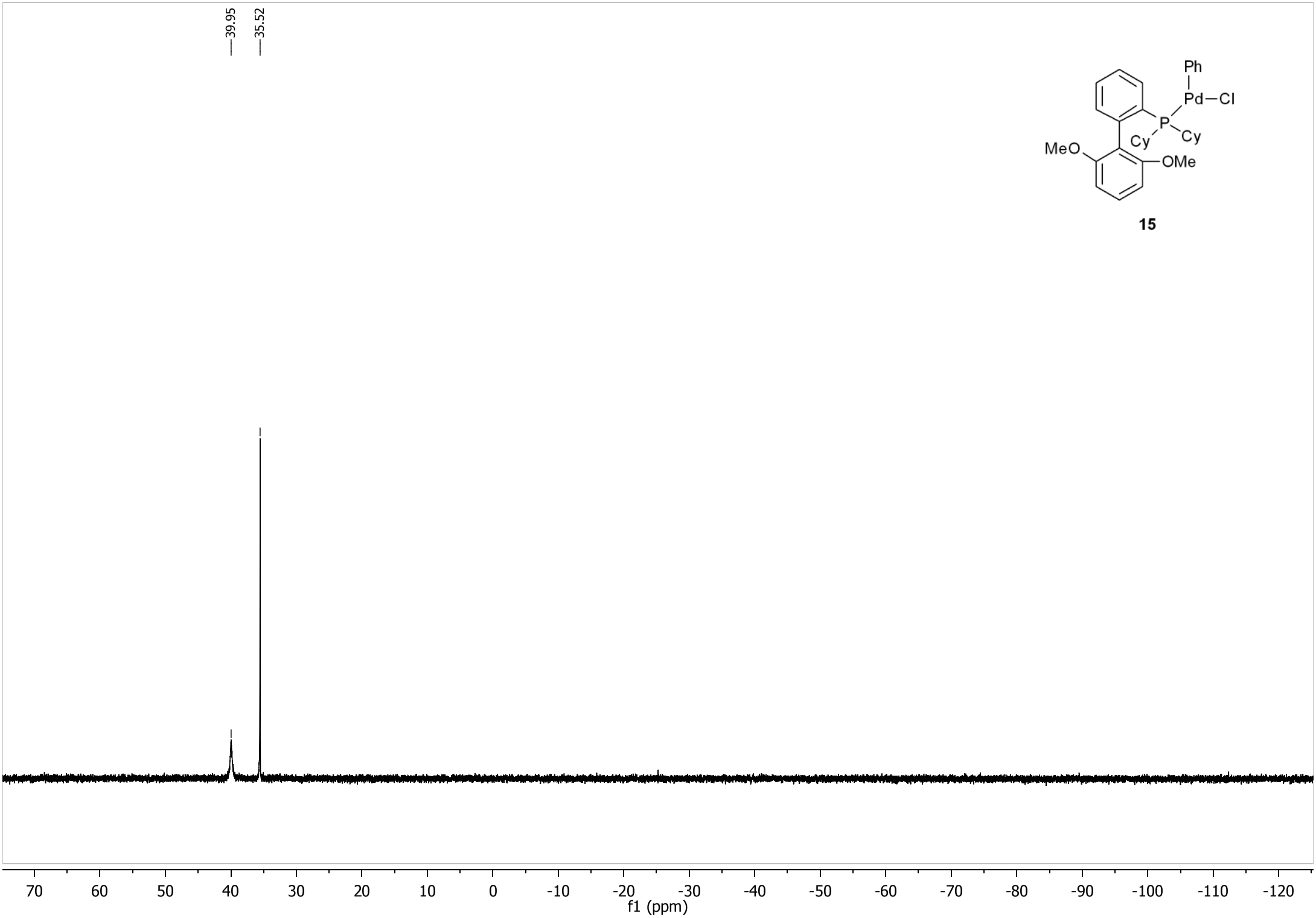

49.84
47.98
45.96
Ph
Pd
N
N
Pd
Ph
P
Cy
Cy
MeO
OMe
Cy
Cy
P
MeO
OMe
14
f1 (ppm)
20
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70

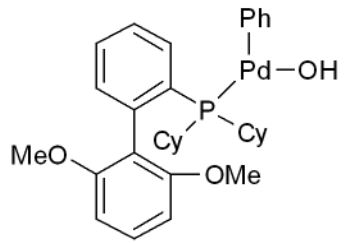


15

f1 (ppm)

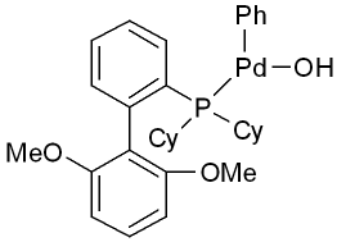

f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
161.13
158.34
138.87
137.44
136.39
134.53
133.63
132.24
131.77
129.88
129.33
127.68
127.41
126.66
126.32
123.97
122.94
106.29
104.48
56.43
38.54
34.77
34.54
30.96
28.61
28.30
28.21
28.09
27.99
27.70
27.60
27.25
MeO
Cy
P
Cy
OMe
Ph
Pd—Cl
15


39.95
35.52
Ph
Pd—Cl
P
Cy
Cy
MeO
OMe
15
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
f1 (ppm)



16

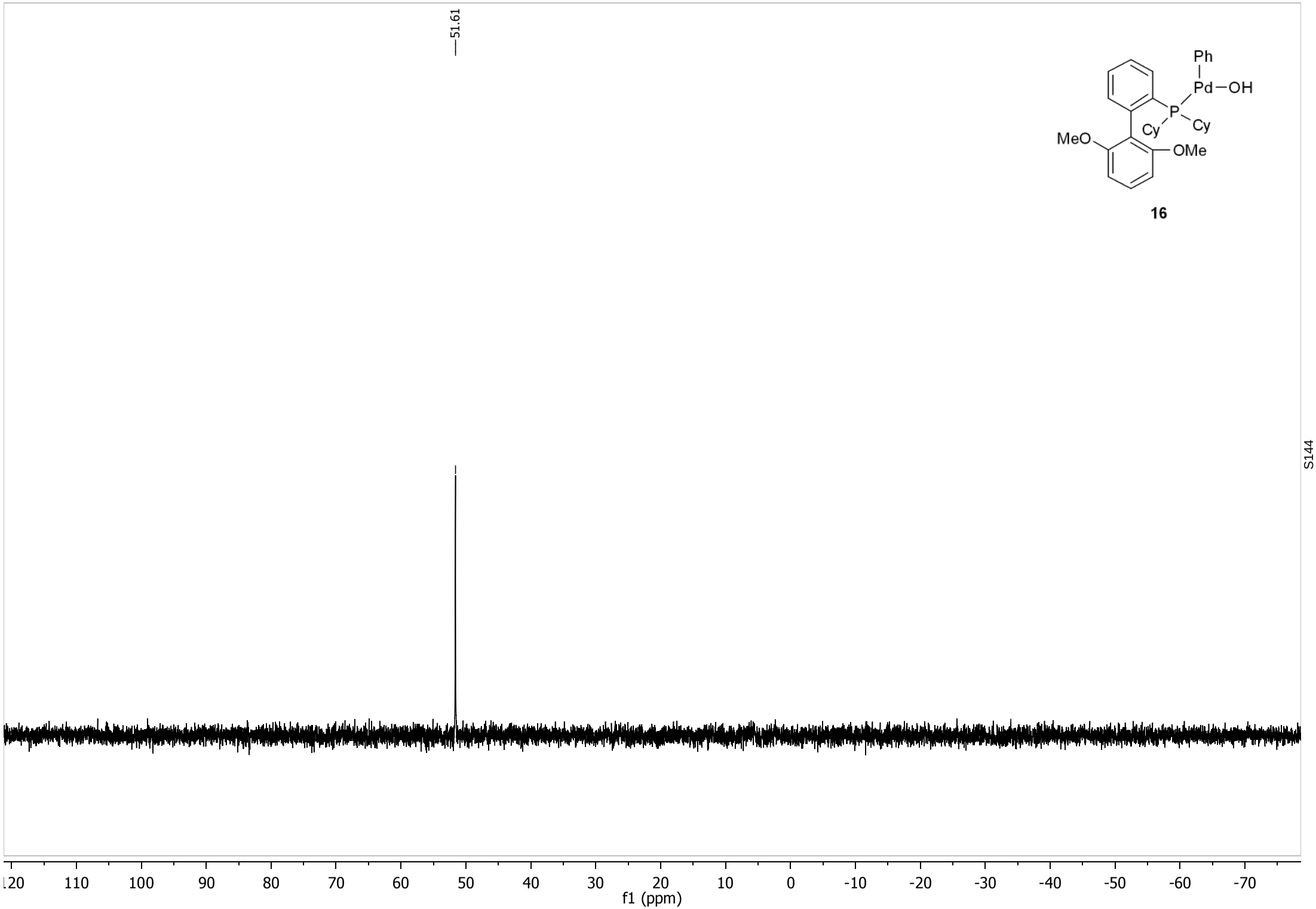
f1 (ppm)



16

159.00
158.73
151.45
137.56
136.90
133.94
133.88
130.00
129.77
129.07
125.90
125.79
121.98
121.93
119.78
104.02
103.86
100.50
55.79
55.34
37.07
36.39
36.19
32.48
32.03
30.88
30.30
28.98
28.85
28.43
28.32
28.18
27.30
27.14

50 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40
f1 (ppm)


51.61
Ph
Pd—OH
P
Cy
Cy
MeO
OMe
16
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
f1 (ppm)