Supporting Information

Deconstructive annulation mediated one-pot synthesis of xanthene derivatives

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Contents

Materials:

β-Naphthol, α-Naphthol, 4-Nitrobenzaldehyde, Anisaldehyde, 2-Chlorobenzaldehyde, 4-Chlorobenzaldehyde, 4-Bromobenzaldehyde, 2-Bromobenzaldehyde, 3-Fluorobenzaldehyde, 4-Fluorobenzaldehyde, 4-Nitrobenzaldehyde and 2,4-Dichlorobenzaldehyde were purchased from Avra chemicals. Benzaldehyde, Pyrrolidine, Piperidine, Salicylaldehyde and Silica gel 100-200 mesh size was purchased from SRL Chemicals Pvt. Ltd. 3-Hydroxybenzaldehyde was purchased from Loba Chemie Pvt Ltd. Dimedone and 1,3-diphenylpropane-1,3-dione, 2-5-dichlorobenzaldehyde and 6-Bromo-2-naphthol was purchased from Aldrich. 3-nitrobenzaldehyde, 4-methoxbenzaldehyde and ethyl-3-oxo-3-phenylpropanoate were purchased from SD fine chemicals. Copper(II) trifluromethanesulfonate was purchased from TCI Chemicals. Melting points were uncorrected. ^{1}H NMR and ^{13}C were recorded JEOL model 600 MHz spectrometer using TMS as an internal standard and $CDCl_3$ and DMSO-d6 as a solvent. All the reactions were carried out in fume hood with necessary safety precautions.

Methods

General procedure for the synthesis of derivatives 12-(2-chlorophenyl)-7a,8,9,10-tetrahydro-12H-naphtho[1,2-e]pyrrolo[2,1-b][1,3]oxazine

Starting material:

The synthesis was carried out by closely following the previously reported procedure[1] (As per reported method Mohit L. Deb et. al). To a stirred solution of 1-((2-chlorophenyl)(pyrrolidin-1-yl)methyl)naphthalen-2-ol (500 mg, 1.48 mmol) in DMF (2 ml), I_2 (5 mol %, 10 mg) and TBHP (70 % in H_2O, 141.9 mg, 1.03 mmol) was added and stirred in the oil bath at 130℃ for stipulated time. After completion of the reaction (monitored by TLC), the reaction mixture was

cooled to room temperature and poured into ice-cold water (20 mL) and extracted with ethyl acetate (2 x 20 mL). The combined organic extracts were dried it over anhydrous Na_2SO_4 and then removed the solvent under reduced pressure. The crude residue obtained was purified by column chromatography (silica gel, 100-200 mesh; ethyl acetate/hexane as eluent).

General procedure for the synthesis of Benzo[a]xanthen-12-one derivatives (one-pot, two-step synthesis) (3a- 3e):

To a stirred solution of 12-(2-chlorophenyl)-7a,8,9,10-tetrahydro-12H-naphtho[1,2-e]pyrrolo[2,1-b][1,3]oxazine (300 mg, 0.89 mmol)) in DMSO (2 ml) was added with $K_2S_2O_8$ (362.2 mg, 1.33 mmol) and $AgNO_3$ (45.5 mg, 0.267 mmol). The reaction mixture was stirred vigoursly at 100 ^oC for an hour. To the same reaction tube, K_2CO_3 (370 mg, 2.67 mmol), copper powder (4.5 mg, 0.07 mmol) and Cu_2O (5.6 mg, 0.04 mmol) was added and stirred in the oil bath at 130 ^oC for 12 hours. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to room temperature and poured into ice-cold water (10 mL) and extracted with ethyl acetate (3 x 5 mL). The combined extracts were dried it over anhydrous Na_2SO_4 and then removed the solvent under reduced pressure. The crude was purified by column chromatography (silica gel, 100-200 mesh; ethyl acetate/hexane as eluent).

12H-benzo[a]xanthen-12-one (3a) : White solid, Reaction carried out with 0.893 mmol of oxazine substrate. Yield = 61% (133.8 mg), Mp: 153- 154 ^oC (152- 154 ^oC [10]); ^1H NMR (600 MHz, $CDCl_3$): 7.33-7.36 (m, 1H), 7.44-7.46 (m, 2H), 7.49- 7.52 (m, 1H), 7.62- 7.64 (m, 1H), 7.68- 7.71 (m, 1H), 7.80 (d, *J* = 7.8 Hz, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 8.35 (dd, *J* = 7.8 Hz, *J* = 1.8 Hz, 1H), 9.99 (d, *J* = 6.0 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 114.6, 117.5, 118.0, 123.6, 124.3, 126.1, 126.7, 127.0, 128.4, 129.6, 130.1, 131.2, 133.9, 136.7, 154.7, 157.6, 178.5.

9-chloro-12H-benzo[a]xanthen-12-one (3b): Reaction carried out with 1.343 mmol of oxazine substrate. Pale yellow semi-solid[11], Yield = 66% (248.25 mg), ^{1}H NMR (600 MHz, $CDCl_3$): 7.43- 7.46 (m, 1H), 7.55- 7.58 (m, 1H), 7.59- 7.62 (m, 1H), 7.72- 7.75 (m, 1H), 7.77- 7.80 (m, 1H), 7.91 (d, *J* =6.6 Hz, 1H), 8.13 (d, *J* = 9.0 Hz , 1H), 8.45 (dd, J_1 = 8.4 Hz, J_2 = 1.8 Hz, 1H), 10.10 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 114.6, 117.5, 118.0, 123.6, 124.3, 126.1, 126.7, 127.0, 128.3, 129.6, 130.1, 131.2, 134.0, 136.7, 154.7, 157.6, 178.5.

7H-benzo[c]xanthen-7-one (3c): White solid, Reaction carried out with 0.297 mmol of oxazine substrate. Yield = 63% (46.3 mg), Mp: 154- 157 ºC (159- 161 ºC [10]); ^{1}H NMR (600 MHz, $CDCl_3$): 7.38-7.41 (m, 1H), 7.50- 7.57 (m, 3H), 7.67- 7.74 (m, 2H), 7.86 (d, *J* = 9.6 Hz, 1H), 8.09 (d, *J* = 9.0 Hz, 1H), 8.39 (d, *J* = 9.6 Hz, 1H), 10.04 (d, *J* = 9.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 114.6, 117.5, 118.1, 123.6, 124.3, 126.2, 126.6, 126.9, 128.3, 129.6, 130.1, 131.2, 133.9, 136.7, 154.7, 157.6, 178.5.

2-Bromo-7H-benzo[c]xanthen-7-one (3d): White solid, Reaction carried out with 0.120 mmol of oxazine substrate. Yield = 63% (24.87 mg), Mp: 219- 221 ºC (218- 221 ºC [10]); ^{1}H NMR (600 MHz, $CDCl_3$): 7.45- 7.48 (m, 1H), 7.56- 7.61 (m, 2H), 7.74- 7.77 (m, 1H), 7.84 (dd, J_1 = 9.0 Hz, J_2 = 1.8 Hz, 1H), 8.03- 8.05 (m, 2H), 8.43 (dd, J_1 = 7.8 Hz, J_2 = 0.9 Hz, 1H), 10.00 (d, *J* = 9.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 114.6, 117.6, 119.4, 120.2, 123.4, 124.5, 126.7, 128.8, 129.7, 130.3, 131.5, 132.5, 134.2, 135.4, 154.6, 157.5, 178.2.

9-Chloro-7H-benzo[c]xanthen-7-one (3e): Pale yellow solid, Reaction carried out with 0.135 mmol of oxazine substrate. Yield = 53% (20.02 mg), Mp: 220- 222 ºC (224- 226 ºC [10]); ^{1}H NMR (600 MHz, $CDCl_3$): 7.43- 7.46 (m, 1H), 7.56- 7.58 (m, 1H), 7.59- 7.62 (m, 1H), 7.72- 7.75 (m, 1H),7.77- 7.80 (m, 1H), 7.91 (d, *J* = 6.6 Hz, 1H), 8.13 (d, *J* = 9.0 Hz, 1H), 8.45 (dd, J_1 = 8.4 Hz, J_2 = 1.8 Hz, 1H), 10.10 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 114.6,

117.5, 118.0, 123.6, 124.3, 126.1, 126.7, 127.0, 128.3, 129.6, 130.1, 131.2, 133.9, 136.7, 154.7, 157.6, 178.5.

General procedure for the synthesis of 12H-Benzo[a]xanthen-12-one derivatives (one-pot procedure):

To a stirred solution of 12-(2-chlorophenyl)-7a,8,9,10-tetrahydro-12H-naphtho[1,2-e]pyrrolo[2,1-b][1,3]oxazine (10 mg, 0.03 mmol)) in DMF (1 ml), Cs_2CO_3 (38 mg, 0.12 mmol) and copper powder (1.44mg, 0.02 mmol) was added and stirred in the oil bath at 130 ^oC for 20 hours. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to room temperature and poured into ice-cold water (10 mL) and extracted with ethyl acetate (3 x 5 mL). The combined extracts were dried over anhydrous Na_2SO_4 and then removed the solvent under reduced pressure. Purified the crude by column chromatography (silica gel, 100-200 mesh; ethyl acetate/hexane as eluent).

The synthesized compounds were crosschecked with the previously obtained product. They are matching satisfactorily.

12H-benzo[a]xanthen-12-one (3a): White solid, Reaction carried out with 0.0297 mmol of oxazine substrate. Yield = 81% (5.9 mg)

9-chloro-12H-benzo[a]xanthen-12-one (3b): Reaction carried out with 0.270 mmol of oxazine substrate. Half white solid, Yield = 64% (48 mg),

General procedure for the synthesis of 9,9-dimethyl-12-phenyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one derivatives (4a-s)

To a stirred solution of 12-phenyl-7a,8,9,10-tetrahydro-12H-naphtho[1,2-e]pyrrolo[2,1-b][1,3]oxazine (50 mg, 0.165 mmol) in 1,2-dichloroethane (5 ml) , $K_2S_2O_8$ (64.8 mg, 0.24 mmol.) and $AgNO_3$ (8.2 mg, 0.048 mmol) was added and stirred in the oil bath at 100℃ for 1.5 hours. After 1.5 hours, 5,5-dimethylcyclohexane-1,3-dione (33.6 mg, 0.24 mmol) and copper(II) triflate (5.78 mg, 0.016 mmol)is added in the reaction mixture and stirred at 90℃ for 4 hours. After completion of the reaction, the reaction mixture was cooled oto room temperature, quenched with water (10 mL) and extracted with ethyl acetate (2×20 mL). The combined organic extracts were dried over anhydrous Na_2SO_4, concentrated under reduced pressure and the crude sample was purified by silica gel (100-200 mesh) column chromatography with ethyl acetate:hexane(1:10 v/v) as eluent.

9,9-dimethyl-12-phenyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4a):

Reaction carried out with 0.165 mmol of oxazine substrate. White Solid, Yield = 80% (46.6 mg) Mp: 152-154 °C (154-155°C[2]) ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.89 (s, 3H), 1.03 (s, 3H), 2.18 (d, *J*= 16.2 Hz, 1H), 2.24 (d, *J*= 16.2 Hz, 1H), 2.48 (s, 2H), 5.71 (s, 1H), 6.99-7.02 (m, 1H), 7.13-7.18 (m, 2H), 7.27-7.37 (m, 5H), 7.67-7.70 (m, 2H), 7.98 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 26.9, 29.1, 31.9, 34.6, 41.2, 50.7, 114.1, 116.9, 117.5, 123.5, 124.7, 126.1, 126.8, 128.1, 128.2, 128.3, 128.7, 131.2, 131.3, 144.6, 147.6, 163.6, 196.6.

9,9-dimethyl-12-(p-tolyl)-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4b) :

Reaction carried out with 0.475 mmol of oxazine substrate. White Crystals, Yield = 81 % (142.3 mg), Mp: 173-176 °C (175-177°C[3]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.97 (s, 3H), 1.11 (s, 3H), 2.19 (s, 3H), 2.24 (d, *J* = 16.8 Hz, 1H), 2.29 (d, *J* = 16.2 Hz, 1H), 2.56 (s, 2H), 5.66 (s, 1H), 6.96 (d, *J* = 7.8 Hz, 2H), 7.21-7.43 (m, 5H), 7.72-7.76 (m, 2H), 8.00 (d, *J* = 8.4 Hz, 1H).

^{13}C NMR (150 MHz, $CDCl_3$): δ 20.9, 27.2, 29.2, 32.2, 34.3, 41.4, 50.9, 114.4, 117.0, 117.9, 123.7, 124.8, 126.9, 128.2, 128.3, 128.7, 128.9, 131.4, 131.5, 135.6, 141.8, 147.7, 163.7, 196.9.

12-(4-methoxyphenyl)-9,9-dimethyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4c): Reaction carried out with 0.301 mmol of oxazine substrate. White Crystals, Yield = 76% (88.3 mg), Mp: 202-205 °C (205-206 °C[2]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.96 (s, 3H), 1.10 (s, 3H), 2.24 (d, *J* = 16.2 Hz, 1H), 2.29 (d, *J* = 16.2 Hz, 1H), 2.55 (s, 2H), 3.67 (s, 3H), 5.66 (s, 1H), 6.69-6.71 (m, 2H), 7.24-7.43 (m, 5H), 7.73-7.77 (m, 2H), 7.98 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 27.2, 29.3, 32.2, 33.8, 41.4, 50.9, 55.0, 113.6, 114.4, 117.0, 117.9, 123.7, 124.8, 126.9, 128.3, 128.7, 129.3, 131.4, 131.5, 137.1, 147.7, 157.7, 163.6, 197.0.

9,9-dimethyl-12-(4-nitrophenyl)-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4d): Reaction carried out with 0.433 mmol of oxazine substrate. Pale yellow Solid, Yield = 89% (154.0 mg), Mp: 174-177 °C (176-178 °C[3]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.94 (s, 3H), 1.13 (s, 3H), 2.25 (d, *J* = 16.2 Hz, 1H), 2.33 (d, *J* = 16.2 Hz, 1H), 2.60 (s, 2H), 5.81 (s, 1H), 7.35-7.45 (m, 3H), 7.51-7.52 (m, 2H), 7.80-7.84 (m, 3H), 8.03 (d, *J* = 6.6 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 27.0, 29.3, 32.2, 34.8, 41.4, 50.7, 112.9, 116.0, 117.1, 123.1, 123.6, 125.2, 127.3, 128.6, 129.3, 129.6, 131.0, 131.5, 146.3, 147.8, 151.8, 164.6, 196.7.

12-(4-fluorophenyl)-9,9-dimethyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4e): Reaction carried out with 0.313 mmol of oxazine substrate. White Solid, Yield = 76 % (89.16 mg), Mp: 186-188 °C (185-186 °C[3]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.93 (s, 3H), 1.09 (s, 3H), 2.25 (d, *J* = 16.8 Hz, 1H), 2.28 (d, *J* = 16.8 Hz, 1H), 2.53 (s, 2H), 5.69 (s, 1H), 6.82-6.86 (m, 2H), 7.28-7.42 (m, 5H), 7.73-7.76 (m, 2H), 7.91 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (150

MHz, $CDCl_3$): δ 27.0, 29.2, 32.1, 33.9, 41.3, 50.8, 114.0, 114.9, 115.0, 117.0, 117.3, 123.4, 124.9, 127.0, 128.4, 128.9, 129.8, 129.9, 131.2, 131.5, 140.5, 147.7, 160.3, 161.9, 163.8, 196.8.

12-(4-bromophenyl)-9,9-dimethyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4f): Reaction carried out with 0.210 mmol of oxazine substrate. White Solid, Yield = 85 % (78.2 mg), Mp: 188-189 °C (187-189 °C[3]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.97 (s, 3H), 1.12 (s, 3H), 2.25 (d, *J* = 16.2 Hz, 1H), 2.31 (d, *J* = 16.2 Hz, 1H), 2.57 (s, 2H), 5.67 (s, 1H), 7.20-7.23 (m, 2H), 7.27-7.33 (m, 3H), 7.38-7.45(m, 2H), 7.77-7.80 (m, 2H), 7.89 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 27.1, 29.3, 32.3, 34.2, 41.4, 50.8, 113.7, 116.9, 117.0, 120.1, 123.4, 125.0, 127.1, 128.5, 129.1, 130.2, 131.2, 131.3, 131.5, 143.7, 147.7, 164.1, 196.9.

12-(4-chlorophenyl)-9,9-dimethyl-8,9,10,12-tetrahydro-11H benzo[a]xanthen-11-one (4g): Reaction carried out with 0.297 mmol of oxazine substrate. White Crystals, Yield = 80% (92.2 mg), Mp: 182-184°C (181-182°C[2]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.94 (s, 3H), 1.10 (s, 3H), 2.23 (d, *J* = 16.2 Hz, 1H), 2.29 (d, *J* = 16.2 Hz, 1H), 2.54 (s, 2H), 5.68 (s, 1H), 7.11-7.13 (m, 2H), 7.26-7.43 (m, 5H), 7.74-7.77 (m, 2H), 7.89 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 27.0, 29.2, 32.2, 34.1, 41.3, 50.8, 113.8, 117.0, 123.4, 125.0, 127.1, 128.3, 128.4, 129.0, 129.7, 131.2, 131.5, 131.9, 143.2, 147.7, 164.0, 196.8.

12-(2-bromophenyl)-9,9-dimethyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4h): Reaction carried out with 0.210 mmol of oxazine substrate. White Solid, Yield = 78 % (70.8 mg), Mp: 171-173 °C (169- 171 °C[4]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.98 (s, 3H), 1.12 (s, 3H), 2.22 (d, *J* = 16.2 Hz, 1H), 2.30 (d, *J* = 16.2 Hz, 1H), 2.59 (s, 2H), 5.95 (s, 1H), 6.87-6.91 (m, 1H), 7.05- 7.08 (m, 1H), 7.20-7.29 (m, 2H), 7.36-7.50 (m, 3H), 7.72-7.76 (m, 2H), 8.30 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 27.1, 29.3, 32.1, 35.3, 41.5, 50.9,

113.7, 117.1, 117.7, 123.5, 124.4, 124.9, 127.0, 127.5, 127.8, 128.3, 129.1, 131.4, 131.7, 133.3, 144.0, 147.6, 164.0, 196.7.

12-(2-chlorophenyl)-9,9-dimethyl-8,9,10,12-tetrahydro-11H benzo[a]xanthen-11-one (4i): Reaction carried out with 0.297 mmol of oxazine substrate. White Crystals, Yield = 62.6 % (72.0 mg), Mp: 174-176 °C (175-176 °C[3]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.98 (s, 3H), 1.12 (s, 3H), 2.22 (d, *J* = 16.2 Hz, 1H), 2.30 (d, *J* = 16.2 Hz, 1H), 2.55-2.62 (m, 2H), 5.99 (s, 1H), 6.96-7.05 (m, 2H), 7.25-7.48 (m, 5H), 7.72-7.75 (m, 2H), 8.22 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 27.1, 29.3, 32.1, 32.9, 41.4, 50.8, 113.4, 117.0, 117.4, 123.9, 124.9, 126.8, 127.1, 127.6, 128.3, 129.1, 129.9, 131.3, 131.6, 132.9, 142.1, 147.6, 164.2, 196.7.

12-(2-hydroxyphenyl)-9,9-dimethyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4j): Reaction carried out with 0.315 mmol of oxazine substrate. White Solid, Yield = 76 % (89.1 mg), Mp: 131-133 °C (132-133 °C [3]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.99 (s, 3H), 1.15 (s, 3H), 2.36 (d, *J* = 16.2 Hz, 1H), 2.41 (d, *J* = 16.2 Hz, 1H), 2.61 (s, 2H), 5.77 (s, 1H), 6.59-6.63 (m, 2H), 6.98-7.02 (m, 2H), 7.32-7.41 (m, 3H), 7.67 (d, *J* = 9.6 Hz, 1H), 7.76-7.79 (m, 2H), 9.26 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 27.3, 28.0, 29.0, 32.4, 41.6, 50.2, 113.9, 116.6, 117.5, 118.8, 121.5, 123.5, 125.3, 127.5, 127.9, 128.2, 128.7, 129.1, 131.1, 131.5, 132.7, 147.8, 152.8, 166.8, 200.6.

9,9-dimethyl-12-(3-nitrophenyl)-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4k): Reaction carried out with 0.288 mmol of oxazine substrate. White Solid, Yield = 85% (98.5 mg), Mp: 168-171 °C (169-170 °C[2]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.95 (s, 3H), 1.13 (s, 3H), 2.24 (d, *J* = 16.2 Hz, 1H), 2.32 (d, *J* = 16.2 Hz, 1H), 2.60 (s, 2H), 5.81 (s, 1H), 7.34-7.45 (m, 4H), 7.78-7.81 (m, 3H), 7.86 (d, *J* = 7.2 Hz, 1H), 7.91-7.93 (m, 1H), 8.11-8.12 (m, 1H).

^{13}C NMR (150 MHz, $CDCl_3$): δ 27.1, 29.2, 32.3, 34.7, 41.3, 50.7, 113.1, 116.0, 117.2, 121.5, 123.1, 123.2, 125.1, 127.3, 128.6, 129.0, 129.6, 130.9, 131.5, 134.8, 146.7, 147.8, 148.4, 164.5, 196.7.

12-(3-hydroxyphenyl)-9,9-dimethyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4l): Reaction carried out with 0.252 mmol of oxazine substrate. White Solid, Yield = 67.3 % (62.9 mg), Mp: 222-225 °C (225-227 °C [5]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.89 (s, 3H), 1.02 (s, 3H), 2.14 (d, *J* = 16.2 Hz, 1H), 2.20 (d, *J* = 16.2 Hz, 1H), 2.47 (s, 2H), 5.53 (s, 1H), 6.47 (d, *J* = 10.8 Hz, 1H), 6.71-6.91 (m, 3H), 7.22-7.34 (m, 3H), 7.64-7.67 (m, 2H), 7.93 (d, *J* = 10.8 Hz, 1H), 8.52 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 26.8, 28.7, 31.8, 34.1, 40.9, 50.5, 113.2, 113.7, 115.3, 116.7, 117.3, 119.3, 123.3, 124.4, 126.5, 127.9, 128.2, 128.6, 131.0, 145.7, 147.2, 156.6, 163.5, 196.4.

12-(3-methoxyphenyl)-9,9-dimethyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4m): Reaction carried out with 0.302 mmol of oxazine substrate. White Solid, Yield = 68% (79.5 mg), Mp: 219-220 °C (219- 221 °C[6]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.96 (s, 3H), 1.09 (s, 3H), 2.24 (d, *J* = 16.8 Hz, 1H), 2.29 (d, *J* = 16.8 Hz, 1H), 2.54 (s, 2H), 3.69 (s, 3H), 5.69 (s, 1H), 6.58-6.60 (m, 1H), 6.90-6.94 (m, 2H), 7.06-7.09 (m, 1H), 7.30 (d, *J* = 9.0 Hz, 1H), 7.33-7.428 (m, 2H), 7.72-7.76 (m, 2H), 7.99 (d, *J* = 9.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 27.2, 29.2, 32.2, 34.6, 41.3, 50.8, 55.0, 111.2, 114.1, 114.6, 117.0, 117.5, 120.9, 123.6, 124.8, 126.9, 128.3, 128.8, 129.0, 131.4, 146.3, 147.7, 159.4, 163.9, 196.8.

12-(3-chlorophenyl)-9,9-dimethyl-8,9,10,12-tetrahydro-11H benzo[a]xanthen-11-one (4n): Reaction carried out with 0.297 mmol of oxazine substrate. White Crystals, Yield = 85 % (98 mg), Mp: 174-176 °C (173-174 °C [3]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.95 (s, 3H), 1.09

(s, 3H), 2.24 (d, *J* = 17.4 Hz, 1H), 2.29 (d, *J* = 16.2 Hz, 1H), 2.52 (d, *J* = 17.4 Hz, 1H), 2.56 (d, *J* = 17.4 Hz, 1H), 5.68 (s, 1H), 7.01-7.10 (m, 2H), 7.23-7.44 (m, 5H), 7.74-7.77 (m, 2H), 7.91 (d, *J* = 9.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 27.1, 29.2, 32.2, 34.5, 41.3, 50.8, 113.6, 116.8, 117.0, 123.4, 124.9, 126.5, 126.8, 127.1, 128.3, 128.4, 129.1, 129.4, 131.2, 131.5, 134.0, 146.6, 147.7, 164.2, 196.6.

12-(3-fluorophenyl)-9,9-dimethyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4o): Reaction carried out with 0.313 mmol of oxazine substrate. White Solid, Yield = 80 % (93.02 mg), Mp: 220- 223 °C (224- 226 °C[6]); ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.97 (s, 3H), 1.12 (s, 3H), 2.26 (d, *J* = 16.2 Hz, 1H), 2.31 (d, *J* = 16.2 Hz, 1H), 2.57 (s, 2H), 5.72 (s, 1H), 6.73- 6.77 (m, 1H), 6.97- 7.00 (m, 1H), 7.12-7.18 (m, 2H), 7.33 (d, *J* = 9 Hz, 1H), 7.38-7.46 (m, 2H), 7.76- 7.80 (m, 2H), 7.93 (d, *J* = 9.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 27.1, 29.3, 32.2, 34.4, 41.4, 50.8, 113.2, 113.3, 113.8, 115.2, 115.4, 116.9, 117.0, 123.5, 124.2, 125.0, 127.1, 128.5, 129.1, 129.6, 131.3, 131.5, 147.1, 147.7, 162.0, 163.6, 164.1, 196.8.

(1,3-diphenyl-1H-benzo[f]chromen-2-yl)(phenyl)methanone (4p): Reaction carried out with 0.166 mmol of oxazine substrate. White solid, Yield = 71 % (52 mg), Mp: 190- 193 °C (191 °C [7]); ^{1}H NMR (600 MHz, $CDCl_3$): 5.91 (s, 1H), 6.96- 7.18 (m, 9H), 7.31-7.43 (m, 9H), 7.80 (d, *J* = 9.0 Hz, 2H), 7.94 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 41.3, 115.4, 116.3, 117.3, 123.5, 124.6, 126.6, 126.9, 127.6, 127.8, 128.0, 128.5, 128.6, 129.0, 129.2, 129.6, 131.2, 131.4, 131.7, 133.8, 138.6, 144.5, 148.7, 154.2, 198.0.

(1-(4-chlorophenyl)-3-phenyl-1H-benzo[f]chromen-2-yl)(phenyl)methanone (4q): Reaction carried out with 0.297 mmol of oxazine substrate. Pale yellow solid, Yield = 69 % (96 mg), Mp: 207- 209 °C (208 °C [7]); ^{1}H NMR (600 MHz, $CDCl_3$): 5.87 (s, 1H), 7.00-7.03

(m, 2H), 7.08- 7.17 (m, 6H), 7.31-7.46 (m, 9H), 7.83 (d, *J* = 9.0 Hz, 2H), 7.89 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 40.5, 114.7, 116.1, 117.3, 123.2, 124.8, 127.1, 127.7, 127.9, 128.6, 128.8, 129.0, 129.2, 129.3, 129.4, 129.9, 131.0, 131.4, 131.8, 132.4, 133.6, 138.5, 143.2, 148.7, 155.4, 197.7.

12-phenyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one (4r): Reaction carried out with 0.331 mmol of oxazine substrate. White Solid, Yield = 83.11 % (89.79 mg) Mp: 201-203 °C (202- 203 °C[2]) ^{1}H NMR (600 MHz, $CDCl_3$): δ 1.91-2.03 (m, 2H), 2.32- 2.44 (m, 2H), 2.60-2.72 (m, 2H), 5.73 (s, 1H), 7.03-7.06 (m, 1H), 7.15-7.17 (m, 2H), 7.31-7.35 (m, 4H), 7.38-7.41 (m, 1H), 7.73-7.76 (m, 2H), 7.95 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 20.2, 27.7, 34.6, 37.0, 115.5, 116.9, 117.6, 123.6, 124.8, 126.2, 126.9, 128.2, 128.3, 128.4, 128.7, 131.3, 131.4, 145.0, 147.7, 165.5, 197.0.

General procedure for the synthesis of 14-phenyl-14H-dibenzo[a,j]xanthene **(4s):**

To a stirred solution of 12-(4-nitrophenyl)-7a,8,9,10-tetrahydro-12H-naphtho[1,2-e]pyrrolo[2,1-b][1,3]oxazine (50 mg, 0.144 mmol)) in water:acetone mixture (4 ml; 1:1 v/v) and stirred in 100 ºC for an hour. After that the same reaction tube, 21 mg (0.141 mmol) β-naphthol was added along with copper powder (1 mg, 0.014 mmol) and the reaction mixture was stirred vigoursly at 100 ºC for 4 hours. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to room temperature and poured into ice-cold water (10 mL) and extracted with ethyl acetate (3 x 5 mL). The combined extracts were dried it over anhydrous Na_2SO_4 and then removed the solvent under reduced pressure. The crude was purified by column chromatography (silica gel, 100-200 mesh; ethyl acetate/hexane as eluent).

14-(4-nitrophenyl)-14H-dibenzo[a,j]xanthene (4s): Reaction carried out with 0.144 mmol of oxazine substrate. White solid, Yield = 87 % (50.82 mg), Mp: 309- 311 ^{o}C (312- 313 ^{o}C[8]); ^{1}H NMR (600 MHz, $CDCl_3$): 6.59 (s, 1H), 7.42- 7.45 (m, 2H), 7.50 (d, *J* = 7.2 Hz, 2H), 7.58- 7.60 (m, 2H), 7.67 (d, *J* = 7.2 Hz, 2H), 7.82- 7.85 (m, 4H), 8.00 (d, *J* = 7.8 Hz, 2H), 8.28 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 37.9, 115.8, 118.1, 122.0, 123.9, 124.6, 127.2, 128.9, 129.1, 129.6, 131.1, 146.3, 148.8, 152.0.

(2-chlorophenyl)(2-hydroxynaphthalen-1-yl)methanone (2a): [09] White solid, Yield = 83% (As given in Table 1, Entry 4 in the manuscript), Mp: 123-125; ^{1}H NMR (600 MHz, $CDCl_3$): 7.20-7.25 (m, 2H), 7.29-7.31 (m, 2H), 7.39 (d, *J* = 9.0 Hz, 2H), 7.58 (d, *J* = 7.8 Hz, 2H), 7.77 (d, *J* = 9.0 Hz, 1H), 7.95 (d, *J* = 9 Hz, 1H), 11.01 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 114.1, 119.2, 123.9, 126.1, 126.9, 128.5, 128.7, 128.9, 130.9, 132.1, 136.5, 138.5, 139.1, 161.4, 198.9.

1-((2-chlorophenyl)(pyrrolidin-1-yl)methyl)naphthalen-2-ol (IM):

White solid, Yield = 39% (As given in **Scheme 3, (i)a** Entry in the manuscript), Mp: 163-167 (160-164 ^{o}C)[23]; ^{1}H NMR (600 MHz, $CDCl_3$): 1,76- 1.92 (m, 4H), 2.37- 2.42 (m, 1H), 2.51- 2.63 (m, 2H), 3.28- 3.32 (m, 1H), 5.90 (s, 1H), 7.10- 7.16 (m, 3H), 7.20- 7.23 (m, 1H), 7.36- 7.39 (m, 2H), 7.66- 7.72 (m, 3H), 7.86 (d, *J* = 8.4 Hz, 1H).

Single Crystal X-ray Diffraction

Single crystal X-ray diffraction data were collected at 160.0(1) K on a Rigaku OD Synergy/Hypix diffractometer using the copper X-ray radiation (l = 1.54184 Å) from a dual wavelength X-ray source and an Oxford Instruments Cryojet XL cooler. The selected suitable single crystal was mounted using polybutene oil on a flexible loop fixed on a goniometer head and immediately transferred to the diffractometer. Pre-experiment, data collection, data

reduction and analytical absorption correction[12] were performed with the program suite *CrysAlisPro*.[13] Using *Olex2*,[14] the structure was solved with the *SHELXT*[15] small molecule structure solution program and refined with the *SHELXL* program package[16] by full-matrix least-squares minimization on F^2. *PLATON*[17] was used to check the result of the X-ray analysis. For more details about the data collection and refinement parameters, see the CIF file.

Table S1 Crystal data and structure refinement for 4m.	
Empirical formula	$C_{26}H_{24}O_3$
Formula weight	384.45
Temperature/K	160.0(1)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.03740(10)
b/Å	12.74610(10)
c/Å	15.5693(2)
α/°	90
β/°	93.5670(10)
γ/°	90
Volume/Å^3	1988.04(4)
Z	4
ρ_{calc}g/cm^3	1.284
μ/mm^{-1}	0.657
F(000)	816.0
Crystal size/mm^3	0.2 × 0.12 × 0.09
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.974 to 159.668
Index ranges	$-12 \leq h \leq 12$, $-9 \leq k \leq 15$, $-19 \leq l \leq 18$
Reflections collected	24751
Independent reflections	4301 [R_{int} = 0.0192, R_{sigma} = 0.0151]
Data/restraints/parameters	4301/0/266
Goodness-of-fit on F^2	1.056
Final R indexes [I>=2σ (I)]	R_1 = 0.0340, wR_2 = 0.0845
Final R indexes [all data]	R_1 = 0.0357, wR_2 = 0.0859
Largest diff. peak/hole / e Å^{-3}	0.26/-0.16
CCDC No.	2307517

Table S2 Crystal data and structure refinement for 3a.	
Empirical formula	$C_{17}H_{10}O_2$

Formula weight	246.25
Temperature/K	160.0(1)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	7.12120(10)
b/Å	12.50200(10)
c/Å	12.82470(10)
α/°	90
β/°	95.5510(10)
γ/°	90
Volume/Å^3	1136.42(2)
Z	4
ρ_{calc}g/cm^3	1.439
μ/mm^{-1}	0.754
F(000)	512.0
Crystal size/mm^3	0.13 × 0.09 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.904 to 159.026
Index ranges	$-8 \leq h \leq 9$, $-15 \leq k \leq 15$, $-16 \leq l \leq 11$
Reflections collected	13198
Independent reflections	2461 [R_{int} = 0.0160, R_{sigma} = 0.0144]
Data/restraints/parameters	2461/0/173
Goodness-of-fit on F^2	1.097
Final R indexes [I>=2σ (I)]	R_1 = 0.0339, wR_2 = 0.1013
Final R indexes [all data]	R_1 = 0.0363, wR_2 = 0.1034
Largest diff. peak/hole / e Å^{-3}	0.24/-0.15
CCDC No.	2307516

Molecular docking analysis

We performed molecular docking analysis of four drug targets of which three of them are cancer targets (epidermal growth factor receptor, EGFR; cyclin-dependent kinase-6, CDK6 and cyclin-dependent kinase-4, CDK-4 and α-glucosidase from *Saccharomyces cerevisiae*. The 3D-structures of the former three targets (EGFR: 3W2S; CDK-6: 6OQO; CDK-4: 7SJ3) were retrieved from the protein data bank, while the latter target was obtained from ALPHA-FOLD

predicted model in the Uniprot database. The protein structures and the synthesized compounds] were prepared using the protein preparation wizard[18] and ligprep module of Schrödinger suite 2021-3, respectivel.[19] The OPLS-4 force field[20] was used for small molecules and protein targets. The receptor grid for each protein target has been constructed using the position of the ligand molecule complexed in these protein targets. After defining active site, the flexible ligand docking was performed using Glide XP mode[21] to predict the best orientation at the binding pocket of the target protein. The protein-ligand interaction analysis for the best pose was carried out using the PLIP web tool.[22]

Table S3. Glide XP docking score (in kcal mol^{-1})

S. No	Compound No	EGFR	CDK6	CDK4	α-Glucosidase
1	**4a**	-5.169	-4.377	-3.680	-4.812
2	**4b**	-5.614	-2.875	-2.384	-2.227
3	**4c**	-5.419	-2.918	-2.085	-5.075
4	**4d**	-4.901	-3.138	-3.536	-2.898
5	**4e**	-4.807	-2.223	-4.939	-2.340
6	**4f**	-4.782	-3.178	-2.441	-2.568
7	**4g**	-4.922	-3.353	-2.444	-2.710
8	**4i**	-5.112	-1.586	-2.431	-5.611
9	**4j**	-5.559	-3.297	-6.182	-6.558
10	**4k**	-5.310	-2.550	-3.615	-5.620
11	**4l**	-6.279	-4.108	-3.354	-4.222
12	**4n**	-4.886	-3.078	-3.794	-5.777
13	**4m**	-5.037	-3.026	-5.010	-5.387
14	**4p**	-2.606	-4.115	-2.180	-6.485
15	**4q**	-3.676	-3.599	-1.602	-5.666
16	**4r**	-5.195	-5.396	-2.571	-5.309

17	**W2R**	-14.337			
18	**N1J**		-9.298		
19	**6ZV**			-12.017	
20	**GLU**				-8.24

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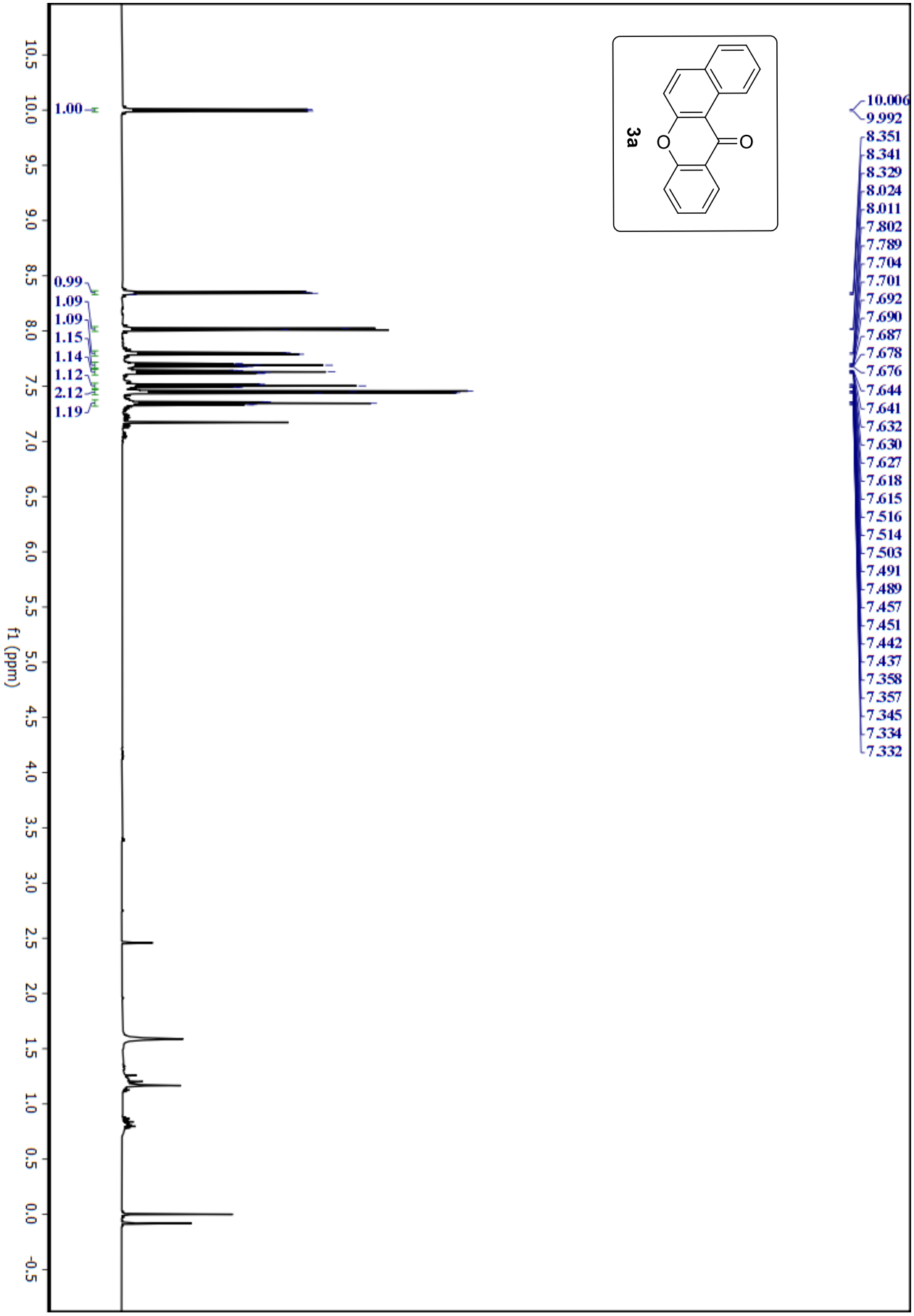
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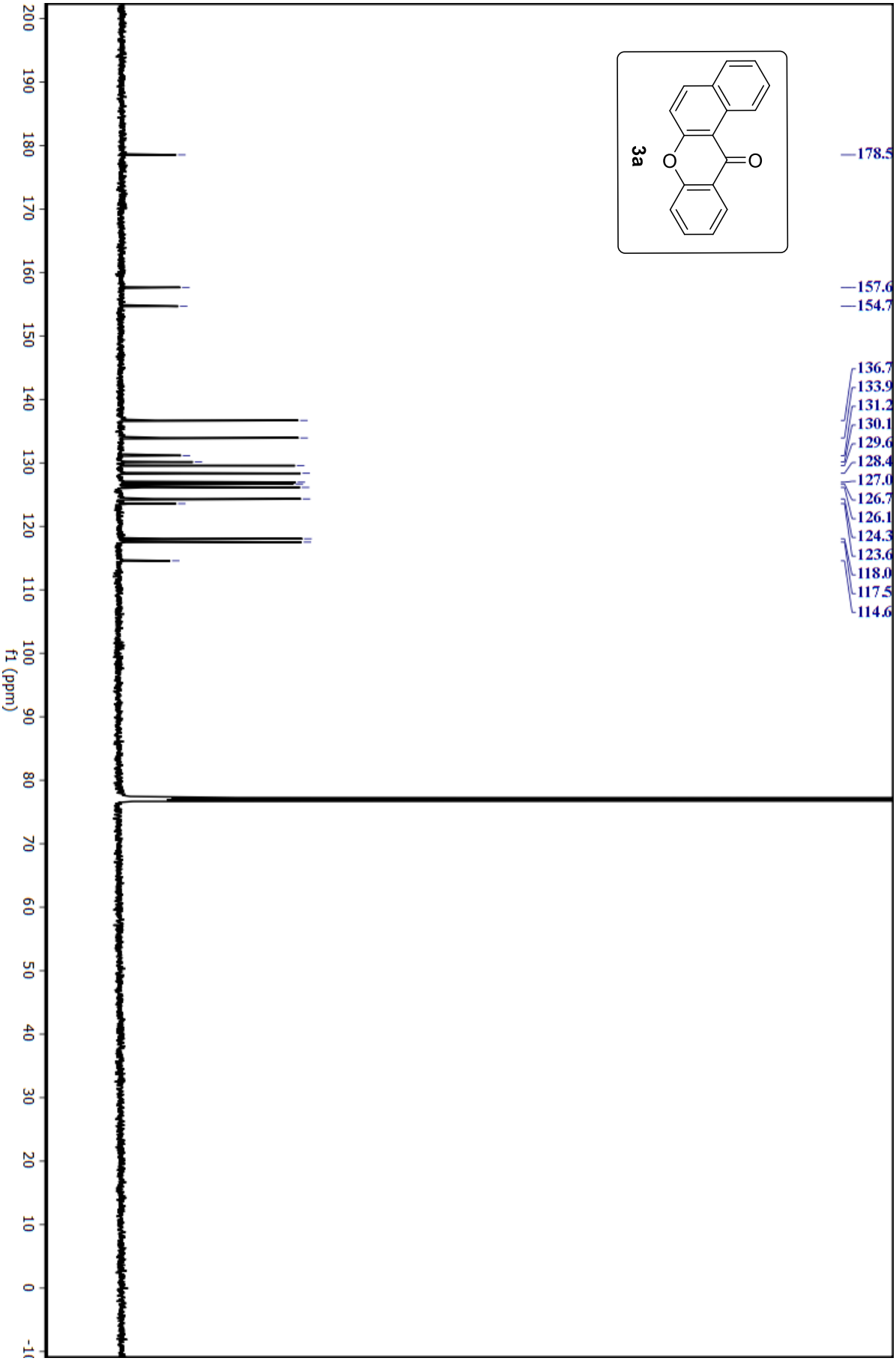
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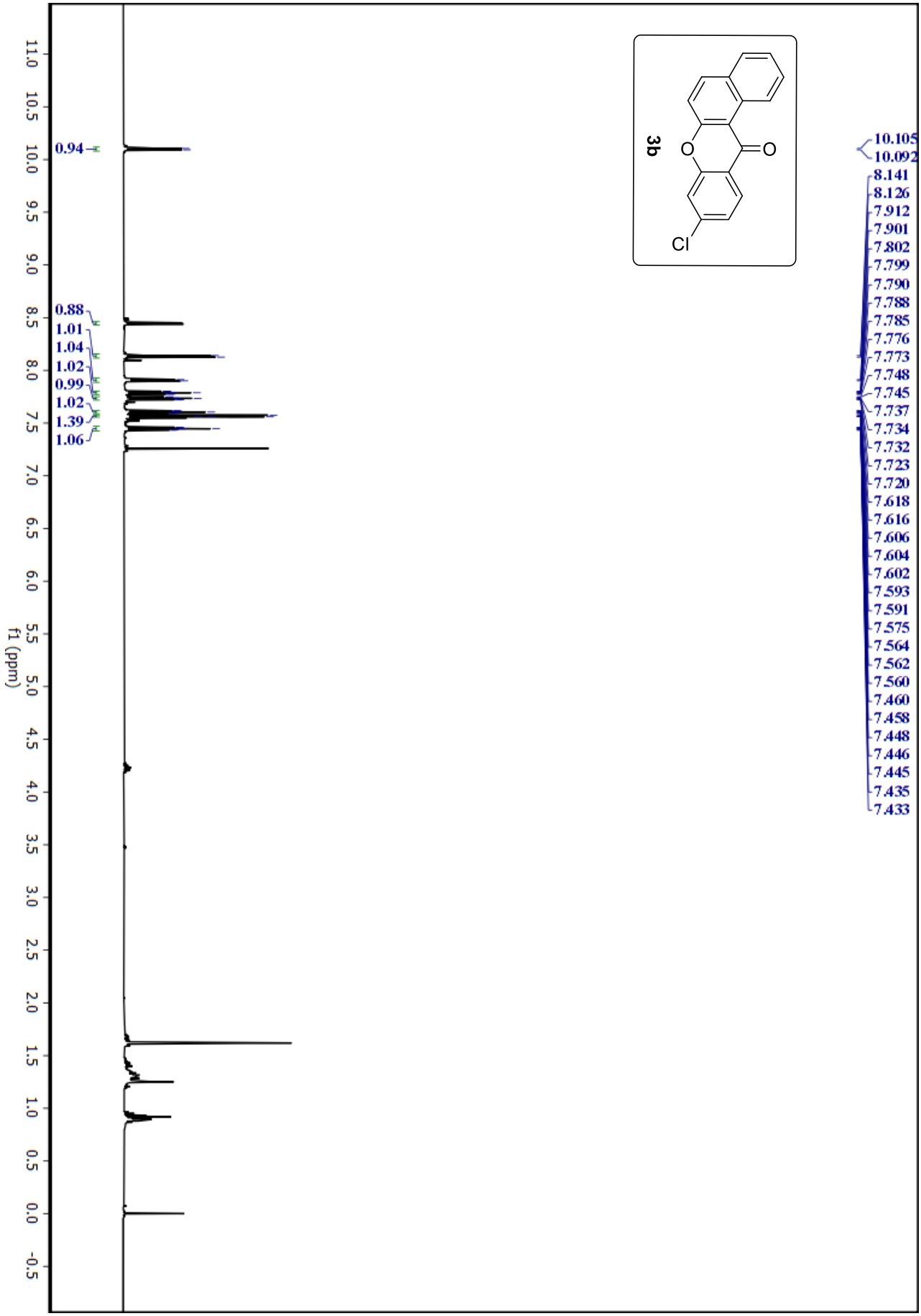
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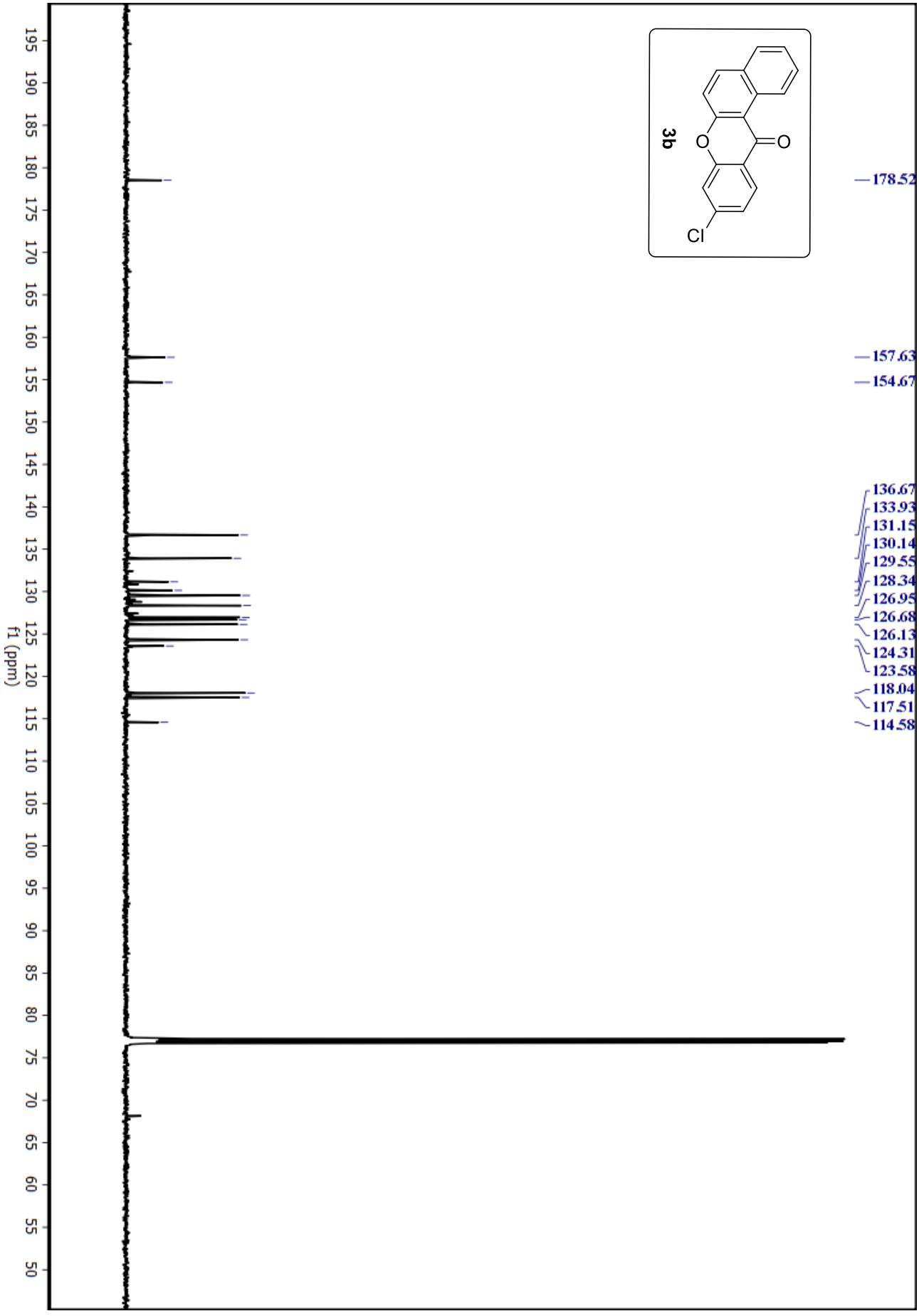
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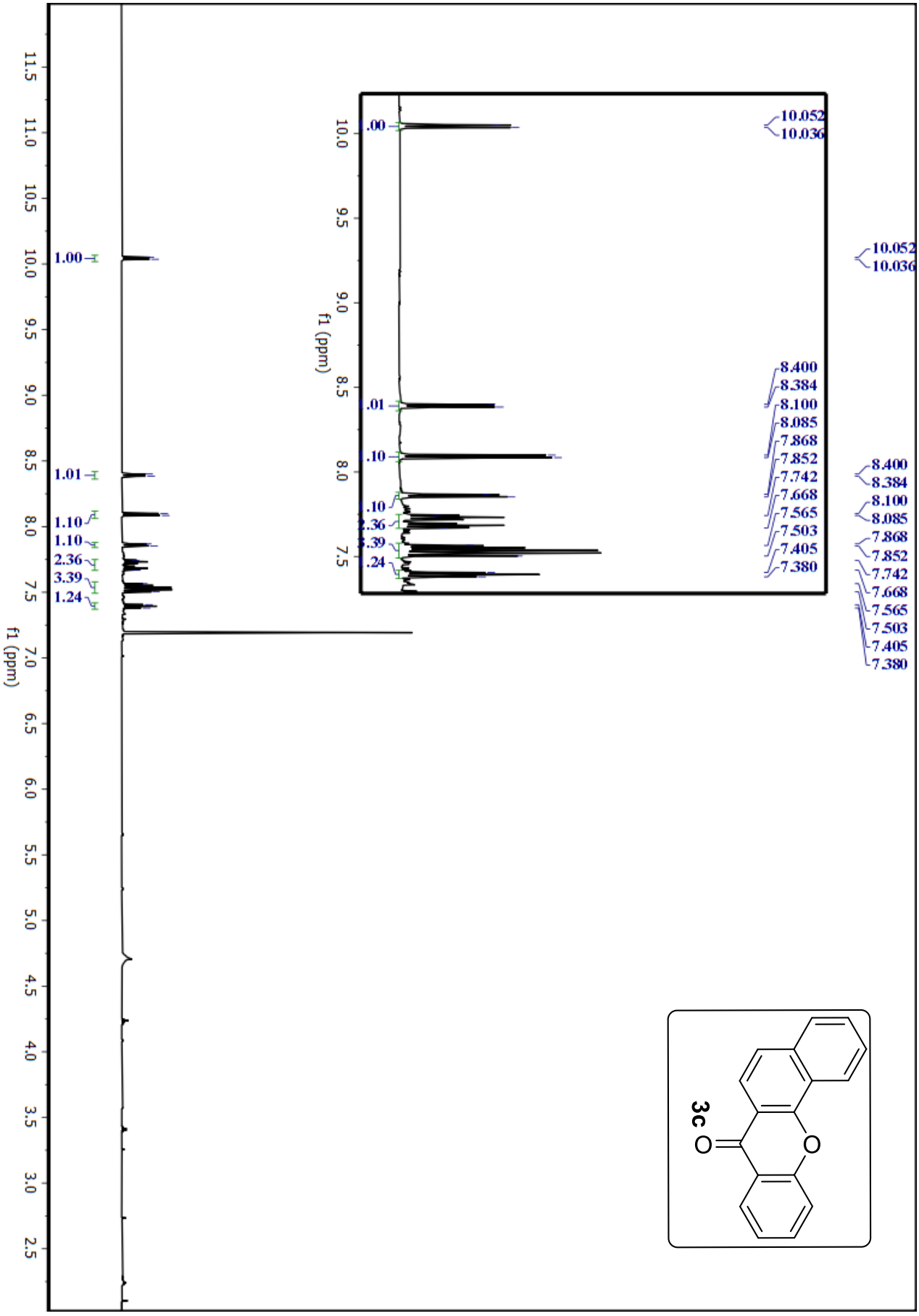
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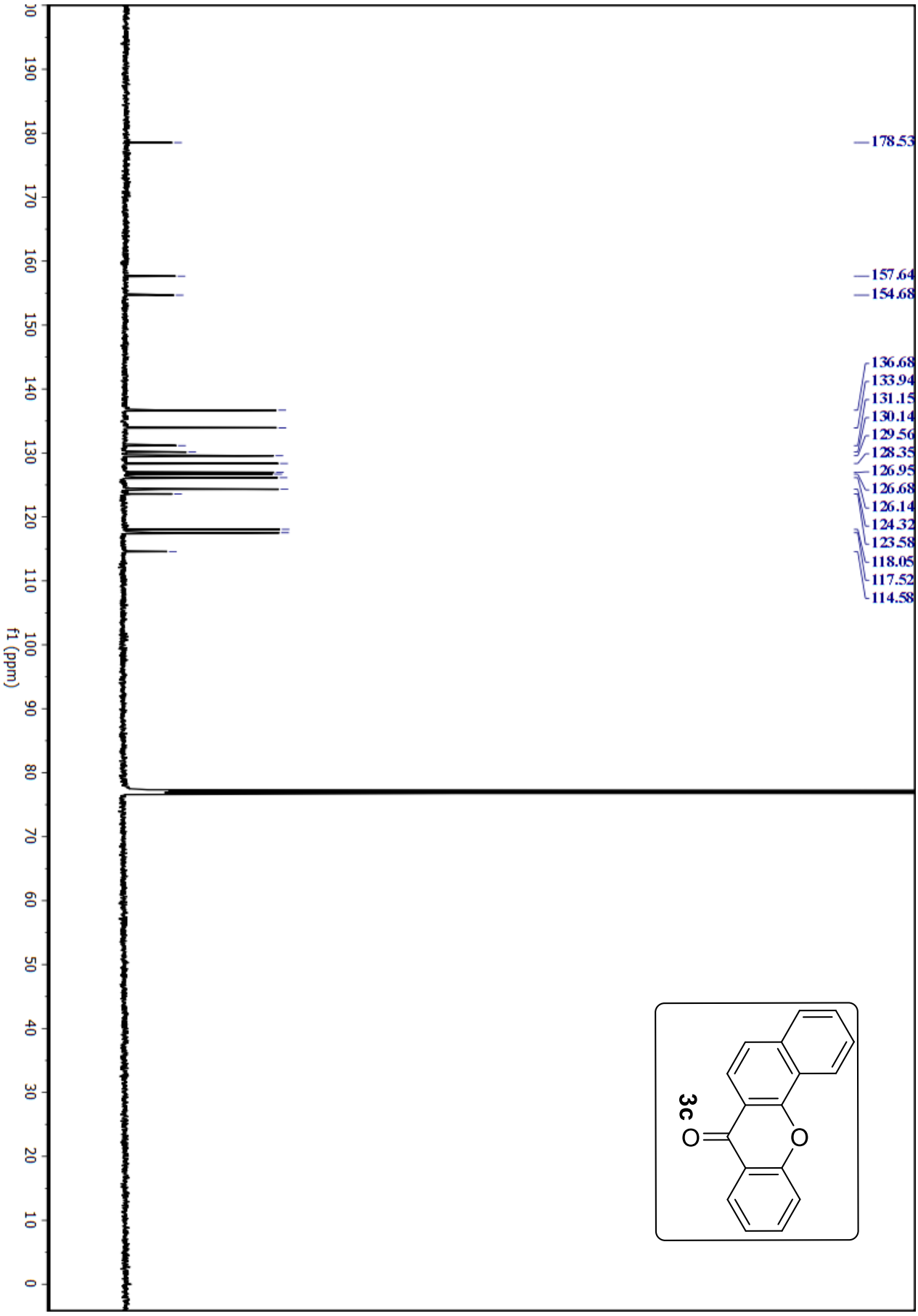
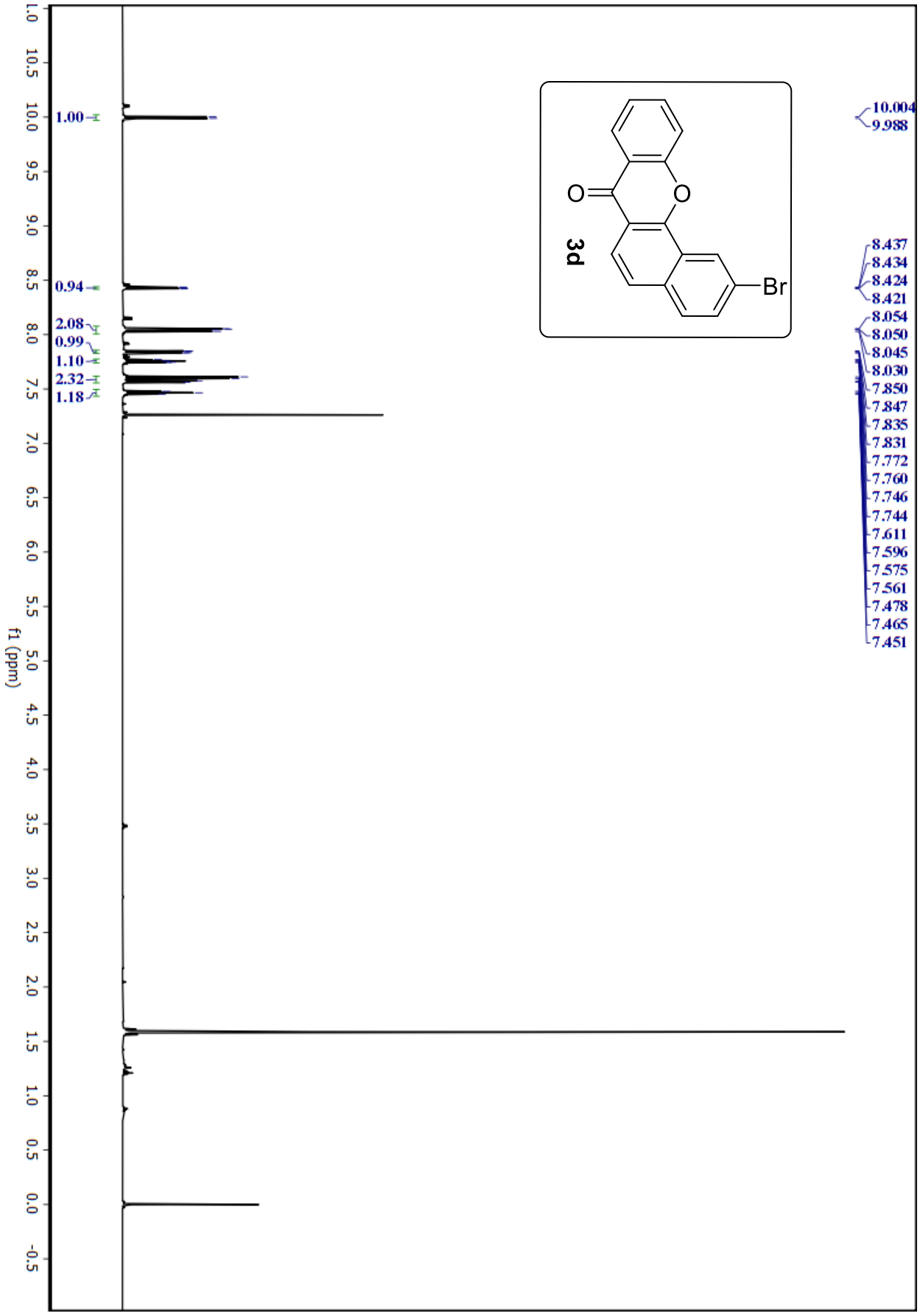
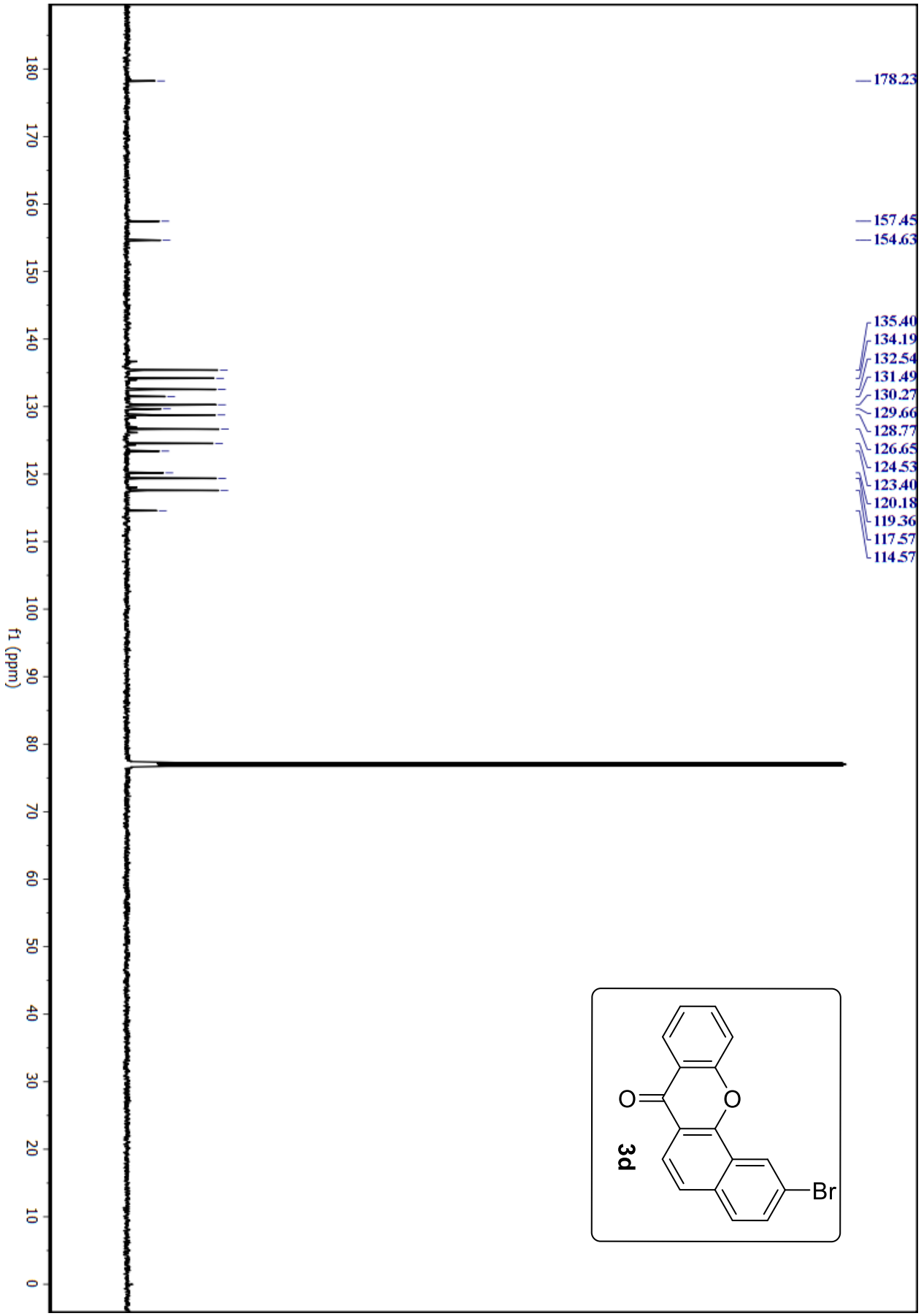
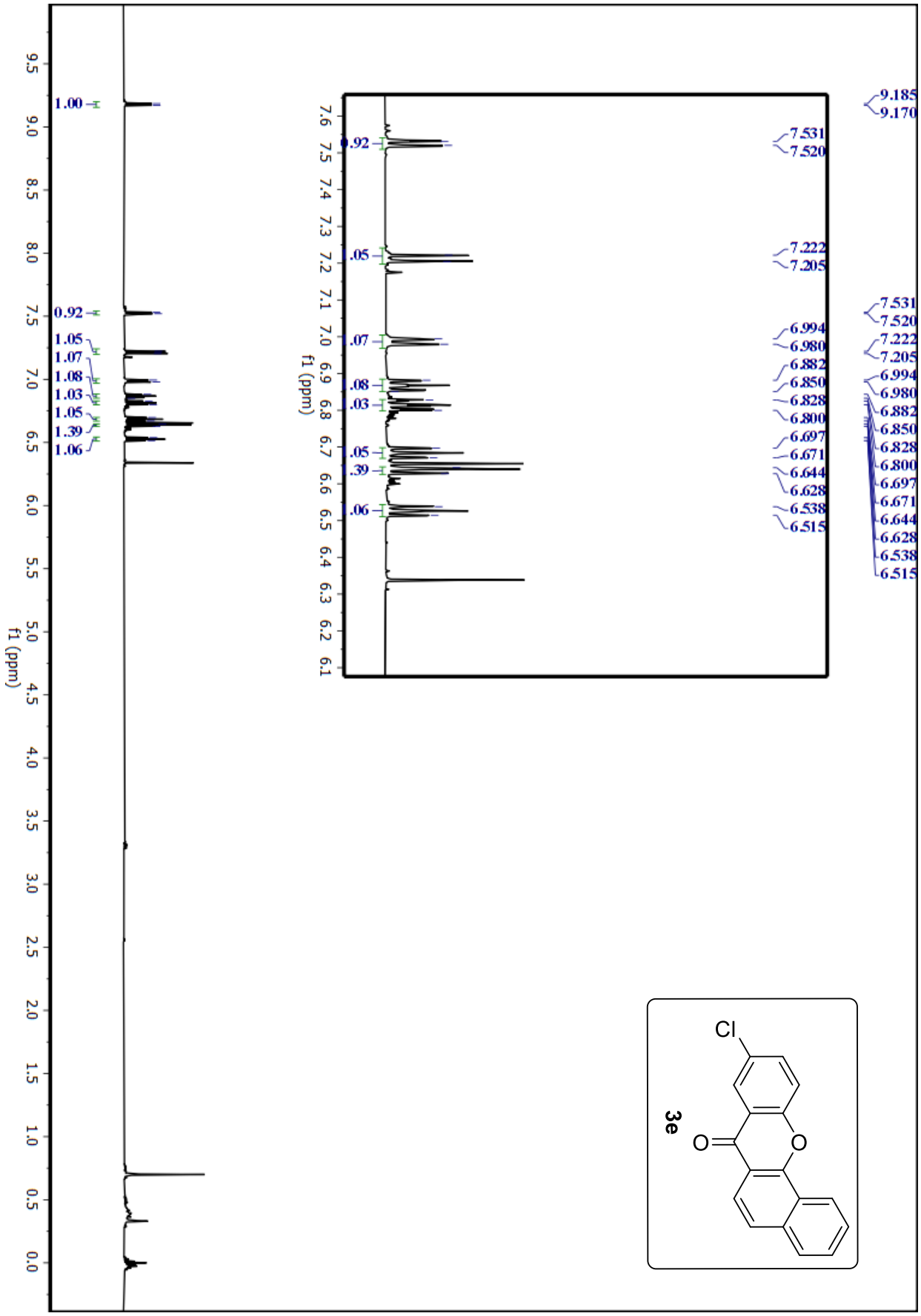
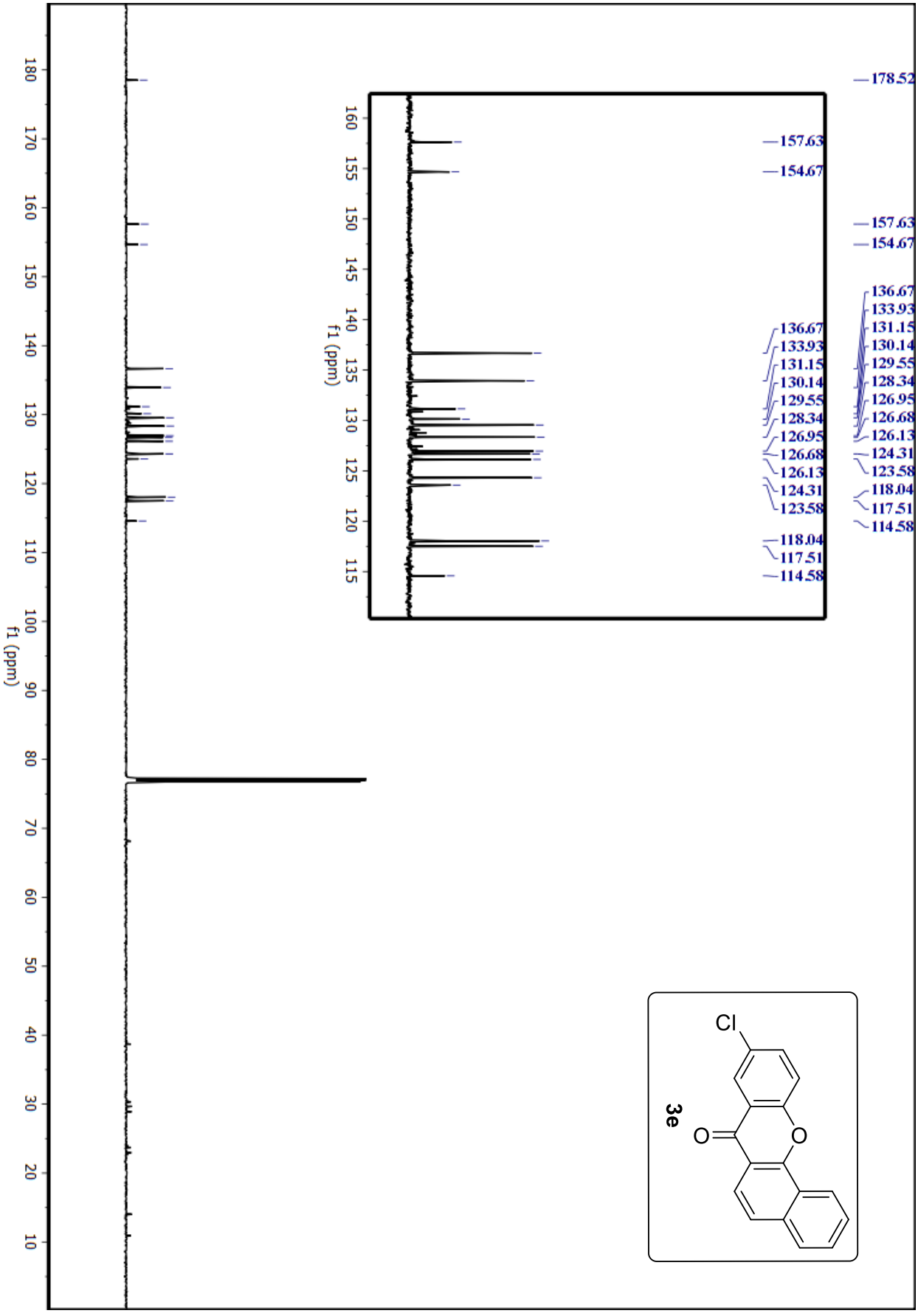
3.39
.24
10.052
10.036
8.400
8.384
8.100
8.085
7.868
7.852
7.742
7.668
7.565
7.503
7.405
7.380
3c
O
O

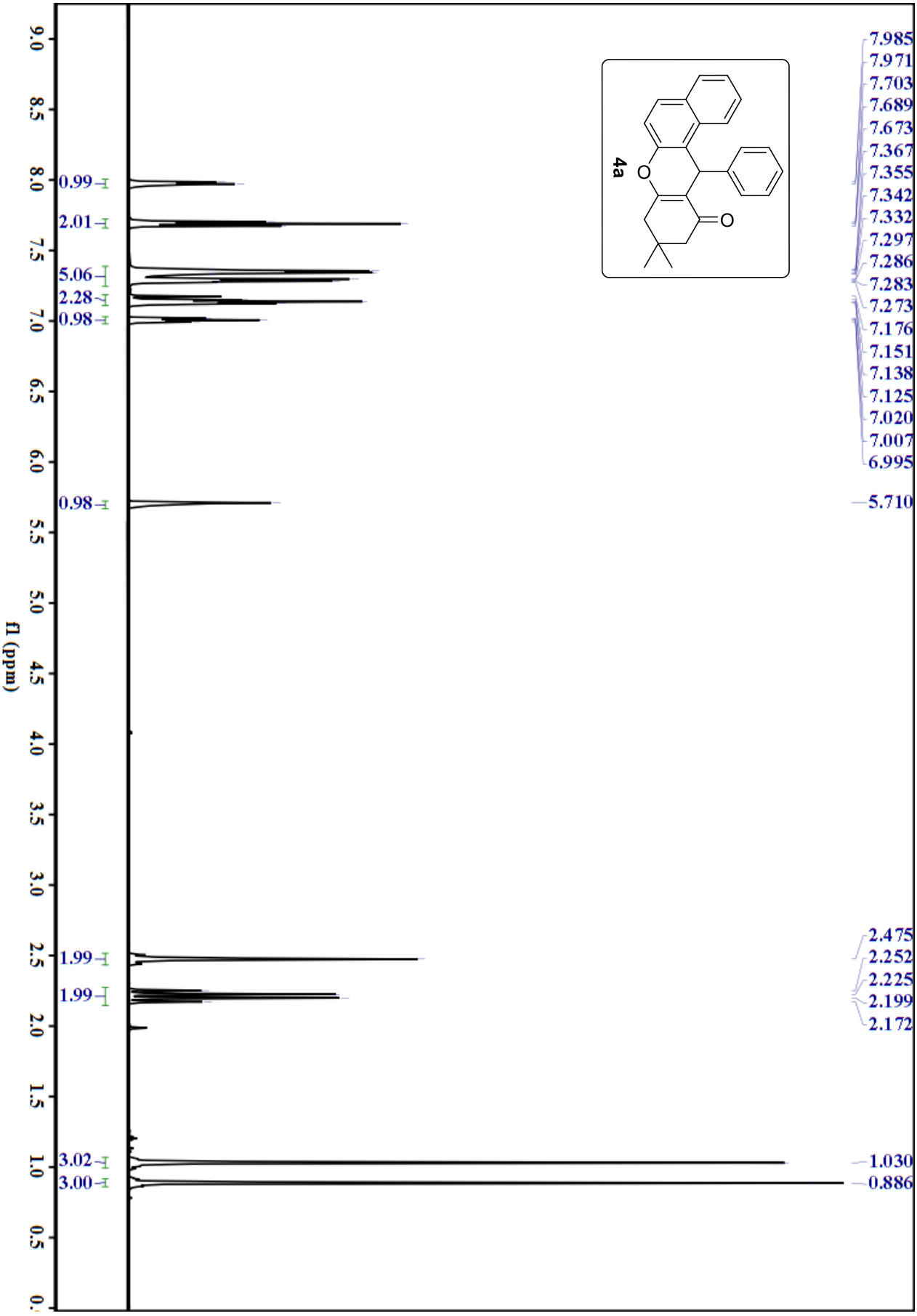

178.53
157.64
154.68
136.68
133.94
131.15
130.14
129.56
128.35
126.95
126.68
126.14
124.32
123.58
118.05
117.52
114.58
f1 (ppm)
3c
O
O

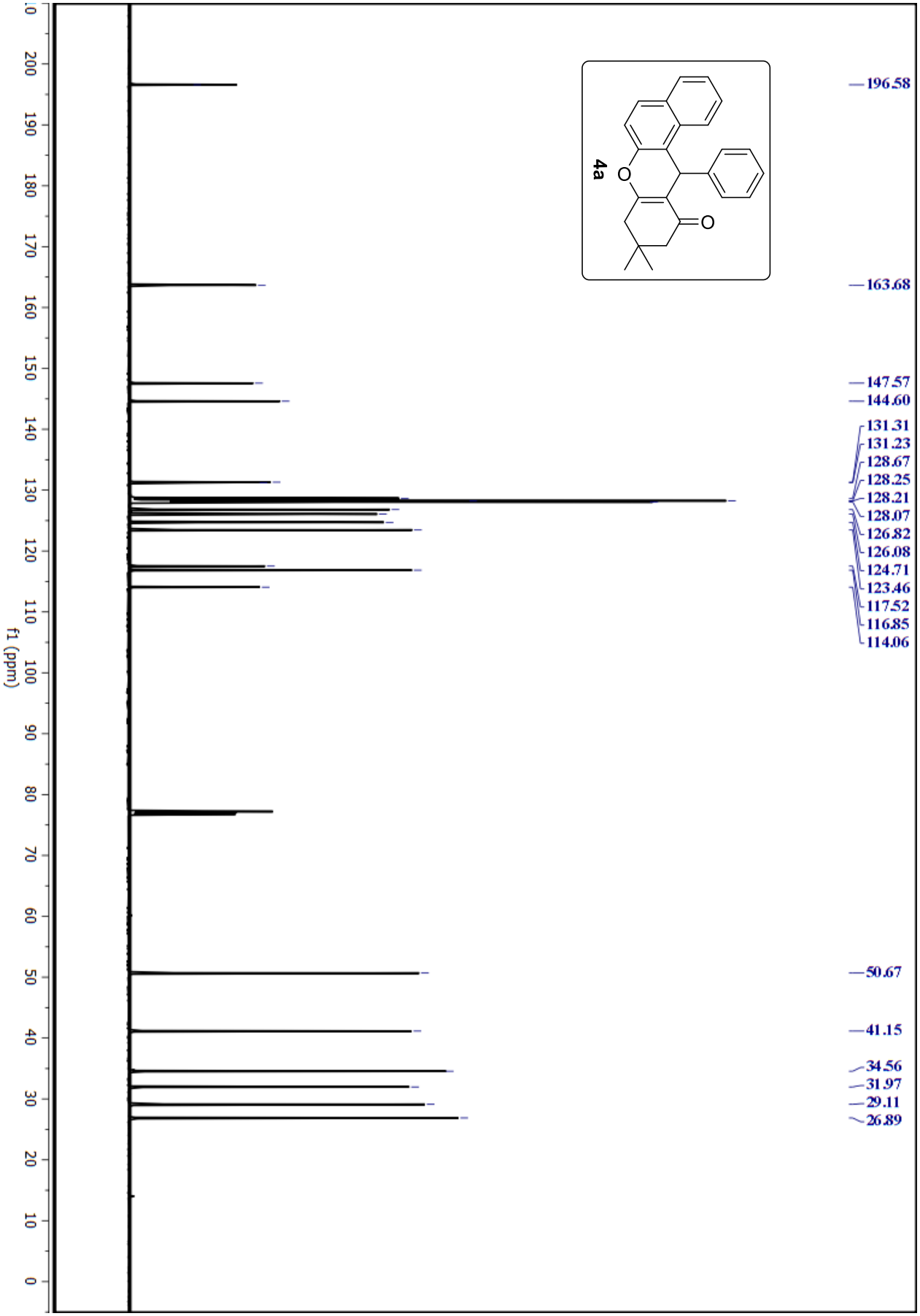

3d
Br
O
O
10.004
9.988
8.437
8.434
8.424
8.421
8.054
8.050
8.045
8.030
7.850
7.847
7.835
7.831
7.772
7.760
7.746
7.744
7.611
7.596
7.575
7.561
7.478
7.465
7.451
1.00
0.94
2.08
0.99
1.10
2.32
1.18
f1 (ppm)

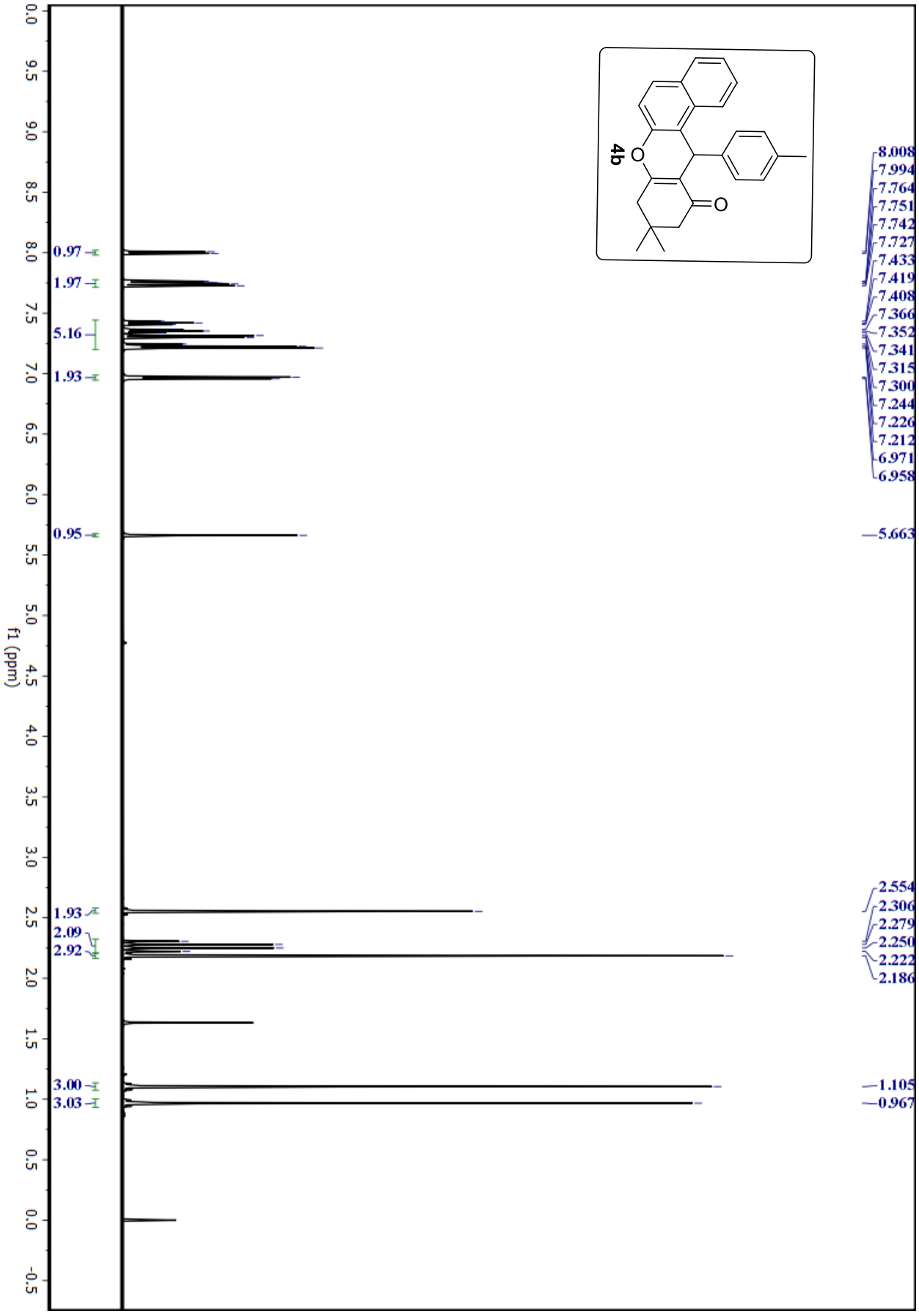

178.23
157.45
154.63
135.40
134.19
132.54
131.49
130.27
129.66
128.77
126.65
124.53
123.40
120.18
119.36
117.57
114.57
f1 (ppm)
O
O
Br
3d

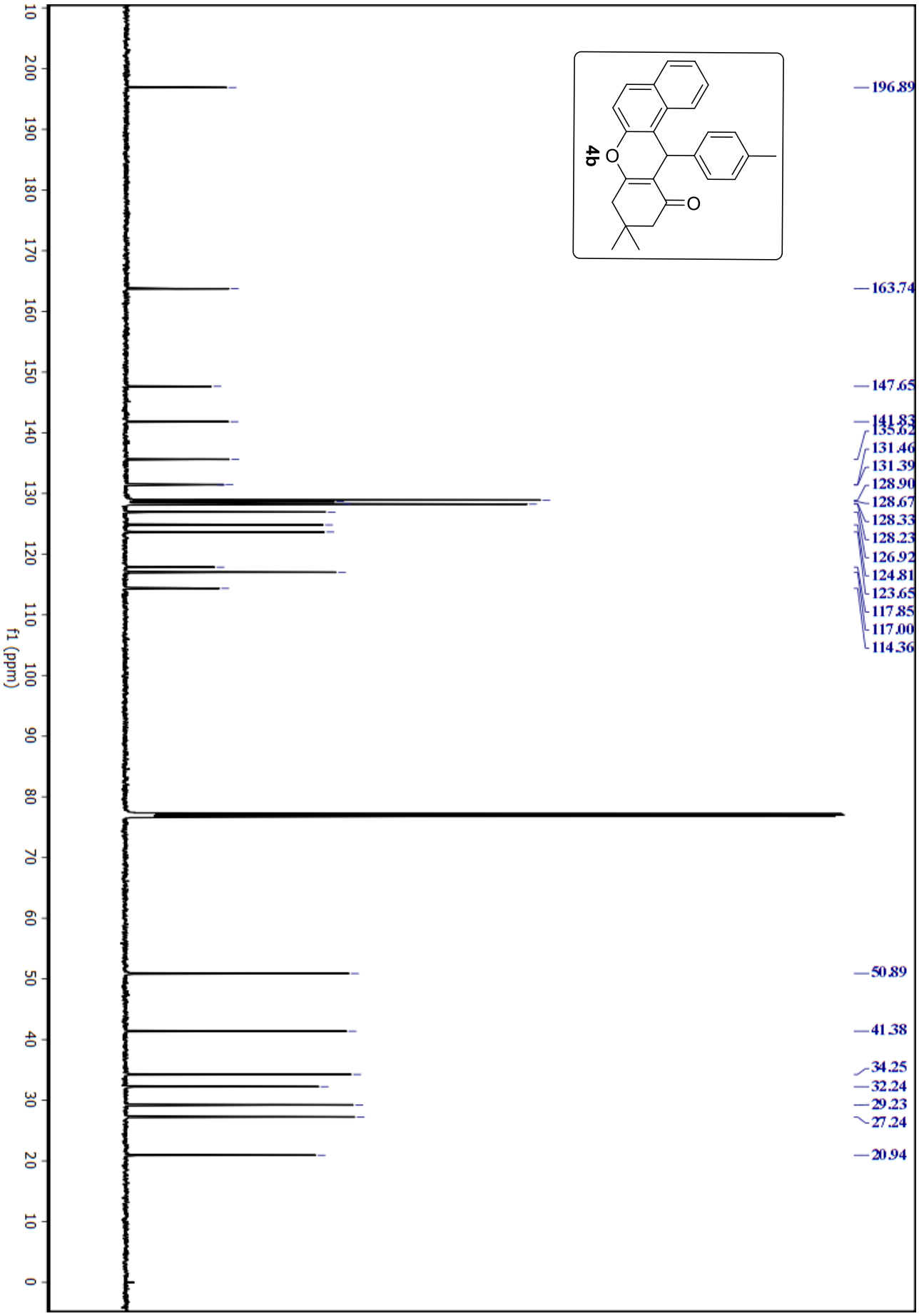

f1 (ppm)
1.00
0.92
1.05
1.07
1.08
1.03
1.05
1.39
1.06
9.185
9.170
7.531
7.520
7.222
7.205
6.994
6.980
6.882
6.850
6.828
6.800
6.697
6.671
6.644
6.628
6.538
6.515
Cl
O
O
3e

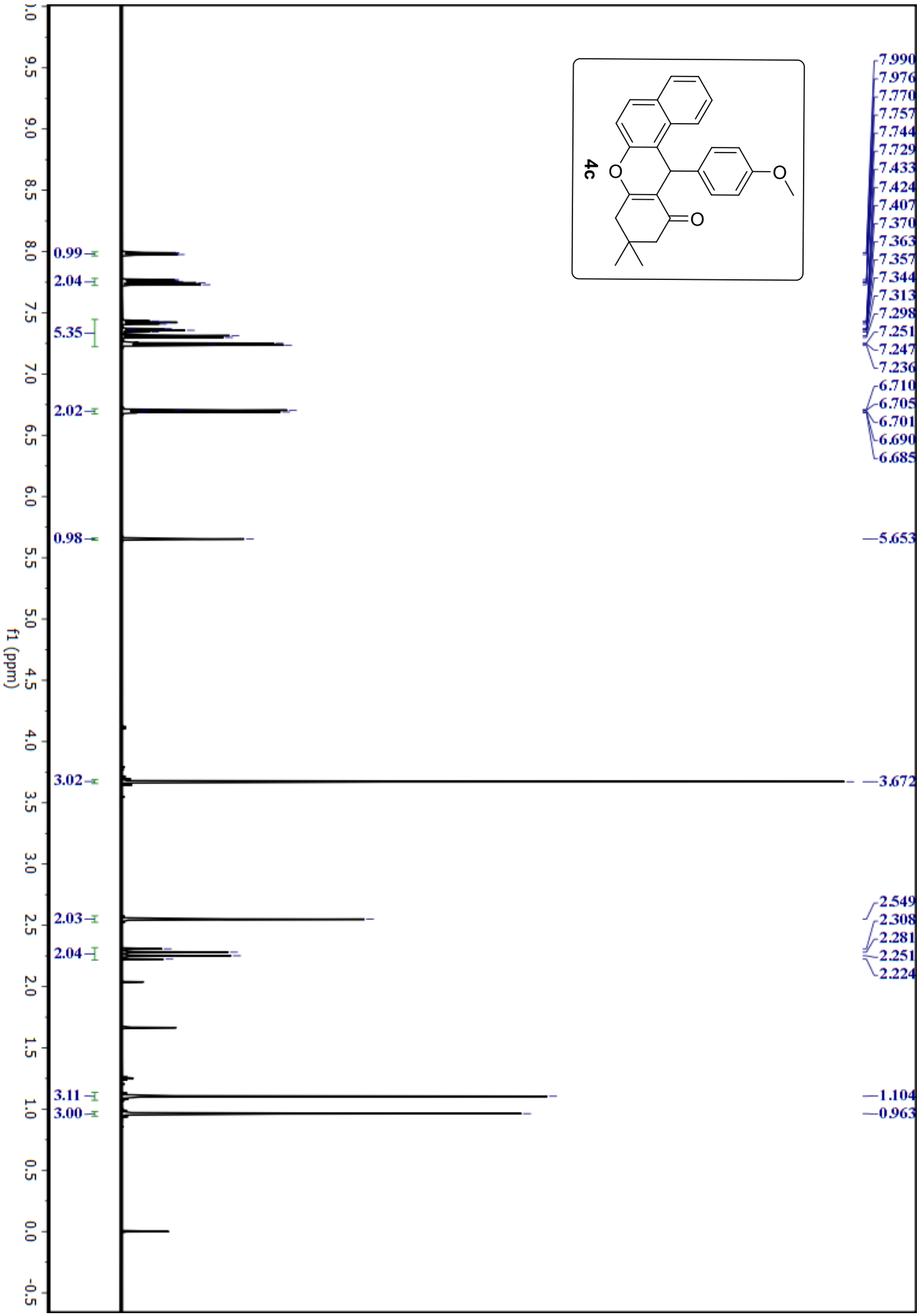

178.52
157.63
154.67
157.63
154.67
136.67
133.93
131.15
130.14
129.55
128.34
126.95
126.68
126.13
124.31
123.58
118.04
117.51
114.58
136.67
133.93
131.15
130.14
129.55
128.34
126.95
126.68
126.13
124.31
123.58
118.04
117.51
114.58
f1 (ppm)
f1 (ppm)
Cl
O
O
3e

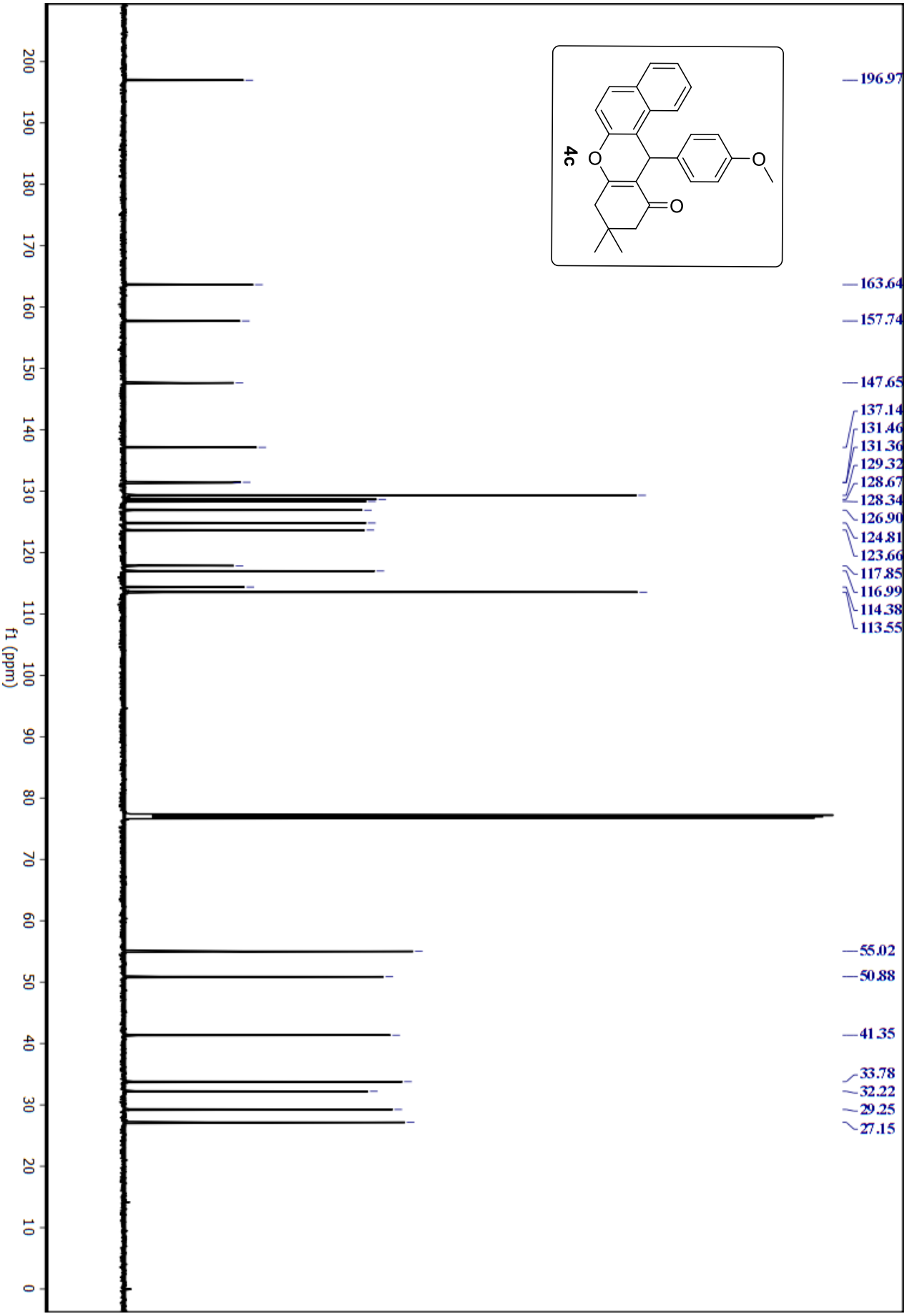

4a
O
O
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
0.99
2.01
5.06
2.28
0.98
0.98
1.99
1.99
3.02
3.00
7.985
7.971
7.703
7.689
7.673
7.367
7.355
7.342
7.332
7.297
7.286
7.283
7.273
7.176
7.151
7.138
7.125
7.020
7.007
6.995
5.710
2.475
2.252
2.225
2.199
2.172
1.030
0.886

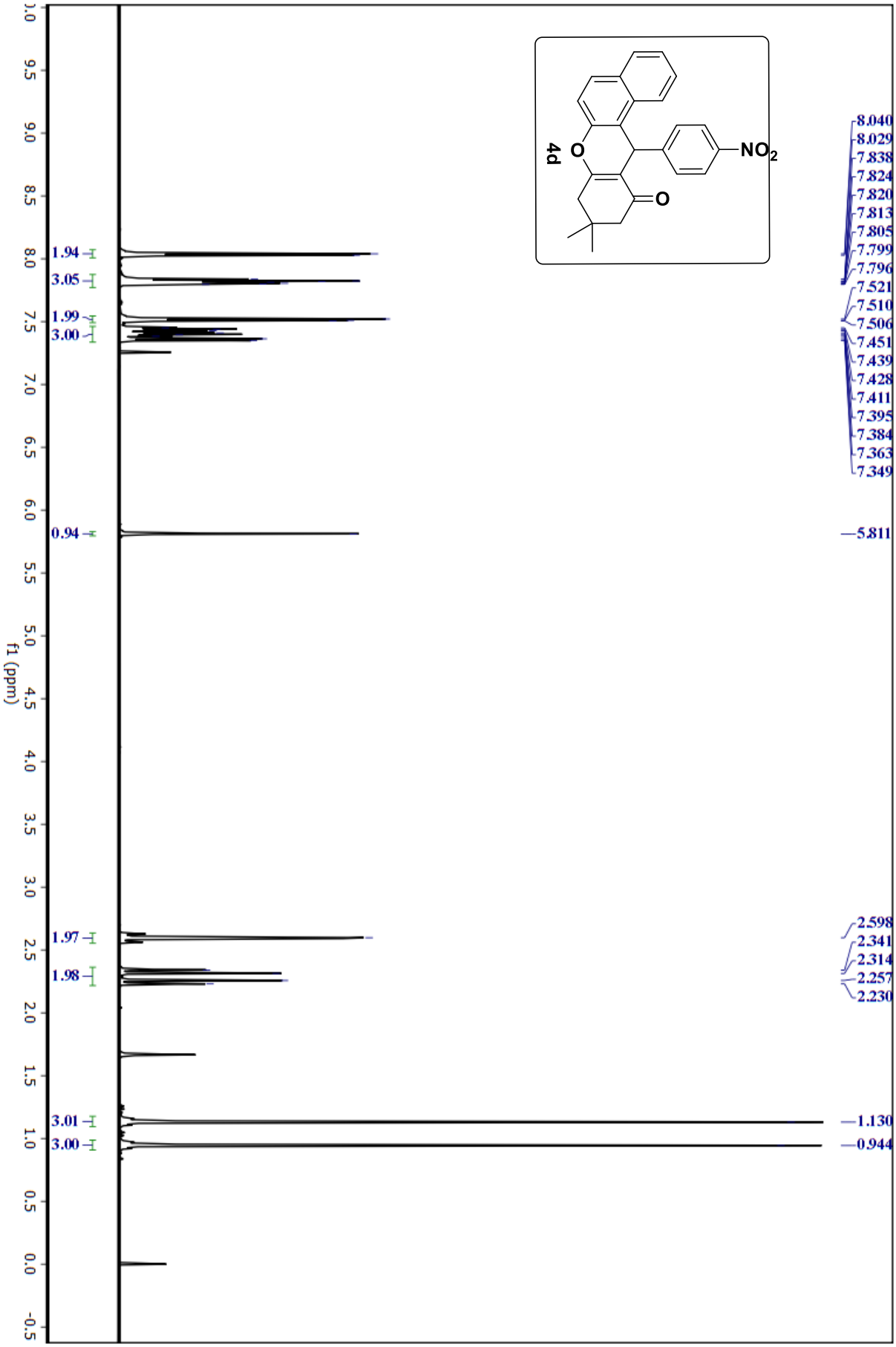

4a
O
O
196.58
163.68
147.57
144.60
131.31
131.23
128.67
128.25
128.21
128.07
126.82
126.08
124.71
123.46
117.52
116.85
114.06
50.67
41.15
34.56
31.97
29.11
26.89
f1 (ppm)

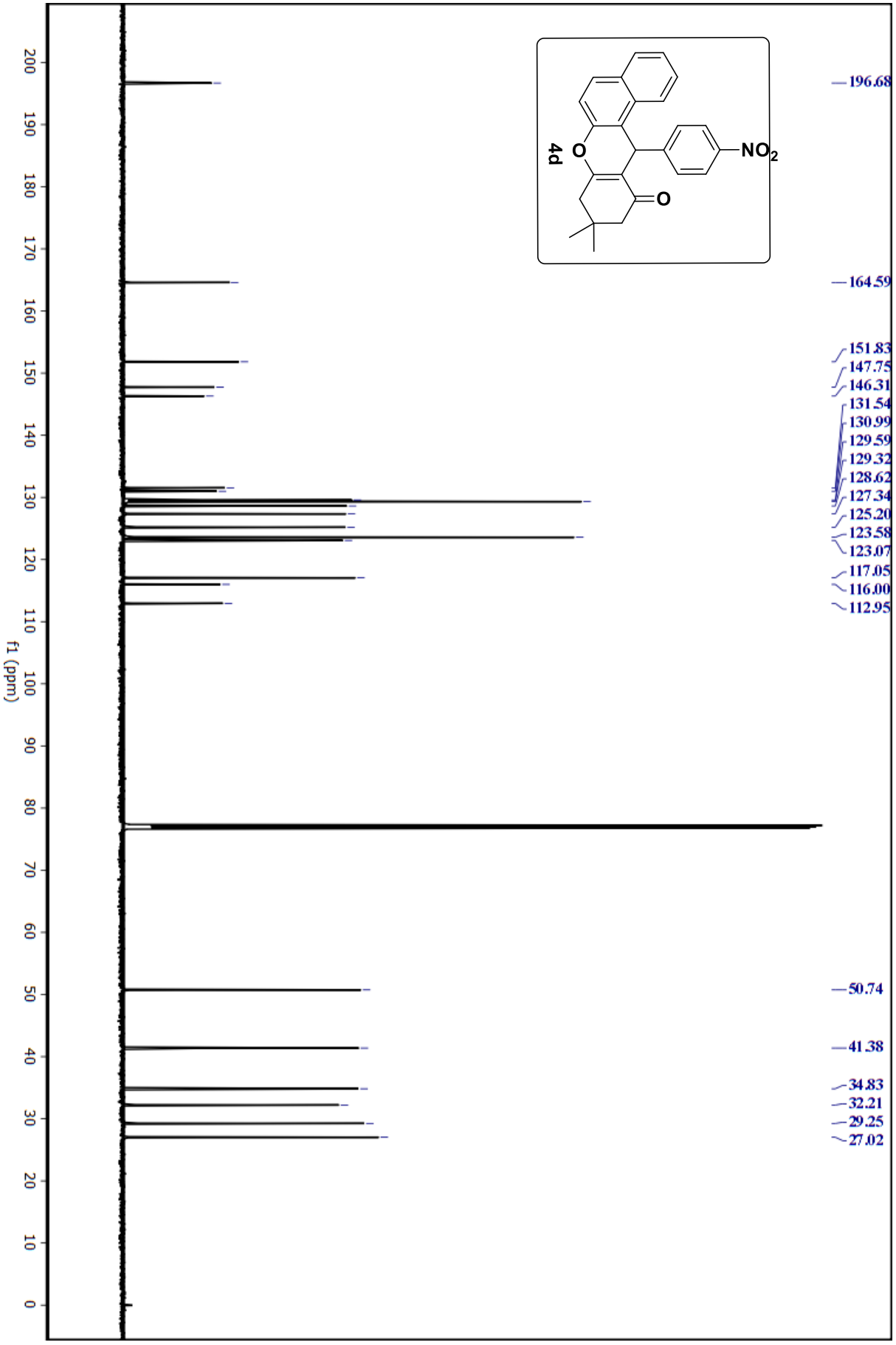

4b
O
O
f1 (ppm)
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
0.97
1.97
5.16
1.93
0.95
1.93
2.09
2.92
3.00
3.03
8.008
7.994
7.764
7.751
7.742
7.727
7.433
7.419
7.408
7.366
7.352
7.341
7.315
7.300
7.244
7.226
7.212
6.971
6.958
5.663
2.554
2.306
2.279
2.250
2.222
2.186
1.105
0.967

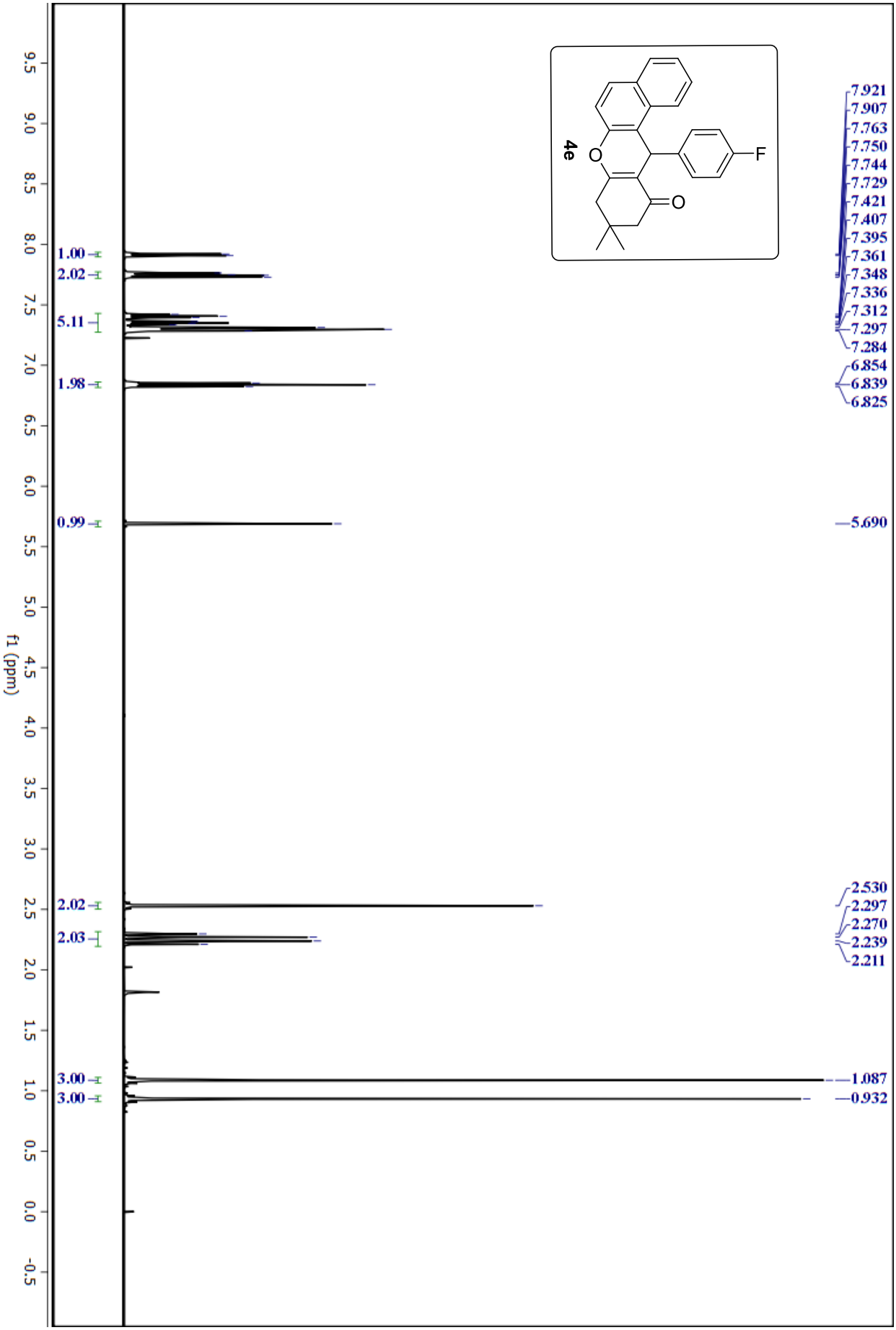

4b
O
O
196.89
163.74
147.65
141.83
135.62
131.46
131.39
128.90
128.67
128.33
128.23
126.92
124.81
123.65
117.85
117.00
114.36
50.89
41.38
34.25
32.24
29.23
27.24
20.94
f1 (ppm)

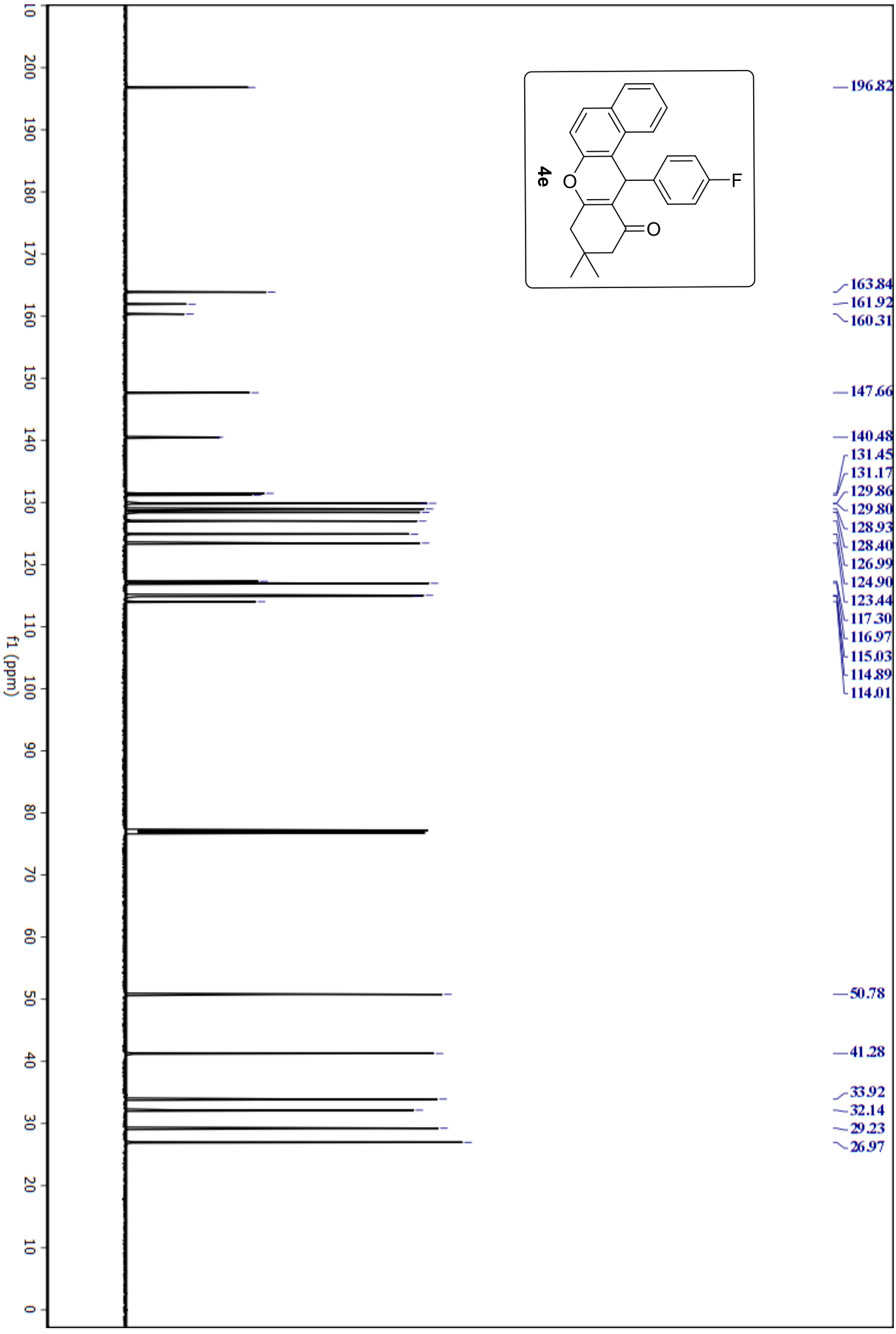

4c
O
O
O
7.990
7.976
7.770
7.757
7.744
7.729
7.433
7.424
7.407
7.370
7.363
7.357
7.344
7.313
7.298
7.251
7.247
7.236
6.710
6.705
6.701
6.690
6.685
5.653
3.672
2.549
2.308
2.281
2.251
2.224
1.104
0.963
0.99
2.04
5.35
2.02
0.98
3.02
2.03
2.04
3.11
3.00
f1 (ppm)

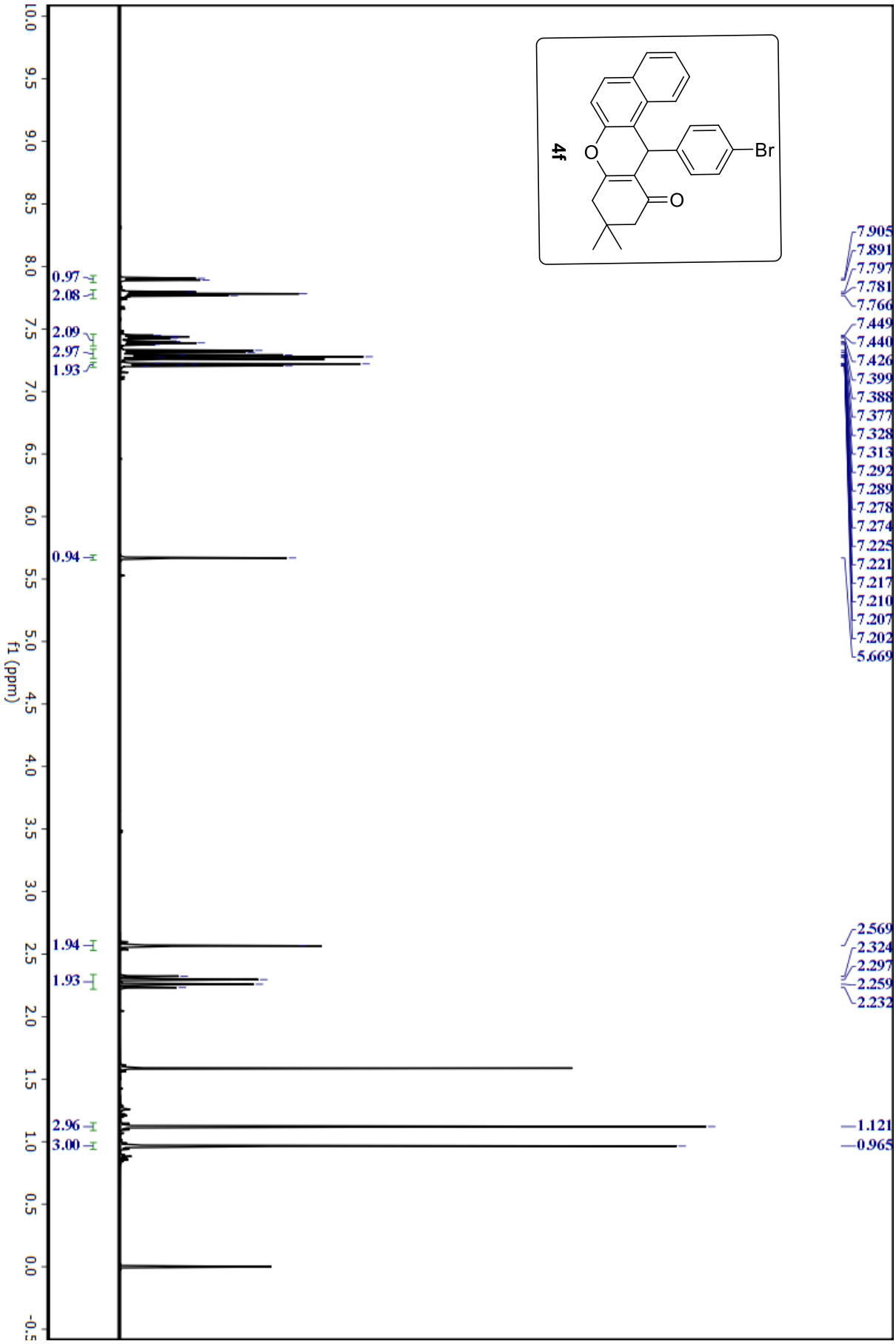

4c
O
O
O
196.97
163.64
157.74
147.65
137.14
131.46
131.36
129.32
128.67
128.34
126.90
124.81
123.66
117.85
116.99
114.38
113.55
55.02
50.88
41.35
33.78
32.22
29.25
27.15
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

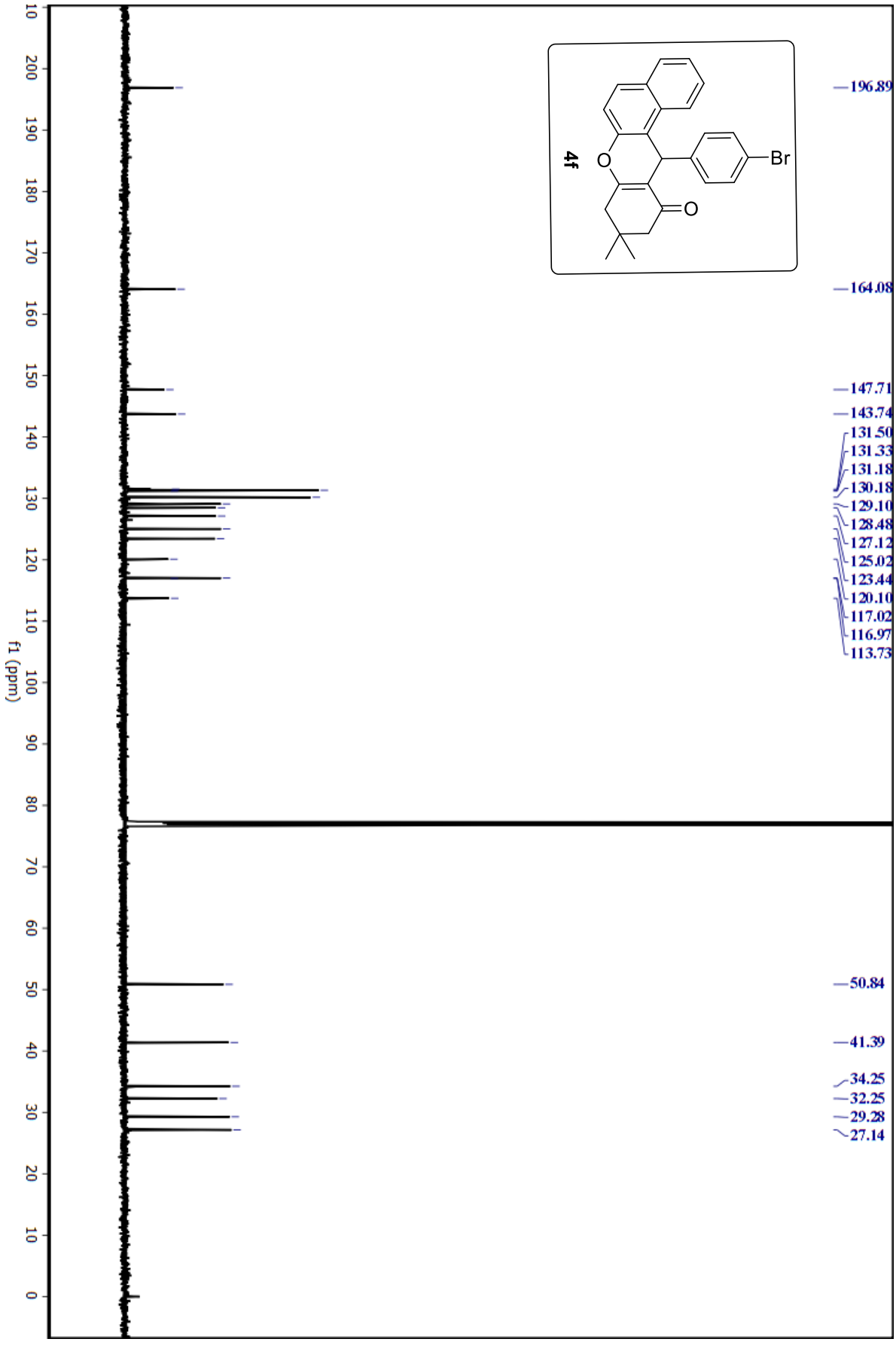

4d
O
NO2
O
8.040
8.029
7.838
7.824
7.820
7.813
7.805
7.799
7.796
7.521
7.510
7.506
7.451
7.439
7.428
7.411
7.395
7.384
7.363
7.349
5.811
2.598
2.341
2.314
2.257
2.230
1.130
0.944
1.94
3.05
1.99
3.00
0.94
1.97
1.98
3.01
3.00
f1 (ppm)

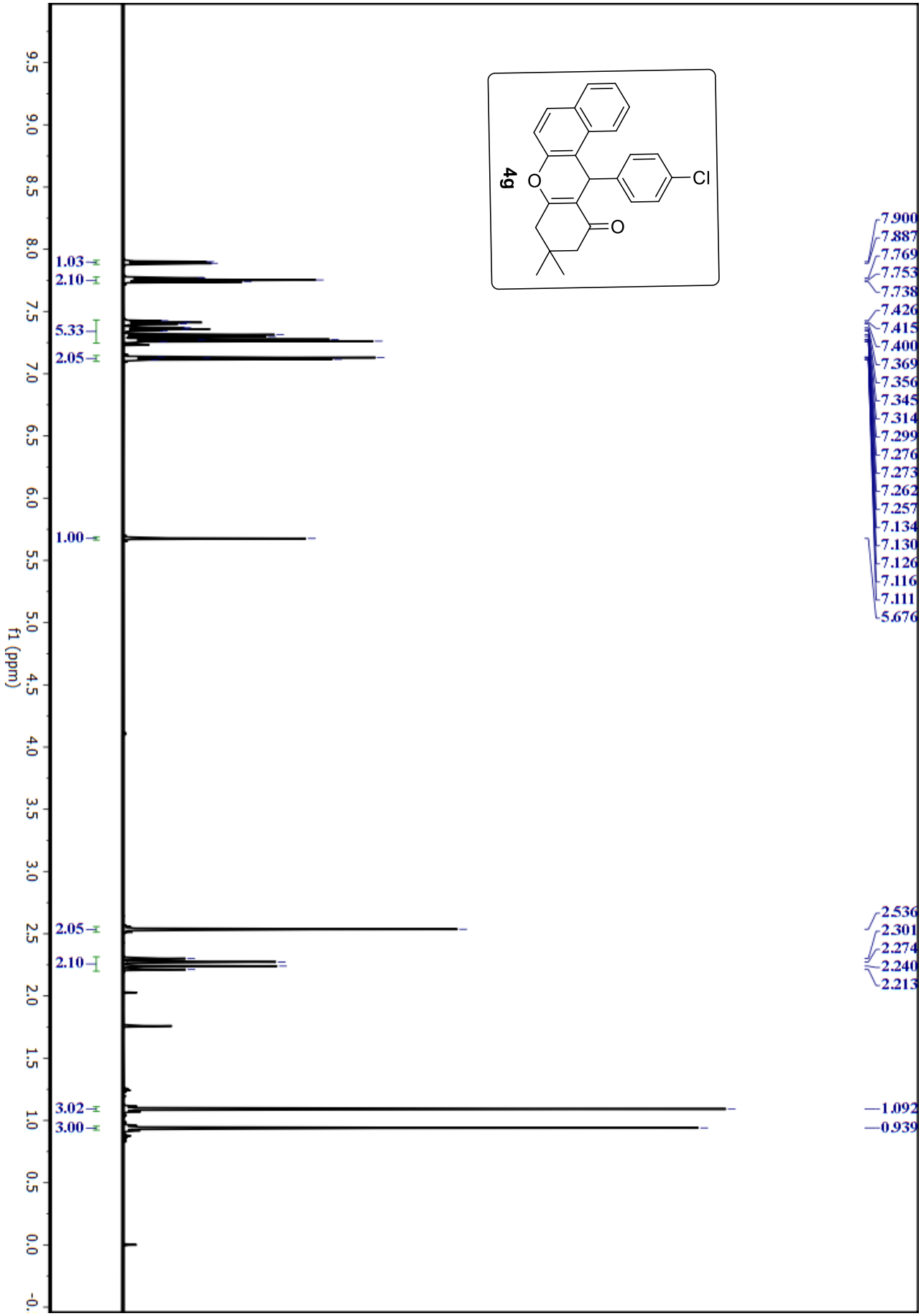

4d
O
NO2
O
196.68
164.59
151.83
147.75
146.31
131.54
130.99
129.59
129.32
128.62
127.34
125.20
123.58
123.07
117.05
116.00
112.95
50.74
41.38
34.83
32.21
29.25
27.02
f1 (ppm)

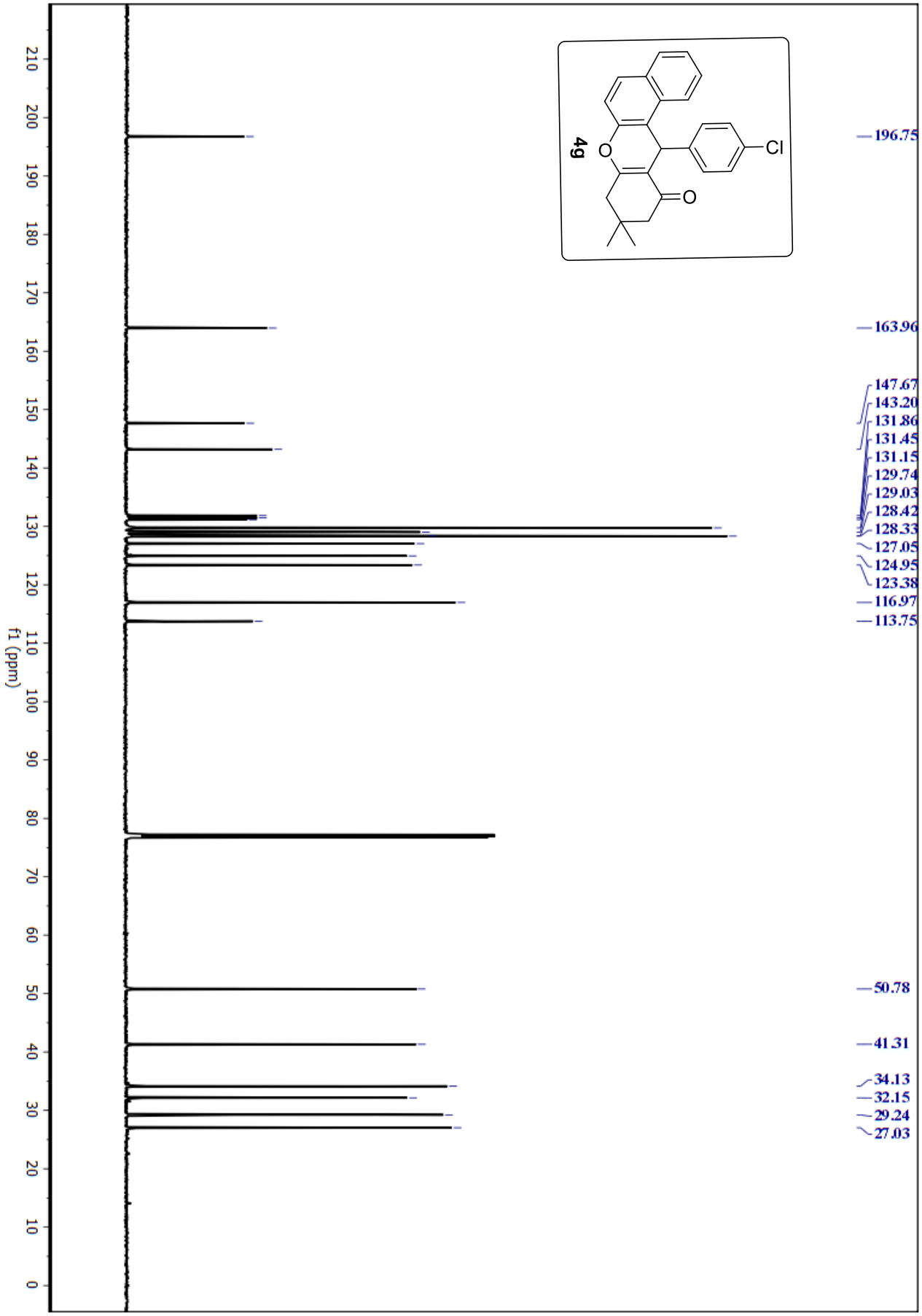

4e
O
F
O
7.921
7.907
7.763
7.750
7.744
7.729
7.421
7.407
7.395
7.361
7.348
7.336
7.312
7.297
7.284
6.854
6.839
6.825
5.690
2.530
2.297
2.270
2.239
2.211
1.087
0.932
1.00
2.02
5.11
1.98
0.99
2.02
2.03
3.00
3.00
f1 (ppm)

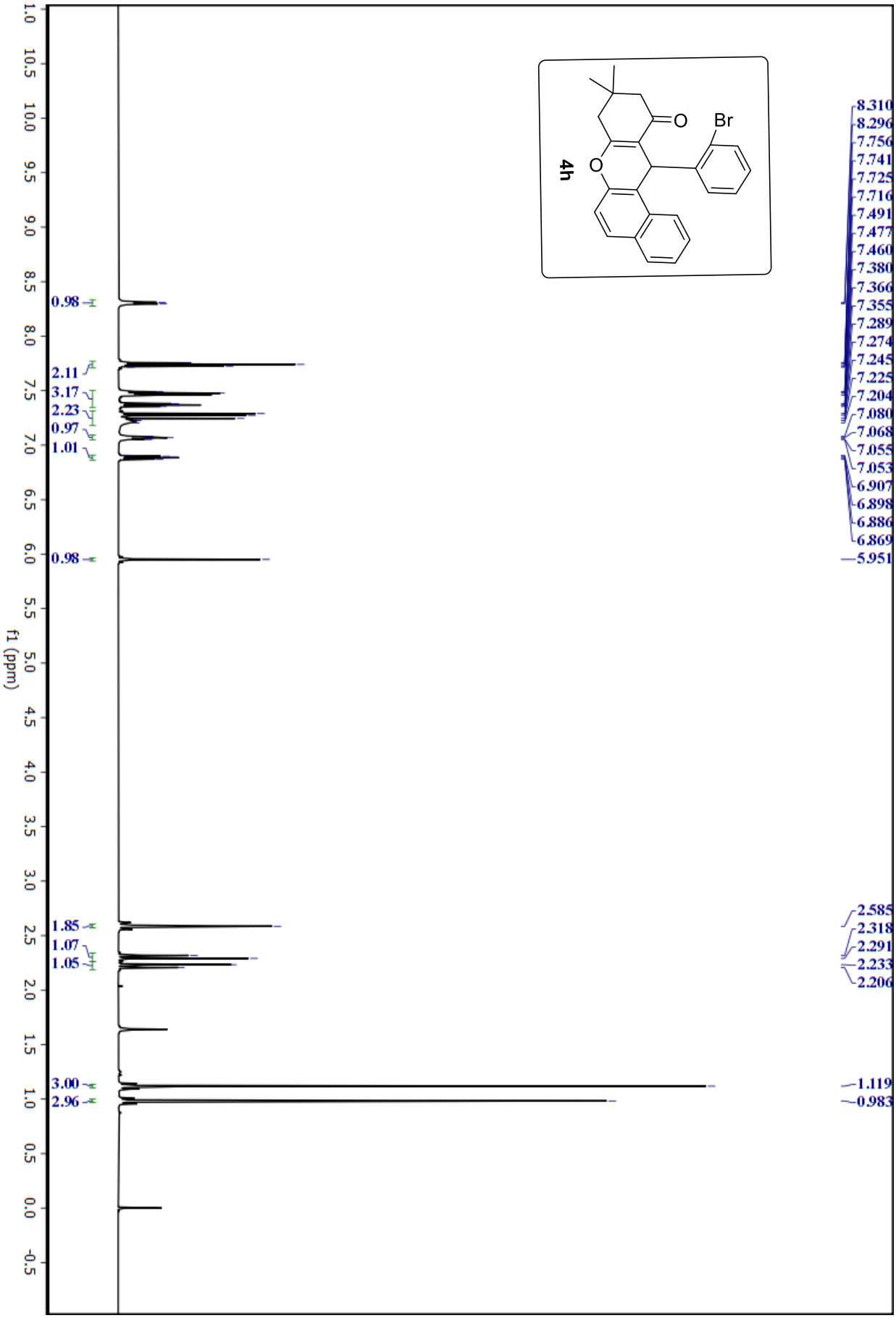

4e
O
F
O
196.82
163.84
161.92
160.31
147.66
140.48
131.45
131.17
129.86
129.80
128.93
128.40
126.99
124.90
123.44
117.30
116.97
115.03
114.89
114.01
50.78
41.28
33.92
32.14
29.23
26.97
f1 (ppm)

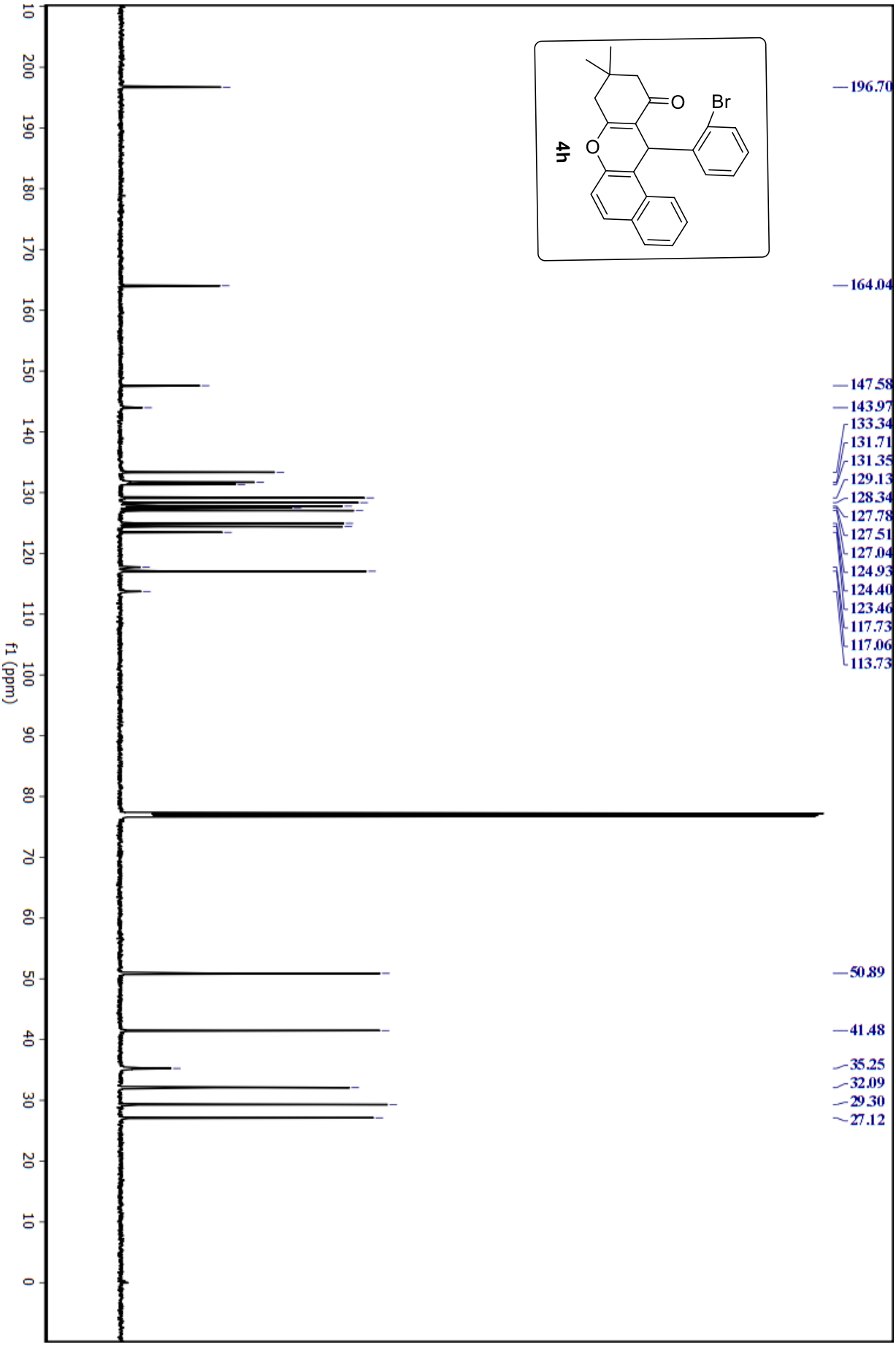

4f
O
Br
O
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
0.97
2.08
2.09
2.97
1.93
0.94
1.94
1.93
2.96
3.00
7.905
7.891
7.797
7.781
7.766
7.449
7.440
7.426
7.399
7.388
7.377
7.328
7.313
7.292
7.289
7.278
7.274
7.225
7.221
7.217
7.210
7.207
7.202
5.669
2.569
2.324
2.297
2.259
2.232
1.121
0.965

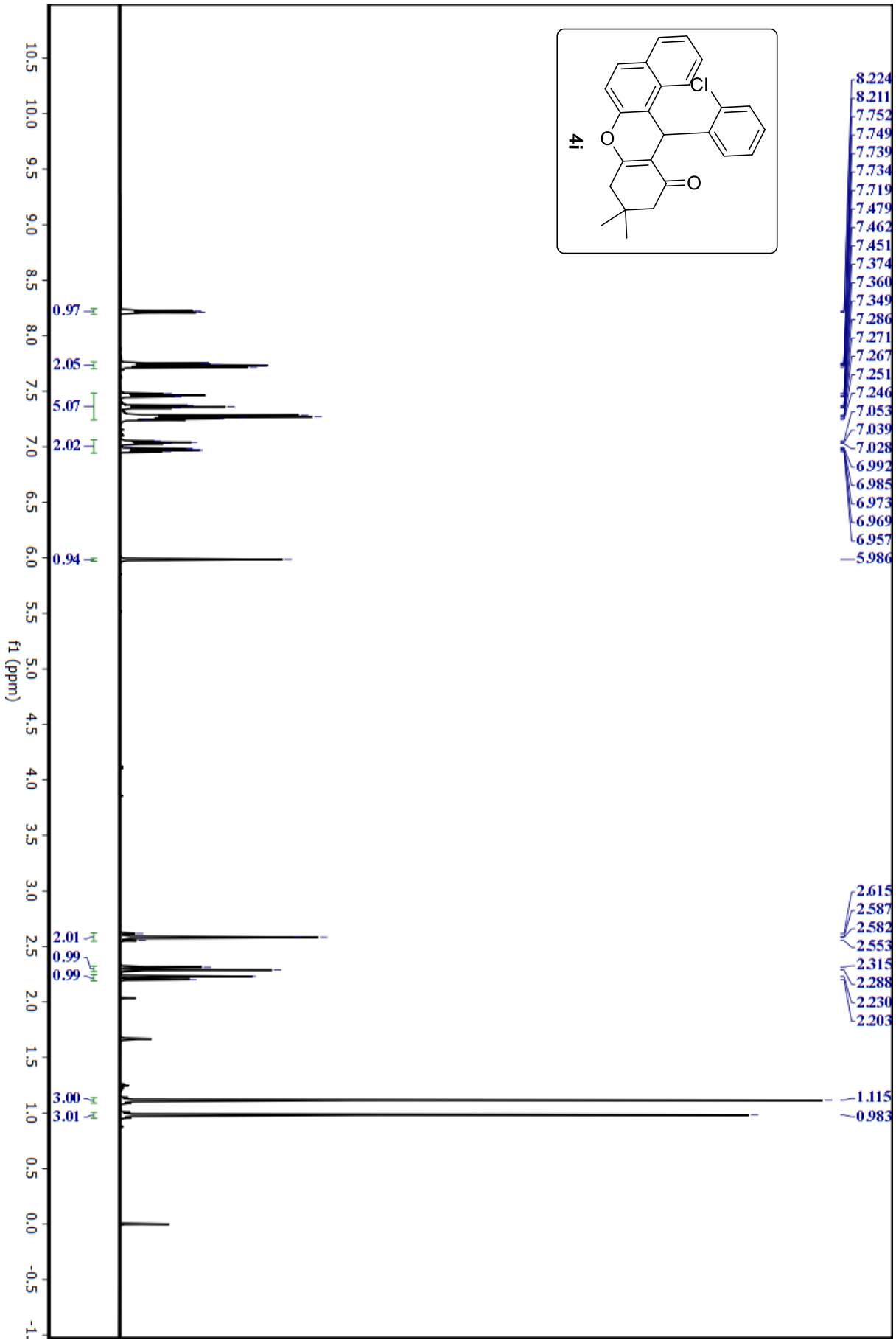

4f
O
Br
O
196.89
164.08
147.71
143.74
131.50
131.33
131.18
130.18
129.10
128.48
127.12
125.02
123.44
120.10
117.02
116.97
113.73
50.84
41.39
34.25
32.25
29.28
27.14
f1 (ppm)

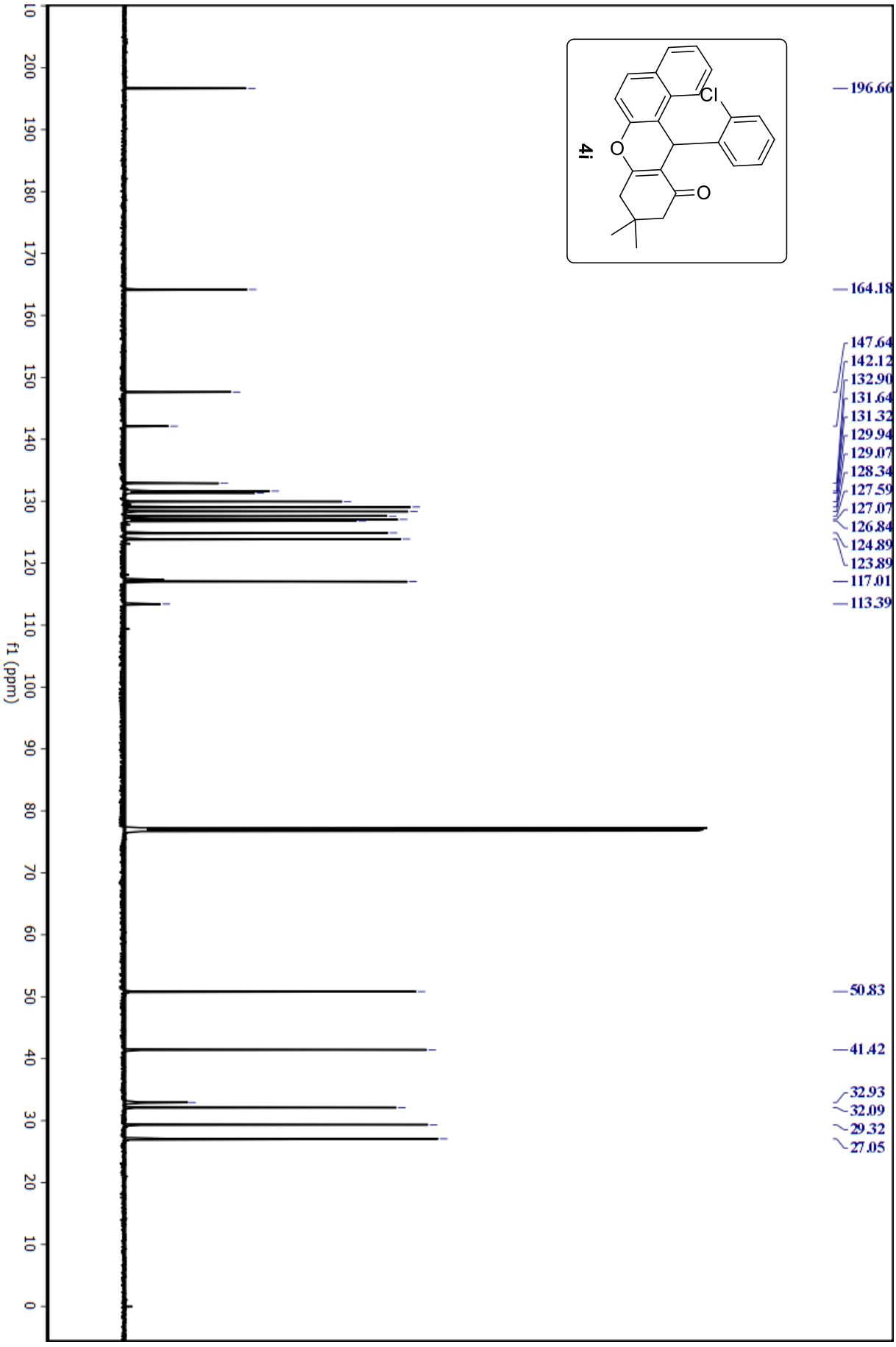

4g
O
Cl
O
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
1.03
2.10
5.33
2.05
1.00
2.05
2.10
3.02
3.00
7.900
7.887
7.769
7.753
7.738
7.426
7.415
7.400
7.369
7.356
7.345
7.314
7.299
7.276
7.273
7.262
7.257
7.134
7.130
7.126
7.116
7.111
5.676
2.536
2.301
2.274
2.240
2.213
1.092
0.939

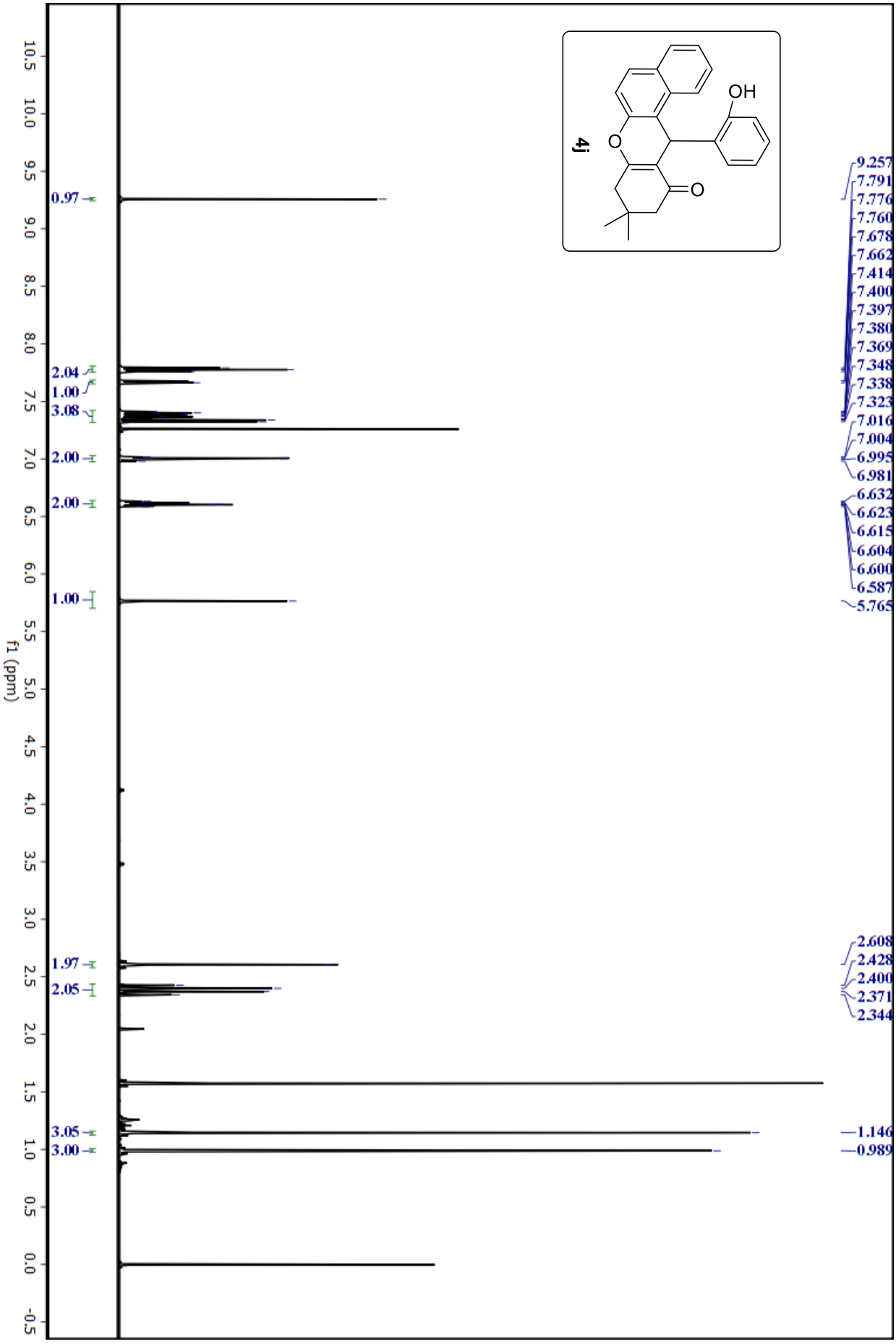

4g
O
Cl
O
196.75
163.96
147.67
143.20
131.86
131.45
131.15
129.74
129.03
128.42
128.33
127.05
124.95
123.38
116.97
113.75
50.78
41.31
34.13
32.15
29.24
27.03
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

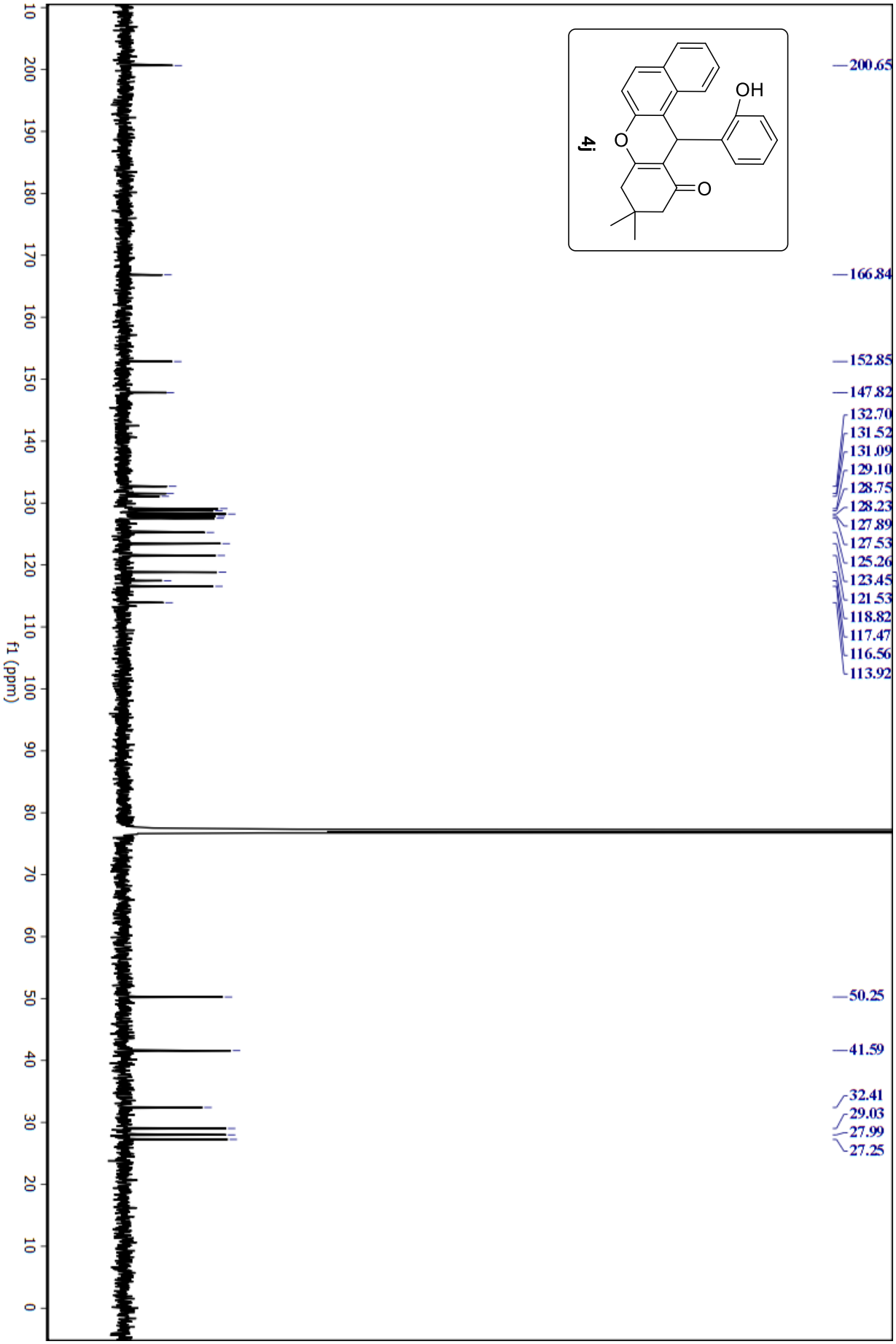

4h
O
Br
O
f1 (ppm)
8.310
8.296
7.756
7.741
7.725
7.716
7.491
7.477
7.460
7.380
7.366
7.355
7.289
7.274
7.245
7.225
7.204
7.080
7.068
7.055
7.053
6.907
6.898
6.886
6.869
5.951
2.585
2.318
2.291
2.233
2.206
1.119
0.983
0.98
2.11
3.17
2.23
0.97
1.01
0.98
1.85
1.07
1.05
3.00
2.96

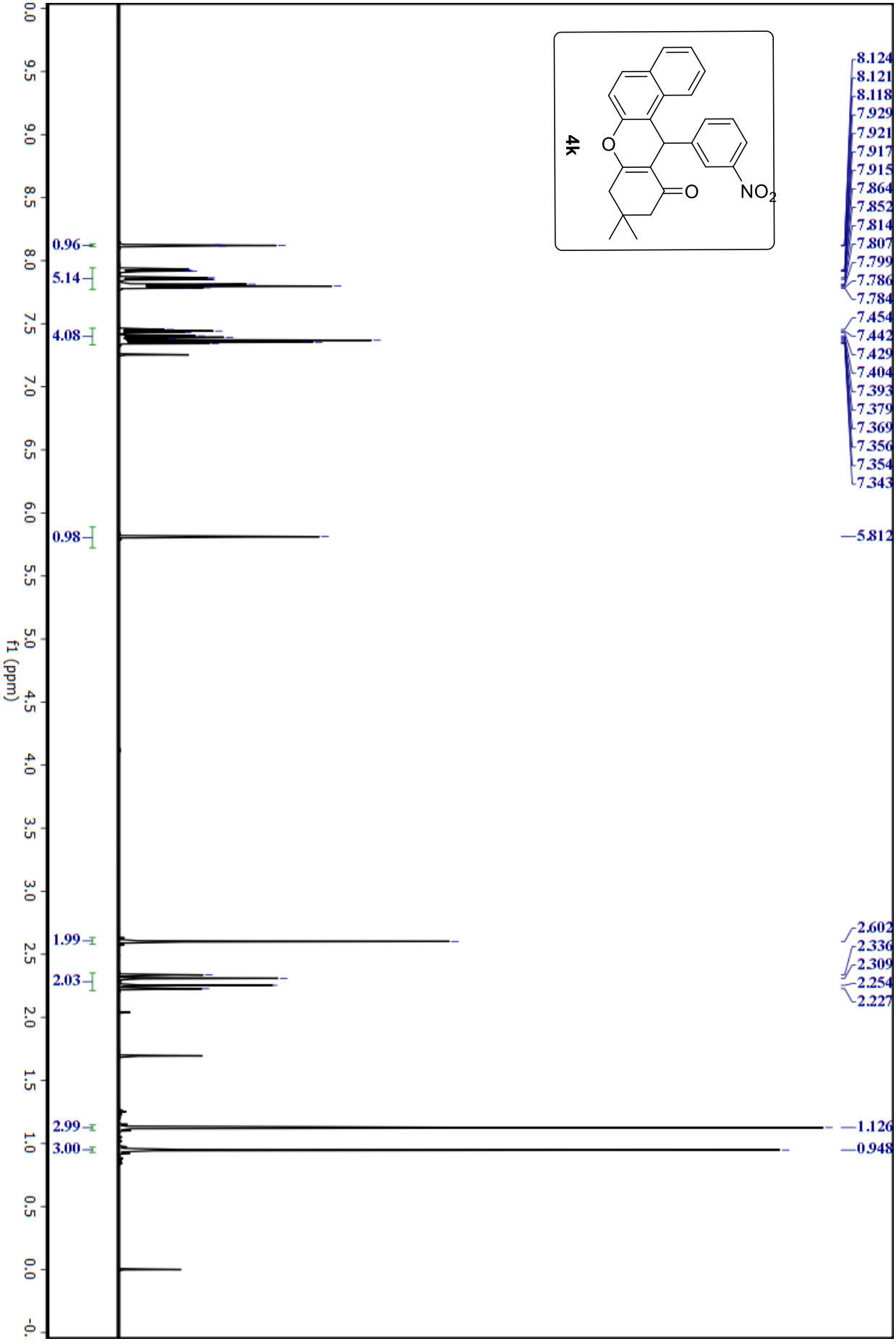

4h
O
Br
O
196.70
164.04
147.58
143.97
133.34
131.71
131.35
129.13
128.34
127.78
127.51
127.04
124.93
124.40
123.46
117.73
117.06
113.73
50.89
41.48
35.25
32.09
29.30
27.12
f1 (ppm)

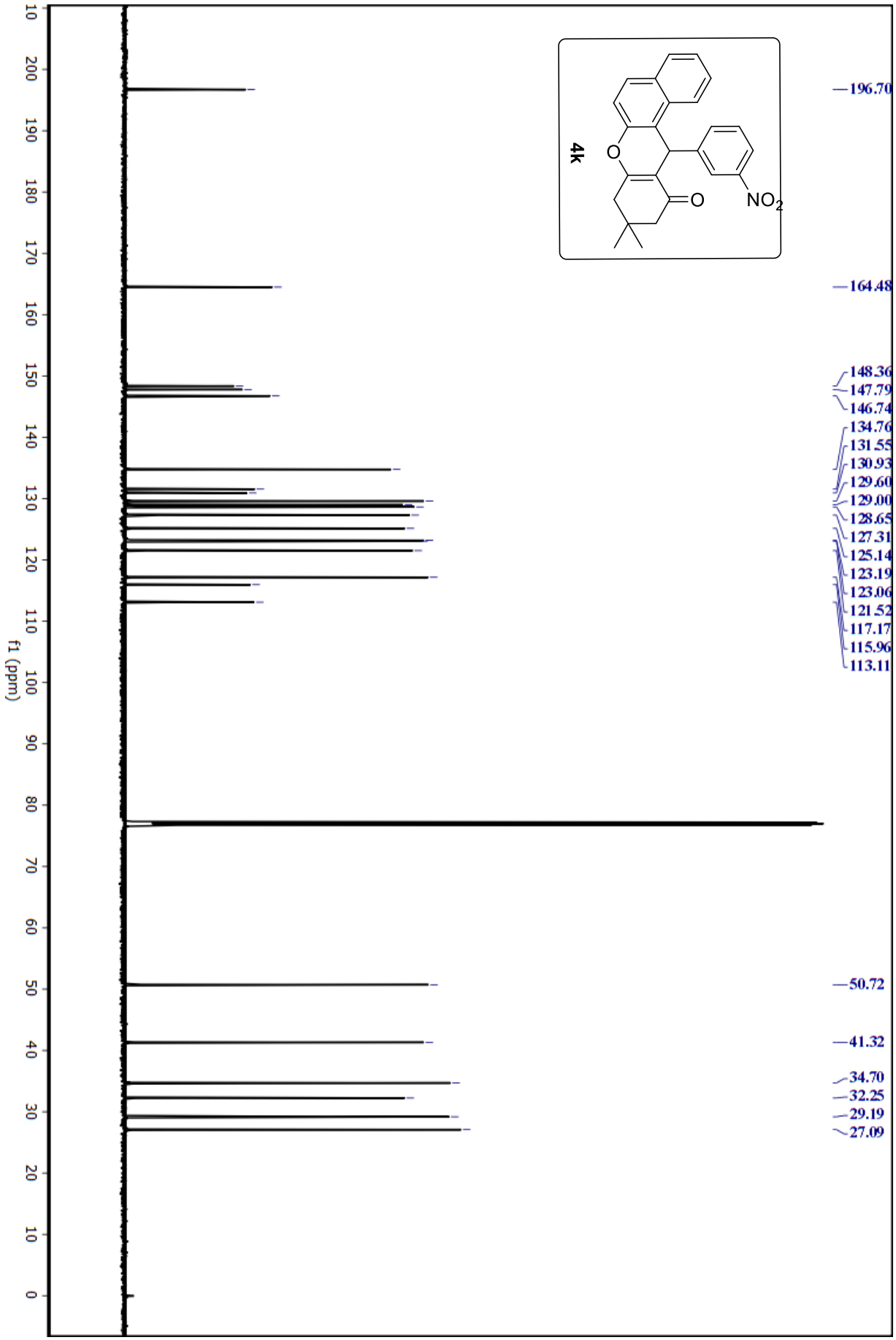

4i
Cl
O
O
8.224
8.211
7.752
7.749
7.739
7.734
7.719
7.479
7.462
7.451
7.374
7.360
7.349
7.286
7.271
7.267
7.251
7.246
7.053
7.039
7.028
6.992
6.985
6.973
6.969
6.957
5.986
2.615
2.587
2.582
2.553
2.315
2.288
2.230
2.203
1.115
0.983
0.97
2.05
5.07
2.02
0.94
2.01
0.99
0.99
3.00
3.01
f1 (ppm)

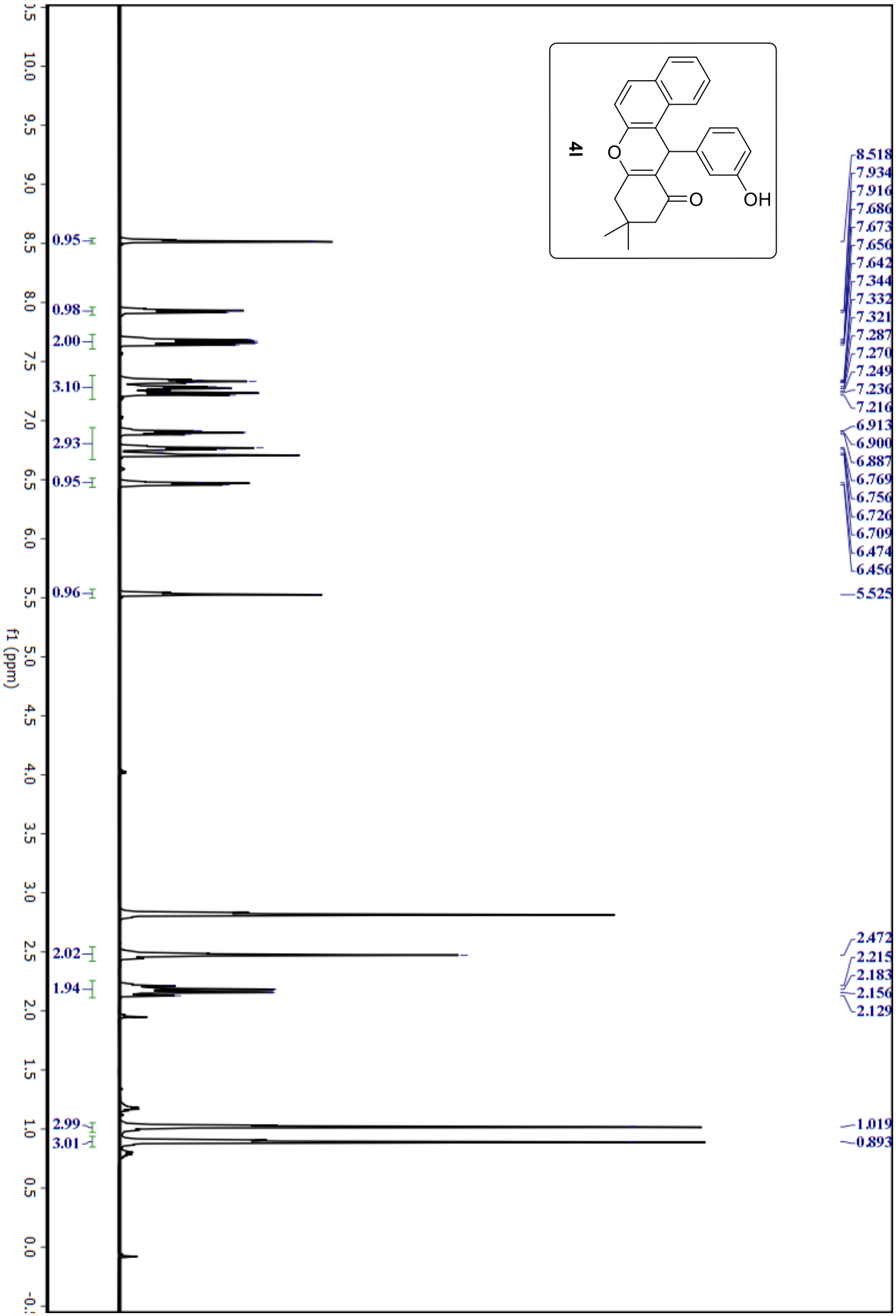

4i
Cl
O
O
196.66
164.18
147.64
142.12
132.90
131.64
131.32
129.94
129.07
128.34
127.59
127.07
126.84
124.89
123.89
117.01
113.39
50.83
41.42
32.93
32.09
29.32
27.05
f1 (ppm)

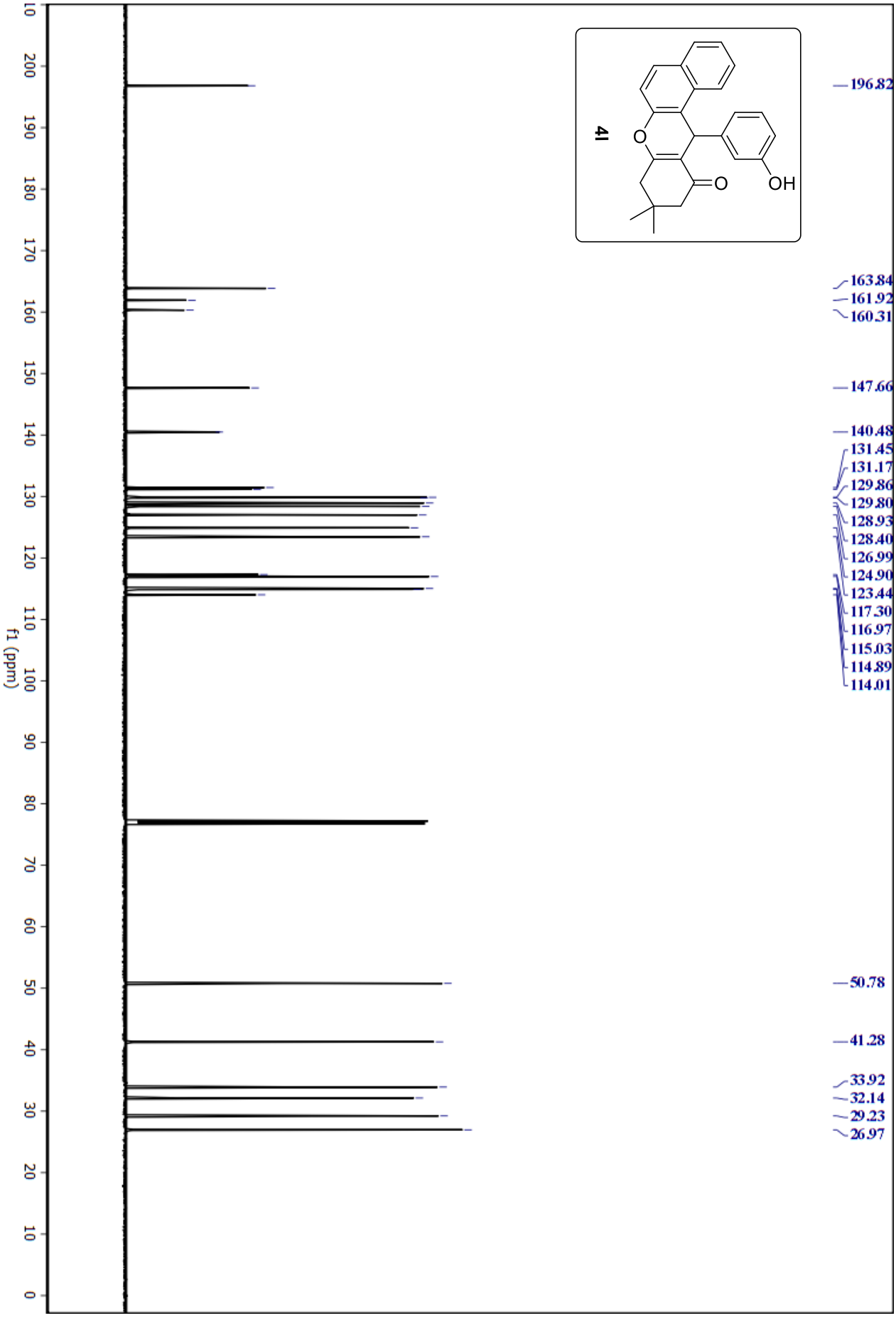

4j
OH
O
O
f1 (ppm)
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
0.97
2.04
1.00
3.08
2.00
2.00
1.00
1.97
2.05
3.05
3.00
9.257
7.791
7.776
7.760
7.678
7.662
7.414
7.400
7.397
7.380
7.369
7.348
7.338
7.323
7.016
7.004
6.995
6.981
6.632
6.623
6.615
6.604
6.600
6.587
5.765
2.608
2.428
2.400
2.371
2.344
1.146
0.989

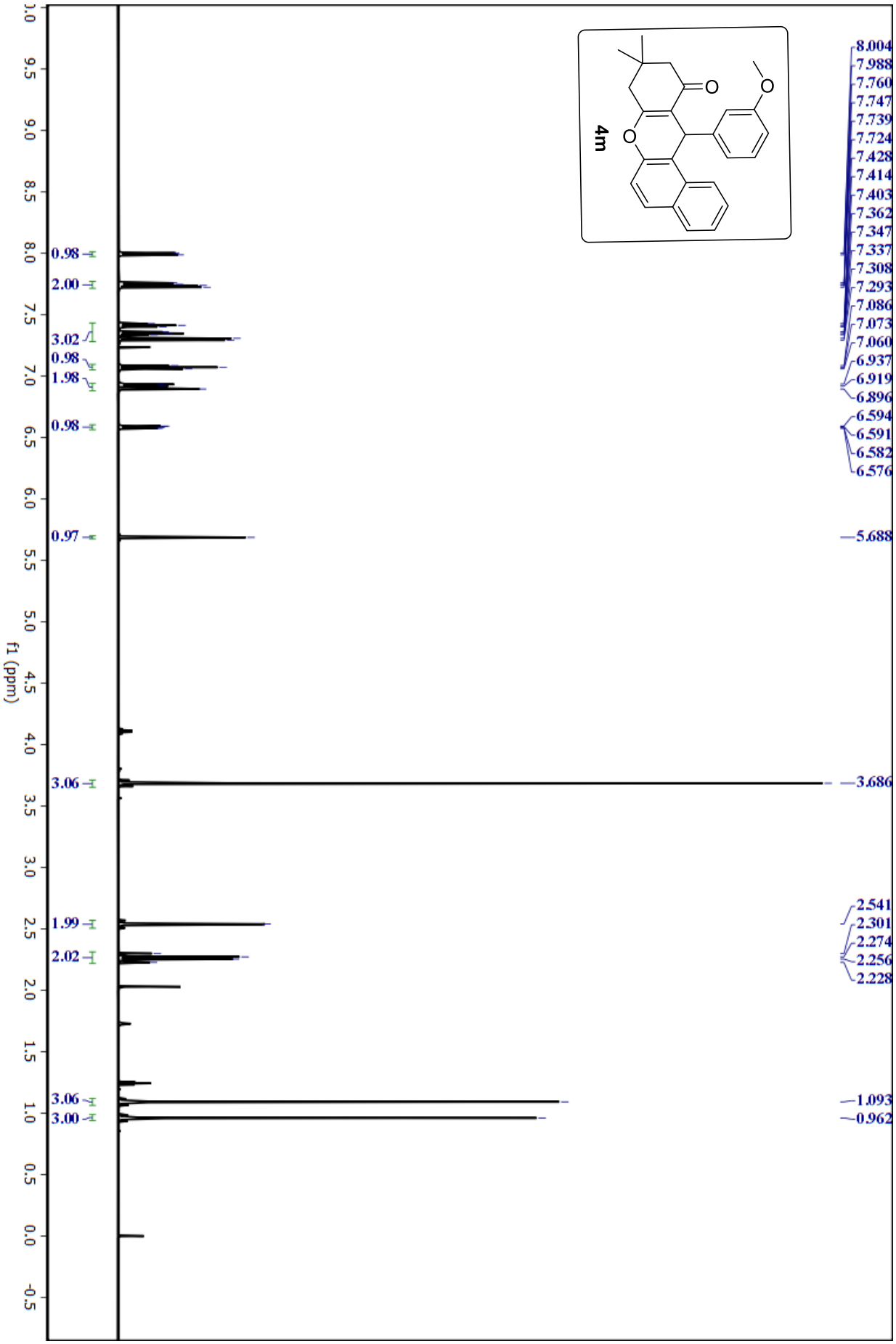

4j
OH
O
O
200.65
166.84
152.85
147.82
132.70
131.52
131.09
129.10
128.75
128.23
127.89
127.53
125.26
123.45
121.53
118.82
117.47
116.56
113.92
50.25
41.59
32.41
29.03
27.99
27.25
f1 (ppm)

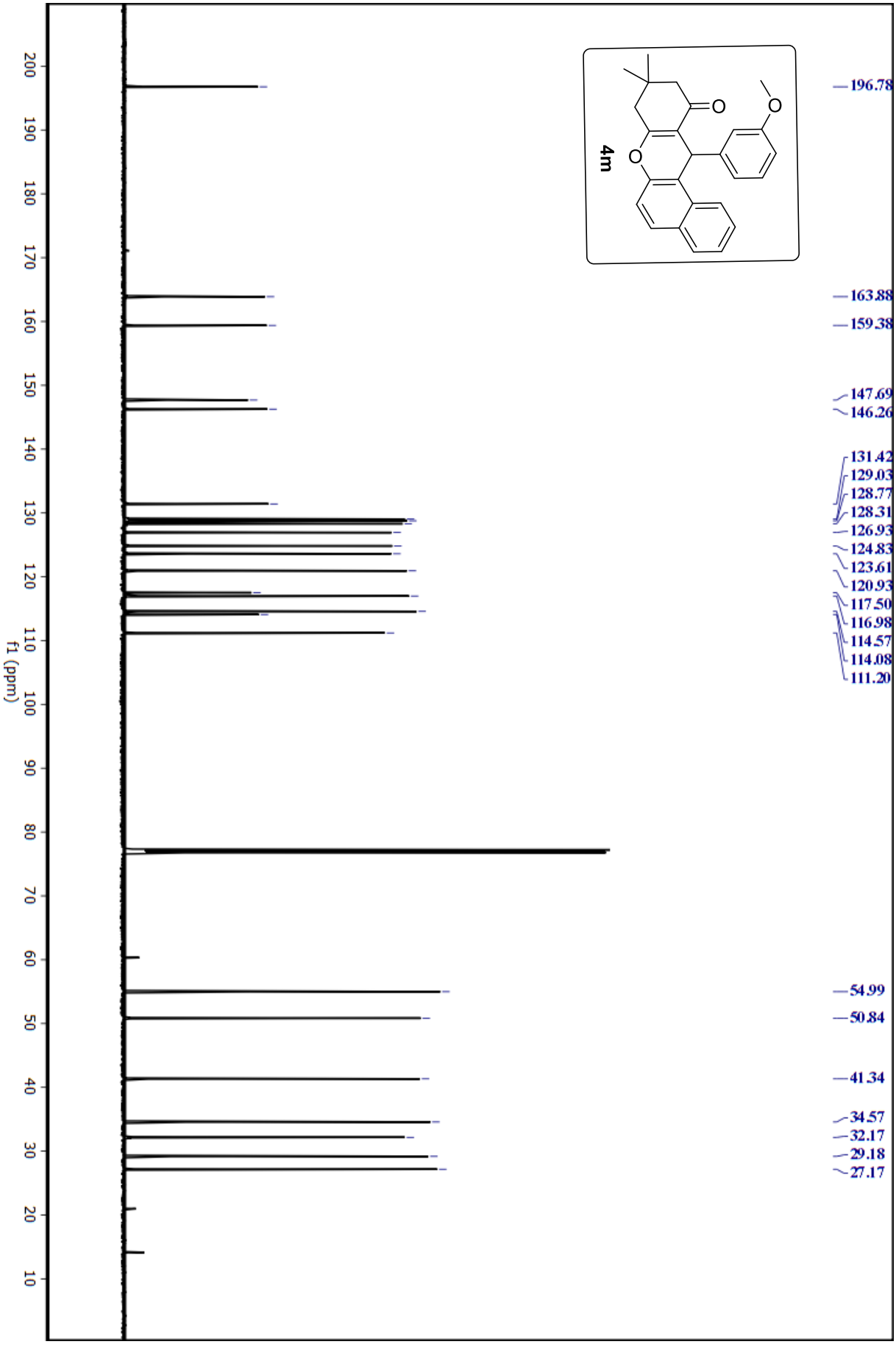

4k
O
O
NO2
f1 (ppm)
0.96
5.14
4.08
0.98
1.99
2.03
2.99
3.00
8.124
8.121
8.118
7.929
7.921
7.917
7.915
7.864
7.852
7.814
7.807
7.799
7.786
7.784
7.454
7.442
7.429
7.404
7.393
7.379
7.369
7.356
7.354
7.343
5.812
2.602
2.336
2.309
2.254
2.227
1.126
0.948

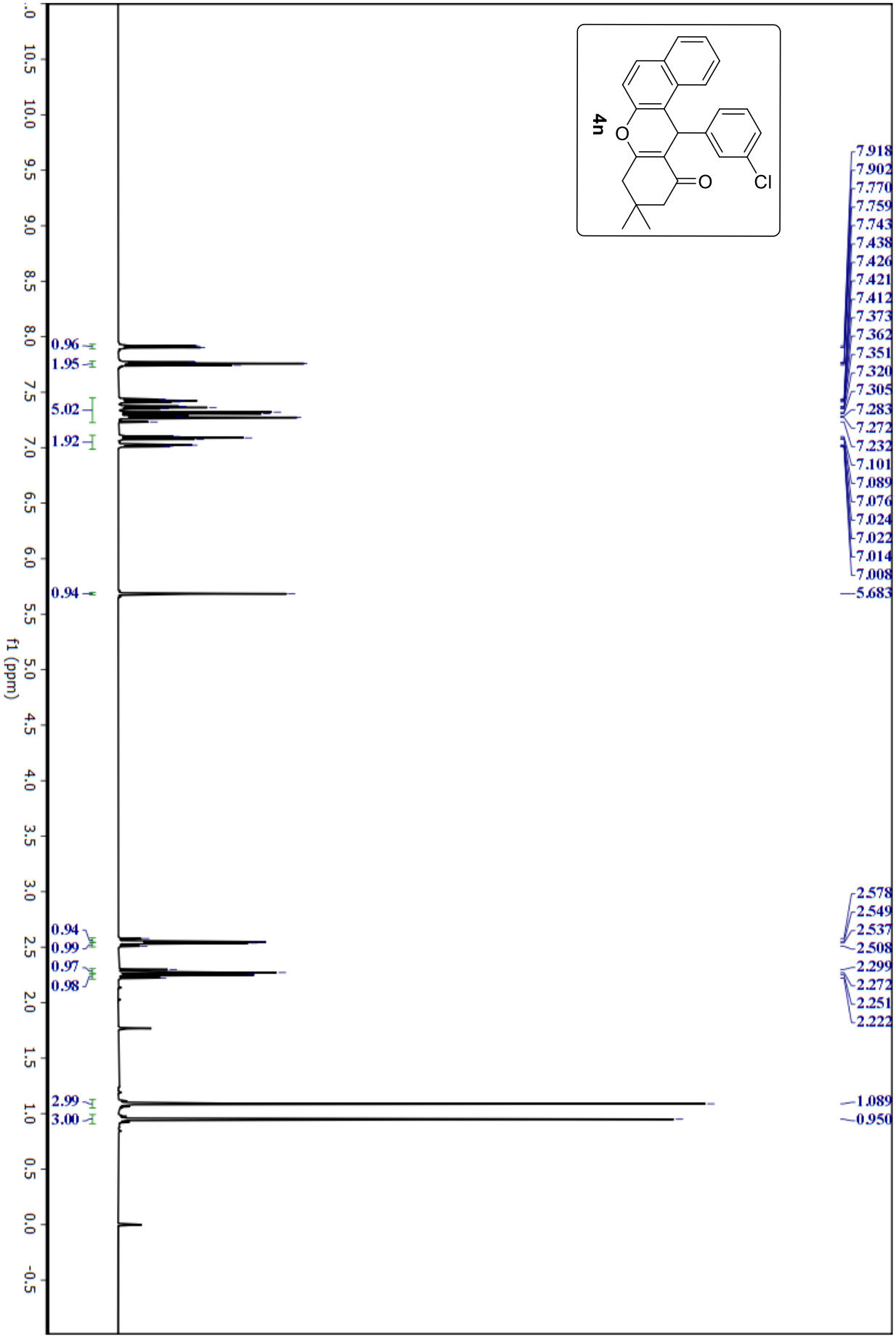

4k
O
O
NO2
196.70
164.48
148.36
147.79
146.74
134.76
131.55
130.93
129.60
129.00
128.65
127.31
125.14
123.19
123.06
121.52
117.17
115.96
113.11
50.72
41.32
34.70
32.25
29.19
27.09
f1 (ppm)

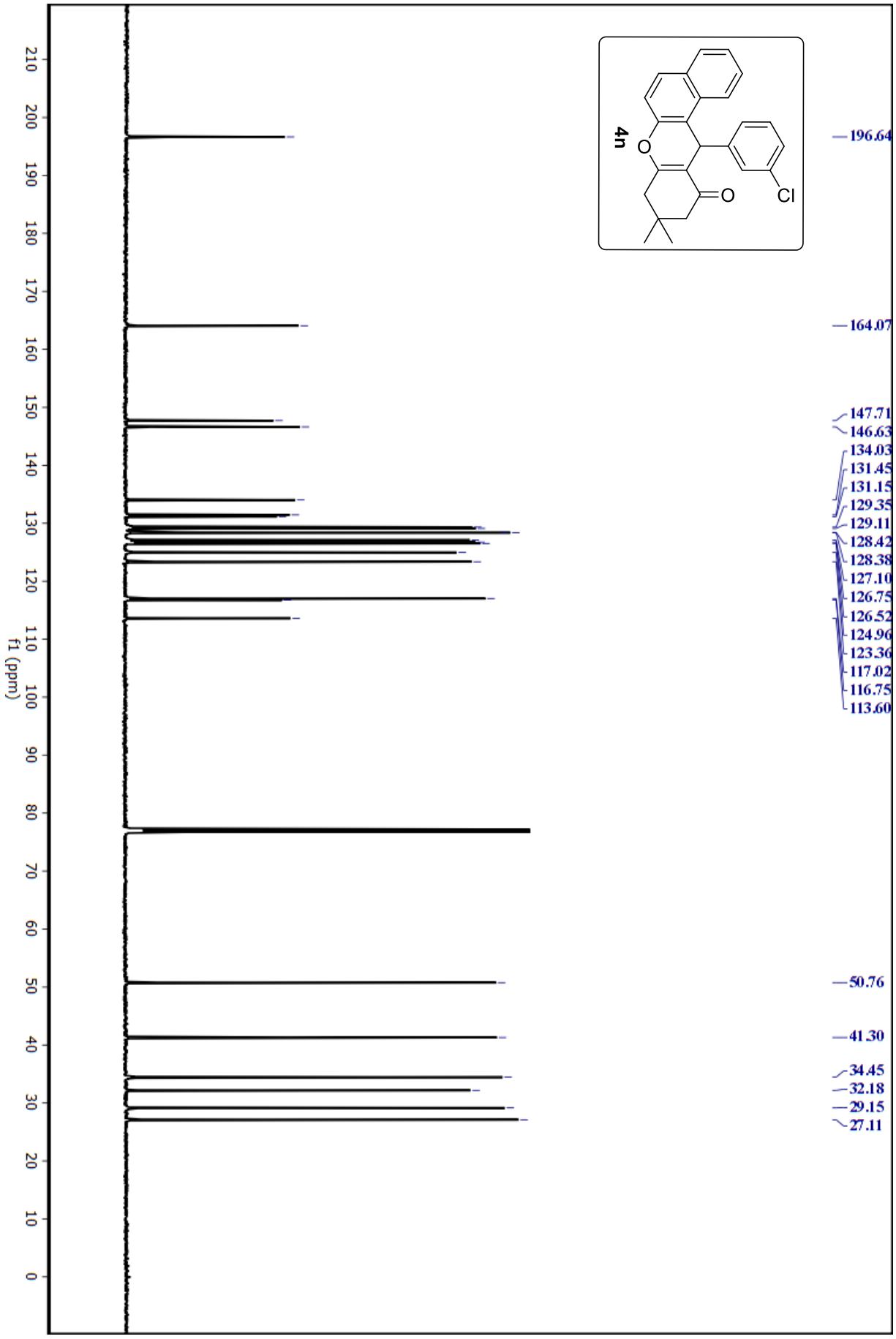

4l
O
O
OH
f1 (ppm)
0.95
0.98
2.00
3.10
2.93
0.95
0.96
2.02
1.94
2.99
3.01
8.518
7.934
7.916
7.686
7.673
7.656
7.642
7.344
7.332
7.321
7.287
7.270
7.249
7.236
7.216
6.913
6.900
6.887
6.769
6.756
6.726
6.709
6.474
6.456
5.525
2.472
2.215
2.183
2.156
2.129
1.019
0.893

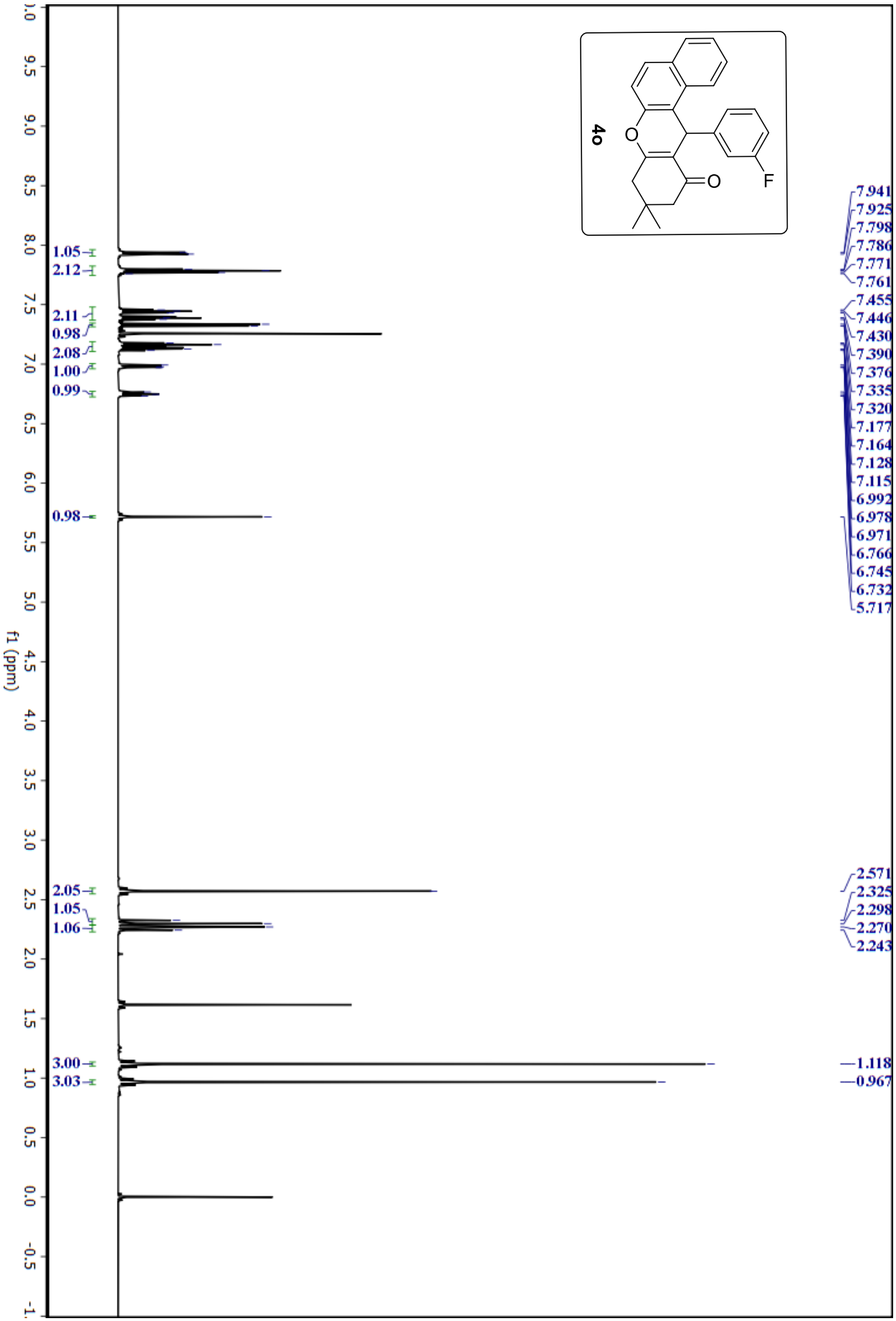

41
O
O
OH
196.82
163.84
161.92
160.31
147.66
140.48
131.45
131.17
129.86
129.80
128.93
128.40
126.99
124.90
123.44
117.30
116.97
115.03
114.89
114.01
50.78
41.28
33.92
32.14
29.23
26.97
f1 (ppm)

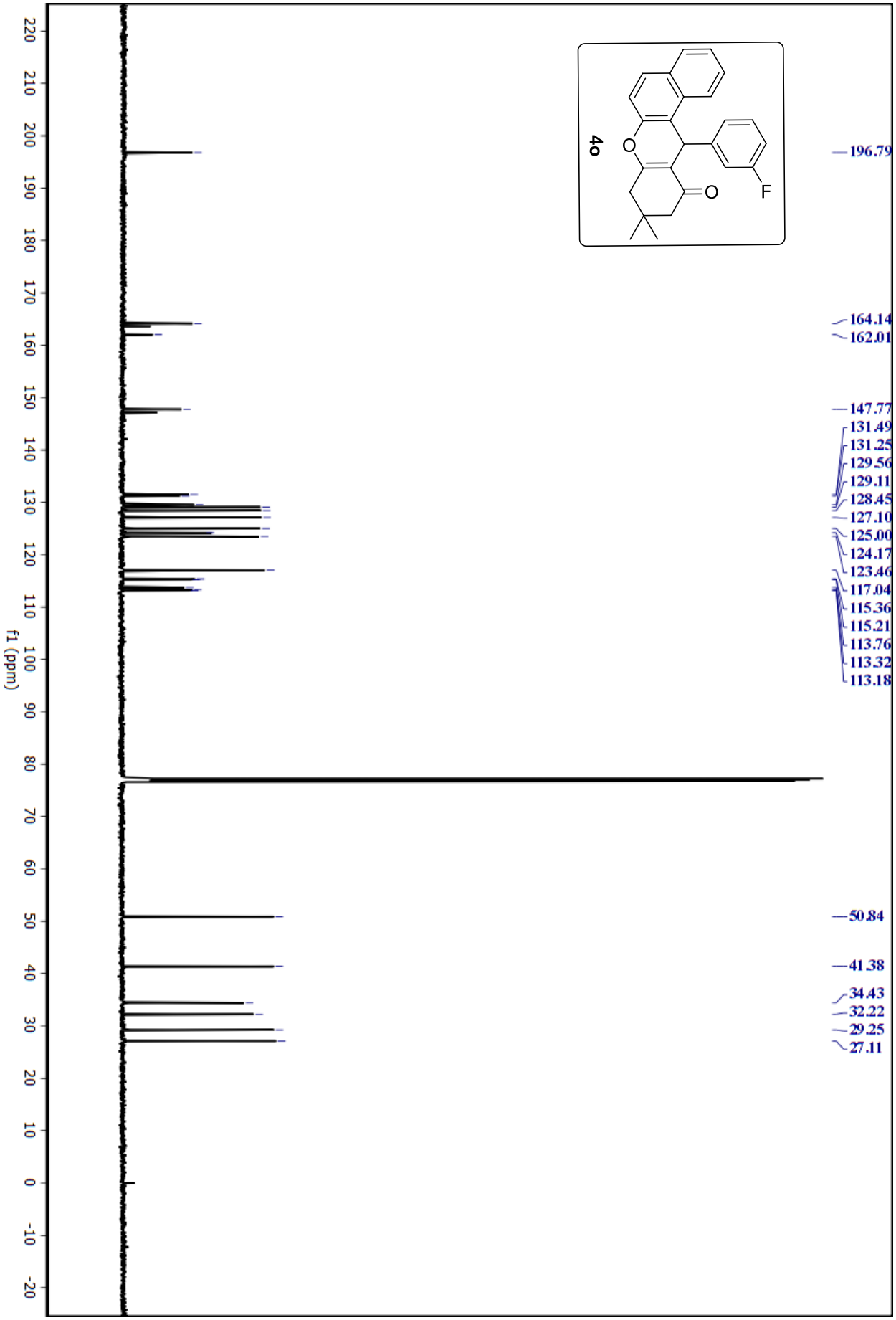

4m
O
O
O
8.004
7.988
7.760
7.747
7.739
7.724
7.428
7.414
7.403
7.362
7.347
7.337
7.308
7.293
7.086
7.073
7.060
6.937
6.919
6.896
6.594
6.591
6.582
6.576
5.688
3.686
2.541
2.301
2.274
2.256
2.228
1.093
0.962
0.98
2.00
3.02
0.98
1.98
0.98
0.97
3.06
1.99
2.02
3.06
3.00
f1 (ppm)

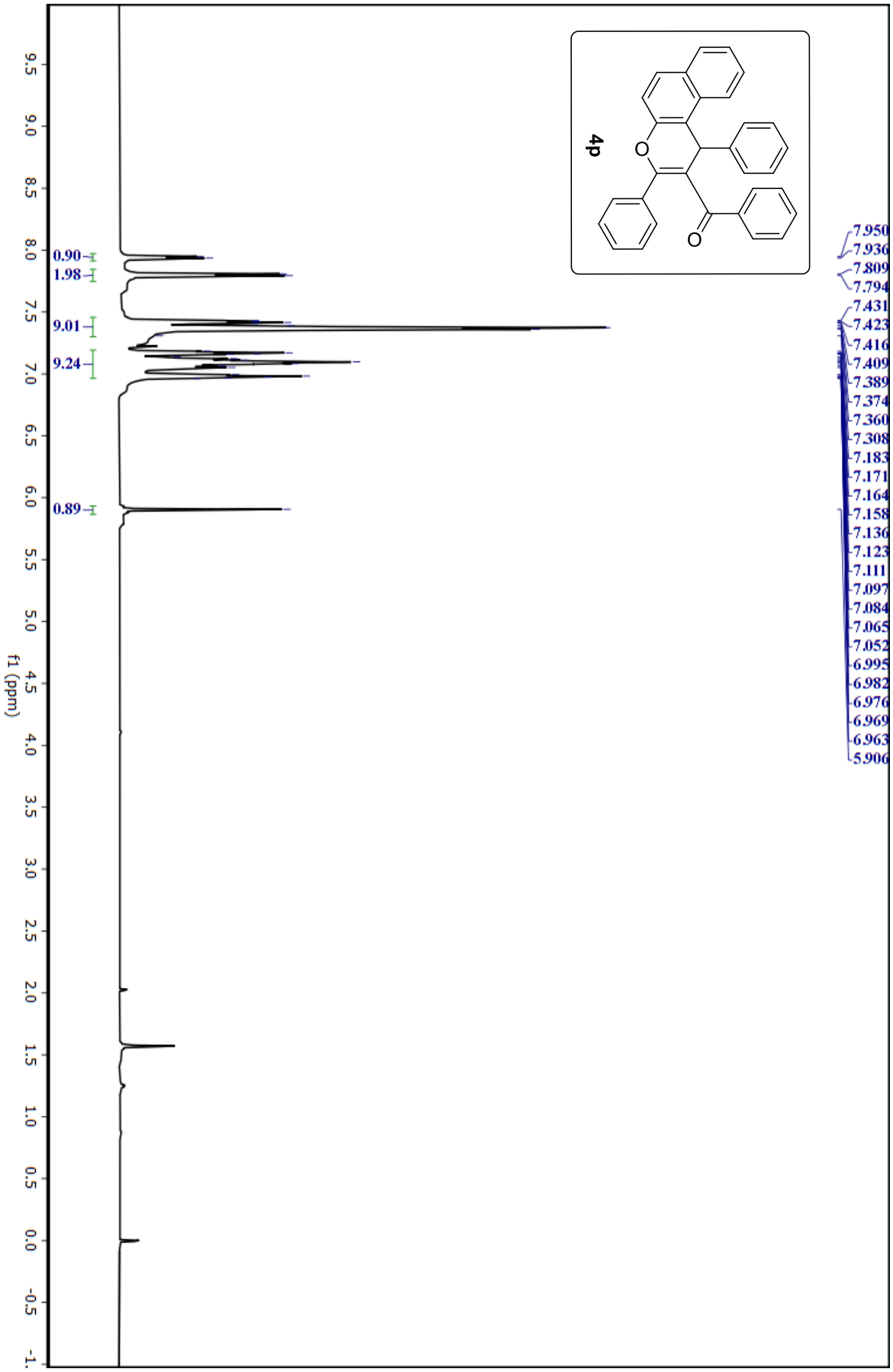

4m
O
O
O
196.78
163.88
159.38
147.69
146.26
131.42
129.03
128.77
128.31
126.93
124.83
123.61
120.93
117.50
116.98
114.57
114.08
111.20
54.99
50.84
41.34
34.57
32.17
29.18
27.17
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

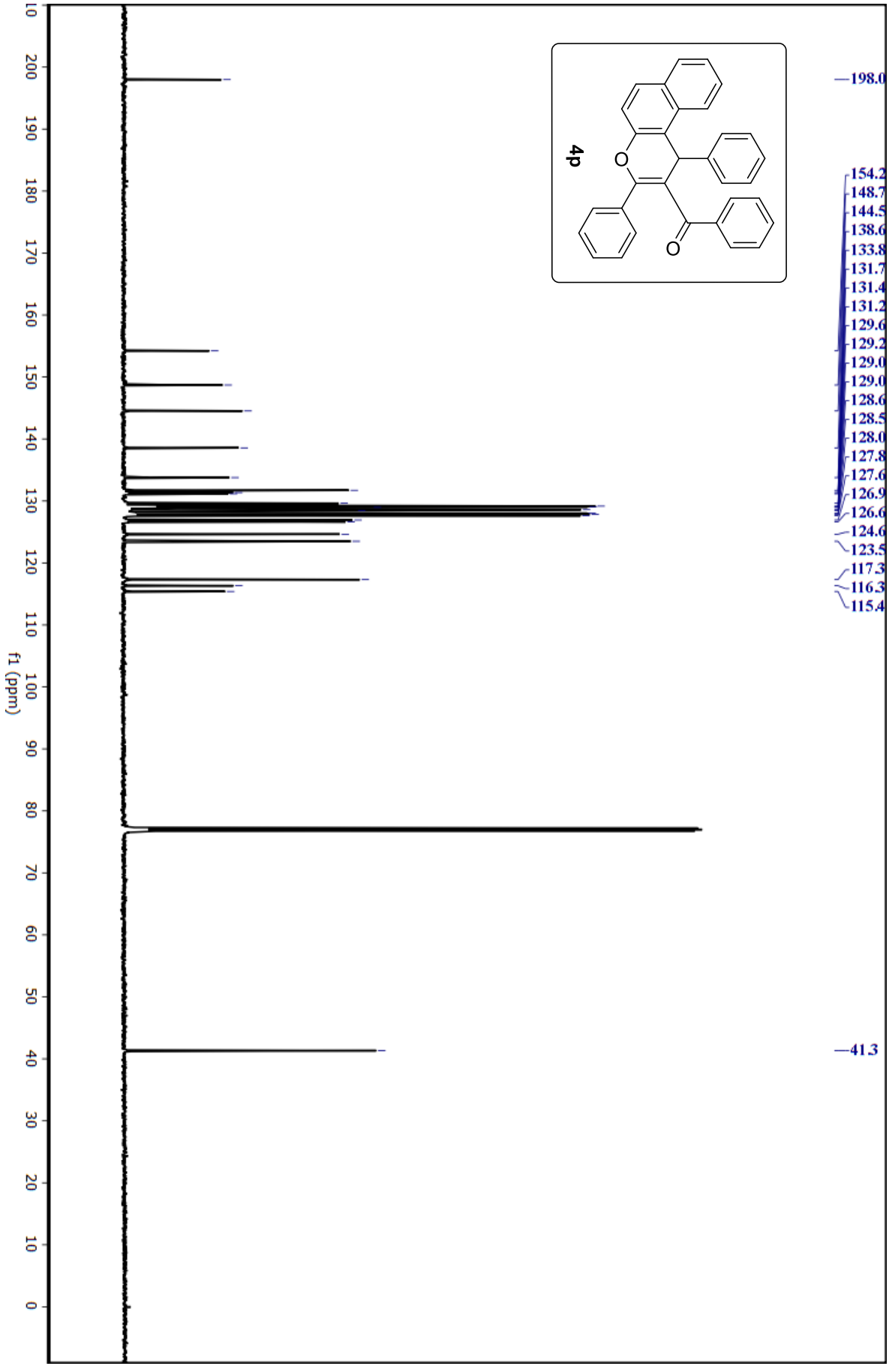

4n
O
O
Cl
f1 (ppm)
0.96
1.95
5.02
1.92
0.94
0.94
0.99
0.97
0.98
2.99
3.00
7.918
7.902
7.770
7.759
7.743
7.438
7.426
7.421
7.412
7.373
7.362
7.351
7.320
7.305
7.283
7.272
7.232
7.101
7.089
7.076
7.024
7.022
7.014
7.008
5.683
2.578
2.549
2.537
2.508
2.299
2.272
2.251
2.222
1.089
0.950

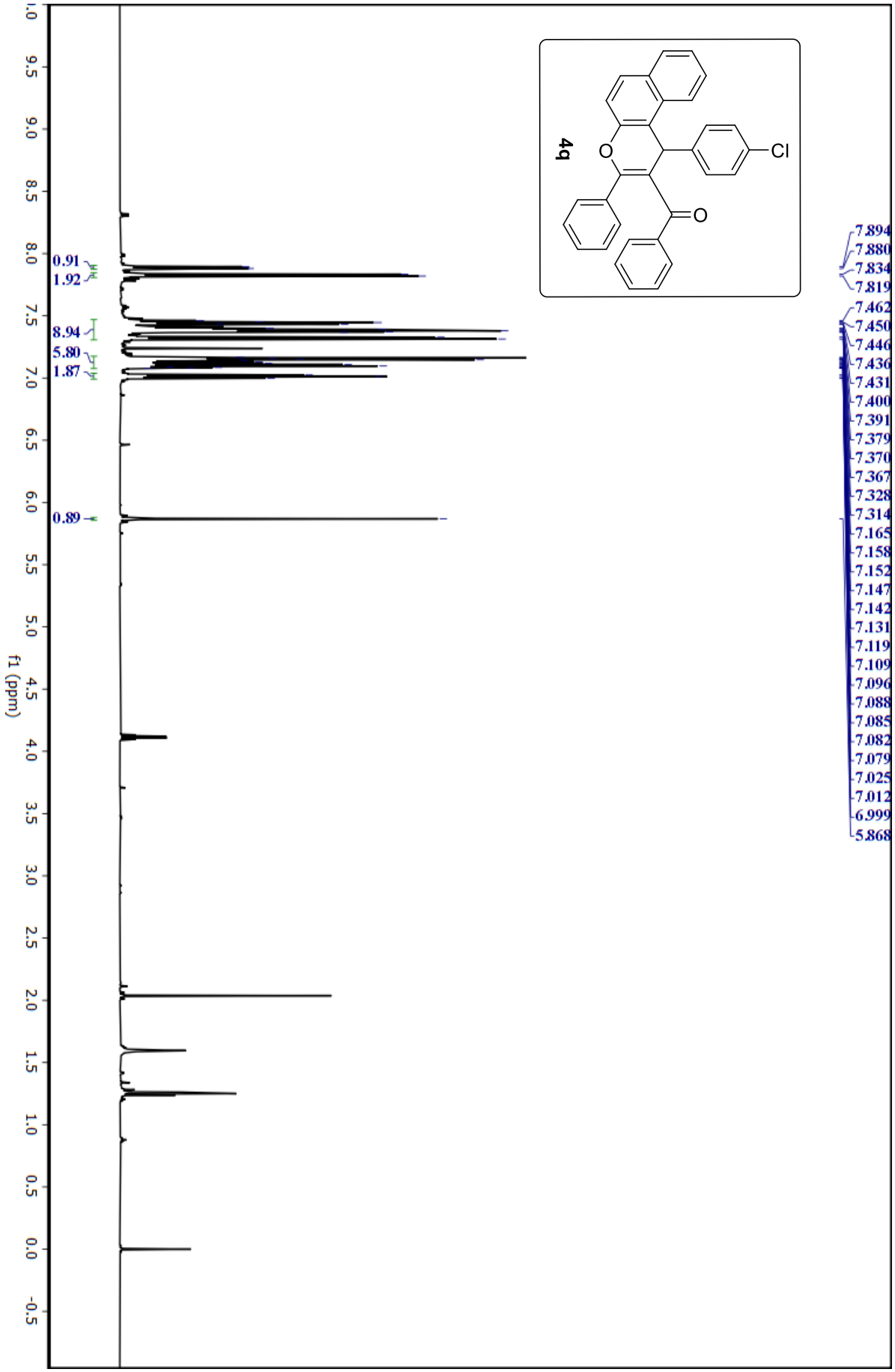

4n
O
O
Cl
196.64
164.07
147.71
146.63
134.03
131.45
131.15
129.35
129.11
128.42
128.38
127.10
126.75
126.52
124.96
123.36
117.02
116.75
113.60
50.76
41.30
34.45
32.18
29.15
27.11
f1 (ppm)

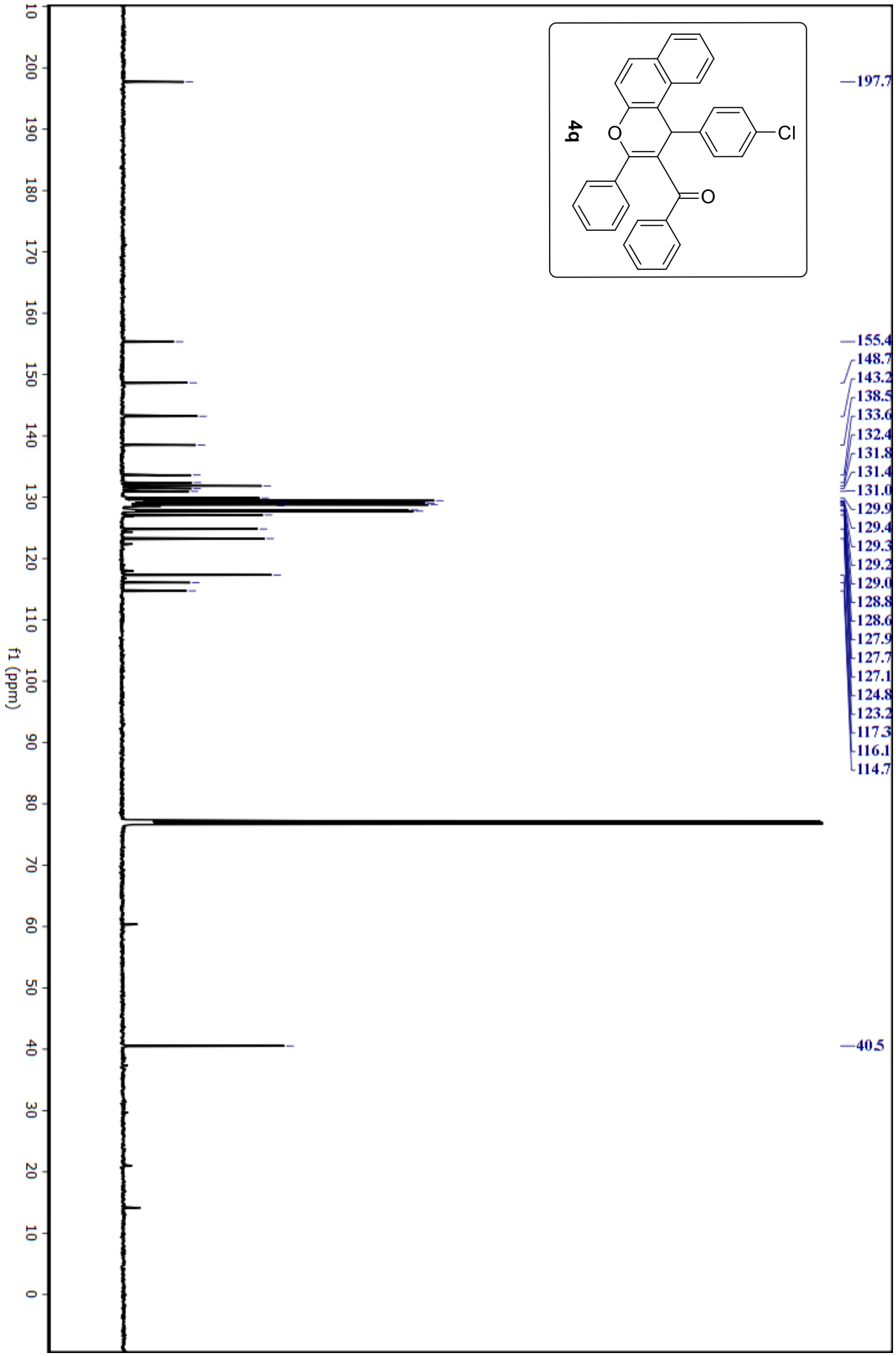

4o
O
O
F
f1 (ppm)
1.05
2.12
2.11
0.98
2.08
1.00
0.99
0.98
2.05
1.05
1.06
3.00
3.03
7.941
7.925
7.798
7.786
7.771
7.761
7.455
7.446
7.430
7.390
7.376
7.335
7.320
7.177
7.164
7.128
7.115
6.992
6.978
6.971
6.766
6.745
6.732
5.717
2.571
2.325
2.298
2.270
2.243
1.118
0.967

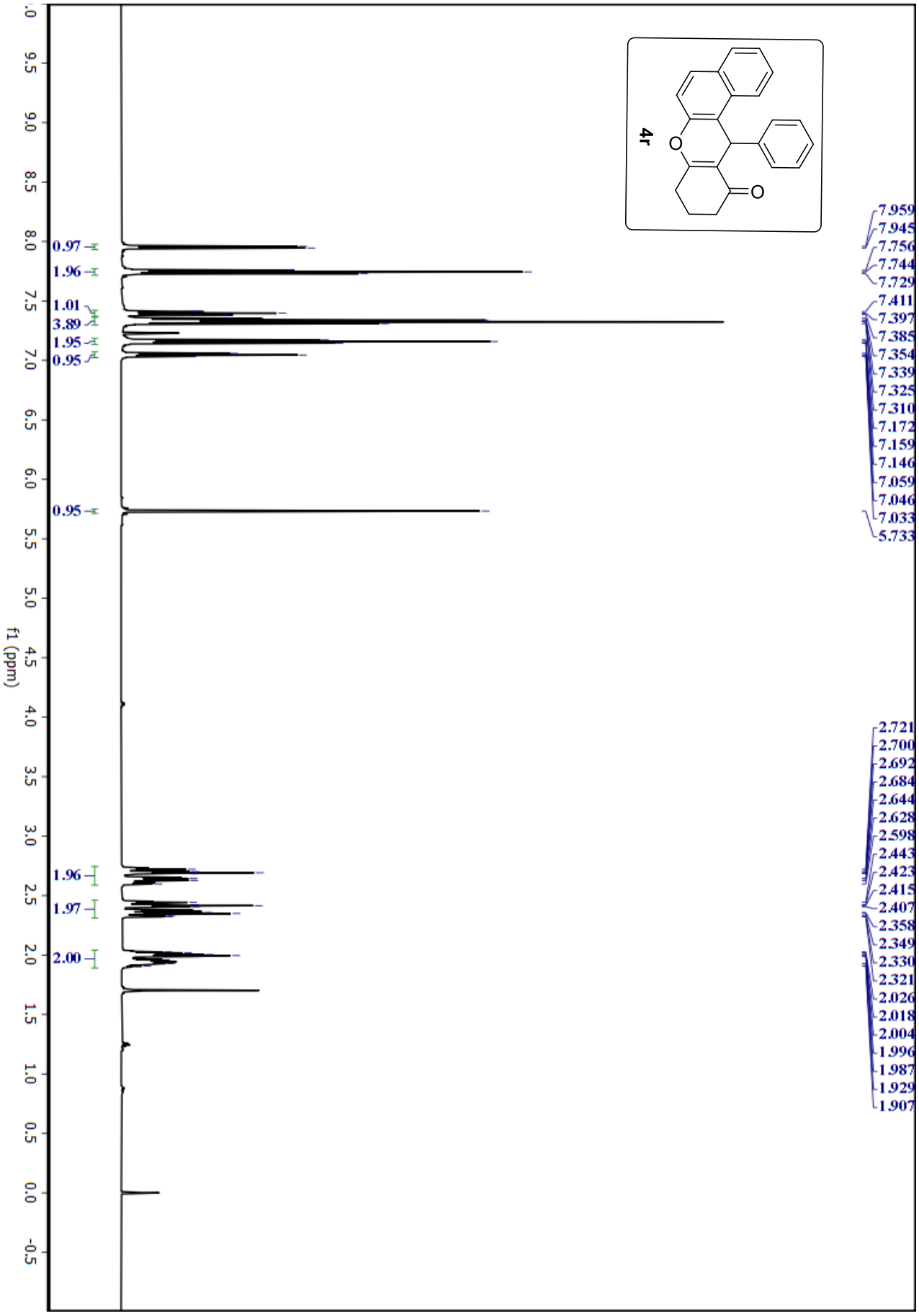

4o
O
O
F
196.79
164.14
162.01
147.77
131.49
131.25
129.56
129.11
128.45
127.10
125.00
124.17
123.46
117.04
115.36
115.21
113.76
113.32
113.18
50.84
41.38
34.43
32.22
29.25
27.11
f1 (ppm)

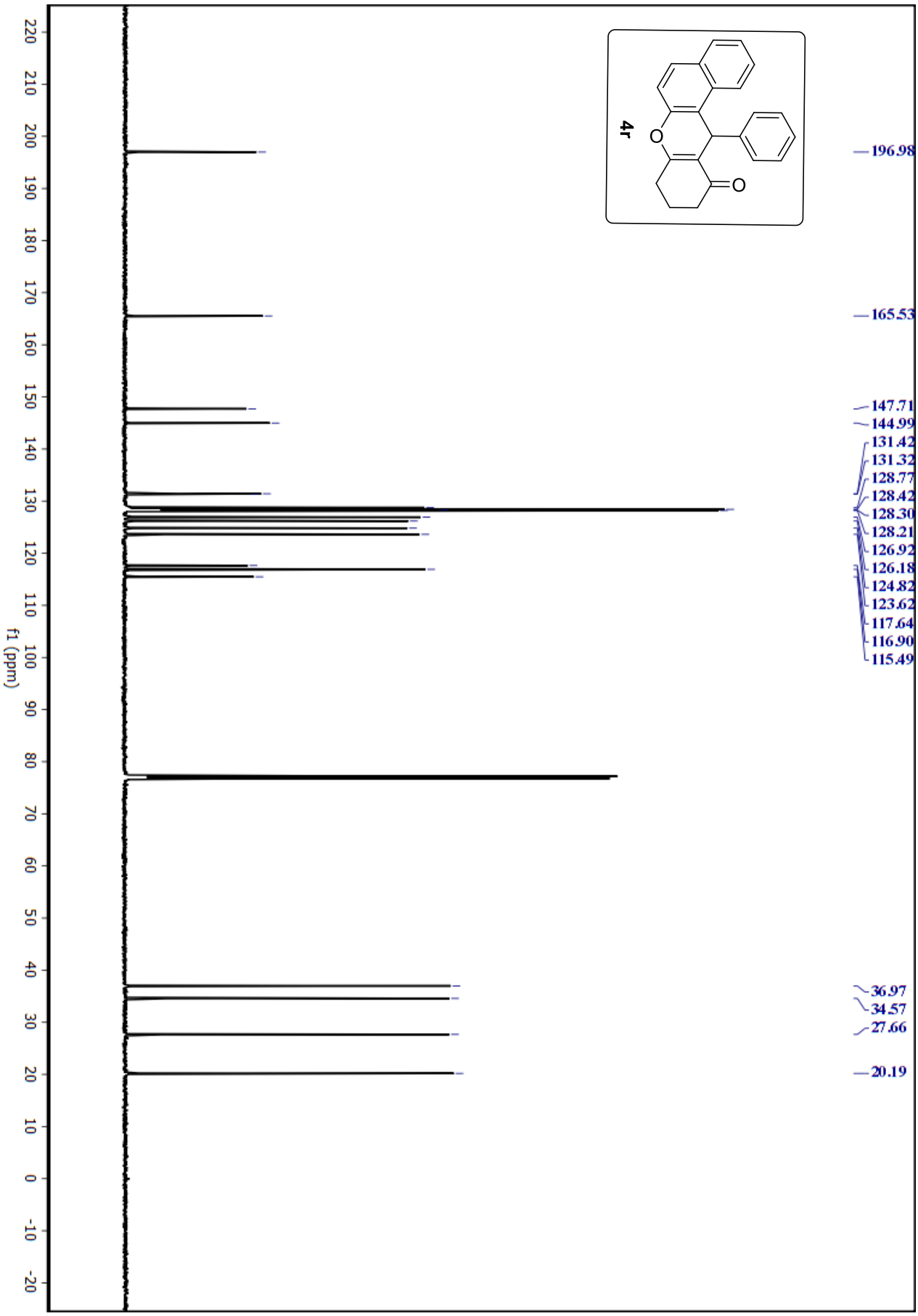

4p
O
O
0.90
1.98
9.01
9.24
0.89
7.950
7.936
7.809
7.794
7.431
7.423
7.416
7.409
7.389
7.374
7.360
7.308
7.183
7.171
7.164
7.158
7.136
7.123
7.111
7.097
7.084
7.065
7.052
6.995
6.982
6.976
6.969
6.963
5.906
f1 (ppm)

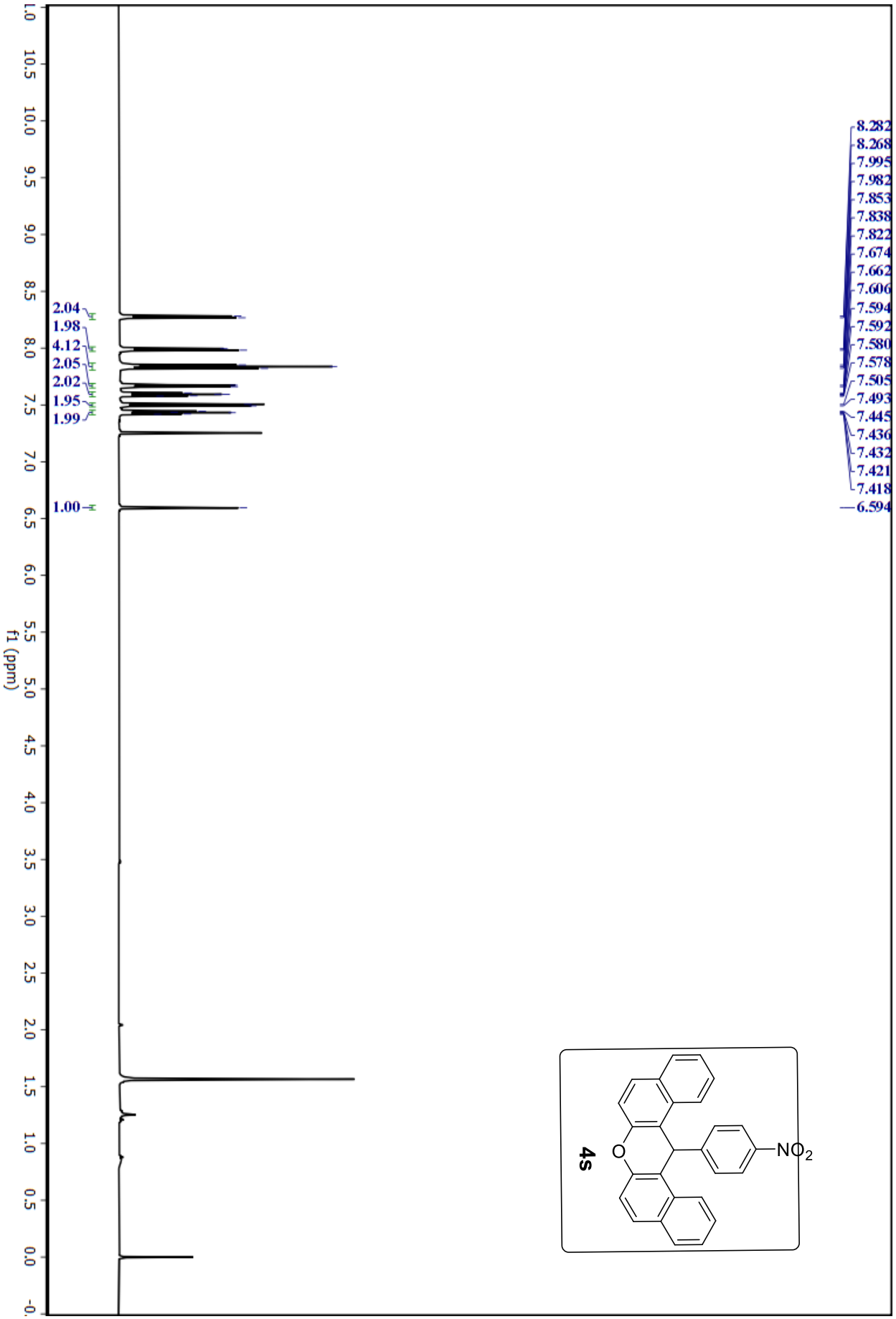

4p
O
O
198.0
154.2
148.7
144.5
138.6
133.8
131.7
131.4
131.2
129.6
129.2
129.0
129.0
128.6
128.5
128.0
127.8
127.6
126.9
126.6
124.6
123.5
117.3
116.3
115.4
41.3
f1 (ppm)

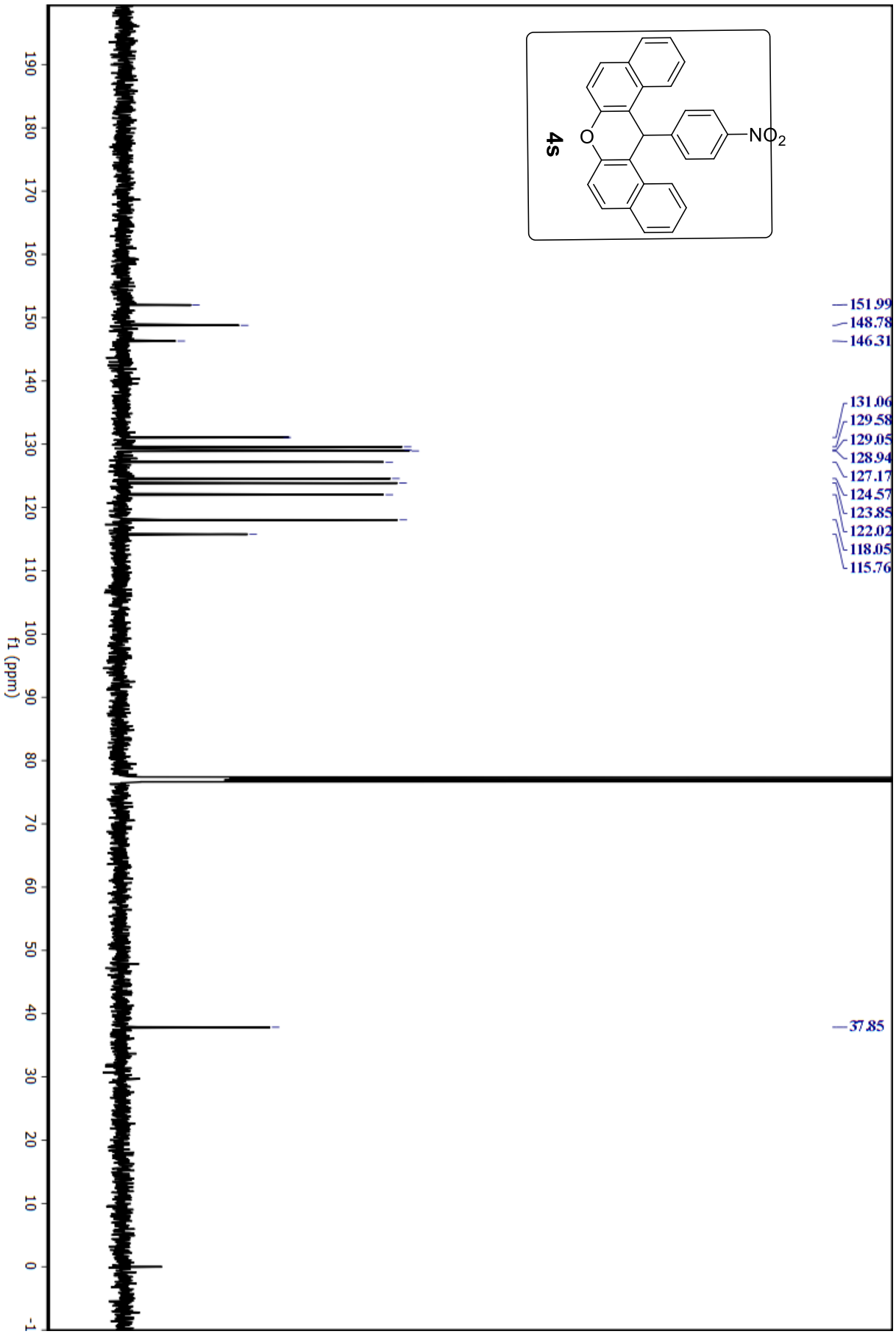

4q
O
Cl
O
0.91
1.92
8.94
5.80
1.87
0.89
7.894
7.880
7.834
7.819
7.462
7.450
7.446
7.436
7.431
7.400
7.391
7.379
7.370
7.367
7.328
7.314
7.165
7.158
7.152
7.147
7.142
7.131
7.119
7.109
7.096
7.088
7.085
7.082
7.079
7.025
7.012
6.999
5.868
f1 (ppm)

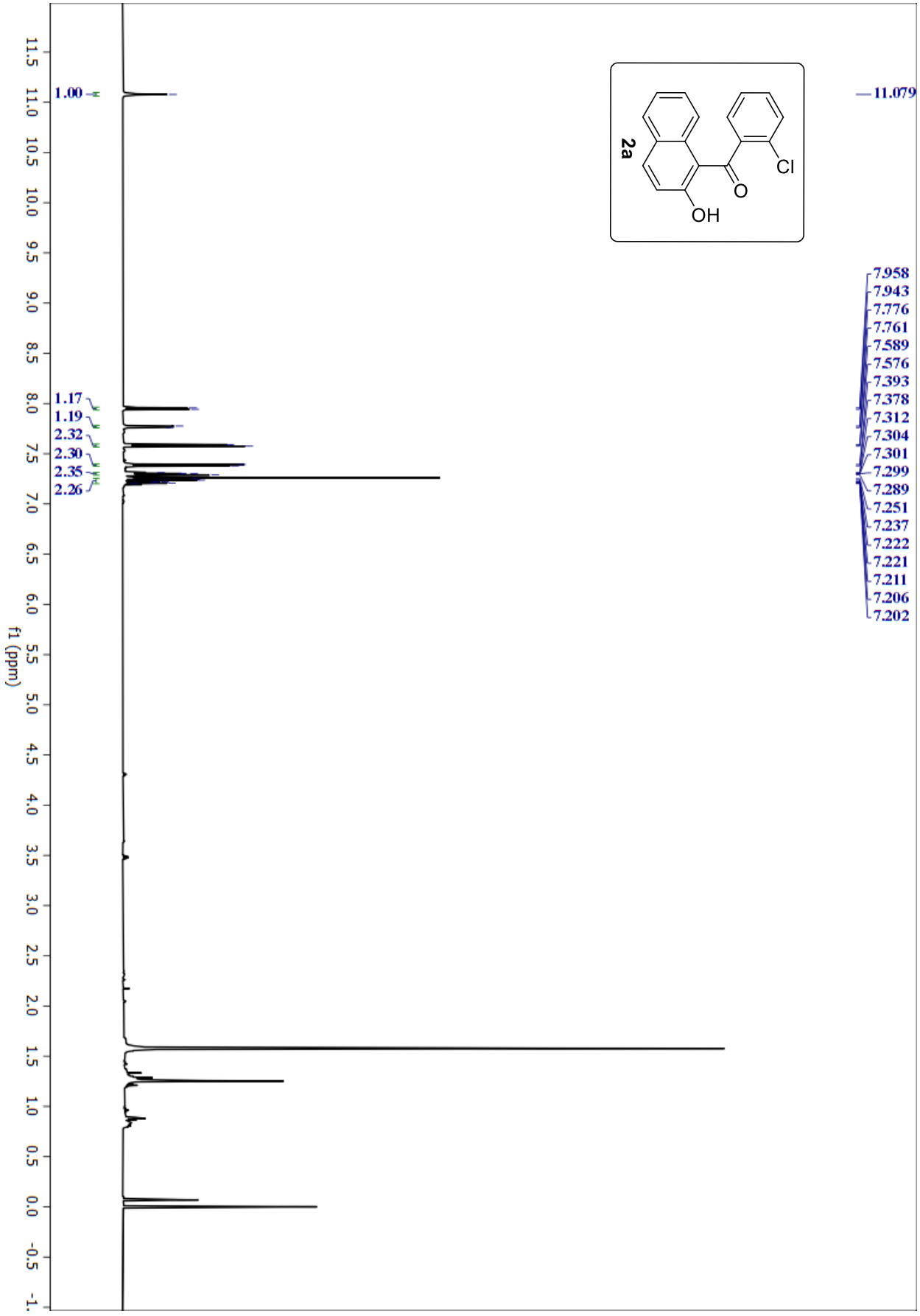

4q
O
Cl
O
197.7
155.4
148.7
143.2
138.5
133.6
132.4
131.8
131.4
131.0
129.9
129.4
129.3
129.2
129.0
128.8
128.6
127.9
127.7
127.1
124.8
123.2
117.3
116.1
114.7
40.5
f1 (ppm)

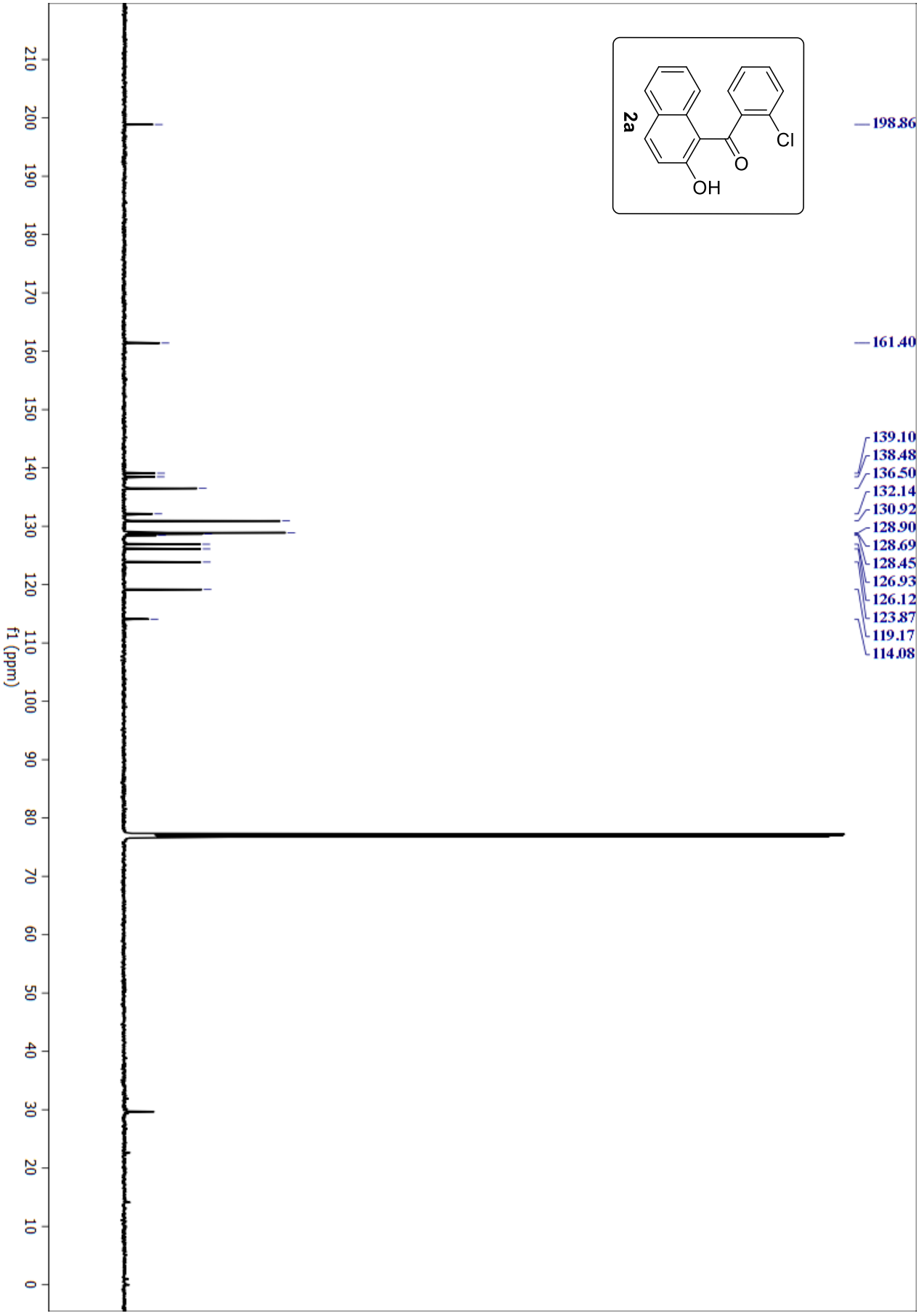

4r
O
O
f1 (ppm)
0.97
1.96
1.01
3.89
1.95
0.95
0.95
1.96
1.97
2.00
7.959
7.945
7.756
7.744
7.729
7.411
7.397
7.385
7.354
7.339
7.325
7.310
7.172
7.159
7.146
7.059
7.046
7.033
5.733
2.721
2.700
2.692
2.684
2.644
2.628
2.598
2.443
2.423
2.415
2.407
2.358
2.349
2.330
2.321
2.026
2.018
2.004
1.996
1.987
1.929
1.907

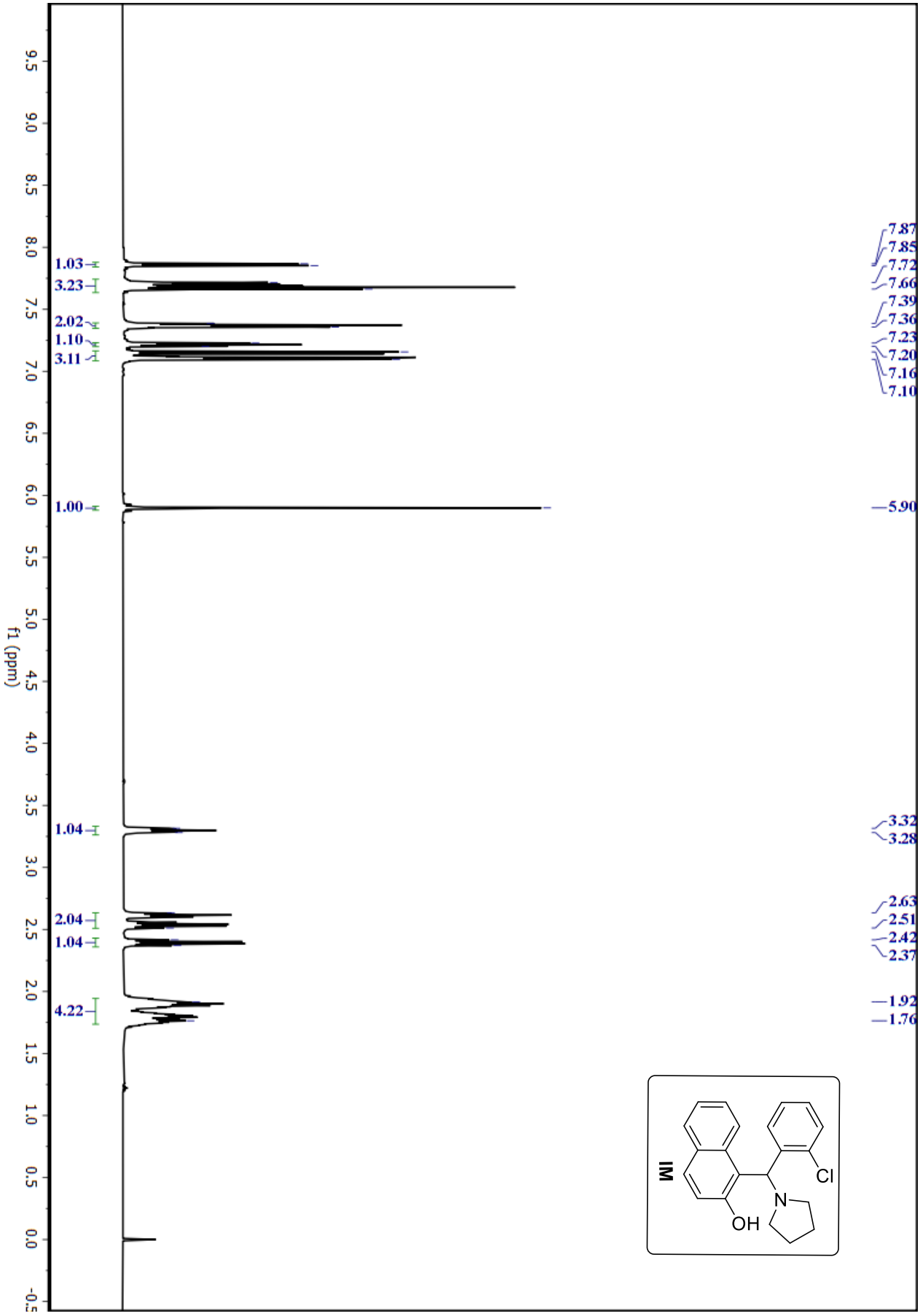

4r
O
O
196.98
165.53
147.71
144.99
131.42
131.32
128.77
128.42
128.30
128.21
126.92
126.18
124.82
123.62
117.64
116.90
115.49
36.97
34.57
27.66
20.19
f1 (ppm)


8.282
8.268
7.995
7.982
7.853
7.838
7.822
7.674
7.662
7.606
7.594
7.592
7.580
7.578
7.505
7.493
7.445
7.436
7.432
7.421
7.418
6.594
2.04
1.98
4.12
2.05
2.02
1.95
1.99
1.00
f1 (ppm)
4s
O
NO2


4s
O
NO2
151.99
148.78
146.31
131.06
129.58
129.05
128.94
127.17
124.57
123.85
122.02
118.05
115.76
37.85
f1 (ppm)


11.079
1.00
1.17
1.19
2.32
2.30
2.35
2.26
7.958
7.943
7.776
7.761
7.589
7.576
7.393
7.378
7.312
7.304
7.301
7.299
7.289
7.251
7.237
7.222
7.221
7.211
7.206
7.202
2a
Cl
O
OH
f1 (ppm)


2a
Cl
O
OH
198.86
161.40
139.10
138.48
136.50
132.14
130.92
128.90
128.69
128.45
126.93
126.12
123.87
119.17
114.08
f1 (ppm)


f1 (ppm)
1.03
3.23
2.02
1.10
3.11
1.00
1.04
2.04
1.04
4.22
7.87
7.85
7.72
7.66
7.39
7.36
7.23
7.20
7.16
7.10
5.90
3.32
3.28
2.63
2.51
2.42
2.37
1.92
1.76
IM
Cl
N
OH

s