Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

NHC/Iron Cooperative Catalysis: Aerobic Oxidative Esterification of Aldehydes with Phenols

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General Remarks

Dioxane was freshly distilled over sodium. All reactions were performed in oven-dried glassware under air or N_2. Preparative thin layer chromatography plates were prepared with silica gel 60 GF254 MercK (Ref. 1.07730.1000). Reaction mixtures were analysed by TLC using ALUGRAM® SIL G/UV254 from MN (Ref. 818133, silica gel 60), and visualisation of TLC spots was effected using UV and $KMnO_4$ solution. NMR spectra were recorded in a Bruker AMX 400 using $CDCl_3$ as solvent and $(CH_3)_4Si$ (1H) as internal standard. All coupling constants are expressed in Hz. Iron sources: $Fe(TfO)_2$ (Solchemar, >99.5 %); carbonyl iron metal powder (Aldrich, 99.5 %, low trace metals). NHC ligands used were prepared following reported procedures: 1,3-bis(*tert*-butyl) imidazolium chloride[1], 1,3-bis(2,6-diisopropylphenyl) imidazolium chloride and 1,3-bis(2,6-diisopropylphenyl) imidazolinium chloride[2], were prepared according to literature procedures, except 1,3-bis(2,4,6-trimethy-phenyl) imidazolinium chloride which was purchased from Aldrich. The aldehydes and phenols were purchased from Aldrich and used without further purification. Potassium *tert*-butoxide was purchased from Aldrich and purified by sublimation prior to use.

Preparation of iron (II) triflate:

To an oven dried round bottom flask previously washed with HNO_3/HCl to remove metal traces, freshly distilled methanol (2 ml) and Fe powder (60 mg, 1.1 mmol) were added under N_2. Then, freshly distilled trifluoromethanesulfonic acid (180 µl, 2 mmol) was slowly added with stirring. The mixture was stirred at room temperature overnight, excess iron filtered out and the solvent removed at reduced pressure. The solvated salt was dried under vacuum at 120 ºC until constant weight. Iron (II) triflate was obtained in approximately quantitative yield and kept stored under N_2

General procedures for oxidative esterification:

[1] Arduengo A. J. III, Dias H. V. R., Harlow R. L., Kline M., *J. Am. Chem. Soc.*, **1992,** *114*, 5530.
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Method A: To a round bottom flask under N_2 were added freshly dried dioxane over sodium (1.5 mL), NHC ligand precursor (20 mol%) and sublimed KO^{t}Bu (0.247 mmol). The mixture was allowed to react at room temperature for 20 min., after which $Fe(TfO)_2$ (20 mol%) was also added. The mixture was left reacting 5 min. at room temperature and then the phenol (0.25 mmol) and the aldehyde (0.25 mmol) were sequentially added. The N_2 atmosphere was removed and the mixture was heated at 90 ºC. Typically, after a reaction time of 24 h the volatiles were removed under reduced pressure and the product isolated by preparative thin layer chromatography (Hexanes:AcOEt).

3b[3], (**3c**, **3d**)[4], (**3e**, **3f**, **3g**, **3n**)[5], **3h**[6], **3i**[7], **3j**[8], **3s**[9].

Method B: To a round bottom flask under N_2 were added freshly dried dioxane over sodium (1.5 mL), NHC ligand precursor (20 mol%) and dried K_2CO_3 (0.247 mmol). The mixture was allowed to react at room temperature for 20 min., after which anhydrous $FeCl_3$ (20 mol%) was also added. The mixture was left reacting 5 min. at room temperature and then the aldehyde (0.25 mmol) and the phenol (0.25 mmol) were sequentially added. The N_2 atmosphere was removed, a drying tube filled with blue silica gel was fitted and the mixture was heated at 90 ºC. Typically, after a reaction time of 24 h the volatiles were removed under reduced pressure and the product isolated by flash column chromatography (Hexanes:AcOEt).

(**3t**, **3v**)[10], **3u**[11], **3v**[12], **3w**[13]

phenyl benzoate (3a)

The title compound was prepared according to method A, in 84% yield.

Yellow crystals, m.p. 69-70 °C; IR (CHCl3): ν 1728 (C=O) cm^{-1}, ν 1077 (C-O) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) 8.19-8.20 (d, 2H), 7.65-7.70 (t, 1H)7.53-7.57 (t, 2H), 7.44-7.50 (t, 2H), 7.29-7.34 (t, 1H), 7.23-7.26 (d, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 165.2, 151.0, 133.6, 130.2, 129.5, 129.6, 128.6, 125.9, 121.7

phenyl 4-chlorobenzoate (3b)

The title compound was prepared according to method A, in 77% yield.

White crystals, m.p. 104-105 °C; IR (CHCl3): ν 1734 (C=O) cm^{-1}, ν 1077 (C-O) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (2H, d, J = 8.4 Hz), 7.52 (2H, d, J = 8.4 Hz), 7.46 (2H, t, J = 7.8 Hz), 7.31 (1H, t, J = 7.8 Hz), 7.23 (2H, d, J = 7.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.8, 140.2, 131.6, 129.6, 129.0, 128.0, 126.1, 121.6.

2-naphtyl 4-methoxybenzoate (3c)

The title compound was prepared according to method A, in 62% yield.

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White crystals, m.p. 107-108 °C; IR ($CHCl_3$): ν 1734 (C=O) cm^{-1}, ν 1070 (C-O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.23 (2H, d, J = 8.8 Hz), 7.92 (1H, d, J = 8.9 Hz), 7.87 (2H, m), 7.71 (1H, d, J = 2.3 Hz), 7.52 (2H, m), 7.38 (1H, dd, J_1 = 8.9 Hz, J_2 = 2.3 Hz), 7.03 (2H, d, J = 8.8 Hz), 3.94 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 164.0, 148.7, 133.9, 132.4, 131.5, 129.4, 127.8, 127.7, 126.5, 125.6, 121.9, 121.4, 118.8, 113.9, 55.6.

phenyl 4-bromobenzoate (3d)

The title compound was prepared according to method A, in 59% yield.

White crystals, m.p. 104-105 °C; IR ($CHCl_3$): ν 1727 (C=O) cm^{-1}, ν 1076 (C-O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.09 (2H, d, J = 8.4 Hz), 7.68 (2H, d, J = 8.4 Hz), 7.46 (2H, t, J = 7.8 Hz), 7.31 (1H, t, J = 7.8 Hz), 7.23 (2H, d, J = 7.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 150.8, 132.0, 131.7, 129.6, 128.9, 128.5, 126.1, 121.6.

phenyl 4-fluorobenzoate (3e)

The title compound was prepared according to method A, in 82% yield.

White crystals, m.p. 59-60 °C; IR ($CHCl_3$): ν 1721 (C=O) cm^{-1}, ν 1064 (C-O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.25 (2H, dd, J_{HH} = 8.7 Hz, J_{HF} = 5.6 Hz), 7.46 (2H, t, J = 7.8 Hz), 7.31 (1H, t, J = 7.8 Hz), 7.23 (2H, d, J = 7.8 Hz), 7.21 (2H, t, J_{HH} = J_{HF} = 8.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2 (d, J_{CF} = 255.4 Hz), 164.3, 150.8, 132.8 (d, J_{CF} = 9.7 Hz), 129.6, 126.0, 125.8 (d, J_{CF} = 2.8 Hz), 121.7, 115.8 (d, J_{CF} = 22.1 Hz).

phenyl 4-cyanobenzoate (3f)

The title compound was prepared according to method A, in 55% yield.

Brown crystals, m.p. 165-166 °C; IR ($CHCl_3$): ν 1728 (C=O) cm^{-1}, ν 1070 (C-O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.34 (2H, d, J = 7.8 Hz), 7.85 (2H, d, J = 7.8 Hz), 7.48 (2H, t, J = 7.8 Hz), 7.33 (1H, t, J = 7.8 Hz), 7.24 (2H, d, J = 7.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 150.5, 133.4, 132.4, 130.7, 129.7, 126.4, 121.5, 117.9, 117.0.

phenyl 4-methylbenzoate (3g)

The title compound was prepared according to method A, in 85% yield.

White crystals, m.p. 76-77 °C; IR ($CHCl_3$): ν 1727 (C=O) cm^{-1}, ν 1077 (C-O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.15 (2H, d, J = 8.1 Hz), 7.47 (2H, t, J = 7.8 Hz), 7.35 (2H, d, J = 8.1 Hz), 7.31 (1H, t, J = 7.8 Hz), 7.26 (2H, d, J = 7.8 Hz), 1.55 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 151.1, 144.5, 130.3, 129.5, 129.3, 126.8, 125.8, 121.8, 21.8.

phenyl 2-naphthenate (3h)

The title compound was prepared according to method A, in 89% yield.

White crystals, m.p. 94-95 °C; IR ($CHCl_3$): ν 1728 (C=O) cm^{-1}, ν 1077 (C-O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.8 (1H, s), 8.24 (1H, d, J = 8.6 Hz), 8.04 (1H, d, J = 8.1 Hz), 7.98 (1H, d, J = 8.8 Hz), 7.95

(1H, d, J = 8.6 Hz), 7.64 (2H, m), 7.50 (2H, t, J = 7.4 Hz), 7.32 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 148.6, 133.8, 133.7, 131.5, 130.2, 129.6, 129.5, 128.6, 127.8, 127.7, 126.6, 125.8, 121.3, 118.7.

2-naphtyl benzoate (3i)

The title compound was prepared according to method A, in 83% yield.

White crystals, m.p. 108-109 °C; IR ($CHCl_3$): ν 1734 (C=O) cm^{-1}, ν 1051 (C-O) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (2H, d, J = 8.2 Hz), 7.96 (1H, d, J = 9.0 Hz), 7.91 (2H, m), 7.76 (1H, d, J = 2.3 Hz), 7.70 (1H, t, J = 7.5 Hz), 7.59 (2H, d, J = 7.9 Hz), 7.57-7.53 (2H, m), 7.43 (1H, dd, J_1 = 8.8 Hz, J_2 = 2.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 151.1, 135.8, 132.5, 132.0, 129.6, 129.5, 128.7, 128.4, 127.9, 126.9, 126.8, 126.0, 125.5, 121.8.

4-methylphenyl 4-bromobenzoate (3j)

The title compound was prepared according to method A, in 65% yield.

white crystals, m.p. 118-119 °C; IR ($CHCl_3$): ν 1727 (C=O) cm^{-1}, ν 1077 (C-O) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (2H, d, J = 8.3 Hz), 7.67 (2H, d, J = 8.3 Hz), 7.25 (2H, d, J = 8.2 Hz), 7.10 (2H, d, J = 8.2 Hz), 2.40 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 148.5, 135.7, 131.9, 131.7, 130.1, 128.7, 128.6, 121.3, 21.0.

4-chlorophenyl benzoate (3k)

The title compound was prepared according to method A, in 82% yield.

White crystals, m.p. 86-88 °C; IR ($CHCl_3$): ν 1734 (C=O) cm^{-1}, ν 1058 (C-O) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (2H, d, J = 8.0 Hz), 7.68 (1H, t, J = 7.4 Hz), 7.55 (2H, t, J = 7.6 Hz), 7.42 (2H, d, J = 8.8 Hz), 7.19 (2H, d, J = 8.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 149.4, 133.8, 131.3, 130.2, 129.6, 129.2, 128.7, 123.1.

4-nitrophenyl benzoate (3l)

The title compound was prepared according to method A, in 88% yield.

Pale Yellow crystals, m.p. 129-130 °C; IR ($CHCl_3$): ν 1741 (C=O) cm^{-1}, ν 1058 (C-O) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (2H, d, J = 9.1 Hz), 8.23 (2H, d, J = 8.0 Hz), 7.71 (1H, t, J = 7.5 Hz), 7.57 (2H, t, J = 7.7 Hz), 7.45 (2H, d, J = 9.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 155.7, 145.4, 134.3, 130.3, 128.8, 128.5, 125.3, 122.7.

2,4-dichlorophenyl benzoate (3m)

The title compound was prepared according to method A, in 51% yield.

White crystals, m.p. 91-92 °C; IR ($CHCl_3$): ν 1740 (C=O) cm^{-1}, ν 1050 (C-O) cm^{-1}, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (2H, d, J = 7.8 Hz), 7.69 (1H, t, J = 7.4 Hz), 7.55 (2H, t, J = 7.7 Hz), 7.52 (1H, d, J = 2.4 Hz), 7.33 (1H, dd, J_1 = 8.7 Hz, J_2 = 2.4 Hz), 7.25 (1H, d, J = 9.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 146.0, 134.1, 132.0, 130.4, 130.2, 128.7, 128.5, 128.0, 124.7.

4-fluorophenyl benzoate (3n)

The title compound was prepared according to method A, in 86% yield.

White crystals, m.p. 55-56 °C; IR ($CHCl_3$): ν 1734 (C=O) cm^{-1}, ν 1050 (C-O) cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$) δ 8.22 (2H, d, J = 7.6 Hz), 7.67 (1H, t, J = 7.4 Hz), 7.54 (2H, t, J = 7.7 Hz), 7.21 (2H, dd, J_{HH} = 9.1 Hz, J_{HF} = 4.6 Hz)), 7.14 (2H, t, J_{HH} = J_{HF} = 8.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 160.3 (d, J_{CF} = 244.2 Hz), 146.8 (d, J_{CF} = 2.9 Hz), 133.8, 130.2, 129.3, 128.6, 123.1 (d, J_{CF} = 8.5 Hz), 116.2 (d, J_{CF} = 23.5 Hz).

4-bromophenyl benzoate (3o)

The title compound was prepared according to method A, in 87% yield.

White crystals, m.p. 103-105 °C; IR ($CHCl_3$): ν 1728 (C=O) cm^{-1}, ν 1058 (C-O) cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$) δ 8.22 (2H, d, J = 7.7 Hz), 7.68 (1H, t, J = 7.1 Hz), 7.57 (2H, d, J = 8.0 Hz), 7.54 (2H, t, J = 7.3 Hz), 7.14 (2H, d, J = 8.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 150.0, 133.8, 132.6, 130.2, 129.2, 128.7, 123.6, 119.0.

4-(trifluoromethyl)-phenyl benzoate (3p)

The title compound was prepared according to method A, in 81% yield.

White solid, m.p. 107-108.5 °C; IR ($CHCl_3$): ν 1734 (C=O) cm^{-1}, ν 1058 (C-O) cm^{-1}, ^1H NMR (400 MHz, $CDCl_3$) δ 8.24 (2H, d, J = 7.4 Hz), 7.74 (2H, d, J = 8.4 Hz), 7.70 (1H, t, J = 7.4 Hz), 7.56 (2H, t, J = 7.7 Hz), 7.38 (2H, d, J = 8.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 153.5, 134.0, 130.3, 129.0, 128.7, 128.0, 126.9 (q, J_{CF} = 3.7 Hz), 122.3.

phenyl 2-chlorobenzoate (3q)

The title compound was prepared according to method A, in 15% yield.

White crystals, IR ($CHCl_3$): ν 1740 (C=O) cm^{-1}, ν 1032 (C-O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.07 (1H, dd, J_1 = 7.7 Hz, J_2 = 1.3 Hz), 7.63-7.38 (5H, m), 7.32 (1H, J = 7.6 Hz), 7.27 (2H, J = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 150.7, 134.4, 133.2, 131.9, 131.4, 129.6, 129.4, 126.8, 126.1, 121.6.

4-cyanophenyl benzoate (3r)

The title compound was prepared according to method A, in 86% yield.

White crystals, m.p. 90-92 °C; IR ($CHCl_3$): ν 1741 (C=O) cm^{-1}, ν 1064 (C-O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.22 (2H, d, J = 8.0 Hz), 7.78 (2H, d, J = 8.4 Hz), 7.70 (1H, t, J = 6.9 Hz), 7.56 (2H, t, J = 7.6 Hz), 7.40 (2H, d, J = 8.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 154.3, 134.2, 133.8, 130.3, 128.8, 128.6, 123.0, 118.3, 109.8.

4-fluorophenyl cyclohexanecarboxylate (3s)

The title compound was prepared according to method A, in 32% yield.

White crystals, m.p. 195-196 °C; IR ($CHCl_3$): ν 1753 (C=O) cm^{-1}, ν 1121 (C-O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.10-7.02 (4H, m), 2.57 (1H, tt, J_1 = 11.2 Hz, J_2 = 3.6 Hz), 2.07 (2H, d, J = 11.0 Hz), 1.87-1.81 (2H, m), 1.74-1.70 (1H, m), 1.65-1.55 (2H, m), 1.43-1.28 (3H, m); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 174.6, 160.1 (d, J_{CF} = 242.5 Hz), 146.7 (d, J_{CF} = 2.8 Hz), 122.9 (d, J_{CF} = 8.5 Hz), 116.0 (d, J_{CF} = 23.3 Hz), 43.1, 28.9, 25.7, 25.4.

Phenyl cynnamate (3t)

The title compound was prepared according to method A, in 46% yield, or method B, in 89% yield.

White crystals, m.p. 74.5-75.5 °C; IR ($CHCl_3$): ν 1728 (C=O) cm^{-1}, ν 1638 (C=C) cm^{-1}, ν 1140 (C-O) cm^{-1} ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (1H, d, *J* = 16.0 Hz), 7.62 (2H, m), 7.47-7.43 (5H, m), 7.29 (1H, t, *J* = 7.6 Hz), 7.21 (2H, d, *J* = 8.0 Hz), 6.68 (1H, d, *J* = 16.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 150.8, 146.6, 134.2, 130.7, 129.5, 129.0, 128.3, 125.8, 121.7, 117.3.

Phenyl 4-methoxycynnamate (3u)

The title compound was prepared according to method B, in 55% yield.

White crystals, m.p. 74-75 °C; IR ($CHCl_3$): ν 1721 (C=O) cm^{-1}, ν 1600 (C=C) cm^{-1}, ν 1140 (C-O) cm^{-1} ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (1H, d, J = 15.9 Hz), 7.48 (2H, d, J = 8.8 Hz), 7.34 (2H, t, J = 7.9 Hz), 7.18 (2H, t, J = 7.4 Hz), 7.10 (2H, d, J = 7.5 Hz), 6.87 (2H, d, J = 8.8 Hz), 6.43 (1H, d, J = 15.9 Hz), 3.79 (3H, s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 161.8, 151.0, 146.4, 130.2, 129.6, 127.0, 125.8, 121.8, 114.8, 114.6, 55.6.

4-Bromophenyl cynnamate (3v)

The title compound was prepared according to method B, in 87% yield.

Colorless solid, m.p. 104-105.5 °C; IR ($CHCl_3$): ν 1734 (C=O) cm^{-1}, ν 1593 (C=C) cm^{-1}, ν 1141 (C-O) cm^{-1} ; ^{1}H NMR (400 MHz, $CDCl_3$) δ ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (1H, d, *J* = 16 Hz), 7.57-7.62 (2H, m), 7.43 (2H, d, J= 8.8 Hz), 7.25 – 7.38 (3H m), 7.06 (2H, d, J = 8.9 Hz), 6.60 (1H, d, *J* = 16.0 Hz); ^{13}C NMR (100 MHz, CDCl3), δ (ppm): 117.1, 119.1, 123.7, 128.6, 129.3, 131.1, 132.7, 134.3, 147.3,150.1, 165.3.

4-Chlorophenyl cynnamate (3w)

The title compound was prepared according to method B, in 73% yield.

White crystals, m.p. 99.5-101 °C; IR ($CHCl_3$): ν 1741 (C=O) cm^{-1}, ν 1632 (C=C) cm^{-1}, ν 1134 (C-O) cm^{-1} ; ^{1}H NMR (400 MHz, $CDCl_3$) δ ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (1H, d, *J* = 16.0 Hz), 7.64 – 7.55 (2H m), 7.48 – 7.40 (3H, m), 7.37 (2H, d, *J* = 8.8 Hz), 7.13 (2H, d, *J* = 8.8 Hz), 6.62 (1H, d, *J* = 16.0 Hz). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 149.4, 147.2, 134.2, 131.3, 131.0, 129.6, 129.2, 128.5, 123.2, 117.0.

4-Chlorophenyl 4-methoxycynnamate (3x)

The title compound was prepared according to method B, in 71% yield.

White crystals, m.p. 99-100 °C; IR ($CHCl_3$): ν 1728 (C=O) cm^{-1}, ν 1600 (C=C) cm^{-1}, ν 1141 (C-O) cm^{-1} ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (1H, d, J = 15.9 Hz), 7.54 (2H, d, J = 8.2 Hz), 7.36 (2H, d, J = 8.2 Hz), 7.11 (2H, d, J = 8.2 Hz), 6.94 (2H, d, J = 8.2 Hz), 6.48 (1H, d, J = 15.9 Hz), 3.86 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 162.0, 149.5, 146.8, 131.1, 130.2, 129.6, 126.9, 123.2, 114.6, 114.3, 55.6.

4-Fluorophenyl cynnamate (3y)

The title compound was prepared according to method B, in 90% yield.

White crystals, m.p. 73-74.5 °C; IR ($CHCl_3$): ν 1728 (C=O) cm^{-1}, ν 1638 (C=C) cm^{-1}, ν 1153 (C-O) cm^{-1} ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (1H, d, J = 16.0 Hz), 7.63-7.56 (2H, m), 7.47-7.38 (3H, m), 7.18-7.05 (4H, m), 6.62 (1H, d, J = 16.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 160.4 (d, J_{CF} = 244.2 Hz), 147.0, 146.7 (d, J_{CF} = 2.9 Hz), 134.2, 131.0, 129.2, 128.5, 123.2 (d, J_{CF} = 8.5 Hz), 117.1, 116.2 (d, J_{CF} = 23.4 Hz).

3-Methylphenyl cynnamate (3z)

The title compound was prepared according to method B, in 84% yield.

Yellow crystals, m.p. 53.5-55 °C; IR ($CHCl_3$): ν 1728 (C=O) cm^{-1}, ν 1632 (C=C) cm^{-1}, ν 1150 (C-O) cm^{-1} ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (1H, d, J = 16.0 Hz), 7.57 – 7.46 (2H, m), 7.40 – 7.33 (3H, m), 7.22 (1H, t, J = 7.8 Hz), 7.00 (1H, d, J = 7.5 Hz), 6.95-6.86 (2H, m), 6.56 (1H, d, J = 16.0 Hz), 2.31 (3H, s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 150.8, 146.6, 139.8, 134.3, 130.8, 129.3, 129.1, 128.4, 126.8, 122.4, 118.7, 117.5, 21.5.

Computational details

All calculations were performed using the GAUSSIAN 03 software package,[14] and the PBE1PBE functional, without symmetry constraints. That functional uses a hybrid generalized gradient approximation (GGA), including 25 % mixture of Hartree-Fock[15] exchange with DFT[16] exchange-correlation, given by Perdew, Burke and Ernzerhof functional (PBE).[17] The optimized geometries were obtained with a standard 6-31G(d,p) basis set.[18] Frequency calculations were performed confirming the stationary points as minima. The energy values reported result from single point calculations using a standard 6-311++G(d,p) basis set[19] and the geometries optimized at the PBE1PBE/6-31G(d,p) level. Solvent (1,4-dioxane) effects were considered in the PBE1PBE/6-311++G(d,p)//PBE1PBE/6-31G(d,p)

[14] *Gaussian 03*, Revision C.02, 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.; 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.; Pople, J. A. Gaussian, Inc., Wallingford CT, 2004.

[15] Hehre, W. J.; Radom, L.; Schleyer, P. v.R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*, John Wiley & Sons, NY, 1986.

[16] Parr, R. G.; Yang, W. in *Density Functional Theory of Atoms and Molecules*; Oxford University Press: New York, **1989.**

[17] (a) Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.* **1997**, *78*, 1396. (b) Perdew, J. P. *Phys. Rev. B* **1986**, *33*, 8822.

[18] (a) Ditchfield, R.; Hehre W. J.; Pople, J. A. *J. Chem. Phys.* **1971**, *54*, 724. (b) Hehre, W. J.; Ditchfield R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257. (c) Hariharan, P. C.; Pople, J. A. *Mol. Phys.* **1974**, *27*, 209. (d) Gordon, M. S. *Chem. Phys. Lett.* **1980**, *76*, 163. (e) Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta* **1973**, *28*, 213.

[19] (a) McClean, A. D.; Chandler, G. S. *J. Chem. Phys.* **1980**, *72*, 5639. (b) Krishnan, R.; Binkley, J. S.; Seeger, R. Pople, J. A. *J. Chem. Phys.* **1980**, *72*, 650.(c) Wachters, A. J. H. *J. Chem. Phys.* **1970**, *52*, 1033. (d) Hay, P. J. *J. Chem. Phys.* **1977**, *66*, 4377. (e) Raghavachari, K.; Trucks, G. W. *J. Chem. Phys.* **1989**, *91*, 1062. (f) Binning Jr., R. C.; Curtiss, L. A. *J. Comp. Chem.*, **1990**, *11*, 1206. (g) McGrath, M. P.; Radom, L. *J. Chem. Phys.* **1991**, *94*, 511. (h) Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. v. R. *J. Comp. Chem.* **1983**, *4*, 294. (i) Frisch, M. J.; Pople, J. A.; Binkley, J. S. *J. Chem. Phys.* **1984**, *80*, 3265.

energy calculations using the Polarizable Continuum Model (PCM) initially devised by Tomasi and coworkers[20] as implemented on Gaussian 03.[21] The molecular cavity was based on the united atom topological model applied on UAHF radii, optimized for the HF/6-31G(d) level. The parameters used for 1,4-dioxane were: $\varepsilon = 2.2094$, $\varepsilon_\infty = 2.0232$, r = 2.53 Å, $\rho = 1.0337$.

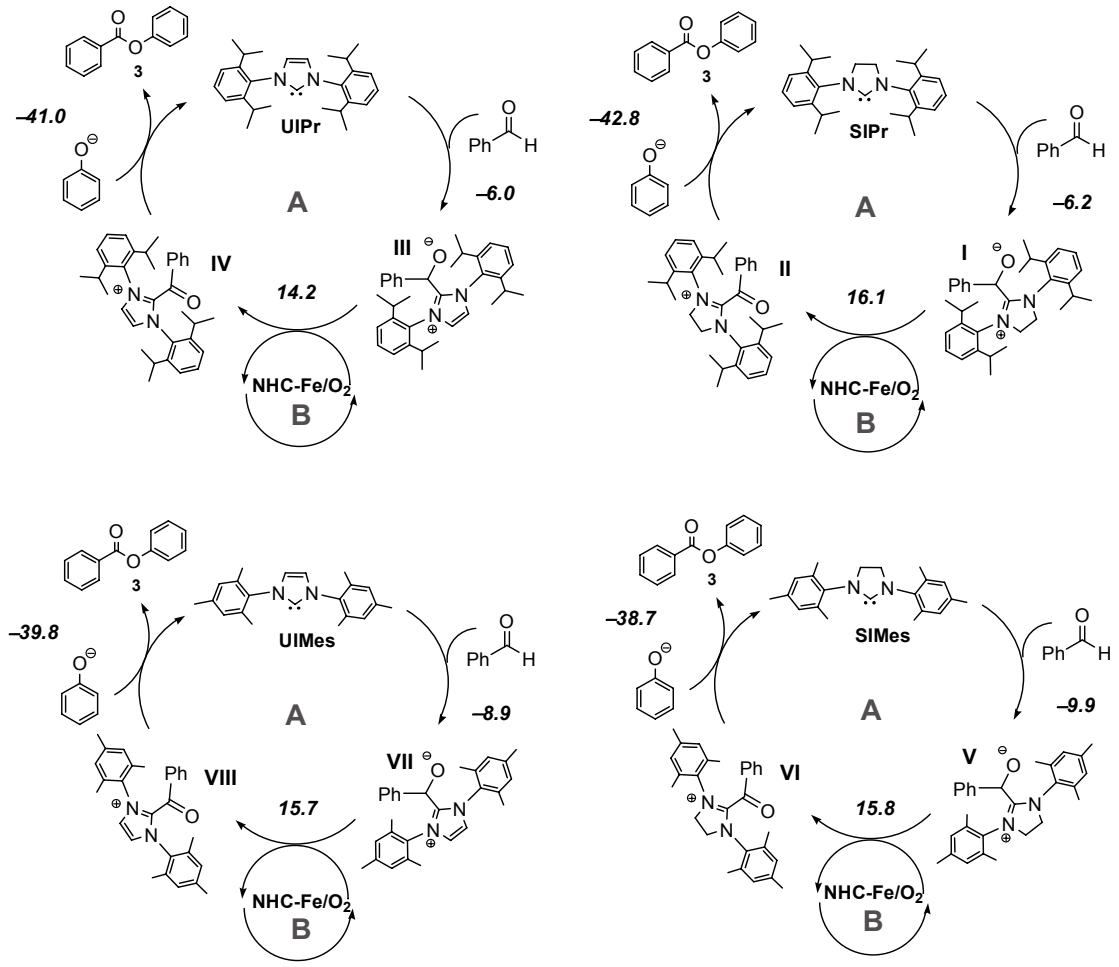
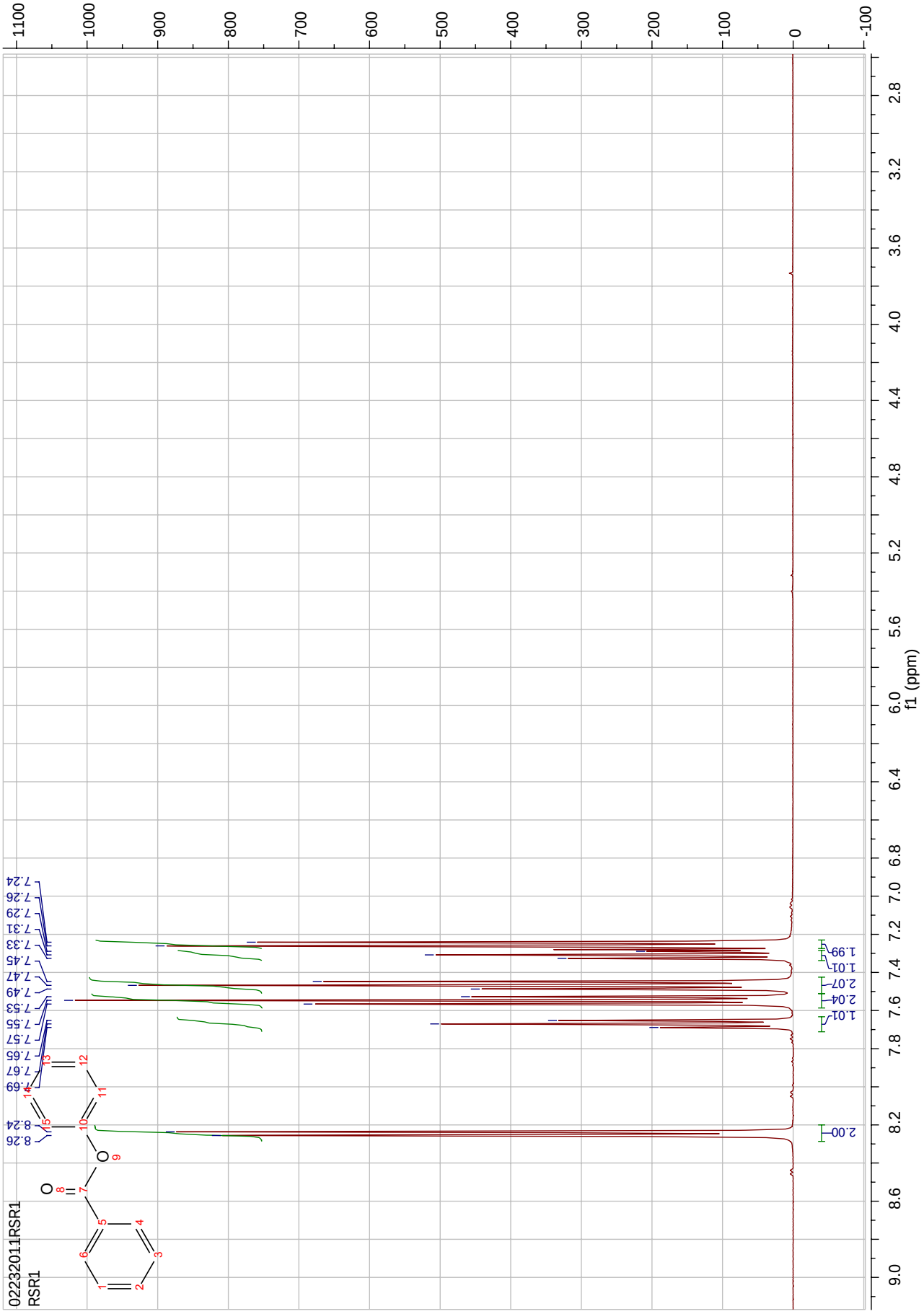


Figure S1. Energy balance (kcal/mol, italics) calculated for the catalytic cycles with NHC from precursors **4** (top left), **5** (top right), **8** (bottom left) and **9** (bottom right).

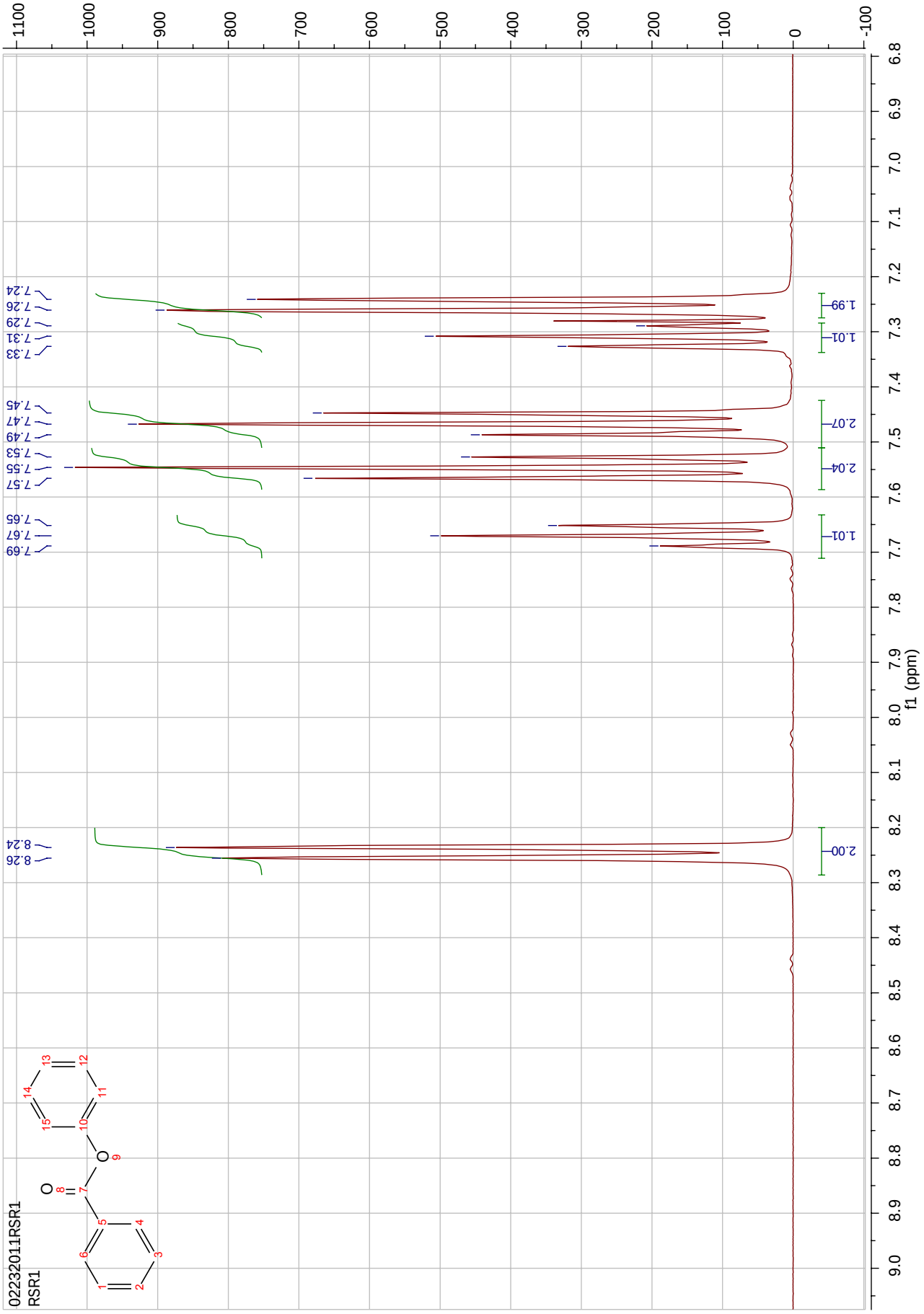
[20] (a) Cancès, M. T.; Mennucci, B.; Tomasi, J. *J. Chem. Phys.* **1997**, *107*, 3032. (b) Cossi, M.; Barone, V.; Mennucci, B.; Tomasi, J. *Chem. Phys. Lett.* **1998**, *286*, 253. (c) Mennucci B.; Tomasi, J. *J. Chem. Phys.* **1997**, *106*, 5151.

[21] (a) Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999. (b) Cossi, M.; Scalmani, G.; Rega, N.; Barone, V. *J. Chem. Phys.* **2002**, *117*, 43.

Appendix A - Spectra



Appendix A - Spectra



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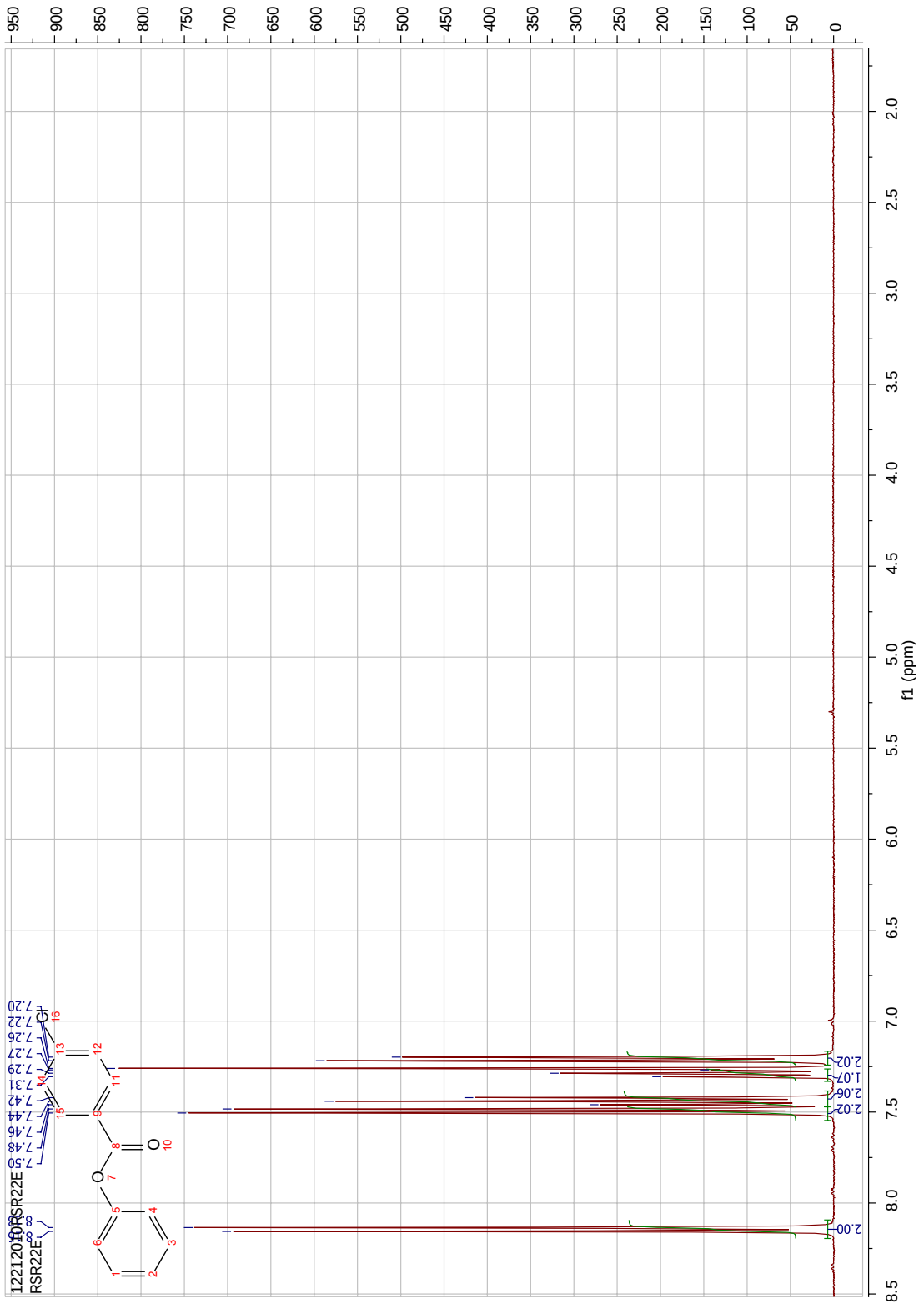

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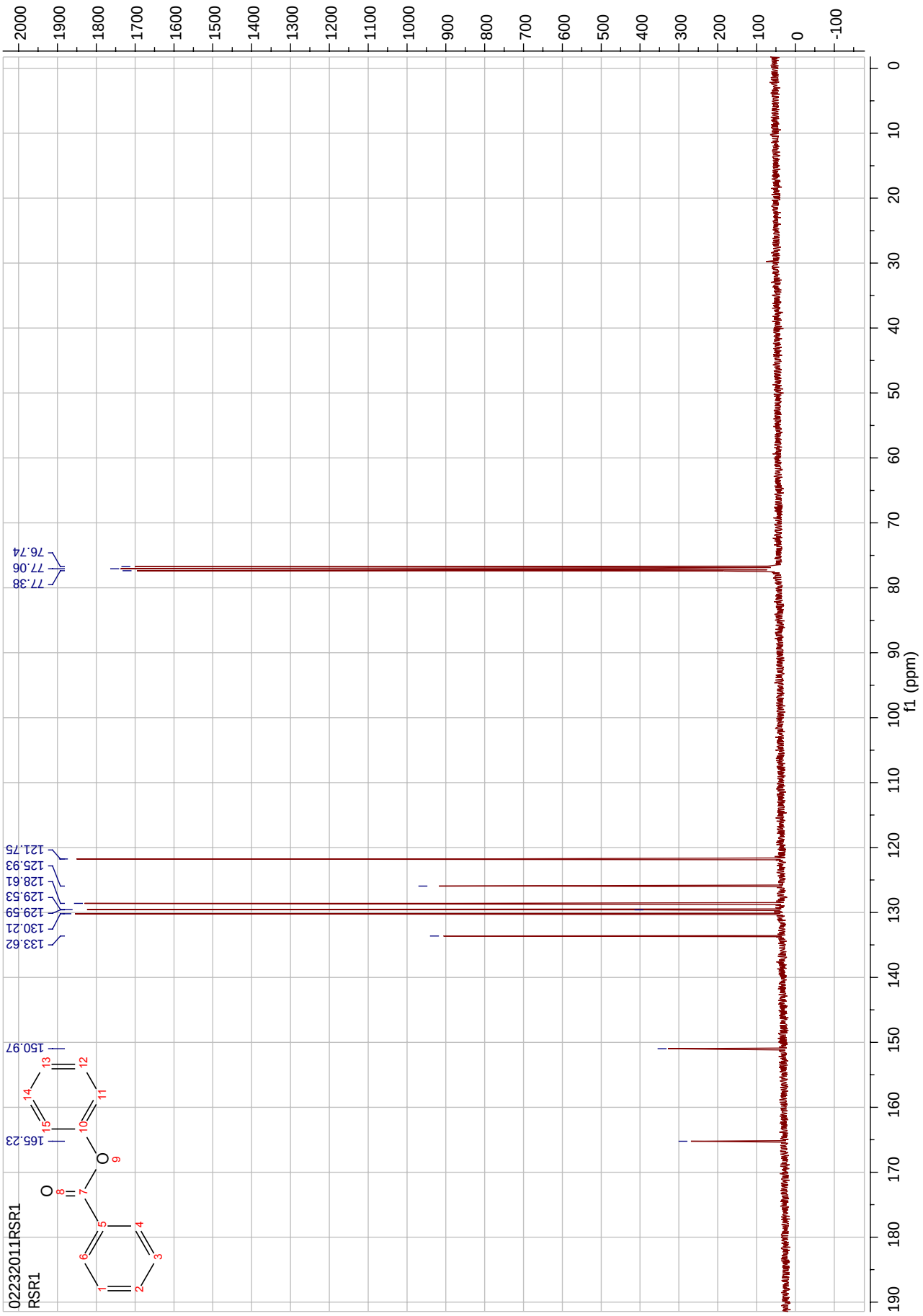
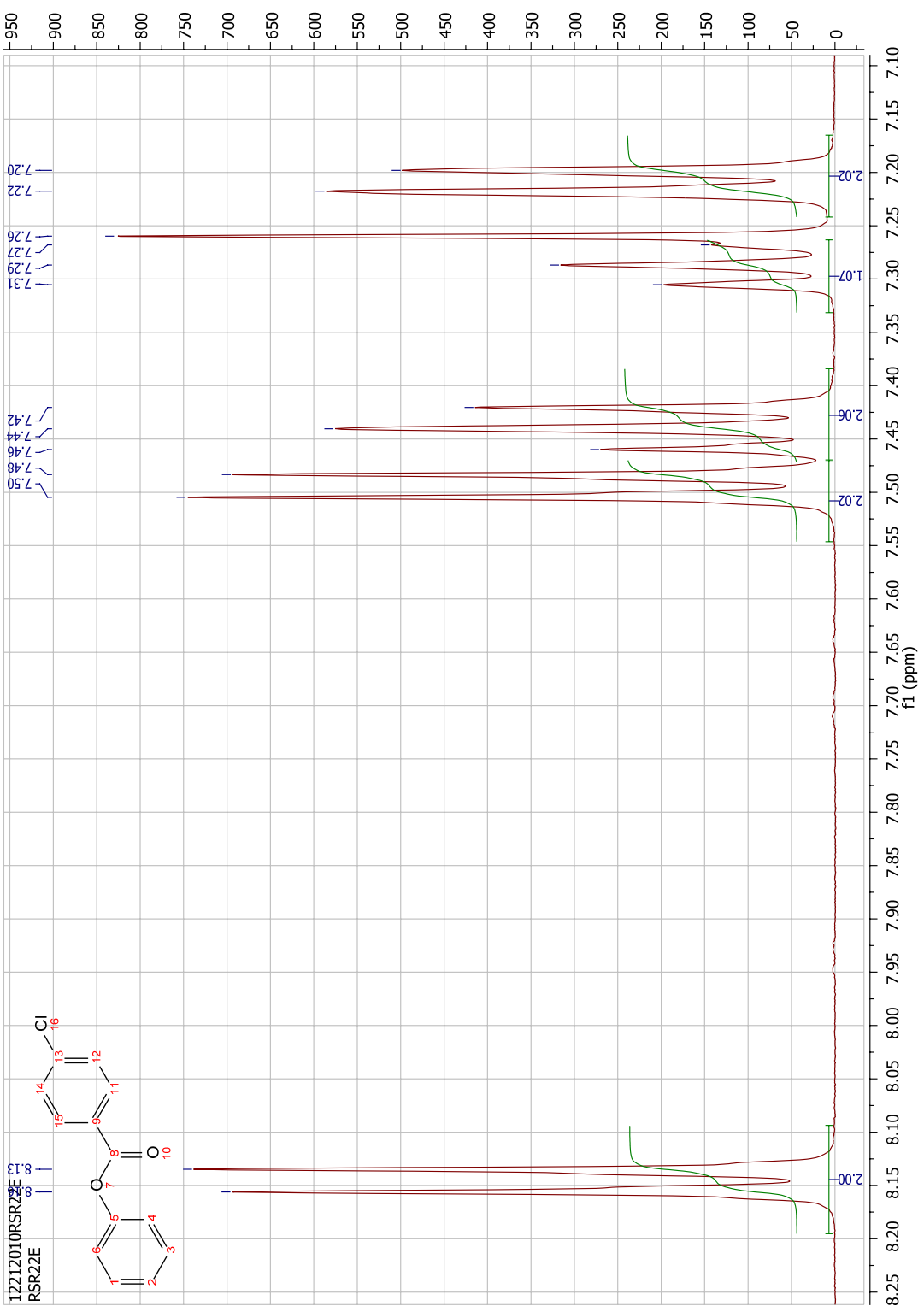
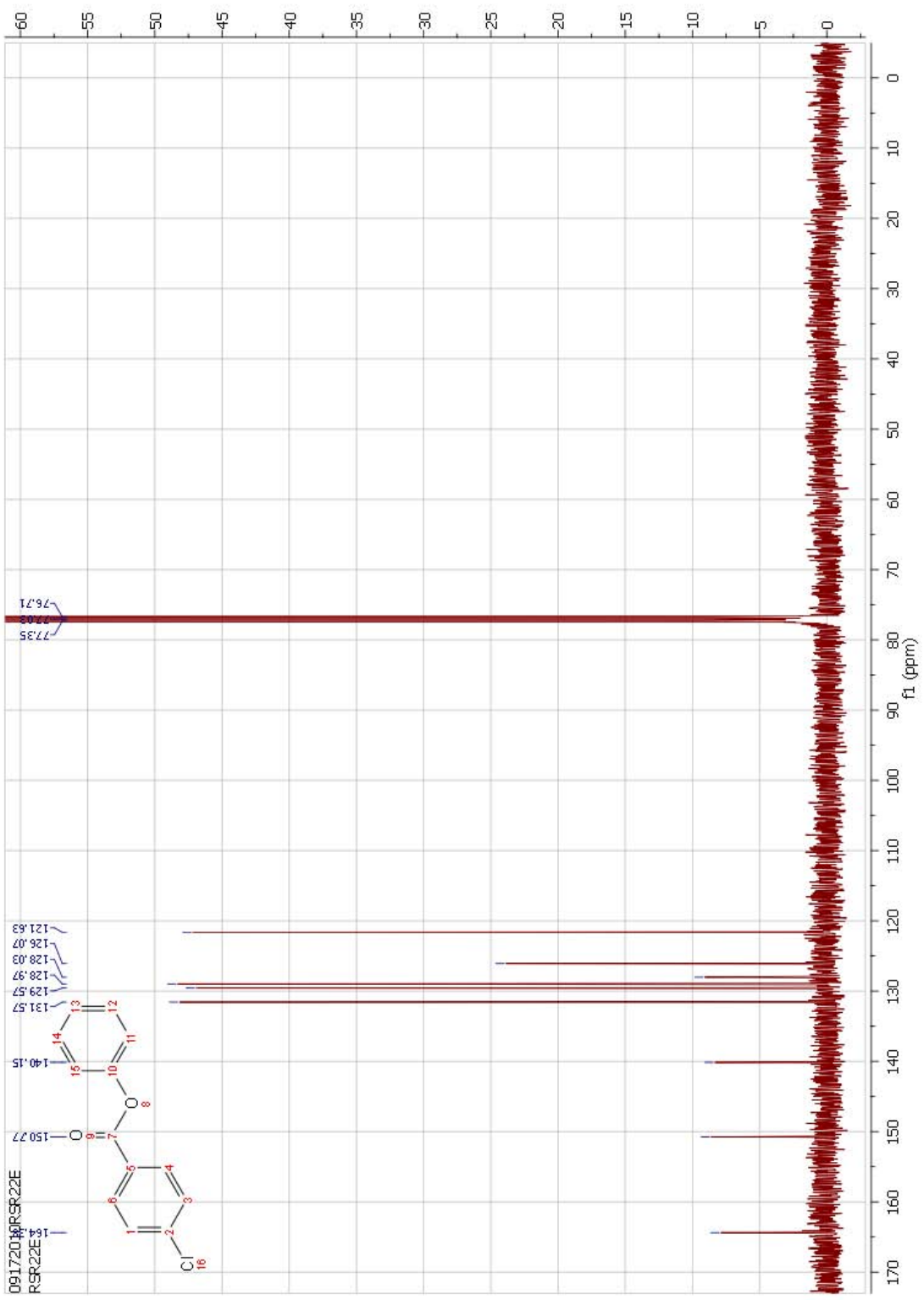


Appendix A - Spectra



Appendix A - Spectra



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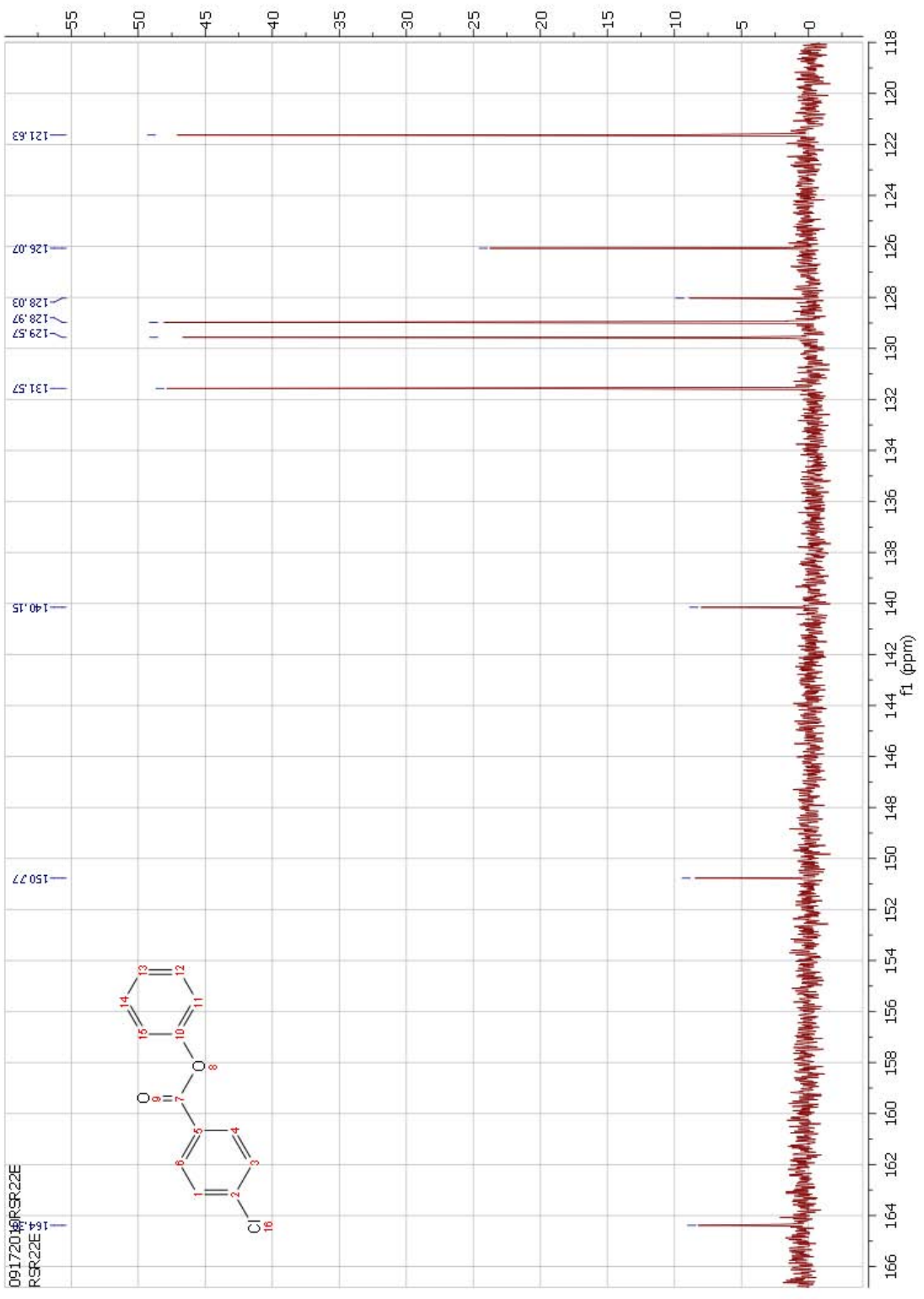

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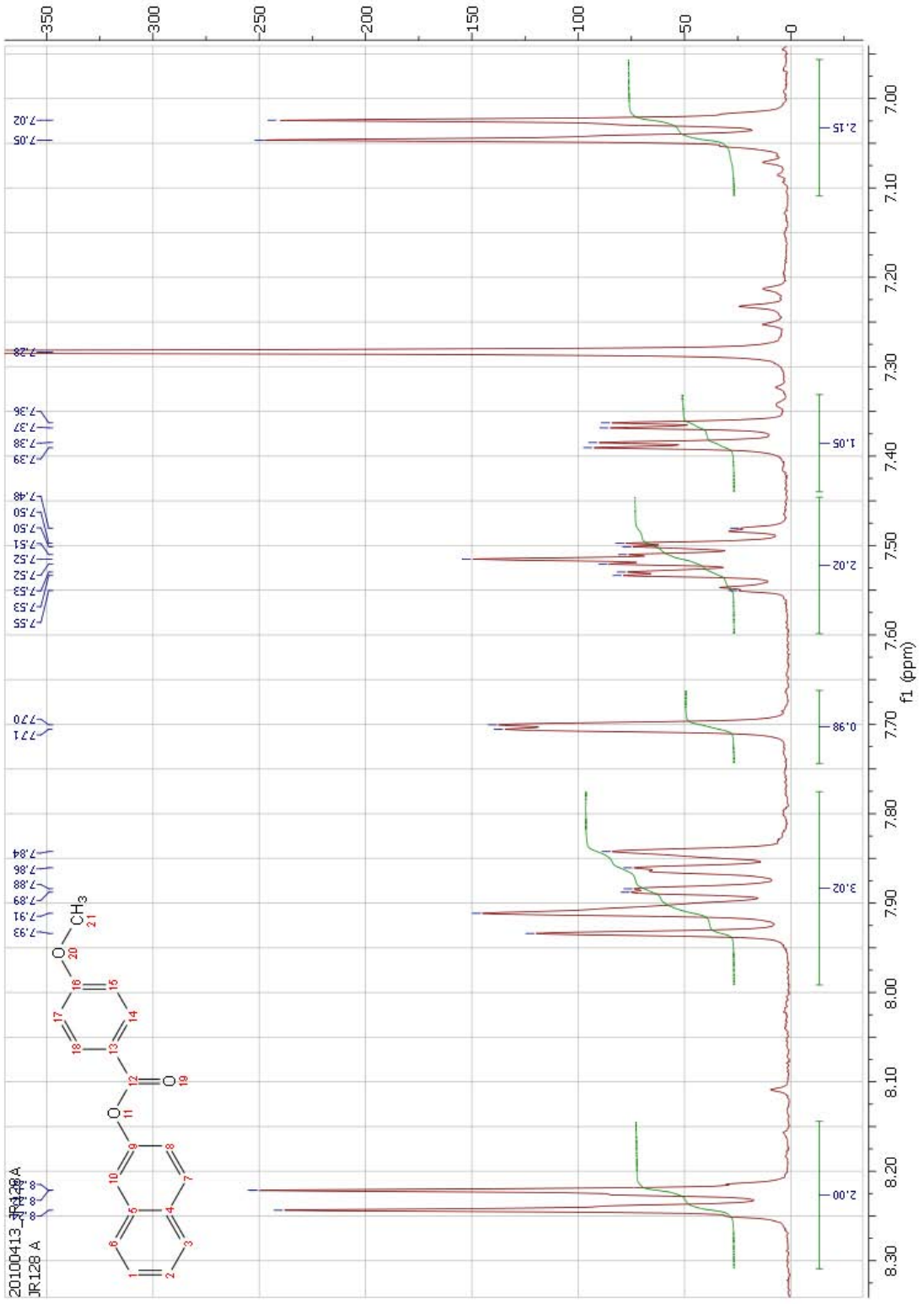

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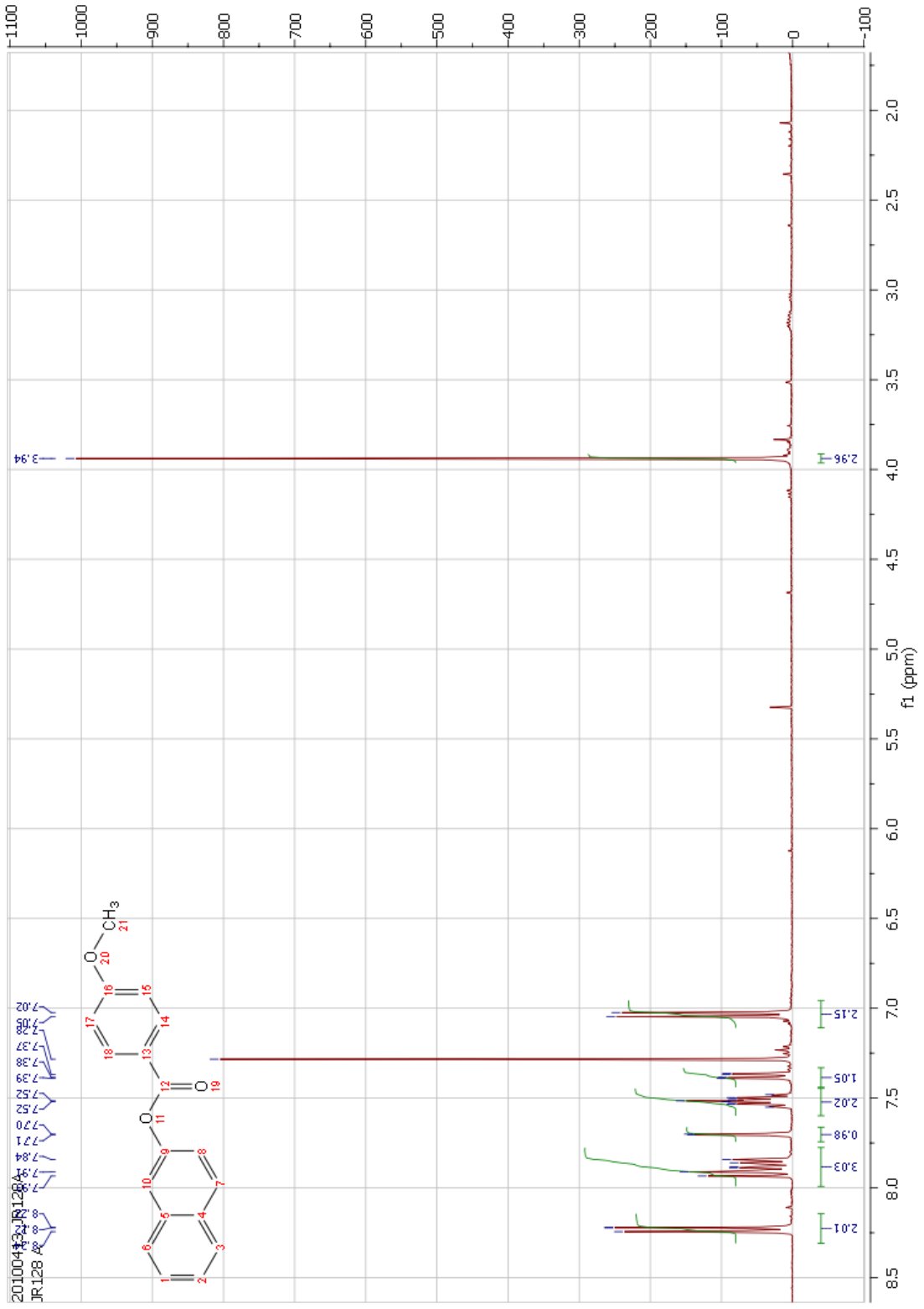

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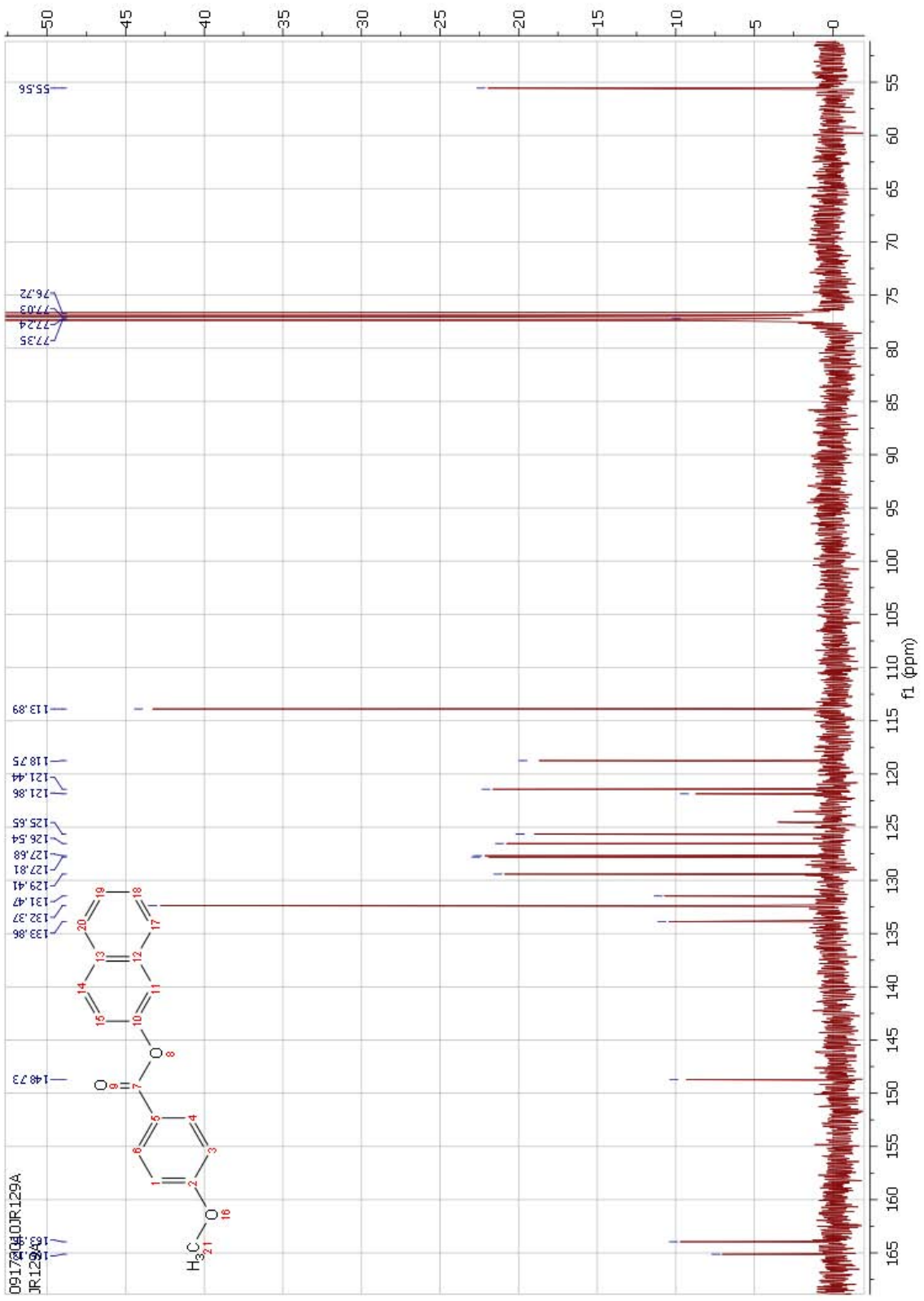

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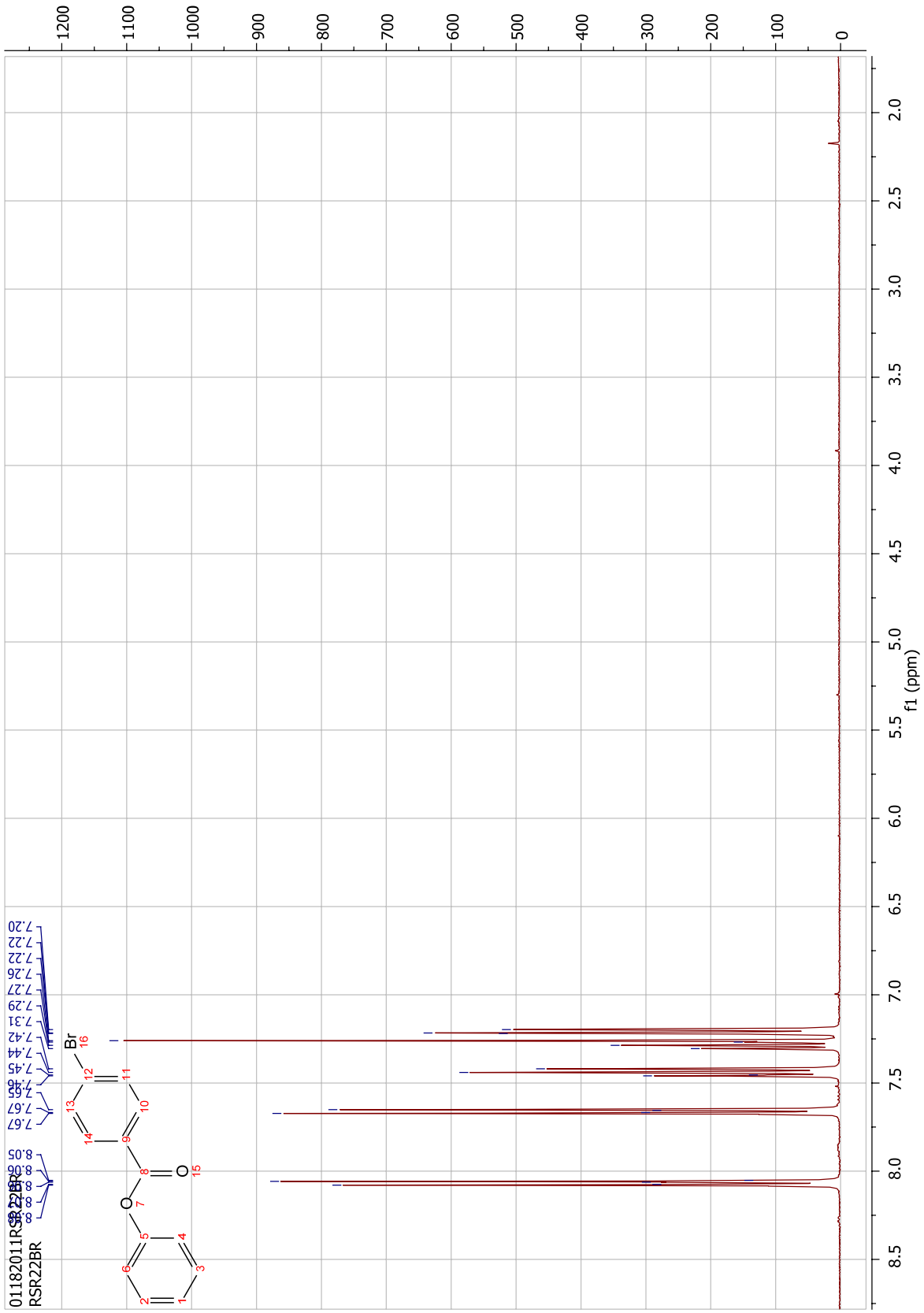

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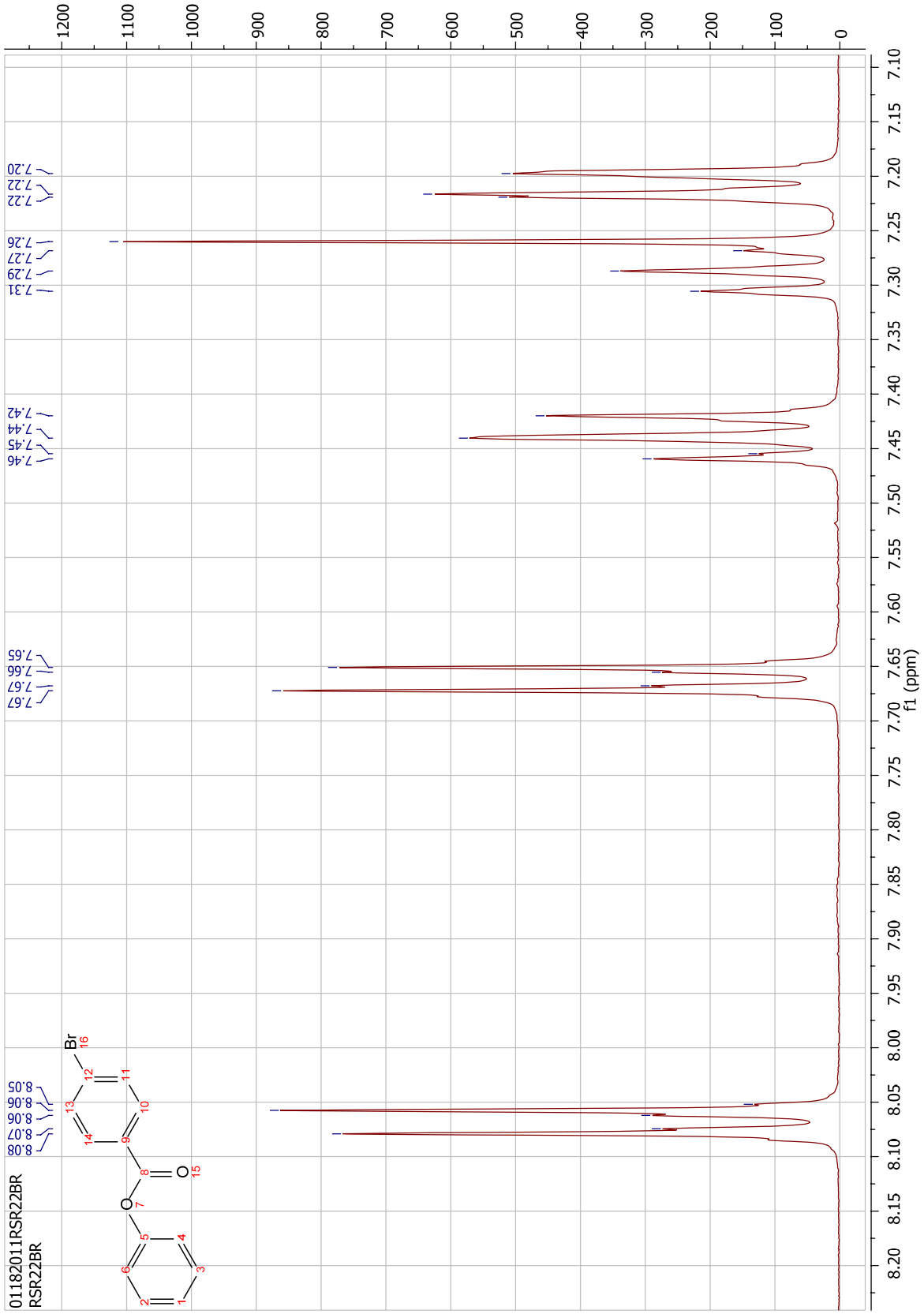

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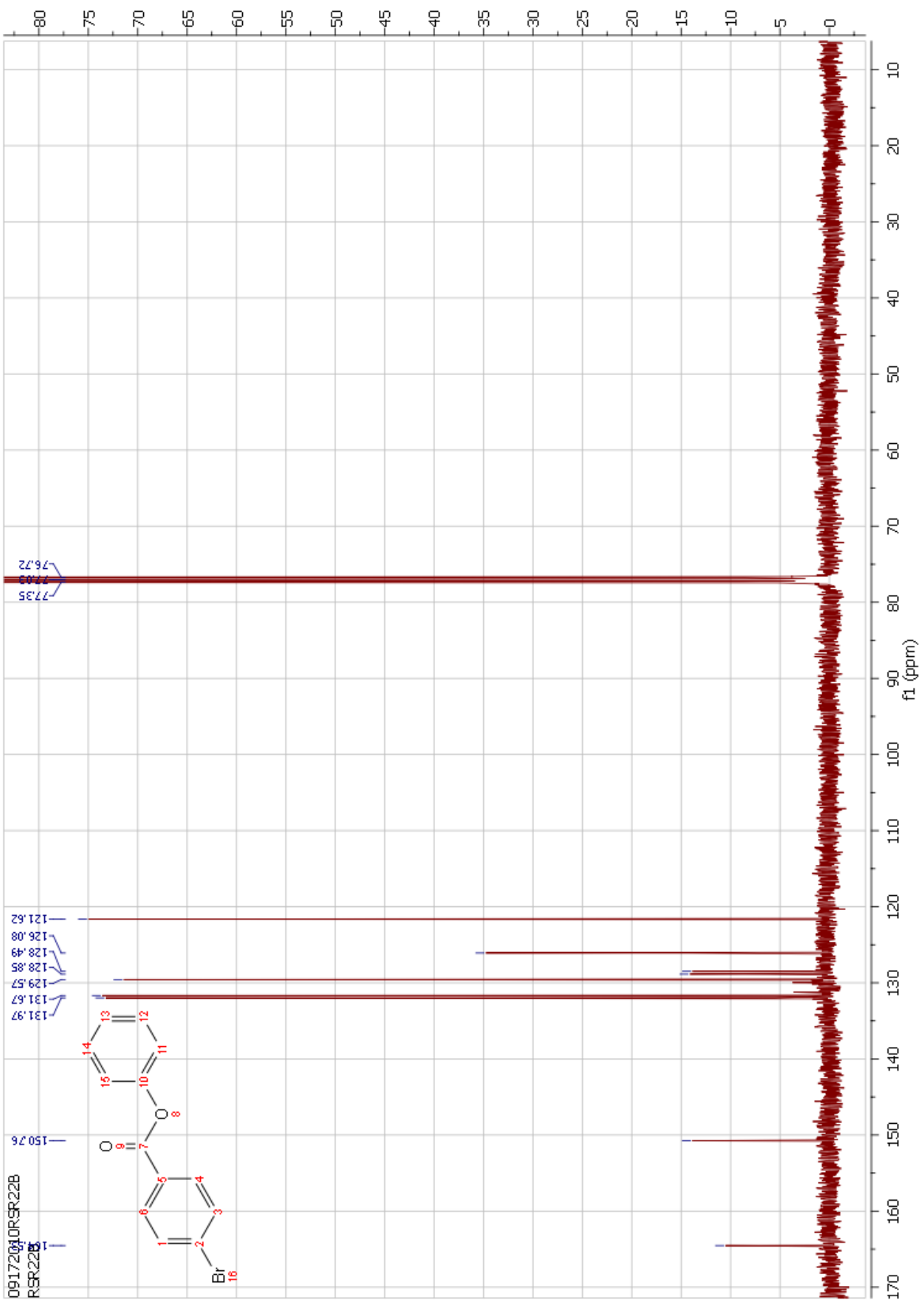

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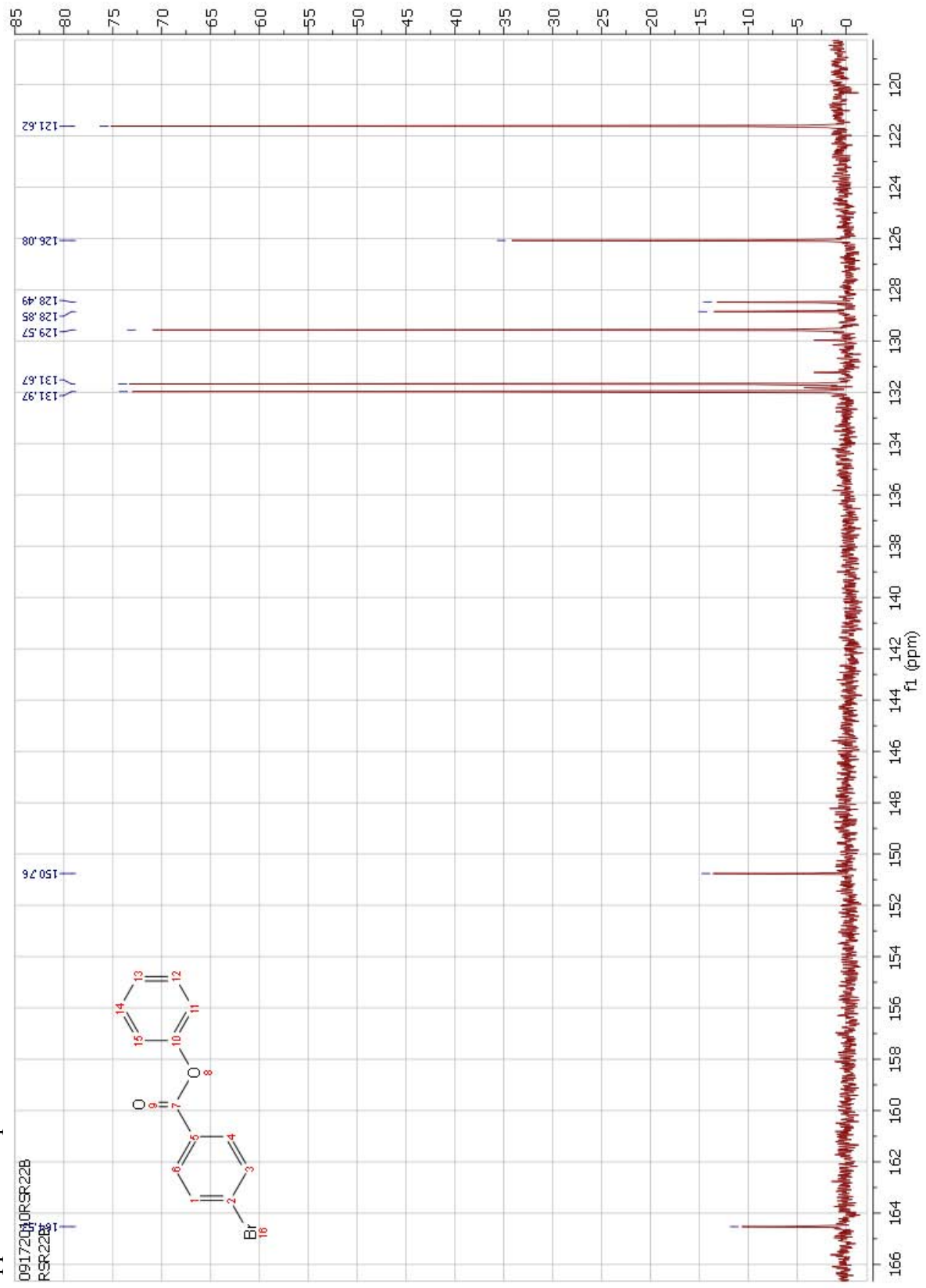

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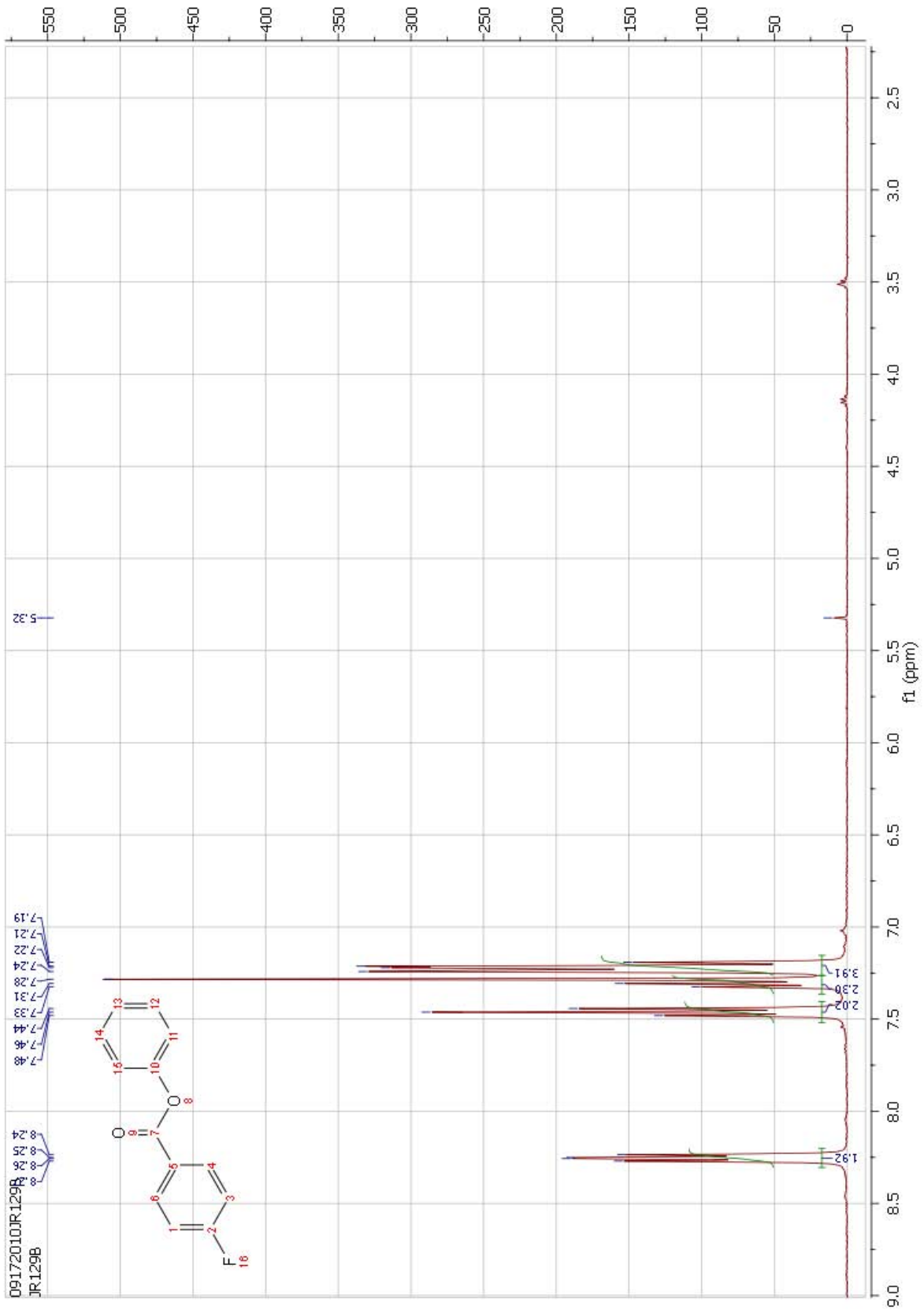

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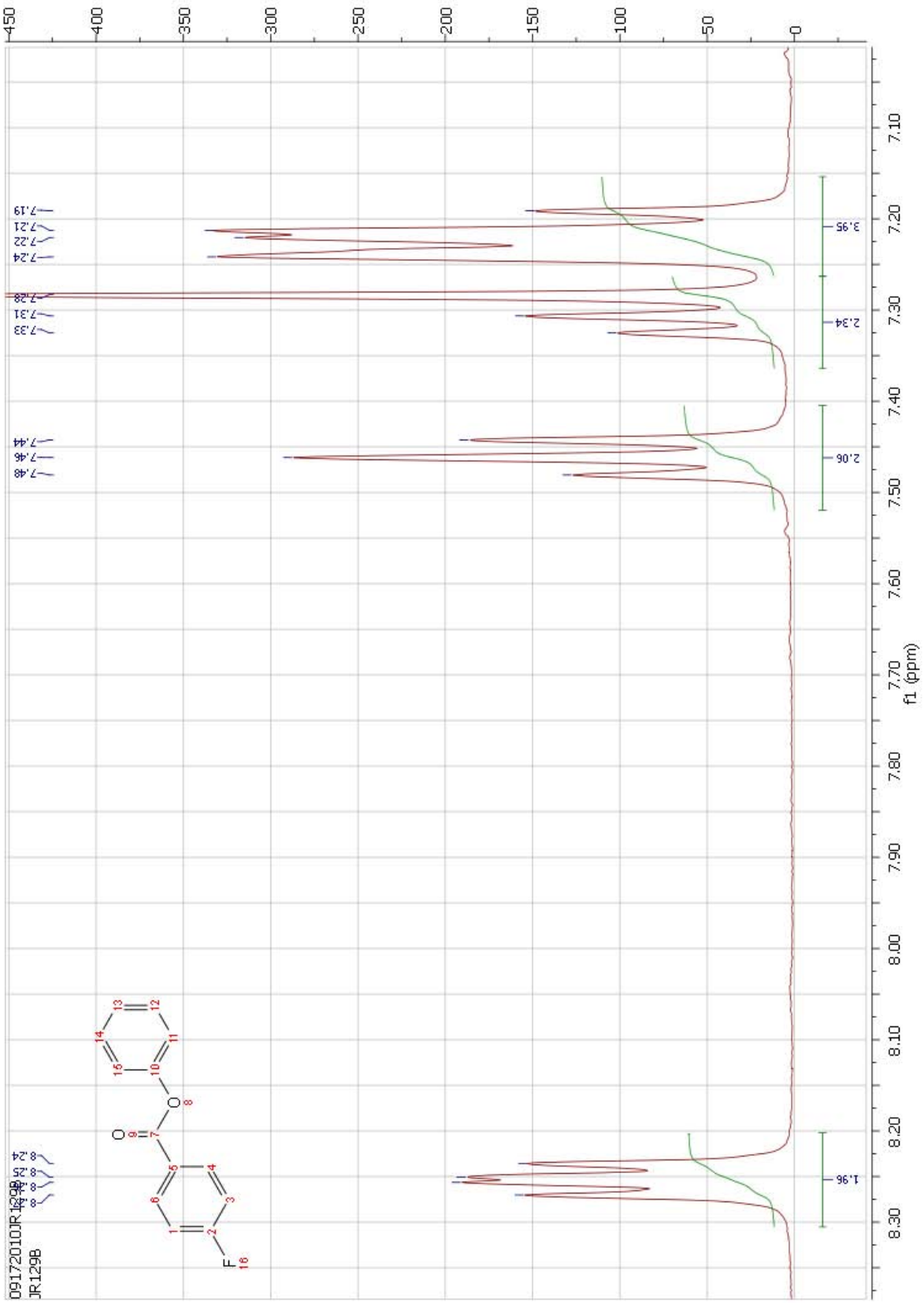

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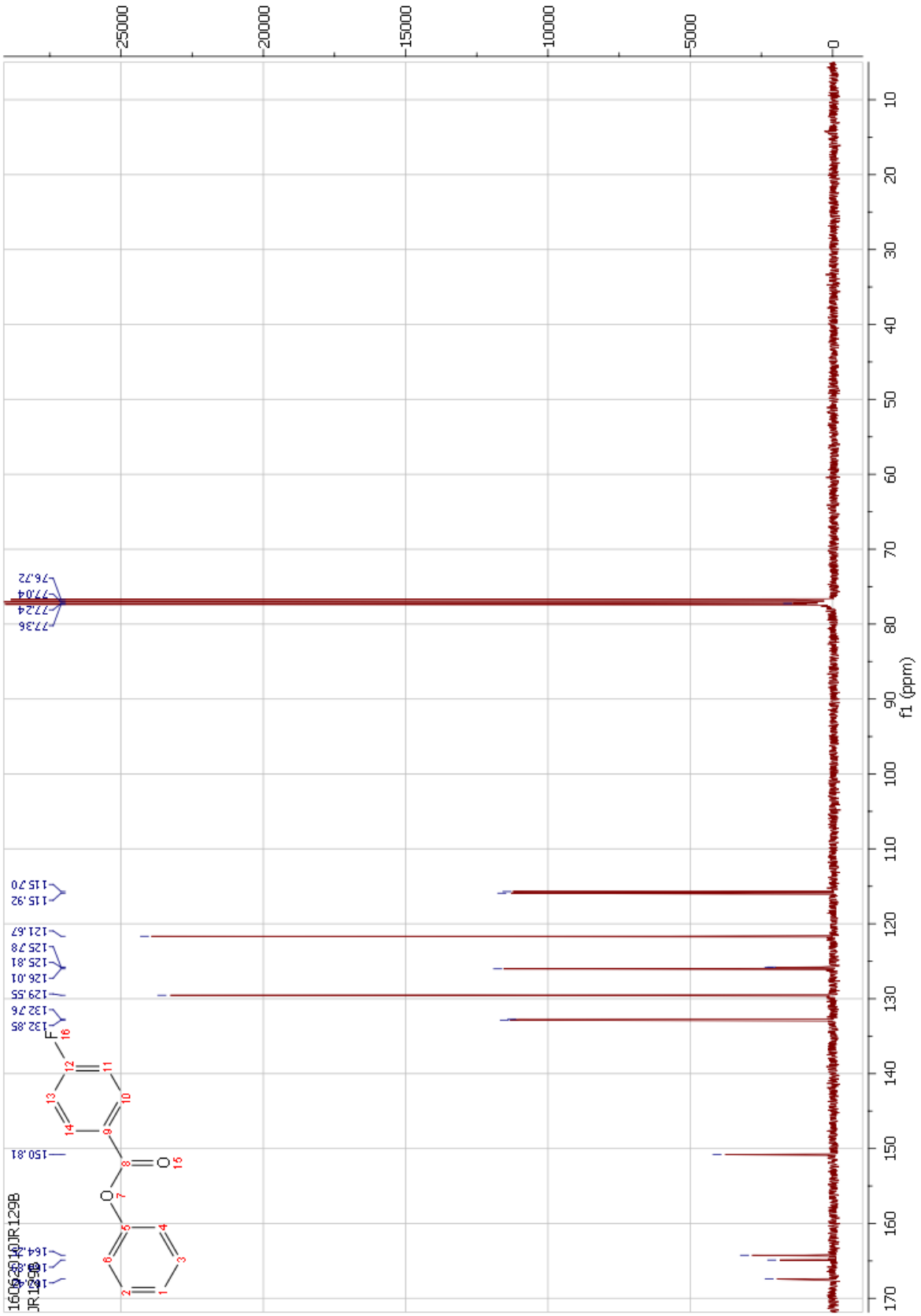

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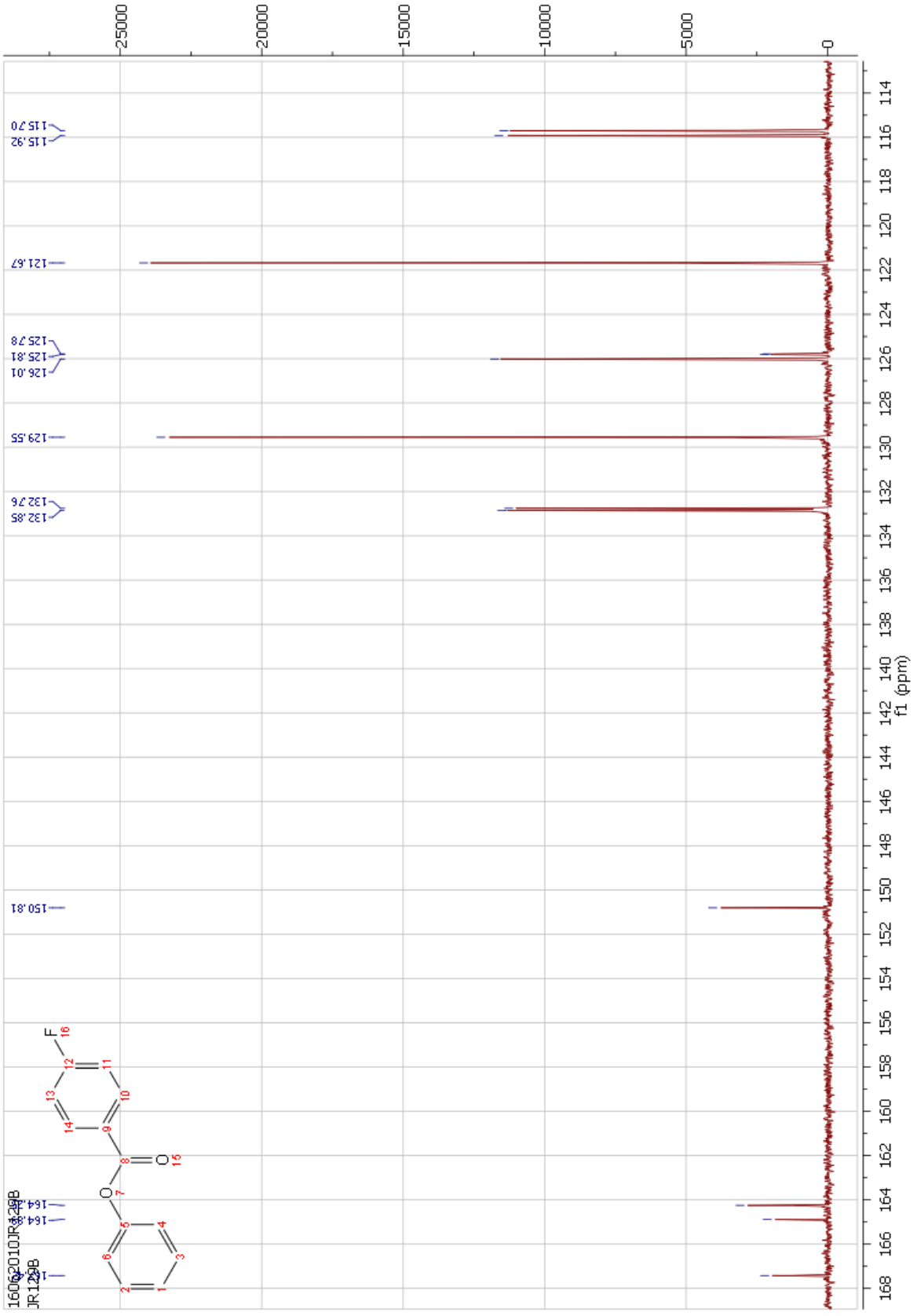

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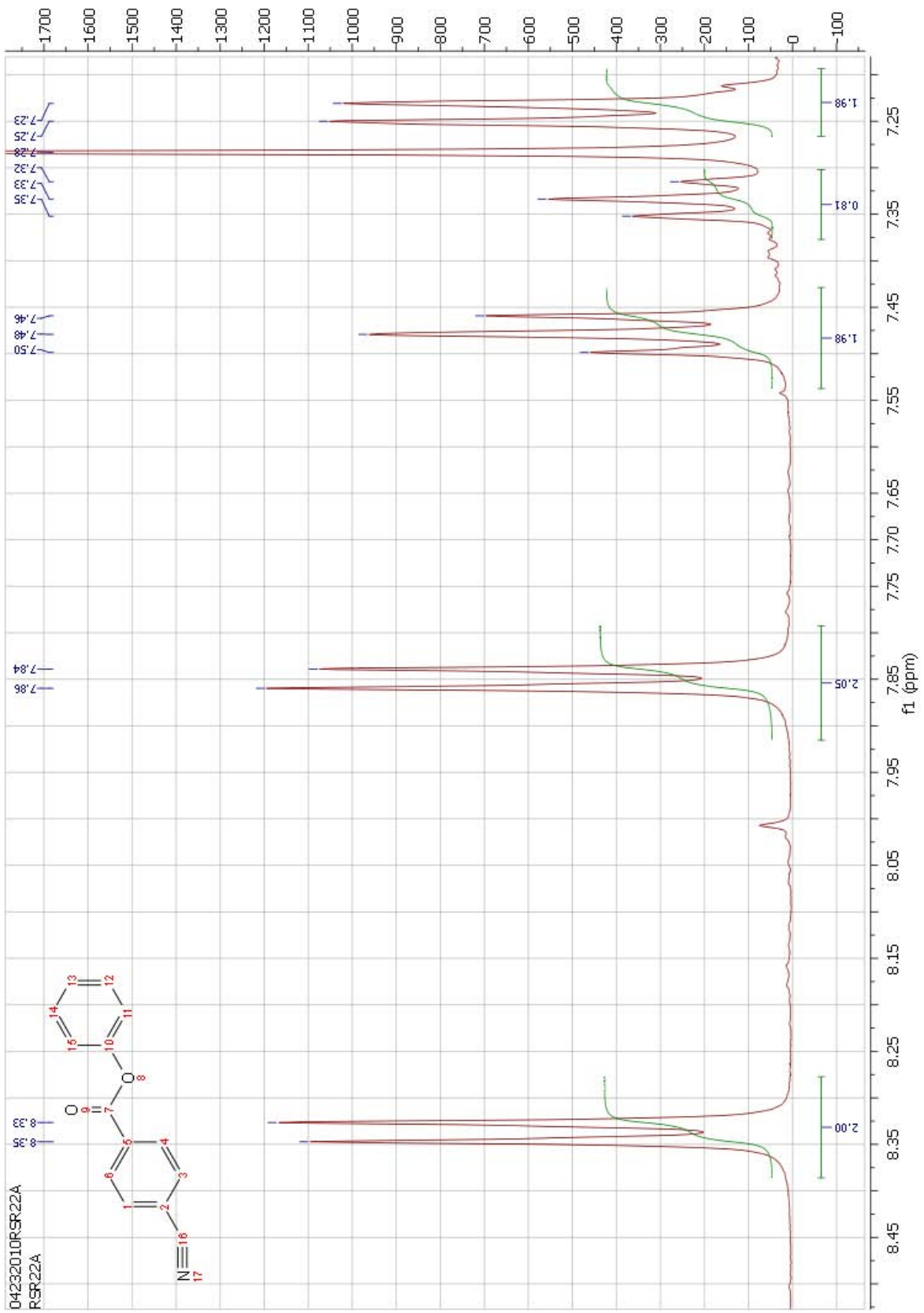

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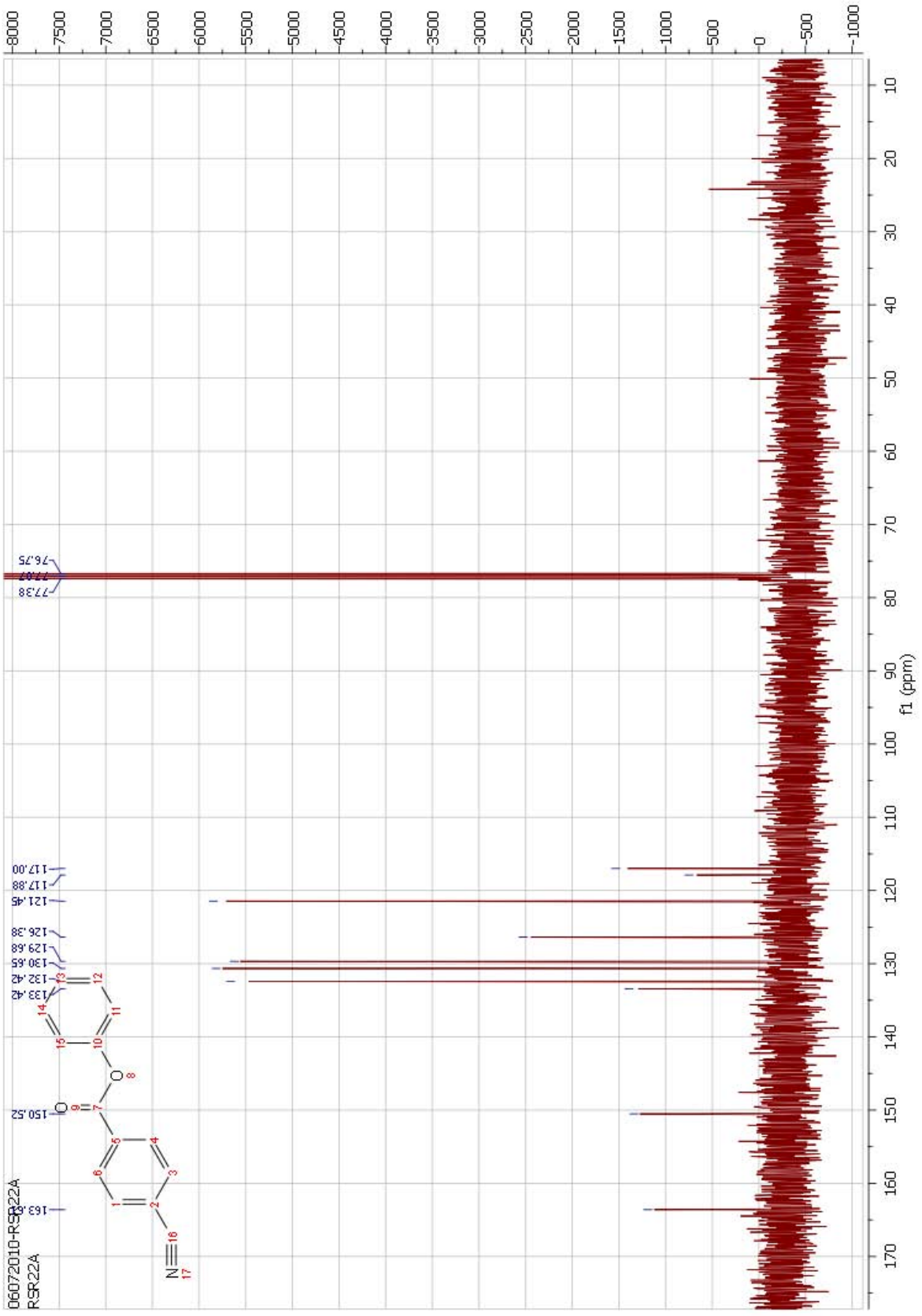

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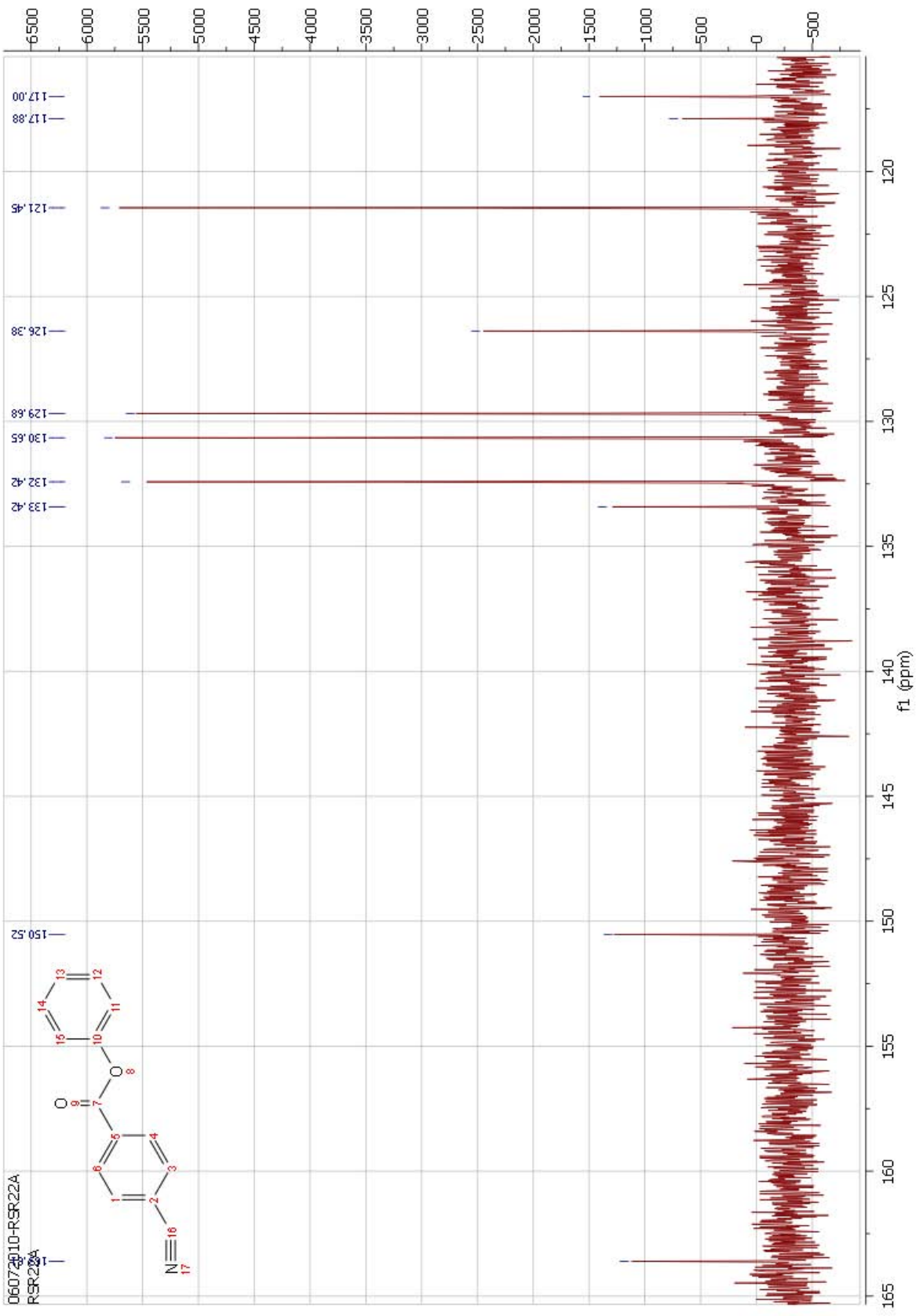

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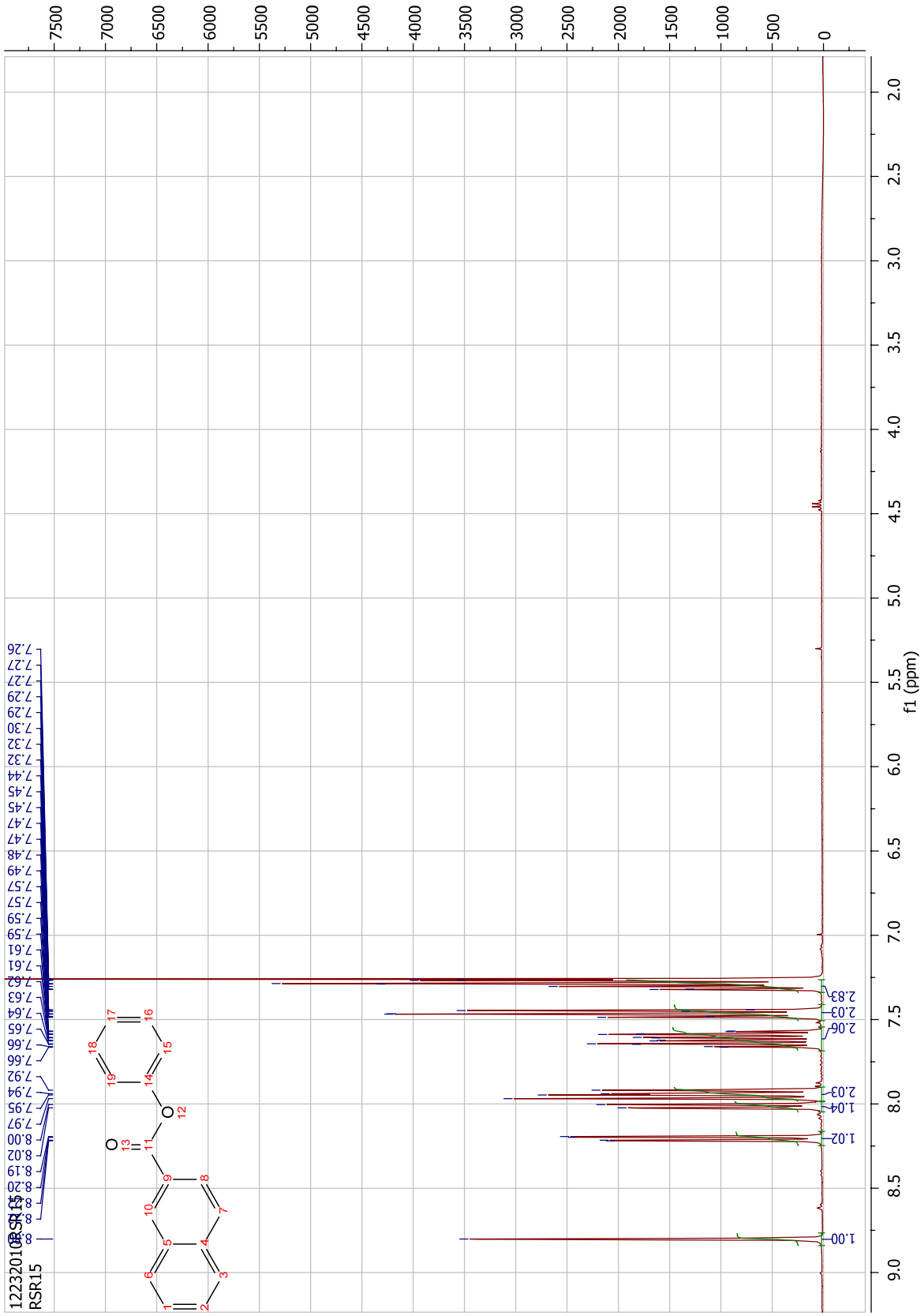

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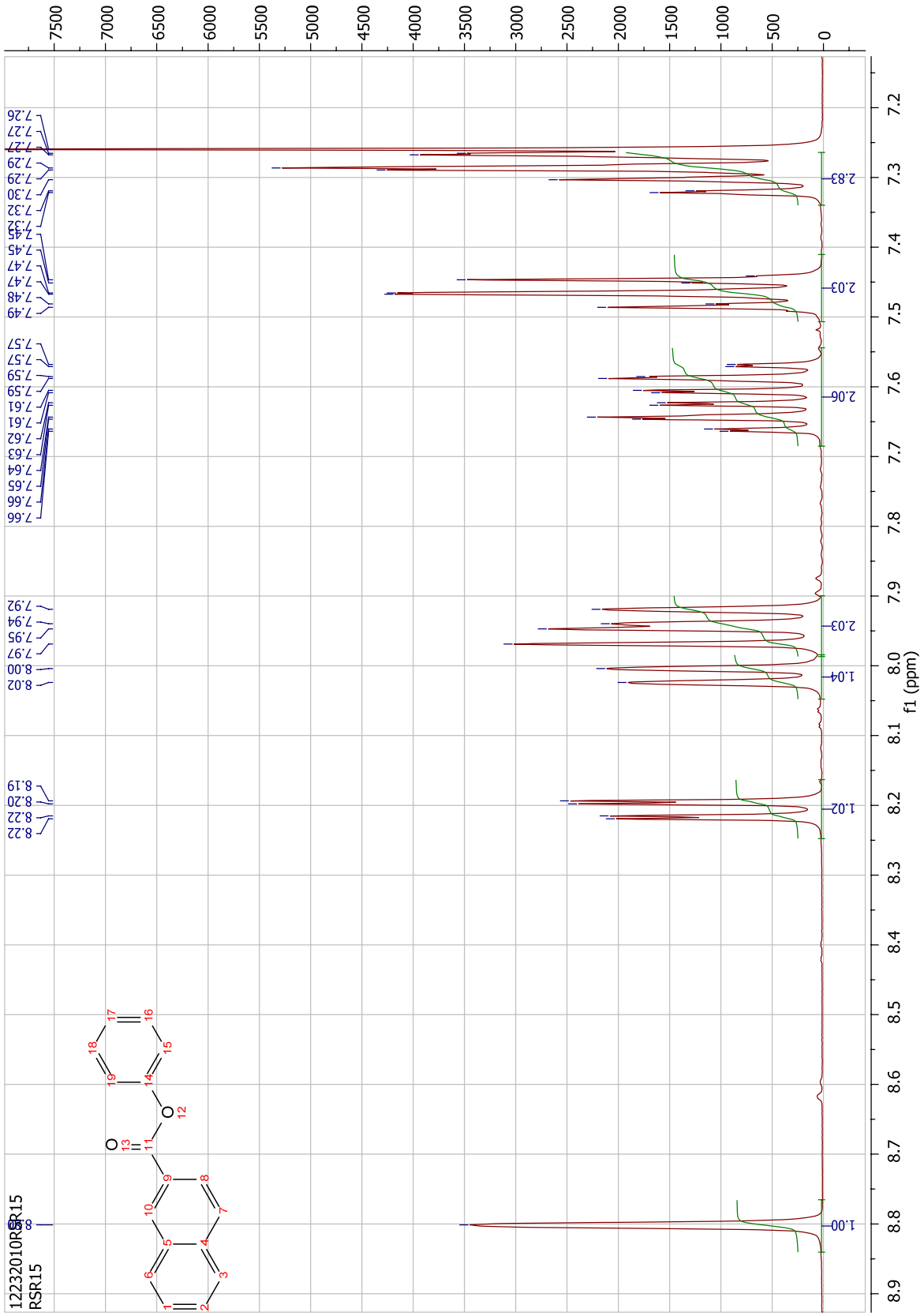

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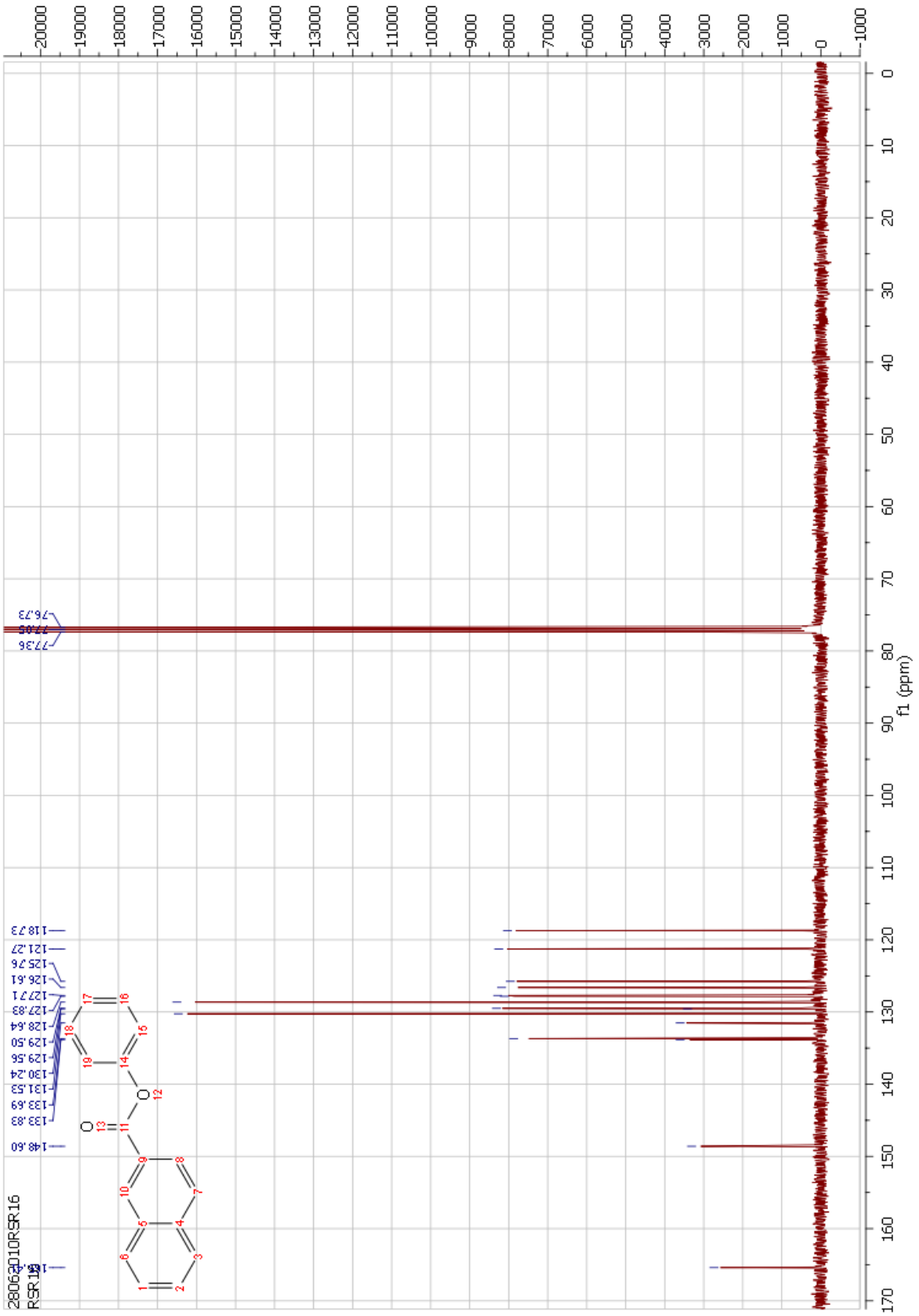

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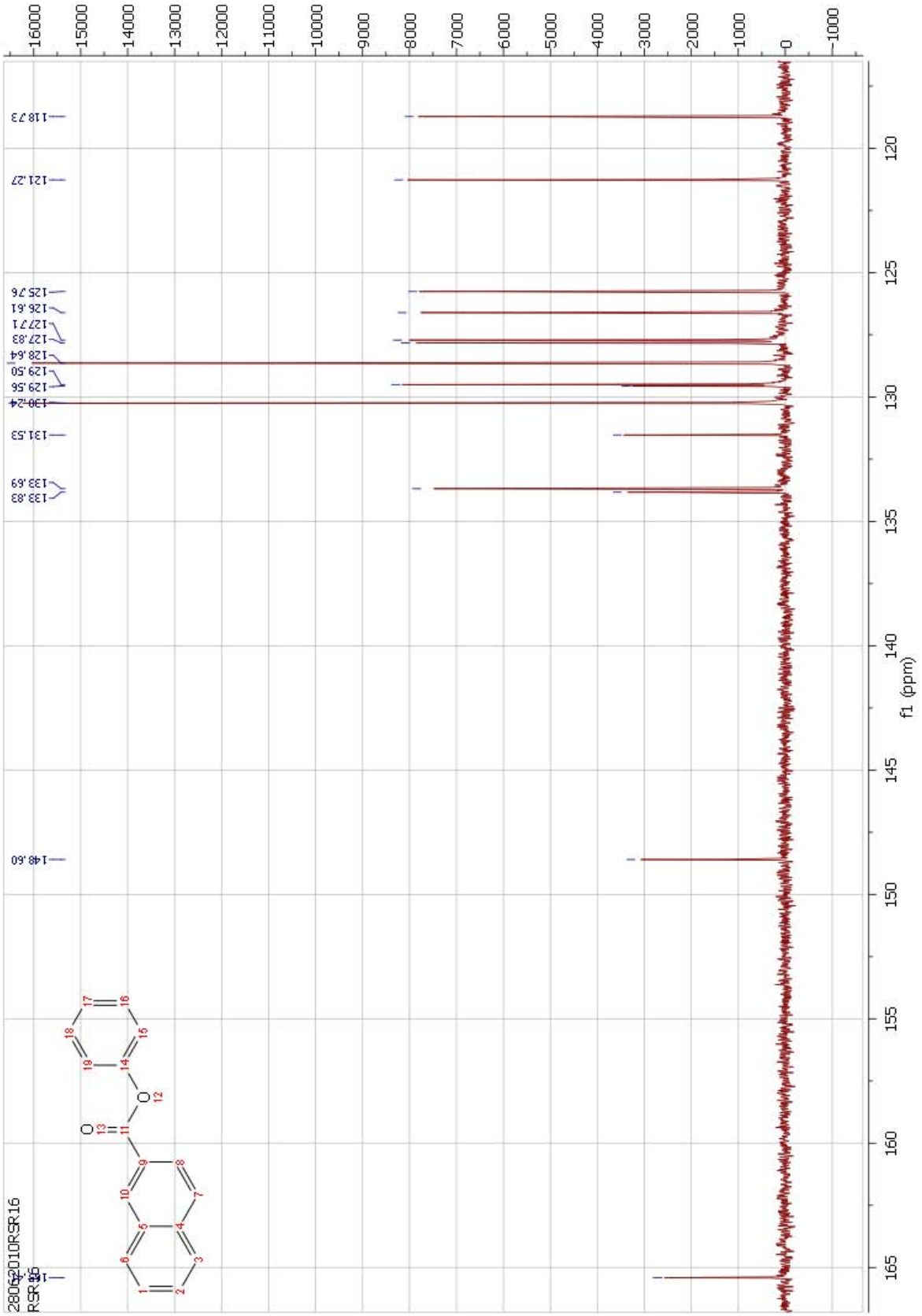

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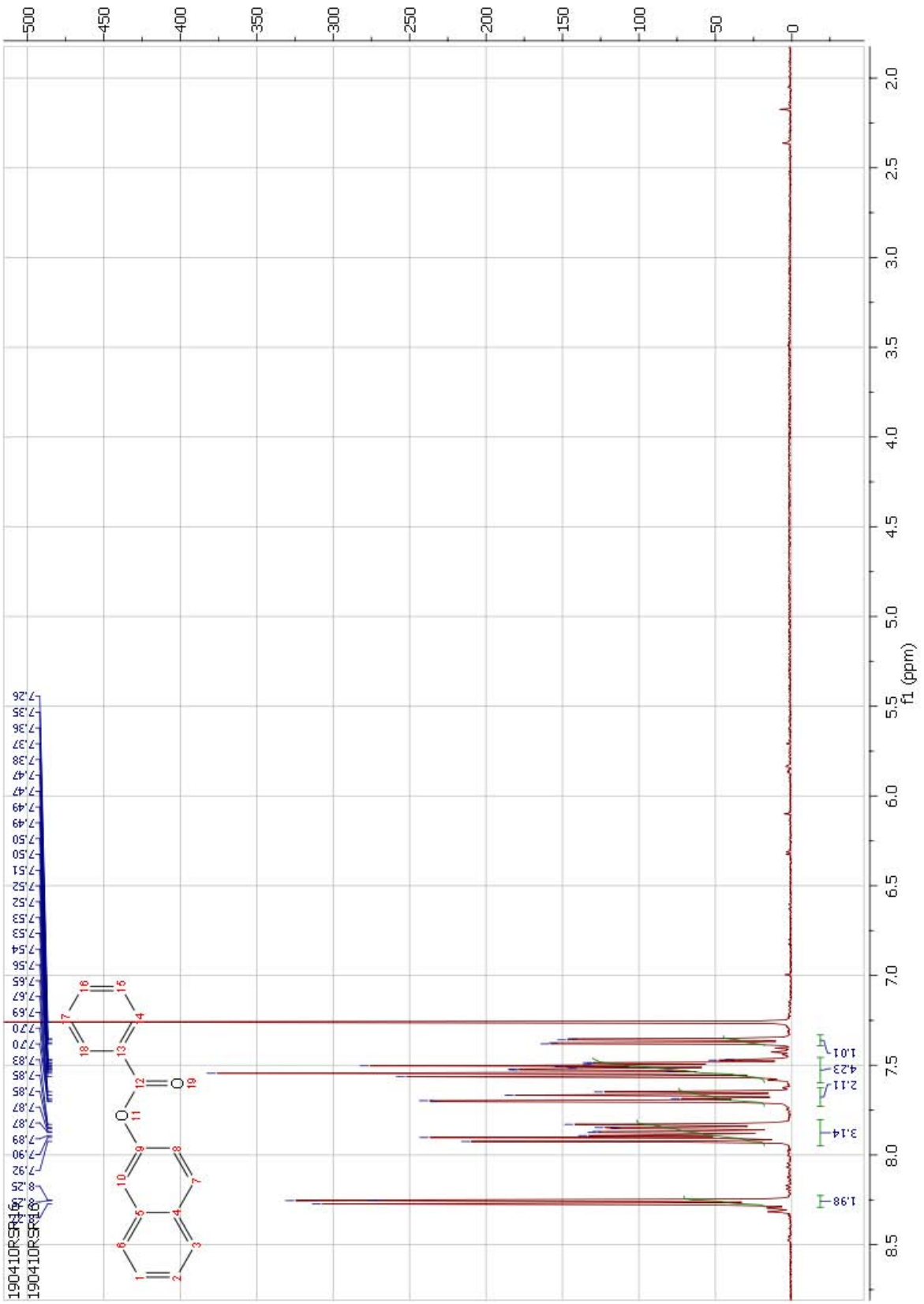

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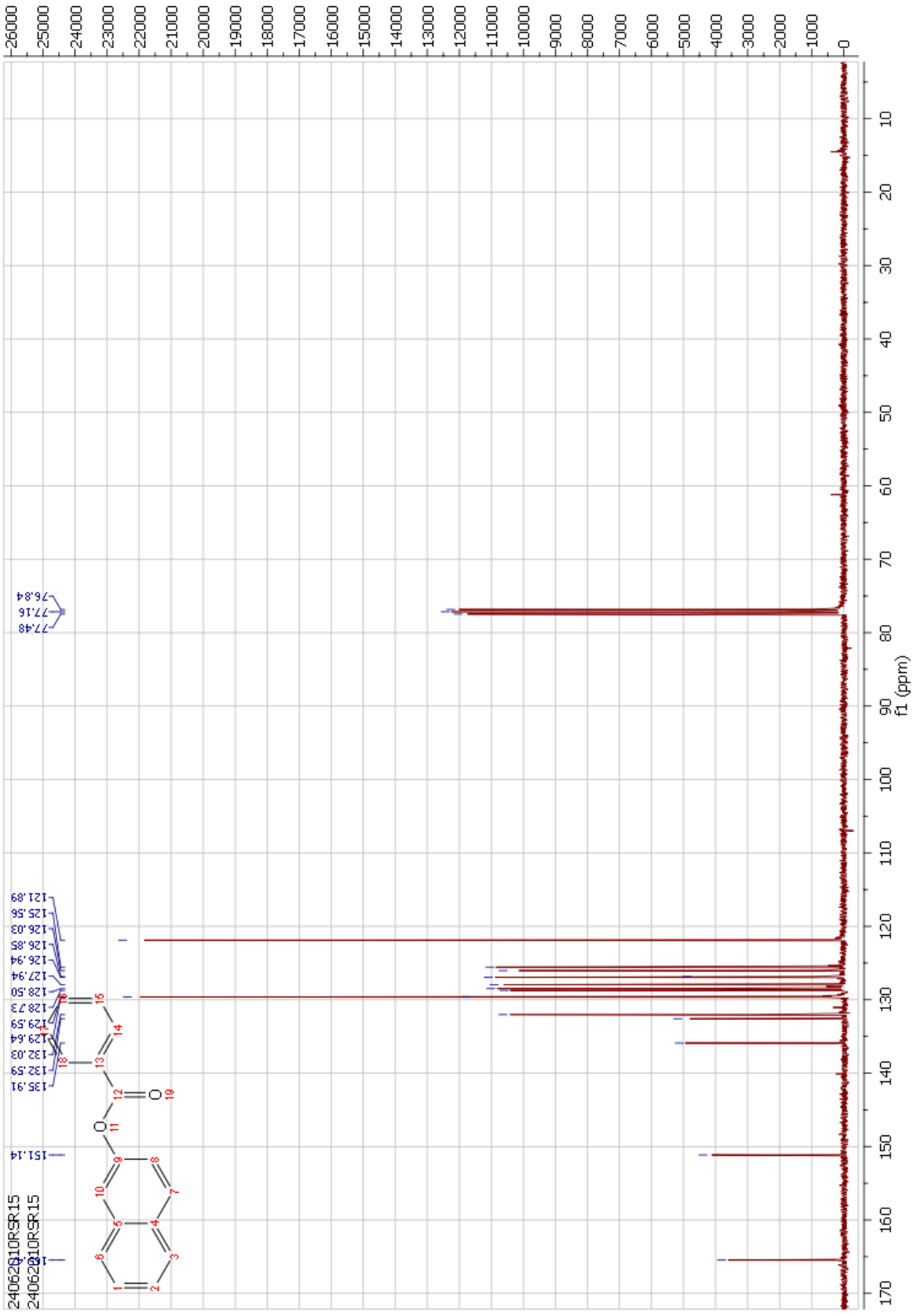

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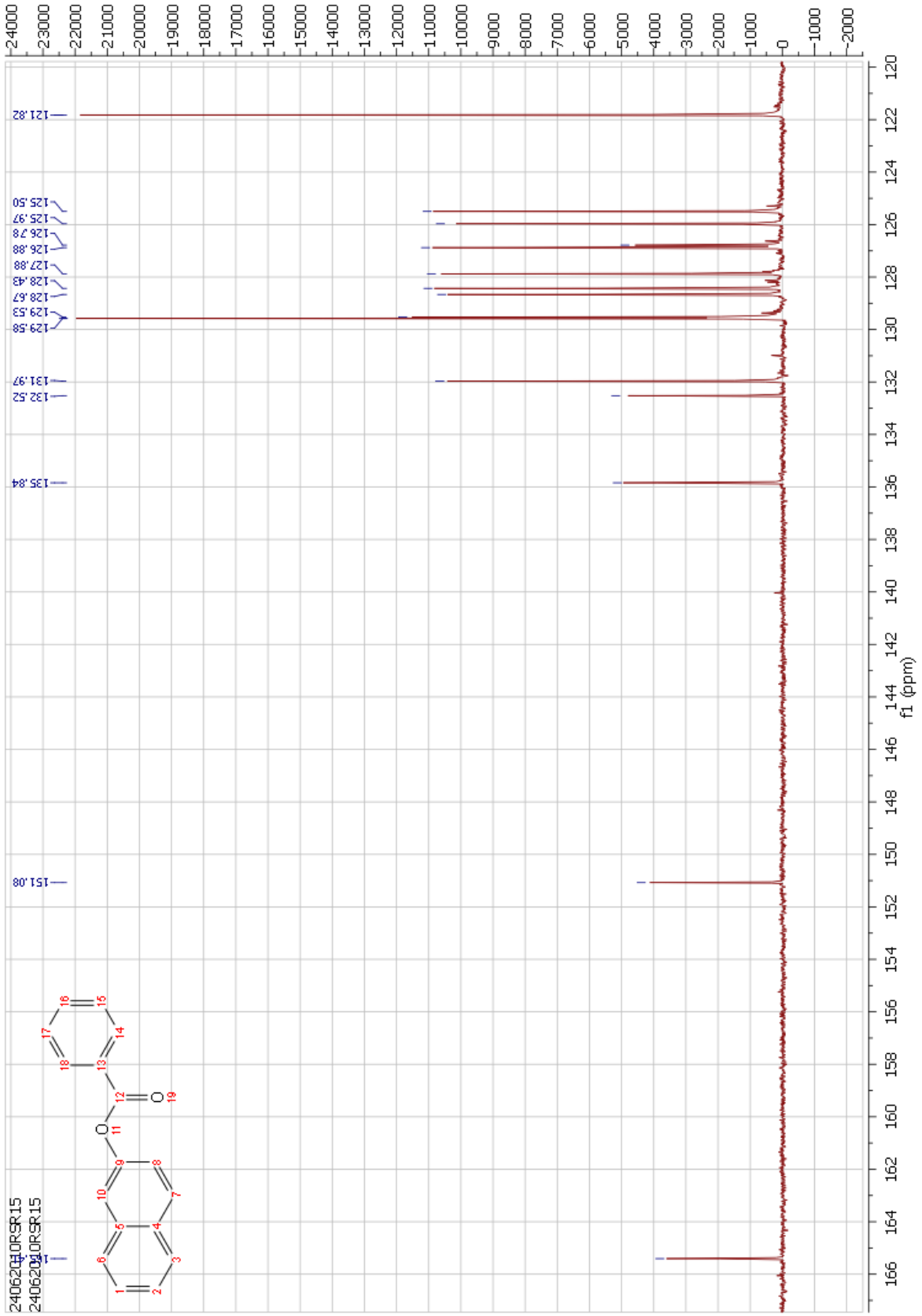

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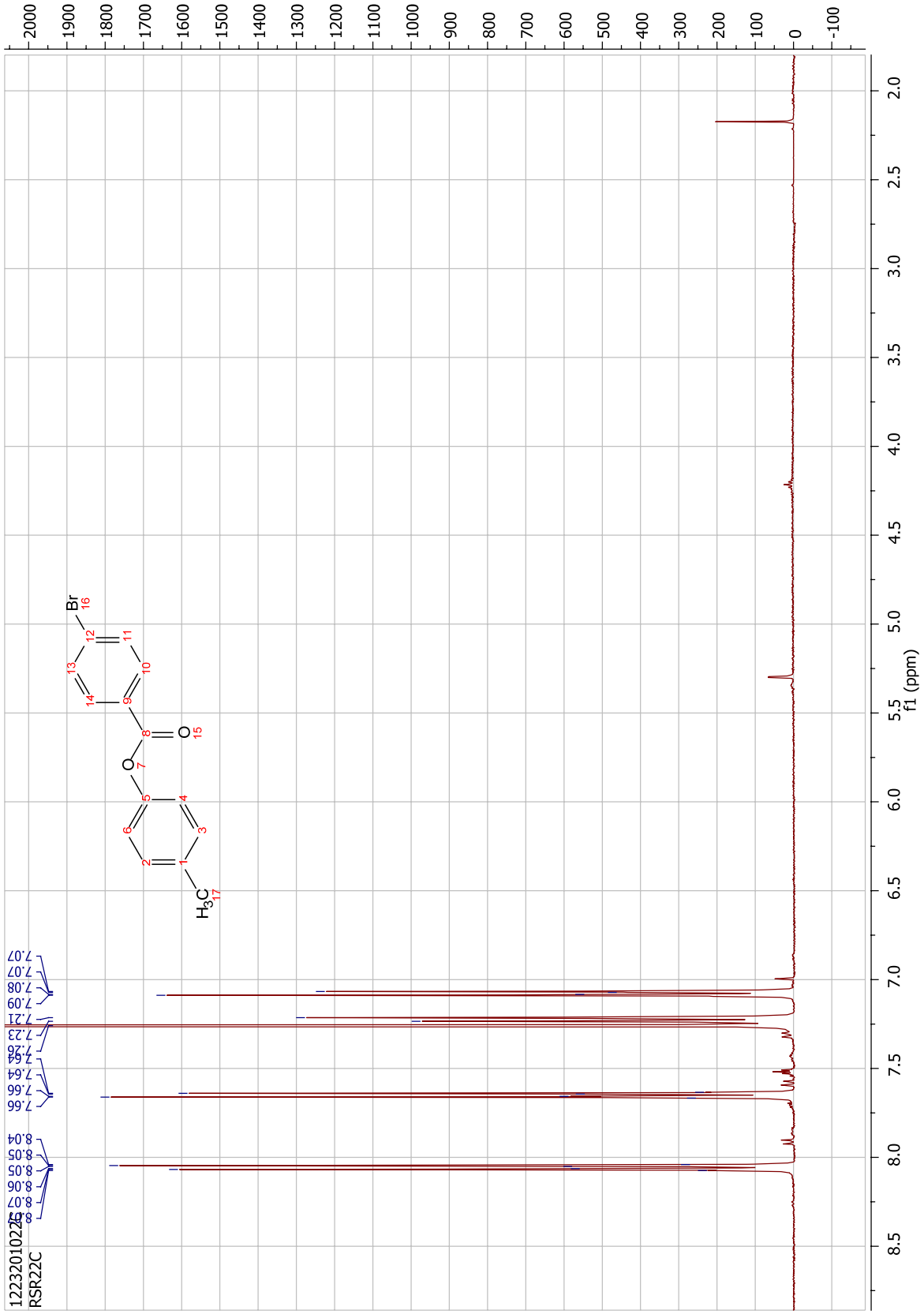

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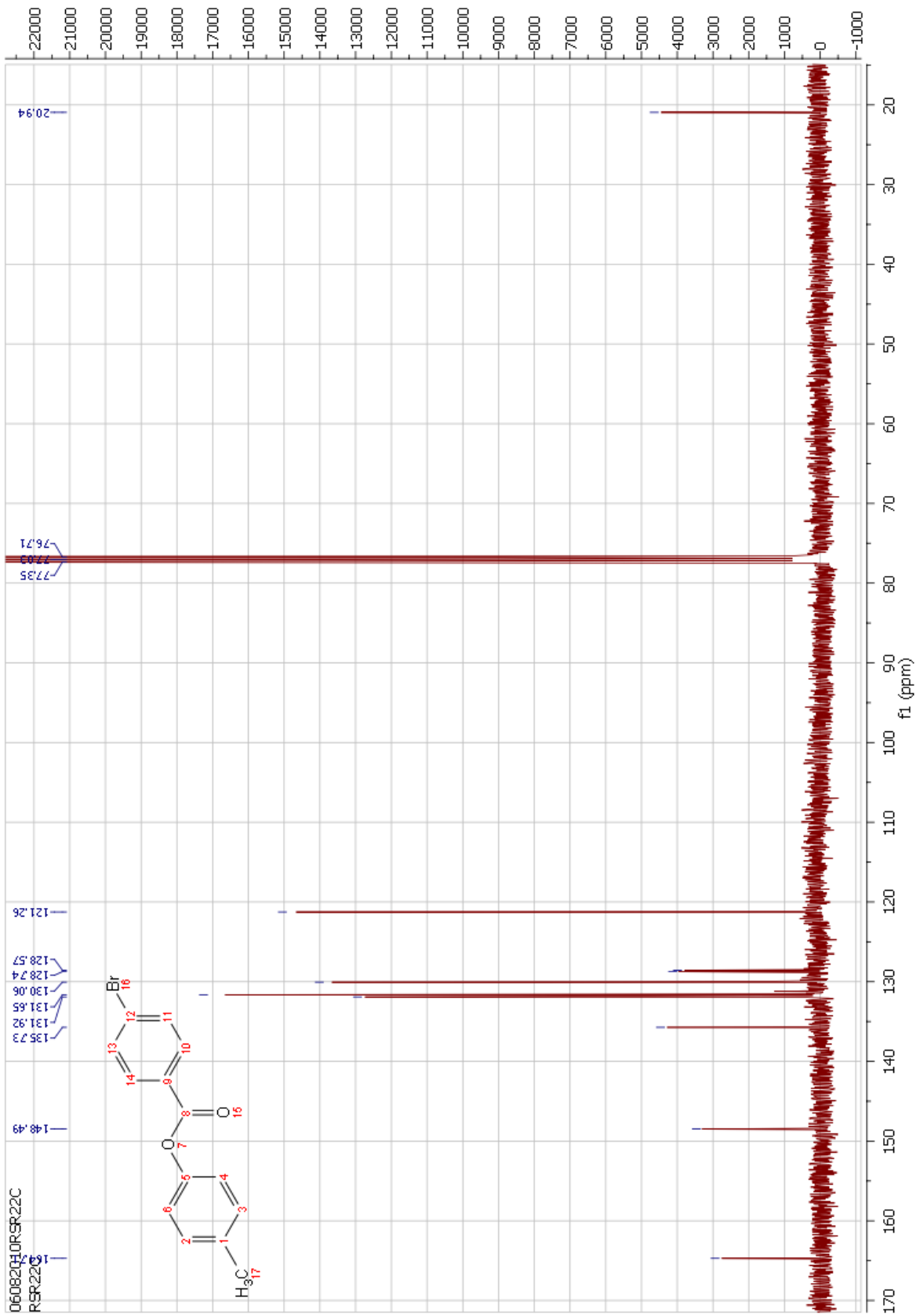

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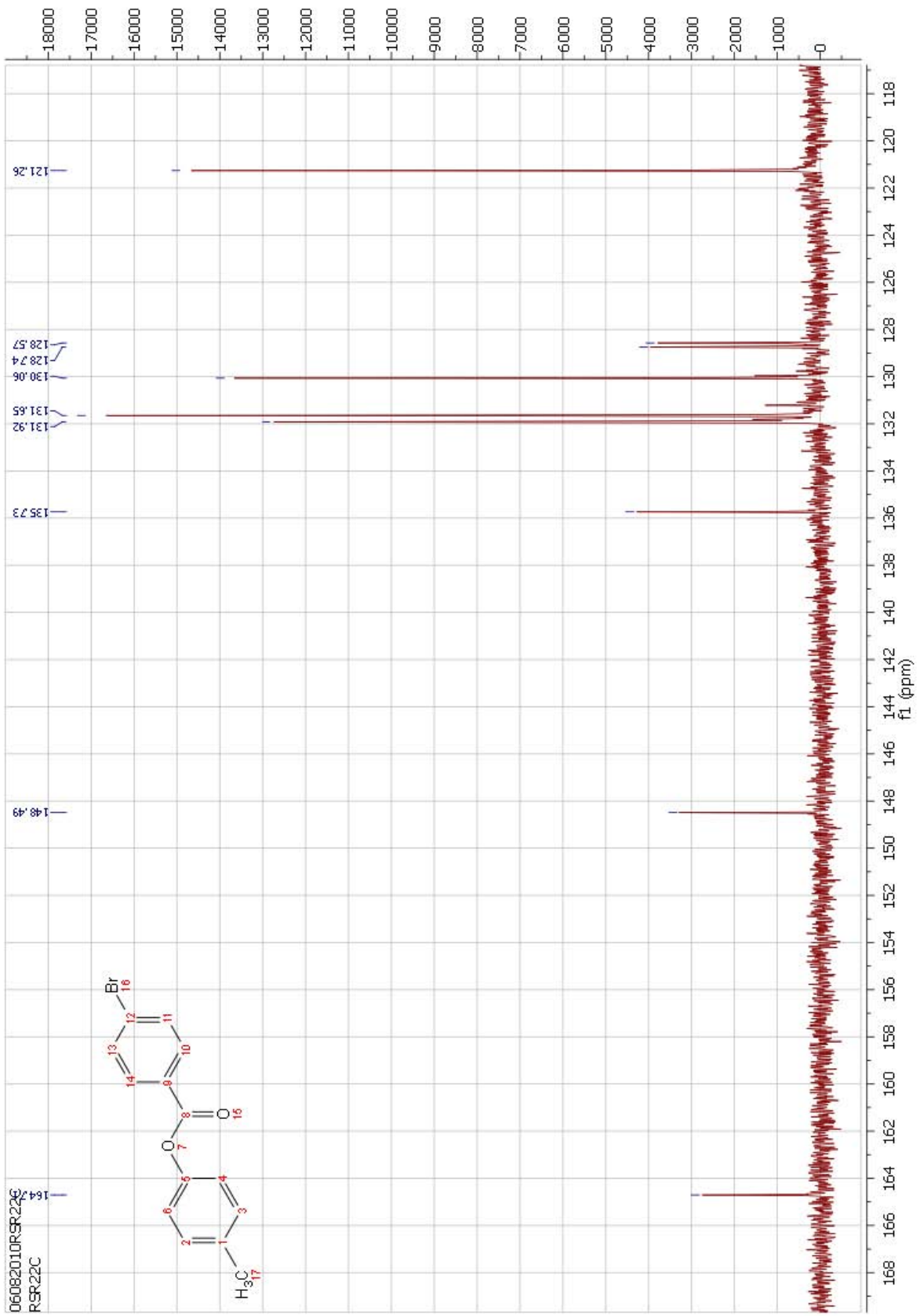

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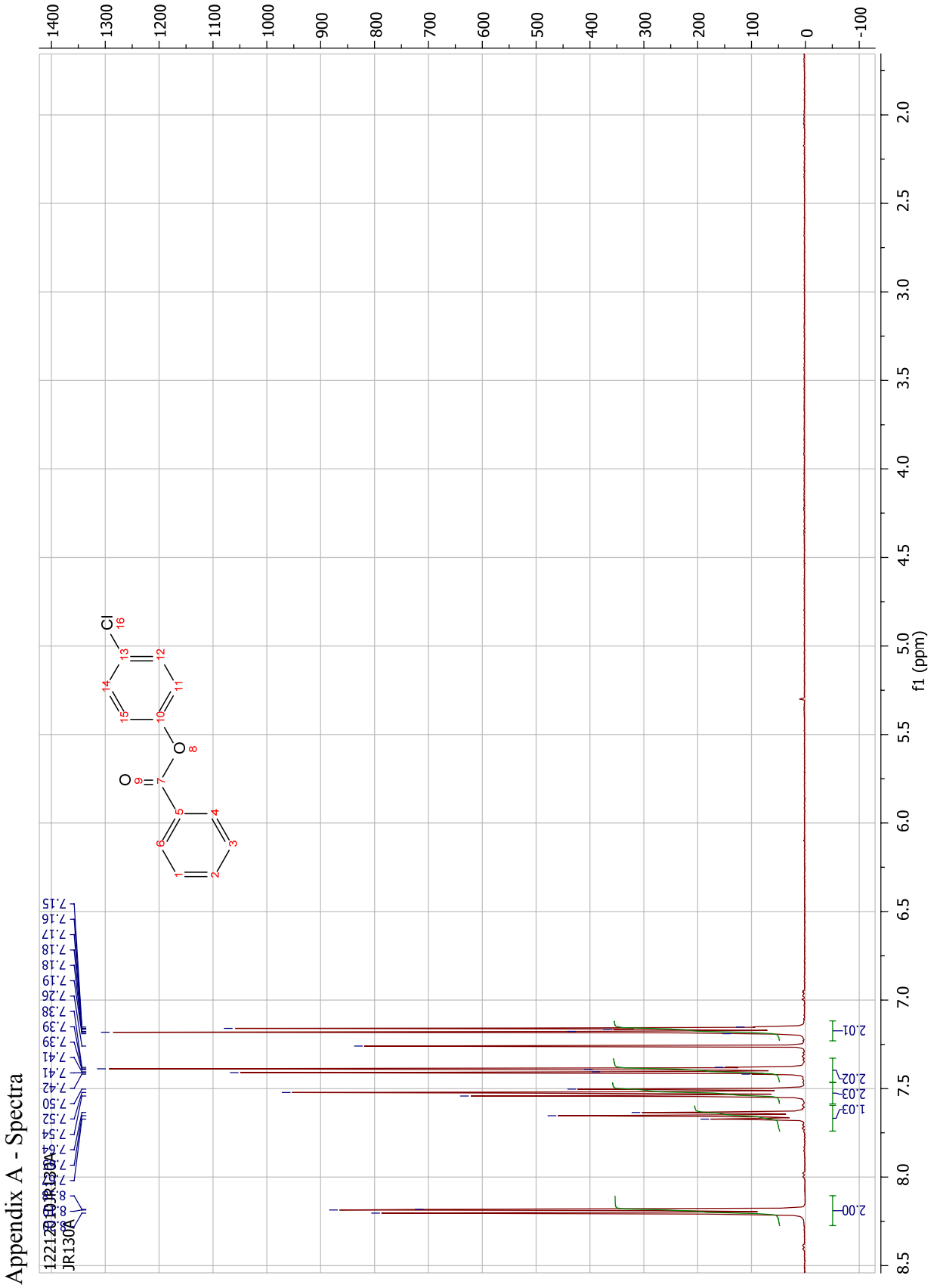

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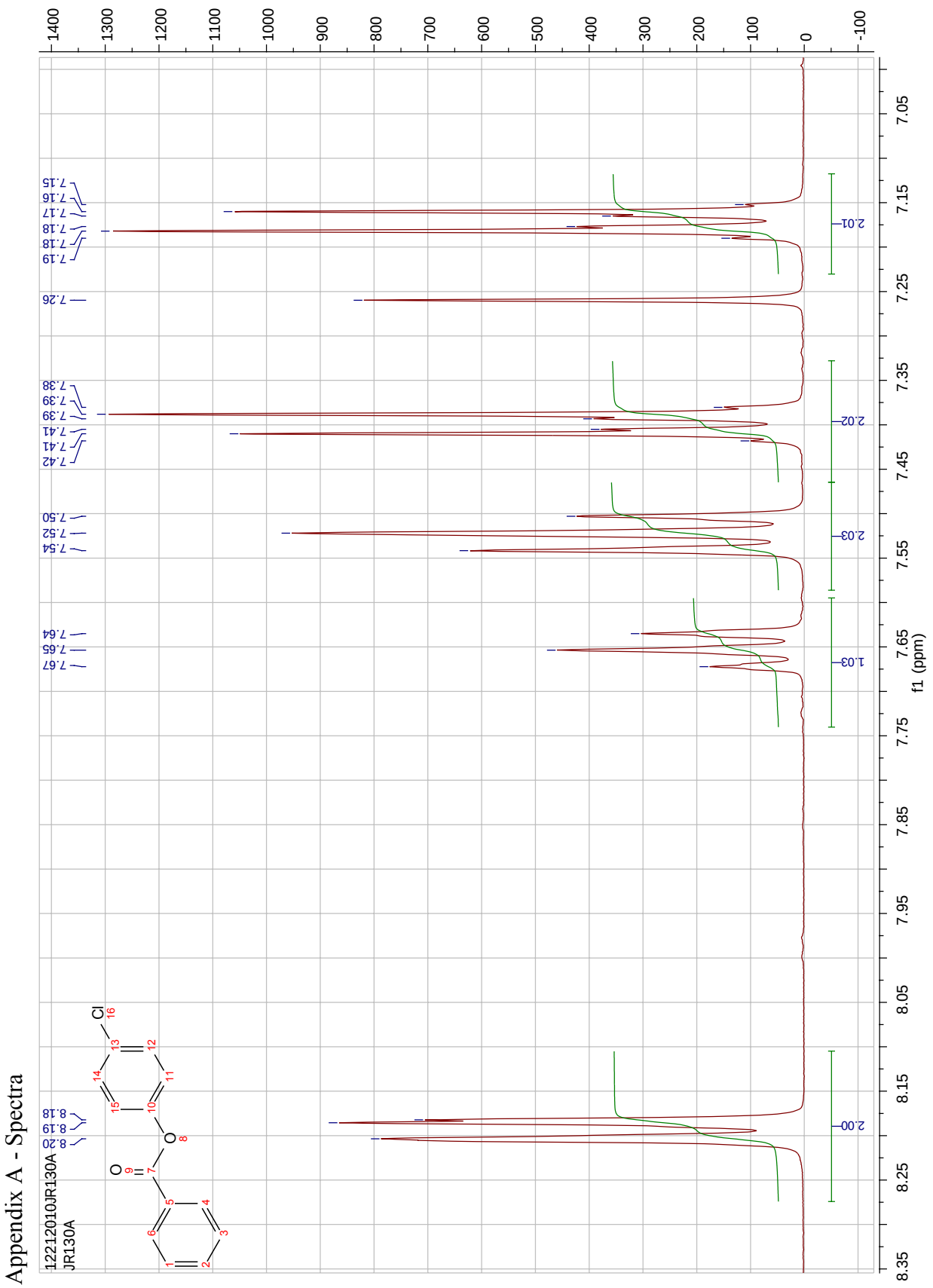

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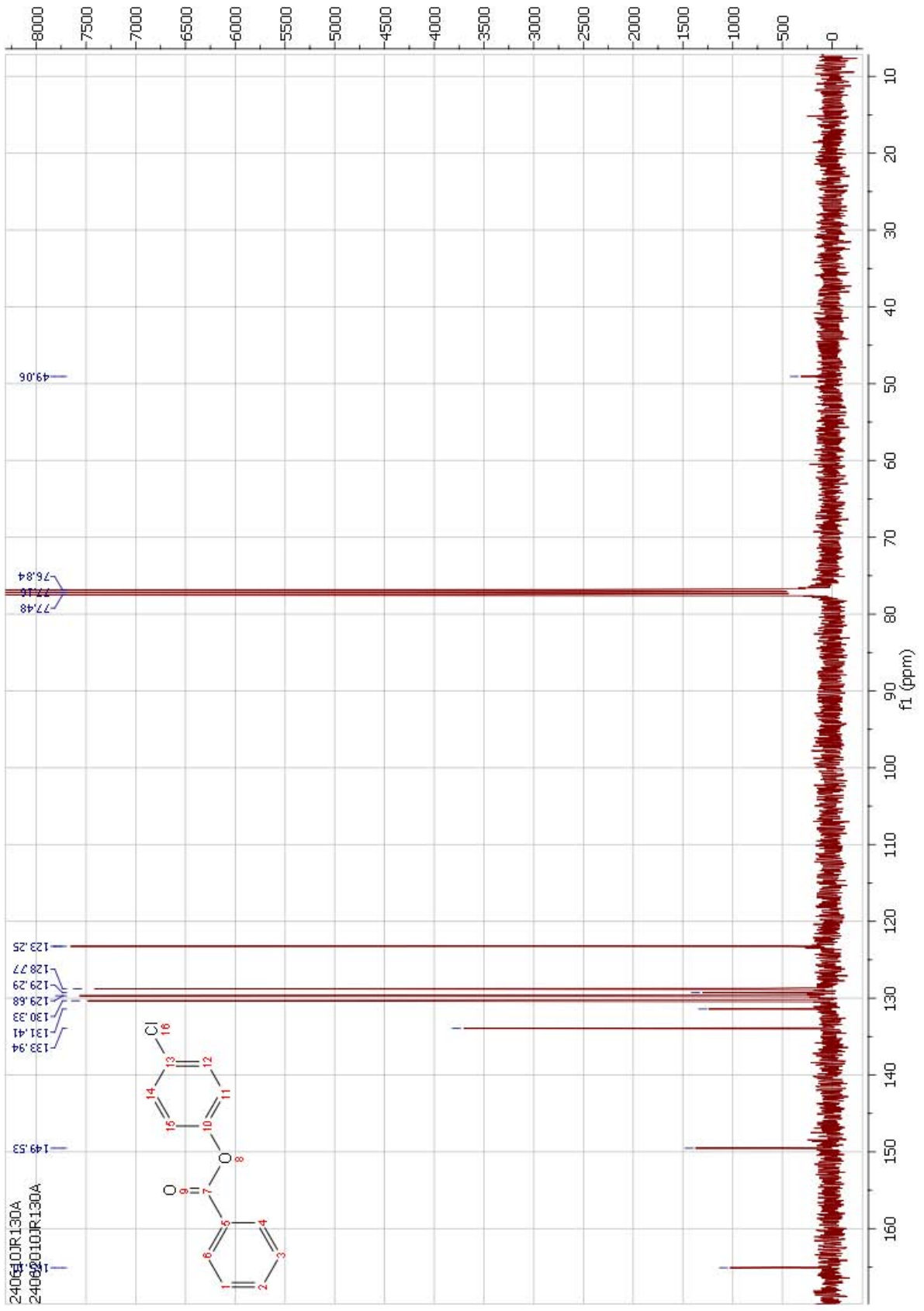

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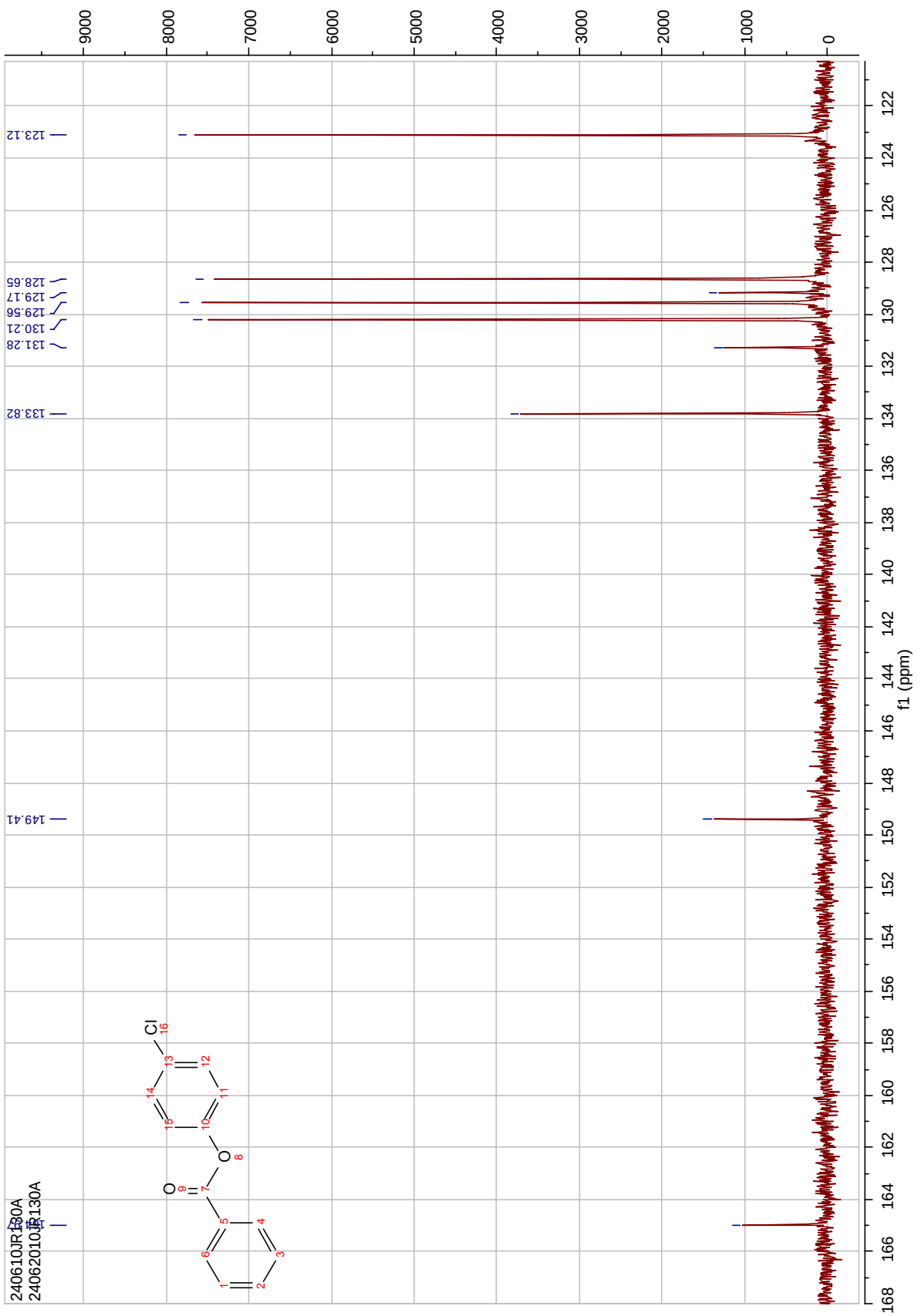

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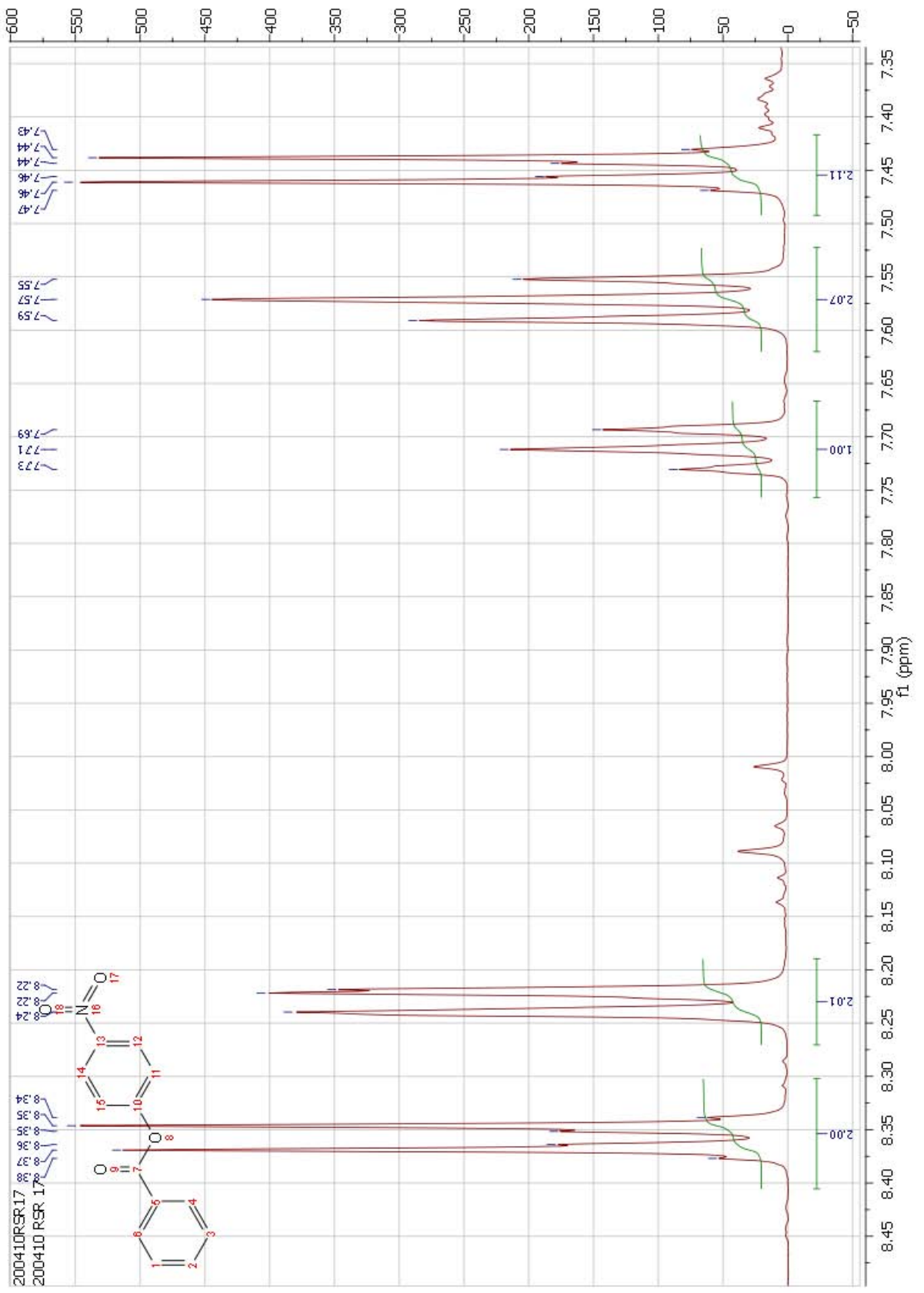

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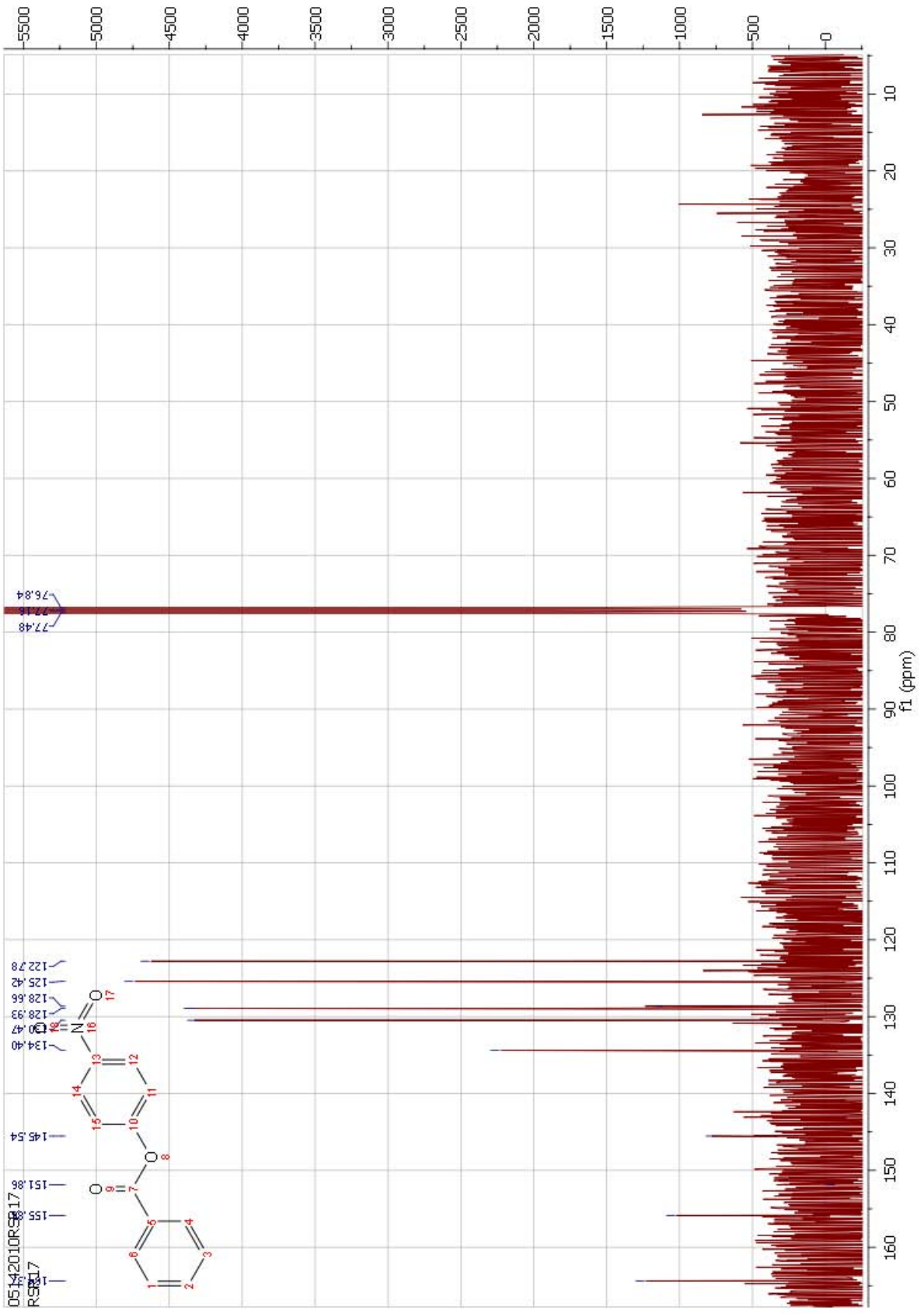

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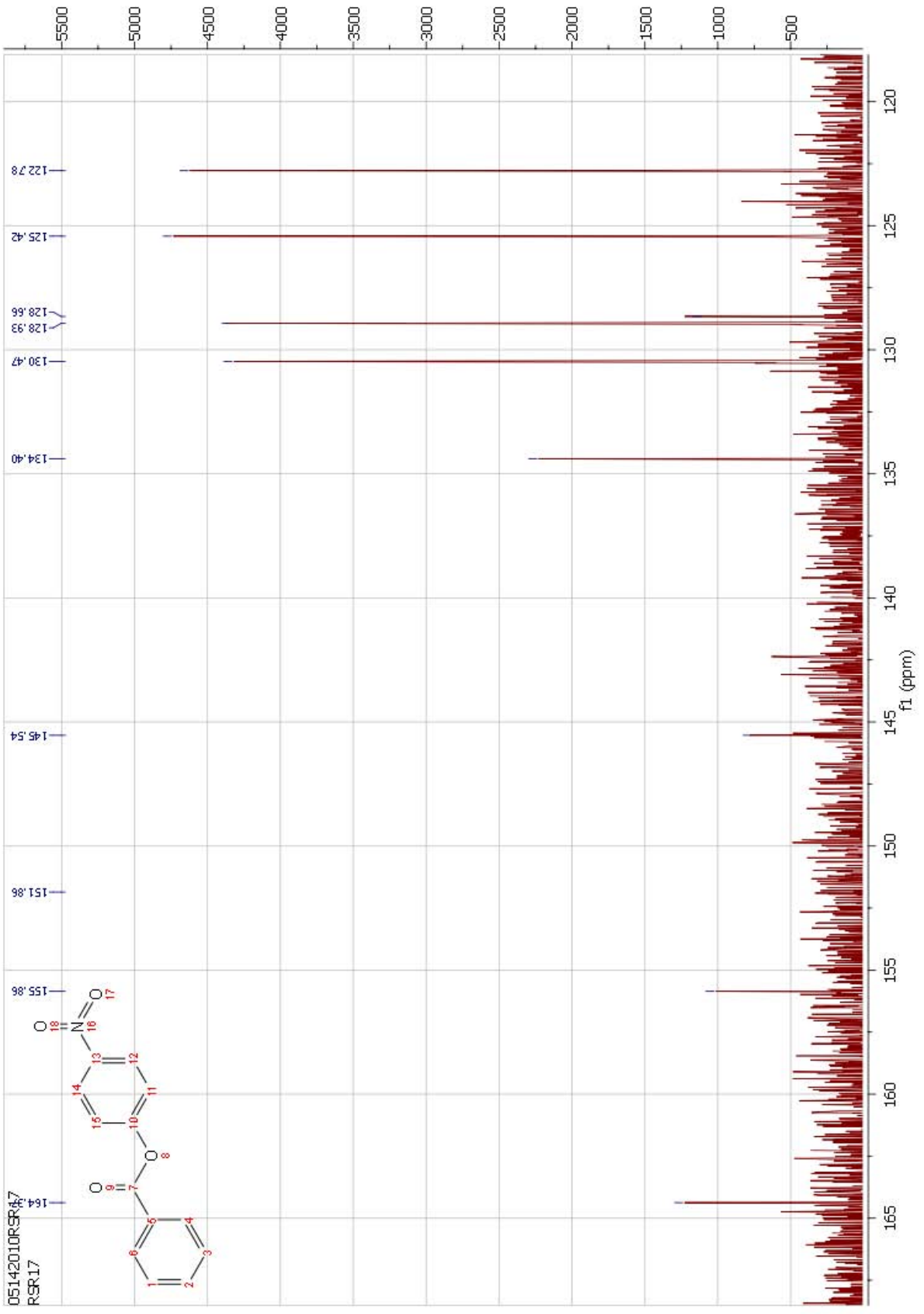

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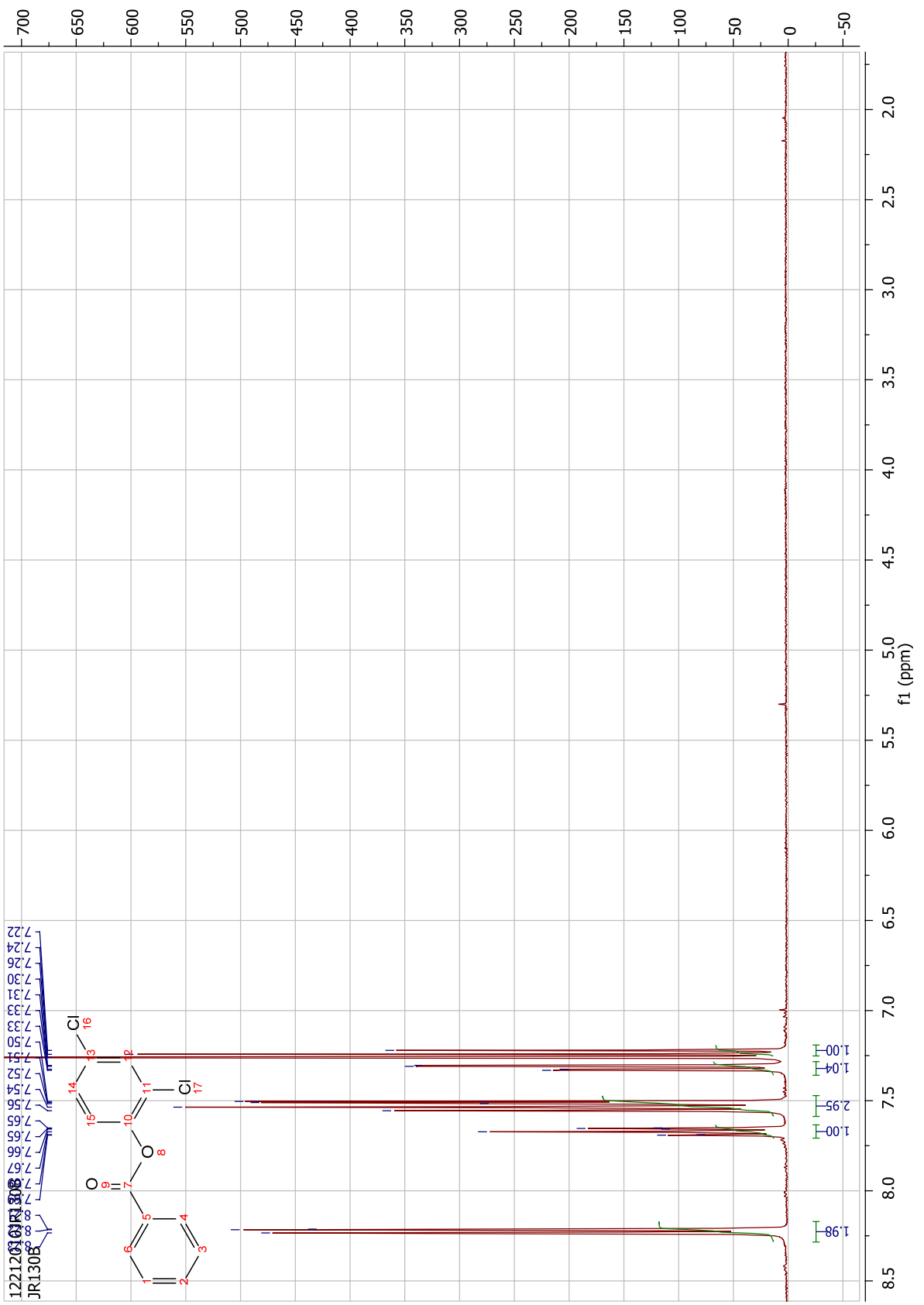

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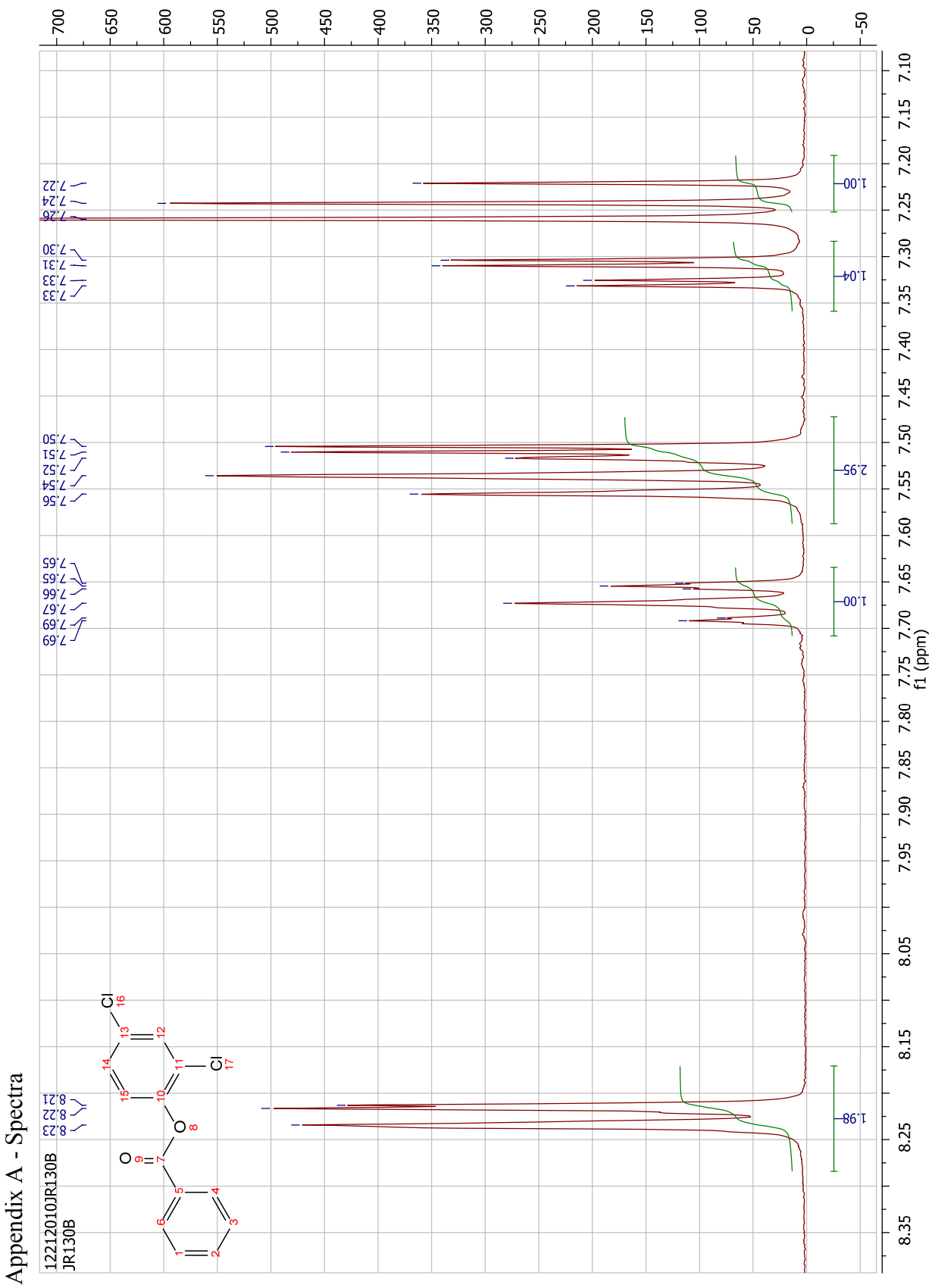

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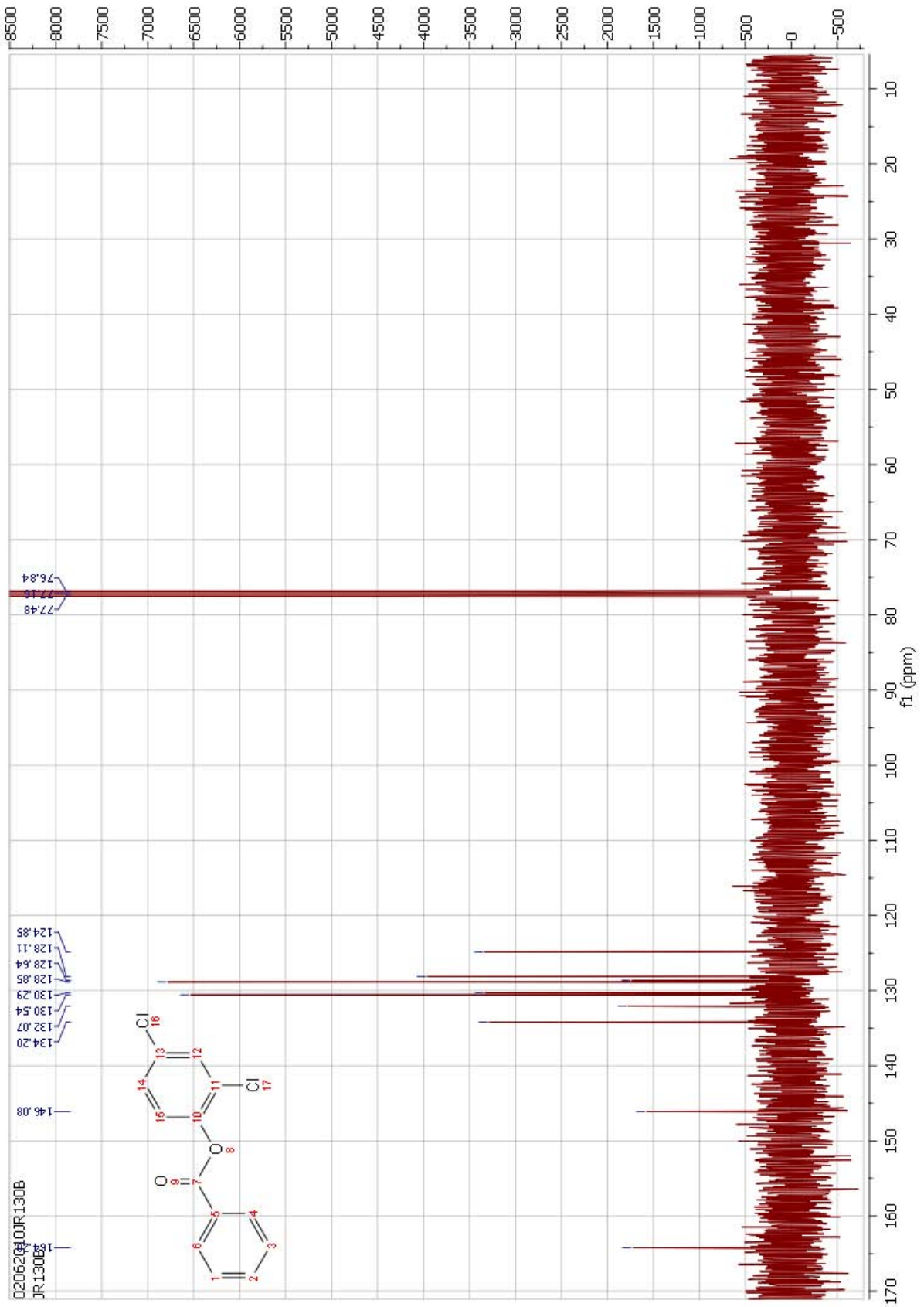

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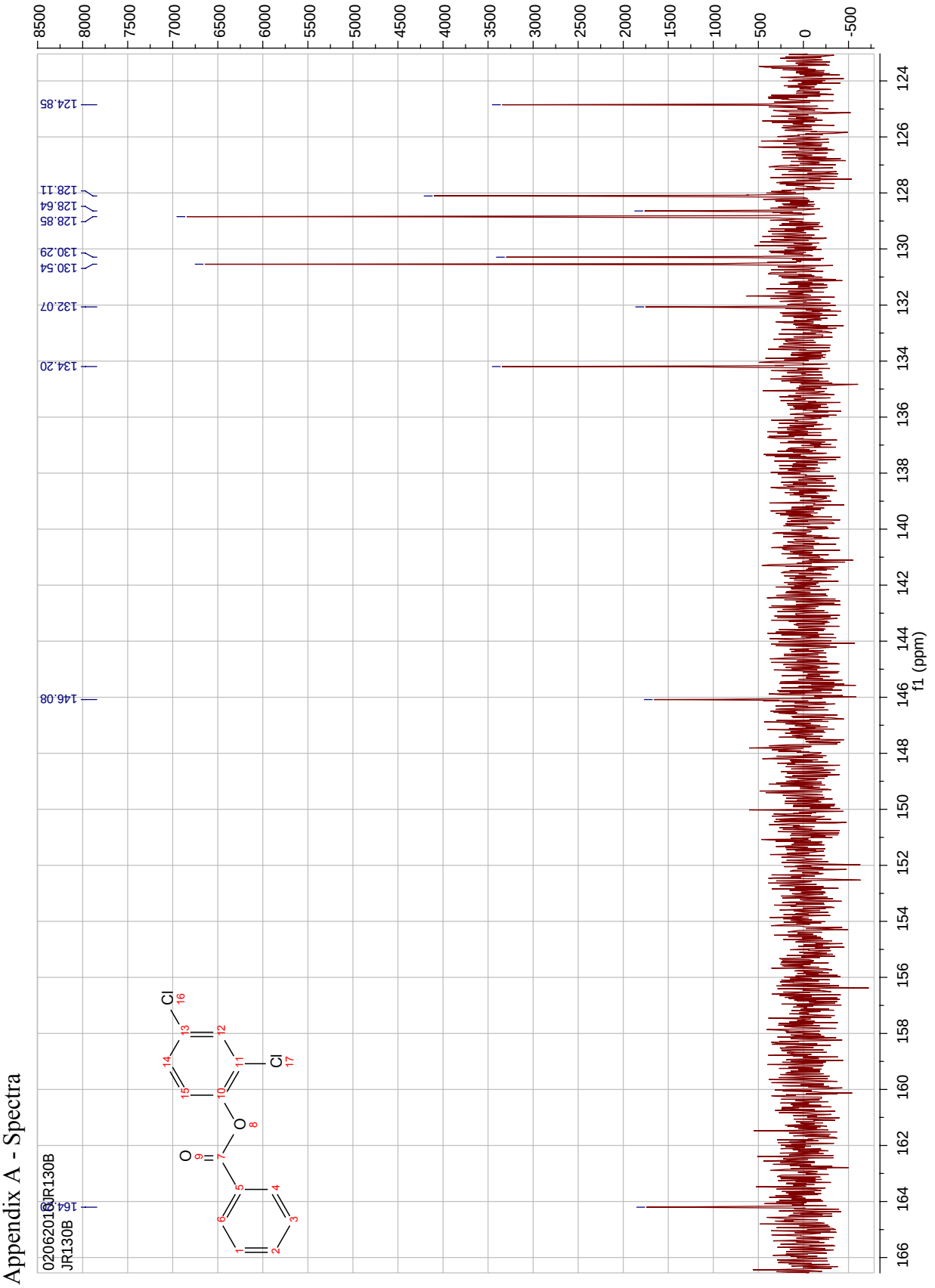

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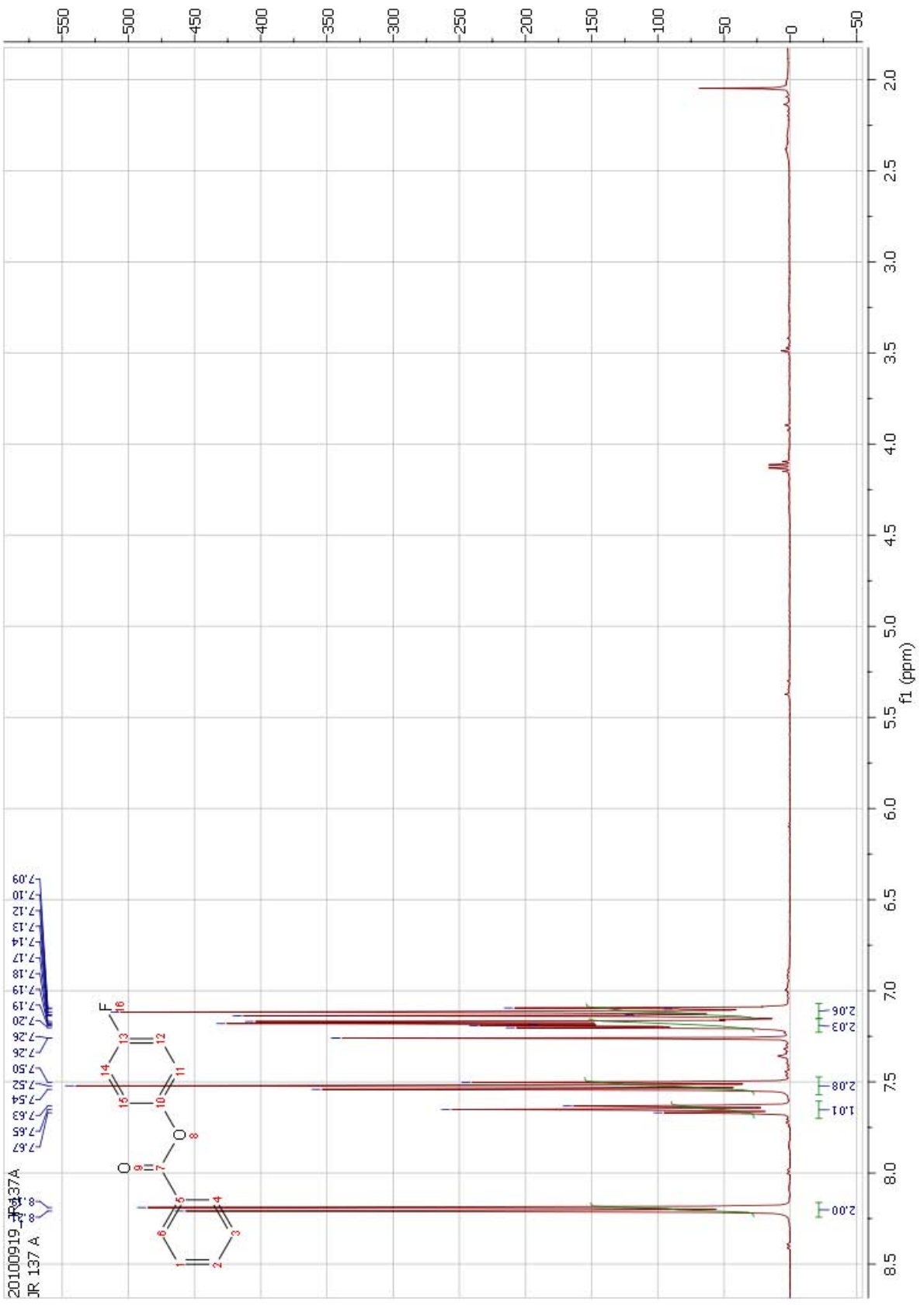
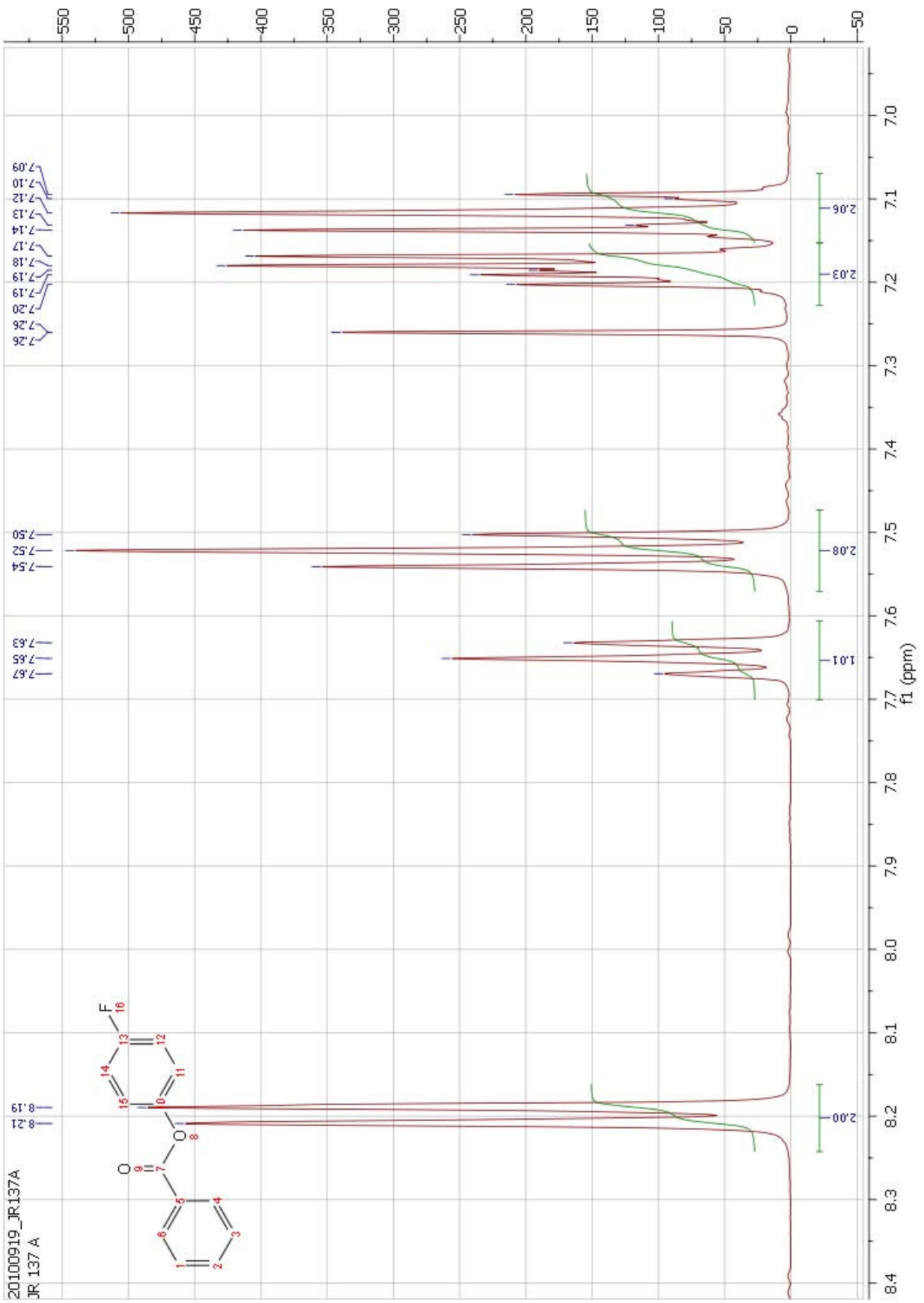
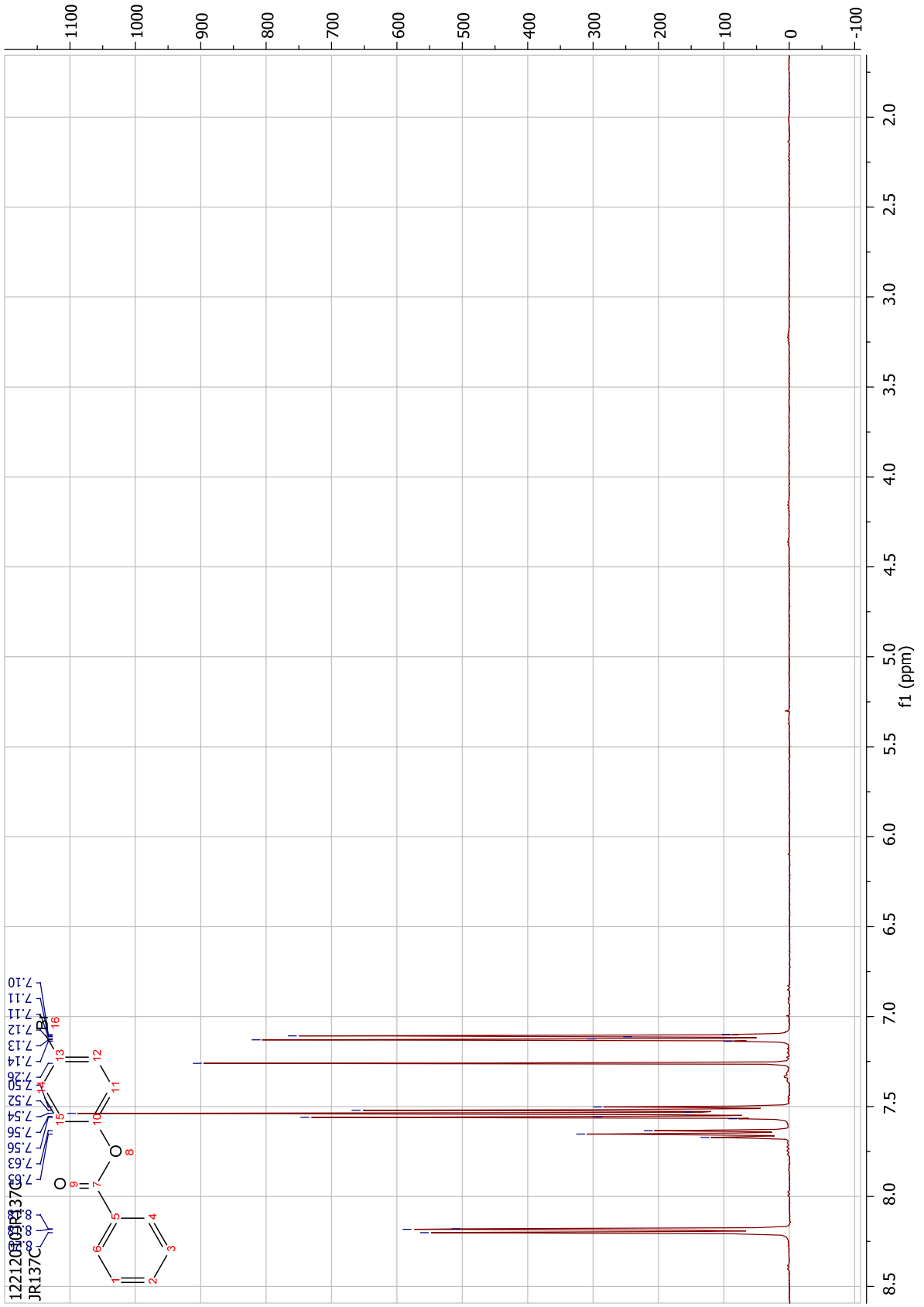


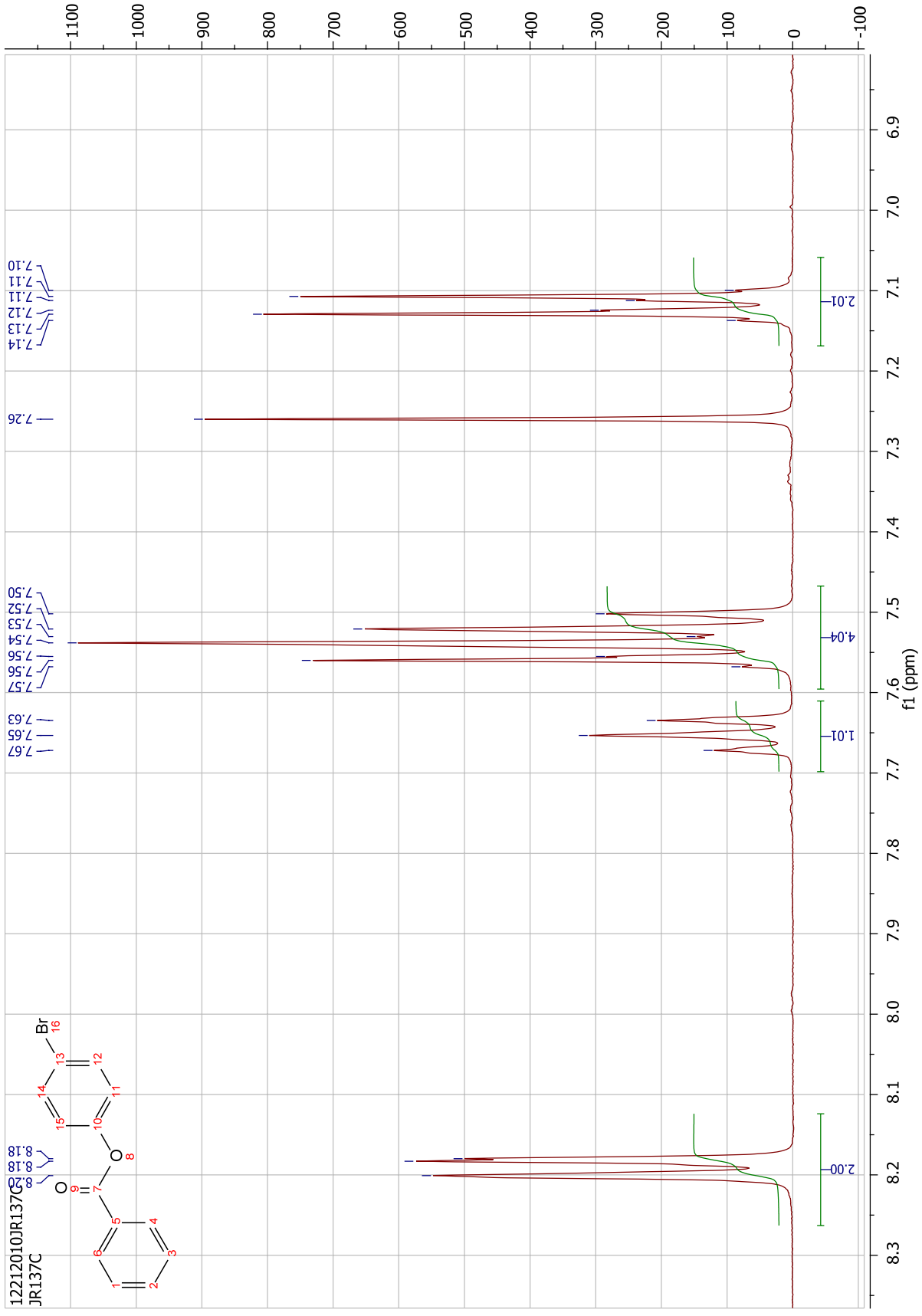
Appendix A - Spectra



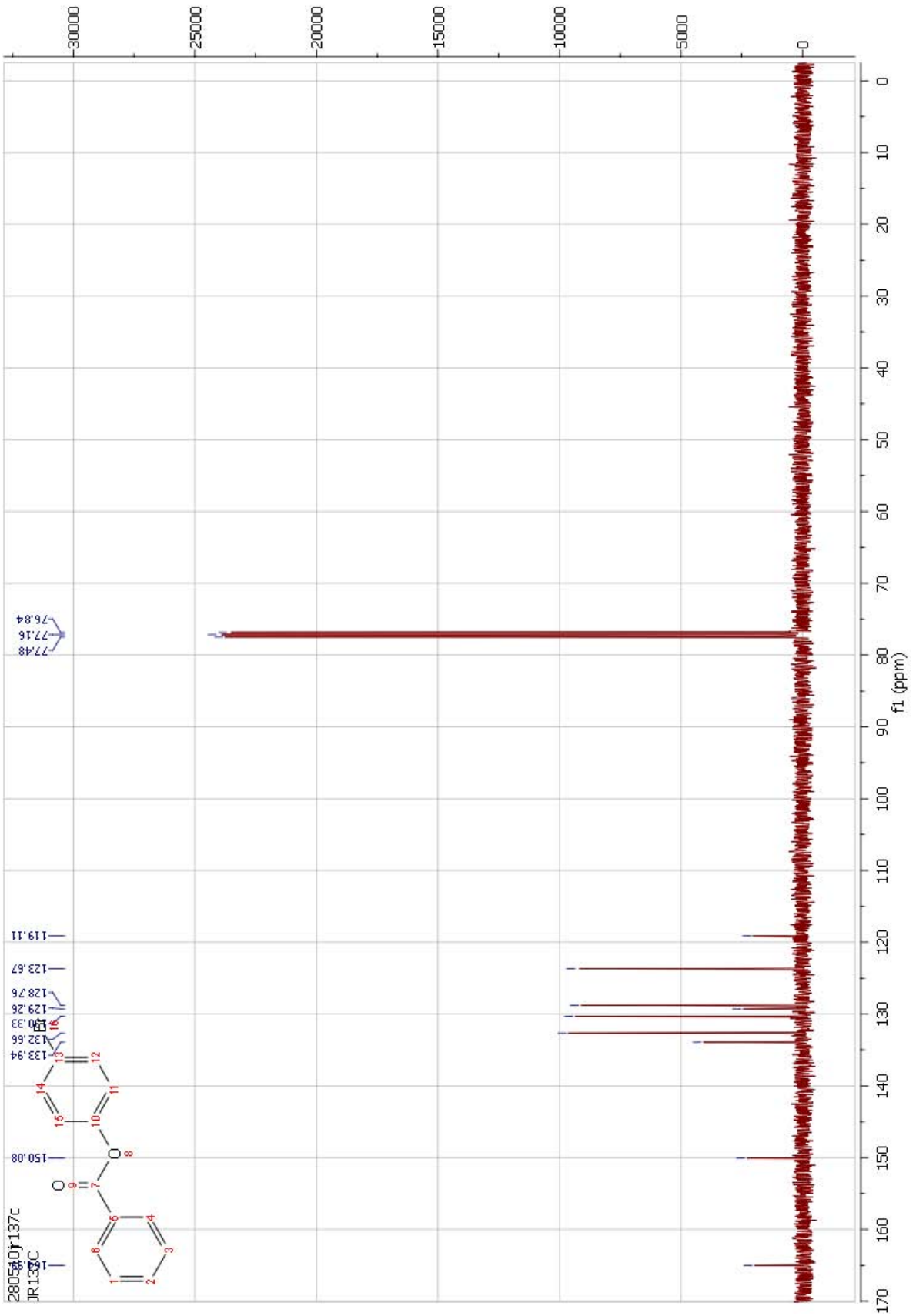
Appendix A - Spectra



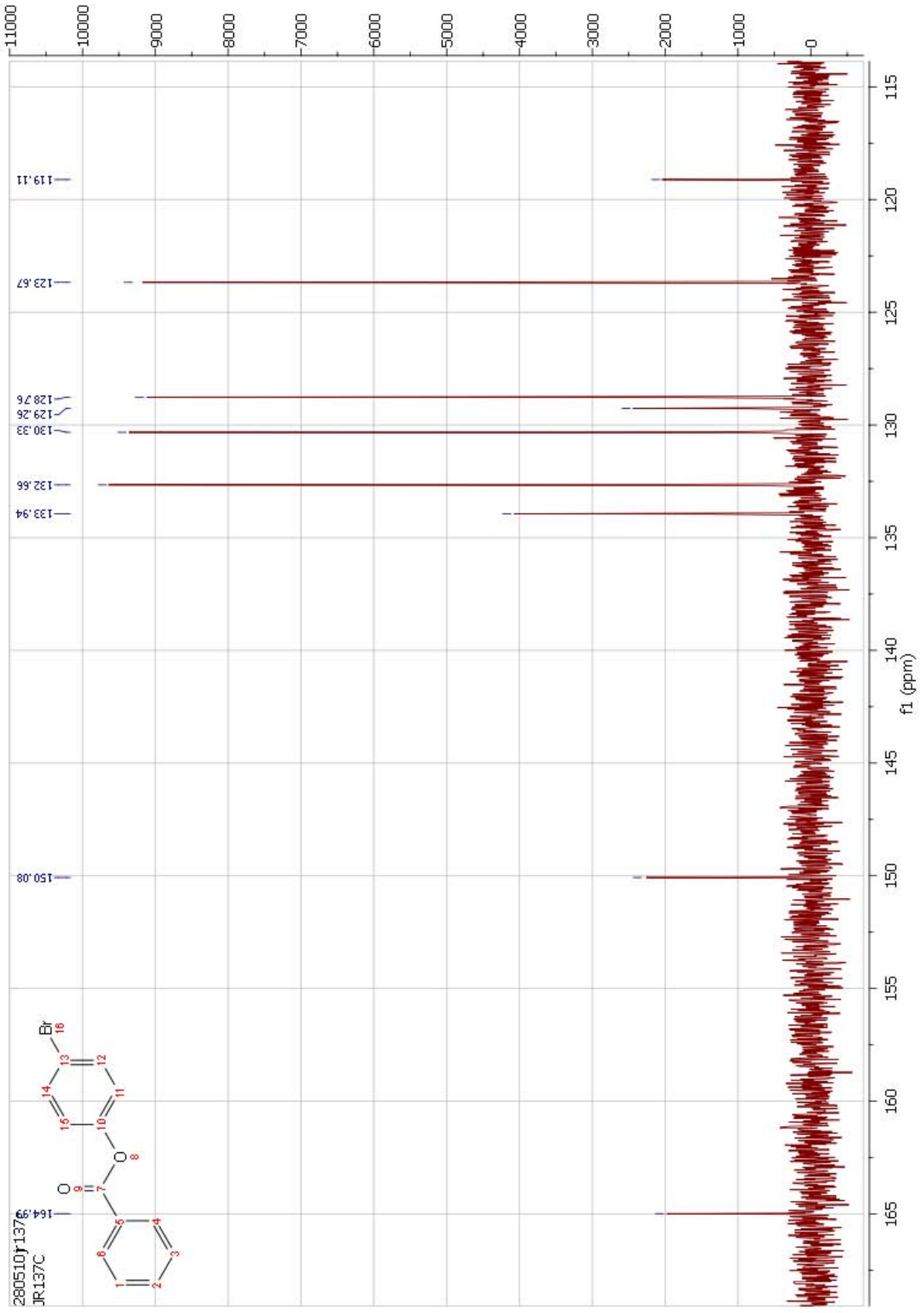
Appendix A - Spectra



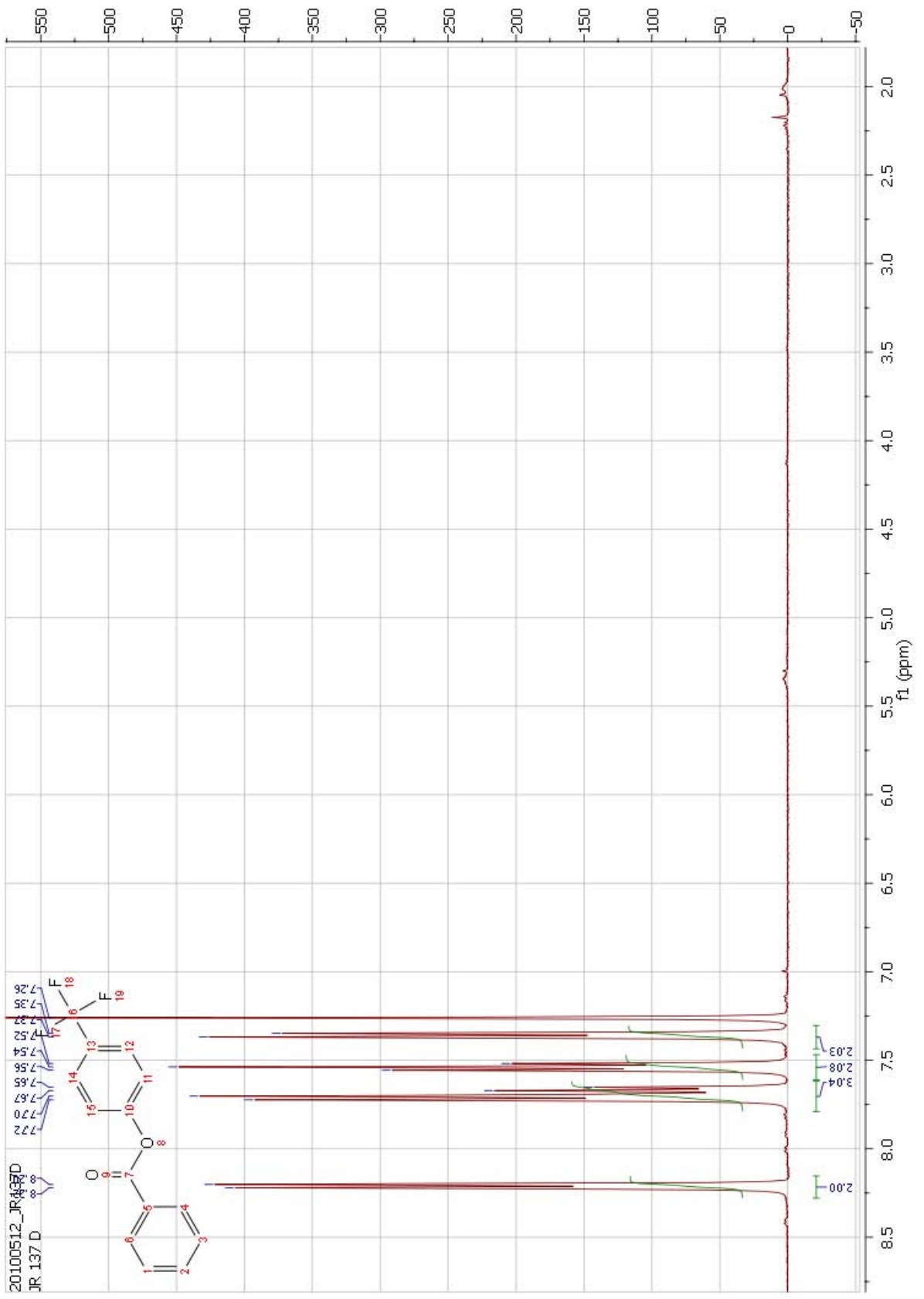
Appendix A - Spectra



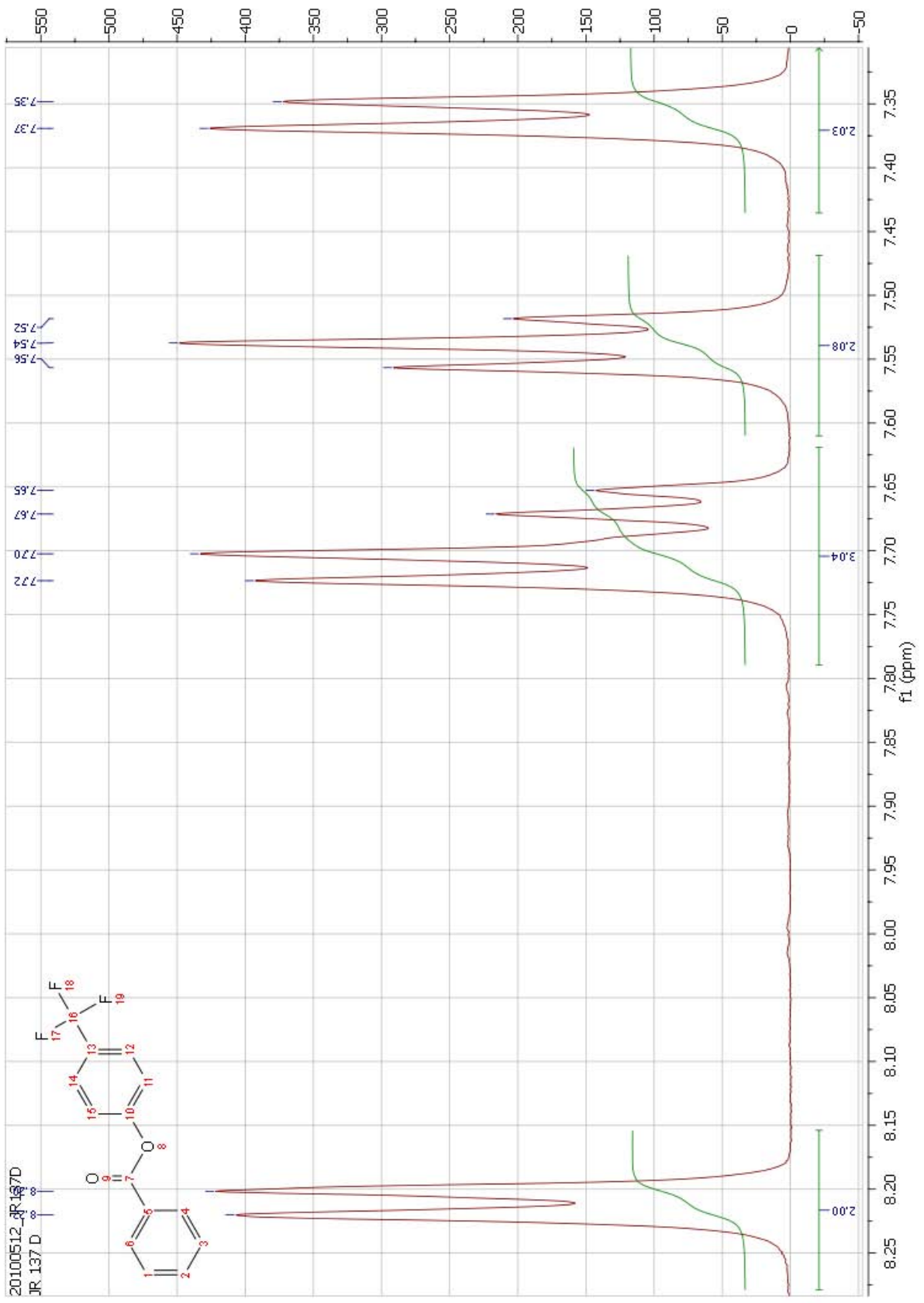
Appendix A - Spectra



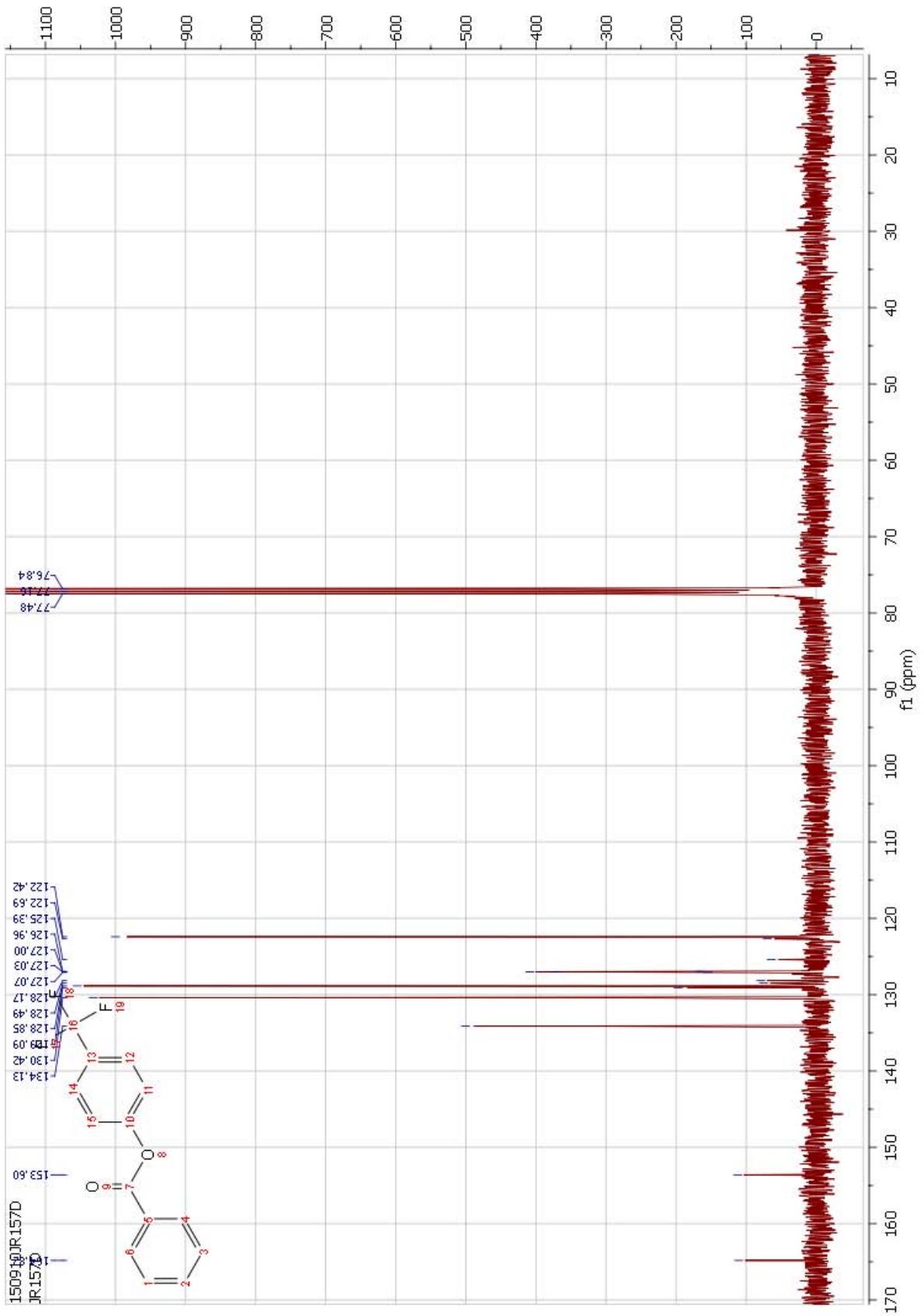
Appendix A - Spectra



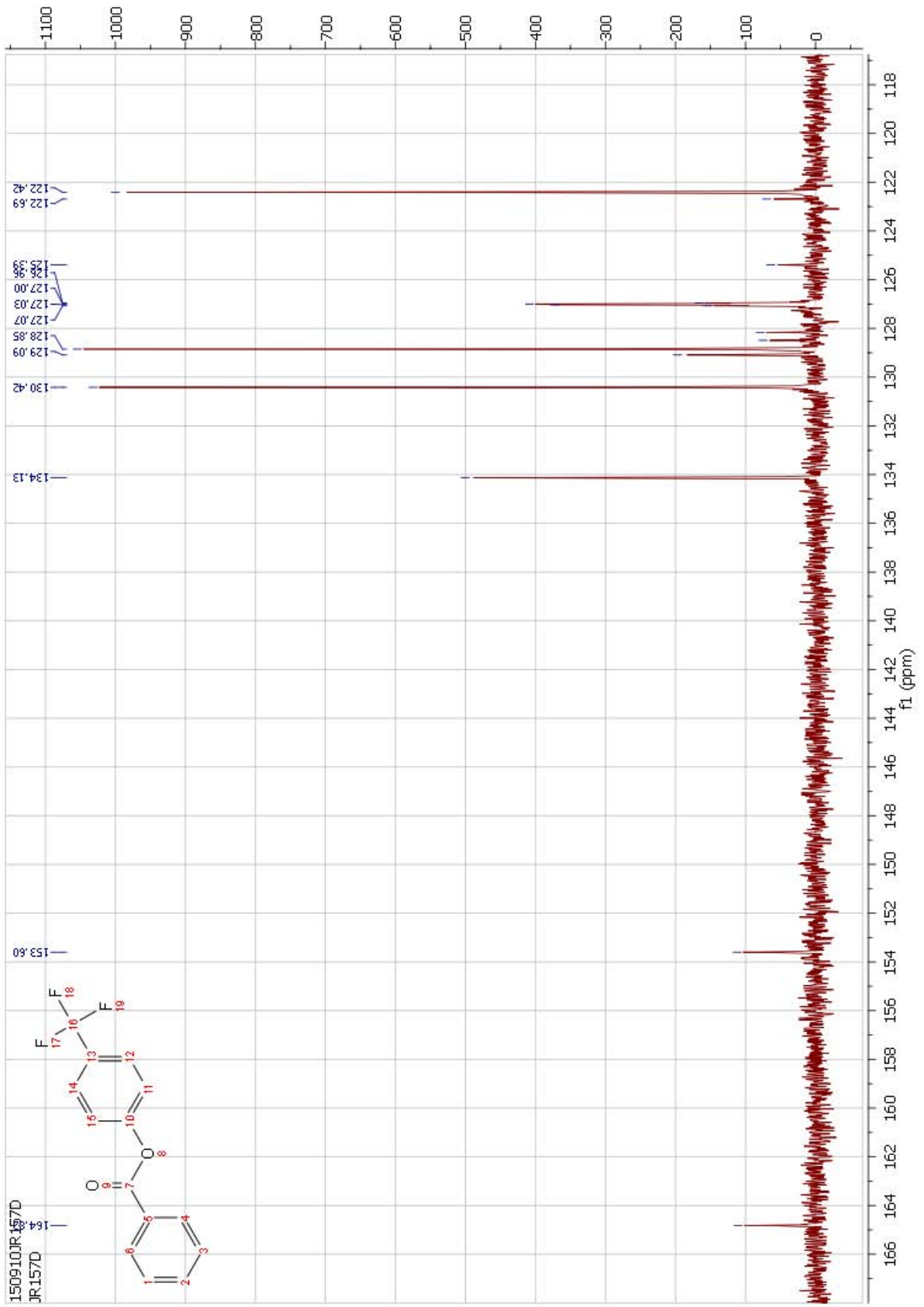
Appendix A - Spectra



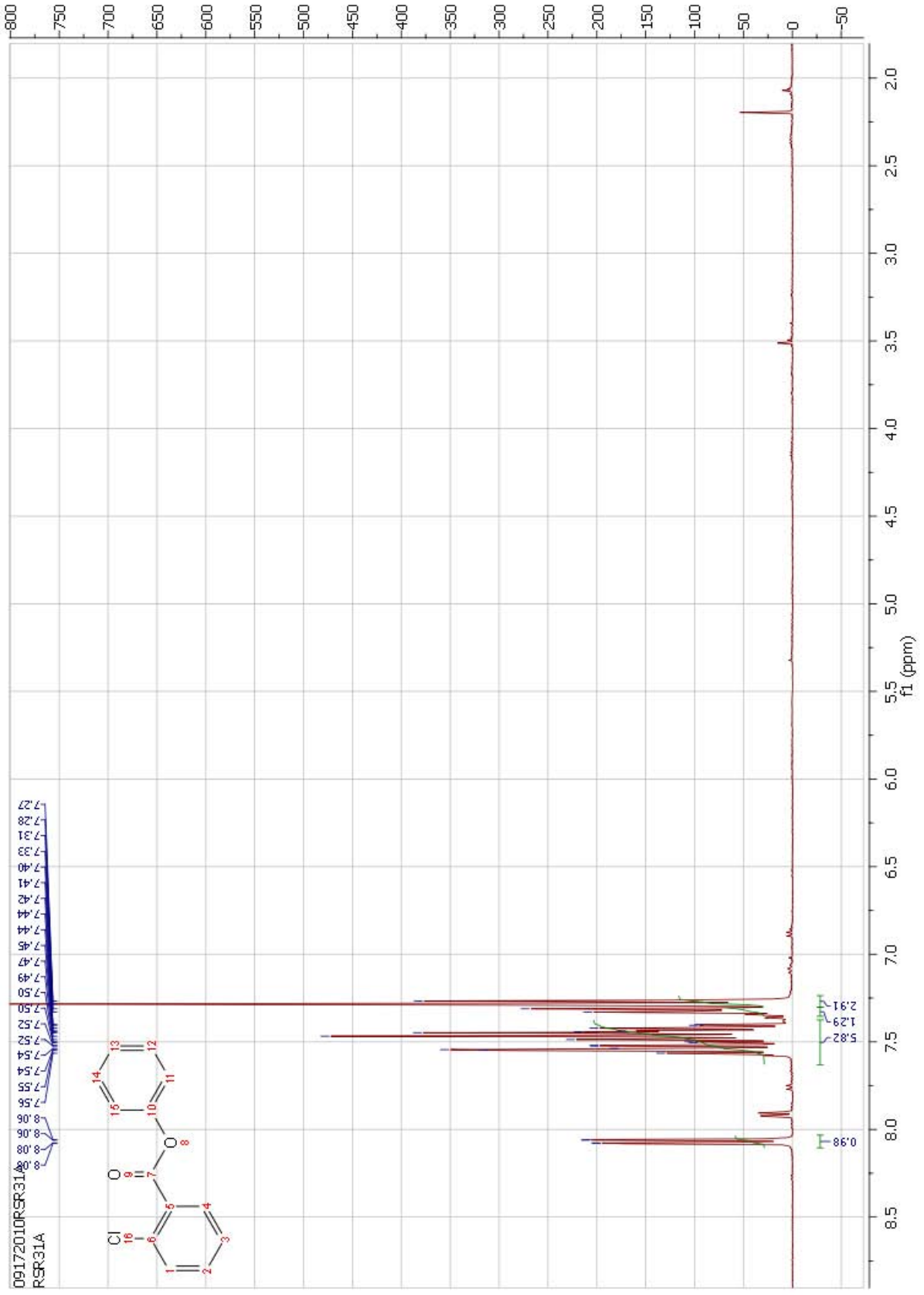
Appendix A - Spectra



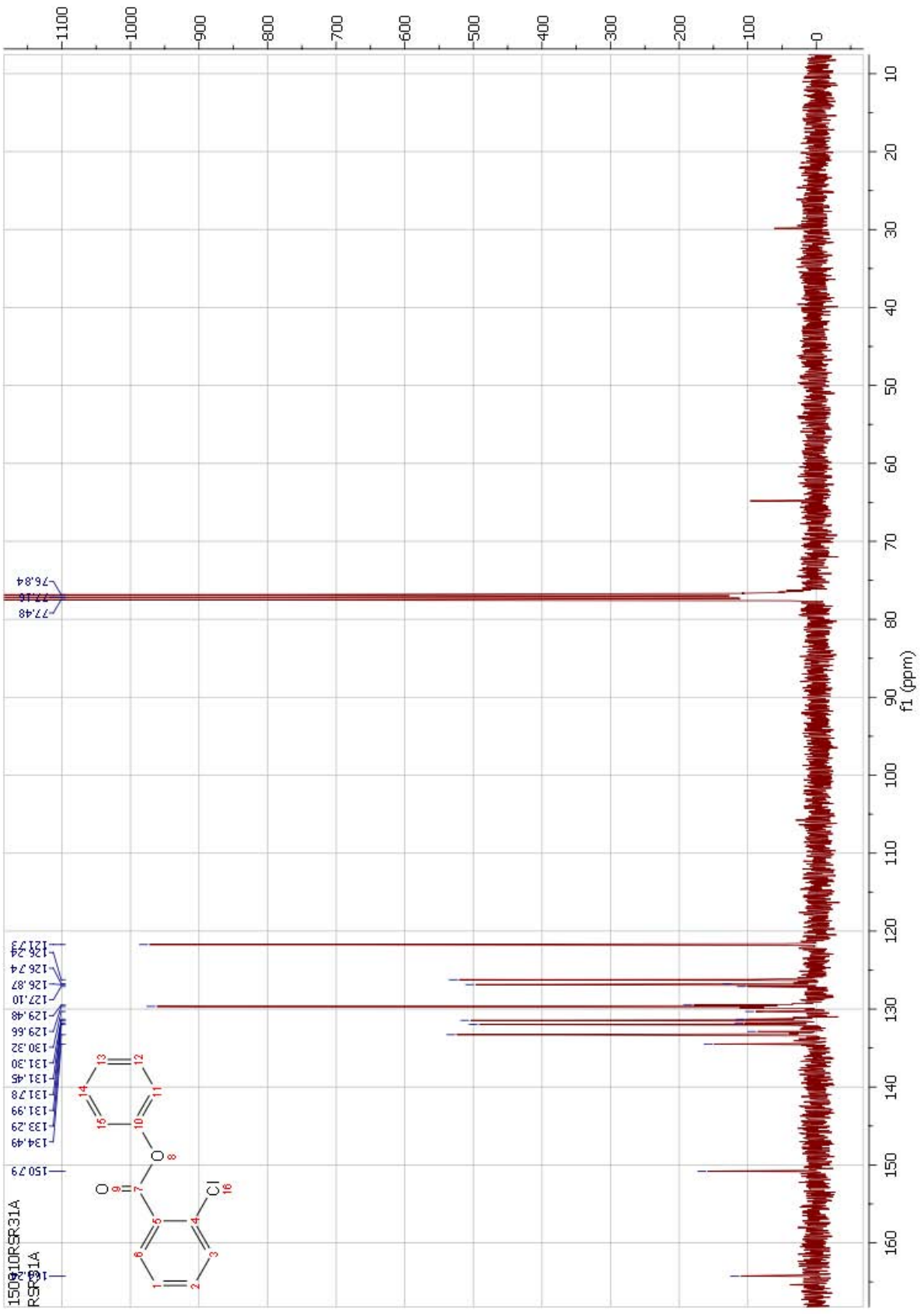
Appendix A - Spectra



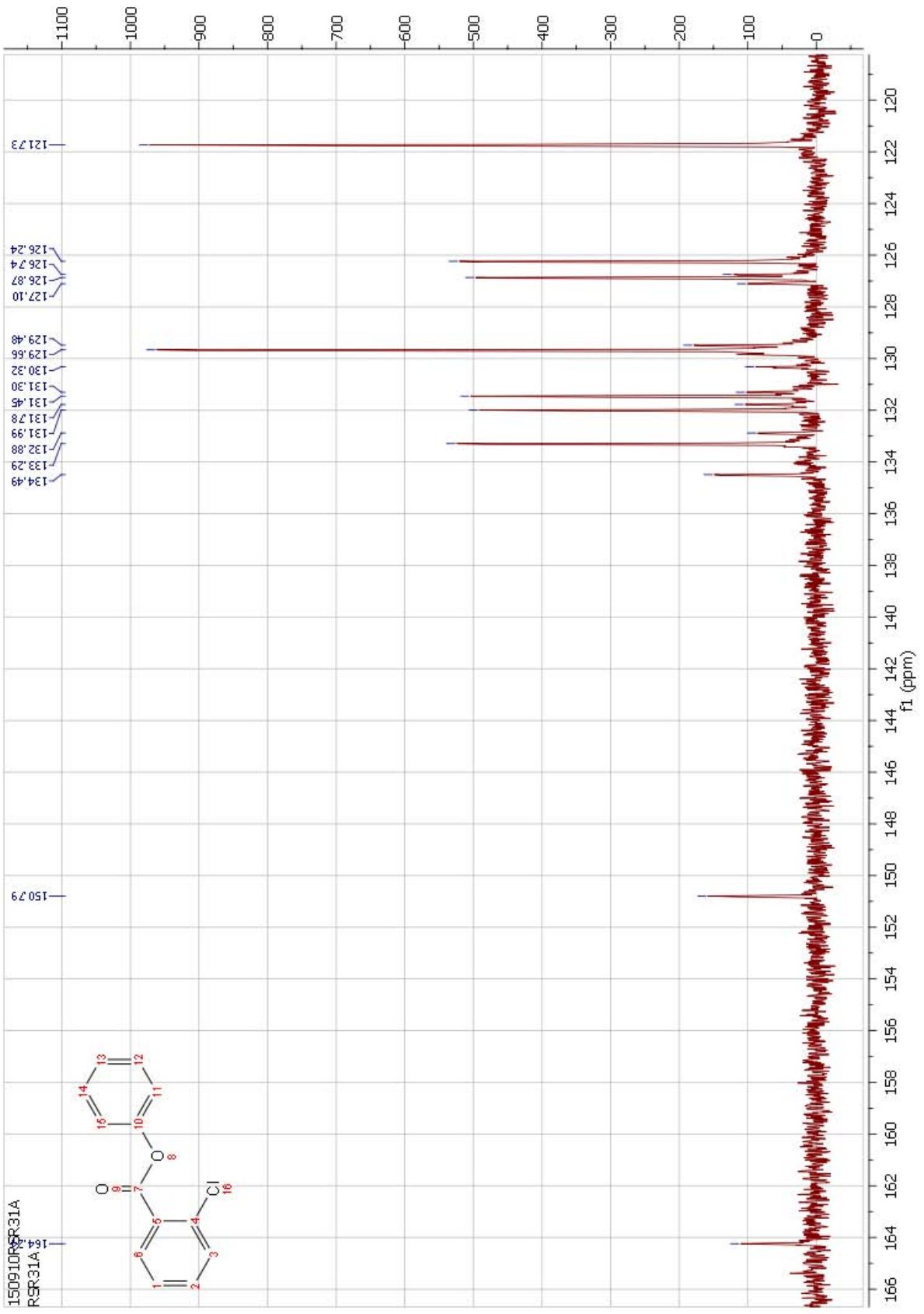
Appendix A - Spectra



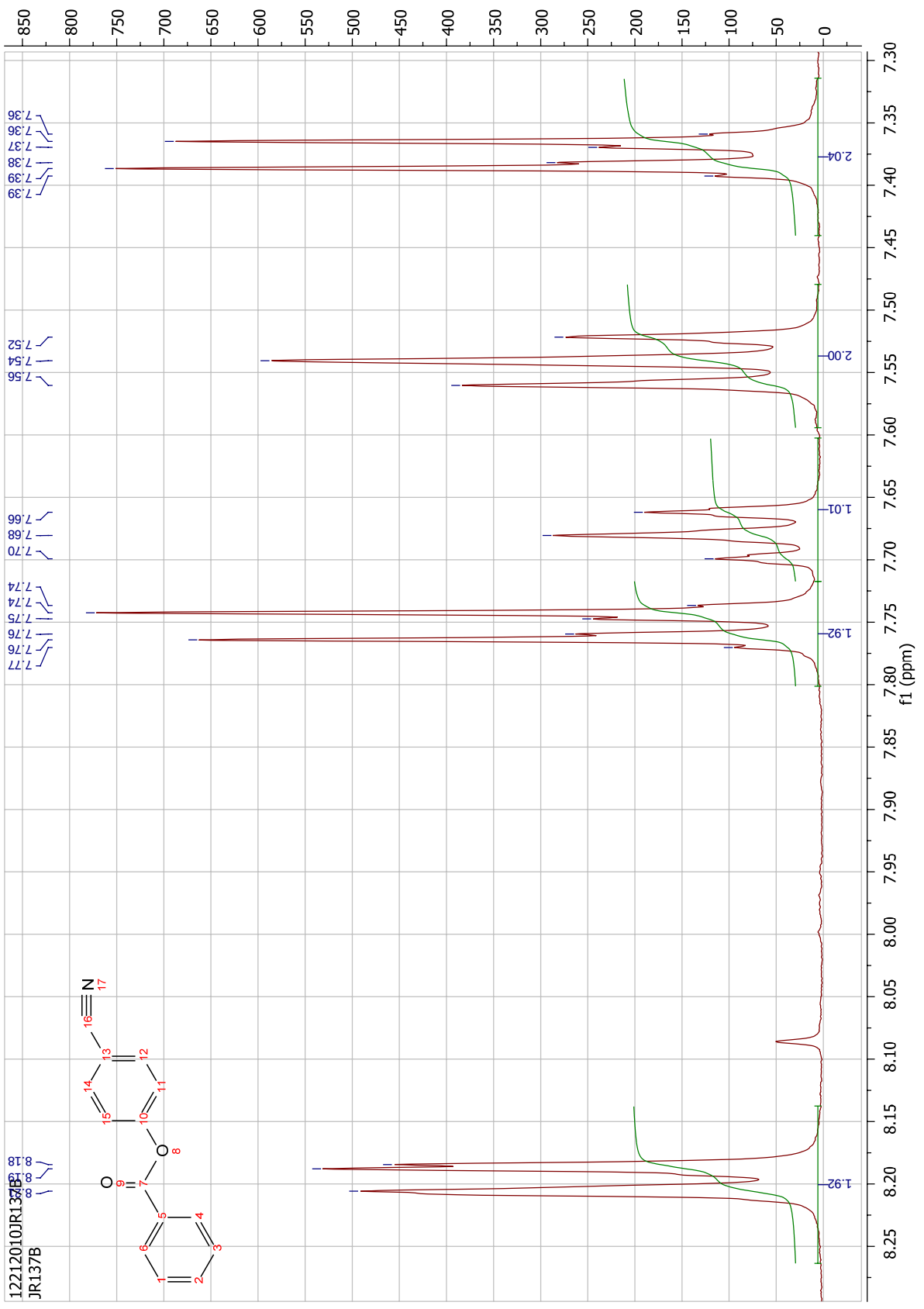
Appendix A - Spectra



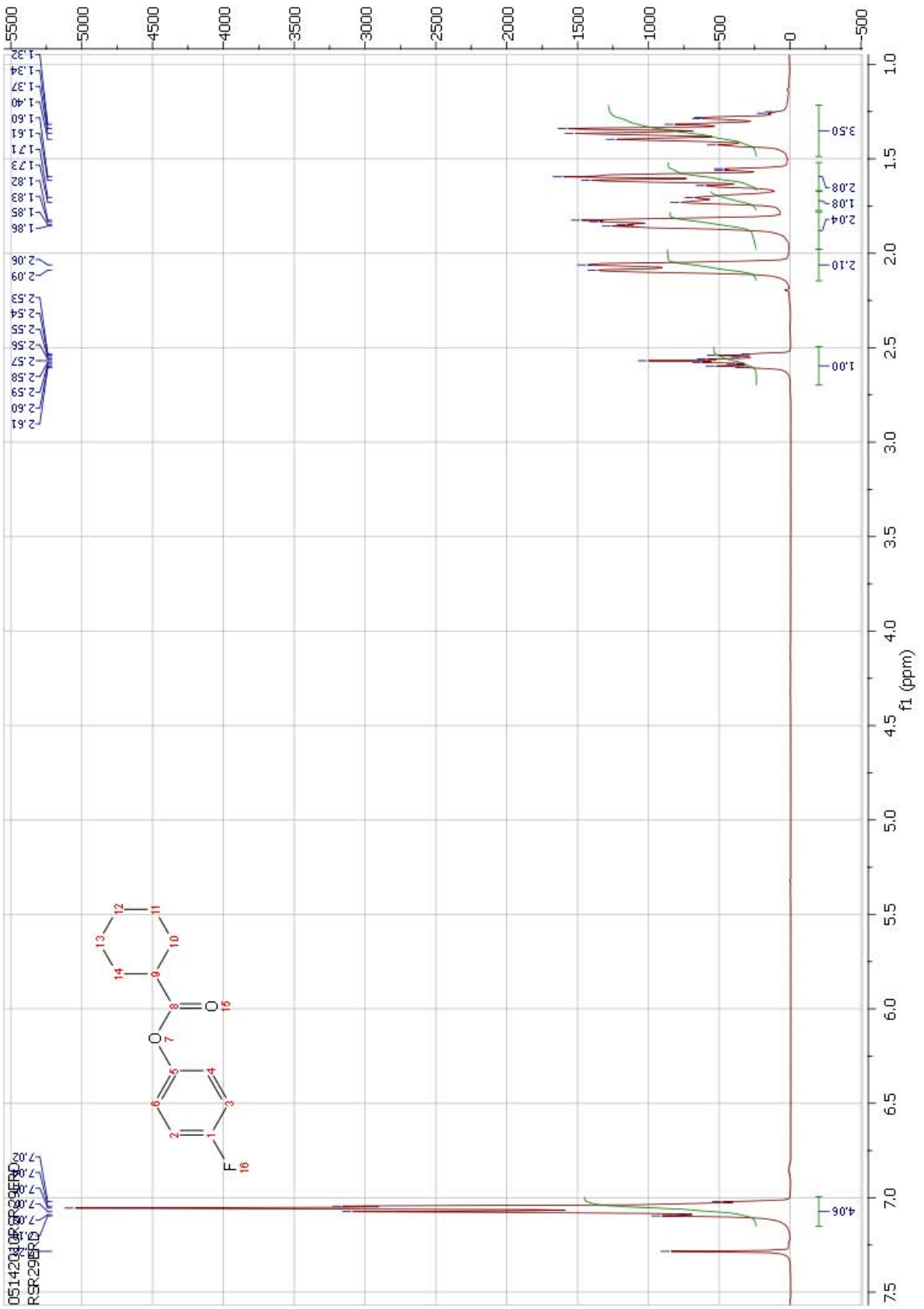
Appendix A - Spectra



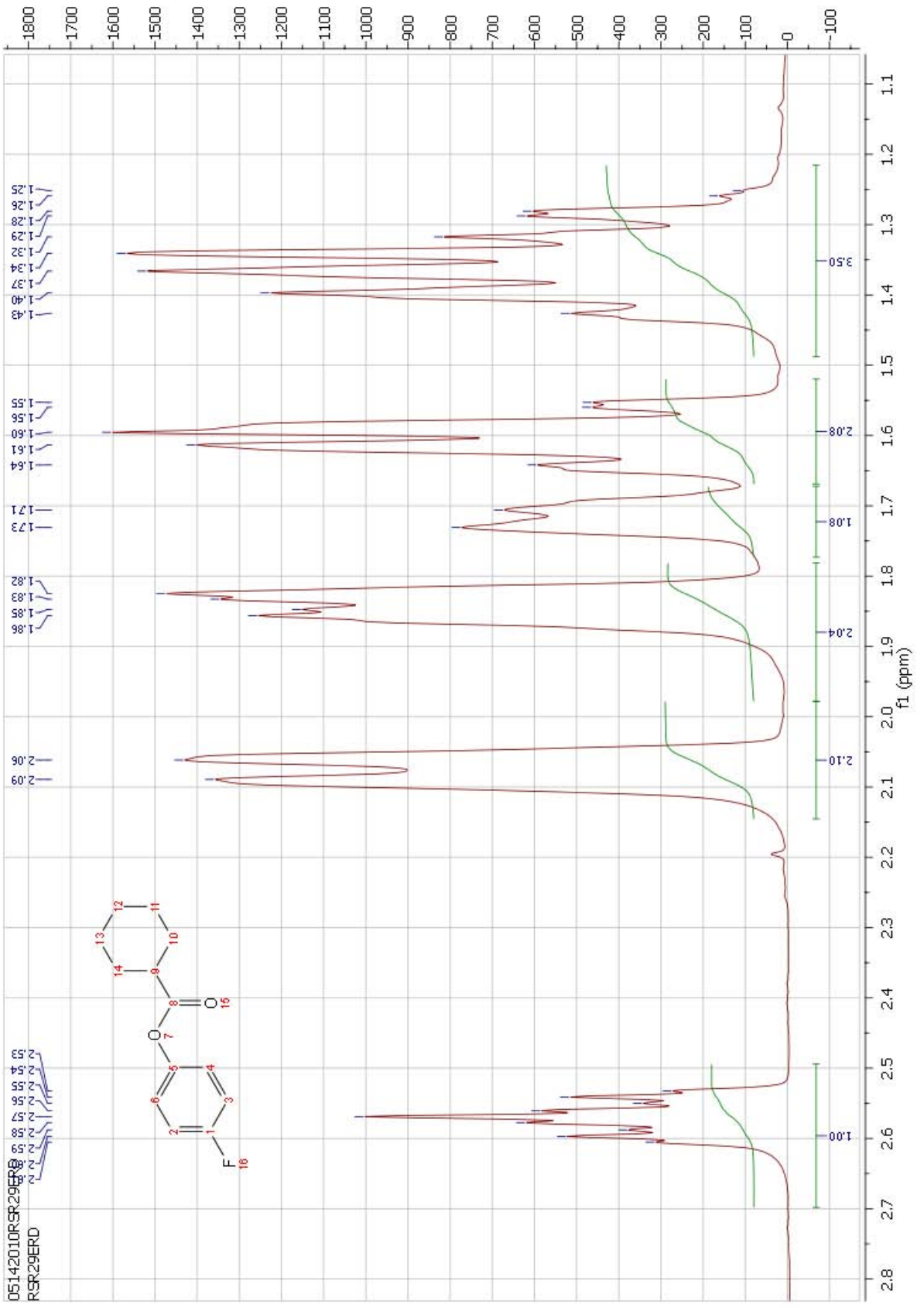
Appendix A - Spectra



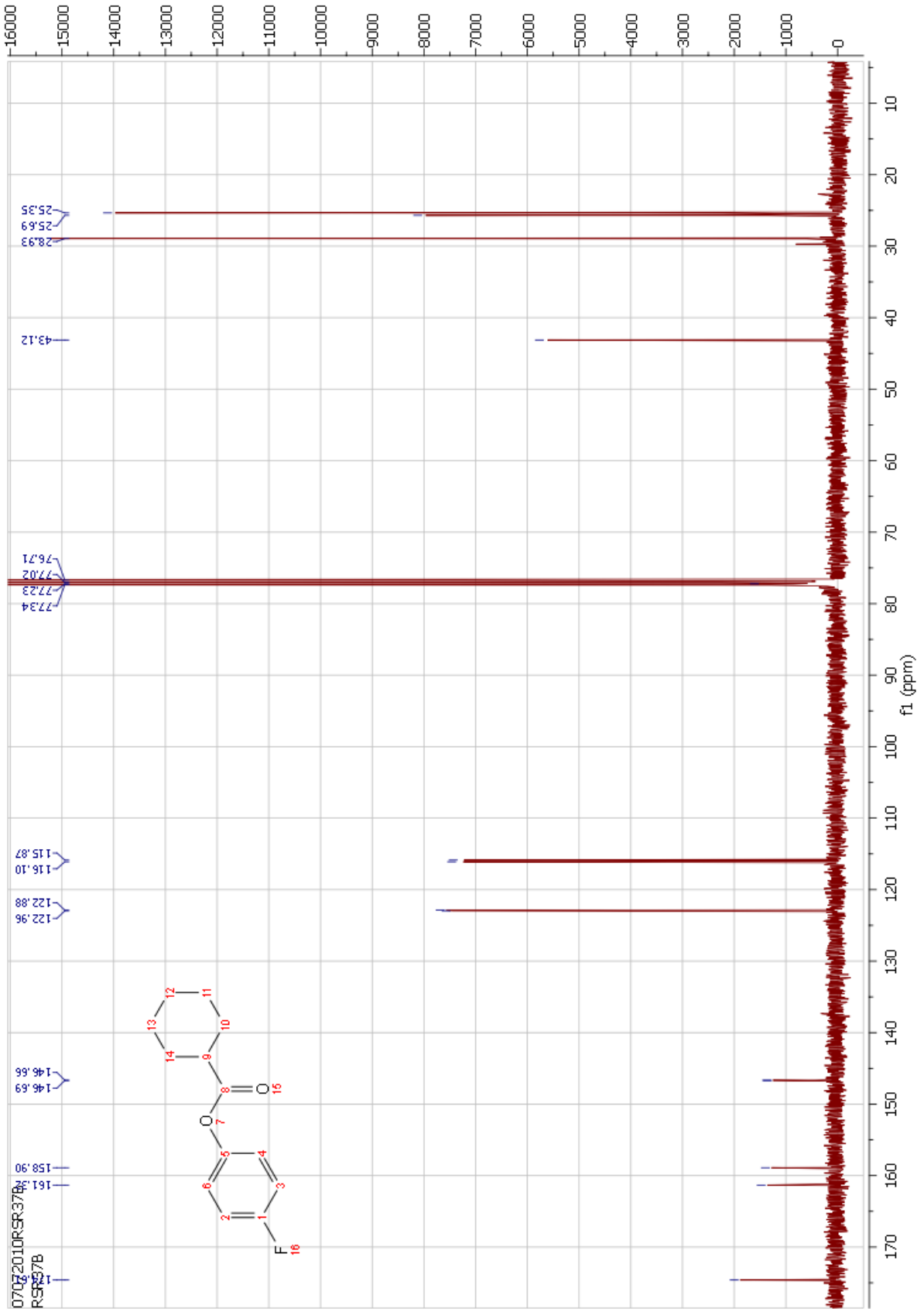
Appendix A - Spectra



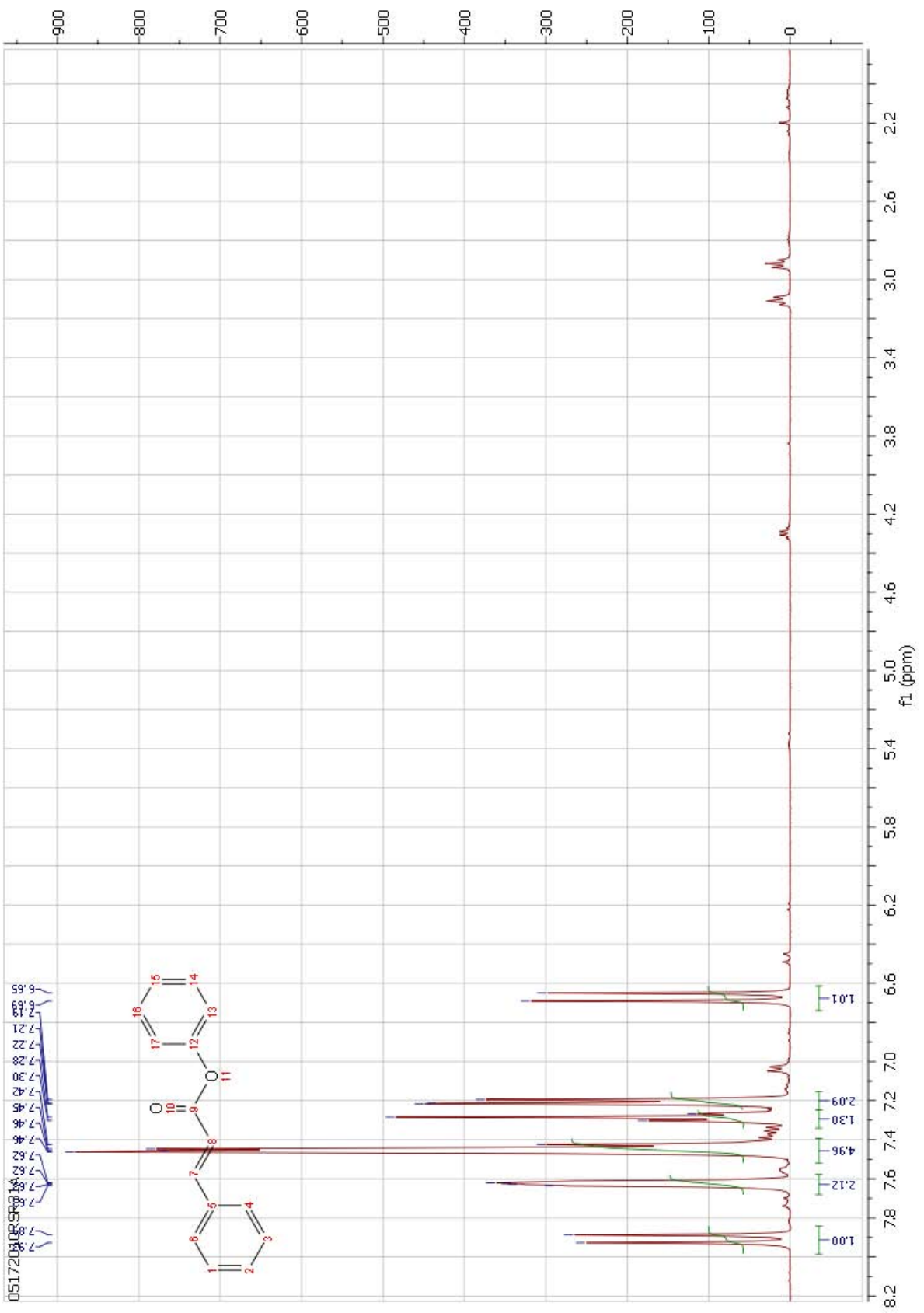
Appendix A - Spectra



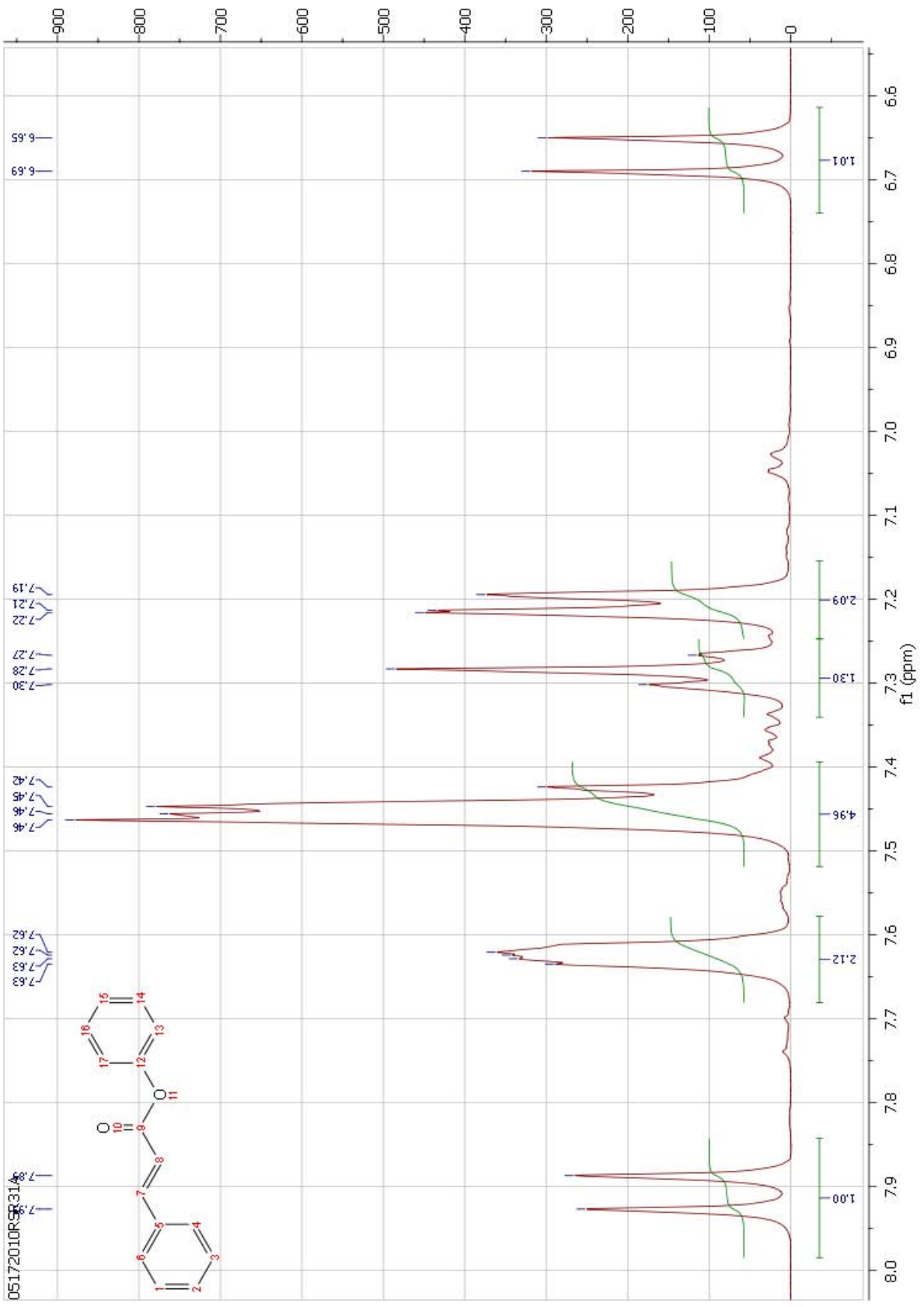
Appendix A - Spectra



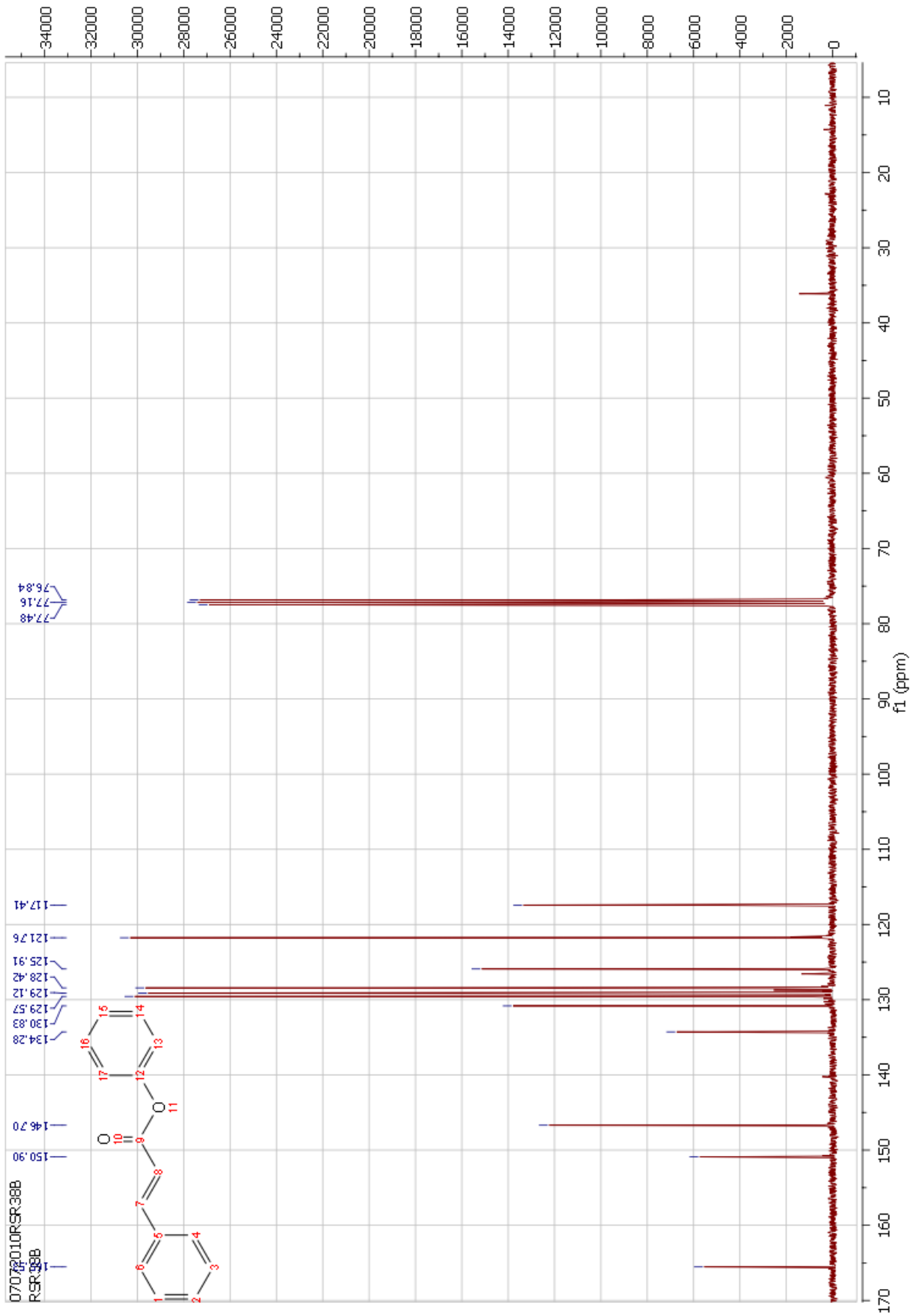
Appendix A - Spectra



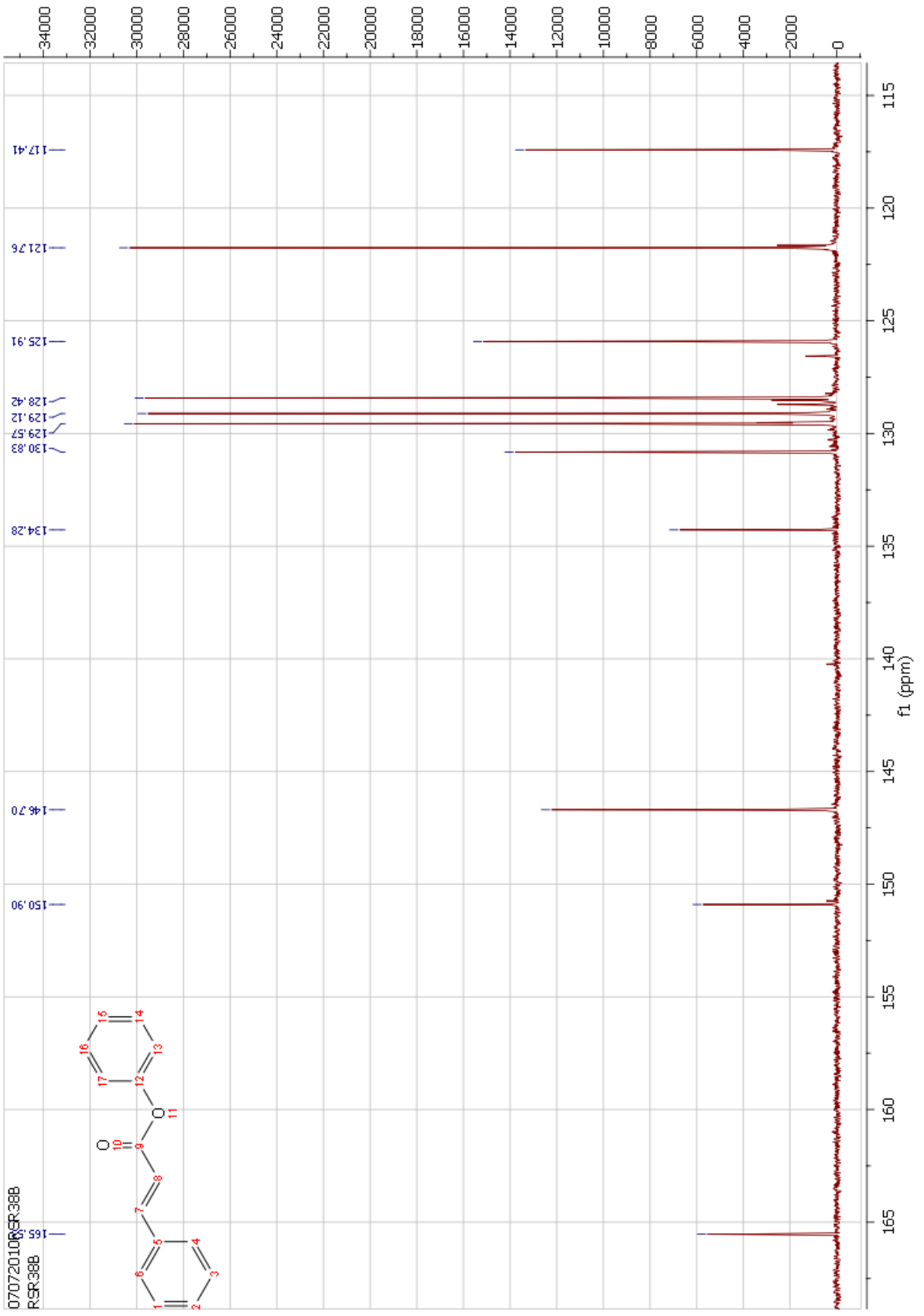
Appendix A - Spectra



Appendix A - Spectra

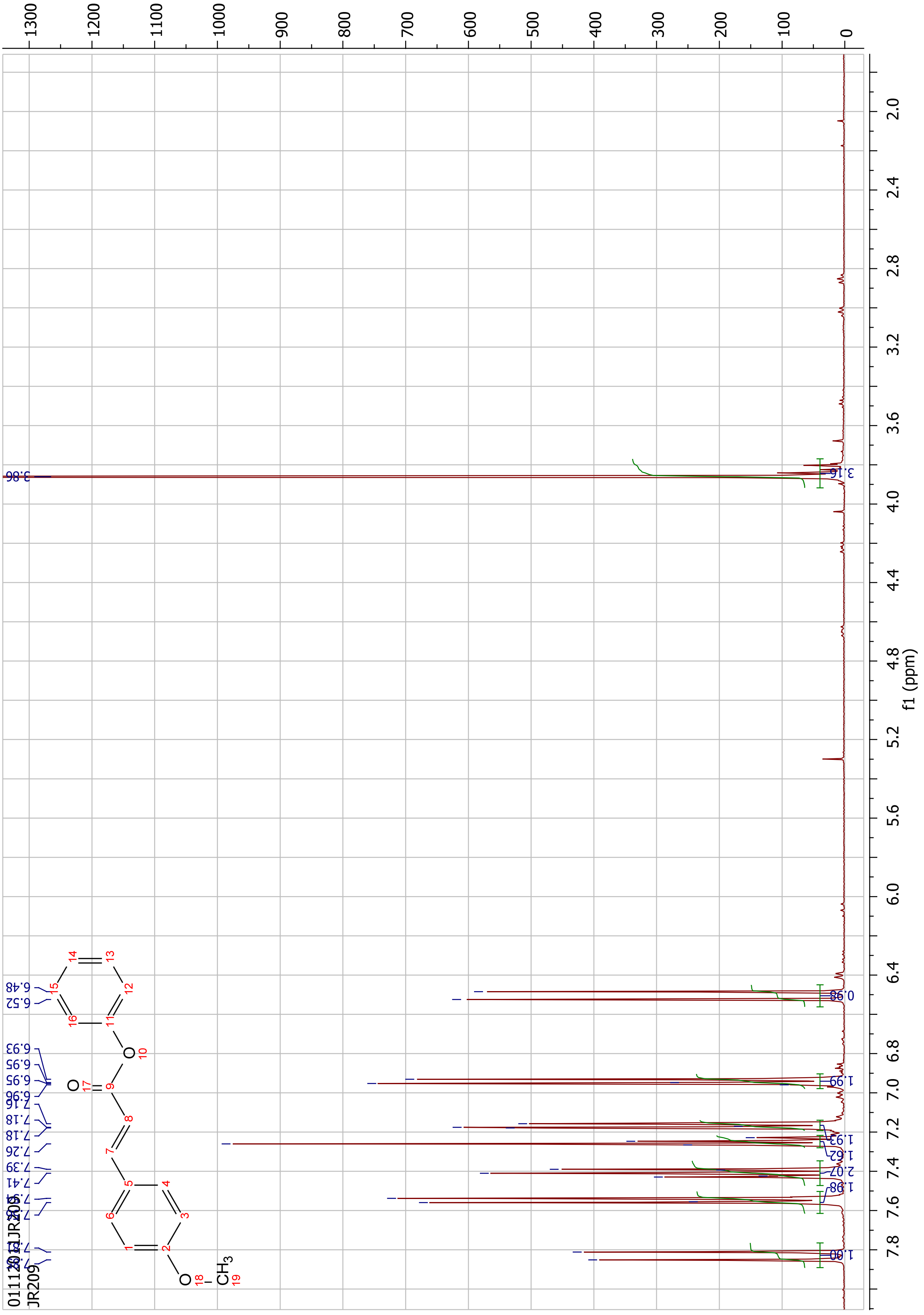


Appendix A - Spectra

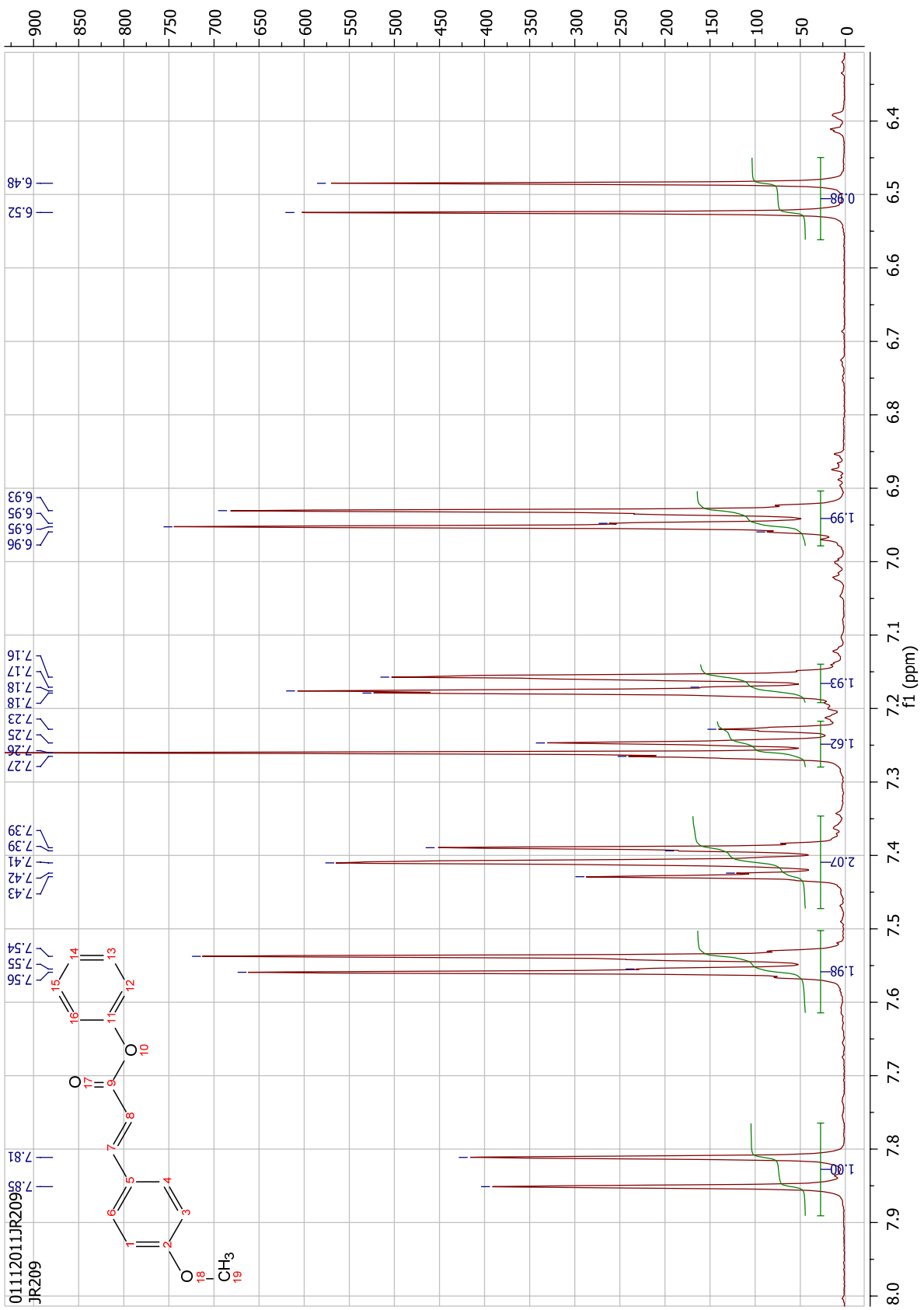


Supplementary Material (ESI) for Organic & Biomolecular Chemistry

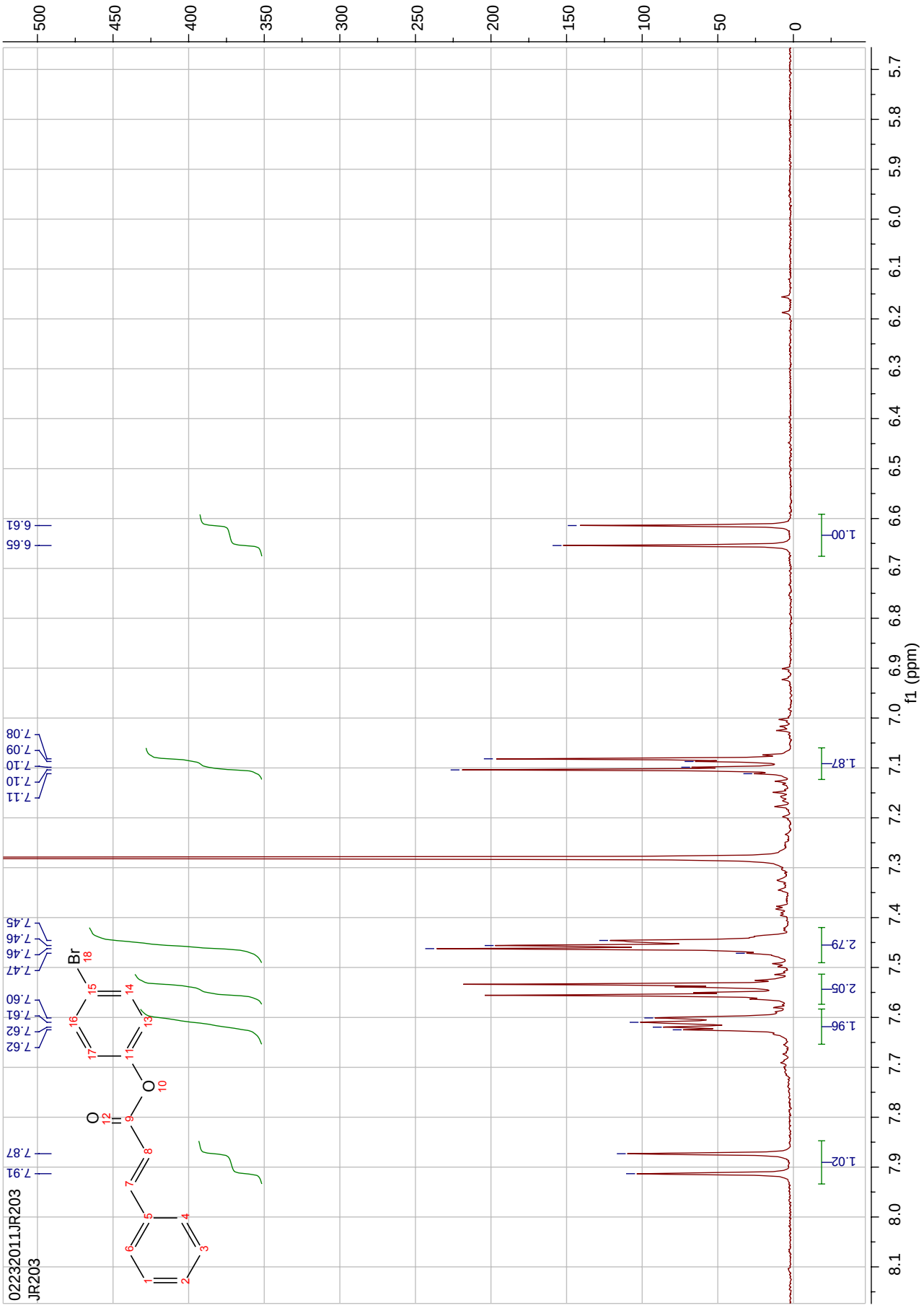
Appendix A - Spectra



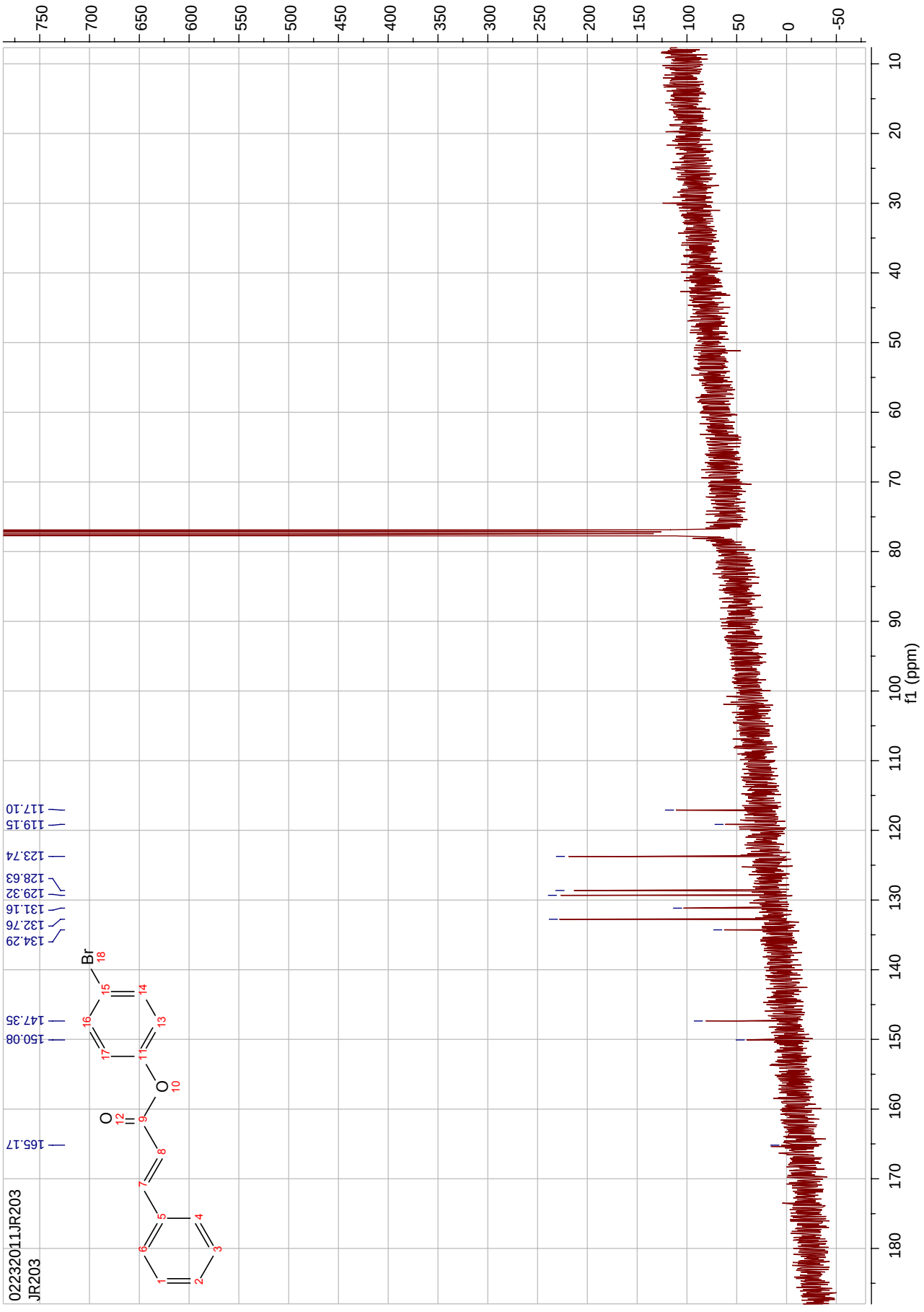
Appendix A - Spectra



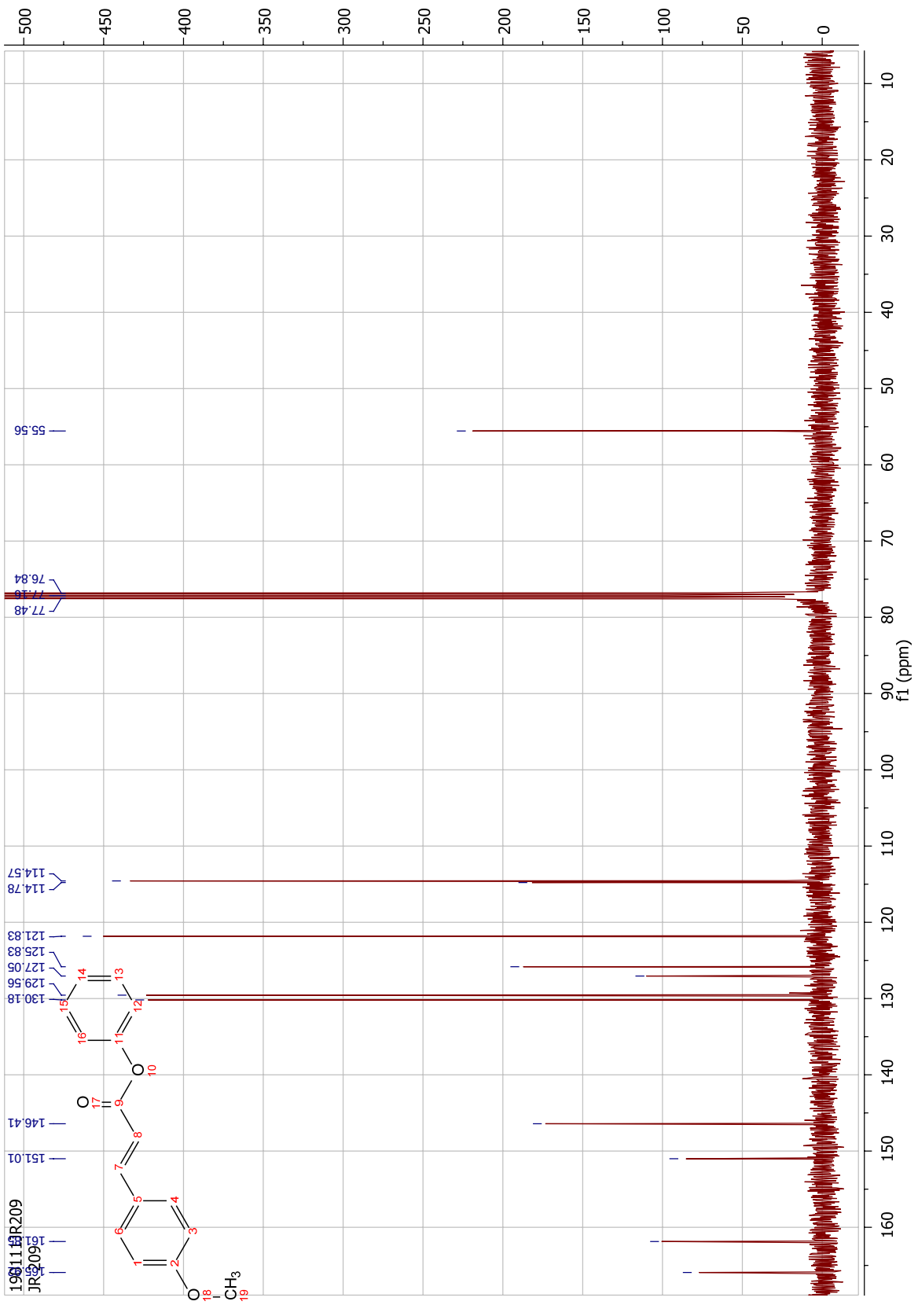
Appendix A - Spectra



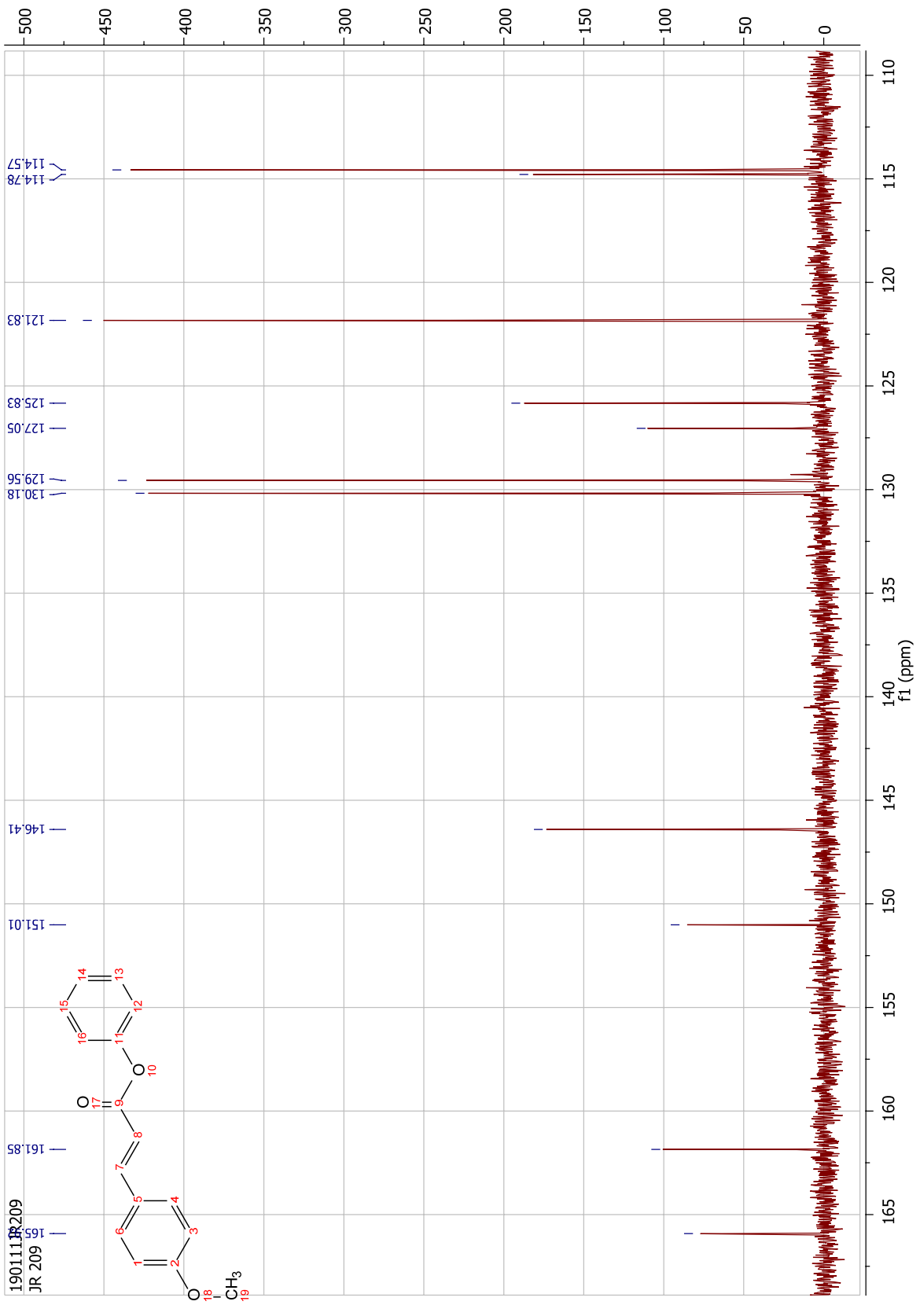
Appendix A - Spectra



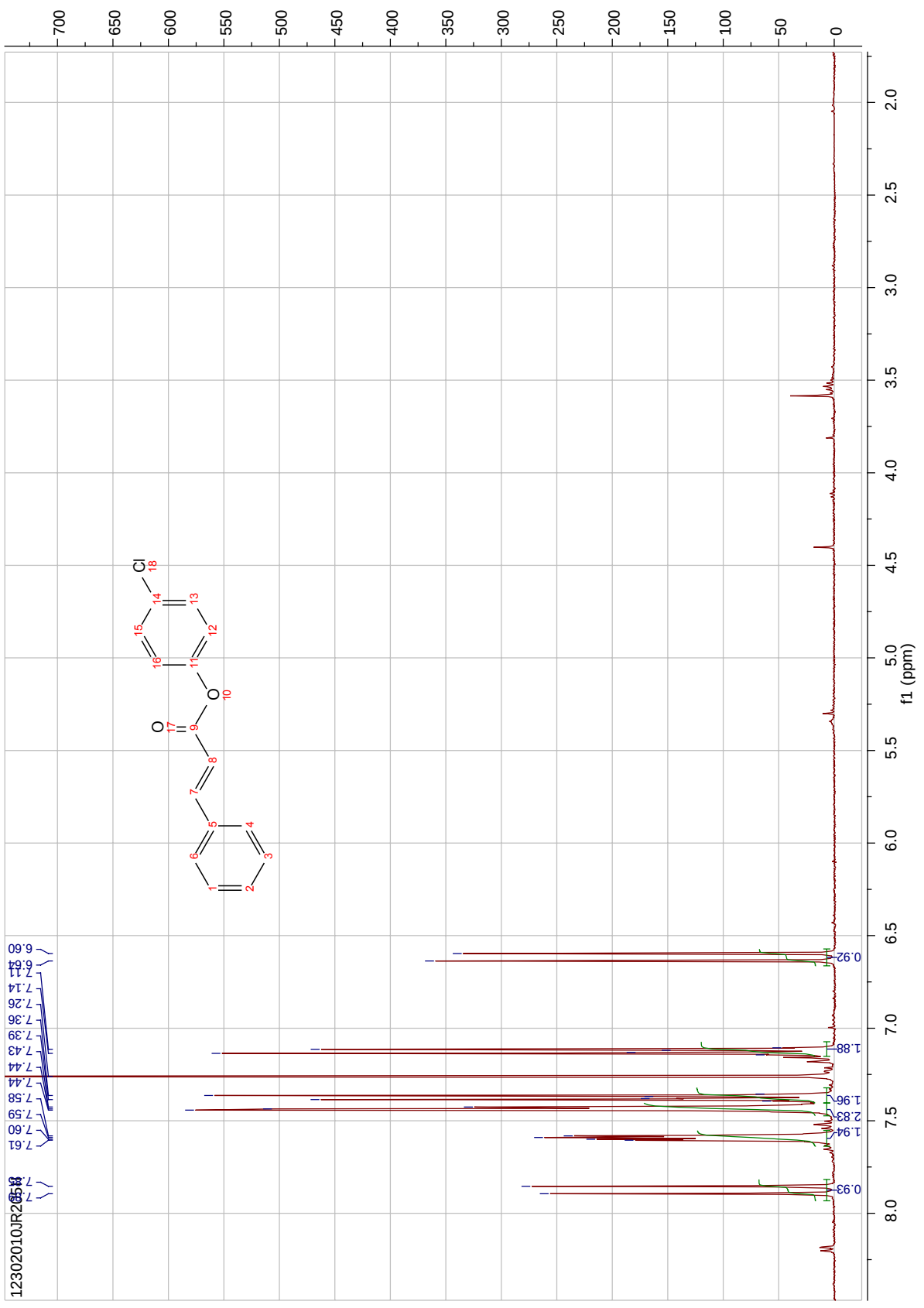
Appendix A - Spectra



Appendix A - Spectra



Appendix A - Spectra



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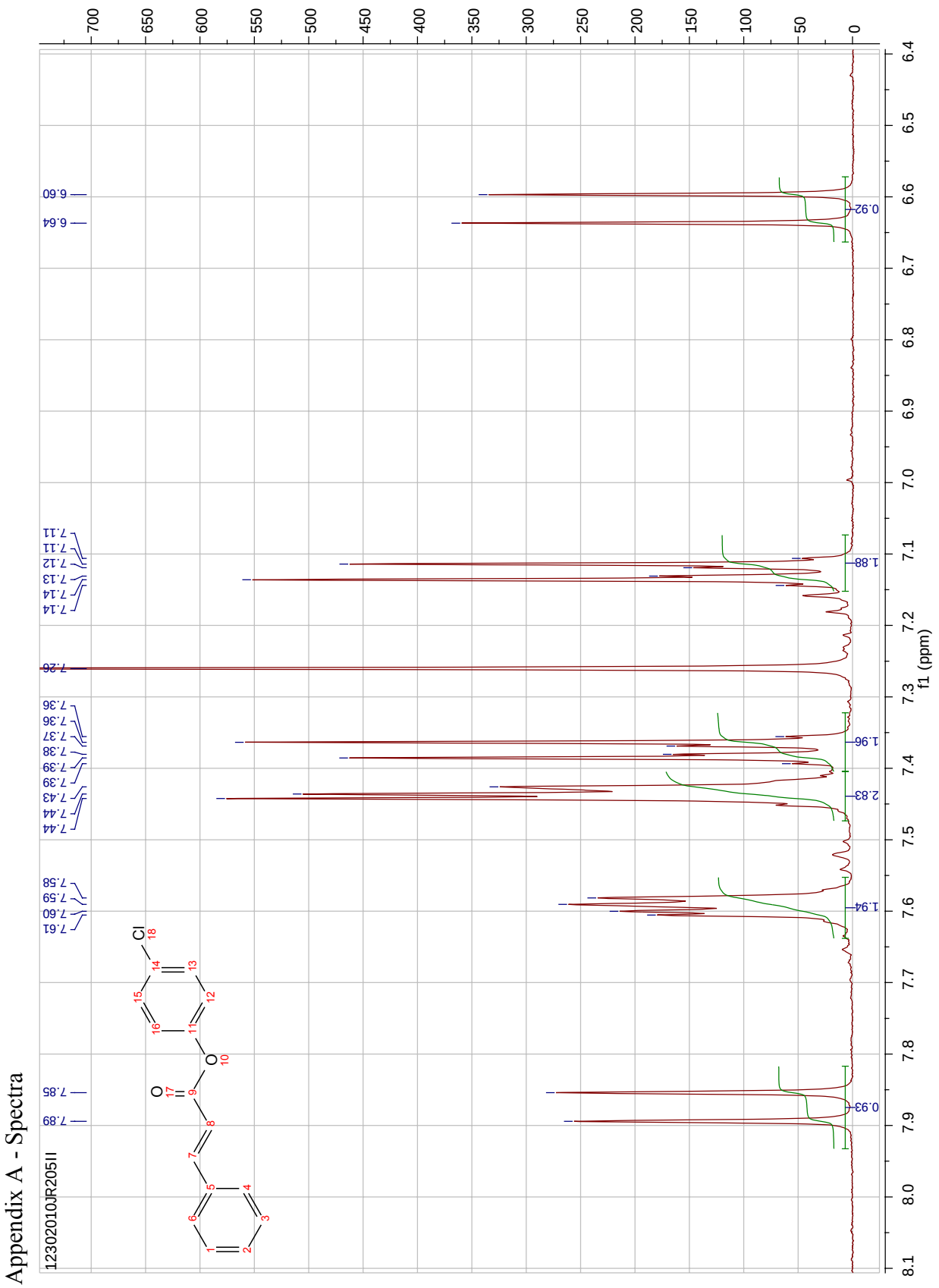
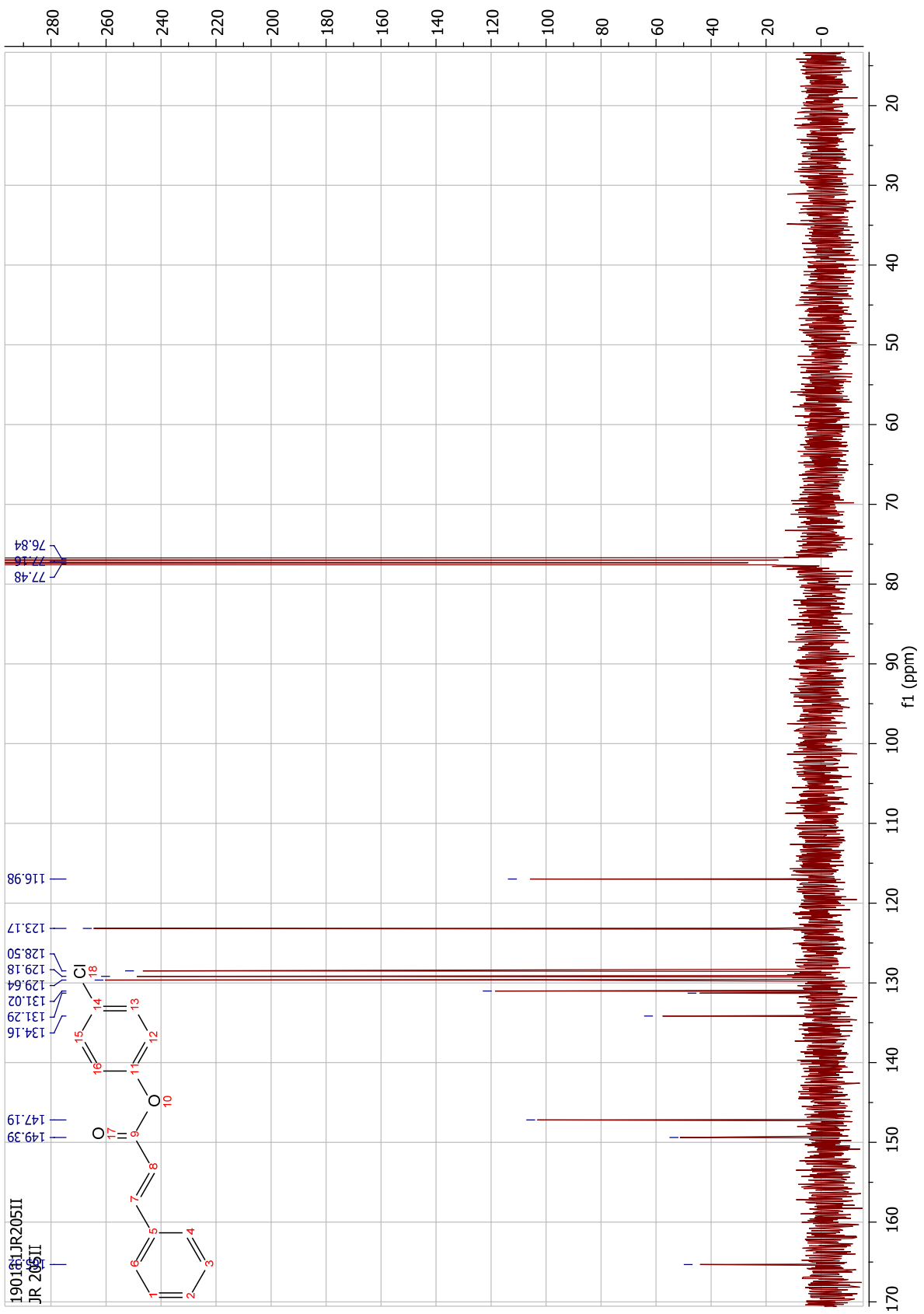
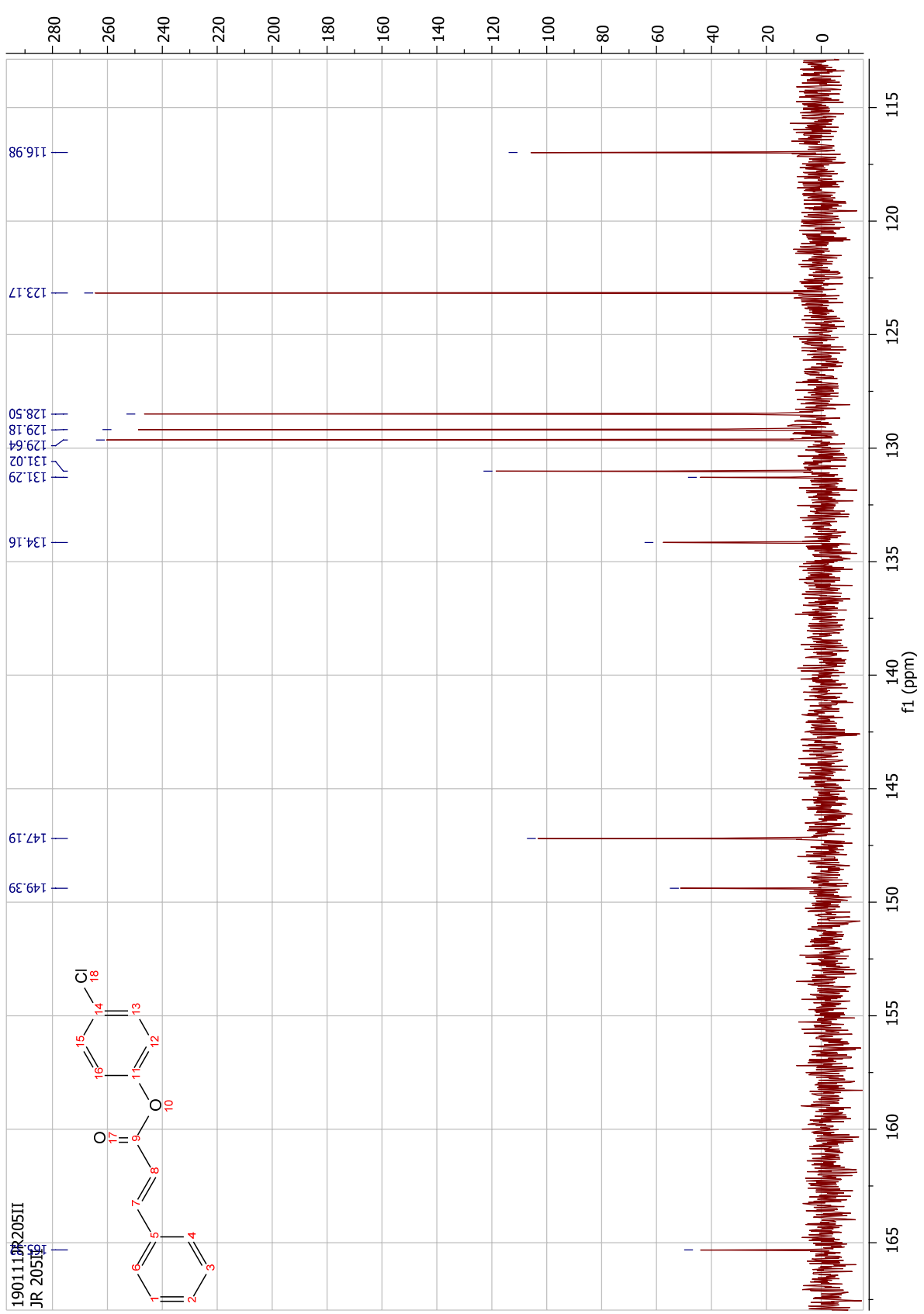


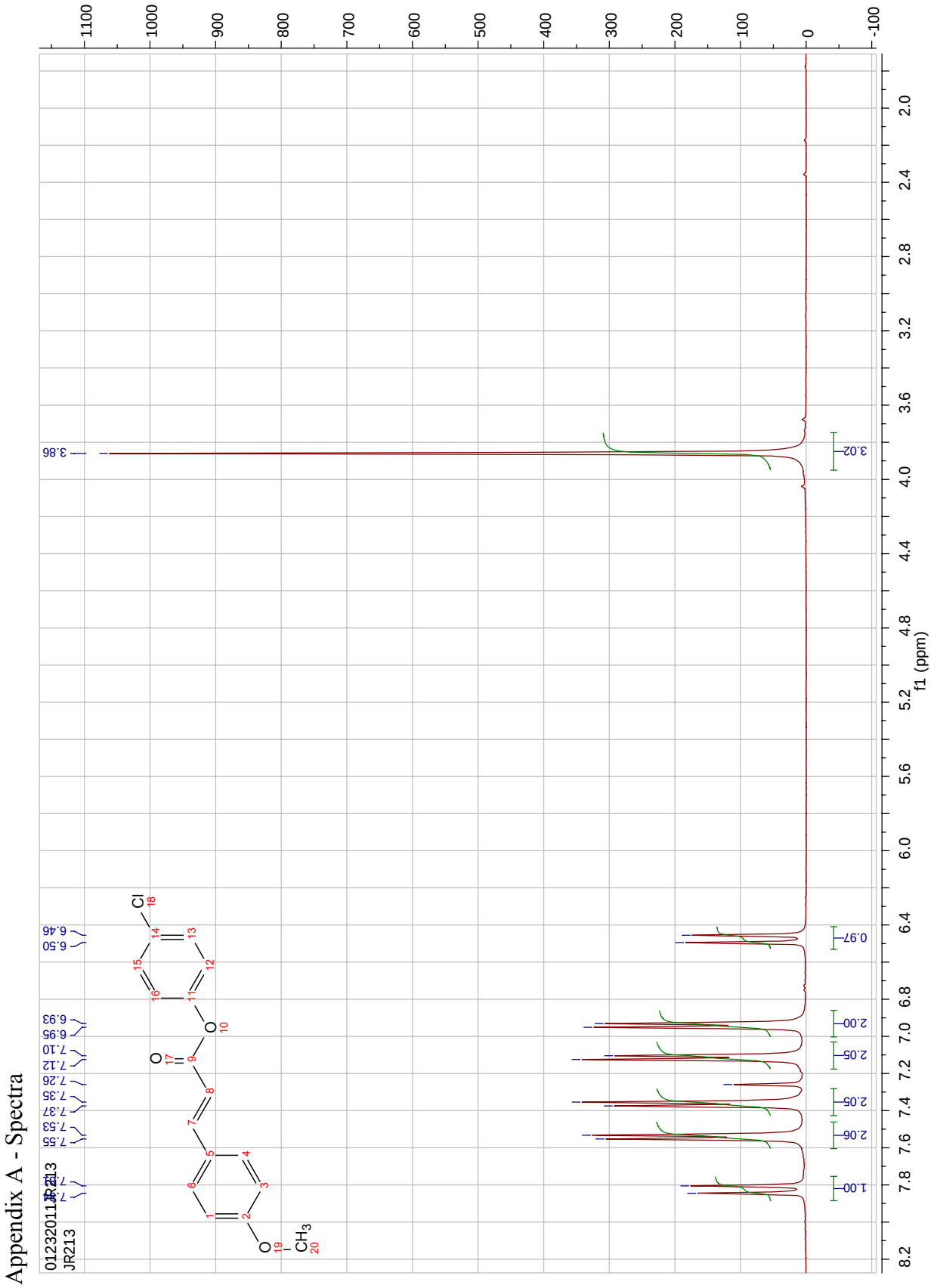
Appendix A - Spectra



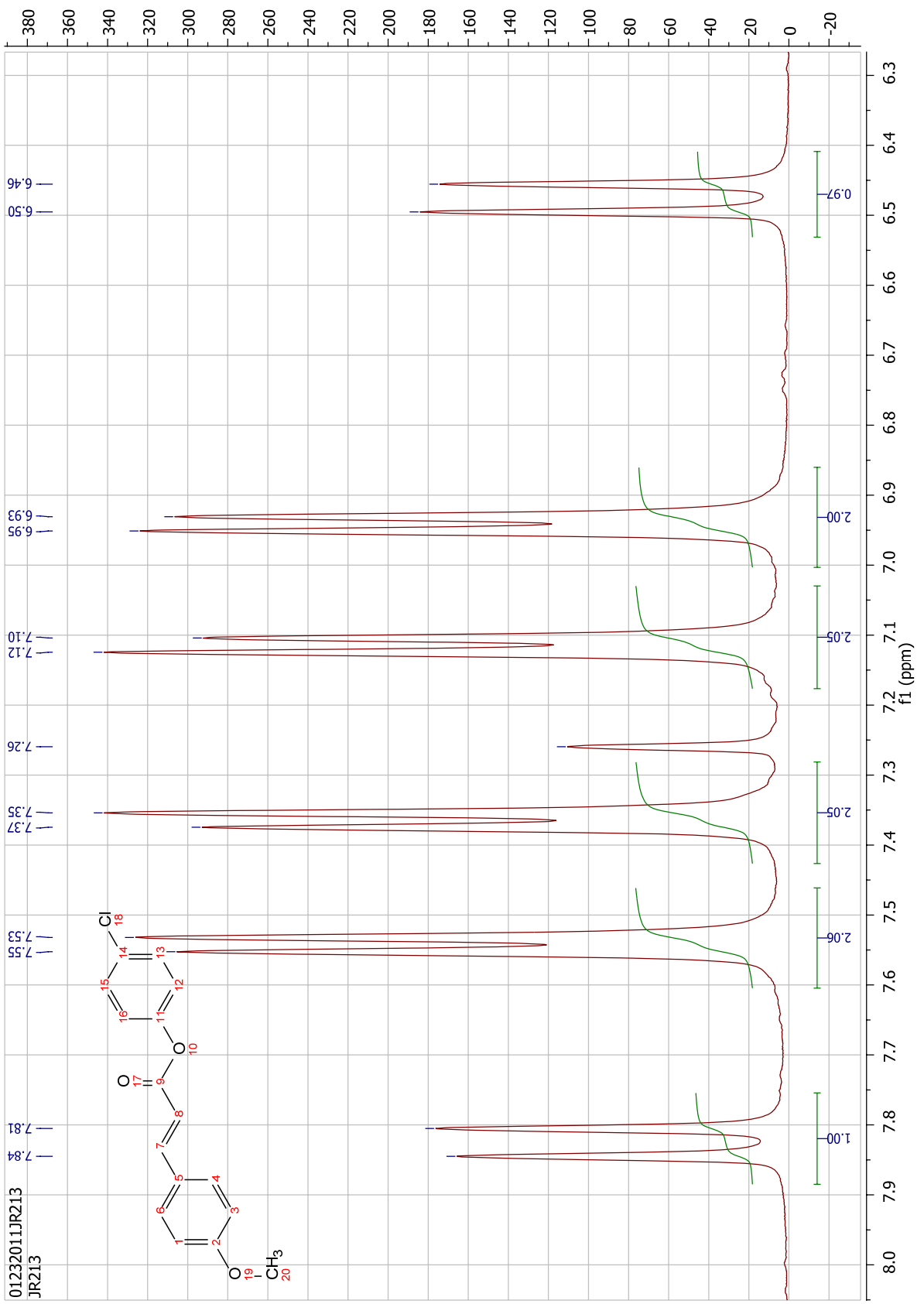
Appendix A - Spectra



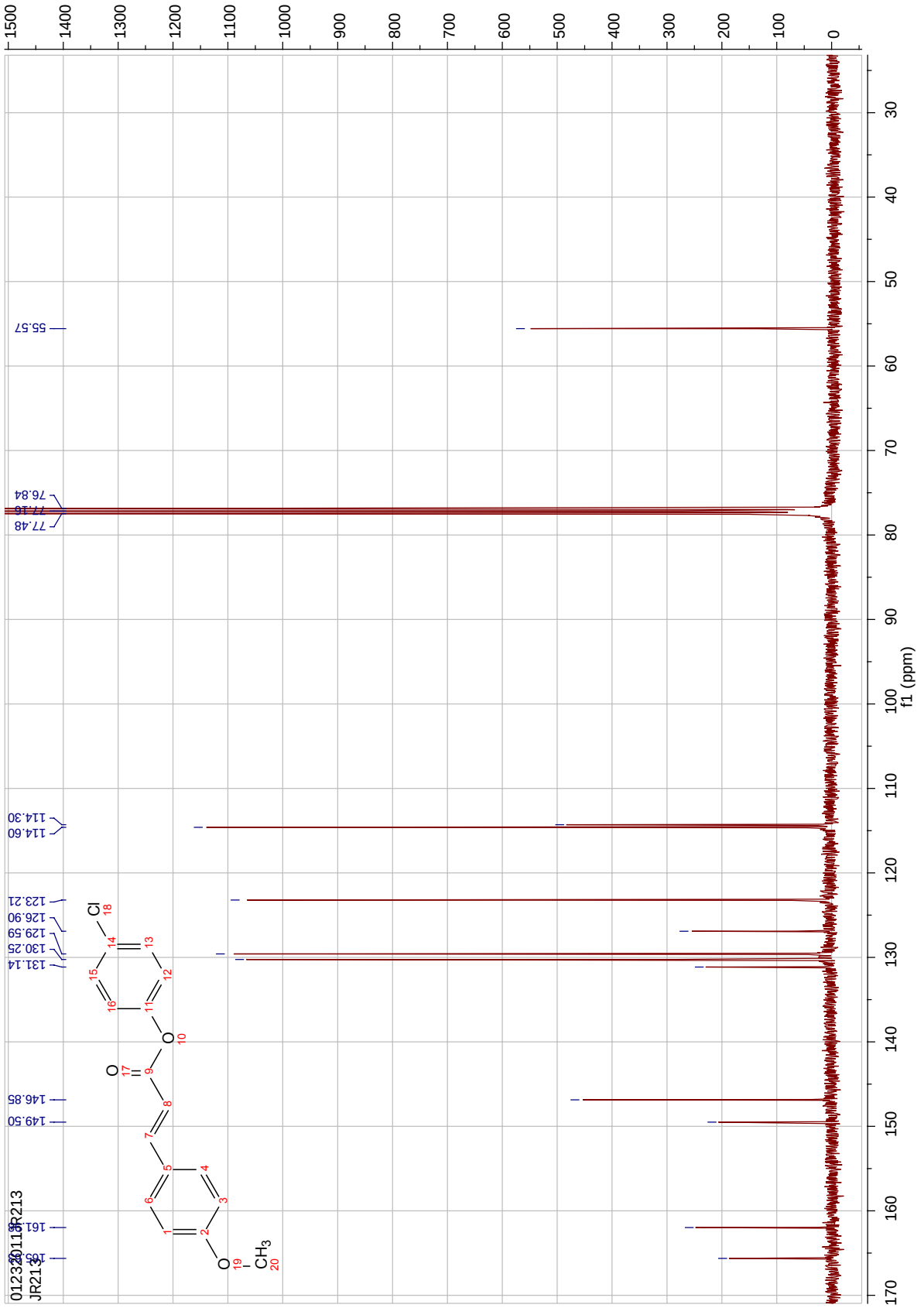
Appendix A - Spectra



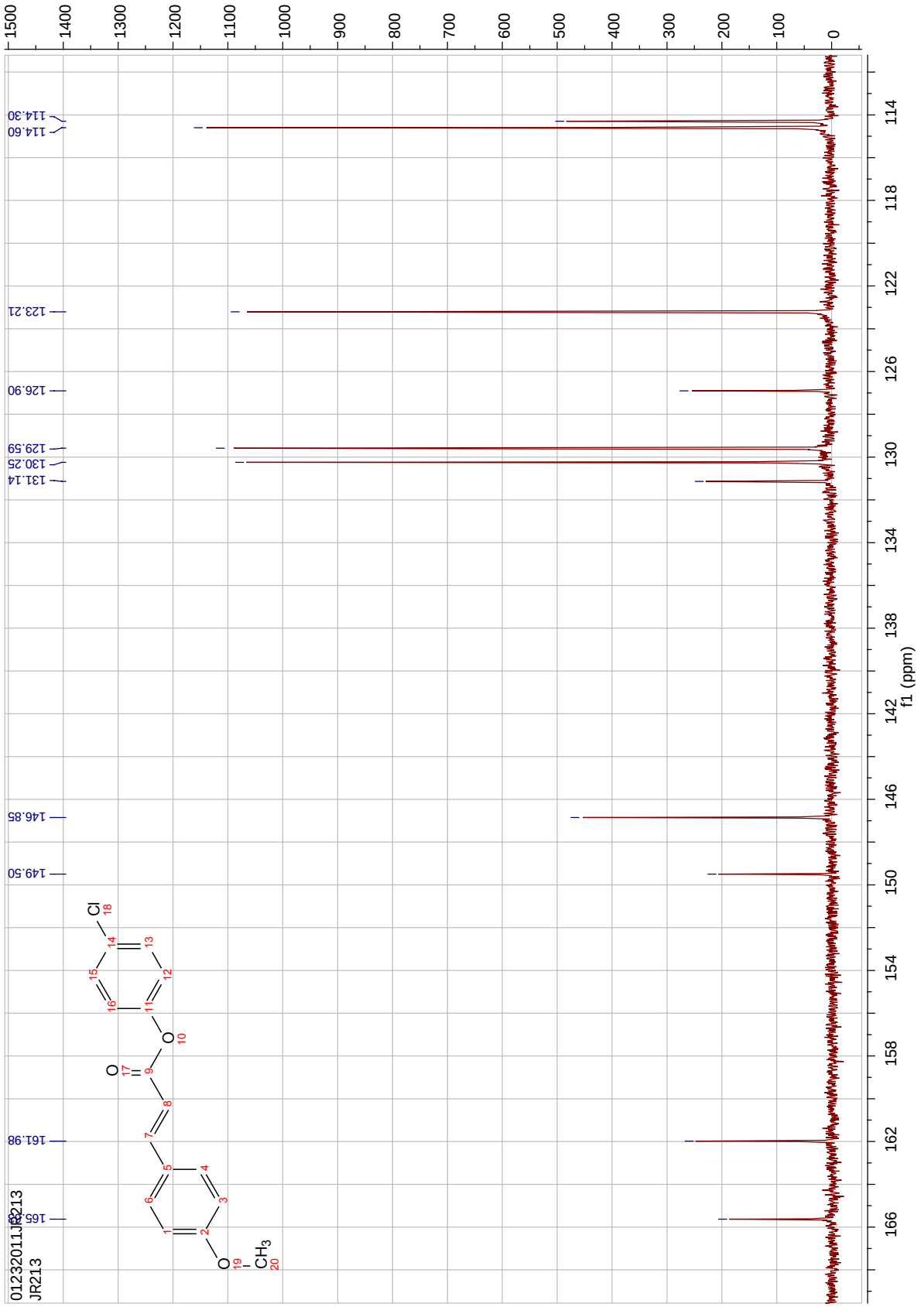
Appendix A - Spectra



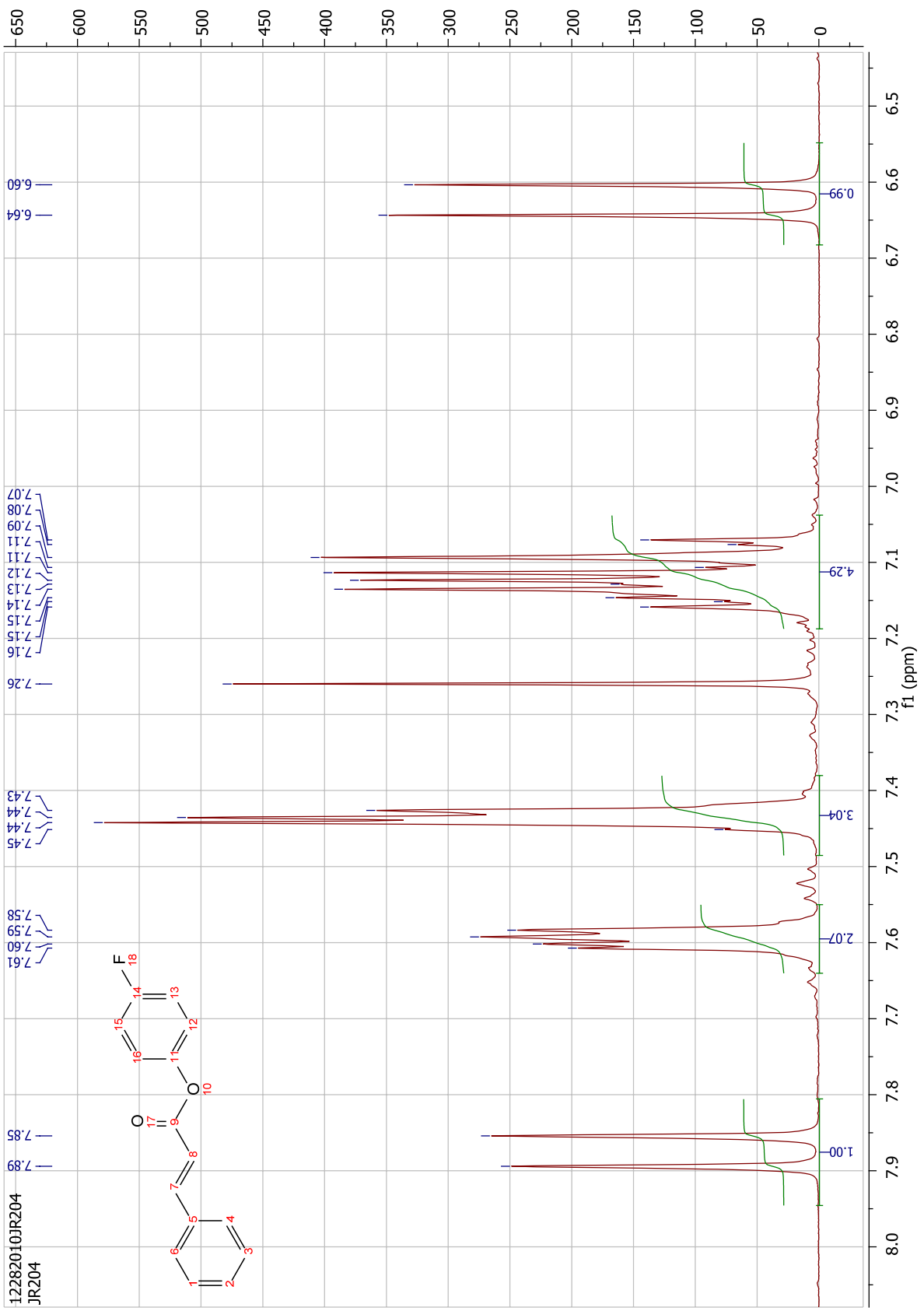
Appendix A - Spectra



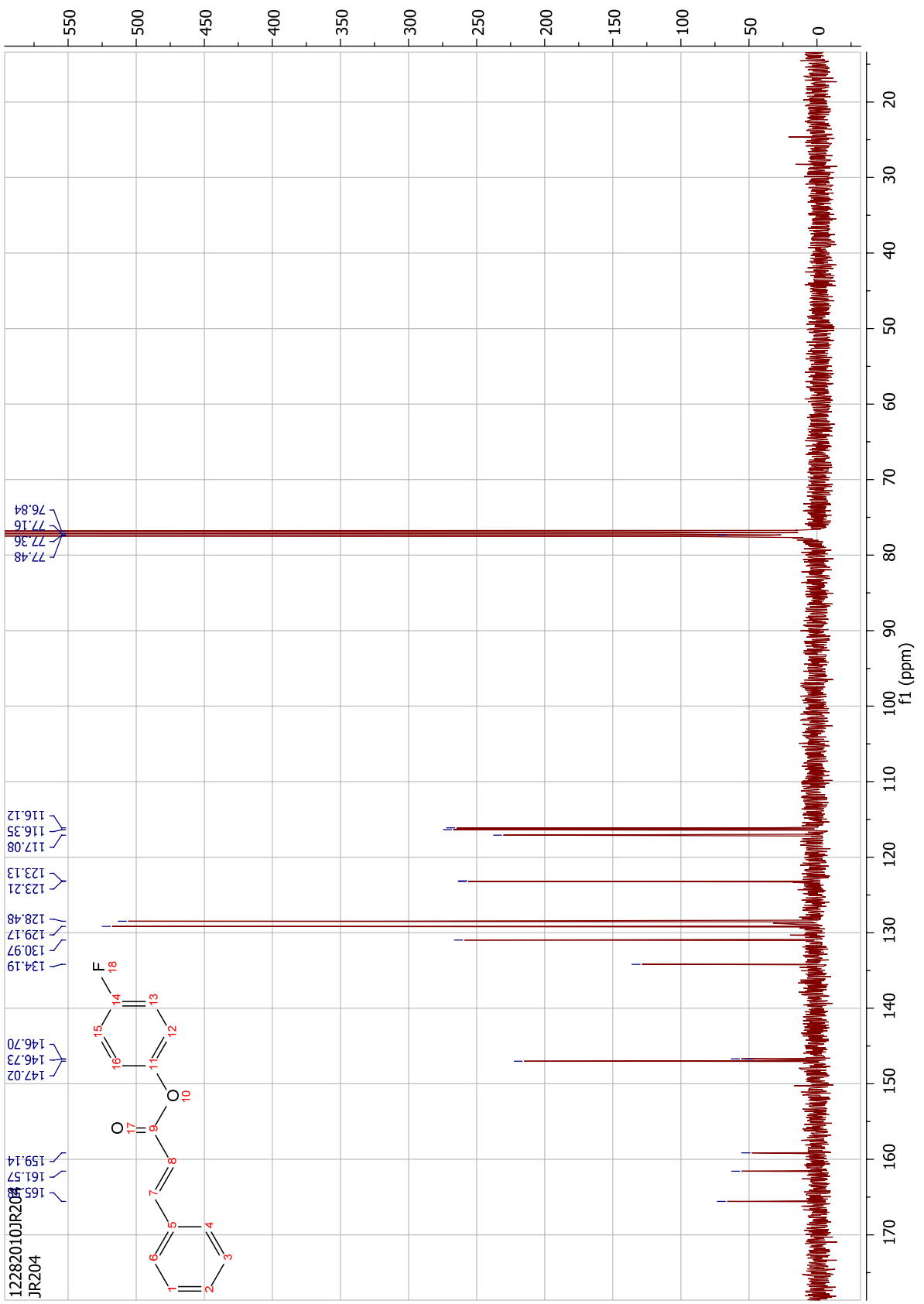
Appendix A - Spectra



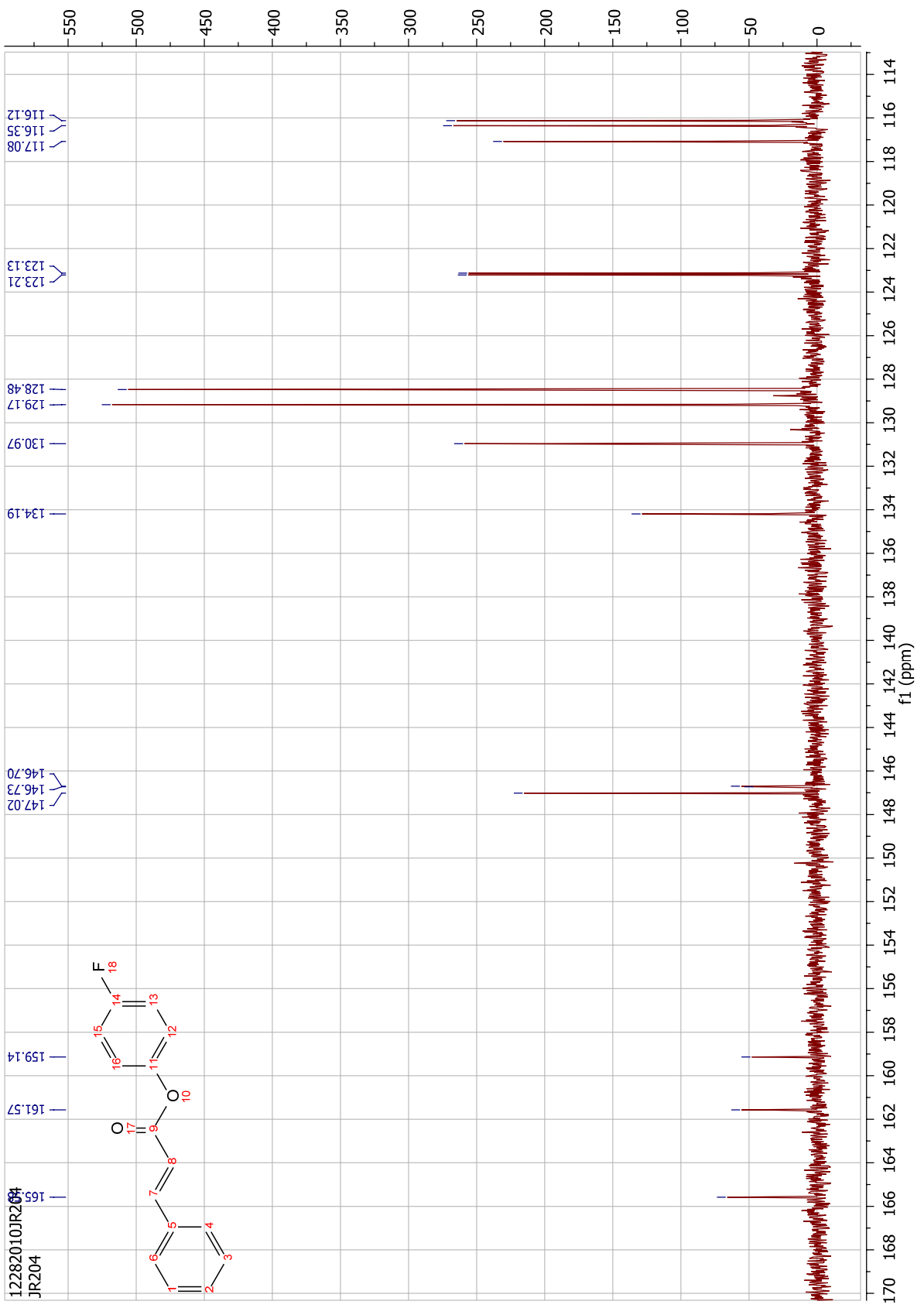
Appendix A - Spectra



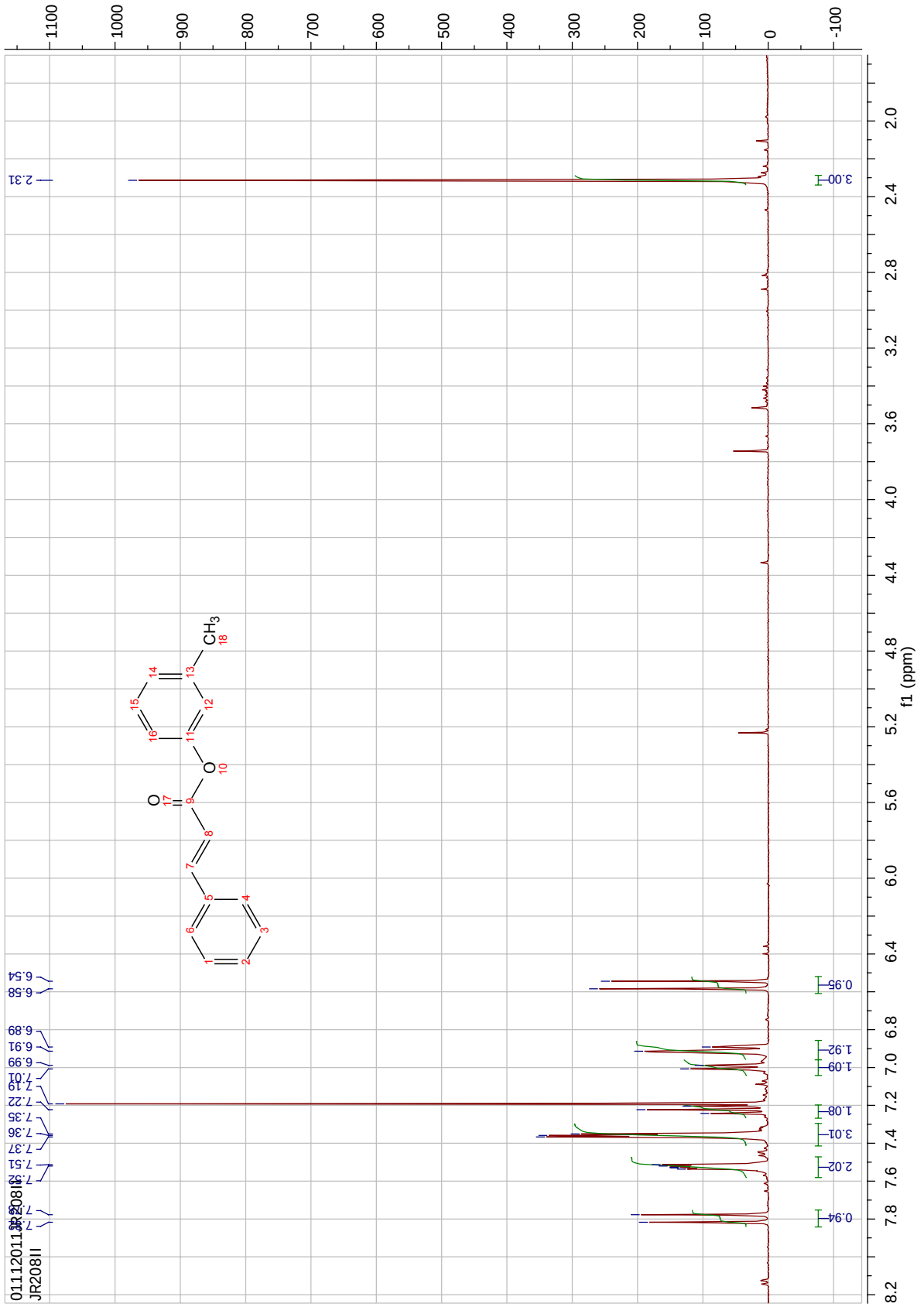
Appendix A - Spectra



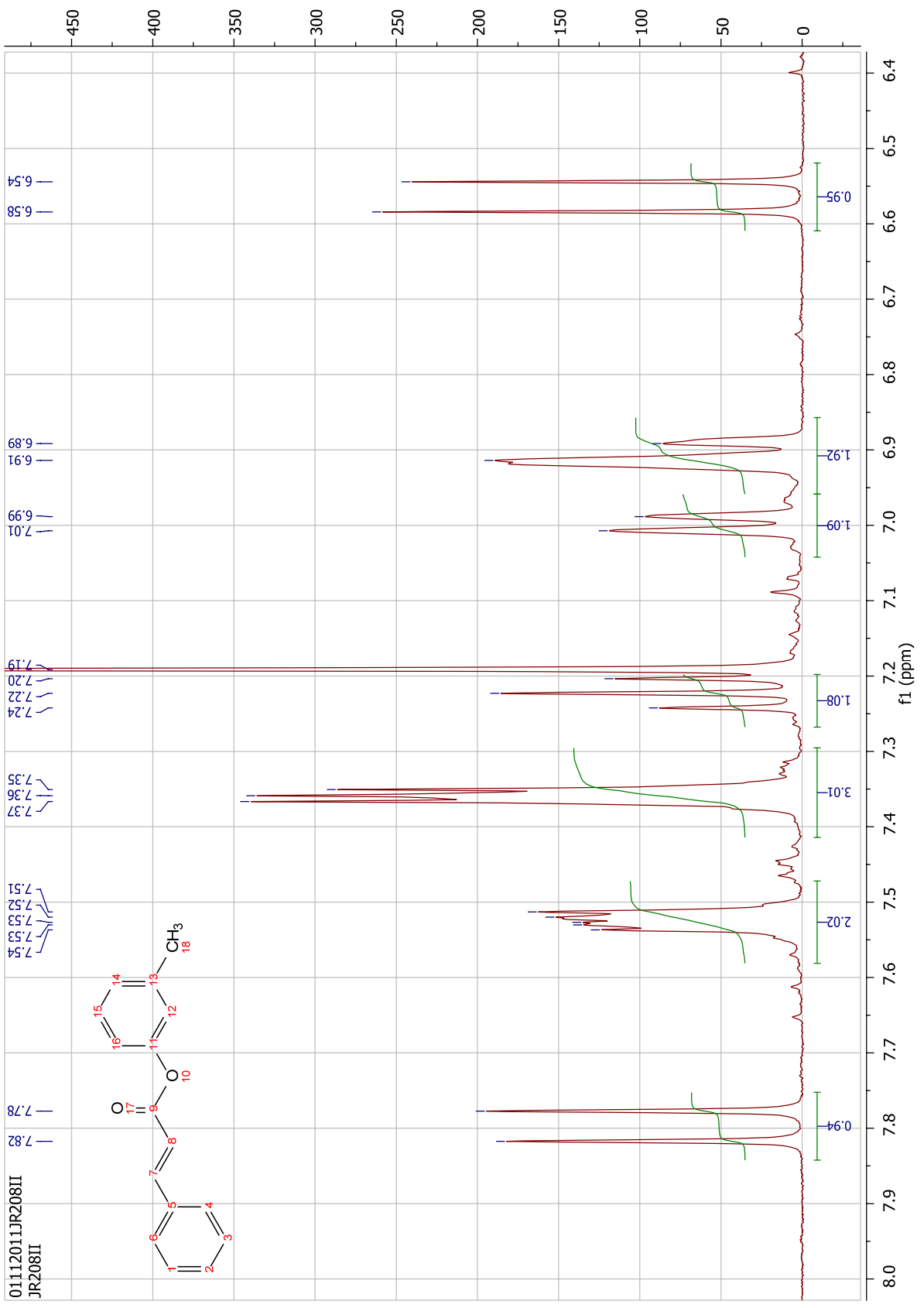
Appendix A - Spectra



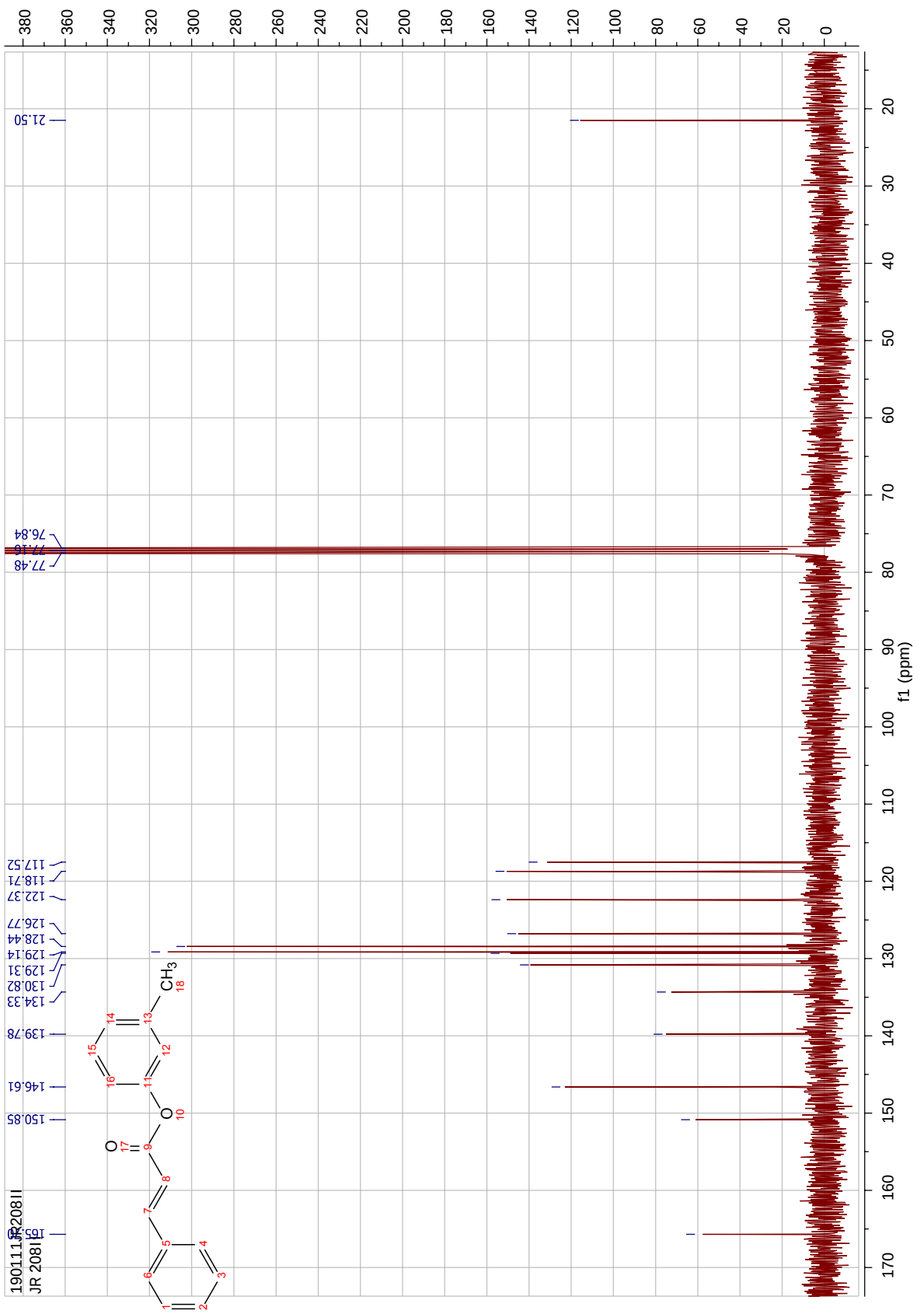
Appendix A - Spectra



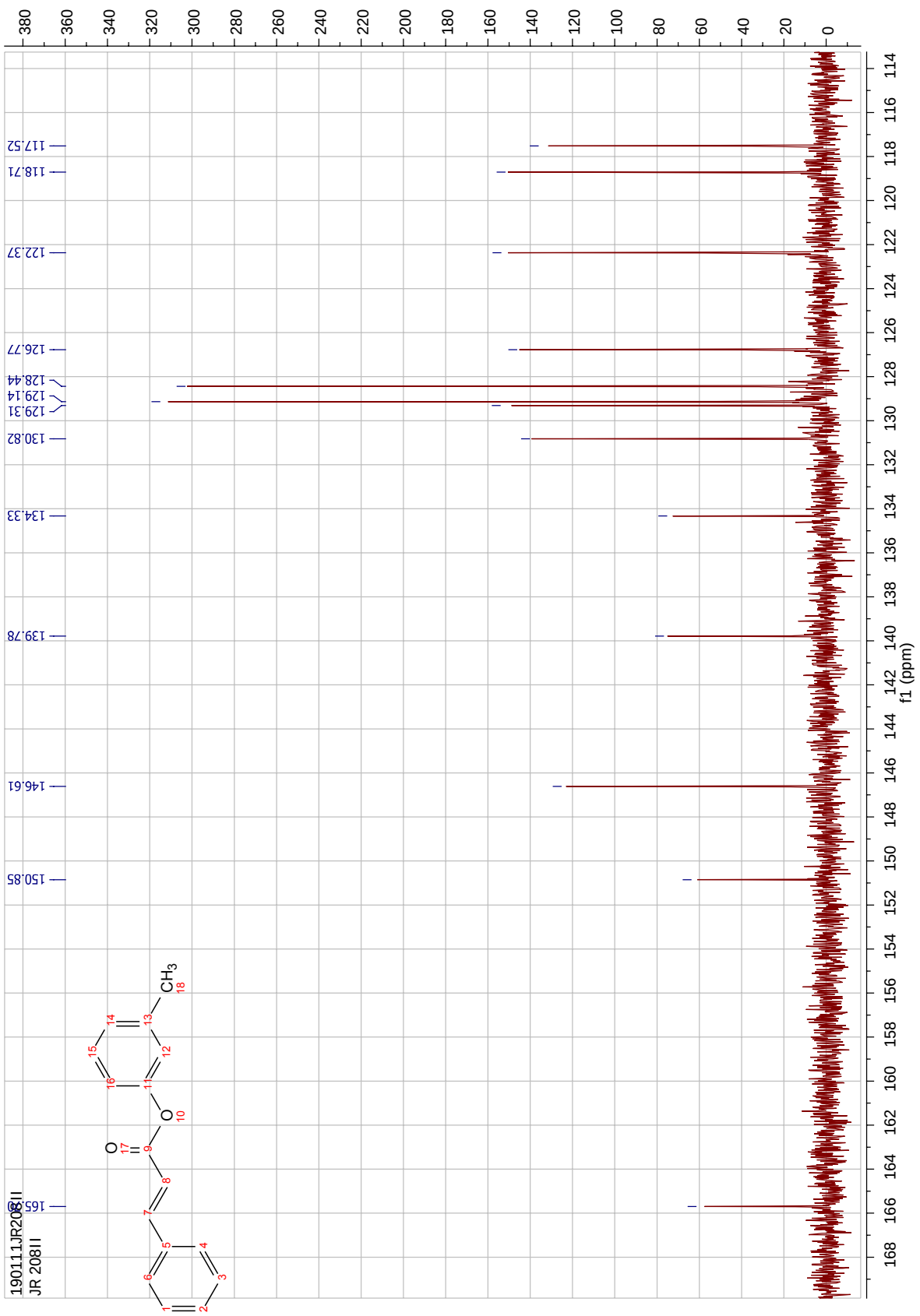
Appendix A - Spectra



Appendix A - Spectra



Appendix A - Spectra



Appendix B – Atomic coordinates

Atomic coordinates of all optimised species

O_2

O	0.000000	0.000000	0.003688
O	0.000000	0.000000	1.206312

OH^-

O	0.000000	0.000000	-0.023270
H	0.000000	0.000000	0.953270

C_6H_5CHO

C	-0.300098	1.015370	-0.268429
C	0.237798	-0.225974	0.063181
C	-0.599108	-1.306163	0.349629
C	-1.976022	-1.145749	0.304658
C	-2.520627	0.099023	-0.027841
C	-1.680327	1.176973	-0.313735
C	-3.985525	0.276736	-0.077347
O	-4.791911	-0.597121	0.154786
H	0.355953	1.851714	-0.490305
H	1.316016	-0.354270	0.099032
H	-0.170781	-2.270349	0.607238
H	-2.656006	-1.964240	0.521774
H	-2.114699	2.140792	-0.571231
H	-4.317566	1.303258	-0.351409

$C_6H_5O^-$

O	2.495195	-0.279957	-0.747900
C	1.287250	-0.153154	-0.410298
C	0.451816	0.948137	-0.838637
C	-0.874418	1.077984	-0.461842
C	-1.500943	0.139874	0.368876
C	-0.731781	-0.944845	0.809313
C	0.595926	-1.093959	0.444736
H	0.917996	1.690785	-1.485780
H	-1.446363	1.936208	-0.823125
H	-2.543341	0.249299	0.659863
H	-1.190437	-1.694768	1.458520
H	1.174099	-1.946603	0.800171

$C_6H_5COOC_6H_5$

C	4.582130	0.289684	0.633741
C	5.250038	-0.920931	0.462847
C	4.539895	-2.071059	0.123298
C	3.162970	-2.010565	-0.044282
C	2.490675	-0.797371	0.126089
C	3.203947	0.355585	0.465822
C	1.018768	-0.801567	-0.064161
O	0.496351	0.441956	0.106097
O	0.366685	-1.779292	-0.337883
C	-0.865848	0.663705	-0.026347
C	-1.227110	1.807393	-0.729012
C	-2.571989	2.143421	-0.840680
C	-3.545036	1.338965	-0.254331
C	-3.165294	0.198451	0.448285
C	-1.823532	-0.148851	0.572340
H	5.137283	1.184555	0.898666
H	6.327307	-0.968097	0.594587
H	5.061503	-3.014057	-0.009848
H	2.584220	-2.890133	-0.307385
H	2.674715	1.292793	0.596873
H	-0.449913	2.418347	-1.176591
H	-2.857283	3.036398	-1.388795
H	-4.595169	1.599639	-0.343644
H	-3.919670	-0.432523	0.908909
H	-1.525285	-1.039322	1.110634

UIPr (from precursor **4**)

C	-1.861224	0.739499	-0.524521
C	-1.916049	-0.556320	-0.142135
N	-0.601110	-0.949544	0.074156
C	0.301673	0.055757	-0.140214
N	-0.516687	1.089064	-0.506329
C	-0.042864	2.376146	-0.929378
C	-0.250751	-2.250548	0.569006
C	-0.392897	-2.485753	1.947649
C	-0.096506	-3.759755	2.437939
C	0.336372	-4.767038	1.590514
C	0.482889	-4.507318	0.234504
C	0.195261	-3.254251	-0.312705
C	0.074448	2.607459	-2.311090
C	0.492036	3.869698	-2.739667
C	0.793095	4.868669	-1.827752
C	0.684810	4.611975	-0.467597
C	0.267064	3.370342	0.018698
C	0.228896	3.194055	1.529686
C	-0.219045	1.534780	-3.343442
C	-0.834316	-1.405307	2.917637
C	0.432389	-3.077745	-1.805480
C	-2.165201	-1.759934	3.586024
C	0.251434	-1.120440	3.958772
C	1.700154	-2.260872	-2.081660
C	-0.771322	-2.558205	-2.595130
C	-1.112864	2.721406	2.093960
C	1.397995	2.336116	2.027513
C	-1.415429	1.912362	-4.220854
C	1.016918	1.228205	-4.193385
H	-2.641194	1.435198	-0.792907
H	-2.752982	-1.226056	-0.017820
H	-0.203496	-3.957380	3.501081
H	0.563421	-5.753854	1.983874
H	0.829721	-5.295697	-0.428725
H	0.585599	4.065458	-3.804426
H	1.116207	5.846499	-2.173499
H	0.929514	5.393512	0.247274
H	0.383171	4.203887	1.932944
H	-0.476051	0.616023	-2.810155
H	-0.984448	-0.483422	2.350021
H	0.620722	-4.092437	-2.181230
H	-2.488604	-0.950700	4.249177
H	-2.952755	-1.926145	2.844277
H	-2.080062	-2.670264	4.189442
H	-0.056009	-0.297665	4.613159
H	1.192057	-0.839896	3.476715
H	0.442890	-1.994025	4.591362
H	1.871388	-2.181139	-3.161297
H	2.574476	-2.743896	-1.634071
H	1.622195	-1.255734	-1.654477
H	-0.566904	-2.640745	-3.668052
H	-1.670898	-3.144599	-2.380466
H	-0.993050	-1.511184	-2.379567
H	-1.940270	3.332459	1.718317
H	-1.325622	1.678957	1.849365
H	-1.100643	2.810008	3.185637
H	1.371190	2.258127	3.120421
H	2.354358	2.785968	1.742811
H	1.362513	1.331183	1.594233
H	-1.635273	1.111010	-4.934163
H	-2.313023	2.086418	-3.619179
H	-1.218520	2.824203	-4.795162
H	0.804103	0.410345	-4.890107
H	1.860601	0.930344	-3.564667
H	1.326006	2.096132	-4.785856

SIPr (from precursor **5**)

C	-1.919422	0.816254	-0.167970
C	-1.994118	-0.593199	0.414049
N	-0.565536	-0.955287	0.504779
C	0.288760	0.072248	0.317923
N	-0.484311	1.128707	-0.009556
C	0.014396	2.402804	-0.424489
C	-0.190619	-2.246671	0.991066
C	-0.249160	-2.491248	2.376484
C	0.040134	-3.774629	2.846055
C	0.389983	-4.792114	1.972848
C	0.469980	-4.528069	0.612219
C	0.184794	-3.264216	0.089414
C	0.215200	2.636854	-1.798381

Appendix B – Atomic coordinates

C	0.625347	3.906542	-2.211918
C	0.845526	4.919894	-1.292796
C	0.672370	4.664689	0.060869
C	0.257180	3.414823	0.527337
C	0.174733	3.232194	2.035350
C	0.044823	1.546223	-2.838960
C	-0.576413	-1.400095	3.378835
C	0.377719	-3.075507	-1.407714
C	-1.848528	-1.714711	4.170961
C	0.606608	-1.143528	4.316830
C	1.647448	-2.268317	-1.702206
C	-0.833262	-2.525274	-2.163690
C	-1.172023	2.737293	2.565952
C	1.338806	2.380084	2.554254
C	-1.042116	1.892039	-3.860412
C	1.375288	1.241475	-3.533891
H	-2.457307	-0.609354	1.409013
H	-2.538370	-1.295618	-0.223196
H	-2.541436	1.538346	0.368059
H	-2.202419	0.846788	-1.228118
H	-0.002694	-3.972504	3.913935
H	0.610547	-5.786773	2.349914
H	0.763800	-5.320339	-0.071944
H	0.781946	4.096369	-3.270591
H	1.162511	5.903881	-1.626669
H	0.865537	5.452752	0.784602
H	0.307921	4.240096	2.450816
H	-0.255204	0.631835	-2.319460
H	-0.742096	-0.473264	2.822591
H	0.543009	-4.086787	-1.802980
H	-2.095391	-0.888666	4.846362
H	-2.704689	-1.882491	3.509515
H	-1.724842	-2.615455	4.781936
H	0.382441	-0.312949	4.994816
H	1.506337	-0.889020	3.750028
H	0.830378	-2.023061	4.930265
H	1.793660	-2.165983	-2.783644
H	2.527176	-2.769394	-1.286560
H	1.592745	-1.271400	-1.252686
H	-0.667014	-2.619312	-3.242232
H	-1.745393	-3.079047	-1.917589
H	-1.001794	-1.467604	-1.950293
H	-2.003455	3.318025	2.152945
H	-1.337693	1.682464	2.337205
H	-1.199903	2.843789	3.655705
H	1.285147	2.283350	3.644750
H	2.297584	2.843356	2.301567
H	1.326954	1.381403	2.105663
H	-1.188186	1.063763	-4.561980
H	-2.001168	2.101017	-3.375388
H	-0.771439	2.776986	-4.446715
H	1.257440	0.411467	-4.238919
H	2.142148	0.964674	-2.805303
H	1.740426	2.107404	-4.096766

UIMes (from precursor **8**)

C	-1.611566	0.686999	-0.355877
C	-1.673893	-0.580755	0.109637
N	-0.360671	-0.960679	0.358773
C	0.552083	0.015870	0.068979
N	-0.263081	1.021588	-0.371948
C	0.229180	2.290299	-0.805991
C	0.007248	-2.245984	0.861289
C	-0.212852	-2.539741	2.211637
C	0.137619	-3.808188	2.674563
C	0.698856	-4.768623	1.834381
C	0.921054	-4.430706	0.499016
C	0.582805	-3.178220	-0.010582
C	0.270411	2.573203	-2.175580
C	0.736791	3.825988	-2.574824
C	1.161437	4.780649	-1.652082
C	1.124143	4.453009	-0.296295
C	0.661411	3.216573	0.150760
C	0.646222	2.874109	1.611938
C	-0.142138	1.544011	-3.188946
C	-0.778147	-1.507408	3.145097
C	0.846553	-2.826719	-1.445668
H	1.020807	3.706975	2.211793
H	1.263823	1.990670	1.801488
H	-0.366487	2.633079	1.954051
H	0.106365	1.874620	-4.200246
H	-1.218641	1.343687	-3.155952
H	0.362694	0.591180	-3.000347
H	-0.704306	-1.842224	4.182527
H	-1.832741	-1.297275	2.935275
H	-2.387738	1.369747	-0.666304
H	-2.514863	-1.235962	0.278206
H	-0.022245	-4.045400	3.724357
C	1.041711	-6.138779	2.348989
H	1.373445	-5.161775	-0.167812
H	0.779275	4.055033	-3.637619
C	1.633372	6.134671	-2.103259
H	1.467614	5.179474	0.437270
H	-0.240415	-0.559228	3.046343
H	1.284051	-3.673031	-1.980602
H	1.528124	-1.972687	-1.508537
H	-0.075913	-2.534745	-1.959900
H	1.920026	-6.548066	1.841615
H	0.214799	-6.840052	2.184595
H	1.247066	-6.122613	3.422973
H	2.436894	6.511504	-1.463755
H	0.818957	6.868193	-2.067908
H	2.003259	6.106830	-3.131920

SIMes (from precursor **9**)

C	-2.009235	0.897294	-0.647994
C	-2.150220	-0.533410	-0.138204
N	-0.737065	-0.943735	-0.020249
C	0.150309	0.070014	-0.091688
N	-0.582205	1.164556	-0.382574
C	-0.013324	2.433283	-0.682088
C	-0.394104	-2.255635	0.409340
C	0.073705	-2.460336	1.719167
C	0.377895	-3.758607	2.120181
C	0.224844	-4.852844	1.266415
C	-0.239175	-4.617282	-0.024405
C	-0.548753	-3.331956	-0.474205
C	0.801258	2.582286	-1.817330
C	1.327444	3.841416	-2.096336
C	1.059818	4.950869	-1.292512
C	0.255798	4.769087	-0.170536
C	-0.286537	3.524362	0.154401
C	-1.120116	3.366938	1.394476
C	1.113777	1.410220	-2.702326
C	0.253230	-1.306906	2.663515
C	-1.016758	-3.121666	-1.886258
H	-0.869705	4.136946	2.128874
H	-0.961556	2.386547	1.852287
H	-2.192538	3.462303	1.181846
H	1.753929	1.711967	-3.535034
H	0.200704	0.969915	-3.120146
H	1.611765	0.620567	-2.131622
H	0.601139	-1.654109	3.639618
H	-0.686053	-0.761701	2.812760
H	-2.657101	1.603853	-0.122474
H	-2.213956	0.983293	-1.723323
H	0.742111	-3.921004	3.132813
C	0.581573	-6.239403	1.724769
H	-0.353882	-5.453975	-0.710862
H	1.964882	3.959047	-2.970566
C	1.614795	6.303991	-1.639834
H	0.053636	5.615305	0.483352
H	0.972491	-0.588336	2.258995
H	-0.657832	-3.924123	-2.536058
H	-0.655951	-2.168021	-2.281553
H	-2.111781	-3.116348	-1.957667
H	0.171966	-7.000094	1.054793
H	0.202625	-6.436746	2.732555
H	1.668686	-6.377695	1.756098
H	1.632244	6.964792	-0.768796
H	1.008618	6.793828	-2.411326
H	2.634685	6.229880	-2.029084
H	-2.702903	-1.178565	-0.826279
H	-2.639875	-0.584861	0.843279

Appendix B – Atomic coordinates

I

C	-2.021677	-0.163473	1.541425
C	-1.473481	-1.595879	1.558780
N	-0.320810	-1.526563	0.659852
C	-0.080767	-0.265262	0.259868
N	-1.069447	0.541630	0.685867
C	-1.165844	1.958913	0.510726
C	0.537790	-2.659372	0.491703
C	1.195362	0.297624	-0.325909
C	1.834343	-0.472751	-1.480413
O	1.870132	0.340266	0.833783
C	2.999002	-1.198224	-1.248136
C	3.635320	-1.865848	-2.290423
C	3.117827	-1.805535	-3.582015
C	1.968043	-1.058053	-3.828876
C	1.340336	-0.386745	-2.783593
C	1.551018	-2.879648	1.450181
C	2.405084	-3.966185	1.263328
C	2.264291	-4.811481	0.172386
C	1.226050	-4.608970	-0.722146
C	0.321268	-3.552122	-0.574670
C	-1.909648	2.463490	-0.573105
C	-2.049959	3.847215	-0.686029
C	-1.475220	4.702711	0.244014
C	-0.752891	4.183933	1.308807
C	-0.585191	2.807005	1.472780
C	-2.571368	1.559027	-1.594695
C	-4.096365	1.581215	-1.442849
C	-2.168621	1.918530	-3.027322
C	0.175736	2.289196	2.678745
C	1.612121	2.814777	2.710733
C	-0.574609	2.620636	3.973411
C	-0.857680	-3.576020	-1.544576
C	-1.877022	-4.623347	-1.070501
C	-1.574509	-2.274127	-1.889683
C	1.695709	-2.043096	2.709972
C	1.229011	-2.854770	3.926118
C	3.116747	-1.520308	2.921485
H	-2.047134	0.288017	2.538807
H	-3.028349	-0.100484	1.114139
H	0.911696	1.288814	-0.756221
H	3.385394	-1.215766	-0.234630
H	4.541552	-2.433402	-2.095672
H	3.615632	-2.324780	-4.396527
H	1.571569	-0.984204	-4.838252
H	0.462872	0.225535	-2.987339
H	3.196070	-4.147103	1.985245
H	2.953183	-5.639182	0.028819
H	1.096596	-5.289964	-1.560050
H	-2.618628	4.259119	-1.515134
H	-1.592483	5.777612	0.138619
H	-0.307108	4.858786	2.034054
H	-2.230154	0.536578	-1.404646
H	-4.564881	0.886255	-2.147834
H	-4.407237	1.301970	-0.430996
H	-4.494911	2.581629	-1.643845
H	-2.570930	1.183280	-3.732024
H	-1.081187	1.945722	-3.142149
H	-2.556410	2.899716	-3.320757
H	0.264726	1.204054	2.577632
H	2.115739	2.458055	3.615945
H	2.153952	2.420675	1.847423
H	1.650794	3.909919	2.719047
H	-0.059544	2.180983	4.833941
H	-1.603251	2.242902	3.963087
H	-0.627339	3.702582	4.138356
H	-0.434959	-3.946999	-2.487620
H	-2.681955	-4.737726	-1.804809
H	-1.409869	-5.600402	-0.918508
H	-2.332072	-4.324857	-0.119074
H	-2.247147	-2.456092	-2.735038
H	-0.871202	-1.493442	-2.183434
H	-2.191119	-1.903590	-1.065447
H	1.069970	-1.154744	2.597224
H	1.261352	-2.239724	4.831976
H	0.208059	-3.234957	3.807793
H	1.877905	-3.722214	4.090777
H	3.162594	-0.945846	3.853248
H	3.381562	-0.853844	2.098696
H	3.849984	-2.330389	3.002497
H	-2.197210	-2.328195	1.186429
H	-1.159203	-1.909182	2.559627

II

C	-2.366421	-0.125739	1.348131
C	-2.060887	-1.624690	1.393506
N	-0.687504	-1.698693	0.867469
C	-0.324081	-0.519613	0.383427
N	-1.259802	0.411816	0.532295
C	-1.144252	1.827208	0.282826
C	0.117963	-2.889205	1.006006
C	1.105539	-0.247912	-0.091932
C	1.413825	0.175332	-1.459205
O	1.941183	-0.412011	0.775174
C	2.766286	0.398938	-1.763607
C	3.132904	0.781416	-3.043259
C	2.157182	0.935651	-4.029111
C	0.813770	0.712515	-3.733792
C	0.438477	0.339039	-2.450137
C	0.882225	-3.012341	2.186501
C	1.670447	-4.152945	2.333229
C	1.693211	-5.139373	1.358920
C	0.893388	-5.014619	0.234254
C	0.067790	-3.903466	0.029941
C	-1.948575	2.389608	-0.729540
C	-1.841919	3.762670	-0.947562
C	-0.986314	4.547907	-0.186796
C	-0.241556	3.976100	0.832883
C	-0.311139	2.608104	1.108507
C	-2.956238	1.587164	-1.534840
C	-4.382554	1.862568	-1.036883
C	-2.878173	1.867092	-3.038895
C	0.428821	2.071670	2.321908
C	1.910627	2.455583	2.328037
C	-0.259568	2.548065	3.607830
C	-0.864500	-4.000619	-1.173727
C	-2.148228	-4.749948	-0.789241
C	-1.179736	-2.726907	-1.950610
C	0.822086	-2.014015	3.329160
C	0.026546	-2.604358	4.501816
C	2.205711	-1.560751	3.800281
H	-2.336035	0.351345	2.333428
H	-3.325934	0.098964	0.881596
H	3.506921	0.261356	-0.982636
H	4.177676	0.955510	-3.279240
H	2.446237	1.228824	-5.033858
H	0.061981	0.827547	-4.508050
H	-0.608608	0.169987	-2.222740
H	2.274257	-4.267737	3.227728
H	2.323122	-6.014785	1.483380
H	0.889618	-5.805313	-0.511150
H	-2.442189	4.225384	-1.724447
H	-0.915286	5.614250	-0.378031
H	0.397001	4.605145	1.444971
H	-2.742193	0.520309	-1.385471
H	-5.104248	1.234525	-1.568352
H	-4.497374	1.684658	0.036812
H	-4.653453	2.907749	-1.217173
H	-3.513856	1.164417	-3.585727
H	-1.857762	1.782423	-3.420117
H	-3.235226	2.873720	-3.276011
H	0.385077	0.978136	2.313679
H	2.414578	1.979280	3.173977
H	2.415686	2.135886	1.413465
H	2.047084	3.536103	2.433936
H	0.236530	2.121246	4.485070
H	-1.315828	2.261423	3.638623
H	-0.214639	3.638097	3.696329
H	-0.331653	-4.650069	-1.879345
H	-2.759959	-4.935284	-1.677610
H	-1.921416	-5.713164	-0.324860
H	-2.758013	-4.180494	-0.079715
H	-1.687973	-2.992595	-2.882596

Appendix B – Atomic coordinates

H	-0.268873	-2.186001	-2.217458
H	-1.850331	-2.049664	-1.410545
H	0.292951	-1.120519	2.980532
H	-0.078706	-1.866170	5.303092
H	-0.975642	-2.931781	4.205475
H	0.538959	-3.476950	4.919247
H	2.101273	-0.788555	4.569364
H	2.791637	-1.152156	2.975465
H	2.768047	-2.384625	4.250488
H	-2.726033	-2.209143	0.751284
H	-2.092035	-2.042921	2.401226

III

C	-1.594288	-0.217346	1.808826
C	-1.110546	-1.479763	1.815655
N	0.046768	-1.482318	1.058248
C	0.299299	-0.230926	0.602983
N	-0.719868	0.541380	1.049046
C	-0.843421	1.966359	0.888245
C	0.879626	-2.646908	0.896252
C	1.622574	0.357106	0.090799
C	2.194830	-0.369805	-1.132201
O	2.371281	0.365185	1.189416
C	3.330978	-1.158368	-0.978895
C	3.905603	-1.790782	-2.077771
C	3.356240	-1.628596	-3.347447
C	2.234730	-0.818478	-3.514301
C	1.665274	-0.188043	-2.411244
C	1.911594	-2.839690	1.834577
C	2.730967	-3.956542	1.667653
C	2.529746	-4.845507	0.621716
C	1.470838	-4.654930	-0.252495
C	0.602575	-3.565276	-0.130674
C	-1.521211	2.466435	-0.237137
C	-1.674972	3.849470	-0.331555
C	-1.168617	4.694903	0.648032
C	-0.497897	4.170855	1.742729
C	-0.319334	2.793140	1.894173
C	-2.101033	1.553071	-1.300240
C	-3.593576	1.309824	-1.048968
C	-1.870778	2.074925	-2.719558
C	0.404234	2.260450	3.116583
C	1.851057	2.756749	3.170156
C	-0.369656	2.602566	4.393782
C	-0.612101	-3.580468	-1.053368
C	-1.738515	-4.402258	-0.409992
C	-1.155783	-2.252560	-1.574937
C	2.086909	-1.949997	3.051857
C	1.465798	-2.631881	4.276828
C	3.542063	-1.564872	3.310219
H	-2.462794	0.219154	2.274521
H	-1.474573	-2.379205	2.284582
H	1.315586	1.362948	-0.297919
H	3.747953	-1.244139	0.019432
H	4.790792	-2.407702	-1.945661
H	3.808336	-2.117081	-4.206451
H	1.814418	-0.666441	-4.505232
H	0.807264	0.469607	-2.548456
H	3.538311	-4.128490	2.372444
H	3.189101	-5.699880	0.497348
H	1.295549	-5.370368	-1.052021
H	-2.194623	4.271025	-1.186348
H	-1.295556	5.769598	0.553137
H	-0.098349	4.839423	2.499720
H	-1.590435	0.587819	-1.224541
H	-4.005526	0.629659	-1.801914
H	-3.770033	0.868600	-0.063200
H	-4.152616	2.250594	-1.099232
H	-2.179612	1.320174	-3.449713
H	-0.816862	2.309999	-2.895391
H	-2.454769	2.978512	-2.923688
H	0.462303	1.171863	3.031514
H	2.322936	2.413186	4.097355
H	2.405984	2.327308	2.330203
H	1.910005	3.850859	3.152632
H	0.126636	2.161574	5.264229
H	-1.397293	2.224526	4.361653
H	-0.420184	3.684799	4.556388
H	-0.278930	-4.140629	-1.936472
H	-2.560271	-4.544088	-1.120269
H	-1.385792	-5.387474	-0.091568
H	-2.146866	-3.890538	0.468287
H	-1.867895	-2.454908	-2.382336
H	-0.358508	-1.624831	-1.978853
H	-1.696876	-1.695541	-0.804386
H	1.575417	-1.006489	2.849643
H	1.542523	-1.980832	5.154250
H	0.406751	-2.866726	4.123942
H	1.980349	-3.570982	4.510572
H	3.596576	-0.925069	4.197371
H	3.918487	-0.990753	2.461448
H	4.186196	-2.431762	3.496189

IV

C	-1.948648	-0.393700	1.106004
C	-1.606029	-1.690958	1.315449
N	-0.345507	-1.870238	0.800635
C	0.077076	-0.707554	0.267077
N	-0.898367	0.204509	0.447042
C	-0.847713	1.621492	0.148065
C	0.400122	-3.110134	0.925204
C	1.505101	-0.462561	-0.185351
C	1.812128	0.148020	-1.484116
O	2.356982	-0.802031	0.614225
C	3.147143	0.516385	-1.714228
C	3.515216	1.060715	-2.933770
C	2.559914	1.226890	-3.937373
C	1.235804	0.852213	-3.719234
C	0.857771	0.320363	-2.493433
C	1.181923	-3.264373	2.084404
C	1.889301	-4.459114	2.219705
C	1.816222	-5.449055	1.251306
C	1.008825	-5.272553	0.137463
C	0.262821	-4.106025	-0.057024
C	-1.690452	2.118692	-0.863427
C	-1.635095	3.490583	-1.110192
C	-0.792200	4.320976	-0.383829
C	0.000247	3.799437	0.627598
C	-0.013094	2.436423	0.932475
C	-2.672056	1.257884	-1.641614
C	-4.100046	1.457726	-1.115484
C	-2.637293	1.532039	-3.148131
C	0.787014	1.938512	2.123871
C	2.258019	2.356318	2.057080
C	0.136964	2.416596	3.428195
C	-0.680843	-4.098643	-1.253720
C	-2.096773	-4.523612	-0.843623
C	-0.715168	-2.834945	-2.110912
C	1.222522	-2.238708	3.202596
C	0.336962	-2.698004	4.367928
C	2.644001	-1.942629	3.683658
H	-2.829720	0.162859	1.380325
H	-2.136588	-2.498127	1.794342
H	3.875007	0.360809	-0.924499
H	4.545953	1.350951	-3.109717
H	2.850557	1.645603	-4.896131
H	0.502347	0.969672	-4.510614
H	-0.171420	0.018229	-2.331347
H	2.506492	-4.612275	3.098832
H	2.382310	-6.367856	1.369385
H	0.939315	-6.062384	-0.605120
H	-2.265518	3.915499	-1.884445
H	-0.765228	5.384878	-0.598357
H	0.633120	4.463266	1.207929
H	-2.404807	0.203794	-1.493635
H	-4.799438	0.809406	-1.651888
H	-4.190369	1.240965	-0.047052
H	-4.421264	2.493536	-1.263261
H	-3.248791	0.794459	-3.675867
H	-1.621937	1.490549	-3.549833
H	-3.047193	2.517981	-3.386667
H	0.766570	0.844295	2.138566
H	2.811543	1.902295	2.883956
H	2.727649	2.039744	1.121980

Appendix B – Atomic coordinates

H	2.374074	3.440996	2.142982
H	0.688514	2.028979	4.290259
H	-0.901759	2.081793	3.509108
H	0.140408	3.509186	3.492600
H	-0.296582	-4.892100	-1.905724
H	-2.714586	-4.682976	-1.732913
H	-2.084003	-5.453375	-0.268646
H	-2.590298	-3.755609	-0.238577
H	-1.215717	-3.054819	-3.058650
H	0.290031	-2.473571	-2.345357
H	-1.283877	-2.027770	-1.636780
H	0.813968	-1.296634	2.822558
H	0.335417	-1.947955	5.164840
H	-0.699693	-2.864307	4.057379
H	0.707441	-3.636638	4.792147
H	2.623001	-1.132435	4.419278
H	3.286035	-1.640792	2.853915
H	3.095840	-2.808455	4.177178

V

C	-2.594770	-0.178533	2.389775
C	-1.989893	-1.587944	2.413479
N	-0.834146	-1.471812	1.521224
C	-0.629829	-0.202780	1.143766
N	-1.641649	0.568145	1.570623
C	-1.827649	1.961780	1.318237
C	-0.046093	-2.631010	1.239118
C	0.656092	0.403227	0.598904
C	1.310204	-0.378288	-0.539161
O	1.344937	0.493498	1.744765
C	2.533174	-0.998929	-0.303945
C	3.189529	-1.671983	-1.329995
C	2.630903	-1.722580	-2.605110
C	1.418954	-1.081153	-2.854115
C	0.768923	-0.404399	-1.825548
C	0.968268	-3.012581	2.129252
C	1.671242	-4.183481	1.847471
C	1.382892	-4.972629	0.734669
C	0.343327	-4.577968	-0.106022
C	-0.387148	-3.414642	0.128055
C	-2.591625	2.348876	0.209064
C	-2.810623	3.710225	0.002325
C	-2.293708	4.673945	0.867493
C	-1.544185	4.248810	1.964878
C	-1.294953	2.899995	2.215411
C	-3.153328	1.329560	-0.741558
H	-3.629956	1.817632	-1.594845
H	-3.907587	0.694932	-0.261734
C	-0.461719	2.460283	3.382444
H	-2.374402	0.662772	-1.125173
H	-0.038556	3.324473	3.900291
C	-1.489208	-3.011350	-0.808189
H	0.348651	1.802596	3.029702
H	-1.060734	1.900675	4.112059
C	1.305128	-2.172393	3.324740
H	-1.762744	-3.842617	-1.462760
H	-1.168080	-2.178206	-1.442931
H	-2.668764	0.263374	3.388559
H	-3.589935	-0.150939	1.932230
H	0.349716	1.378608	0.149522
H	2.943174	-0.918583	0.698501
H	4.143967	-2.155339	-1.137420
H	3.144429	-2.245695	-3.407291
H	0.989983	-1.095671	-3.852805
H	-0.158138	0.130578	-2.031954
H	2.470672	-4.483715	2.521555
C	2.187608	-6.205994	0.436133
H	0.094635	-5.188330	-0.971428
H	-3.396718	4.024278	-0.858603
C	-2.510874	6.138350	0.608915
H	-1.132280	4.988913	2.647517
H	-2.390350	-2.689308	-0.276467
H	2.224080	-2.528395	3.797371
H	0.512531	-2.214953	4.082922
H	1.429560	-1.126087	3.007383
H	1.589335	-6.959675	-0.083803
H	2.585243	-6.656389	1.349921
H	3.041423	-5.965706	-0.208466
H	-2.667649	6.689624	1.540696
H	-3.376432	6.307701	-0.037213
H	-1.638548	6.580480	0.113522
H	-2.676837	-2.354163	2.040700
H	-1.663269	-1.884110	3.416248

VI

C	-2.754531	-0.381679	2.057153
C	-2.309347	-1.851523	2.125140
N	-0.942082	-1.811322	1.572513
C	-0.654492	-0.592596	1.153338
N	-1.638077	0.271013	1.345925
C	-1.595168	1.690077	1.120692
C	-0.087792	-2.967188	1.551385
C	0.734886	-0.199140	0.646603
C	0.973199	-0.031934	-0.786362
O	1.571656	-0.051497	1.515469
C	2.255515	0.366080	-1.193422
C	2.529127	0.528602	-2.541775
C	1.531397	0.292176	-3.489133
C	0.256437	-0.106433	-3.090607
C	-0.024829	-0.266794	-1.740328
C	0.717096	-3.216494	2.676454
C	1.501699	-4.364763	2.664578
C	1.494482	-5.257607	1.589128
C	0.664673	-4.980895	0.505188
C	-0.141795	-3.842562	0.460270
C	-2.265597	2.224902	0.012930
C	-2.226556	3.608400	-0.163442
C	-1.563563	4.449821	0.726613
C	-0.943857	3.877809	1.840621
C	-0.951410	2.505374	2.070030
C	-3.030012	1.387811	-0.974942
H	-2.587512	1.465425	-1.973254
H	-4.063201	1.739597	-1.054306
C	-0.299528	1.943981	3.302336
H	-3.060095	0.329637	-0.706273
H	-0.107570	2.740474	4.023740
C	-1.004271	-3.593488	-0.744905
H	0.657011	1.463418	3.073550
H	-0.927892	1.197681	3.799725
C	0.745359	-2.280720	3.850660
H	-1.347558	-4.539073	-1.171050
H	-0.441695	-3.070798	-1.526600
H	-2.869016	0.078486	3.042943
H	-3.684048	-0.238396	1.501419
H	3.013993	0.540571	-0.437185
H	3.519027	0.838109	-2.860935
H	1.750010	0.418559	-4.545196
H	-0.513154	-0.291475	-3.833237
H	-1.018247	-0.575934	-1.431013
H	2.134361	-4.572198	3.524002
C	2.368053	-6.477834	1.606394
H	0.636324	-5.672739	-0.332994
H	-2.738272	4.037835	-1.021581
C	-1.510835	5.932126	0.499002
H	-0.449277	4.522884	2.562520
H	-1.889456	-2.992103	-0.519176
H	1.406939	-2.664919	4.629180
H	-0.245844	-2.154455	4.301375
H	1.108418	-1.291454	3.555928
H	2.073477	-7.194737	0.836883
H	2.327652	-6.981085	2.576615
H	3.414186	-6.206400	1.426026
H	-1.586090	6.482832	1.440426
H	-2.315479	6.267049	-0.159575
H	-0.561069	6.216260	0.031683
H	-2.927876	-2.515978	1.514620
H	-2.282786	-2.248175	3.142634

VII

C	-2.536522	-0.252407	2.214936
C	-2.035259	-1.507550	2.191712
N	-0.847500	-1.462559	1.482884
C	-0.602068	-0.194725	1.081983
N	-1.646296	0.545937	1.518499

Appendix B – Atomic coordinates

C	-1.838052	1.954942	1.315123
C	-0.048193	-2.636027	1.251544
C	0.722330	0.412145	0.596077
C	1.323707	-0.373356	-0.575619
O	1.471554	0.499482	1.694518
C	2.546237	-1.009712	-0.386129
C	3.153813	-1.693275	-1.435219
C	2.546585	-1.737651	-2.688251
C	1.333627	-1.081809	-2.891626
C	0.731010	-0.397544	-1.839076
C	0.946412	-2.964970	2.179920
C	1.671909	-4.133399	1.948054
C	1.420128	-4.957313	0.851729
C	0.393906	-4.605582	-0.024812
C	-0.360018	-3.447693	0.155074
C	-2.637053	2.369534	0.243651
C	-2.843406	3.738208	0.081551
C	-2.276645	4.672020	0.949968
C	-1.495082	4.210209	2.008793
C	-1.256857	2.851836	2.220019
C	-3.244671	1.377341	-0.706590
H	-3.807263	1.888350	-1.490874
H	-3.926895	0.688748	-0.196165
C	-0.401445	2.365035	3.350083
H	-2.476228	0.762423	-1.187722
H	-0.008994	3.207063	3.924861
C	-1.451583	-3.085974	-0.809621
H	0.433732	1.759784	2.954157
H	-0.976741	1.728666	4.033370
C	1.229359	-2.079485	3.353711
H	-1.663263	-3.921500	-1.480881
H	-1.151805	-2.230049	-1.424112
H	-3.431738	0.153770	2.657526
H	-2.402604	-2.432409	2.606739
H	0.407801	1.391946	0.153092
H	2.992711	-0.929184	0.600793
H	4.108720	-2.188861	-1.278911
H	3.022734	-2.267458	-3.508947
H	0.866362	-1.092742	-3.873139
H	-0.199641	0.144786	-2.008419
H	2.457585	-4.403545	2.649999
C	2.248658	-6.187018	0.608408
H	0.174734	-5.245894	-0.876066
H	-3.458766	4.081637	-0.746945
C	-2.479898	6.144827	0.731694
H	-1.050570	4.926902	2.695357
H	-2.381718	-2.816808	-0.298579
H	2.073092	-2.463033	3.932145
H	0.362724	-2.016207	4.022969
H	1.451060	-1.063372	2.985233
H	1.670124	-6.968347	0.107339
H	2.640487	-6.597753	1.543049
H	3.107280	-5.954807	-0.032629
H	-2.451535	6.696165	1.675524
H	-3.436999	6.350235	0.244267
H	-1.691076	6.555228	0.090380

VIII

C	-2.330934	-0.108466	1.935852
C	-1.910941	-1.391197	2.089594
N	-0.636796	-1.467983	1.570549
C	-0.290584	-0.263544	1.093623
N	-1.312212	0.579579	1.310296
C	-1.312665	1.999845	1.047089
C	0.175248	-2.663671	1.567529
C	1.098645	0.100332	0.593020
C	1.300674	0.426971	-0.820297
O	1.980855	0.087766	1.430503
C	2.570800	0.873498	-1.214898
C	2.813601	1.168302	-2.546707
C	1.798262	1.012213	-3.492067
C	0.536507	0.562042	-3.107402
C	0.285185	0.273019	-1.772659
C	0.957304	-2.928773	2.700135
C	1.703235	-4.103907	2.692175
C	1.678896	-4.991859	1.613790
C	0.870491	-4.686839	0.519374
C	0.101433	-3.524443	0.467787
C	-2.045539	2.495080	-0.036132
C	-2.018858	3.875367	-0.244539
C	-1.309296	4.738526	0.586596
C	-0.626322	4.195985	1.678974
C	-0.616011	2.830109	1.941886
C	-2.859276	1.632535	-0.960959
H	-2.480213	1.702389	-1.985475
H	-3.898488	1.974770	-0.981288
C	0.084723	2.291068	3.157373
H	-2.868224	0.578719	-0.674954
H	0.353228	3.107907	3.829647
C	-0.749831	-3.229042	-0.734450
H	1.005906	1.757068	2.902087
H	-0.551808	1.598073	3.717953
C	1.001486	-1.989733	3.870225
H	-0.943434	-4.143931	-1.297893
H	-0.247455	-2.530064	-1.412945
H	-3.249355	0.382325	2.217104
H	-2.394514	-2.255776	2.516635
H	3.345234	0.979261	-0.462102
H	3.793732	1.517454	-2.855041
H	1.993553	1.240149	-4.535601
H	-0.245631	0.434785	-3.849132
H	-0.696316	-0.081860	-1.473617
H	2.319212	-4.333832	3.557755
C	2.514937	-6.237998	1.633416
H	0.829558	-5.375401	-0.320612
H	-2.578848	4.283434	-1.082509
C	-1.274333	6.215191	0.322203
H	-0.096907	4.859674	2.357757
H	-1.717842	-2.794563	-0.465692
H	1.618589	-2.403560	4.669517
H	0.004697	-1.803316	4.284679
H	1.428803	-1.026144	3.574927
H	2.167422	-6.967362	0.898332
H	2.500955	-6.711022	2.619122
H	3.559841	-6.004027	1.400502
H	-1.338319	6.787362	1.251715
H	-2.093418	6.527185	-0.329547
H	-0.335140	6.496226	-0.167599