Supporting Information for:

One-Pot Synthesis of *N*-Substituted Benzannulated Triazoles via Stable Arene Diazonium Salts

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1. Synthesis of Starting Materials

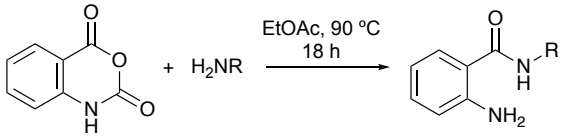
2-Aminobenzamides **6a**–**6e** and **6h**–**6n** were all commercially available.

2-Amino-5-iodobenzamide (6f)[1]

Iodine (0.373 g, 1.47 mmol) was added in portions over 1 h to a stirred solution of 2-aminobenzamide (0.200 g, 1.47 mmol) and sodium hydrogen carbonate (0.123 g, 1.47 mmol) in water (49 mL). The reaction mixture was then heated to 60 °C and stirred for 18 h. The reaction mixture was cooled to room temperature, washed with 1 M aqueous sodium thiosulfate (10 mL) and then extracted with ethyl acetate (3 × 50 mL). The combined organic layers were dried ($MgSO_4$), filtered and concentrated *in vacuo*. Recrystallisation from water:methanol (10:1) gave 2-amino-5-iodobenzamide (**6f**) (0.277 g, 72%) as a brown solid. Mp 191–194 °C (lit.[1] 193–194 °C); δ_H (400 MHz, DMSO-d_6) 6.54 (1H, d, *J* 8.7 Hz, 3-H), 6.69 (2H, br s, NH_2), 7.13 (1H, br s, NH), 7.37 (1H, dd, *J* 8.7, 2.1 Hz, 4-H), 7.80 (1H, d, *J* 2.1 Hz, 6-H); δ_C (101 MHz, DMSO-d_6) 74.4 (C), 116.1 (C), 118.9 (CH), 136.5 (CH), 139.8 (CH), 149.7 (C), 169.9 (C); *m*/*z* (EI) 262 (M^+. 50%), 244 (100), 117 (48), 90 (33).

2-Amino-5-nitrobenzamide (6g)[2]

To a stirred solution of 2-amino-5-nitrobenzoic acid (0.150 g, 0.820 mmol) and hydroxybenzotriazole (0.122 g, 0.910 mmol) in *N*,*N*'-dimethylformamide (3 mL) was added *N*-(3-dimethylaminopropyl)-*N*'-ethylcarbodiimide hydrochloride (0.184 g, 0.910 mmol). The reaction mixture was stirred at room temperature for 2 h, cooled to 0 °C and 28% aqueous ammonia solution (83 μL) was added. The mixture was allowed to warm to room temperature and stirred for a further 2 h. The reaction mixture was diluted in ethyl acetate (30 mL) and washed with 5% aqueous sodium bicarbonate (30 mL). The organic layer was then washed with water (3 × 20 mL) and brine (3 × 20 mL). The organic layer was dried ($MgSO_4$), filtered and concentrated *in vacuo*. The reaction mixture was triturated with ethyl acetate:hexane (1:1) and the resulting solid was filtered to give 2-amino-5-nitrobenzamide (**6g**) (0.116 g, 78%) as a yellow solid. Mp 232–236 °C (lit.[2] 236 °C); δ_H (400 MHz, DMSO-d_6) 6.79 (1H, d, *J* 9.2 Hz, 3-H), 7.42 (1H, br s, NH), 7.91 (2H, br s, NH_2), 8.03 (1H, dd, *J* 9.2, 2.6 Hz, 4-H), 8.22 (1H, br s, NH), 8.55 (1H, d, *J* 2.6 Hz, 6-H); δ_C (101 MHz, DMSO-d_6) 112.1 (C), 116.0 (CH), 126.4 (CH), 127.6 (CH), 134.8 (C), 155.7 (C), 169.7 (C); *m*/*z* (EI) 181 (M^+. 82%), 164 (57), 133 (53), 90 (61), 78 (100), 63 (84).



2-Amino-*N*-benzylbenzamide (6o)[3]

To a stirred solution of benzylamine (0.0910 mL, 0.0830 mmol) in ethyl acetate (0.6 mL) was added isatoic anhydride (0.150 g, 0.910 mmol). The reaction mixture was heated to 90 °C and stirred for 18 h. After cooling to room temperature, the reaction mixture was concentrated *in vacuo*. Purification by flash column chromatography, eluting with 30% ethyl acetate in hexane gave 2-amino-*N*-benzylbenzamide (**6o**) (0.169 g, 90%) as a white solid. Mp 124–127 °C (lit.[3] 123–125 °C); δ_H (400 MHz, $CDCl_3$) 4.61 (2H, d, *J* 5.6 Hz, PhCH_2), 5.56 (2H, br s, NH_2), 6.32 (1H, br s, NH), 6.63 (1H, td, *J* 8.2, 0.9 Hz, 5-H), 6.69 (1H, dd, *J* 8.2, 0.9 Hz, 3-H), 7.21 (1H, td, *J* 8.2, 1.4 Hz, 4-H), 7.27–7.39 (6H, m, 6-H and Ph); δ_C (101 MHz, $CDCl_3$) 43.9 (CH_2), 116.3 (C), 117.1 (CH), 117.8 (CH), 127.2 (CH), 127.7 (CH), 128.0 (2 × CH), 128.9 (2 × CH), 132.6 (CH), 138.4 (C), 148.5 (C), 169.2 (C); *m*/*z* (ESI) 249 (MNa^+. 100%).

2-Amino-*N*-(methoxycarbonylmethyl)benzamide (6p)[4]

To a stirred solution of glycine methyl ester hydrochloride (0.240 g, 1.92 mmol) in ethyl acetate (4.2 mL) was added isatoic anhydride (0.344 g, 2.11 mmol) and triethylamine (0.227 μL, 1.92 mmol). The reaction mixture was heated to 90 °C and stirred for 18 h. After cooling to room temperature, the reaction mixture was concentrated *in vacuo*. Purification by flash column chromatography, eluting with 20% ethyl acetate in dichloromethane gave 2-amino-*N*-(methoxycarbonylmethyl)benzamide (**6p**) (0.320 g, 80%) as a white solid. Mp 73–77 °C (lit.[4] 73–74 °C); δ_H (400 MHz, $CDCl_3$) 3.80 (3H, s OCH_3), 4.20 (2H, d, *J* 5.1 Hz, C$H_2CO_2CH_3$), 5.50 (2H, br s, NH_2), 6.59 (1H, br s, NH), 6.63–6.70 (2H, m, 3-H and 5-H), 7.19–7.25 (1H, m, 4-H), 7.40 (1H, dd, *J* 8.4, 1.6 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 41.6 (CH_2), 52.6 (CH_3), 115.2 (C), 116.8 (CH), 117.5 (CH), 127.6 (CH), 132.8 (CH), 149.0 (C), 169.4 (C), 170.8 (C); *m*/*z* (ESI) 231 (MNa^+. 100%).

2-Amino-*N*-phenylbenzamide (6q)[5]

To a stirred solution of aniline (0.0920 mL, 1.10 mmol) in ethyl acetate (0.6 mL) was added isatoic anhydride (0.150 g, 0.920 mmol). The reaction mixture was heated to 90 °C and stirred for 18 h. After cooling to room temperature, the reaction mixture was concentrated *in vacuo*. Purification by flash column chromatography, eluting with 25–40% ethyl acetate in hexane gave 2-amino-*N*-phenylbenzamide (**6q**) (0.143 g, 73%) as a white solid. Mp 125–127 °C (lit.[5] 125–127 °C); δ_H (500

MHz, CD_3OD) 6.67–6.71 (1H, m, 5-H), 6.79 (1H, dd, *J* 8.2, 0.8 Hz, 3-H), 7.12 (1H, tt, *J* 7.4, 1.1 Hz, 4'-H), 7.20–7.25 (1H, m, 4-H), 7.31–7.36 (2H, m, 3'-H and 5'-H), 7.59 (1H, dd, *J* 7.9, 1.4 Hz, 6-H), 7.60–7.64 (2H, m, 2'-H and 6'-H); δ_C (126 MHz, CD_3OD) 117.4 (CH), 118.0 (C), 118.2 (CH), 122.5 (2 × CH), 125.3 (CH), 129.4 (CH), 129.7 (2 × CH), 133.4 (CH), 140.0 (C), 150.6 (C), 170.5 (C); *m*/*z* (ESI) 235 (MNa^+. 100%).

2-Amino-*N*-(2'-methylphenyl)benzamide (6r)[6]

To a stirred solution of *o*-toluamide (0.236 mL, 2.21 mmol) in ethyl acetate (4 mL) was added isatoic anhydride (0.400 g, 2.45 mmol). The reaction mixture was heated to 90 °C and stirred for 18 h. After cooling to room temperature, the reaction mixture was concentrated *in vacuo*. Purification by flash column chromatography, eluting with 20% ethyl acetate in hexane gave 2-amino-*N*-(2'-methylphenyl)benzamide (**6r**) (0.252 g, 50%) as a white solid. Mp 115–120 °C (lit.[6] 113–115 °C); δ_H (400 MHz, $CDCl_3$) 2.33 (3H, s, 2'-CH_3), 5.54 (2H, br s, NH_2), 6.69–6.78 (2H, m, 3-H and 5'-H), 7.13 (1H, td, *J* 7.6, 1.2 Hz, 4-H), 7.20–7.32 (3H, m, 5-H, 3'-H and 4'-H), 7.50 (1H, dd, *J* 8.4, 1.2 Hz, 6'-H), 7.60 (1H, br s, NH), 7.83 (1H, br d, *J* 8.4 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 18.1 (CH_3), 116.3 (C), 117.0 (CH), 117.8 (CH), 123.7 (CH), 125.6 (CH), 127.0 (CH), 127.3 (CH), 130.0 (C), 130.8 (CH), 132.9 (CH), 135.9 (C), 149.3 (C), 167.7 (C); *m*/*z* (ESI) 225 ($[M–H]^-$. 100%).

2-Amino-*N*-(4'-methylphenyl)benzamide (6s)[3]

To a stirred solution of *p*-toluidine (0.0890 mL, 0.830 mmol) in ethyl acetate (0.6 mL) was added isatoic anhydride (0.150 g, 0.920 mmol). The reaction mixture was heated to 90 °C and stirred for 18 h. After cooling to room temperature, the reaction mixture was concentrated *in vacuo*. Purification by flash column chromatography, eluting with 20–30% ethyl acetate in hexane gave 2-amino-*N*-(4'-methylphenyl)benzamide (**6s**) (0.157 g, 84%) as a white solid. Mp 149–152 °C (lit.[3] 148–150 °C); δ_H (500 MHz, $CDCl_3$) 2.34 (3H, s, 4'-CH_3), 5.49 (2H, br s, NH_2), 6.69–6.74 (2H, m, 3-H and 5-H), 7.17 (2H, br d, *J* 8.3 Hz, 3'-H and 5'-H), 7.23–7.28 (1H, m, 4-H), 7.42–7.48 (3H, m, 6-H, 2'-H and 6'-H), 7.67 (1H, br s, NH); δ_C (126 MHz, $CDCl_3$) 21.0 (CH_3), 116.5 (C), 116.9 (CH), 117.6 (CH), 120.8 (2 × CH), 127.3 (CH), 129.6 (2 × CH), 132.7 (CH), 134.3 (C), 135.4 (C), 149.0 (C), 167.7 (C); *m*/*z* (ESI) 249 (MNa^+. 100%).

2-Amino-*N*-(4'-methoxyphenyl)benzamide (6t)[3]

To a stirred solution of 4-methoxyaniline (0.103 g, 0.830 mmol) in ethyl acetate (0.6 mL) was added isatoic anhydride (0.150 g, 0.910 mmol). The reaction mixture was heated to 90 °C and stirred for 18 h. After cooling to room temperature, the reaction mixture was concentrated *in vacuo*. Purification

by flash column chromatography, eluting with 40% ethyl acetate in hexane gave 2-amino-*N*-(4'-methoxyphenyl)benzamide (**6t**) (0.170 g, 84%) as a brown solid. Mp 113–116 °C (lit.[3] 114–116 °C); δ_H (400 MHz, $CDCl_3$) 3.81 (3H, s, 4'-OCH_3), 5.49 (2H, br s, NH_2), 6.68–6.74 (2H, m, 3-H and 5-H), 6.88–6.94 (2H, m, 3'-H and 5'-H), 7.22–7.28 (1H, m, 4-H), 7.43–7.49 (3H, m, 6-H, 2'-H and 6'-H), 7.64 (1H, br s, NH); δ_C (101 MHz, $CDCl_3$) 55.7 (CH_3), 114.4 (2 × CH), 116.5 (C), 117.0 (CH), 117.7 (CH), 122.7 (2 × CH), 127.2 (CH), 131.0 (C), 132.8 (CH), 149.1 (C), 156.9 (C), 167.7 (C); *m*/*z* (ESI) 265 (MNa^+. 100%).

2-Amino-*N*-(4'-fluorophenyl)benzamide (6u)[6]

To a stirred solution of 4-fluoroaniline (0.0800 mL, 0.830 mmol) in ethyl acetate (0.6 mL) was added isatoic anhydride (0.150 g, 0.920 mmol). The reaction mixture was heated to 90 °C and stirred for 18 h. After cooling to room temperature, the reaction mixture was concentrated *in vacuo*. Purification by flash column chromatography, eluting with 25% ethyl acetate in hexane gave 2-amino-*N*-(4'-fluorophenyl)benzamide (**6u**) (0.143 g, 75%) as a white solid. Mp 122–125 °C (lit.[6] 125–127 °C); δ_H (400 MHz, DMSO-d_6) 6.31 (2H, br s, NH_2), 6.59 (1H, td, *J* 8.0, 1.0 Hz, 5-H), 6.75 (1H, dd, *J* 8.2, 1.0 Hz, 3-H), 7.12–7.23 (3H, m, 4-H, 2'-H and 6'-H), 7.61 (1H, dd, *J* 8.0, 1.3 Hz, 6-H), 7.68–7.76 (2H, m, 3'-H and 5'-H), 10.03 (1H, br s, NH); δ_C (101 MHz, DMSO-d_6) 114.8 (2 × CH, d, $^2J_{CF}$ = 23.8 Hz), 115.0 (C), 115.1 (CH), 116.4 (CH), 122.3 (2 × CH, d, $^3J_{CF}$ = 7.7 Hz), 128.6 (CH), 132.1 (CH), 135.5 (C, d, $^4J_{CF}$ = 2.6 Hz), 149.7 (C), 158.1 (C, d, $^1J_{CF}$ = 240.1 Hz), 167.7 (C); *m*/*z* (ESI) 253 (MNa^+. 100%).

2-Amino-*N*-(4'-chlorophenyl)benzamide (6v)[7]

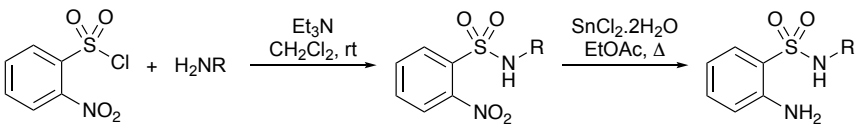
To a stirred solution of 4-chloroaniline (0.212 g, 1.64 mmol) in ethyl acetate (1.2 mL) was added isatoic anhydride (0.300 g, 1.84 mmol). The reaction mixture was heated to 90 °C and stirred for 18 h. After cooling to room temperature, the reaction mixture was concentrated *in vacuo*. Purification by flash column chromatography, eluting with 20–40% ethyl acetate in hexane gave 2-amino-*N*-(4'-chlorophenyl)benzamide (**6v**) (0.277 g, 69%) as a white solid. Mp 197–200 °C (lit.[7] 198–200 °C); δ_H (500 MHz, DMSO-d_6) 6.32 (2H, br s, NH_2), 6.59 (1H, br t, *J* 7.9 Hz, 5-H), 6.75 (1H, br d, *J* 8.2 Hz, 3-H), 7.18–7.23 (1H, m, 4-H), 7.35–7.41 (2H, m, 2'-H and 6'-H), 7.61 (1H, dd, *J* 7.9, 1.1 Hz, 6-H), 7.72–7.78 (2H, m, 3'-H and 5'-H), 10.10 (1H, br s, NH); δ_C (126 MHz, DMSO-d_6) 114.7 (CH), 114.9 (C), 116.4 (CH), 122.0 (2 × CH), 126.9 (C), 128.4 (2 × CH), 128.7 (CH), 132.3 (CH), 138.3 (C), 149.8 (C), 167.9 (C); *m*/*z* (ESI) 269 (MNa^+. 100%).

2-Amino-*N*-(4'-iodophenyl)benzamide (6w)

To a stirred solution of 4-iodoaniline (0.181 g, 0.830 mmol) in ethyl acetate (0.6 mL) was added isatoic anhydride (0.150 g, 0.920 mmol). The reaction mixture was heated to 90 °C and stirred for 18 h. An additional portion of isatoic anhydride (0.0300 g, 0.180 mmol) was then added. After 3 h, a final portion of isatoic anhydride (0.0300 g, 0.180 mmol) was added and the reaction mixture was stirred for 2.5 h. After cooling to room temperature, the reaction mixture was concentrated *in vacuo*. Purification by flash column chromatography, eluting with 25% ethyl acetate in hexane gave 2-amino-*N*-(4'-iodophenyl)benzamide (**6w**) (0.145 g, 52%) as a yellow solid. Mp 120–122 °C; ν_{max}/cm^{-1} (neat) 3285 (NH), 2529 (CH), 1622 (C=O), 1574 (C=C), 1522, 1481, 1385, 812; δ_H (500 MHz, CD_3OD) 6.64–6.70 (1H, m, 5-H), 6.78 (1H, br d, *J* 8.1 Hz, 3-H), 7.19–7.25 (1H, m, 4-H), 7.45–7.50 (2H, m, 2'-H and 6'-H), 7.58 (1H, dd, *J* 7.9, 1.3 Hz, 6-H), 7.63–7.68 (2H, m, 3'-H and 5'-H); δ_C (126 MHz, CD_3OD) 87.8 (C), 117.3 (CH), 117.6 (C), 118.2 (CH), 124.1 (2 × CH), 129.4 (CH), 133.6 (CH), 138.8 (2 × CH), 140.1 (C), 150.8 (C), 170.4 (C); *m*/*z* (ESI) 360.9809 (MNa^+. $C_{13}H_{11}IN_2NaO$ requires 360.9808).

***N*-(2-Aminobenzoyl)-2'-aminothiazole (6x)[8]**

To a stirred solution of 2-aminothiazole (0.166 g, 1.65 mmol) in ethyl acetate (1.2 mL) was added isatoic anhydride (0.300 g, 1.84 mmol). The reaction mixture was heated to 90 °C and stirred for 18 h. After cooling to room temperature, the reaction mixture was concentrated *in vacuo*. Purification by flash column chromatography, eluting with 20–30% ethyl acetate in hexane gave *N*-(2-aminobenzoyl)-2'-aminothiazole (**6x**) (0.300 g, 83%) as an orange solid. Mp 157–159 °C (lit.[8] 151–153 °C); δ_H (500 MHz, $CDCl_3$) 5.68 (2H, br s, NH_2), 6.67–6.72 (1H, m, 5-H), 6.76 (1H, dd, *J* 8.2, 0.7 Hz, 3-H), 6.90 (1H, d, *J* 3.7 Hz, 5'-H), 7.12 (1H, d, *J* 3.7 Hz, 4'-H), 7.29–7.34 (1H, m, 4-H), 7.70 (1H, dd, *J* 8.0, 1.3 Hz, 6-H), 12.26 (1H, br s, NH); δ_C (126 MHz, $CDCl_3$) 113.1 (CH), 113.7 (C), 116.8 (CH), 117.5 (CH), 128.8 (CH), 133.8 (CH), 137.5 (CH), 149.9 (C), 160.1 (C), 167.4 (C); *m*/*z* (ESI) 242 (MNa^+. 100%).



2-Nitro-*N*-methylbenzenesulfonamide[9]

2-Nitrobenzenesulfonyl chloride (0.500 g, 2.26 mmol) was added in portions to a mixture of methylamine hydrochloride (0.183 g, 2.71 mmol) and triethylamine (0.626 mL, 4.51 mmol) in dichloromethane (25 mL) at 0 °C. The reaction mixture was warmed to room temperature and stirred

for 2 h. Methanol (5 mL) was then added and the reaction mixture stirred for a further 1 h. The reaction mixture was concentrated *in vacuo*, diluted with dichloromethane (25 mL) and washed with brine (2 × 25 mL). The organic layer was dried ($MgSO_4$), filtered and concentrated *in vacuo*. Purification by flash column chromatography, eluting with 25% ethyl acetate in hexane gave 2-nitro-*N*-methylbenzenesulfonamide (0.342 g, 70%) as a yellow solid. Mp 100–104 °C (lit.[9] 106 °C); δ_H (400 MHz, $CDCl_3$) 2.80 (3H, d, *J* 5.2 Hz, NCH_3), 5.22 (1H, br s, NH), 7.72–7.79 (2H, m, 4-H and 5-H), 7.84–7.90 (1H, m, 6-H), 8.11–8.17 (1H, m, 3-H); δ_C (101 MHz, $CDCl_3$) 29.9 (CH_3), 125.6 (CH), 131.7 (CH), 132.7 (C), 132.8 (CH), 133.8 (CH), 148.5 (C); *m*/*z* (ESI) 239 (MNa^+. 100%).

2-Nitro-*N*-ethylbenzenesulfonamide[10]

2-Nitrobenzenesulfonyl chloride (0.500 g, 2.26 mmol) was dissolved in dichloromethane (2 mL) and added dropwise to a stirred solution of ethylamine (0.125 mL, 1.88 mmol) and triethylamine (0.315 mL, 2.26 mmol) in dichloromethane (4 mL) at 0 °C. The reaction mixture was warmed to room temperature and stirred for 4 h. The reaction mixture was then concentrated *in vacuo*. Purification by flash column chromatography, eluting with 70% diethyl ether in hexane gave 2-nitro-*N*-ethylbenzenesulfonamide (0.433 g, 100%) as a white solid. Mp 96–98 °C (lit.[10] 98–100 °C); δ_H (400 MHz, $CDCl_3$) 1.17 (3H, t, *J* 7.3 Hz, NCH_2CH_3), 3.16 (2H, qd, *J* 7.3, 6.0 Hz, NCH_2CH_3), 5.22 (1H, d, *J* 6.0 Hz, NH), 7.71–7.78 (2H, m, 4-H and 5-H), 7.83–7.89 (1H, m, 6-H), 8.11–8.17 (1H, m, 3-H); δ_C (101 MHz, $CDCl_3$) 15.3 (CH_3), 39.0 (CH_2), 125.5 (CH), 131.2 (CH), 132.9 (CH), 133.7 (CH), 133.9 (C), 148.2 (C); *m*/*z* (ESI) 253 (MNa^+. 100%).

2-Nitro-*N*-propylbenzenesulfonamide[11]

2-Nitrobenzenesulfonyl chloride (0.500 g, 2.26 mmol) was dissolved in dichloromethane (2 mL) and added dropwise to a stirred solution of *n*-propylamine (0.161 mL, 1.96 mmol) and triethylamine (0.315 mL, 2.26 mmol) in dichloromethane (4 mL) at 0 °C. The reaction mixture was warmed to room temperature and stirred for 2 h. The reaction mixture was then concentrated *in vacuo*, diluted with dichloromethane (25 mL) and washed with water (3 × 30 mL), sodium bicarbonate (2 × 20 mL), 1 M hydrochloric acid (2 × 15 mL) and brine (2 × 15 mL). The organic layer was dried ($MgSO_4$), filtered and concentrated *in vacuo* to give 2-nitro-*N*-propylbenzenesulfonamide (0.392 g, 82%) as a white solid. Mp 72–76 °C (lit.[11] 70 °C); δ_H (400 MHz, $CDCl_3$) 0.91 (3H, t, *J* 7.4 Hz, 3'-H_3), 1.55 (2H, sextet, *J* 7.4 Hz, 2'-H_2), 3.07 (2H, td, *J* 7.4, 6.2 Hz, 1'-H_2), 5.25 (1H, br t, *J* 6.3 Hz, NH), 7.70–7.77 (2H, m, 4-H and 5-H), 7.83–7.89 (1H, m, 6-H), 8.11–8.18 (1H, m, 3-H); δ_C (101 MHz, $CDCl_3$) 11.2 (CH_3), 23.1 (CH_2), 45.7 (CH_2), 125.5 (CH), 131.2 (CH), 132.9 (CH), 133.6 (CH), 134.0 (C), 148.3 (C); *m*/*z* (ESI) 267 (MNa^+. 100%).

2-Nitro-*N*-(*tert*-butyl)benzenesulfonamide

2-Nitrobenzenesulfonyl chloride (0.500 g, 2.26 mmol) was dissolved in dichloromethane (2 mL) and added dropwise to a stirred solution of *tert*-butylamine (0.197 mL, 1.88 mmol) and triethylamine (0.315 mL, 2.26 mmol) in dichloromethane (4 mL) at 0 °C. The reaction mixture was stirred at 0 °C for 1 h, warmed to room temperature and stirred for a further 5 h. The reaction mixture was concentrated *in vacuo*, diluted with dichloromethane (25 mL) and washed with water (3 × 30 mL), sodium bicarbonate (2 × 20 mL), 1 M hydrochloric acid (2 × 15 mL) and brine (2 × 15 mL). The organic layer was dried ($MgSO_4$), filtered and concentrated *in vacuo* to give 2-nitro-*N*-(*tert*-butyl)benzenesulfonamide (0.243 g, 50%) as a white solid. Mp 121–123 °C; ν_{max}/cm^{-1} (neat) 3264 (NH), 2974 (CH), 1541, 1368, 1323, 1153, 997; δ_H (400 MHz, $CDCl_3$) 1.32 (9H, s, NHC(CH_3)$_3$), 5.25 (1H, br s, NH), 7.66–7.76 (2H, m, 4-H and 5-H), 7.85 (1H, dd, *J* 7.3, 2.0 Hz, 6-H), 8.20 (1H, dd, *J* 7.3, 2.0 Hz, 3-H); δ_C (101 MHz, $CDCl_3$) 30.4 (3 × CH_3), 55.9 (C), 125.4 (CH), 130.6 (CH), 133.0 (CH), 133.2 (CH), 137.4 (C), 148.0 (C); *m/z* (ESI) 281.0566 (MNa^+. $C_{10}H_{14}N_2NaO_4S$ requires 281.0566).

***N*-Benzyl-2-nitrobenzenesulfonamide[12]**

2-Nitrobenzenesulfonyl chloride (0.500 g, 2.26 mmol) was dissolved in dichloromethane (2 mL) and added dropwise to a stirred solution of benzylamine (0.206 mL, 1.88 mmol) and triethylamine (0.315 mL, 2.26 mmol) in dichloromethane (4 mL) at 0 °C. The reaction mixture was warmed to room temperature and stirred for 2 h. The reaction mixture was concentrated *in vacuo*, diluted with dichloromethane (20 mL) and washed with water (3 × 20 mL), sodium bicarbonate (2 × 10 mL), 1 M hydrochloric acid (2 × 15 mL) and brine (2 × 15 mL). The organic layer was dried ($MgSO_4$), filtered and concentrated *in vacuo*. Purification by flash column chromatography, eluting with 60% diethyl ether in hexane gave *N*-benzyl-2-nitrobenzenesulfonamide (0.415 g, 75%) as a white solid. Mp 86–91 °C (lit.[12] 92 °C); δ_H (400 MHz, $CDCl_3$) 4.32 (2H, d, *J* 6.3 Hz, PhCH_2), 5.71 (1H, t, *J* 6.3 Hz, NH), 7.17–7.25 (5H, m, Ph), 7.63 (1H, td, *J* 7.8, 1.6 Hz, 5-H), 7.68 (1H, td, *J* 7.8, 1.5 Hz, 4-H), 7.82 (1H, dd, *J* 7.8, 1.5 Hz, 6-H), 8.01 (1H, dd, *J* 7.8, 1.6 Hz, 3-H); δ_C (101 MHz, $CDCl_3$) 48.0 (CH_2), 125.4 (CH), 128.0 (2 × CH), 128.2 (CH), 128.8 (2 × CH), 131.2 (CH), 132.8 (CH), 133.5 (CH), 134.2 (C), 135.8 (C), 148.0 (C); *m/z* (ESI) 315 (MNa^+. 100%).

***N*-(4'-Methoxybenzyl)-2-nitrobenzenesulfonamide[13]**

2-Nitrobenzenesulfonyl chloride (0.500 g, 2.26 mmol) was dissolved in dichloromethane (2 mL) and added dropwise to a stirred solution of 4-methoxybenzylamine (0.246 mL, 1.88 mmol) and triethylamine (0.315 mL, 2.26 mmol) in dichloromethane (4 mL) at 0 °C. The reaction mixture was

warmed to room temperature and stirred for 2 h. The reaction mixture was concentrated *in vacuo*, diluted with dichloromethane (20 mL) and washed with water (3 × 20 mL), sodium bicarbonate (2 × 10 mL), 1 M hydrochloric acid (2 × 15 mL) and brine (2 × 15 mL). The organic layer was dried ($MgSO_4$), filtered and concentrated *in vacuo*. Purification by flash column chromatography, eluting with 50–70% dichloromethane in hexane gave *N*-(4'-methoxybenzyl)-2-nitrobenzenesulfonamide (**X**) (0.458 g, 76%) as a white solid. Mp 112–116 °C (lit.[13] 117–119 °C); δ_H (400 MHz, $CDCl_3$) 3.75 (3H, s, OCH_3), 4.24 (2H, d, *J* 6.2 Hz, NHCH_2), 5.64 (1H, t, *J* 6.2 Hz, NH), 6.75 (2H, br d, *J* 8.4 Hz, 3'-H and 5'-H), 7.12 (2H, d, *J* 8.4 Hz, 2'-H and 6'-H), 7.64 (1H, td, *J* 7.6, 1.7 Hz, 5-H), 7.68 (1H, td, *J* 7.6, 1.5 Hz, 4-H), 7.82 (1H, dd, *J* 7.6, 1.5 Hz, 6-H), 8.01 (1H, dd, *J* 7.6, 1.7 Hz, 3-H); δ_C (101 MHz, $CDCl_3$) 47.6 (CH_2), 55.4 (CH_3), 114.2 (2 × CH), 125.4 (CH), 127.8 (C), 129.4 (2 × CH), 131.2 (CH), 132.8 (CH), 133.5 (CH), 134.2 (C), 148.0 (C), 159.5 (C); *m*/*z* (ESI) 345 (MNa^+. 100%).

_N_-Phenyl-2-nitrobenzenesulfonamide[14]

2-Nitrobenzenesulfonyl chloride (0.300 g, 1.35 mmol) was added in portions over 0.5 h to a stirred solution of aniline (0.148 mL, 1.62 mmol) in 50% aqueous methanol (3 mL) and sodium acetate (0.156 g, 1.90 mmol). The reaction mixture was then heated to 60 °C and stirred for 1 h. The reaction mixture was allowed to cool to room temperature, diluted in water (7 mL) and acidified to pH 2 using 1 M hydrochloric acid. The precipitate was filtered, washed with excess water and then recrystallised from 4:1 ethanol:water to give *N*-phenyl-2-nitrobenzenesulfonamide (0.295 g, 79%) as a white solid. Mp 106–110 °C (lit.[14] 109–110 °C); δ_H (400 MHz, $CDCl_3$) 7.15–7.31 (6H, m, Ph and NH), 7.57 (1H, td, *J* 7.9, 1.3 Hz, 5-H), 7.69 (1H, td, *J* 7.9, 1.3 Hz, 4-H), 7.82 (1H, dd, *J* 7.9, 1.3 Hz, 6-H), 7.86 (1H, dd, *J* 7.9, 1.3 Hz, 3-H); δ_C (101 MHz, $CDCl_3$) 123.5 (2 × CH), 125.4 (CH), 126.8 (CH), 129.6 (2 × CH), 132.0 (CH), 132.4 (C), 132.7 (CH), 134.1 (CH), 135.7 (C), 148.4 (C); *m*/*z* (ESI) 301 (MNa^+. 100%).

_N_-(4'-Methylphenyl)-2-nitrobenzenesulfonamide[15]

2-Nitrobenzenesulfonyl chloride (0.500 g, 2.26 mmol) was dissolved in dichloromethane (2 mL) and added dropwise to a stirred solution of *p*-toluidine (0.227 g, 2.12 mmol) and triethylamine (0.315 mL, 2.26 mmol) in dichloromethane (4 mL) at 0 °C. The reaction mixture was stirred at 0 °C for 1 h, warmed to room temperature and stirred for a further 5 h. The reaction mixture was concentrated *in vacuo*, diluted with dichloromethane (20 mL) and washed with water (3 × 30 mL), sodium bicarbonate (2 × 20 mL), 1 M hydrochloric acid (2 × 15 mL) and brine (2 × 15 mL). The organic layer was dried ($MgSO_4$), filtered and concentrated *in vacuo* to give *N*-(4'-methylphenyl)-2-nitrobenzenesulfonamide (0.390 g, 63%) as a yellow solid. Mp 104–108 °C (lit.[15] 110 °C); δ_H (400

MHz, $CDCl_3$) 2.28 (3H, s, 4'-CH_3), 7.06 (4H, br s, 2'-H, 3'-H, 5'-H and 6'-H), 7.15 (1H, br s, NH), 7.56 (1H, td, *J* 7.9, 1.3 Hz, 5-H), 7.68 (1H, td, *J* 7.9, 1.3 Hz, 4-H), 7.80 (1H, dd, *J* 7.9, 1.3 Hz, 6-H), 7.85 (1H, dd, *J* 7.9, 1.3 Hz, 3-H); δ_C (101 MHz, $CDCl_3$) 21.1 (CH_3), 123.9 (2 × CH), 125.4 (CH), 130.2 (2 × CH), 132.1 (CH), 132.5 (C), 132.6 (CH), 132.9 (C), 133.9 (CH), 136.9 (C), 148.4 (C); *m*/*z* (ESI) 315 (MNa^+. 100%).

_N_-(4'-Methoxyphenyl)-2-nitrobenzenesulfonamide[16]

2-Nitrobenzenesulfonyl chloride (0.500 g, 2.26 mmol) was dissolved in dichloromethane (2 mL) and added dropwise to a stirred solution of *p*-anisidine (0.261 g, 2.12 mmol) and triethylamine (0.315 mL, 2.26 mmol) in dichloromethane (4 mL) at 0 °C. The reaction mixture was warmed to room temperature and stirred for 6 h. The reaction mixture was concentrated *in vacuo*, diluted with dichloromethane (30 mL) and washed with water (3 × 50 mL), sodium bicarbonate (2 × 30 mL), 1 M hydrochloric acid (2 × 30 mL) and brine (2 × 30 mL). The organic layer was dried ($MgSO_4$), filtered and concentrated *in vacuo* to give *N*-(4'-methoxyphenyl)-2-nitrobenzenesulfonamide (0.403 g, 62%) as a brown solid. Mp 106–108 °C (lit.[16] 106–107 °C); δ_H (400 MHz, $CDCl_3$) 3.76 (3H, s, OCH_3), 6.75–6.80 (2H, m, 3'-H and 5'-H), 7.06–7.12 (3H, m, NH, 2'-H and 6'-H), 7.56 (1H, td, *J* 7.8, 1.3 Hz, 5-H), 7.70 (1H, td, *J* 7.8, 1.4 Hz, 4-H), 7.74 (1H, dd, *J* 7.8, 1.4 Hz, 6-H), 7.86 (1H, dd, *J* 7.8, 1.3 Hz, 3-H); δ_C (101 MHz, $CDCl_3$) 55.6 (CH_3), 114.7 (2 × CH), 125.3 (CH), 126.4 (2 × CH), 128.0 (C), 132.1 (CH), 132.4 (C), 132.6 (CH), 133.9 (CH), 148.4 (C), 158.7 (C); *m*/*z* (ESI) 331 (MNa^+. 100%).

_N_-(4'-Bromophenyl)-2-nitrobenzenesulfonamide[15]

2-Nitrobenzenesulfonyl chloride (0.500 g, 2.26 mmol) was dissolved in dichloromethane (2 mL) and added dropwise to a stirred solution of 4-bromoaniline (0.364 g, 2.12 mmol) and triethylamine (0.315 mL, 2.26 mmol) in dichloromethane (4 mL) at 0 °C. The reaction mixture was warmed to room temperature and stirred for 18 h. The reaction mixture was concentrated *in vacuo*, diluted with dichloromethane (20 mL) and washed with water (3 × 20 mL), sodium bicarbonate (2 × 10 mL), 1 M hydrochloric acid (2 × 15 mL) and brine (2 × 15 mL). The organic layer was dried ($MgSO_4$), filtered and concentrated *in vacuo*. Purification by flash column chromatography, eluting with 60% diethyl ether in hexane gave *N*-(4'-bromophenyl)-2-nitrobenzenesulfonamide (0.348 g, 46%) as an off-white solid. Mp 106–110 °C (lit.[15] 105 °C); δ_H (400 MHz, $CDCl_3$) 7.06–7.12 (2H, m, 2'-H and 6'-H), 7.26 (1H, br s, NH), 7.36–7.42 (2H, m, 3'-H and 5'-H), 7.61 (1H, td, *J* 7.8, 1.3 Hz, 5-H), 7.71 (1H, td, *J* 7.8, 1.3 Hz, 4-H), 7.83 (1H, dd, *J* 7.8, 1.3 Hz, 6-H), 7.86 (1H, dd, *J* 7.8, 1.3 Hz, 3-H); δ_C (101 MHz, $CDCl_3$) 120.3 (C), 125.0 (2 × CH), 125.6 (CH), 132.0 (CH), 132.1 (C), 132.7 (2 × CH), 132.9 (CH), 134.3 (CH), 134.8 (C), 148.4 (C); *m*/*z* (ESI) 381 (MNa^+. 100%).

_N_-(4'-Iodophenyl)-2-nitrobenzenesulfonamide[17]

2-Nitrobenzenesulfonyl chloride (0.500 g, 2.26 mmol) was added in portions to a stirred solution of 4-iodoaniline (0.495 g, 2.26 mmol) in dry pyridine (1.5 mL) at 0 °C. The reaction mixture was warmed to room temperature and stirred for 2 h. The reaction mixture was diluted with 2 M aqueous hydrochloric acid (50 mL) and extracted with chloroform (2 × 50 mL). The organic layers were combined and washed with brine (2 × 50 mL). The organic layer was dried ($MgSO_4$), filtered and concentrated *in vacuo*. Purification by flash column chromatography, eluting with 60% diethyl ether in hexane gave *N*-(4'-iodophenyl)-2-nitrobenzenesulfonamide (0.766 g, 84%) as an orange solid. Mp 95–100 °C (lit.[17] 92–94 °C); δ_H (400 MHz, $CDCl_3$) 6.93–7.00 (2H, m, 2'-H and 6'-H), 7.23 (1H, br s, NH), 7.56–7.65 (3H, m, 5-H, 3'-H and 5'-H), 7.71 (1H, td, *J* 7.8, 1.4 Hz, 4-H), 7.82–7.88 (2H, m, 3-H and 6-H); δ_C (101 MHz, $CDCl_3$) 91.2 (C), 125.1 (2 × CH), 125.6 (CH), 132.0 (CH), 132.2 (C), 132.9 (CH), 134.3 (CH), 135.5 (C), 138.7 (2 × CH), 148.4 (C); *m*/*z* (ESI) 427 (MNa^+. 100%).

2-Amino-*N*-methylbenzenesulfonamide (8a)[18]

To a stirred solution of 2-nitro-*N*-methylbenzenesulfonamide (0.126 g, 0.583 mmol) in ethyl acetate (6 mL) was added tin(II) dichloride dihydrate (0.658 g, 2.91 mmol). The reaction mixture was heated under reflux for 18 h. The mixture was cooled to room temperature and sodium bicarbonate (100 mL) was added. The reaction mixture was filtered through a pad of Celite® and diluted with ethyl acetate (40 mL). The organic layer was washed with sodium bicarbonate (3 × 60 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo.* Purification by flash column chromatography, eluting with 65% diethyl ether in hexane gave 2-amino-*N*-methylbenzenesulfonamide (**8a**) (0.0850 g, 78%) as a yellow oil. Spectroscopic data were consistent with the literature.[18] δ_H (400 MHz, $CDCl_3$) 2.58 (3H, d, *J* 5.5 Hz, NCH_3), 4.66 (1H, br s, NH), 4.85 (2H, br s, NH_2), 6.77 (1H, dd, *J* 8.1, 1.0 Hz, 3-H), 6.79–6.86 (1H, m, 5-H), 7.31–7.37 (1H, m, 4-H), 7.71 (1H, dd, *J* 8.0, 1.5 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 29.5 (CH_3), 117.9 (CH), 118.1 (CH), 120.7 (C), 130.2 (CH), 134.4 (CH), 145.2 (C); *m*/*z* (ESI) 209 (MNa^+. 100%).

2-Amino-*N*-ethylbenzenesulfonamide (8b)

To a stirred solution of 2-nitro-*N*-ethylbenzenesulfonamide (0.142 g, 0.617 mmol) in ethyl acetate (6 mL) was added tin(II) dichloride dihydrate (0.696 g, 3.08 mmol). The reaction mixture was heated under reflux for 18 h. The mixture was cooled to room temperature and sodium bicarbonate (150 mL) was added. The reaction mixture was filtered through a pad of Celite® and diluted with ethyl acetate (50 mL). The organic layer was washed with sodium bicarbonate (3 × 50 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo.* Purification by flash column chromatography, eluting with 60% diethyl ether in hexane gave 2-amino-*N*-ethylbenzenesulfonamide (**8b**) (0.104 g, 84%) as a yellow oil.

ν_{max}/cm^{-1} (neat) 3377 (NH), 2980 (CH), 1618 (C=C), 1483, 1454, 1315, 1140, 752; δ_H (400 MHz, $CDCl_3$) 1.07 (3H, t, *J* 7.3 Hz, 2'-H_3), 2.94 (2H, qd, *J* 7.3, 6.2 Hz, 1'-H_2), 4.61 (1H, br d, *J* 6.2 Hz, NH), 4.82 (2H, br s, NH_2), 6.77 (1H, dd, *J* 8.1, 0.9 Hz, 3-H), 6.79–6.84 (1H, m, 5-H), 7.30–7.36 (1H, m, 4-H), 7.71 (1H, dd, *J* 8.0, 1.5 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 15.1 (CH_3), 38.5 (CH_2), 117.9 (CH), 118.1 (CH), 122.0 (C), 129.9 (CH), 134.2 (CH), 145.1 (C); *m/z* (ESI) 223.0509 (MNa^+. $C_8H_{12}N_2NaO_2S$ requires 223.0512).

2-Amino-*N*-propylbenzenesulfonamide (8c)

To a stirred solution of 2-nitro-*N*-propylbenzenesulfonamide (0.200 g, 0.819 mmol) in ethyl acetate (8 mL) was added tin(II) dichloride dihydrate (0.924 g, 4.09 mmol). The reaction mixture was heated under reflux for 18 h. The mixture was cooled to room temperature and sodium bicarbonate (150 mL) was added. The reaction mixture was filtered through a pad of Celite® and diluted with ethyl acetate (60 mL). The organic layer was washed with sodium bicarbonate (3 × 60 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo.* Purification by flash column chromatography, eluting with 60% diethyl ether in hexane gave 2-amino-*N*-propylbenzenesulfonamide (**8c**) (0.138 g, 79%) as a yellow oil. ν_{max}/cm^{-1} (neat) 3379 (NH), 2967 (CH), 1618 (C=C), 1481, 1454, 1315, 1134, 748; δ_H (400 MHz, $CDCl_3$) 0.83 (3H, t, *J* 7.4 Hz, 3'-H_3), 1.37–1.49 (2H, m, 2'-H_2), 2.82 (2H, q, *J* 6.9 Hz, 1'-H_2), 4.82–4.96 (3H, m, NH and NH_2), 6.72–6.81 (2H, m 3-H and 5-H), 7.27–7.33 (1H, m, 4-H), 7.69 (1H, dd, *J* 8.0, 1.4 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 11.2 (CH_3), 22.8 (CH_2), 45.1 (CH_2), 117.8 (CH), 117.8 (CH), 121.7 (C), 129.7 (CH), 134.1 (CH), 145.1 (C); *m/z* (ESI) 237.0664 (MNa^+. $C_9H_{14}N_2NaO_2S$ requires 237.0668).

2-Amino-*N*-(*tert*-butyl)benzenesulfonamide (8d)

To a stirred solution of 2-nitro-*N*-(*tert*-butyl)benzenesulfonamide (0.222 g, 0.859 mmol) in ethyl acetate (9 mL) was added tin(II) dichloride dihydrate (0.970 g, 4.30 mmol). The reaction mixture was heated under reflux for 18 h. The mixture was cooled to room temperature and sodium bicarbonate (150 mL) was added. The reaction mixture was filtered through a pad of Celite® and diluted with ethyl acetate (100 mL). The organic layer was washed with sodium bicarbonate (3 × 60 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo.* Purification by flash column chromatography, eluting with 20% ethyl acetate in hexane gave 2-amino-*N*-(*tert*-butyl)benzenesulfonamide (**8d**) (0.0330 g, 17%) as a beige solid. Mp 83–87 °C; ν_{max}/cm^{-1} (neat) 3383 (NH), 2974 (CH), 1620 (C=C), 1483, 1315, 1136, 752; δ_H (400 MHz, $CDCl_3$) 1.18 (9H, s, NHC(CH_3)$_3$), 4.75–4.90 (3H, m, NH and NH_2), 6.73 (1H, br d, *J* 8.1 Hz, 3-H), 6.76–6.82 (1H, m, 5-H), 7.26–7.32 (1H, m, 4-H), 7.74 (1H, dd, *J* 8.0,

1.4 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 30.0 (3 × CH_3), 54.8 (C), 117.8 (CH), 118.0 (CH), 125.3 (C), 129.4 (CH), 133.8 (CH), 144.9 (C); *m/z* (ESI) 251.0824 (MNa^+. $C_{10}H_{16}N_2NaO_2S$ requires 251.0825).

2-Amino-*N*-benzylbenzenesulfonamide (8e)

To a stirred solution of 2-nitro-*N*-benzylbenzenesulfonamide (0.176 g, 0.602 mmol) in ethyl acetate (6 mL) was added tin(II) dichloride dihydrate (0.679 g, 3.01 mmol). The reaction mixture was heated under reflux for 18 h. The mixture was cooled to room temperature and sodium bicarbonate (60 mL) was added. The reaction mixture was filtered through a pad of Celite® and diluted with ethyl acetate (30 mL). The organic layer was washed with sodium bicarbonate (3 × 60 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo.* Purification by flash column chromatography, eluting with 30% ethyl acetate in hexane gave 2-amino-*N*-benzylbenzenesulfonamide (**8e**) (0.134 g, 85%) as a yellow oil; ν_{max}/cm^{-1} (neat) 3375 (NH), 1616 (C=C), 1481, 1454, 1315, 1138, 841; δ_H (400 MHz, $CDCl_3$) 4.05 (2H, d, *J* 6.2 Hz, PhCH_2), 4.84 (2H, br s, NH_2), 4.96 (1H, t, *J* 6.2 Hz, NH), 6.77 (1H, dd, *J* 8.1, 0.8 Hz, 3-H), 6.79–6.85 (1H, m, 5-H), 7.16–7.20 (2H, m, 2'-H and 6'-H), 7.24–7.37 (4H, m, 4-H, 3'-H, 4'-H and 5'-H), 7.74 (1H, dd, *J* 8.0, 1.5 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 47.5 (CH_2), 117.9 (CH), 118.2 (CH), 121.8 (C), 128.0 (2 × CH), 128.0 (CH), 128.8 (2 × CH), 129.9 (CH), 134.4 (CH), 136.4 (C), 145.2 (C); *m/z* (ESI) 285.0670 (MNa^+. $C_{13}H_{14}N_2NaO_2S$ requires 285.0668).

2-Amino-*N*-(4'-methoxybenzyl)benzenesulfonamide (8f)

To a stirred solution of 2-nitro-*N*-(4'-methoxybenzyl)benzenesulfonamide (0.250 g, 0.776 mmol) in ethyl acetate (7.5 mL) was added tin(II) dichloride dihydrate (0.875 g, 3.88 mmol). The reaction mixture was heated under reflux for 18 h. The mixture was cooled to room temperature and sodium bicarbonate (100 mL) was added. The reaction mixture was filtered through a pad of Celite® and diluted with ethyl acetate (60 mL). The organic layer was washed with sodium bicarbonate (3 × 60 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo.* Purification by flash column chromatography, eluting with 65% diethyl ether in hexane gave 2-amino-*N*-(4'-methoxybenzyl)benzenesulfonamide (**8f**) (0.0760 g, 33%) as a colourless oil; ν_{max}/cm^{-1} (neat) 3372 (NH), 1612 (C=C), 1514, 1483, 1317, 1248, 1142, 752; δ_H (400 MHz, $CDCl_3$) 3.77 (3H, s, 4'-OCH_3), 3.98 (2H, d, *J* 6.1 Hz, NHCH_2), 4.83 (2H, br s, NH_2), 4.87 (2H, t, *J* 6.1 Hz, N*H*CH_2), 6.75–6.85 (4H, m, 3-H, 5-H, 3'-H and 5'-H), 7.06–7.12 (2H, m, 2'-H and 6'-H), 7.31–7.37 (1H, m, 4-H), 7.74 (1H, dd, *J* 8.0, 1.5 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 47.0 (CH_2), 55.4 (CH_3), 114.2 (2 × CH), 117.9 (CH), 118.1 (CH), 121.8 (C), 128.4 (C), 129.4 (2 × CH), 130.0 (CH), 134.4 (CH), 145.1 (C), 159.4 (C); *m/z* (ESI) 315.0770 (MNa^+. $C_{14}H_{16}N_2NaO_3S$ requires 315.0774).

2-Amino-*N*-phenylbenzenesulfonamide (8g)[19]

To a stirred solution of 2-nitro-*N*-phenylbenzenesulfonamide (0.265 g, 0.952 mmol) in ethyl acetate (10 mL) was added tin(II) dichloride dihydrate (1.07 g, 4.76 mmol). The reaction mixture was heated under reflux for 18 h. The mixture was cooled to room temperature and sodium bicarbonate (150 mL) was added. The reaction mixture was filtered through a pad of Celite® and diluted with ethyl acetate (100 mL). The organic layer was washed with sodium bicarbonate (3 × 50 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo.* Purification by flash column chromatography, eluting with 60% diethyl ether in hexane gave 2-amino-*N*-phenylbenzenesulfonamide (**8g**) (0.195 g, 83%) as a white solid. Mp 120–122 °C (lit.[19] 123–124 °C); δ_H (400 MHz, $CDCl_3$) 4.86 (2H, br s, NH_2), 6.63–6.70 (1H, m, 5-H), 6.74 (1H, dd, *J* 8.2, 1.0 Hz, 3-H), 6.77 (1H, br s, NH), 7.01–7.06 (2H, m, 2'-H and 6'-H), 7.12 (1H, tt, *J* 6.7, 1.2 Hz, 4'-H), 7.17–7.22 (2H, m, 3'-H and 5'-H), 7.24–7.28 (1H, m, 4-H), 7.48 (1H, dd, *J* 8.0, 1.5 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 117.8 (CH), 118.1 (CH), 121.2 (C), 123.0 (2 × CH), 126.1 (CH), 129.3 (2 × CH), 130.1 (CH), 134.6 (CH), 136.4 (C), 145.1 (C); *m*/*z* (ESI) 271 (MNa^+. 100%).

2-Amino-*N*-(4'-methylphenyl)benzenesulfonamide (8h)[20]

To a stirred solution of *N*-(4'-methylphenyl)-2-nitrobenzenesulfonamide (0.193 g, 0.660 mmol) in ethyl acetate (7 mL) was added tin(II) dichloride dihydrate (0.745 g, 3.30 mmol). The reaction mixture was heated under reflux for 18 h. The mixture was cooled to room temperature and sodium bicarbonate (100 mL) was added. The reaction mixture was filtered through a pad of Celite® and diluted with ethyl acetate (30 mL). The organic layer was washed with sodium bicarbonate (3 × 50 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo.* Purification by flash column chromatography, eluting with 60% diethyl ether in hexane gave 2-amino-*N*-(4'-methylphenyl)lbenzenesulfonamide (**8h**) (0.134 g, 77%) as a beige solid. Mp 123–125 °C (lit.[20] 125–126 °C); δ_H (400 MHz, $CDCl_3$) 2.25 (3H, s, 4'-CH_3), 4.85 (2H, br s, NH_2), 6.63–6.71 (2H, m, 5-H and NH), 6.74 (1H, dd, *J* 8.1, 0.8 Hz, 3-H), 6.88–6.94 (2H, m, 2'-H and 6'-H), 6.97–7.02 (2H, m, 3'-H and 5'-H), 7.23–7.29 (1H, m, 4-H), 7.46 (1H, dd, *J* 8.0, 1.5 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 21.0 (CH_3), 117.8 (CH), 118.1 (CH), 121.3 (C), 123.6 (2 × CH), 129.9 (2 × CH), 130.2 (CH), 133.7 (C), 134.5 (CH), 136.1 (C), 145.1 (C); *m*/*z* (ESI) 285 (MNa^+. 100%).

2-Amino-*N*-(4'-methoxyphenyl)benzenesulfonamide (8i)[21]

To a stirred solution of *N*-(4'-methoxyphenyl)-2-nitrobenzenesulfonamide (0.133 g, 0.431 mmol) in ethyl acetate (5 mL) was added tin(II) dichloride dihydrate (0.487 g, 2.16 mmol). The reaction mixture was heated under reflux for 18 h. The mixture was cooled to room temperature and sodium

bicarbonate (100 mL) was added. The reaction mixture was filtered through a pad of Celite® and diluted with ethyl acetate (50 mL). The organic layer was washed with sodium bicarbonate (3 × 50 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo.* Purification by flash column chromatography, eluting with 60% diethyl ether in hexane gave 2-amino-*N*-(4'-methoxyphenyl)benzenesulfonamide (**8i**) (0.110 g, 92%) as an off-white solid. Mp 98–103 °C (lit.[21] 98–99 °C); δ_H (400 MHz, $CDCl_3$) 3.73 (3H, s, 4'-OCH_3), 4.84 (2H, br s, NH_2), 6.59 (1H, br s, NH), 6.63–6.77 (4H, m, 3-H, 5-H, 3'-H and 5'-H), 6.90–6.97 (2H, m, 2'-H and 6'-H), 7.26–7.31 (1H, m, 4-H), 7.40 (1H, dd, *J* 8.0, 1.4 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 55.5 (CH_3), 114.4 (2 × CH), 117.7 (CH), 118.1 (CH), 121.1 (C), 126.5 (2 × CH), 128.8 (C), 130.2 (CH), 134.5 (CH), 145.0 (C), 158.4 (C); *m*/*z* (ESI) 301 (MNa^+. 100%).

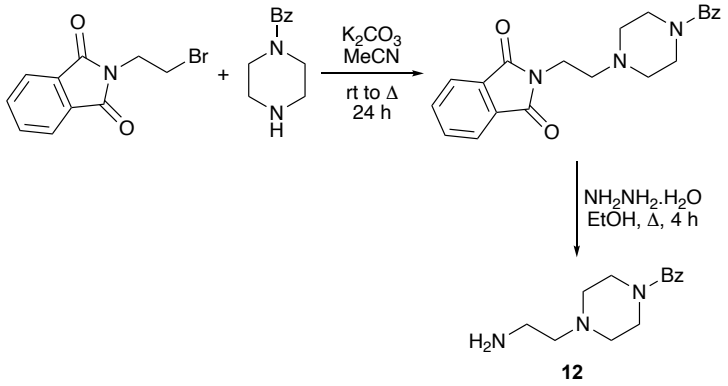
2-Amino-*N*-(4'-bromophenyl)benzenesulfonamide (8j)

To a stirred solution of *N*-(4'-bromophenyl)-2-nitrobenzenesulfonamide (0.0940 g, 0.263 mmol) in ethyl acetate (3 mL) was added tin(II) dichloride dihydrate (0.297 g, 1.32 mmol). The reaction mixture was heated under reflux for 18 h. The mixture was cooled to room temperature and sodium bicarbonate (100 mL) was added. The reaction mixture was filtered through a pad of Celite® and diluted with ethyl acetate (50 mL). The organic layer was washed with sodium bicarbonate (3 × 50 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo.* Purification by flash column chromatography, eluting with 60% diethyl ether in hexane gave 2-amino-*N*-(4'-bromophenyl)benzenesulfonamide (**8j**) (0.0730 g, 85%) as a white solid. Mp 105–110 °C; ν_{max}/cm^{-1} (neat) 3225 (NH), 1616 (C=C), 1481, 1312, 1134, 910; δ_H (400 MHz, $CDCl_3$) 4.84 (2H, br s, NH_2), 6.67–6.72 (1H, m, 5-H), 6.75 (1H, dd, *J* 8.2, 0.8 Hz, 3-H), 6.83 (1H, br s, NH), 6.89–6.94 (2H, m, 2'-H and 6'-H), 7.26–7.34 (3H, m, 4-H, 3'-H and 5'-H), 7.48 (1H, dd, *J* 8.0, 1.5 Hz, 6-H); δ_C (101 MHz, $CDCl_3$) 118.0 (CH), 118.4 (CH), 119.4 (C), 121.0 (C), 124.6 (2 × CH), 130.1 (CH), 132.4 (2 × CH), 134.8 (CH), 135.6 (C), 145.0 (C); *m*/*z* (ESI) 348.9615 (MNa^+. $C_{12}H_{11}{}^{79}BrN_2NaO_2S$ requires 348.9617).

2-Amino-*N*-(4'-iodophenyl)benzenesulfonamide (8k)

To a stirred solution of *N*-(4'-iodophenyl)-2-nitrobenzenesulfonamide (0.200 g, 0.495 mmol) in ethyl acetate (5 mL) was added tin(II) dichloride dihydrate (0.558 g, 2.47 mmol). The reaction mixture was heated under reflux for 18 h. The mixture was cooled to room temperature and sodium bicarbonate (150 mL) was added. The reaction mixture was filtered through a pad of Celite® and diluted with ethyl acetate (60 mL). The organic layer was washed with sodium bicarbonate (3 × 60 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo.* Purification by flash column chromatography, eluting

with 60% diethyl ether in hexane gave 2-amino-*N*-(4'-iodophenyl)benzenesulfonamide (**8k**) (0.149 g, 80%) as a yellow solid. Mp 116–120 °C; ν_{max}/cm^{-1} (neat) 3383 (NH), 2916 (CH), 1620 (C=C), 1485, 1319, 1141; δ_H (400 MHz, $CDCl_3$) 4.84 (2H, br s, NH_2), 6.70 (1H, td, *J* 8.2, 1.0 Hz, 5-H), 6.73 (1H, dd, *J* 8.1, 1.0 Hz, 3-H), 6.77–6.84 (3H, m, NH, 2'-H and 6'-H), 7.26–7.32 (1H, m, 4-H), 7.47–7.53 (3H, m, 6-H, 3'-H and 5'-H); δ_C (101 MHz, $CDCl_3$) 90.2 (C), 118.0 (CH), 118.4 (CH), 121.0 (C), 124.6 (2 × CH), 130.1 (CH), 134.8 (CH), 136.4 (C), 138.4 (2 × CH), 145.0 (C); *m/z* (ESI) 396.9481 (MNa^+. $C_{12}H_{11}IN_2NaO_2S$ requires 396.9478).



12

2-[2'-(4''-Benzoylpiperazin-1-yl)ethyl]isoindole-1,3-dione

To an oven dried flask containing *N*-benzoylpiperazine (0.900 g, 4.73 mmol) in acetonitrile (30 mL) was added 2-(2-bromoethyl)isoindoline-1,3-dione (1.20 g, 4.73 mmol) and potassium carbonate (2.29 g, 16.6 mmol). The reaction mixture was heated under reflux for 24 h. The reaction mixture was cooled to room temperature and concentrated *in vacuo*. The reaction mixture was diluted with water (60 mL) and extracted with ethyl acetate (5 × 60 mL). The organic layer was dried ($MgSO_4$), filtered and concentrated *in vacuo*. Purification by flash column chromatography, eluting with 70–80% ethyl acetate in hexane gave 2-[2'-(4''-benzoylpiperazin-1-yl)ethyl]isoindole-1,3-dione (1.09 g, 63%) as a white solid. Mp 151–156 °C; ν_{max}/cm^{-1} (neat) 2813 (CH), 2359, 1765, 1702 (C=O), 1617, 1578 (C=C), 1432, 1399, 1288, 1009, 709; δ_H (500 MHz, CD_3OD) 2.50 (2H, br s, 2''-H_2), 2.63 (2H, br s, 6''-H_2), 2.69 (2H, br t, *J* 6.3 Hz, 2'-H_2), 3.38 (2H, br s, 3''-H_2), 3.70 (2H, br s, 5''-H_2), 3.84 (2H, br t, *J* 6.3 Hz, 1'-H_2), 7.36–7.49 (5H, m, Ph), 7.77–7.88 (4H, m, 4-H, 5-H, 6-H and 7-H); δ_C (126 MHz, CD_3OD) 35.9 (CH_2), 43.2 (CH_2), 53.7 (CH_2), 54.2 (CH_2), 56.6 (2 × CH_2), 124.1 (2 × CH), 128.0 (2 × CH), 129.7 (2 × CH), 131.1 (CH), 133.5 (2 × C), 135.3 (2 × CH), 136.8 (C), 169.9 (2 × C), 172.4 (C); *m/z* (ESI) 386.1476 (MNa^+. $C_{21}H_{21}N_3NaO_3$ requires 386.1475).

1-Benzoyl-4-[2'-aminoethyl]piperazine (12)

To a stirred solution of 2-[2'-(4''-benzoylpiperazin-1-yl)ethyl]isoindole-1,3-dione (0.200 g, 0.550 mmol) in ethanol (5.5 mL) was added hydrazine monohydrate (0.149 mL, 0.605 mmol). The reaction was heated under reflux for 4 h. The reaction mixture was cooled to room temperature. The resulting white solid was filtered and washed with ethanol (50 mL). The filtrate was concentrated *in vacuo*. The solid was dissolved in 1 M aqueous sodium hydroxide (25 mL) and saturated with sodium chloride. The mixture was extracted with ethyl acetate (5 × 25 mL). The combined organic layers were dried ($MgSO_4$), filtered and concentrated *in vacuo* to give 1-benzoyl-4-[2'-aminoethyl]piperazine (**12**) (0.110 g, 86%) as a yellow oil. ν_{max}/cm^{-1} (neat) 3372 (NH), 2941 (CH), 1628 (C=O), 1576 (C=C), 1433, 1293, 1002, 761; δ_H (500 MHz, CD_3OD) 2.44 (2H, br s, 3-H_2), 2.50 (2H, br t, *J* 6.2 Hz, 1'-H_2), 2.57 (2H, br s, 5-H_2), 2.77 (2H, br t, *J* 6.2 Hz, 2'-H_2), 3.47 (2H, br s, 2-H_2), 3.79 (2H, br s, 6-H_2), 7.38–7.51 (5H, m, Ph); δ_C (126 MHz, CD_3OD) 38.8 (CH_2), 43.2 (CH_2), 53.9 (CH_2), 54.4 (CH_2), 60.7 (2 × CH_2), 128.0 (2 × CH), 129.7 (2 × CH), 131.1 (CH), 136.8 (C), 172.4 (C); *m/z* (ESI) 256.1418 (MNa^+. $C_{13}H_{19}N_3NaO$ requires 256.1420).

2. References

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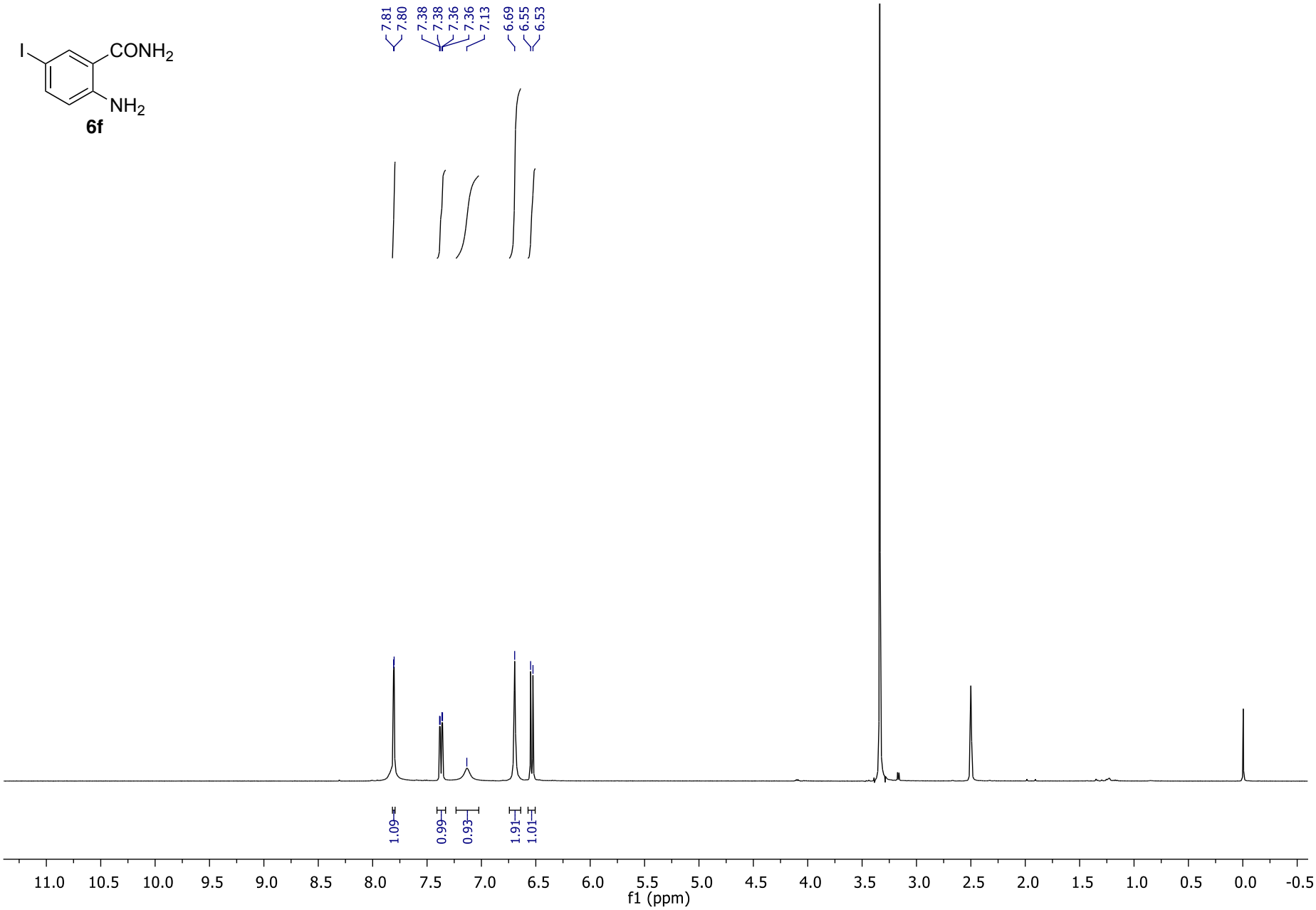
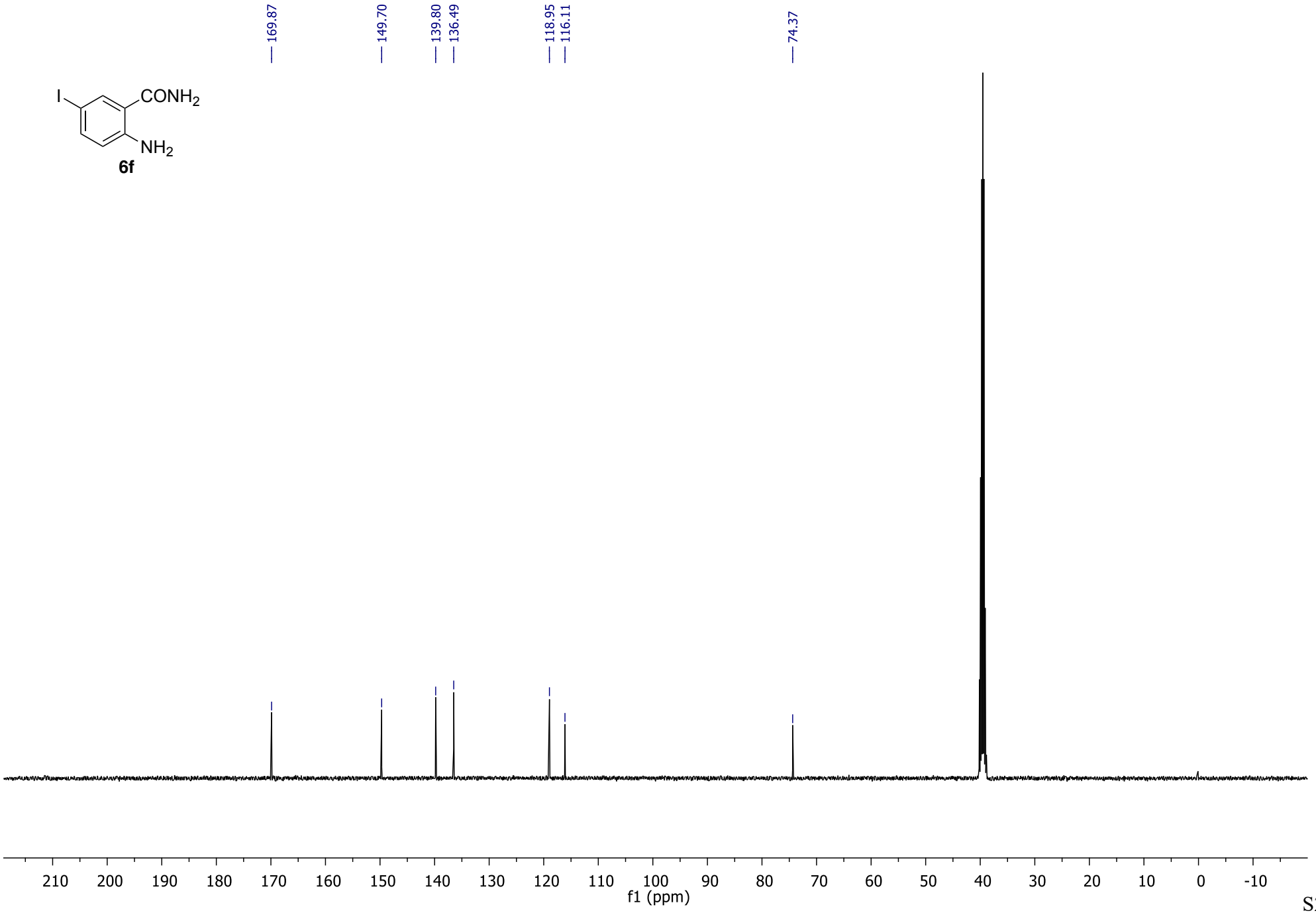
3. ^{1}H NMR and ^{13}C NMR Spectra of All Compounds

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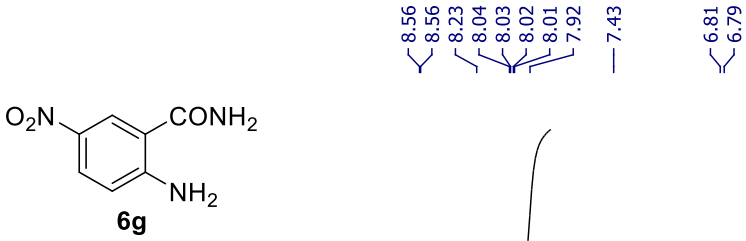
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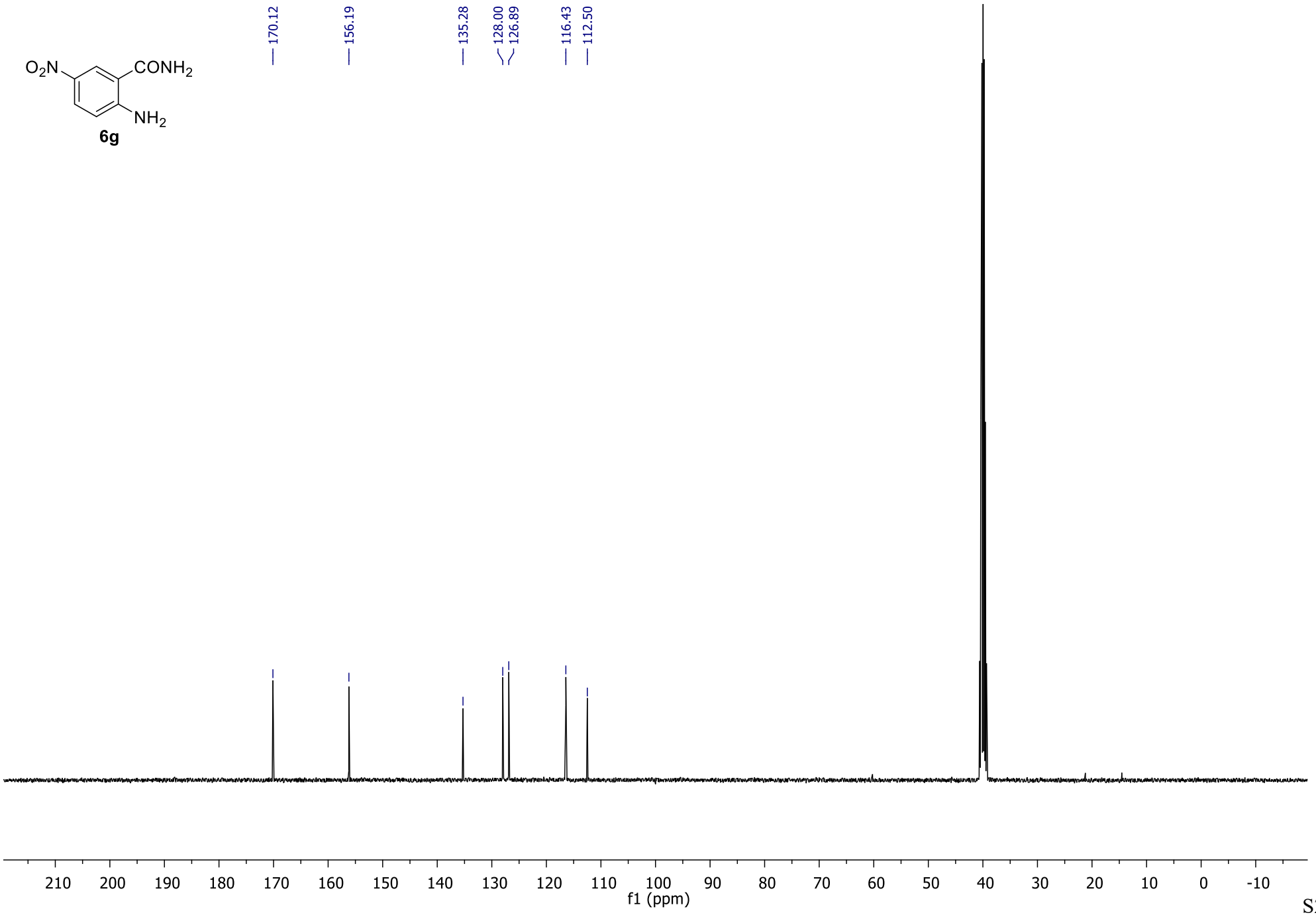
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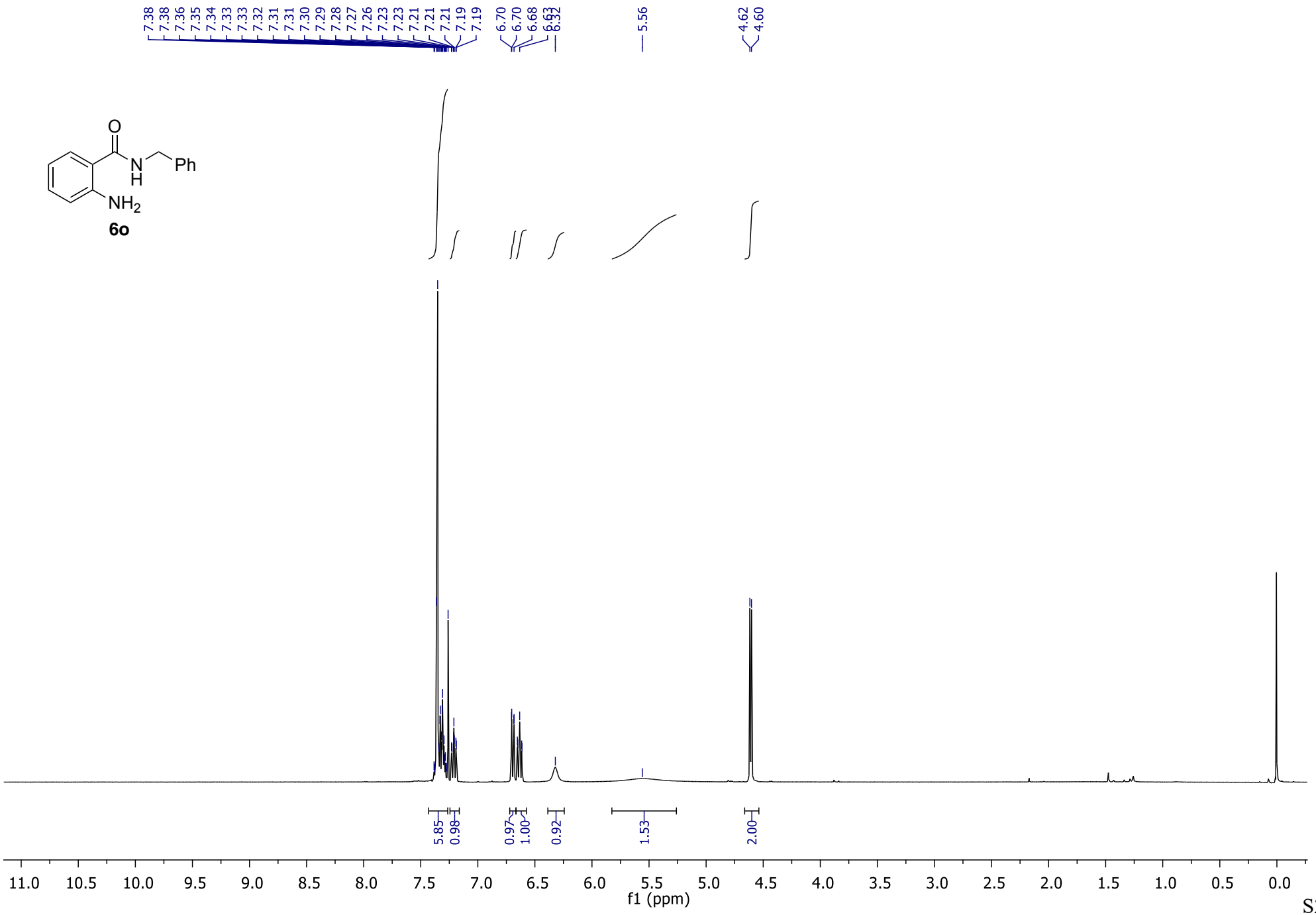
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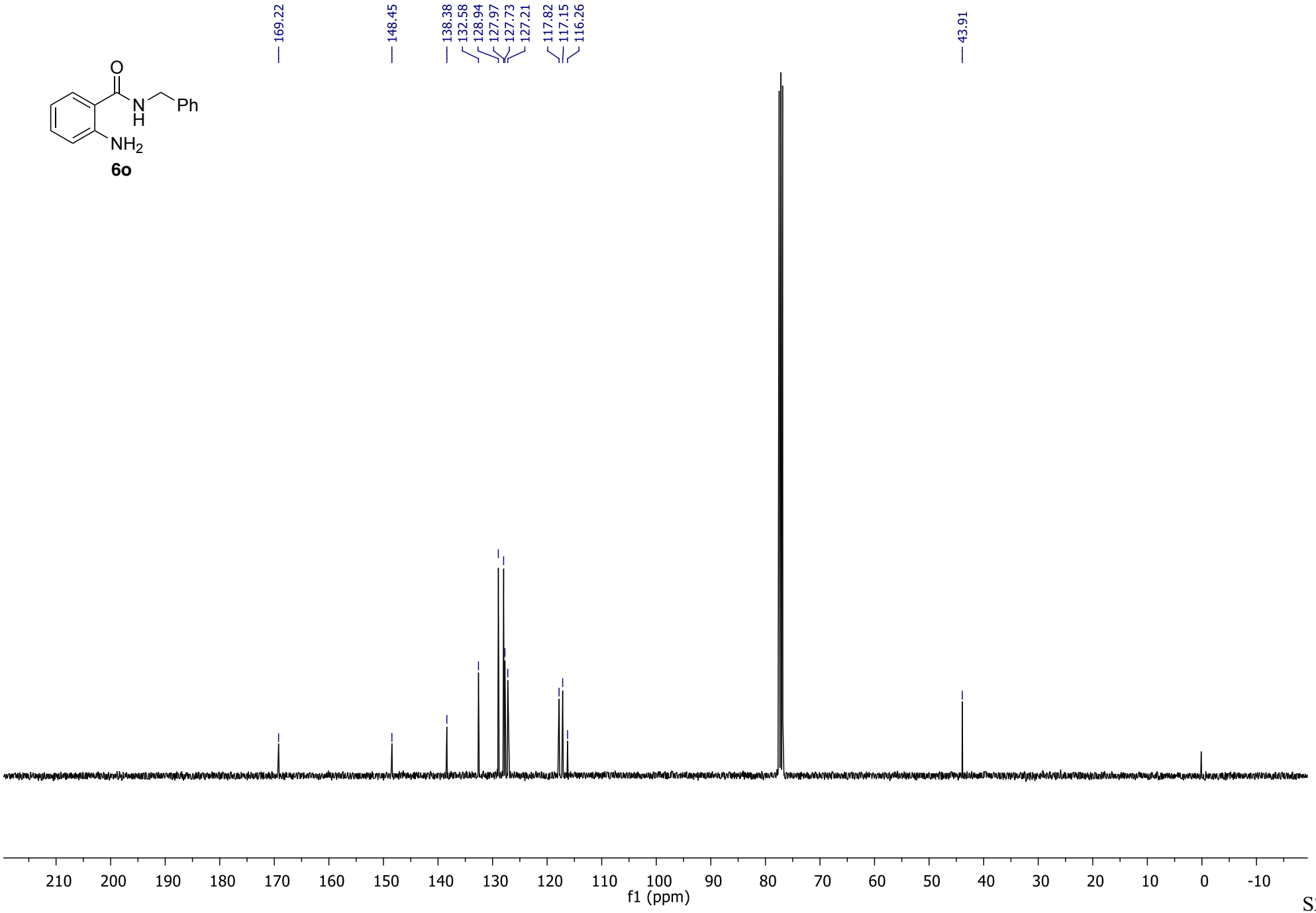
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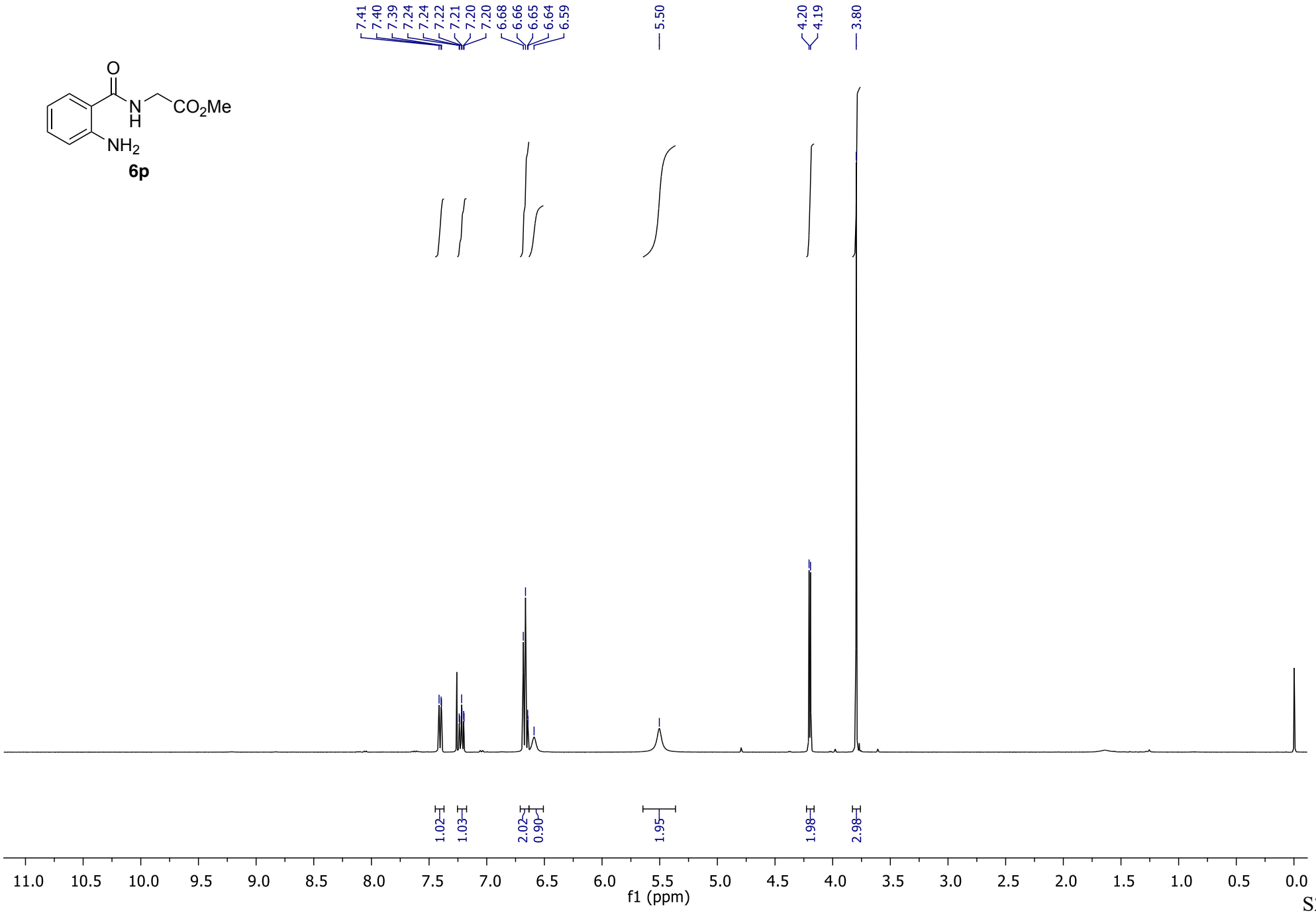
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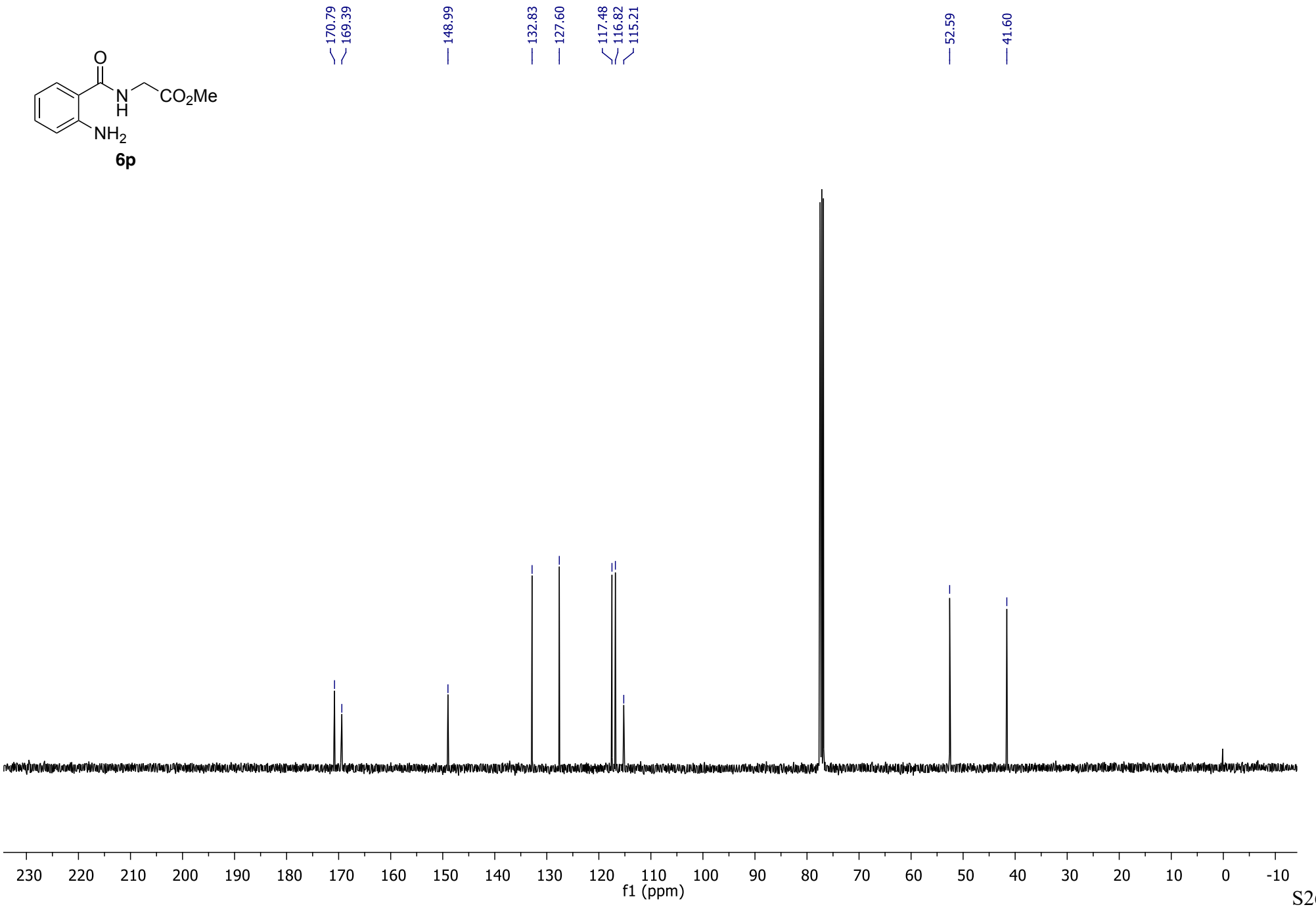
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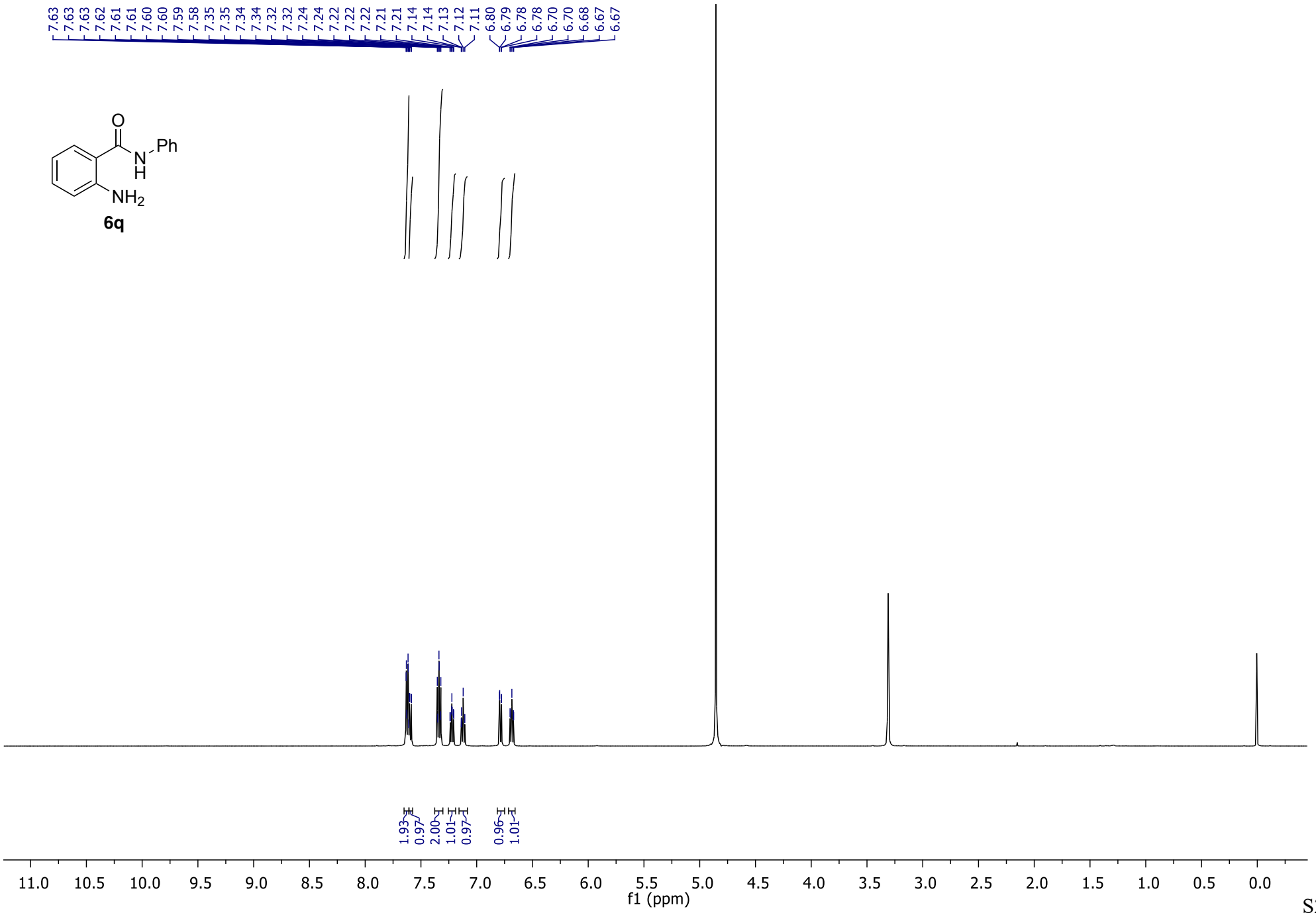
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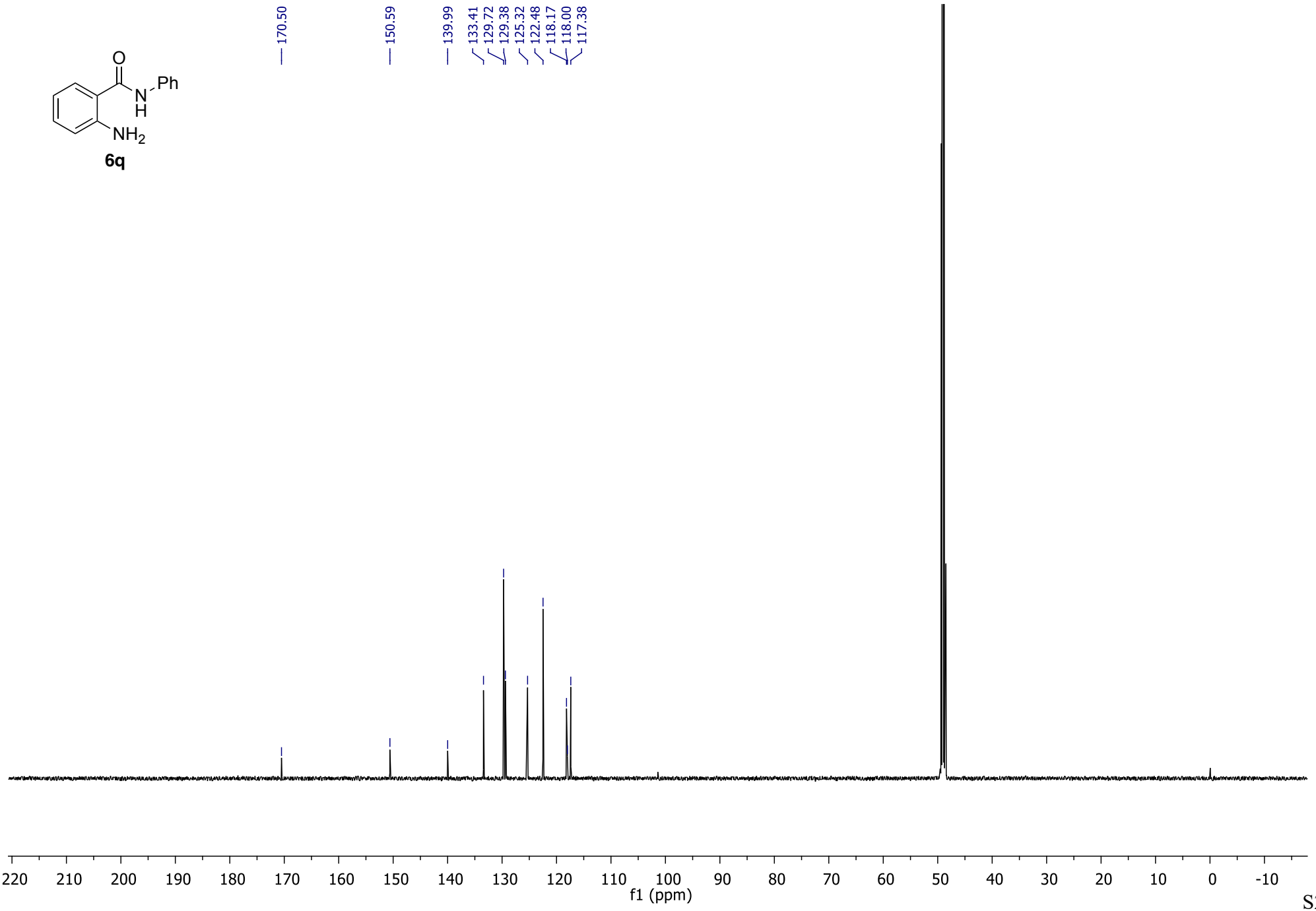
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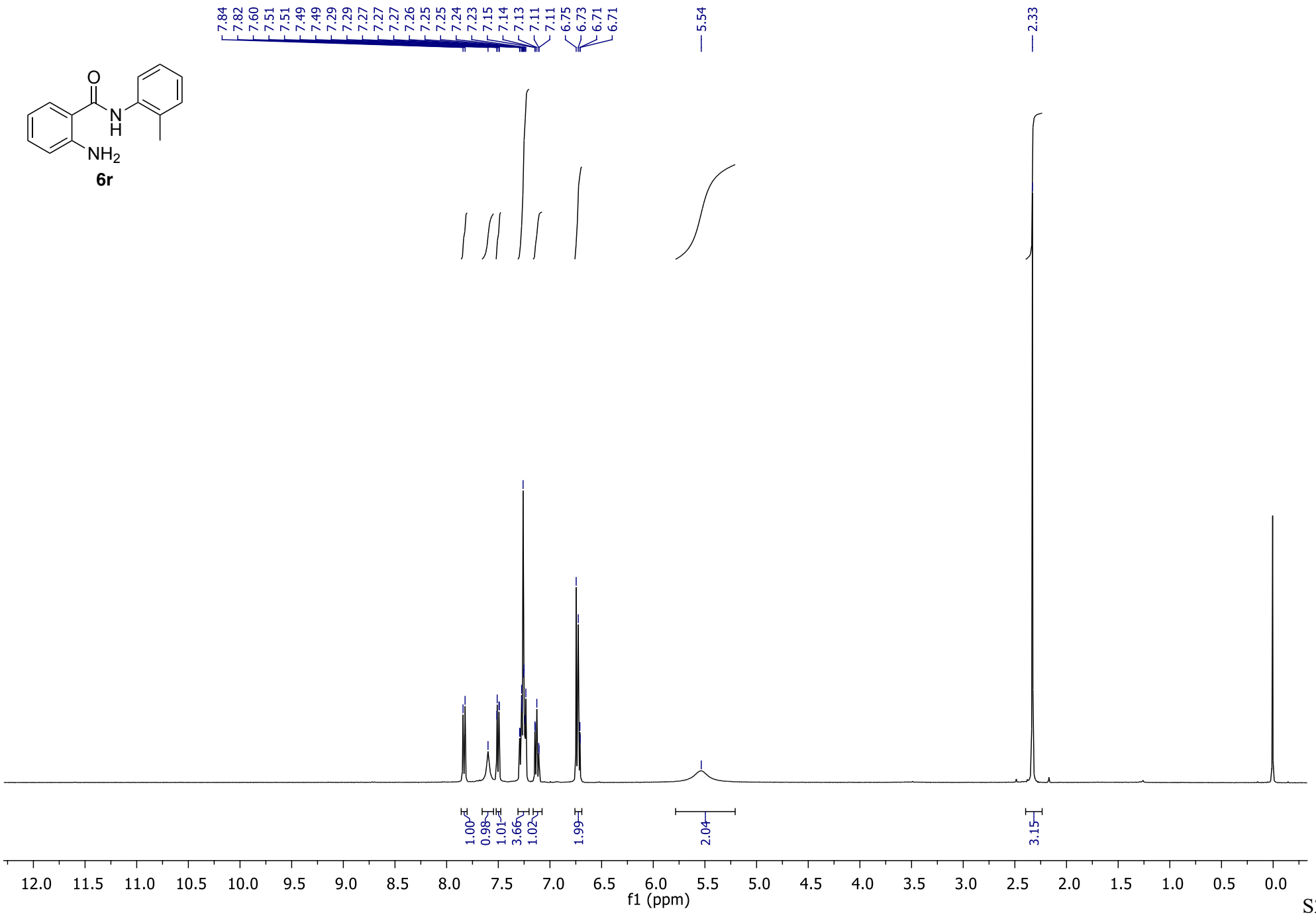
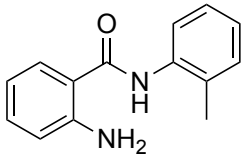
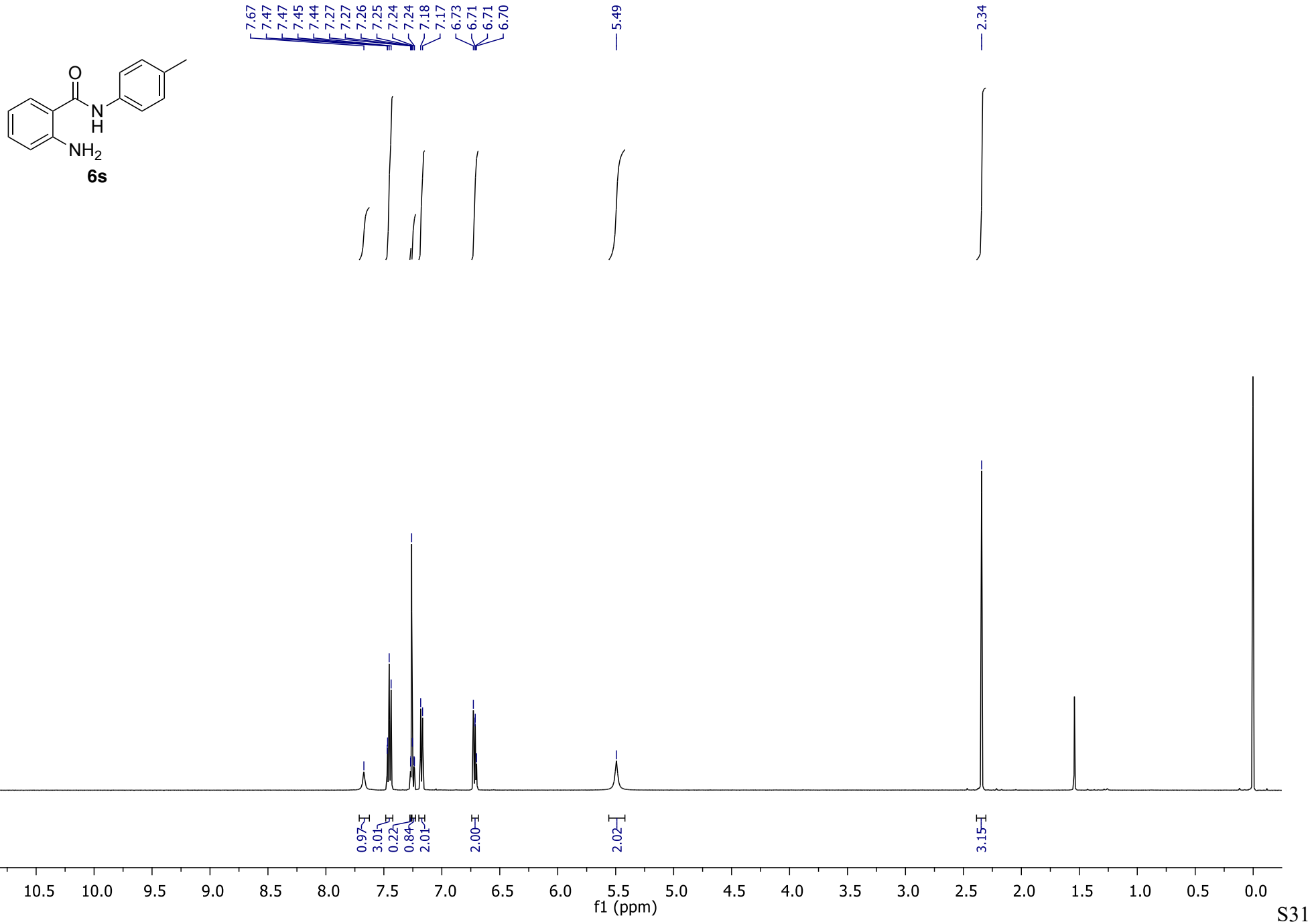
f1 (ppm)

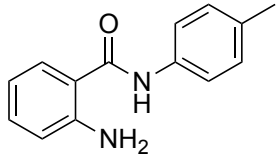

7.84
7.82
7.60
7.51
7.51
7.49
7.49
7.29
7.29
7.27
7.27
7.27
7.26
7.25
7.25
7.24
7.23
7.15
7.14
7.13
7.11
7.11
6.75
6.73
6.71
6.71
5.54
2.33
O
N
H
NH2
6r
1.00
0.98
1.01
3.66
1.02
1.99
2.04
3.15
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
N
H
NH2

6r

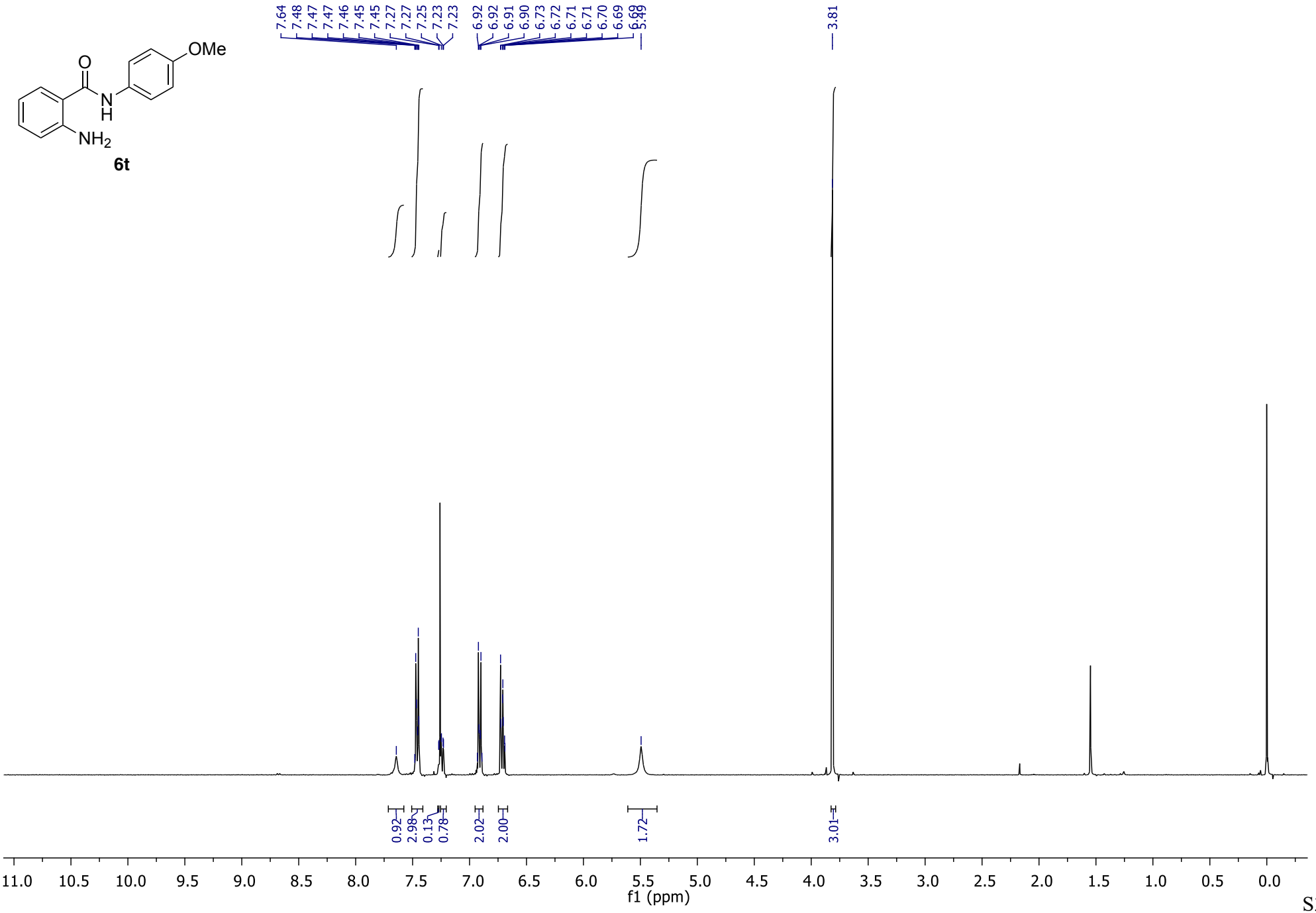
167.70
149.29
135.87
132.90
130.76
130.01
127.28
126.95
125.56
123.69
117.76
116.99
116.28
18.07
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

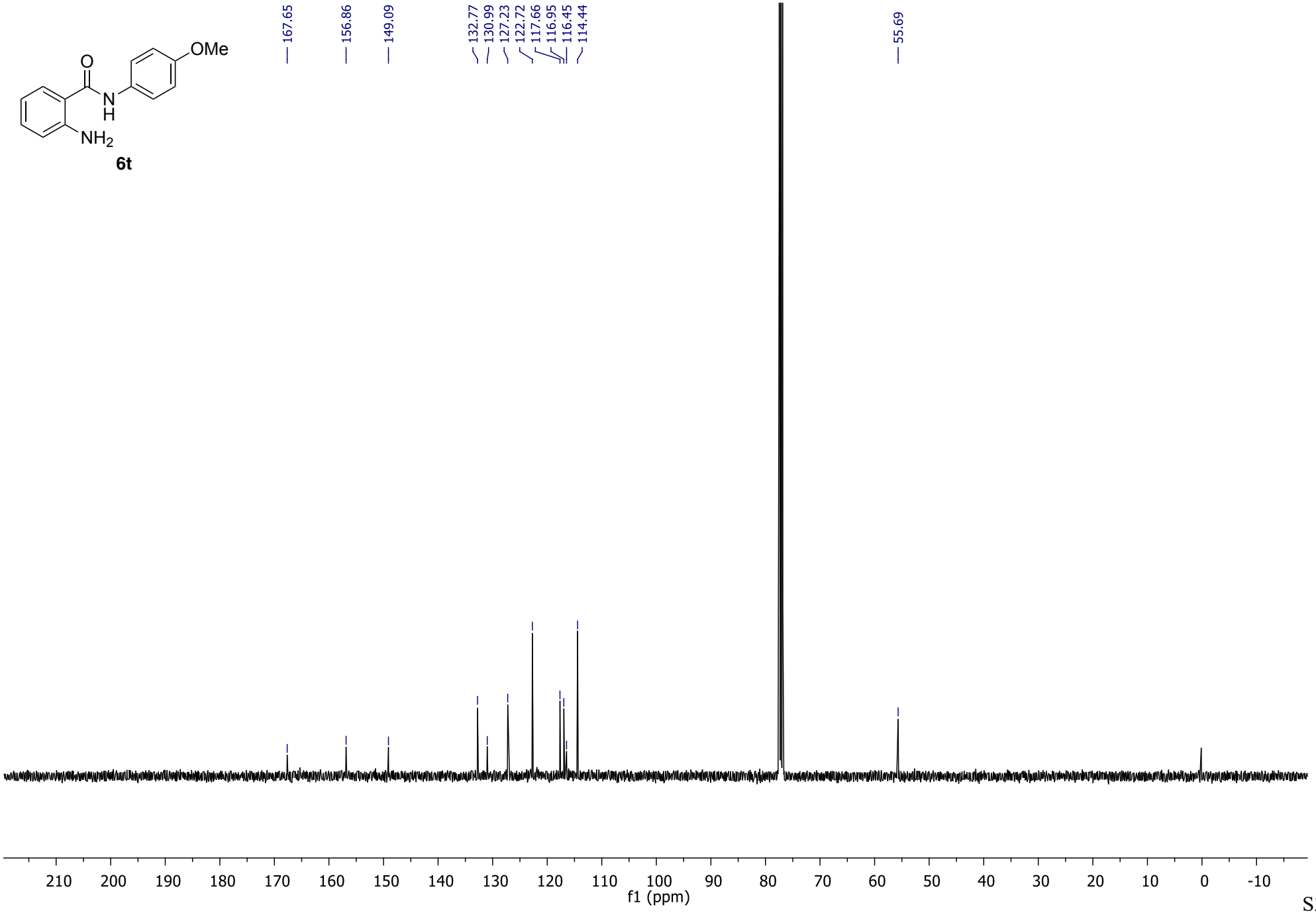

7.67
7.47
7.47
7.45
7.44
7.27
7.27
7.26
7.25
7.24
7.24
7.18
7.17
6.73
6.71
6.71
6.70
5.49
2.34
O
N
H
NH2
6s
0.97
3.01
0.22
0.84
2.01
2.00
2.02
3.15
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

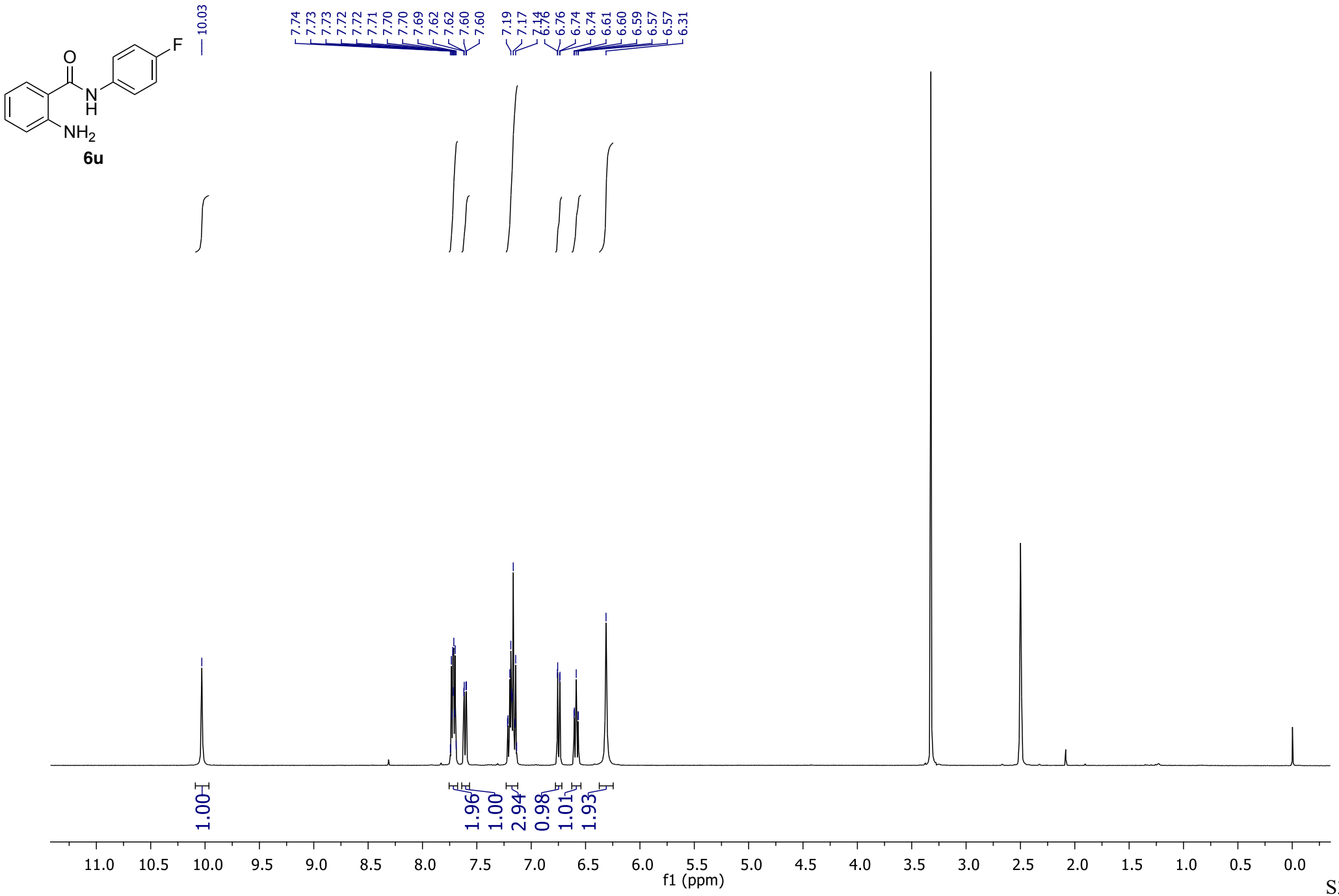

O
N
H
NH2

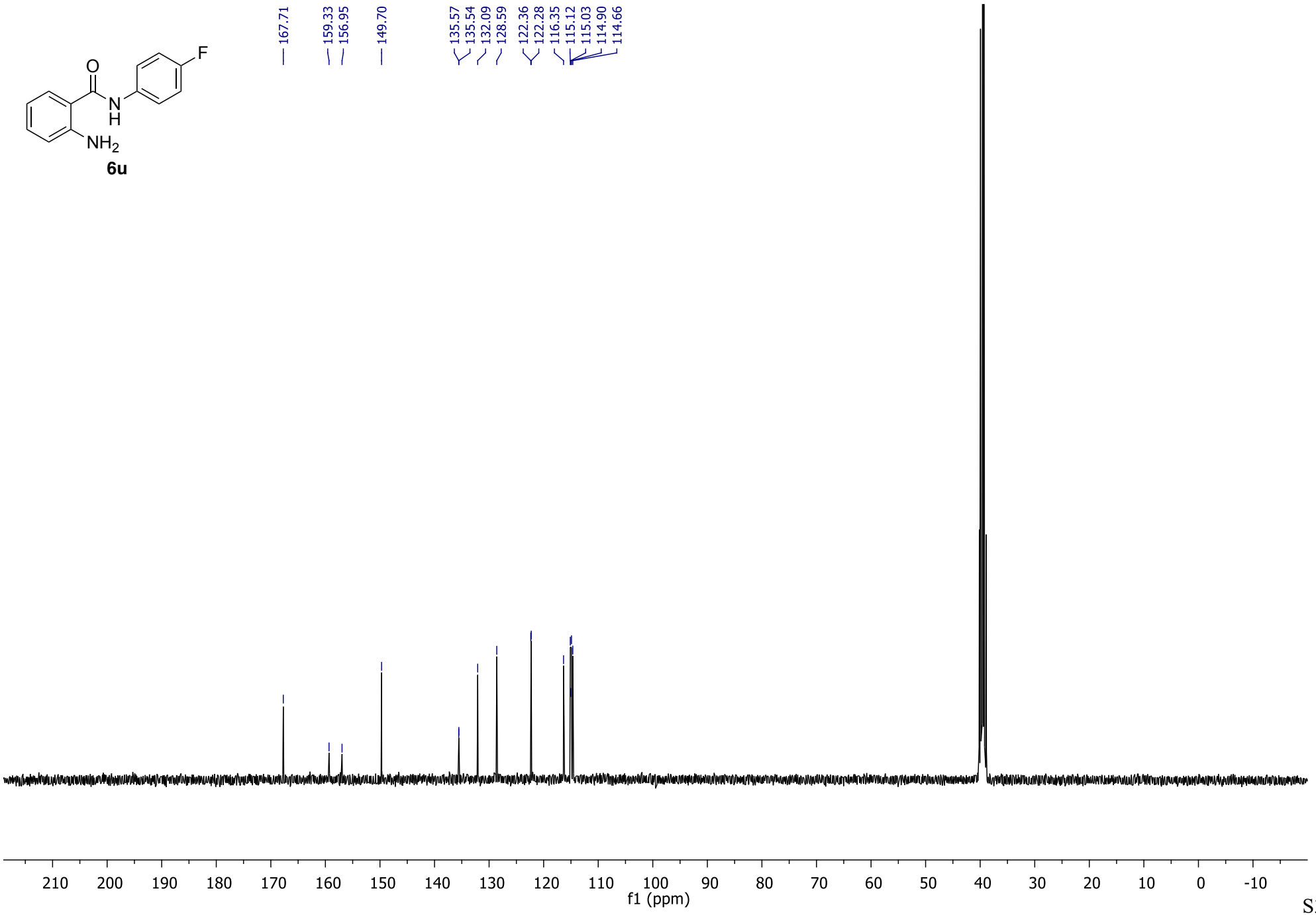
6s

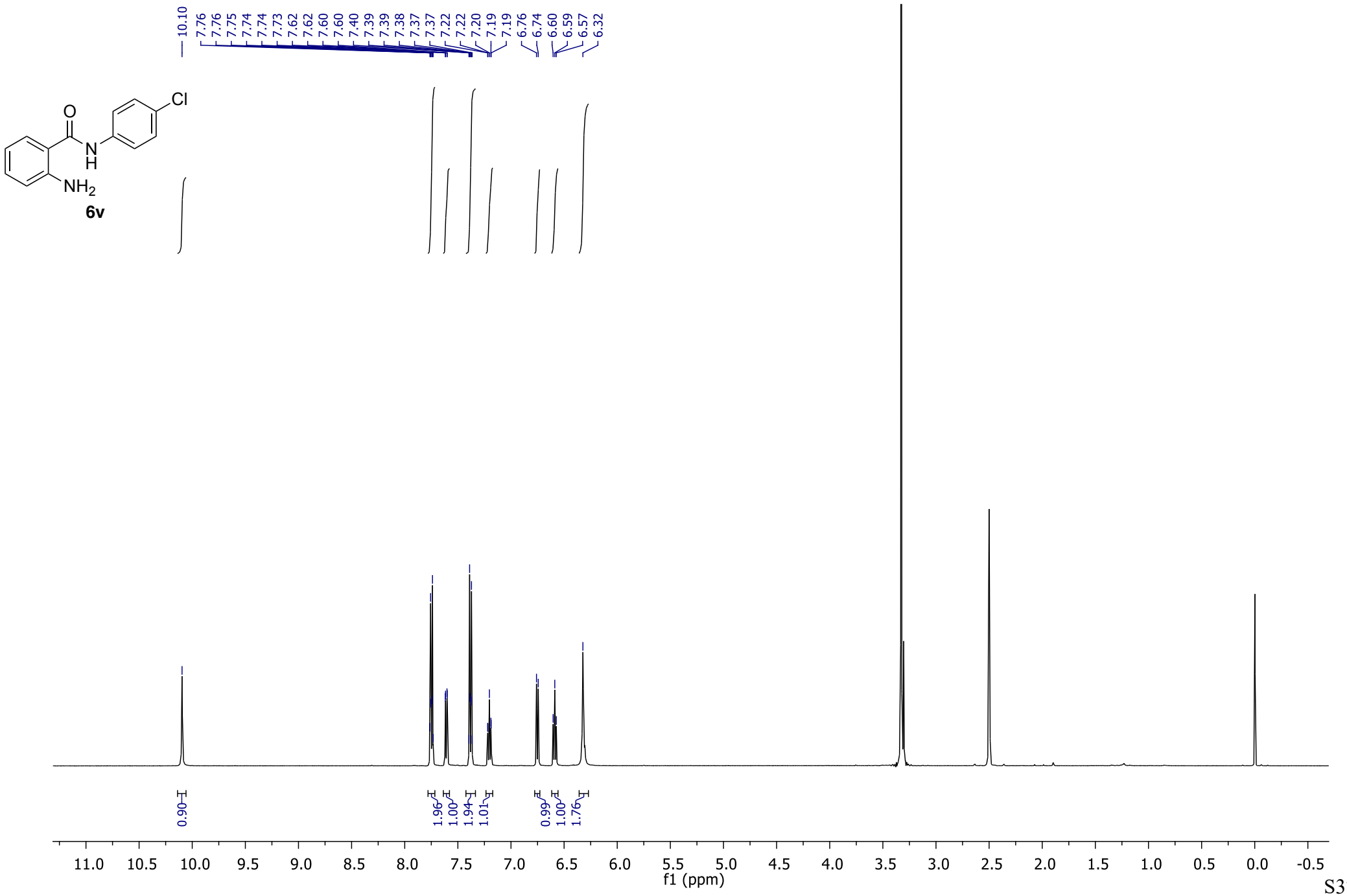
167.65
149.02
135.37
134.28
132.71
129.64
127.29
120.84
117.60
116.90
116.53
21.00
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

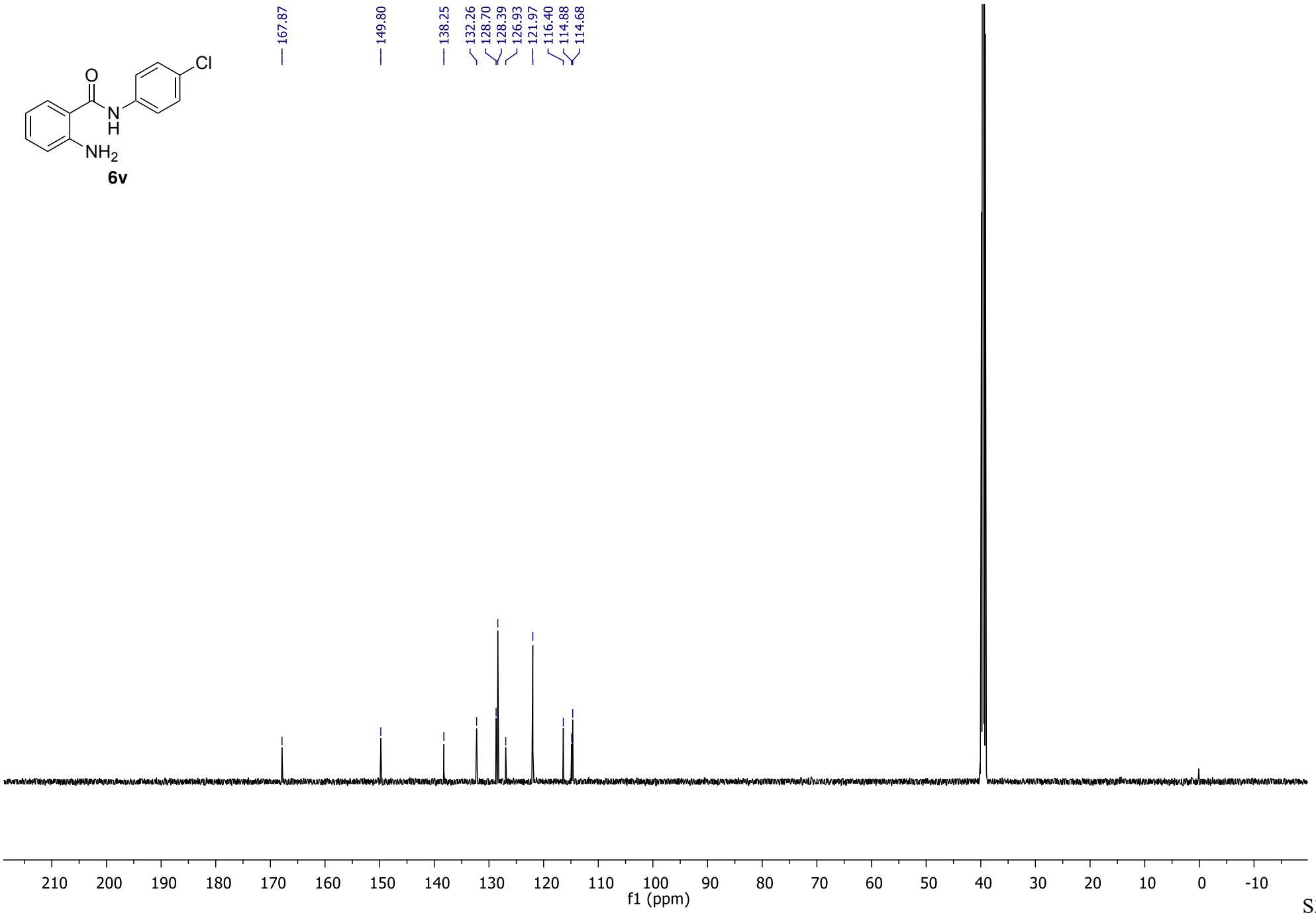

O
N
H
NH2
OMe
6t
7.64
7.48
7.47
7.47
7.46
7.45
7.45
7.27
7.27
7.25
7.23
7.23
6.92
6.92
6.91
6.90
6.73
6.72
6.71
6.71
6.70
6.69
6.69
3.81
0.92
2.98
0.13
0.78
2.02
2.00
1.72
3.01
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

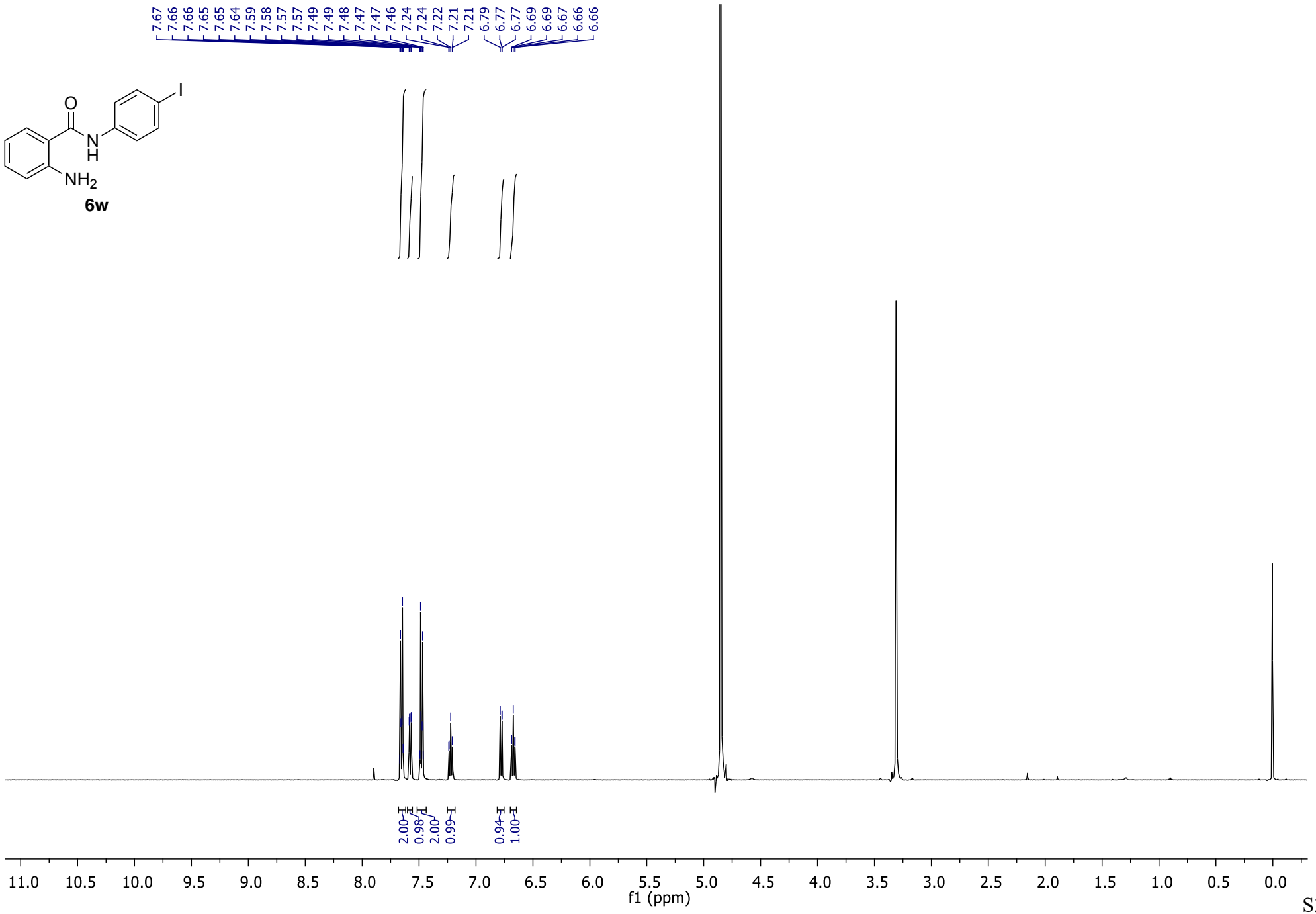

O
N
H
NH2
OMe
6t
167.65
156.86
149.09
132.77
130.99
127.23
122.72
117.66
116.95
116.45
114.44
55.69
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

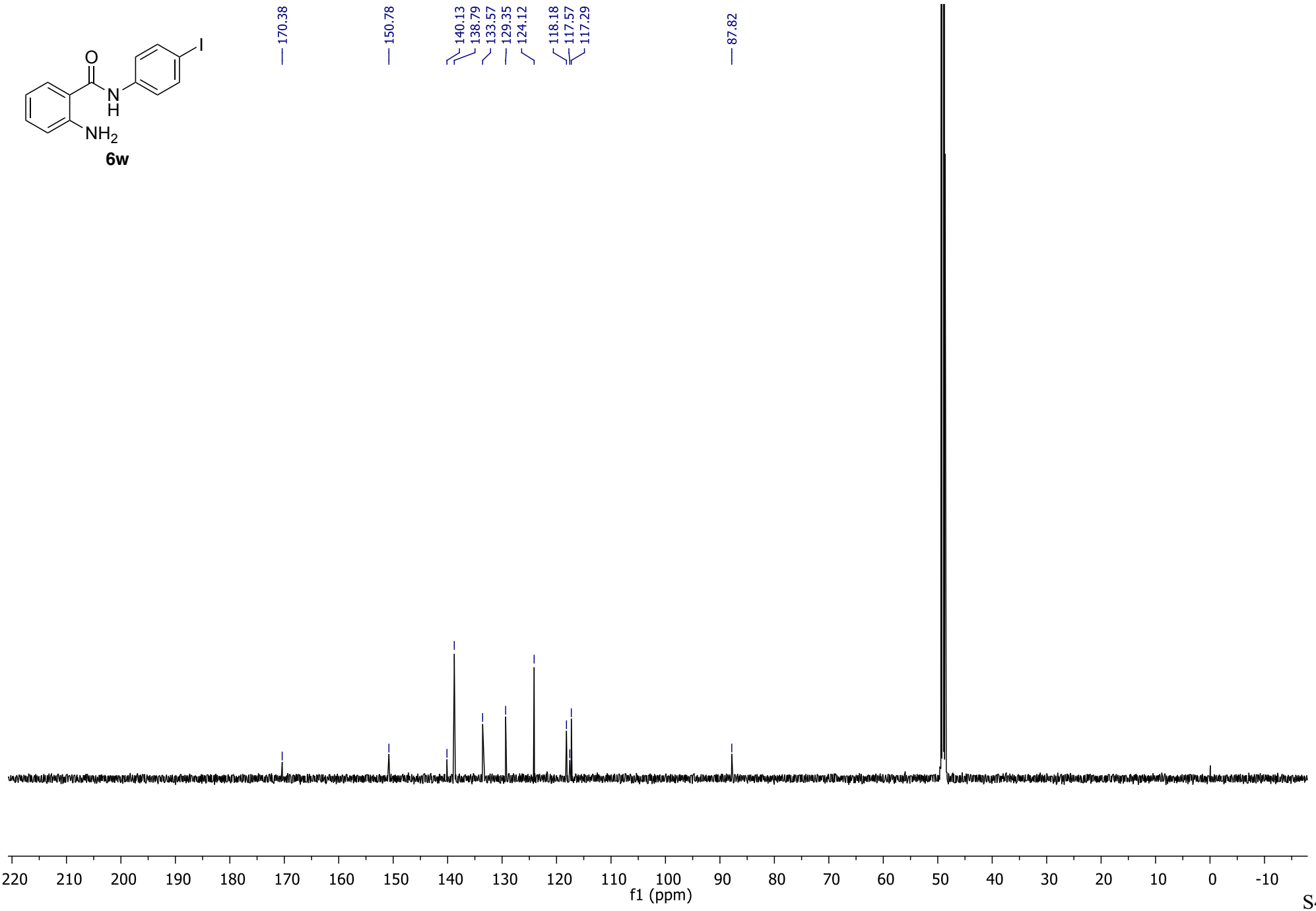

O
N
H
F
NH2
6u
10.03
7.74
7.73
7.73
7.72
7.72
7.71
7.70
7.70
7.69
7.62
7.62
7.60
7.60
7.19
7.17
7.14
6.76
6.74
6.74
6.61
6.60
6.59
6.57
6.57
6.31
1.00
1.96
1.00
2.94
0.98
1.01
1.93
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

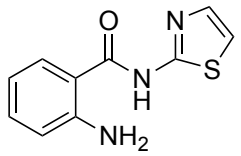

167.71
159.33
156.95
149.70
135.57
135.54
132.09
128.59
122.36
122.28
116.35
115.12
115.03
114.90
114.66
O
N
H
F
NH2
6u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


10.10
7.76
7.76
7.75
7.74
7.74
7.73
7.62
7.62
7.60
7.60
7.40
7.39
7.39
7.38
7.37
7.37
7.22
7.22
7.20
7.19
7.19
6.76
6.74
6.60
6.59
6.57
6.32
O
N
H
Cl
NH2
6v
0.90
1.96
1.00
1.94
1.01
0.99
1.00
1.76
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


167.87
149.80
138.25
132.26
128.70
128.39
126.93
121.97
116.40
114.88
114.68
O
N
H
Cl
NH2
6v
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

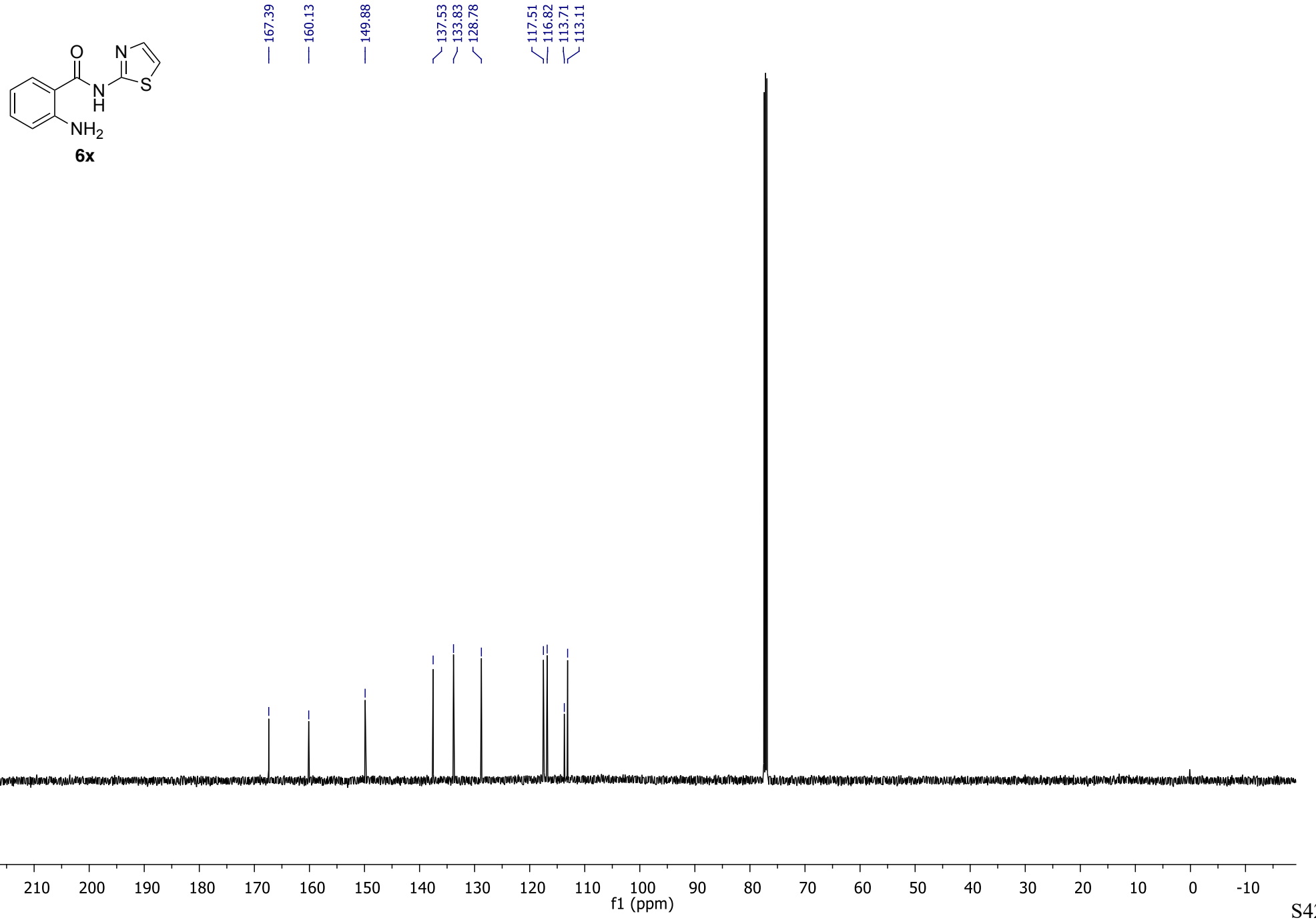

7.67
7.66
7.66
7.65
7.65
7.64
7.59
7.58
7.57
7.57
7.49
7.49
7.48
7.47
7.47
7.46
7.24
7.24
7.22
7.21
7.21
6.79
6.77
6.77
6.69
6.69
6.67
6.66
6.66
O
N
H
NH2
I
6w
2.00
0.98
2.00
0.99
0.94
1.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

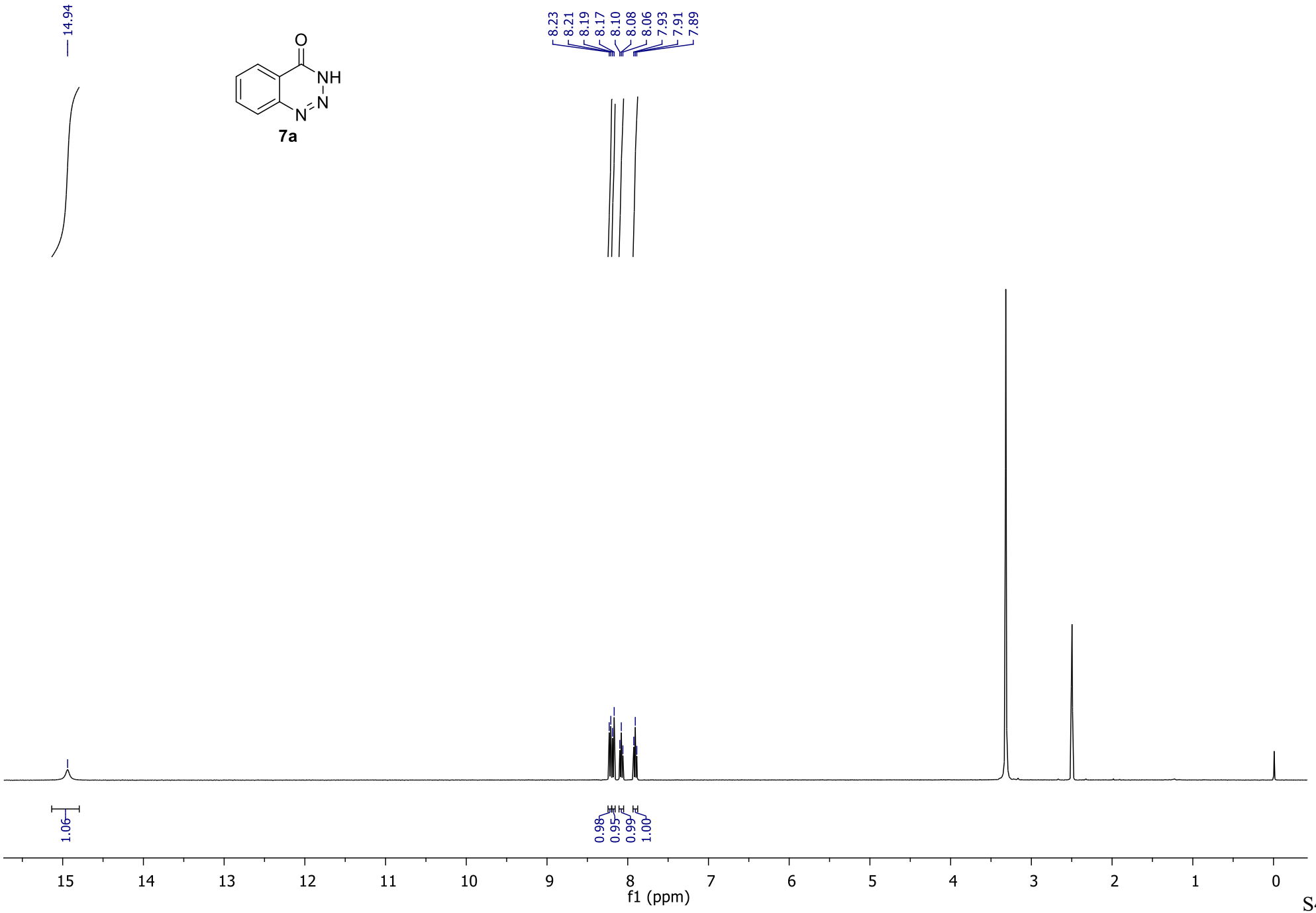

O
N
H
NH2
I
6w
170.38
150.78
140.13
138.79
133.57
129.35
124.12
118.18
117.57
117.29
87.82
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

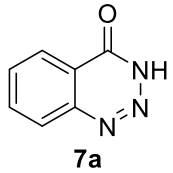

O
N
N
H
S
NH2

6x

12.26
7.71
7.71
7.69
7.69
7.33
7.33
7.32
7.31
7.31
7.31
7.30
7.13
7.12
6.91
6.90
6.76
6.76
6.75
6.75
6.71
6.71
6.69
6.68
6.68
5.68
0.87
1.00
1.01
0.99
0.96
0.99
1.01
1.92
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

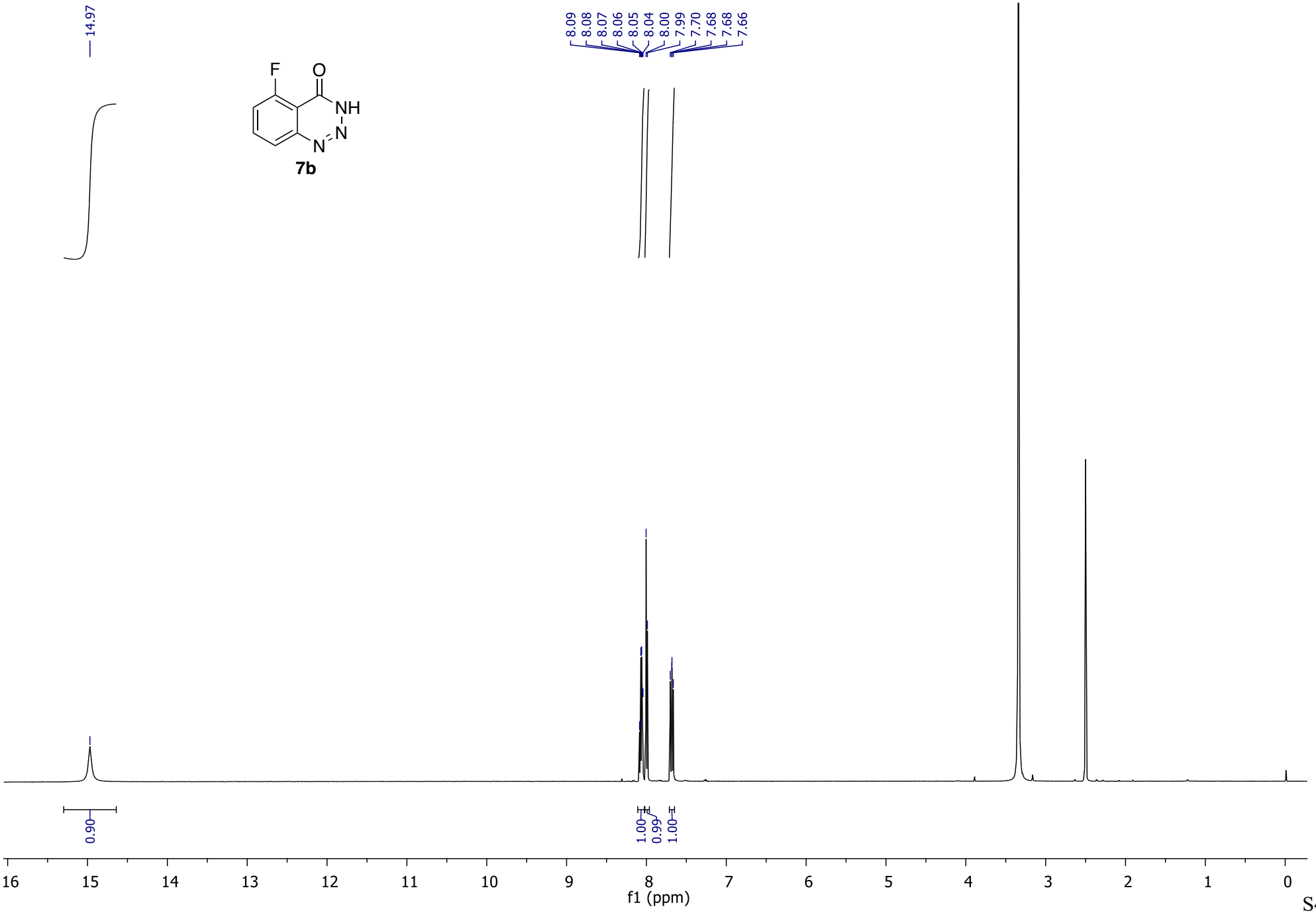

O
N
N
H
S
NH2
6x
167.39
160.13
149.88
137.53
133.83
128.78
117.51
116.82
113.71
113.11
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

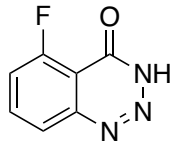

14.94
8.23
8.21
8.19
8.17
8.10
8.08
8.06
7.93
7.91
7.89
O
NH
N
N
7a
1.06
0.98
0.95
0.99
1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


O
NH
N
N

7a

155.59
144.18
135.48
132.55
127.85
124.27
120.18
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


14.97
8.09
8.08
8.07
8.06
8.05
8.04
8.00
7.99
7.70
7.68
7.68
7.66
F
O
NH
N
N
7b
0.90
1.00
0.99
1.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

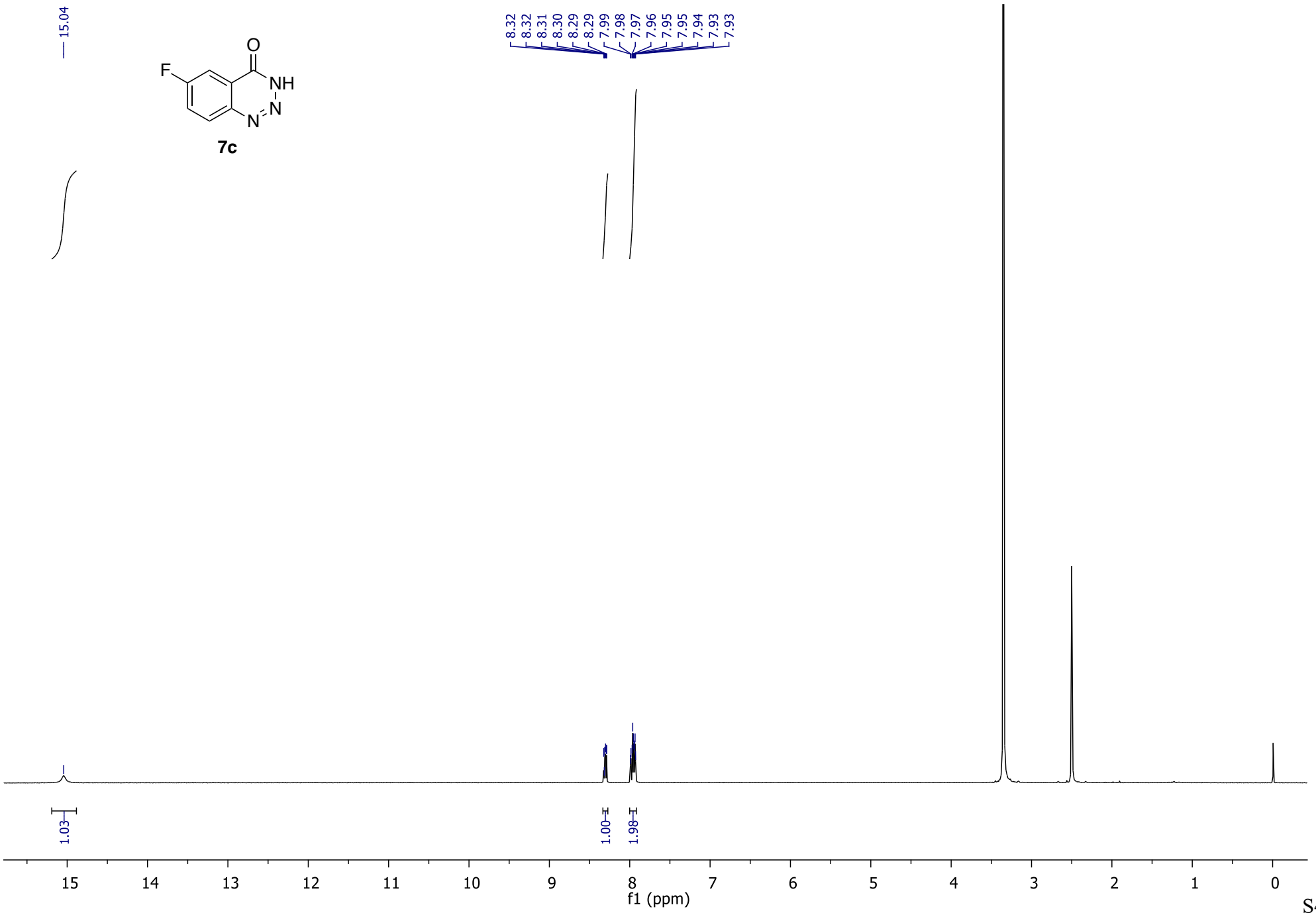


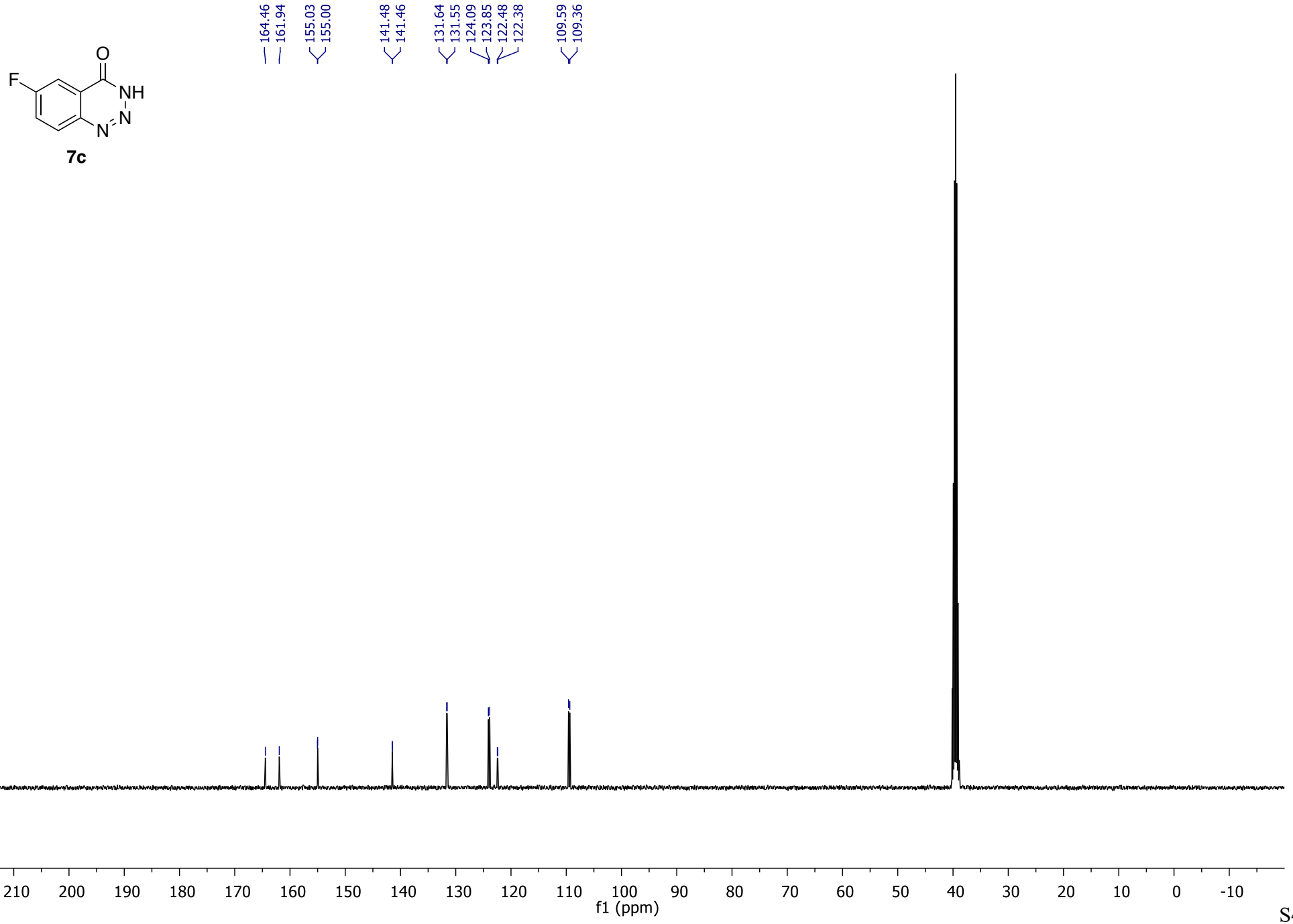
7b

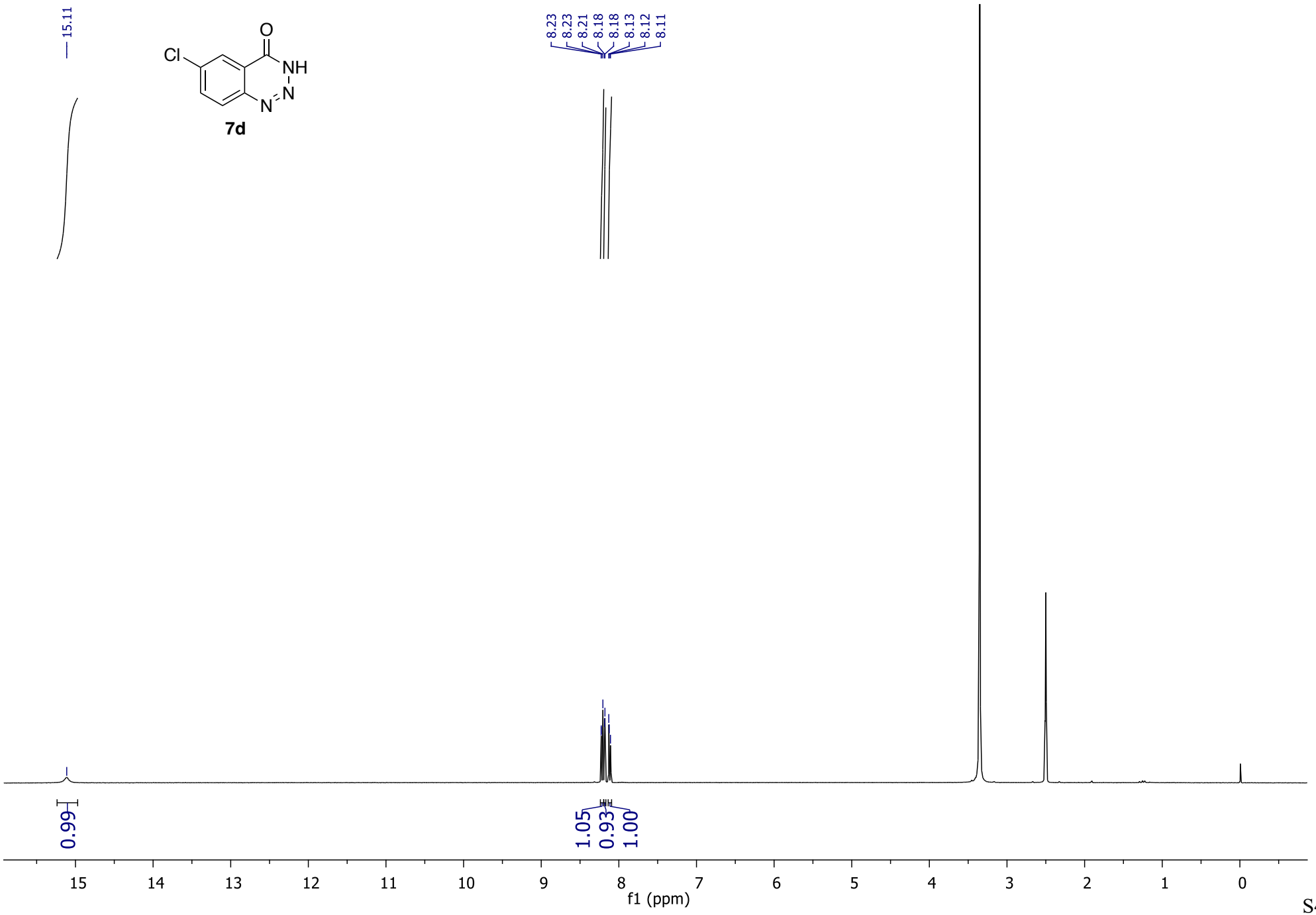
159.77
157.67
152.69
145.73
136.55
136.47
124.05
118.71
118.55
109.85

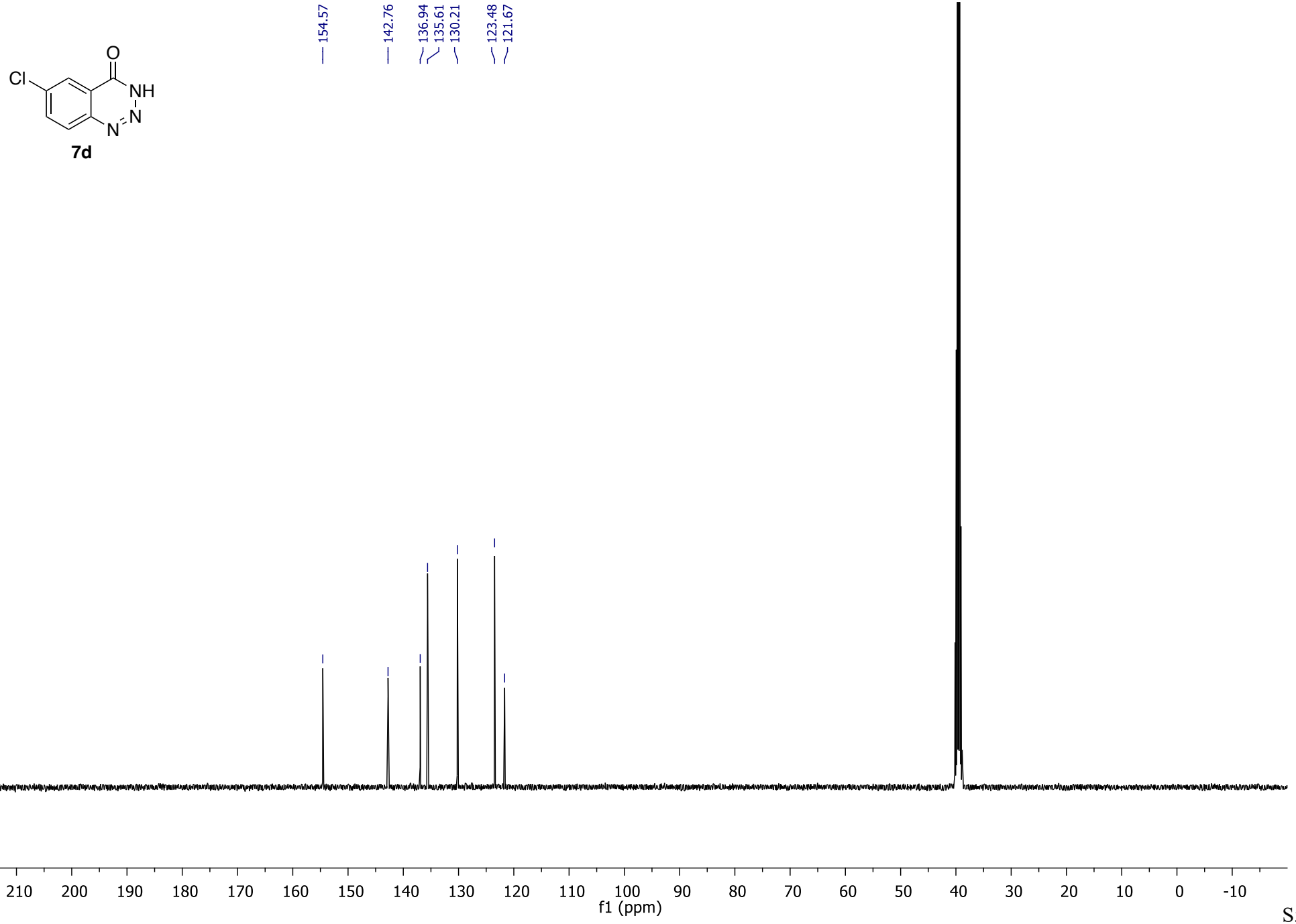
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

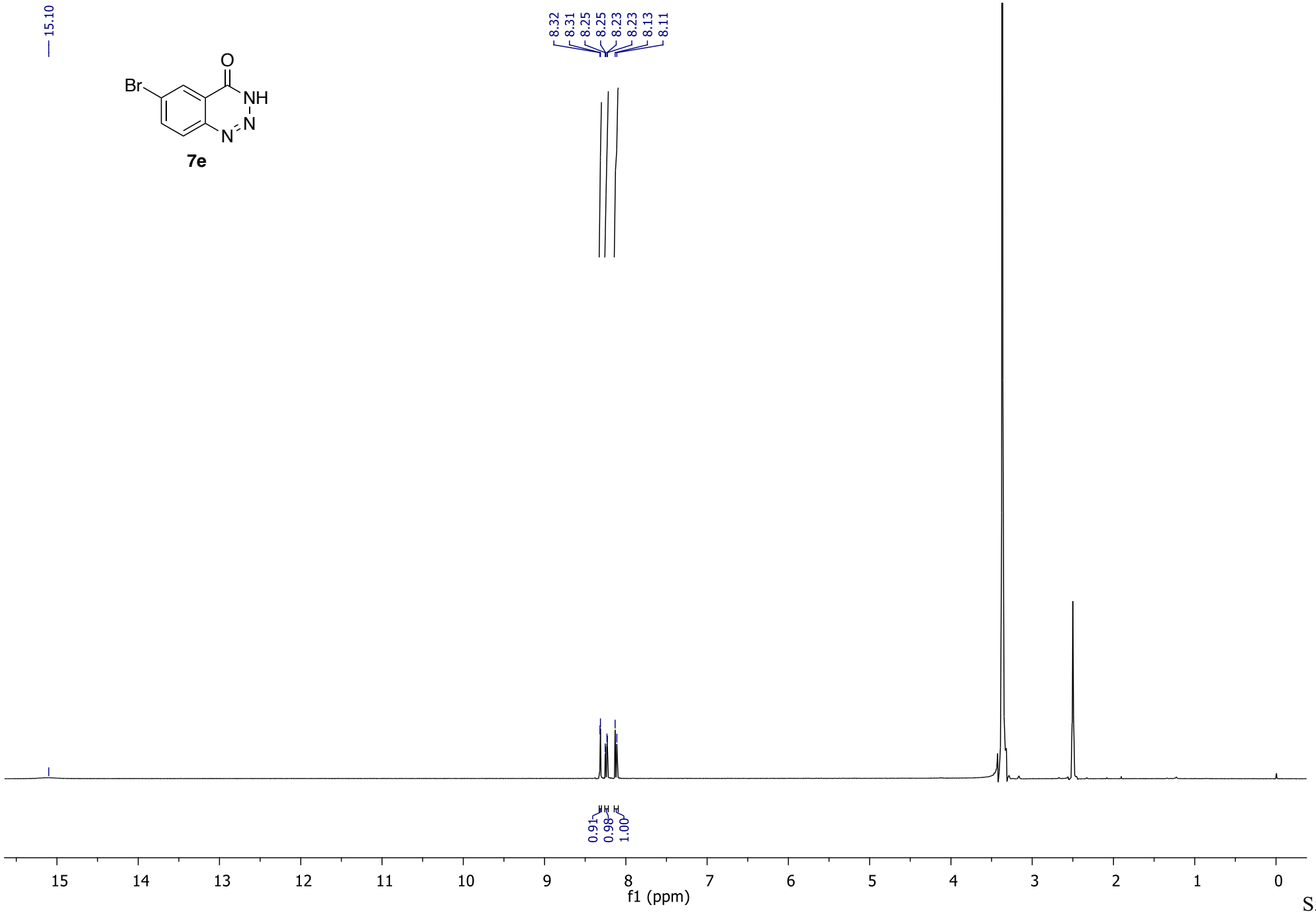
f1 (ppm)

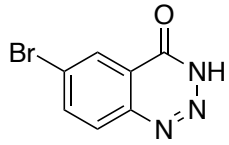

15.04
8.32
8.32
8.31
8.30
8.29
8.29
7.99
7.98
7.97
7.96
7.95
7.95
7.94
7.93
7.93
O
F
NH
N
N
7c
1.03
1.00
1.98
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


164.46
161.94
155.03
155.00
141.48
141.46
131.64
131.55
124.09
123.85
122.48
122.38
109.59
109.36
O
NH
N
N
F
7c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


15.11
8.23
8.23
8.21
8.18
8.18
8.13
8.12
8.11
Cl
O
NH
N
N
7d
0.99
1.05
0.93
1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

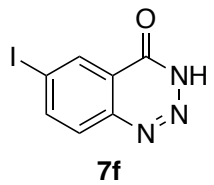

154.57
142.76
136.94
135.61
130.21
123.48
121.67
Cl
O
NH
N
N
7d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


15.10
8.32
8.31
8.25
8.25
8.23
8.23
8.13
8.11
Br
O
NH
N
N
7e
0.91
0.98
1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


O
Br
NH
N
N

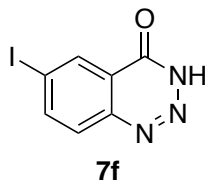
7e

154.30
142.88
138.29
130.05
126.50
125.64
121.66
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
I
NH
N
N

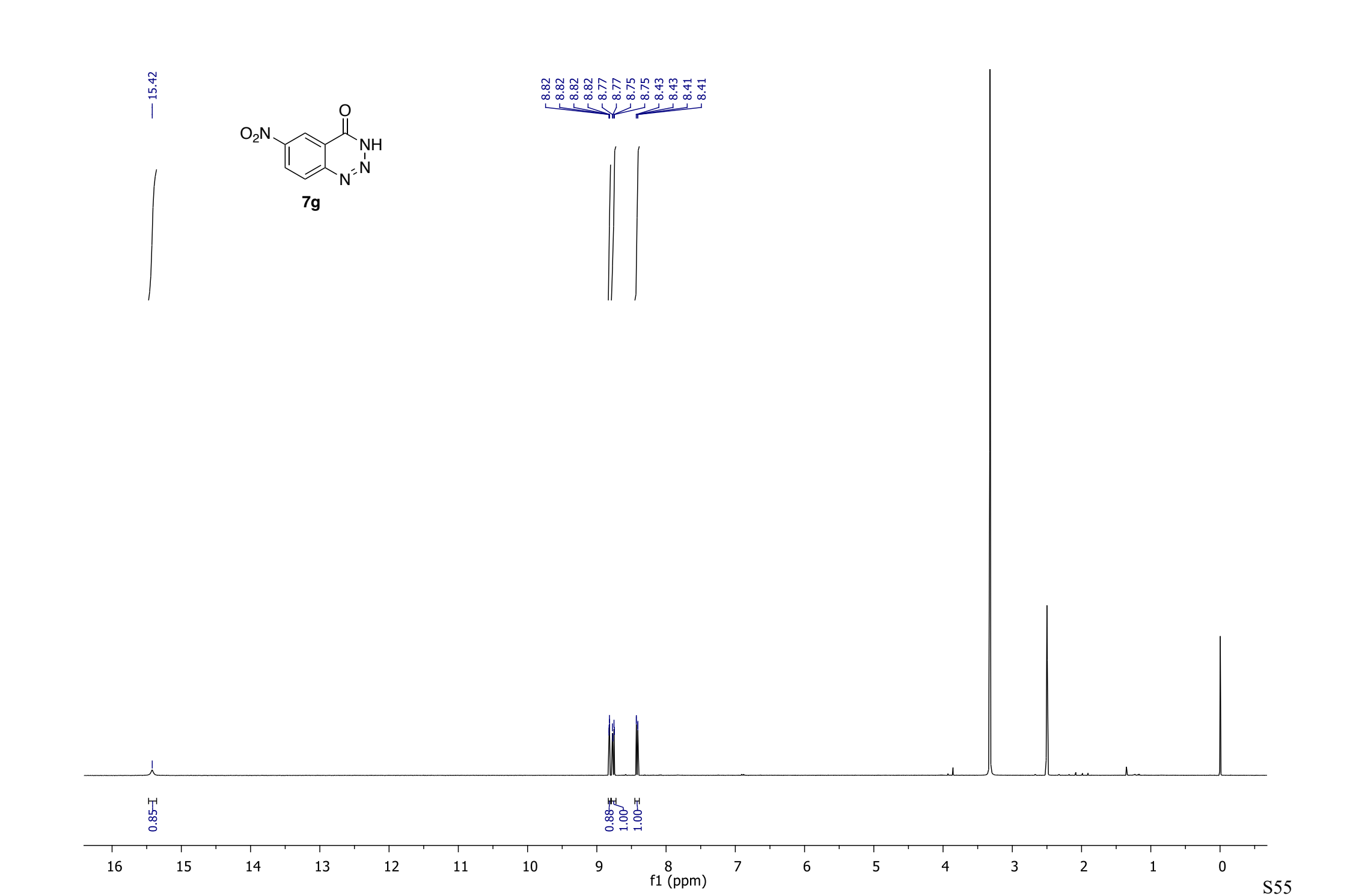
7f

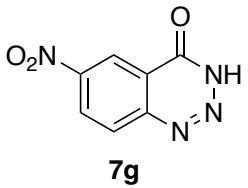
8.64
8.64
8.39
8.38
8.36
8.36
7.91
7.89
7.89
1.00
1.01
1.08
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
I
NH
N
N

7f

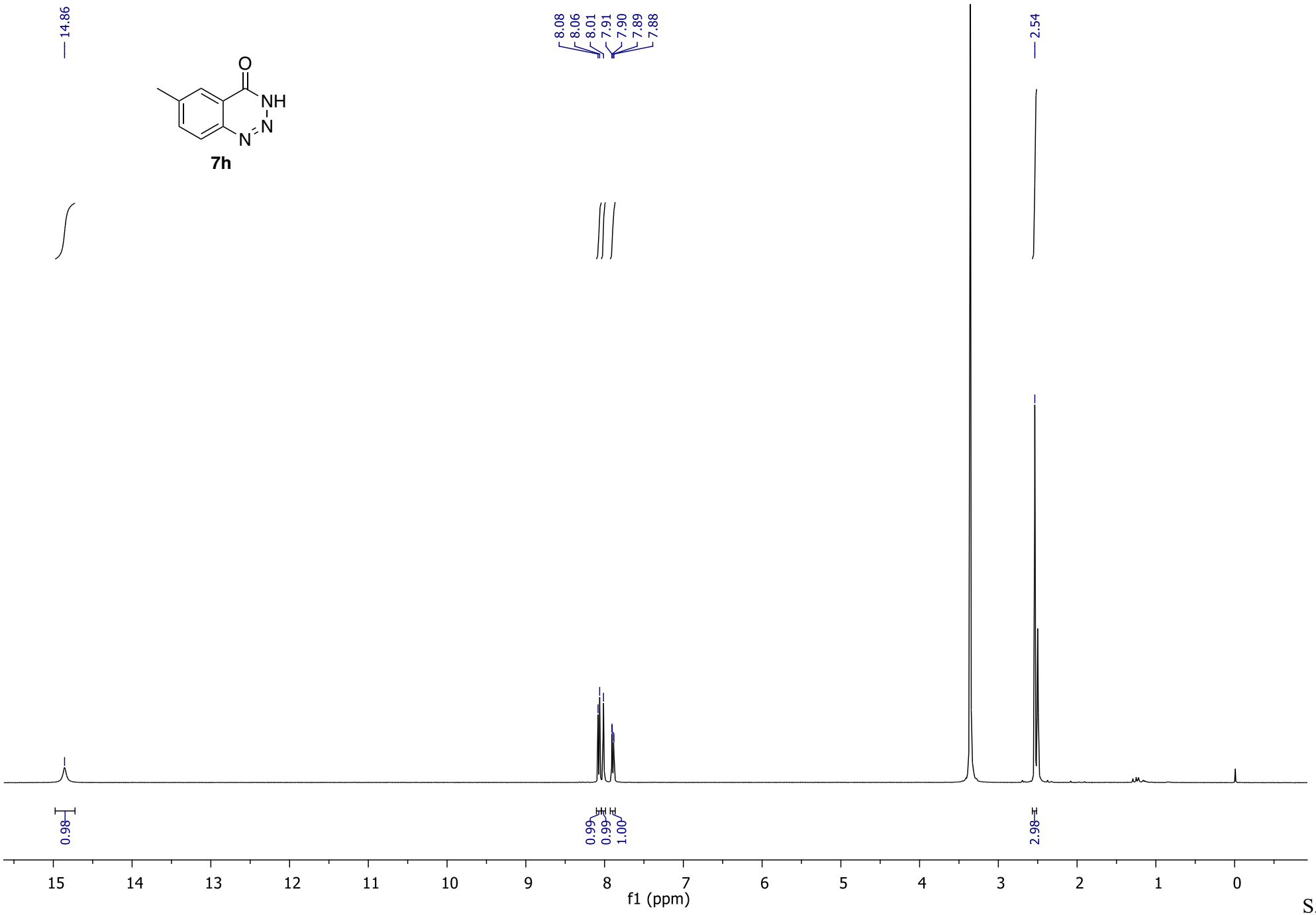
156.60
145.61
145.20
134.61
130.54
122.81
99.49
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

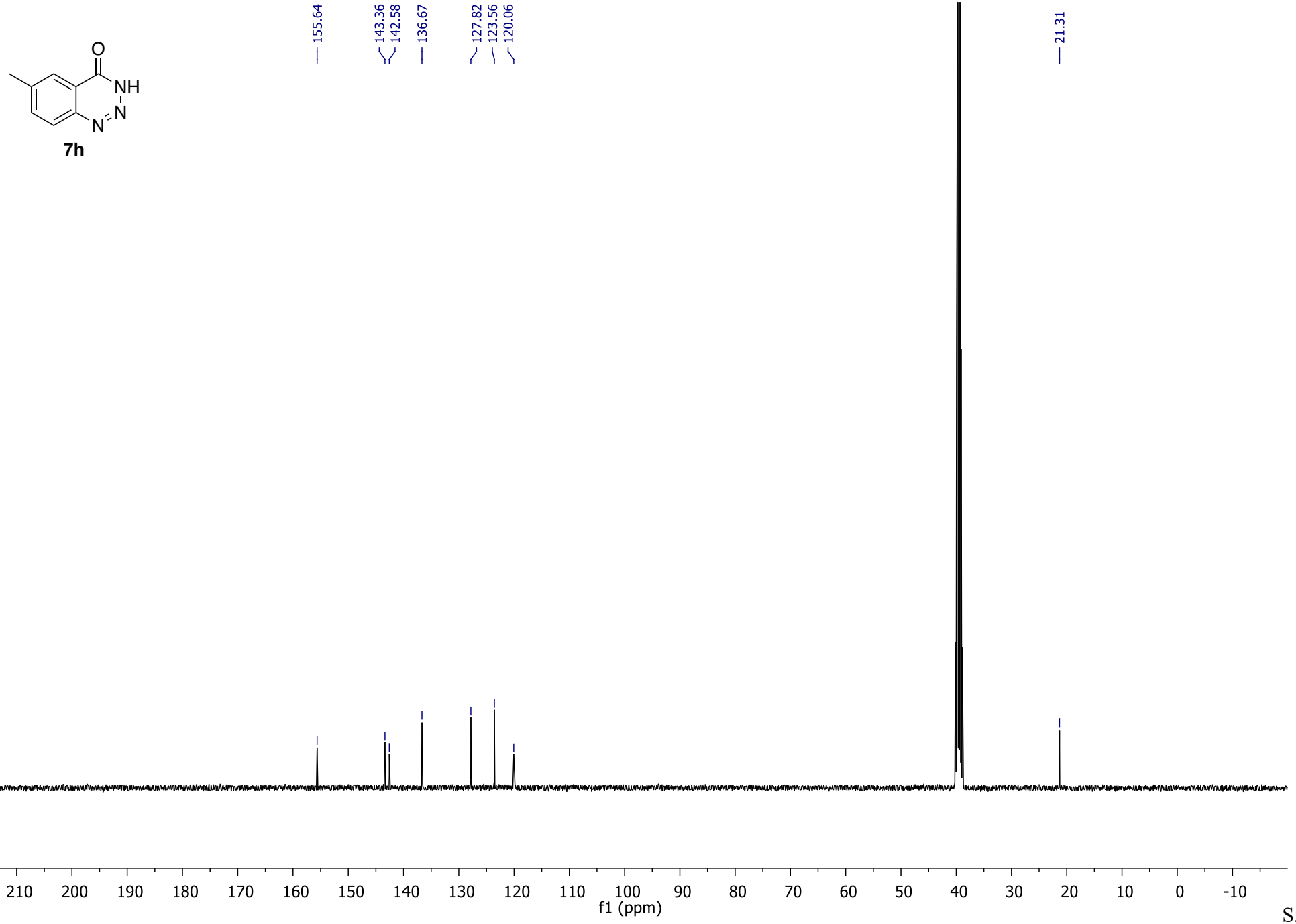

15.42
8.82
8.82
8.82
8.82
8.77
8.77
8.75
8.75
8.43
8.41
8.41
O
O2N
NH
N
N
7g
0.85
0.88
1.00
1.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

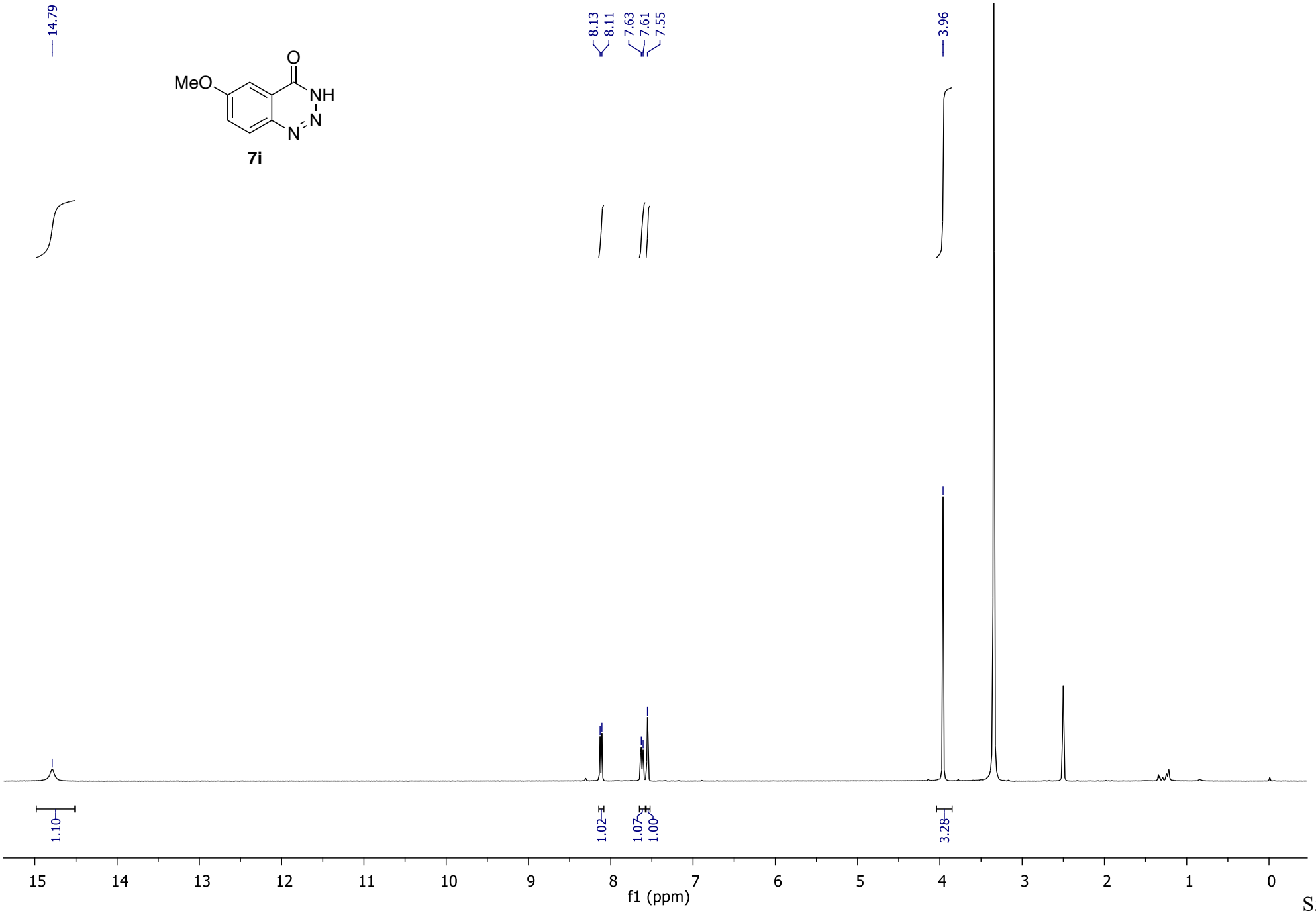

O
O2N
NH
N
N

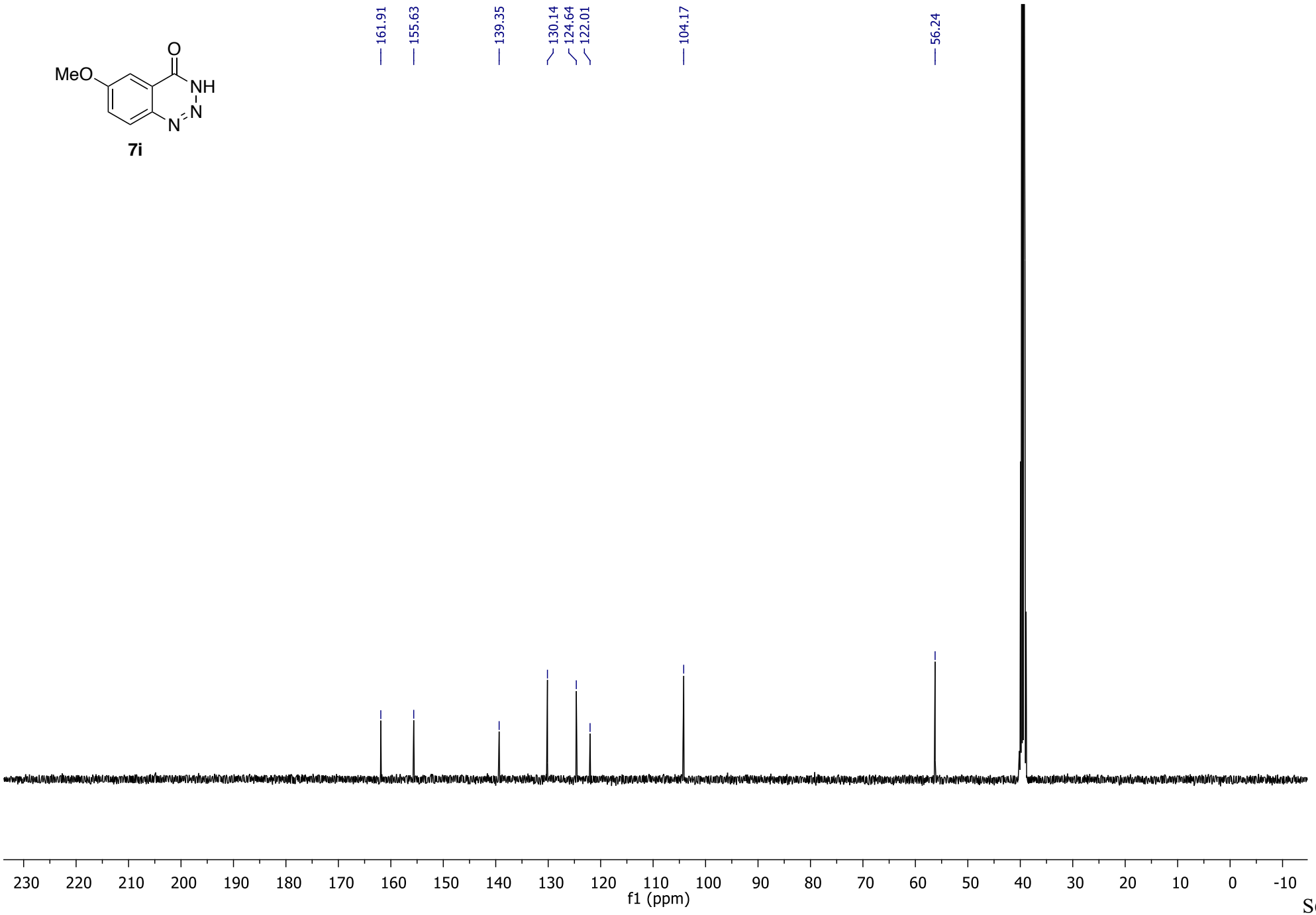
7g

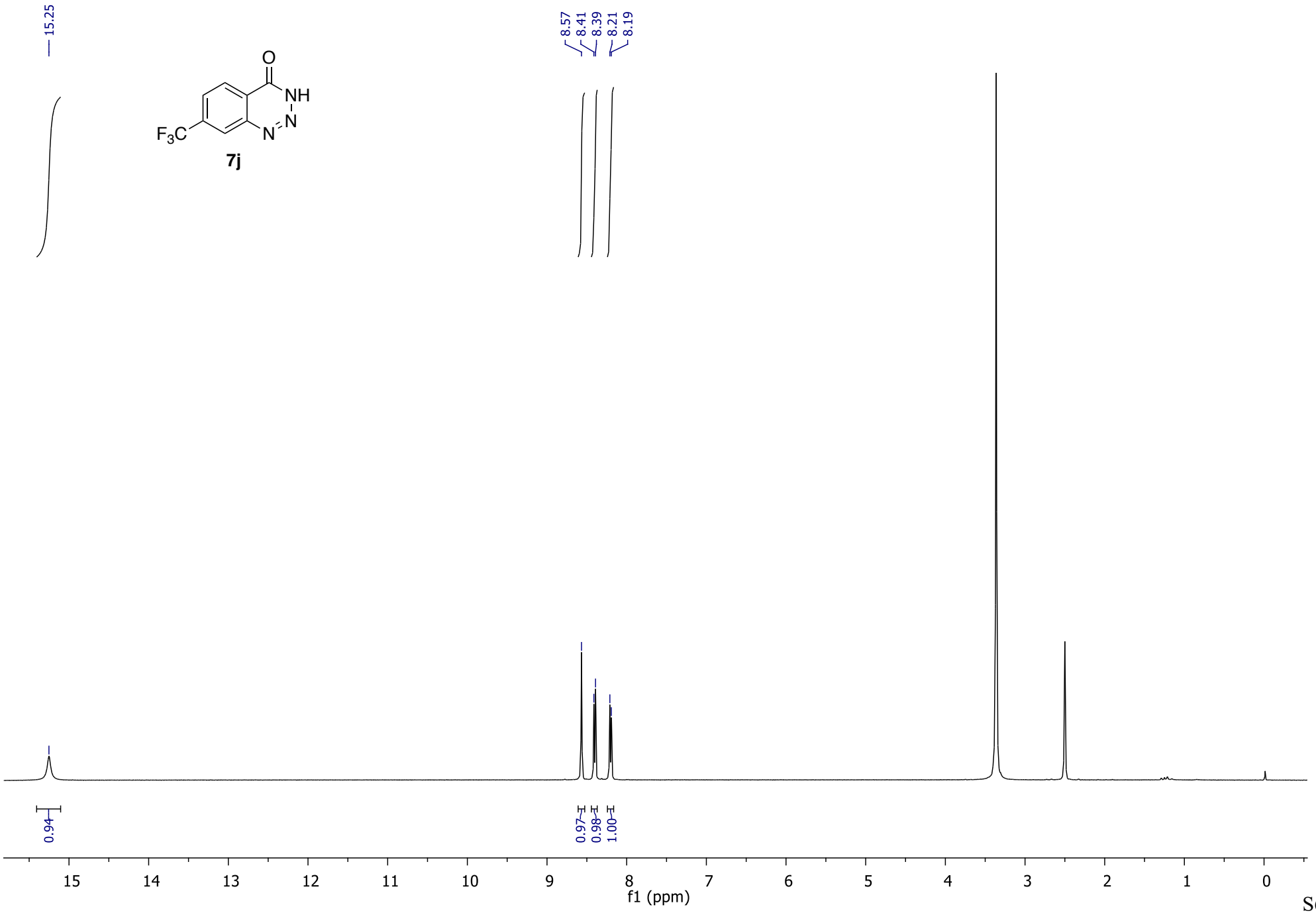
154.84
148.50
146.44
130.15
129.35
121.09
120.27
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

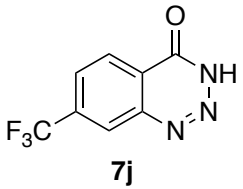

14.86
8.08
8.06
8.01
7.91
7.90
7.89
7.88
2.54
O
NH
N
N
7h
0.98
0.99
0.99
1.00
2.98
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


O
NH
N
N
7h
155.64
143.36
142.58
136.67
127.82
123.56
120.06
21.31
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


14.79
8.13
8.11
7.63
7.61
7.55
3.96
MeO
O
NH
N
N
7i
1.10
1.02
1.07
1.00
3.28
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

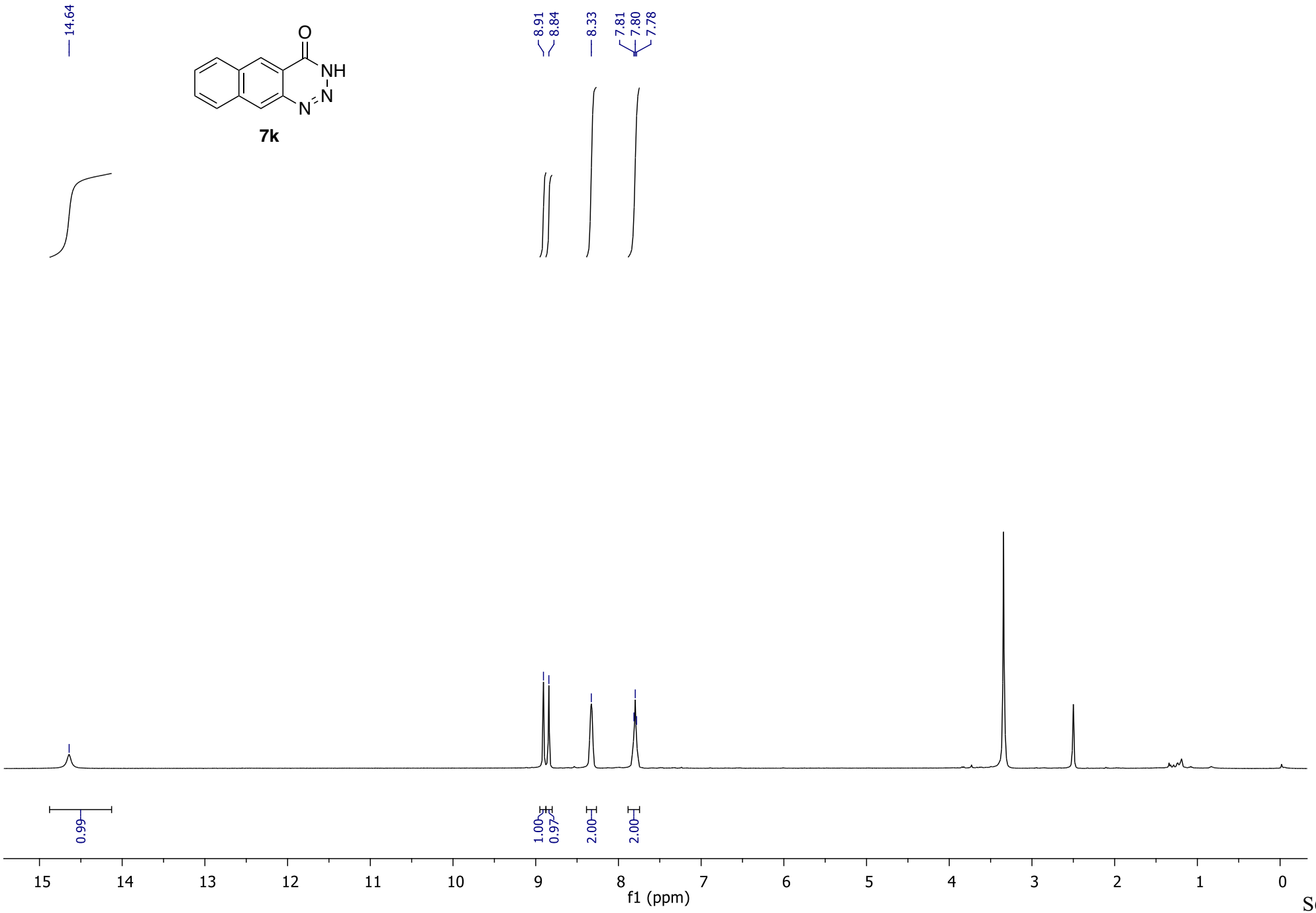

MeO
O
NH
N
N
7i
161.91
155.63
139.35
130.14
124.64
122.01
104.17
56.24
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

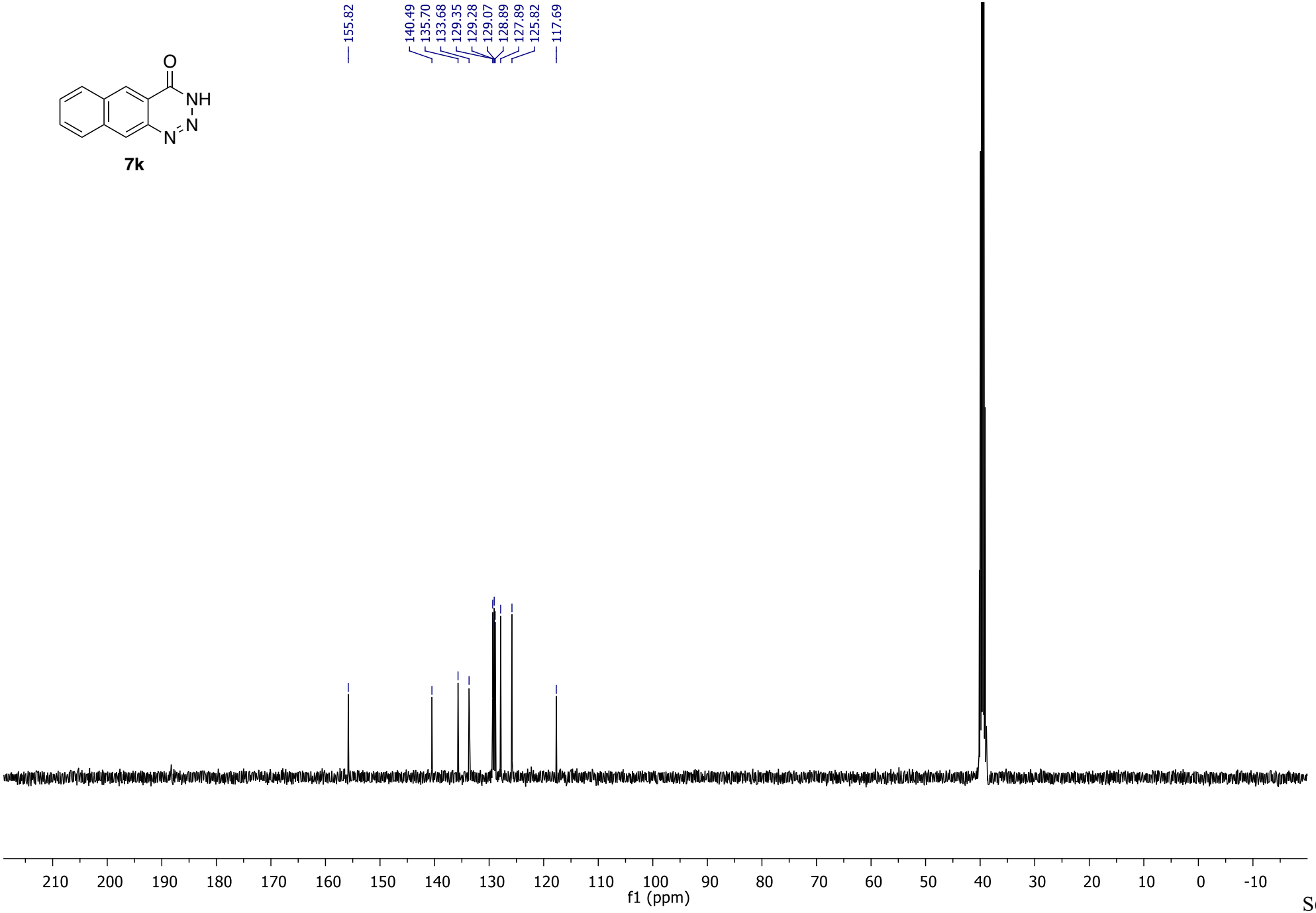

15.25
8.57
8.41
8.39
8.21
8.19
O
NH
N
N
F3C
7j
0.94
0.97
0.98
1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

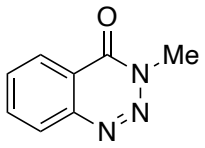

O
NH
N
N
F3C

7j

154.76
143.94
134.91
134.59
134.26
128.12
128.09
127.13
126.30
125.25
125.21
124.41
123.13
121.70
118.98
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

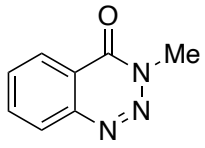

14.64
8.91
8.84
8.33
7.81
7.80
7.78
O
NH
N
N
7k
0.99
1.00
0.97
2.00
2.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


155.82
140.49
135.70
133.68
129.35
129.28
129.07
128.89
127.89
125.82
117.69
O
NH
N
N
7k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
N
Me
N
N

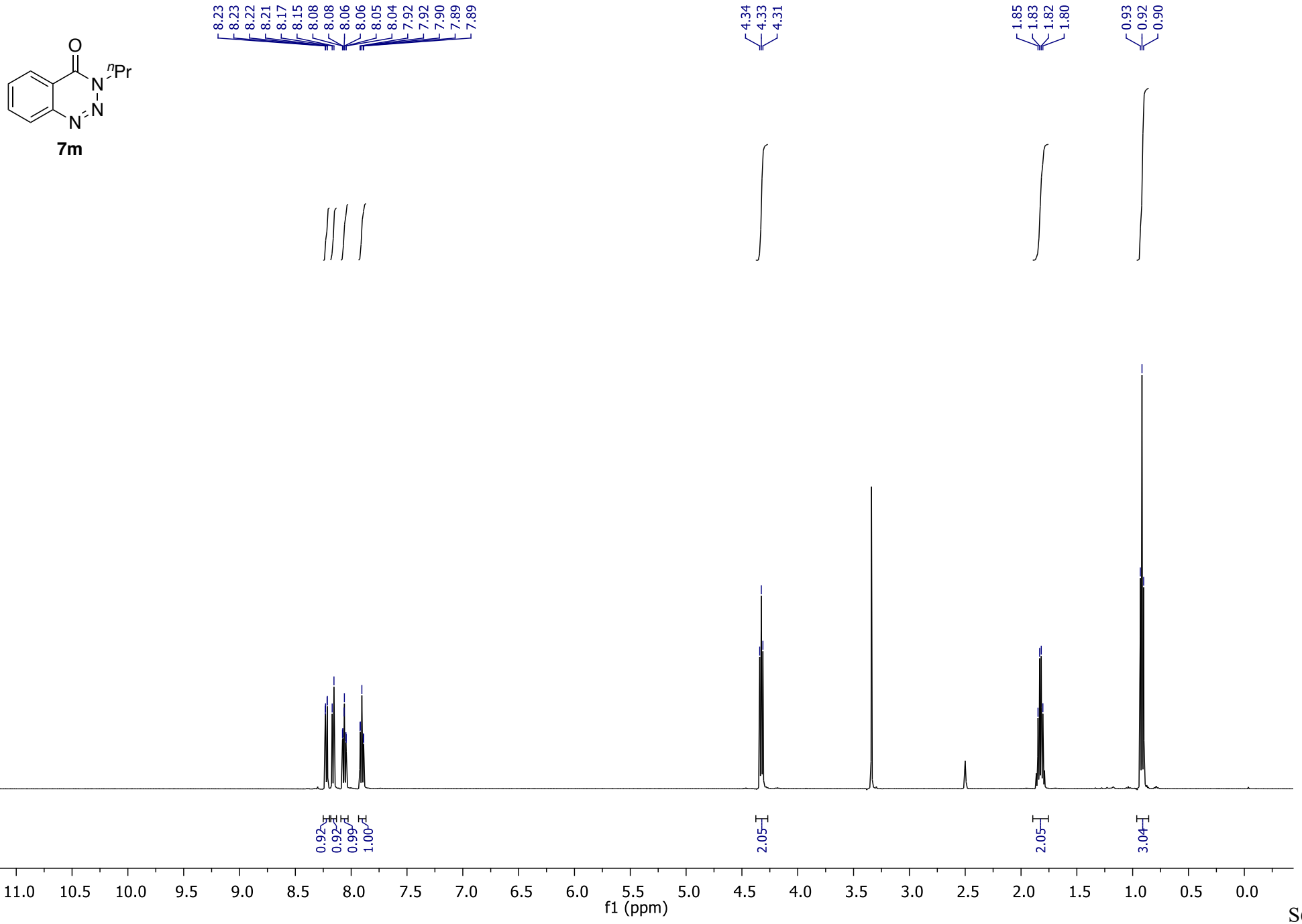
7l

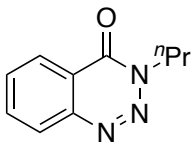
8.25
8.25
8.24
8.23
8.19
8.18
8.09
8.09
8.08
8.07
8.06
8.06
7.94
7.93
7.92
7.91
7.90
3.93
0.94
0.92
0.99
1.00
3.09
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
Me
N
N
N

7l

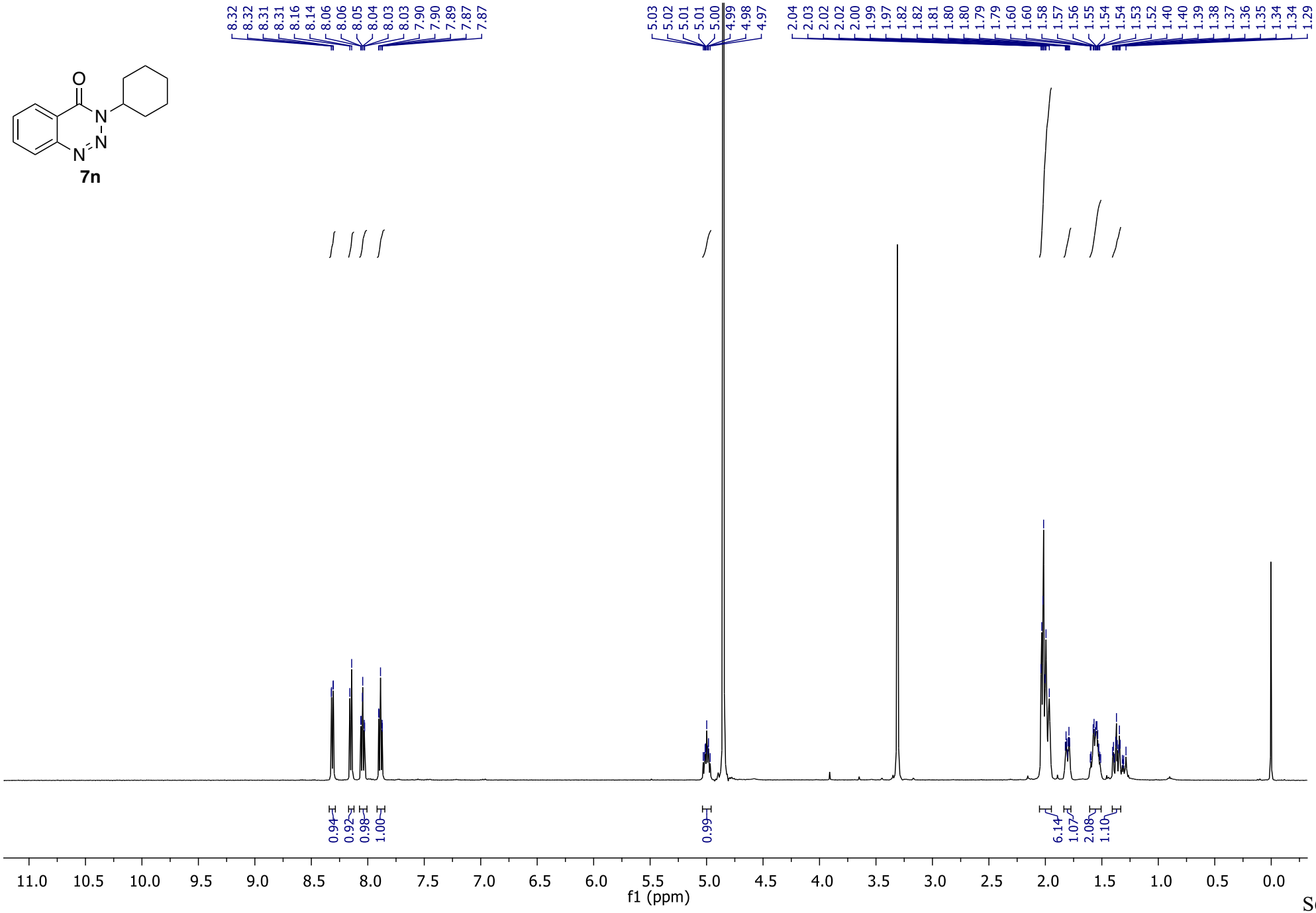
155.06
143.93
135.22
132.81
127.90
124.35
119.15
37.04
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

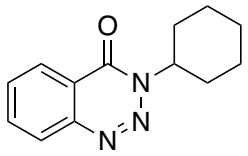

O
nPr
N
N
N
7m
8.23
8.23
8.22
8.21
8.17
8.15
8.08
8.08
8.06
8.06
8.05
8.04
7.92
7.92
7.90
7.89
7.89
4.34
4.33
4.31
1.85
1.83
1.82
1.80
0.93
0.92
0.90
0.92
0.92
0.99
1.00
2.05
2.05
3.04
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
N
nPr
N
N

7m

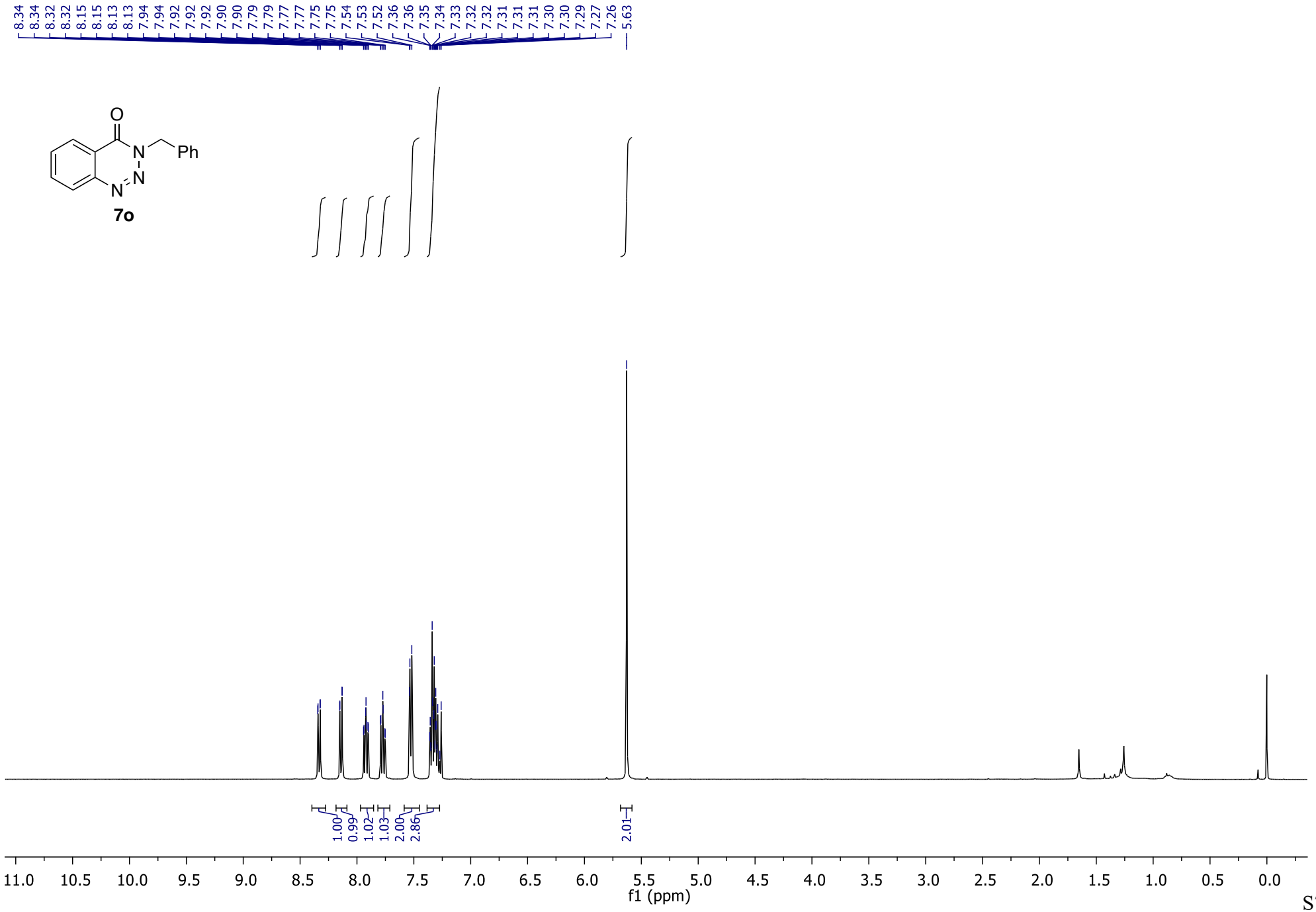
154.67
143.65
135.26
132.79
127.88
124.50
119.15
50.65
21.67
10.94
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

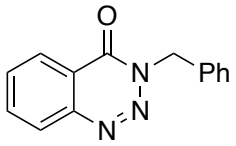

7n
8.32 8.32 8.31 8.31 8.16 8.14 8.06 8.06 8.05 8.04 8.03 8.03 7.90 7.89 7.87 7.87
5.03 5.02 5.01 5.01 5.00 4.99 4.98 4.97
2.04 2.03 2.02 2.02 2.00 1.99 1.97 1.82 1.81 1.80 1.80 1.79 1.79 1.60 1.60 1.58 1.57 1.56 1.55 1.54 1.54 1.53 1.52 1.40 1.40 1.39 1.38 1.37 1.36 1.35 1.34 1.34 1.29
0.94 0.92 0.98 1.00
0.99
6.14 1.07 2.08 1.10
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


O
N
N
N

7n

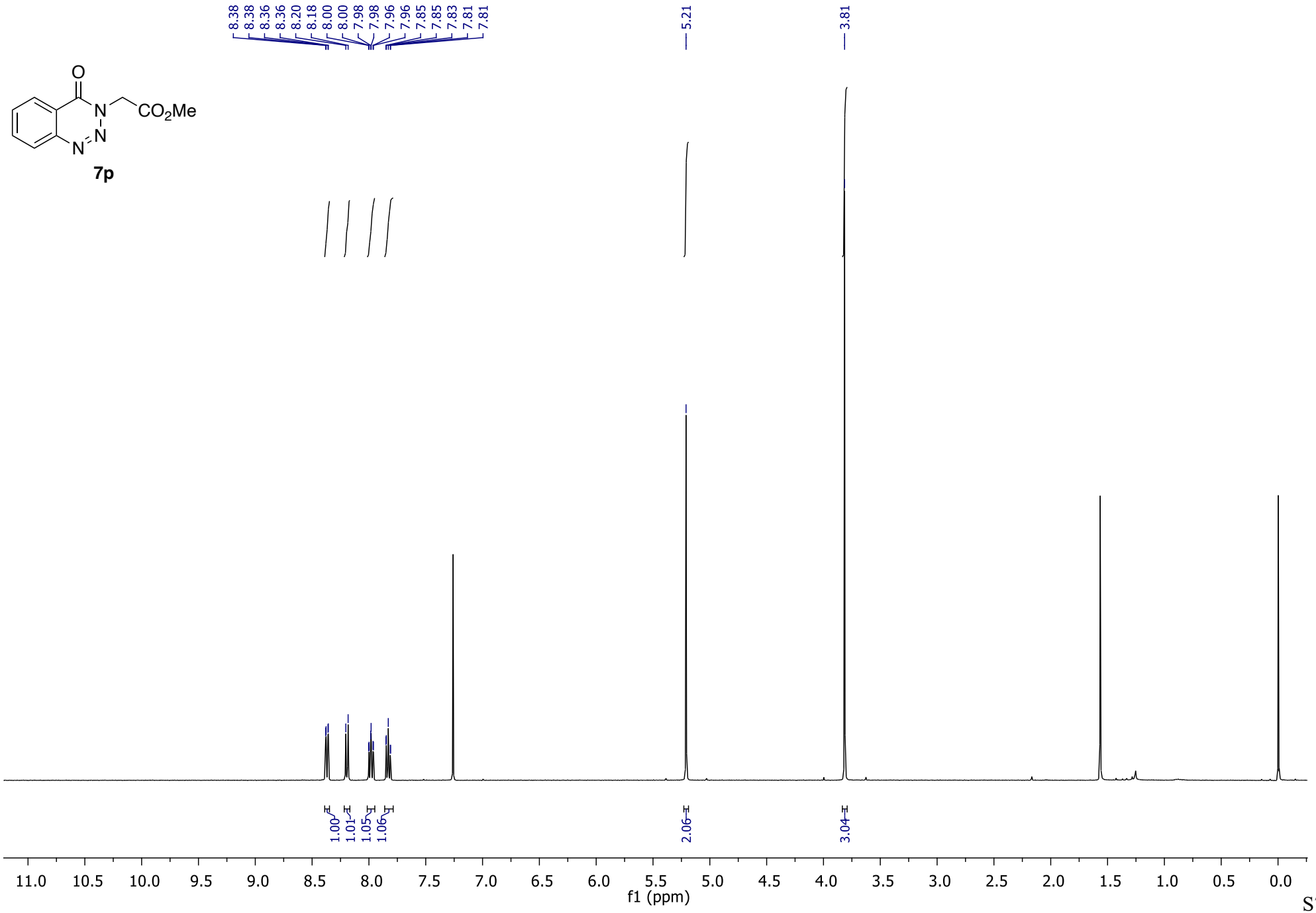
156.61
145.16
136.38
133.71
128.97
126.00
120.58
58.18
32.94
26.90
26.51
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

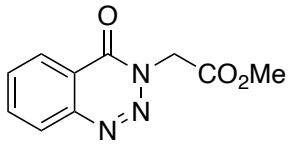

8.34
8.34
8.32
8.32
8.15
8.15
8.13
8.13
7.94
7.94
7.92
7.92
7.92
7.90
7.90
7.79
7.79
7.77
7.77
7.75
7.75
7.54
7.53
7.52
7.36
7.36
7.35
7.34
7.33
7.32
7.32
7.31
7.31
7.31
7.30
7.30
7.29
7.27
7.26
5.63
O
N
N
N
Ph
7o
1.00
0.99
1.02
1.03
2.00
2.86
2.01
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
N
N
N
Ph

7o

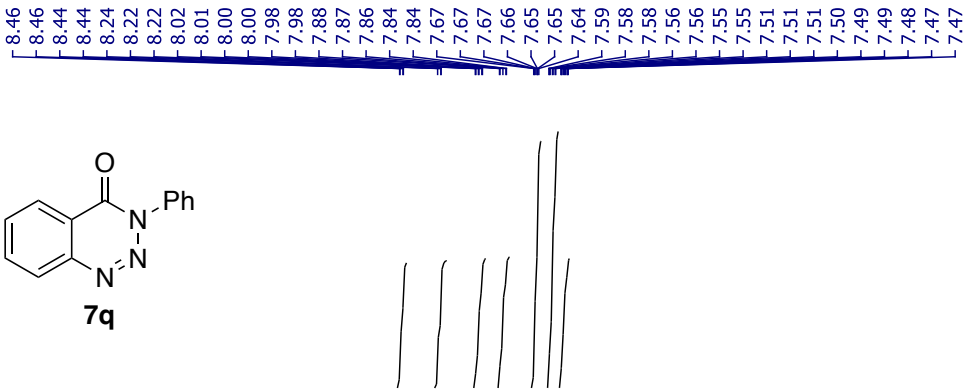
155.50
144.48
135.91
134.92
132.46
128.98
128.85
128.46
128.34
125.31
120.25
53.50
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

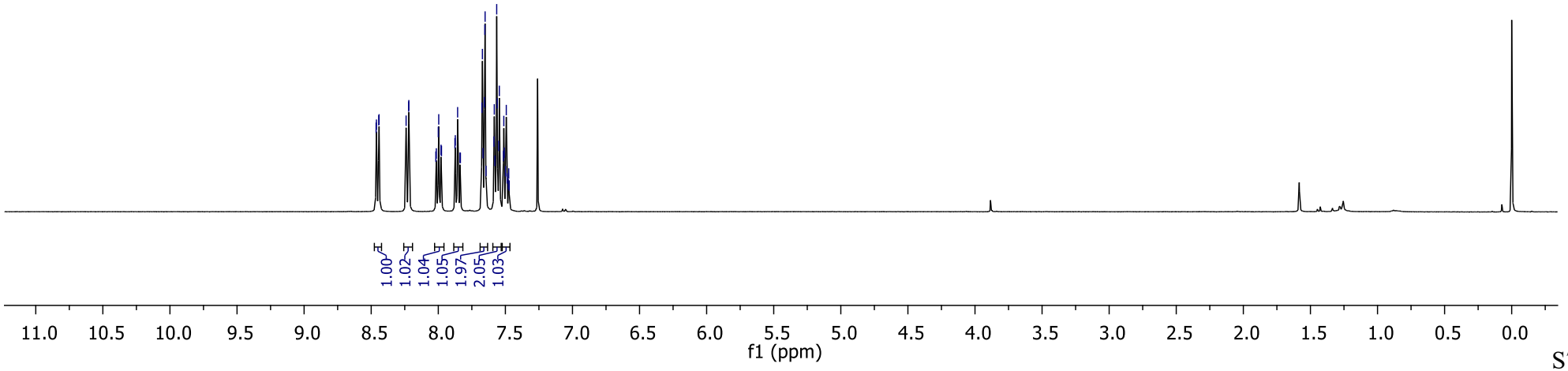

8.38
8.38
8.36
8.36
8.20
8.18
8.00
8.00
7.98
7.98
7.96
7.96
7.85
7.85
7.83
7.81
7.81
5.21
3.81
O
N
N
N
CO2Me
7p
1.00
1.01
1.05
1.06
2.06
3.04
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

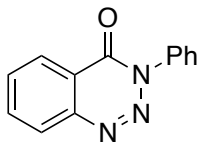

O
N
N
N
CO2Me

7p

167.69
155.71
144.53
135.31
132.84
128.77
125.36
119.93
52.94
50.86
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

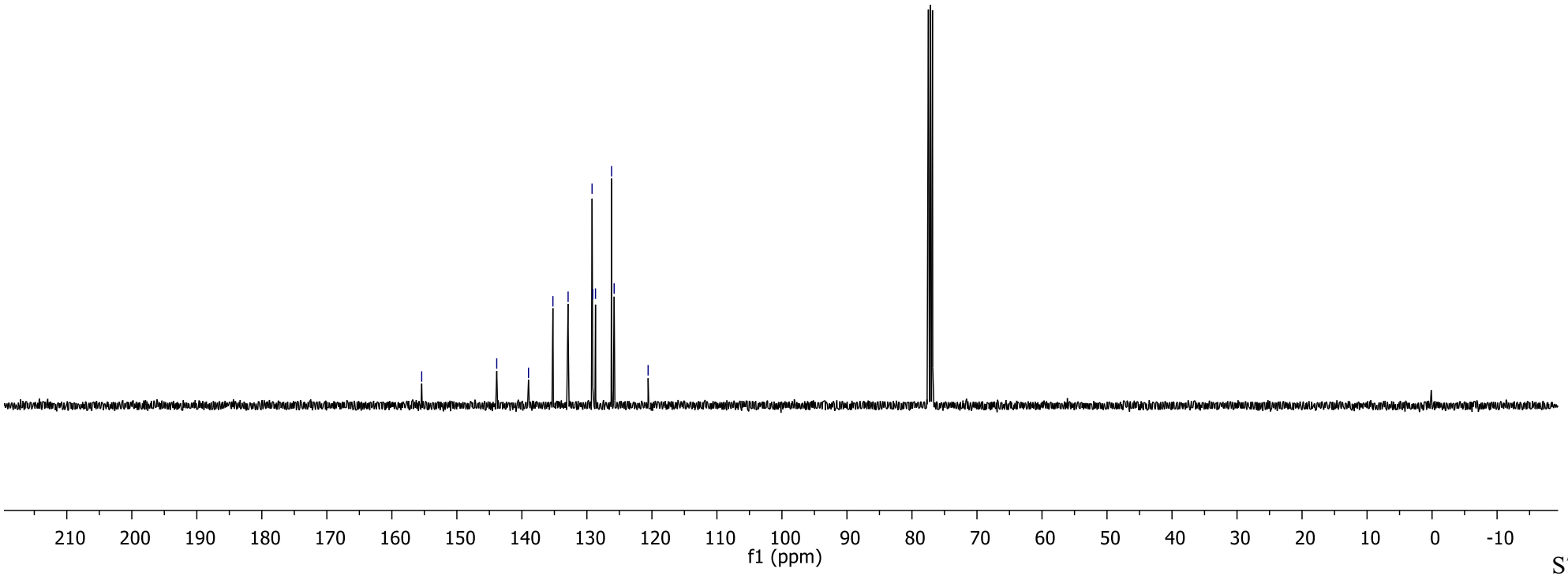

8.46
8.46
8.44
8.44
8.24
8.22
8.22
8.02
8.01
8.00
8.00
7.98
7.98
7.88
7.87
7.86
7.84
7.84
7.67
7.67
7.67
7.66
7.65
7.65
7.64
7.59
7.58
7.58
7.56
7.56
7.55
7.55
7.51
7.51
7.51
7.50
7.49
7.49
7.48
7.47
7.47
O
N
Ph
N
N
7q

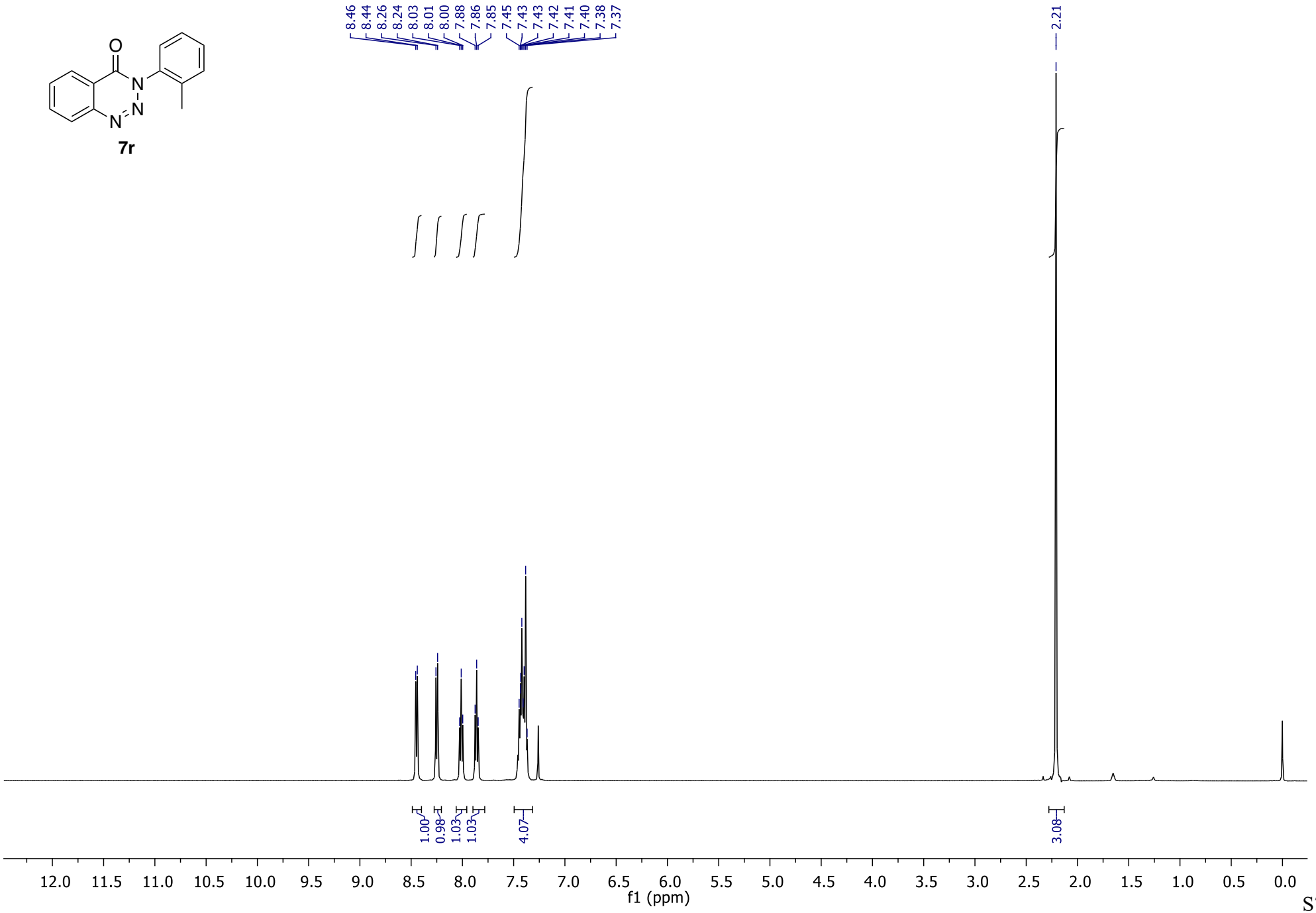

1.00
1.02
1.04
1.05
1.97
2.05
1.03
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

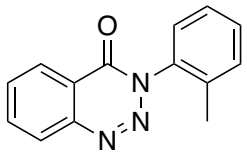


7q

155.41
143.87
138.98
135.23
132.89
129.21
129.10
128.68
126.21
125.81
120.59

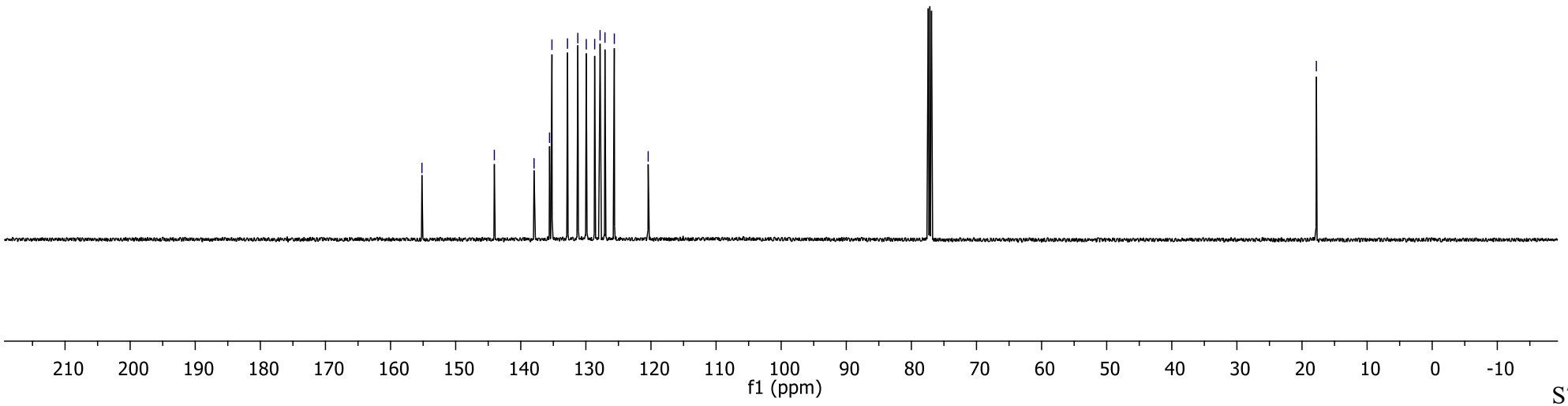


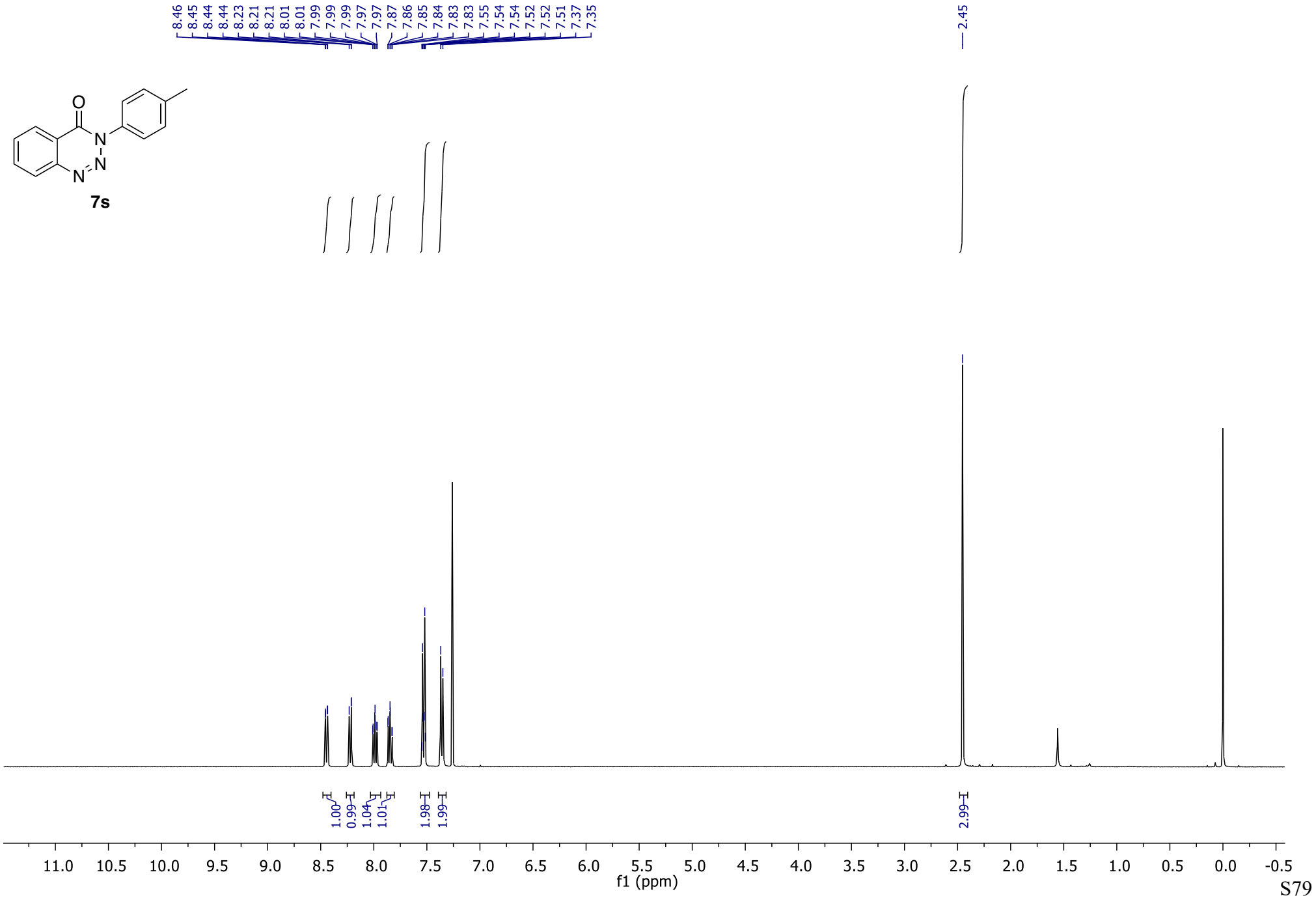

O
N
N
N
7r
8.46
8.44
8.26
8.24
8.03
8.01
8.00
7.88
7.86
7.85
7.45
7.43
7.43
7.42
7.41
7.40
7.38
7.37
2.21
1.00
0.98
1.03
1.03
4.07
3.08
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



7r

155.18
144.06
137.96
135.58
135.21
132.82
131.24
129.94
128.65
127.82
127.07
125.63
120.43
17.79

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7.99
7.99
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7.97
7.87
7.86
7.85
7.84
7.83
7.83
7.55
7.54
7.54
7.52
7.52
7.51
7.37
7.35
2.45
O
N
N
N
7s
1.00
0.99
1.04
1.01
1.98
1.99
2.99
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
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6.5
6.0
5.5
5.0
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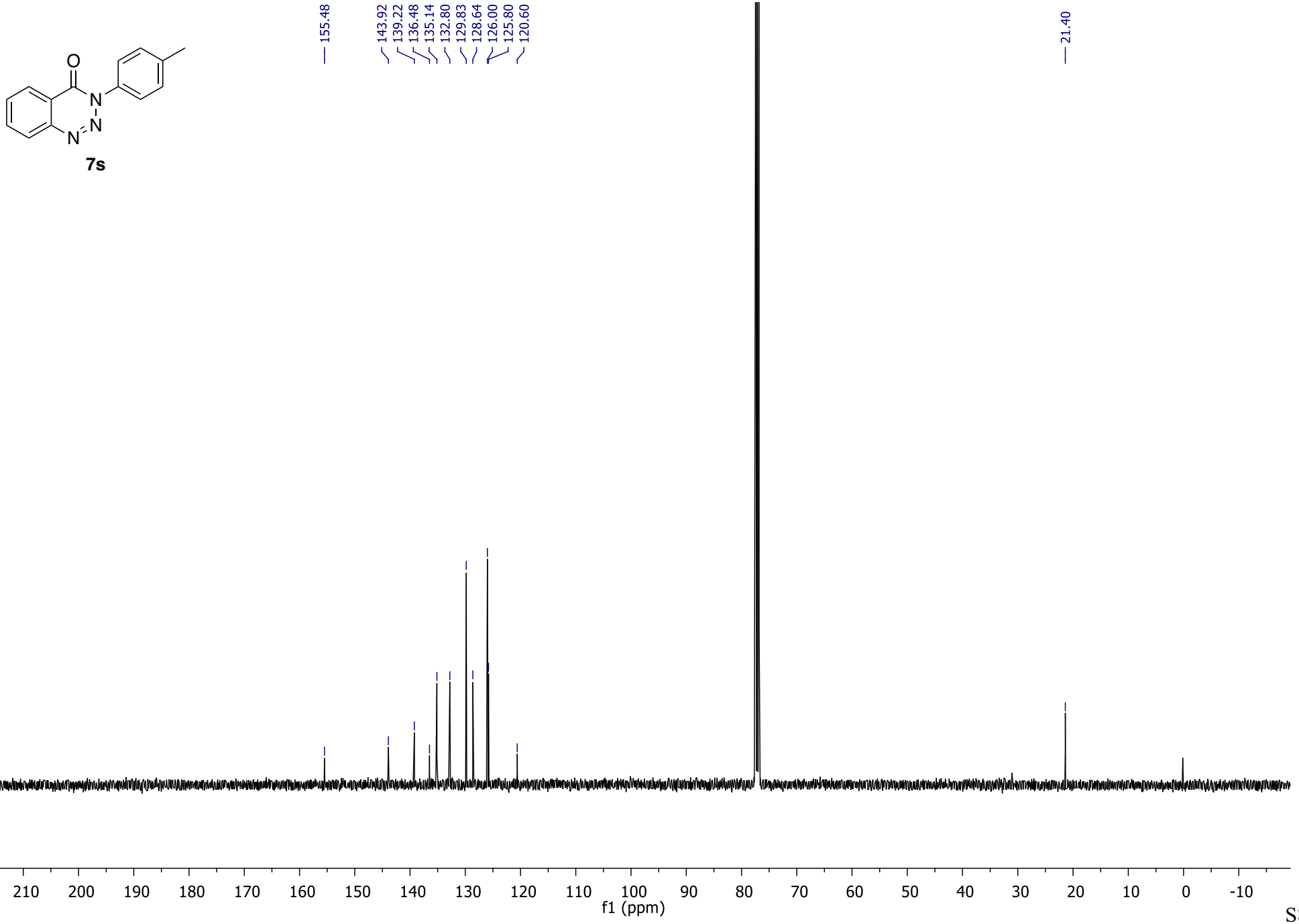
f1 (ppm)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N
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136.48
135.14
132.80
129.83
128.64
126.00
125.80
120.60
21.40
210
200
190
180
170
160
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140
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120
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100
90
80
70
60
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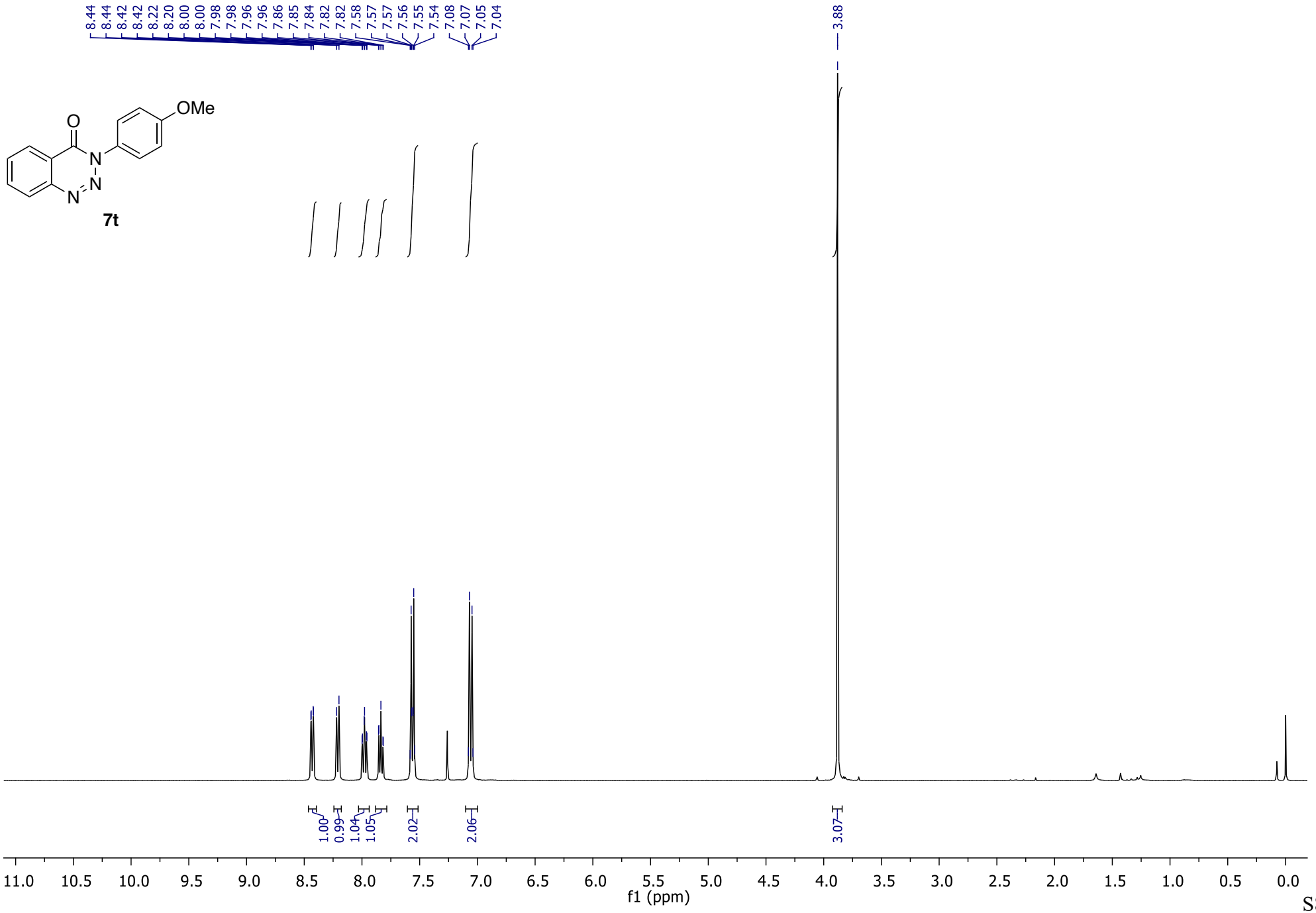
40
30
20
10
0
-10
f1 (ppm)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7.96
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7.84
7.82
7.82
7.58
7.57
7.57
7.56
7.55
7.54
7.08
7.07
7.05
7.04
3.88
OMe
O
N
N
N
7t
1.00
0.99
1.04
1.05
2.02
2.06
3.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
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6.5
6.0
5.5
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3.0
2.5
2.0
1.5
1.0
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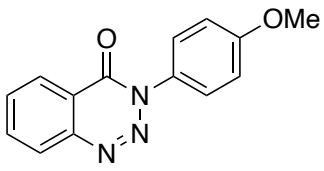
0.0
f1 (ppm)


O
N
N
N
OMe

7t

160.01
155.52
143.87
135.10
132.76
131.87
128.60
127.43
125.74
120.53
114.42
55.71
210
200
190
180
170
160
150
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120
110
100
90
80
70
60
50
40
30
20
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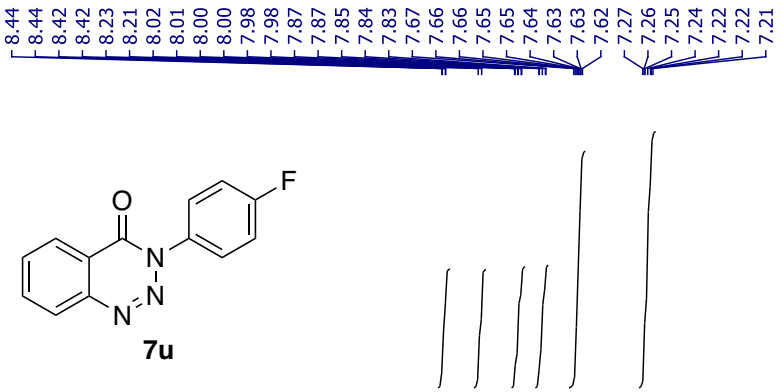
0
-10
f1 (ppm)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8.44
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8.01
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8.00
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7.98
7.87
7.87
7.85
7.84
7.83
7.67
7.66
7.66
7.65
7.65
7.64
7.63
7.63
7.62
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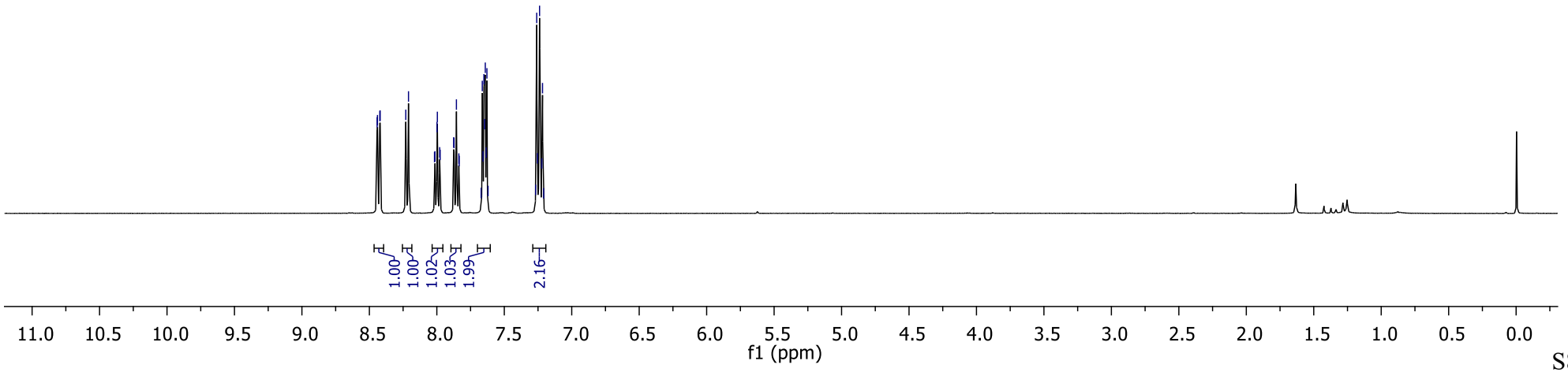
7.26
7.25
7.24
7.22
7.22
7.21
O
N
N
N
F
7u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1.99
2.16
11.0
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10.0
9.5
9.0
8.5
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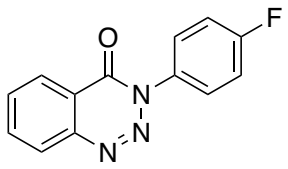
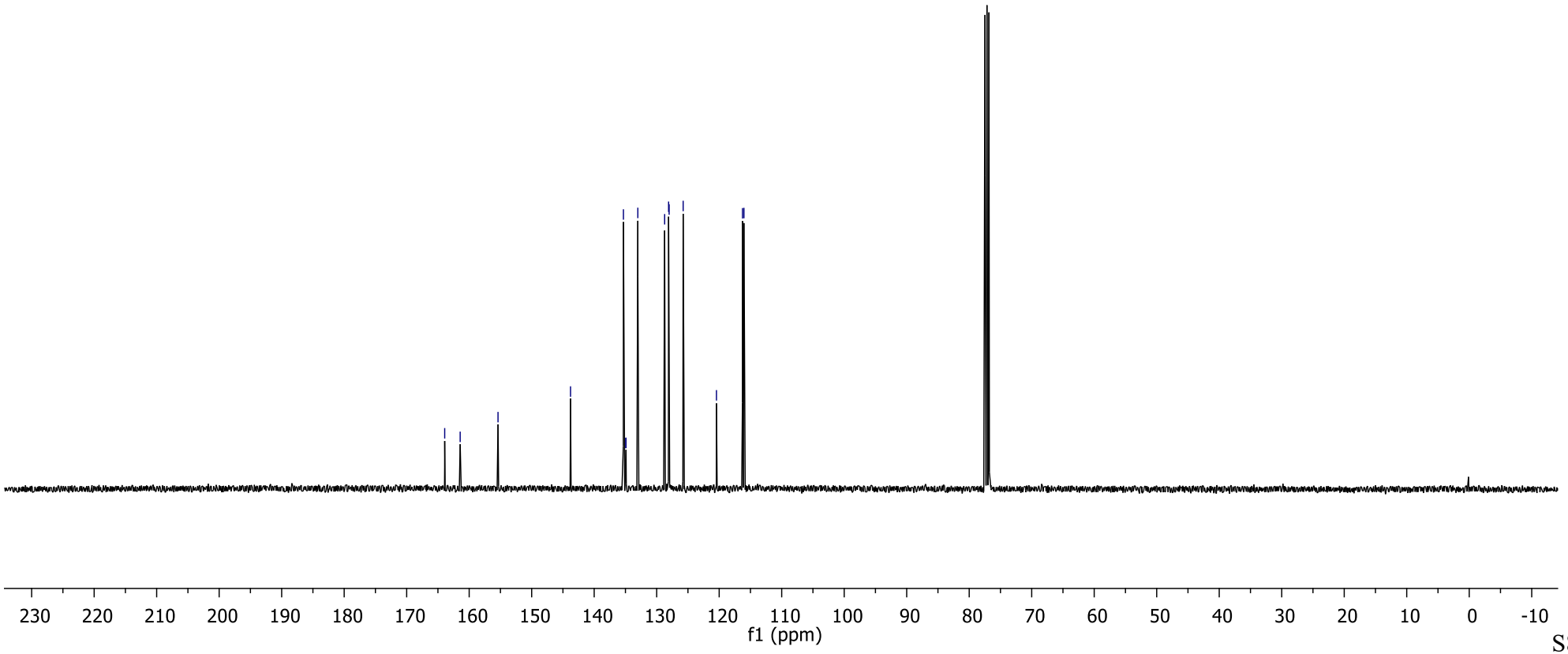
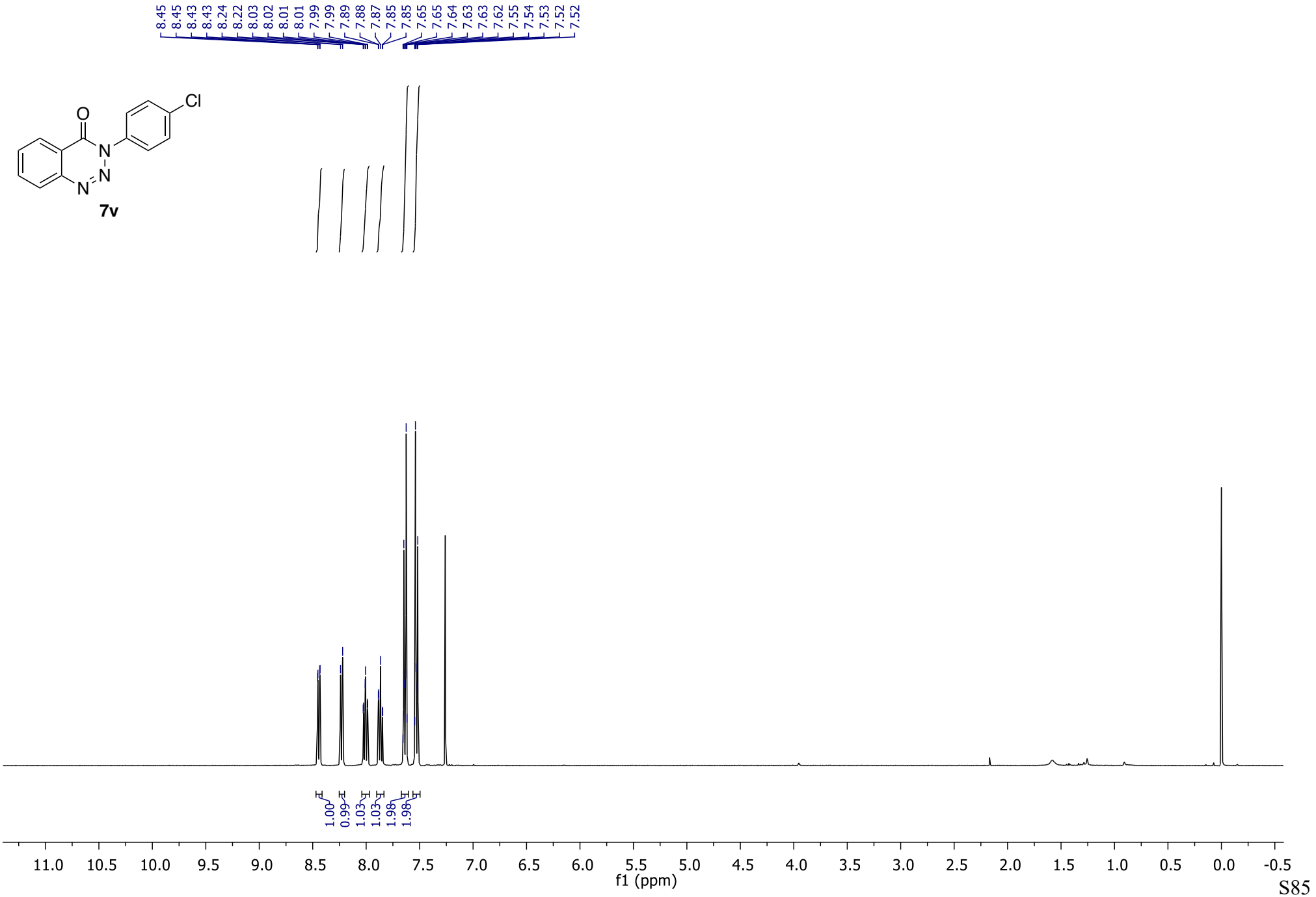
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



7u

163.92
161.44
155.39
143.79
135.32
134.94
134.91
133.02
128.73
128.10
128.01
125.77
120.44
116.27
116.04

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8.45
8.43
8.43
8.24
8.22
8.03
8.02
8.01
8.01
7.99
7.99
7.89
7.88
7.87
7.85
7.85
7.65
7.65
7.64
7.63
7.63
7.62
7.55
7.54
7.53
7.52
7.52
O
N
N
N
Cl
7v
1.00
0.99
1.03
1.03
1.98
1.98
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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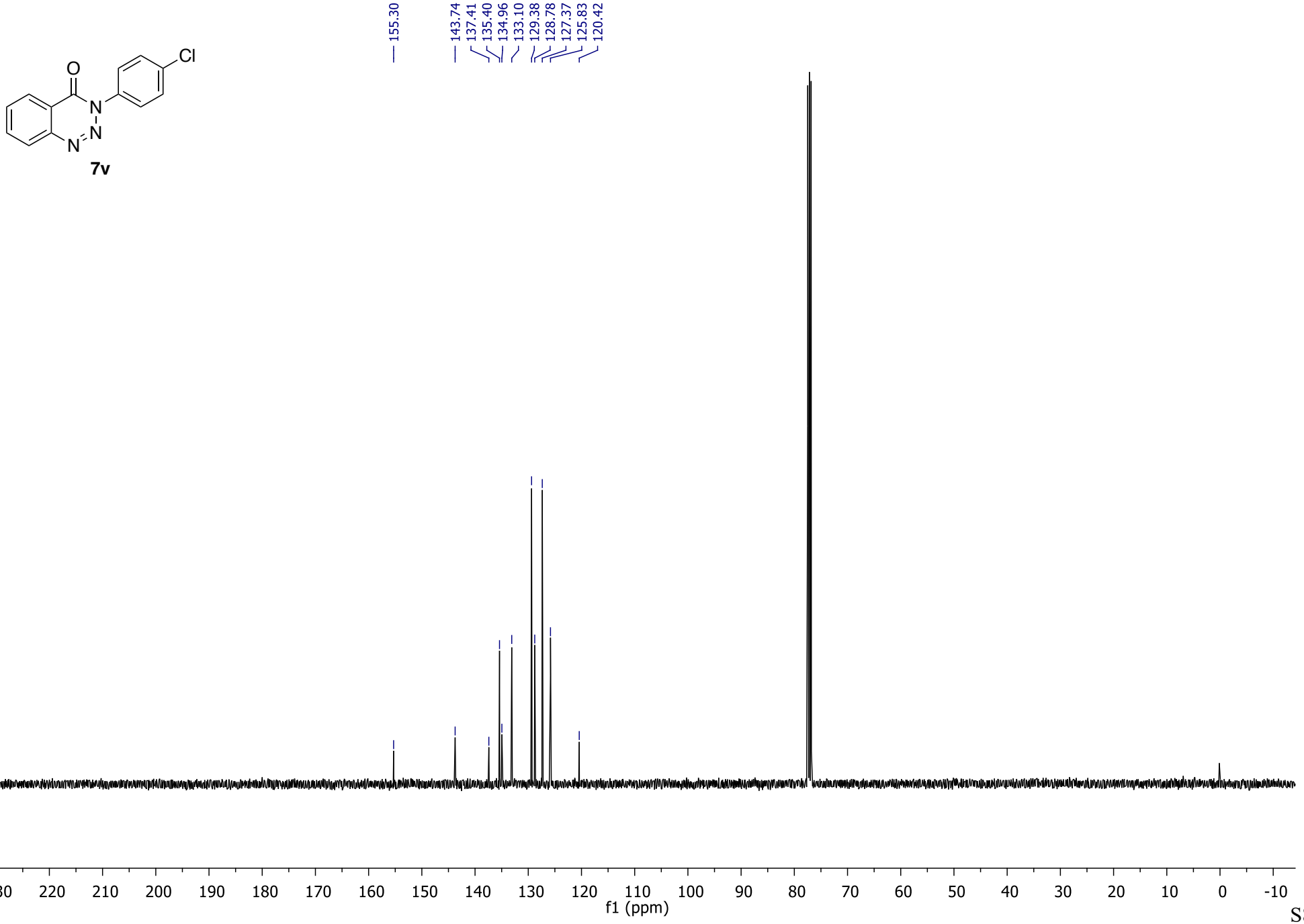
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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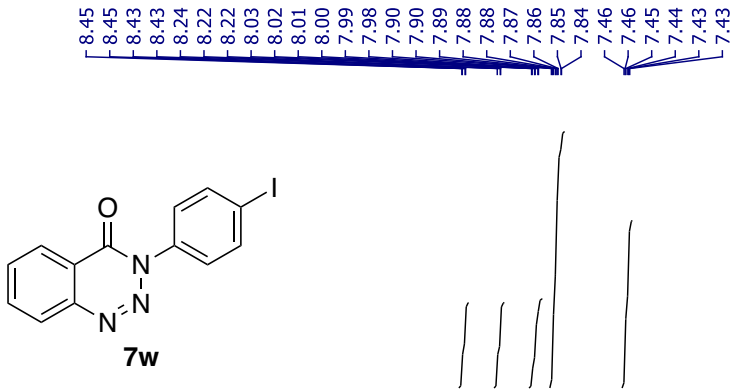
135.40
134.96
133.10
129.38
128.78
127.37
125.83
120.42
O
N
N
N
Cl
7v
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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8.45
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8.43
8.24
8.22
8.22
8.03
8.02
8.01
8.00
7.99
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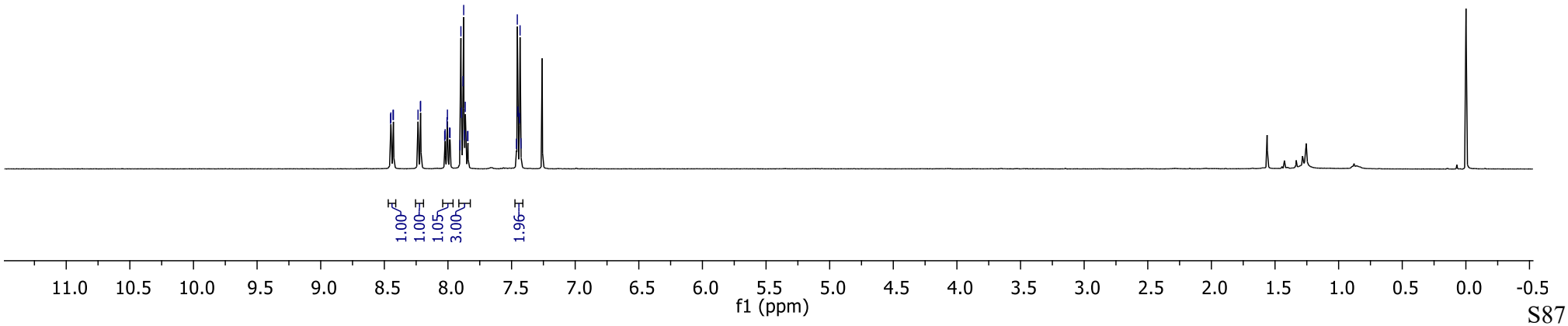
7.90
7.90
7.89
7.88
7.88
7.87
7.86
7.85
7.84
7.46
7.46
7.45
7.44
7.43
7.43
O
N
N
N
I
7w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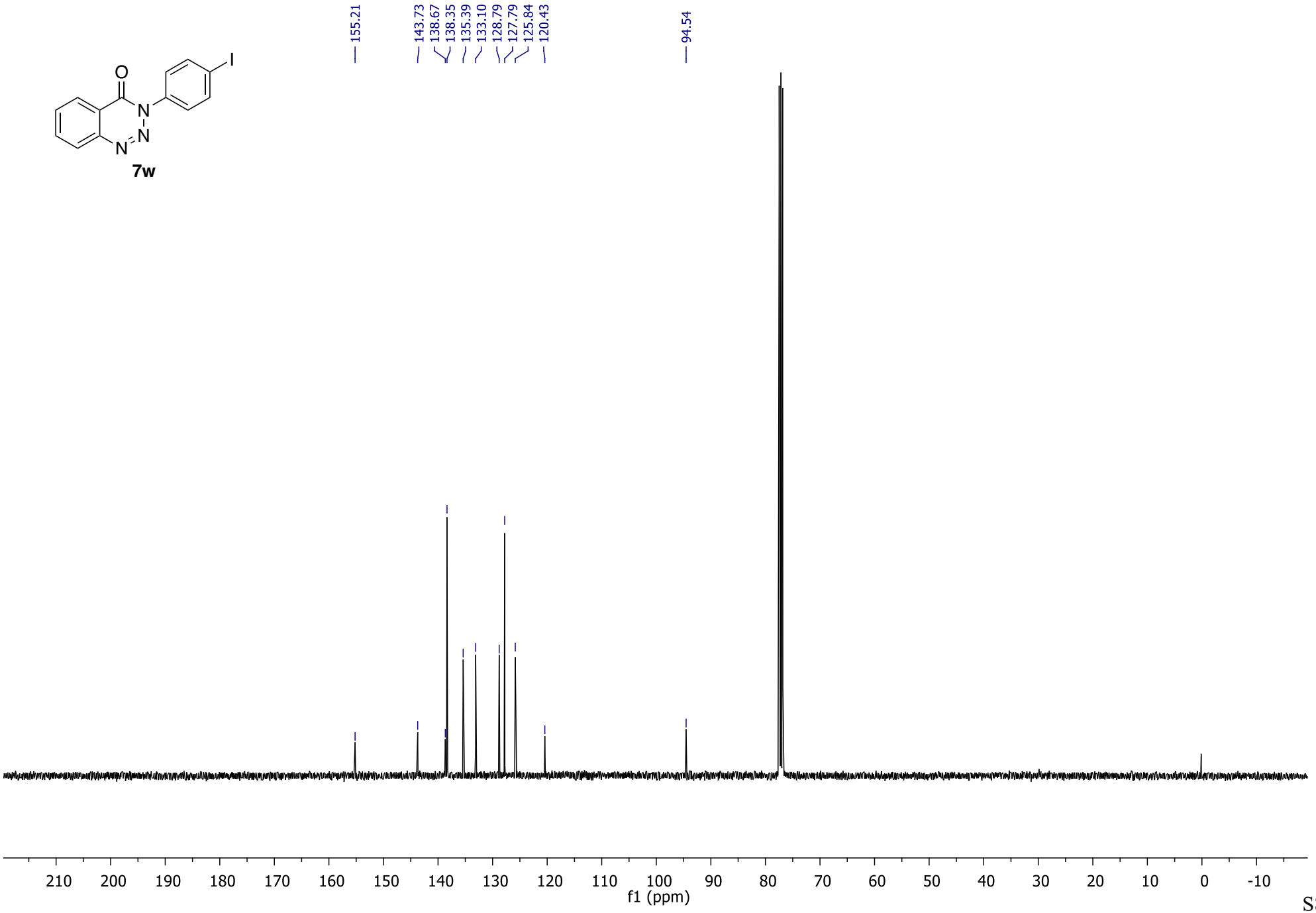
1.00
1.05
3.00
1.96
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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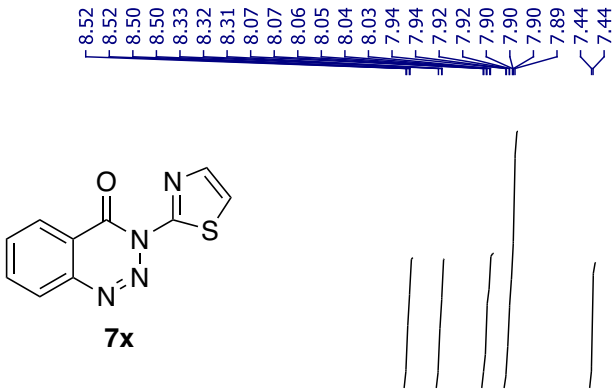
138.67
138.35
135.39
133.10
128.79
127.79
125.84
120.43
94.54
O
N
N
N
I
7w
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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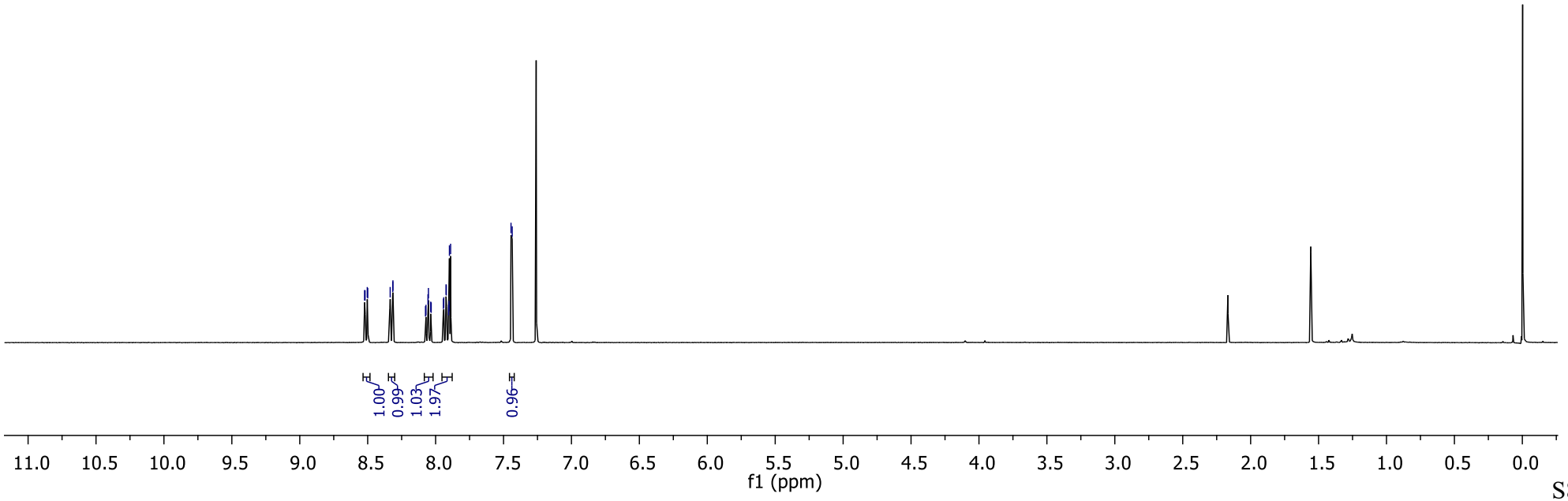
8.50
8.50
8.33
8.32
8.31
8.07
8.07
8.06
8.05
8.04
8.03
7.94
7.94
7.92
7.92
7.90
7.90
7.90
7.89
7.44
7.44
O
N
N
S
N
N
7x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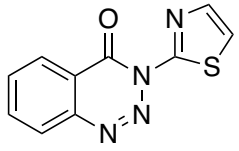
0.99
1.03
1.97
1
0.96
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

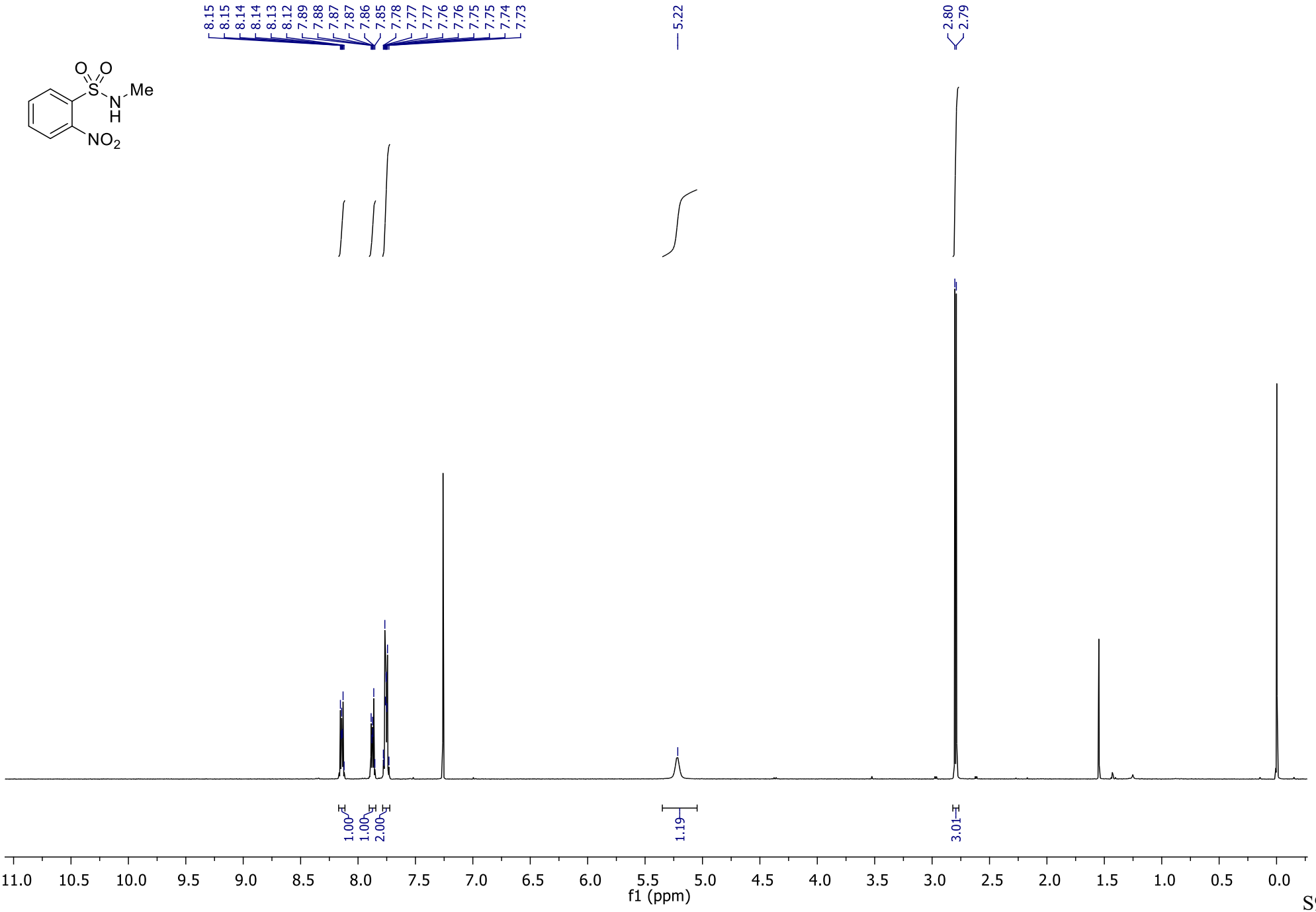


7x

156.34
154.26
142.59
140.18
135.92
133.81
129.50
126.00
119.42
119.14

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

f1 (ppm)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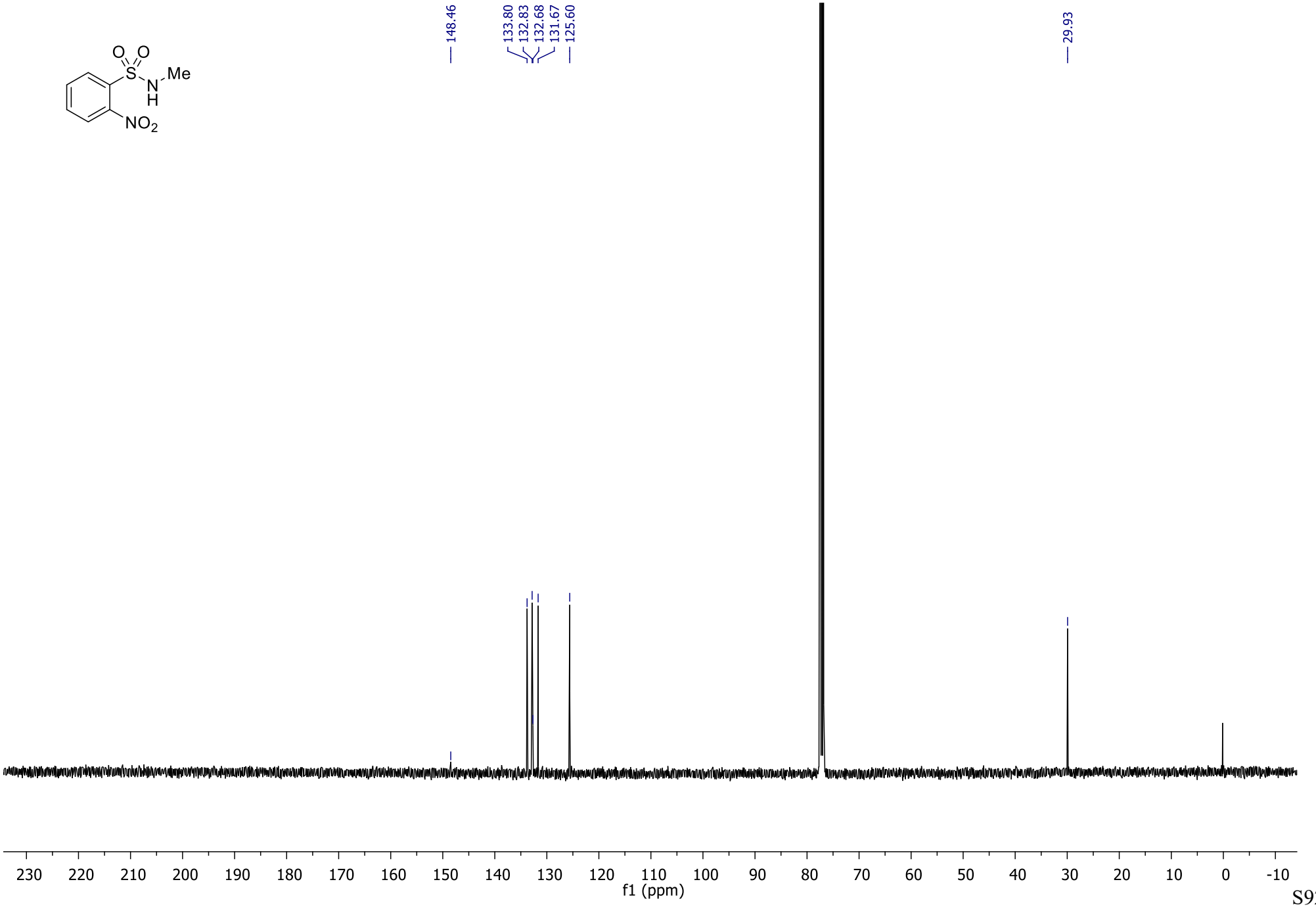
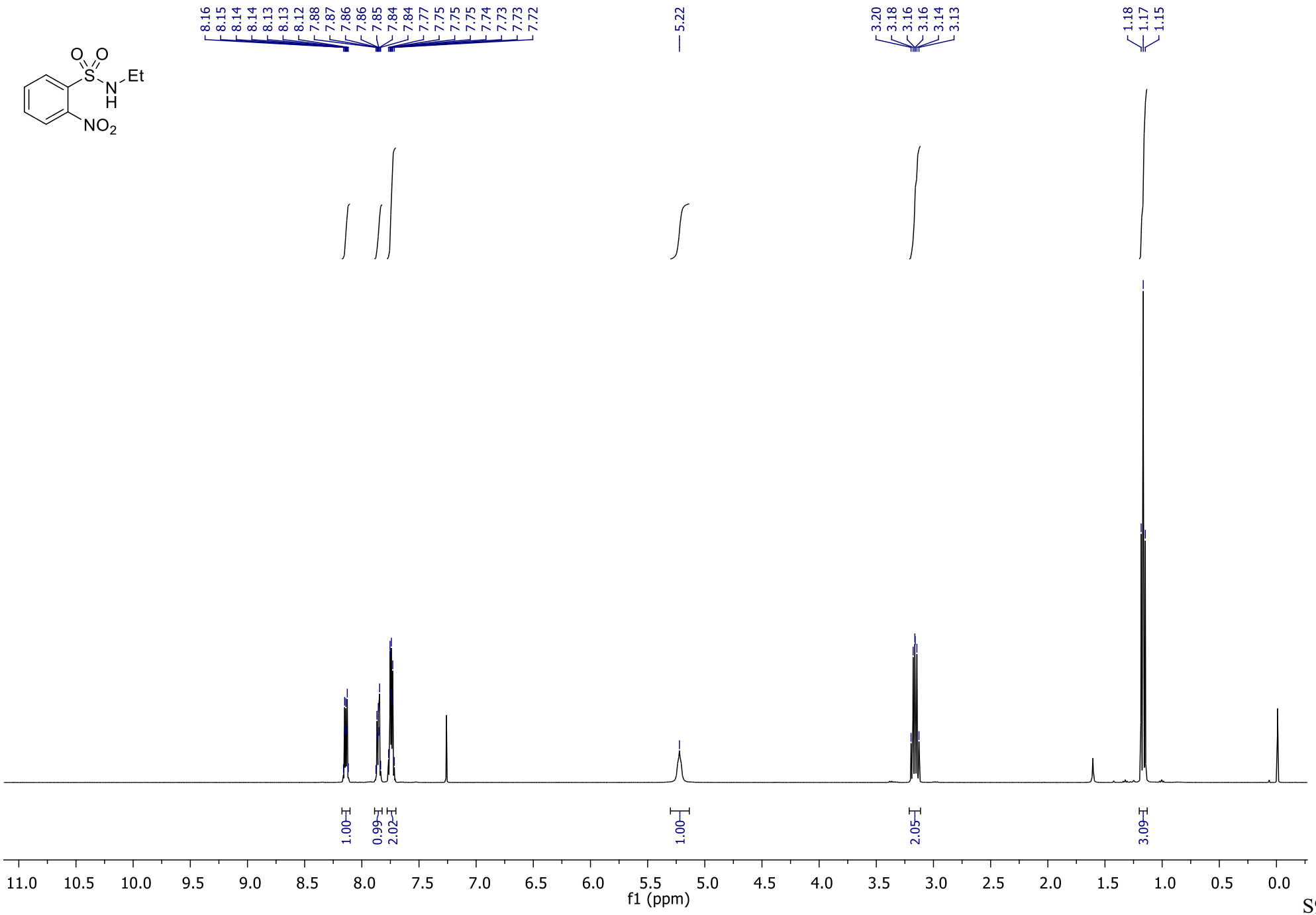
7.88
7.87
7.87
7.86
7.85
7.78
7.77
7.77
7.76
7.76
7.75
7.75
7.74
7.73
5.22
2.80
2.79
O
O
S
N
H
Me
NO2
1.00
1.00
2.00
1.19
3.01
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


148.46
133.80
132.83
132.68
131.67
125.60
29.93
O
O
S
N
H
Me
NO2
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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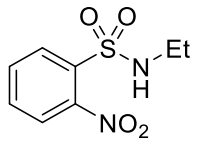
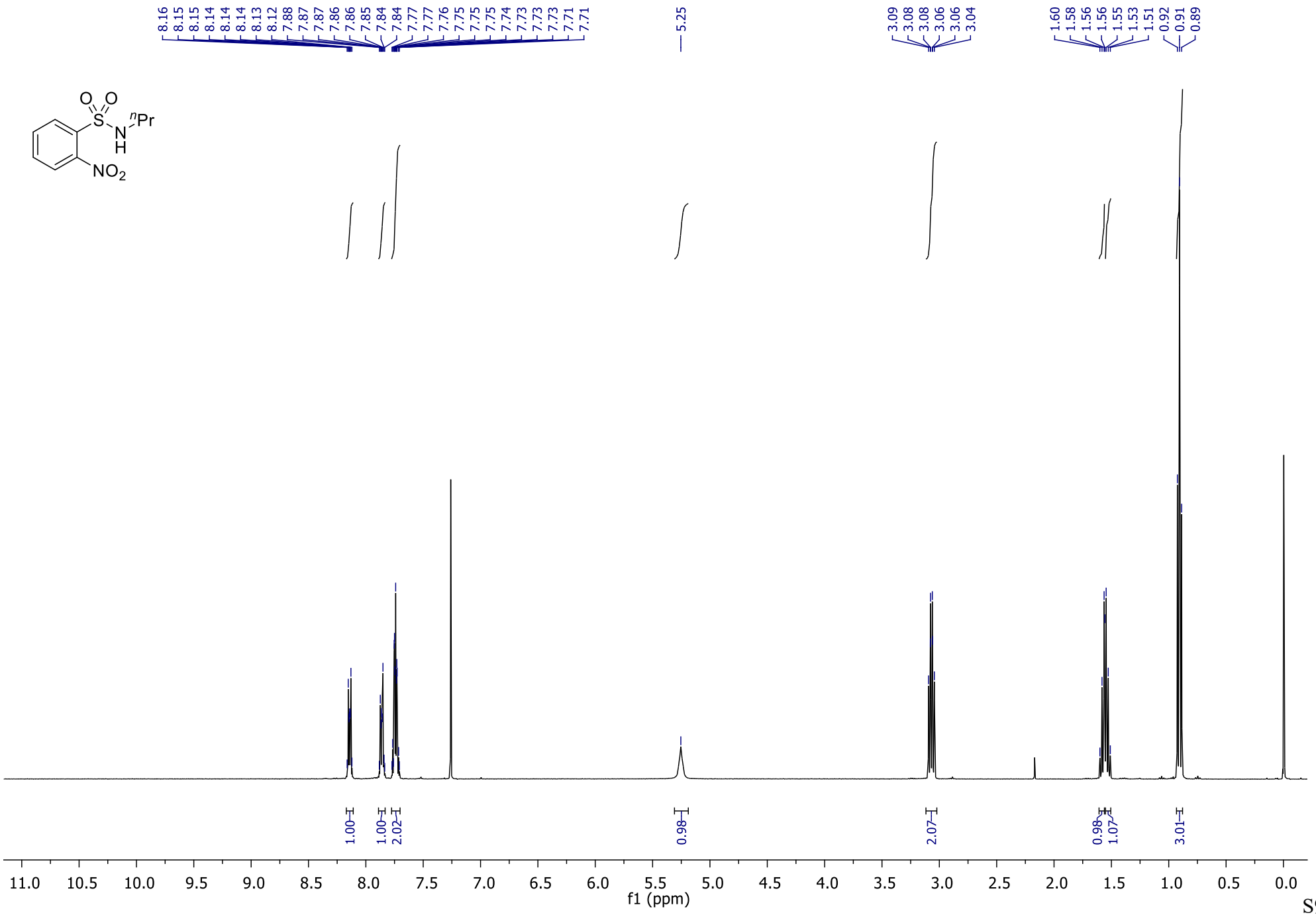
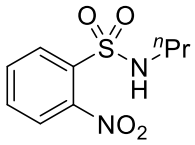
8.14
8.13
8.13
8.12
7.88
7.87
7.86
7.86
7.85
7.84
7.84
7.77
7.75
7.75
7.75
7.74
7.73
7.73
7.72
5.22
3.20
3.18
3.16
3.16
3.14
3.13
1.18
1.17
1.15
O
O
S
N
H
Et
NO2
1.00
0.99
2.02
1.00
2.05
3.09
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
Et
H
NO2

148.23
133.91
133.69
132.91
131.22
125.51
39.04
15.26
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.16 8.15 8.15 8.14 8.14 8.14 8.13 8.12 7.88 7.87 7.87 7.86 7.86 7.85 7.84 7.84 7.77 7.77 7.76 7.75 7.75 7.75 7.74 7.73 7.73 7.73 7.71 7.71
5.25
3.09 3.08 3.08 3.06 3.06 3.04
1.60 1.58 1.56 1.56 1.55 1.53 1.51 0.92 0.91 0.89
O O
S
N
H
nPr
NO2
1.00 1.00 2.02 0.98 2.07 0.98 1.07 3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



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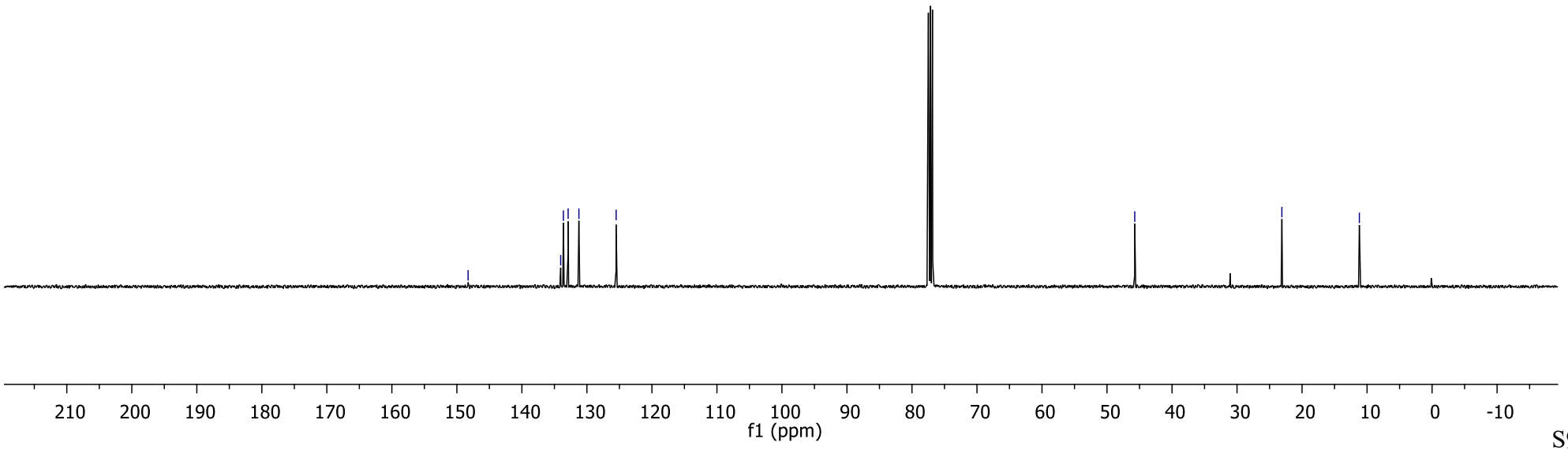
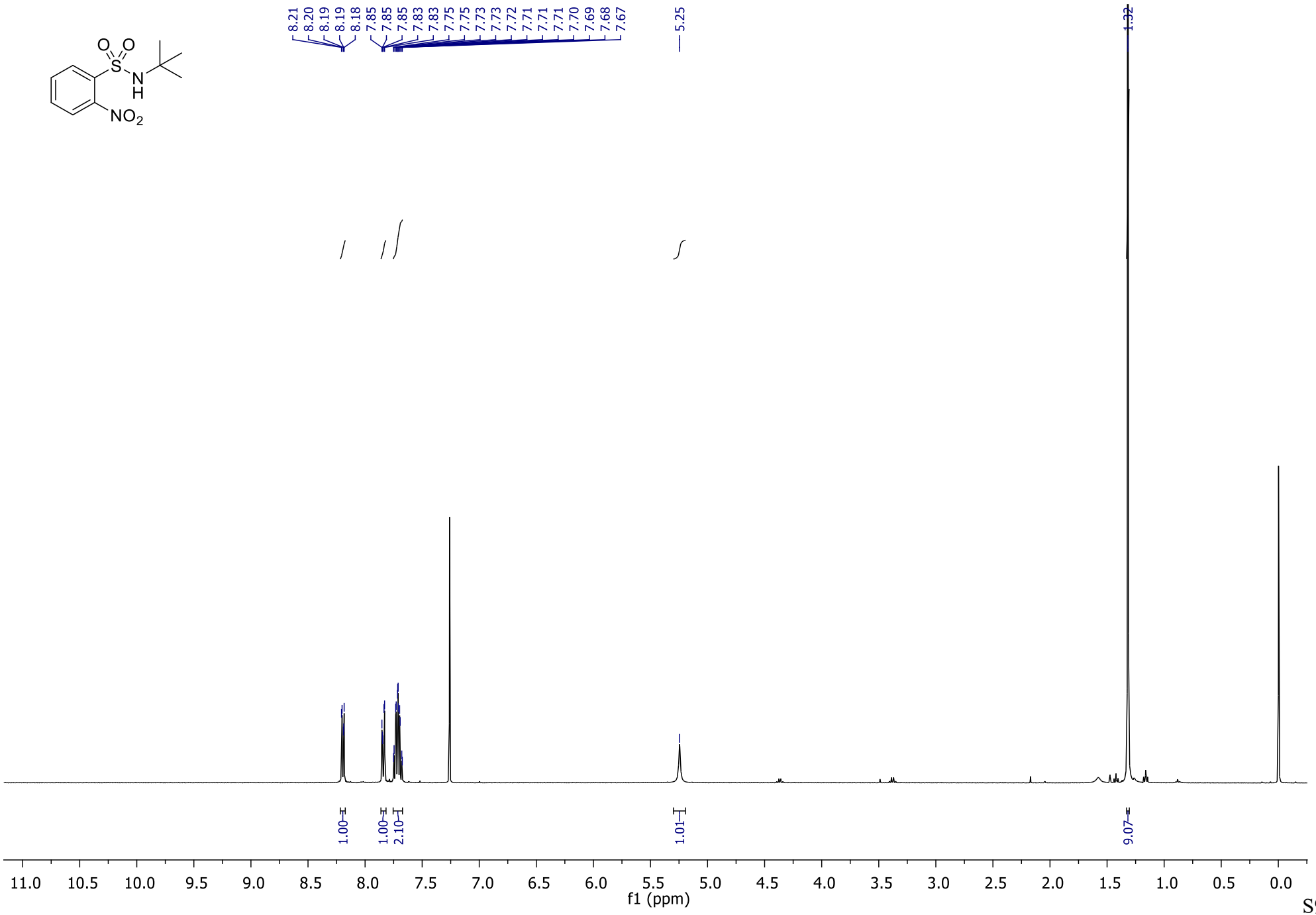
133.61
132.88
131.23
125.50
45.73
23.10
11.19

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8.19
8.18
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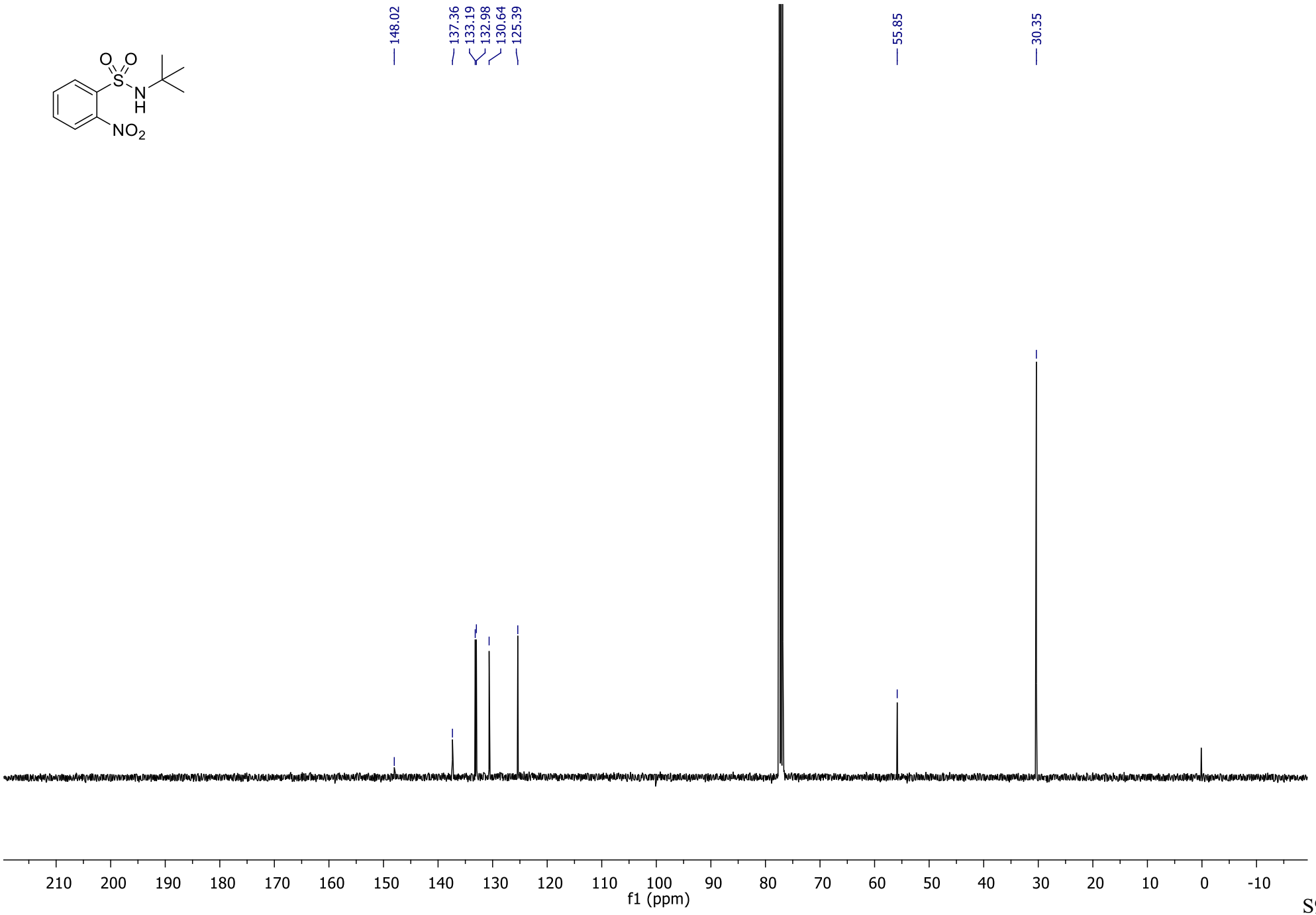
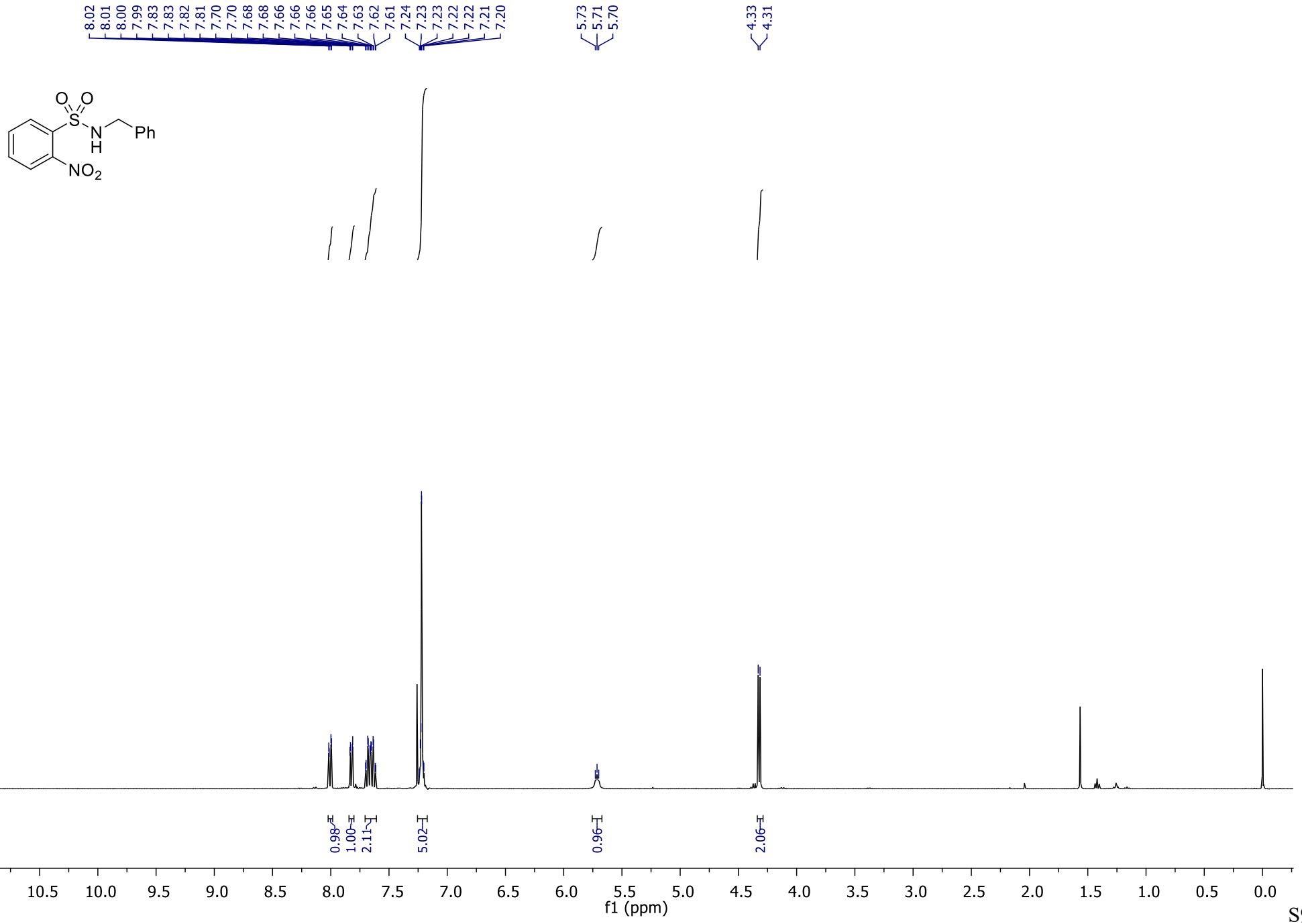
7.85
7.85
7.83
7.83
7.75
7.75
7.73
7.73
7.72
7.71
7.71
7.71
7.70
7.69
7.68
7.67
5.25
1.32
1.00
1.00
2.10
1.01
9.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


148.02
137.36
133.19
132.98
130.64
125.39
55.85
30.35
O
O
S
N
H
NO2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.02
8.01
8.00
7.99
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7.83
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7.81
7.70
7.70
7.68
7.68
7.66
7.66
7.66
7.65
7.64
7.63
7.62
7.61
7.24
7.23
7.23
7.22
7.22
7.21
7.20
5.73
5.71
5.70
4.33
4.31
O
O
S
N
H
Ph
NO2
0.98
1.00
2.11
5.02
0.96
2.06
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
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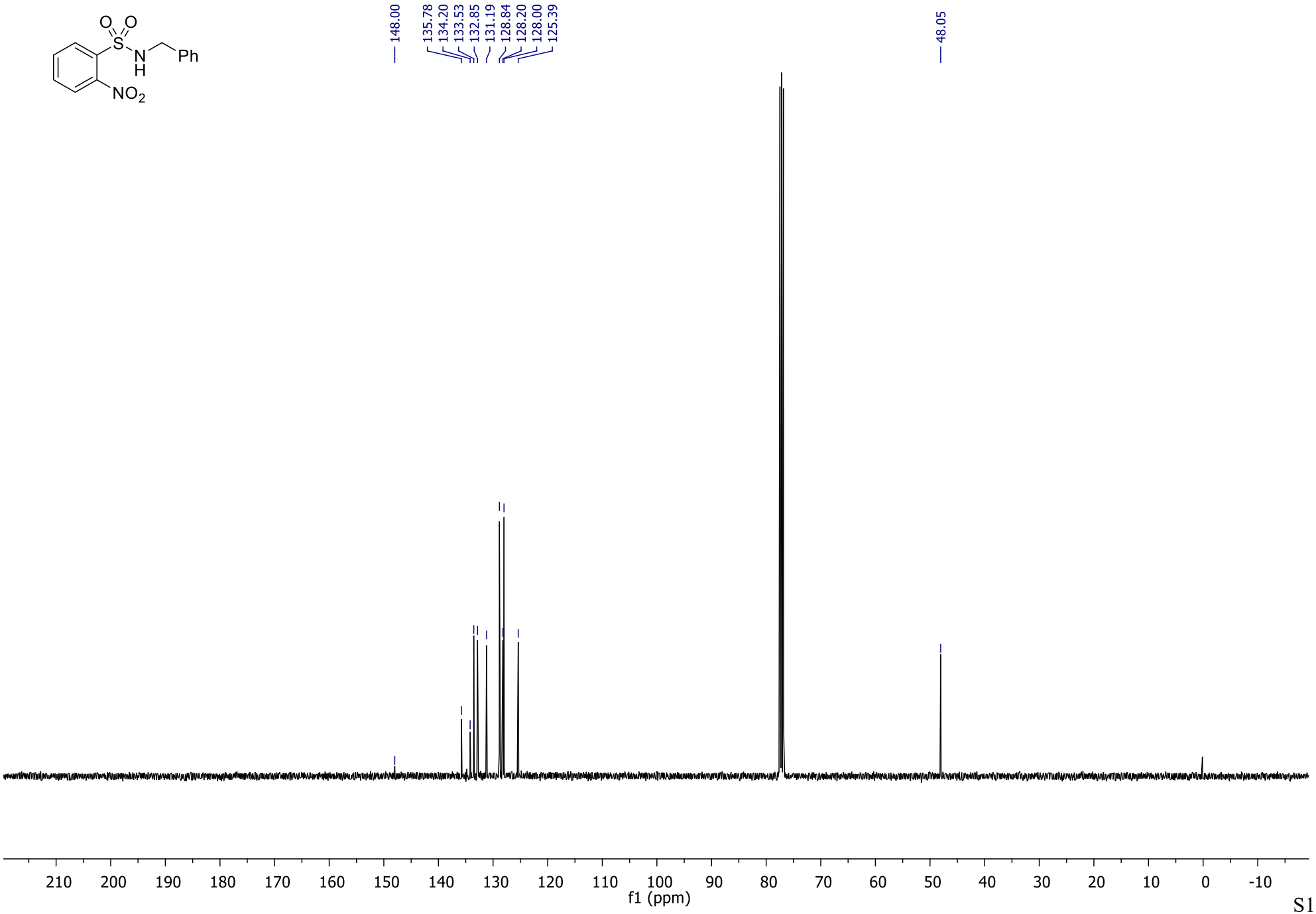
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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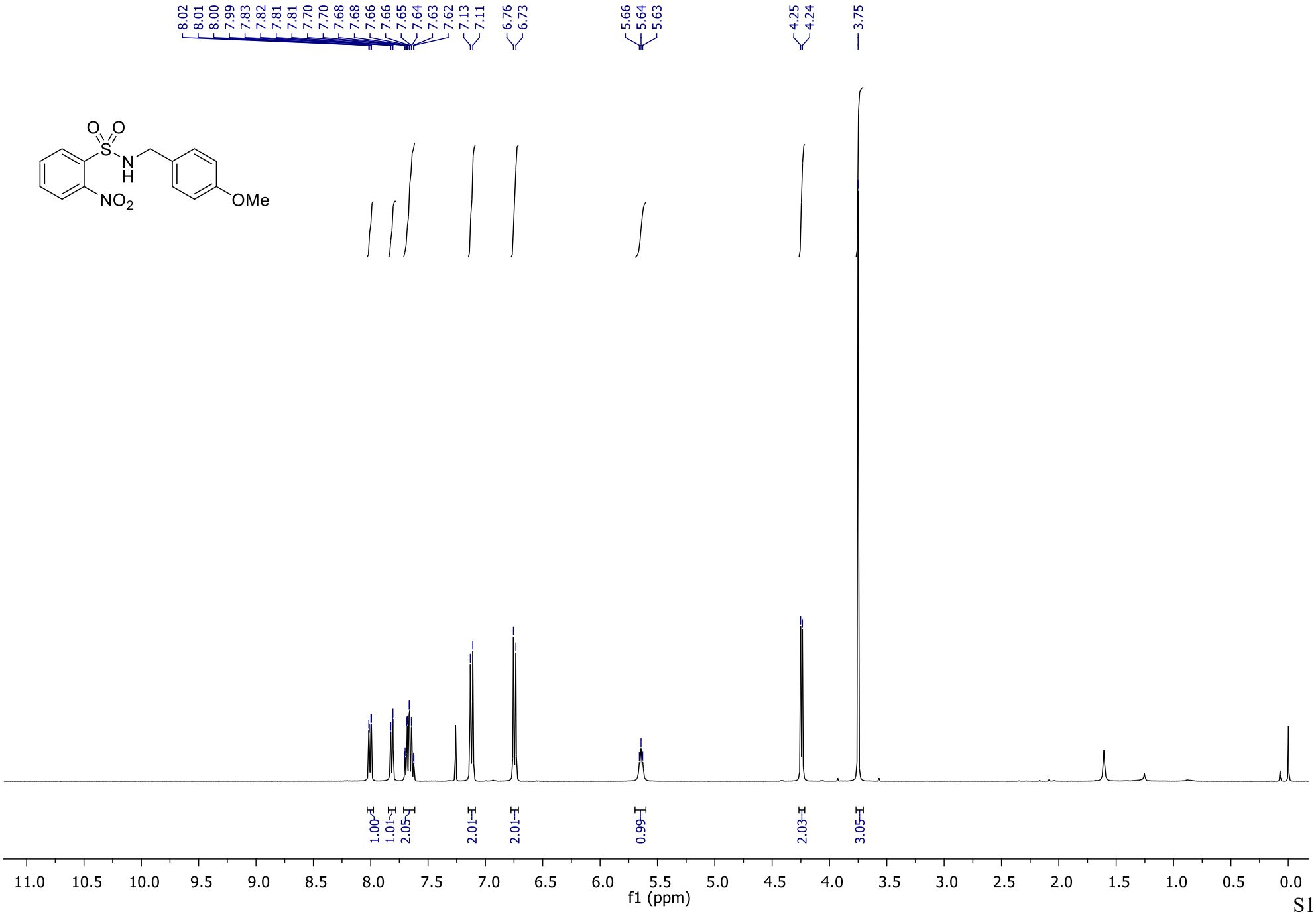
133.53
132.85
131.19
128.84
128.20
128.00
125.39
48.05
O
O
S
N
H
Ph
NO2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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8.00
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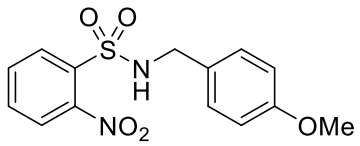
7.81
7.70
7.70
7.68
7.68
7.66
7.66
7.65
7.64
7.63
7.62
7.13
7.11
6.76
6.73
5.66
5.64
5.63
4.25
4.24
3.75
O
O
S
N
H
NO2
OMe
1.00
1.01
2.05
2.01
2.01
0.99
2.03
3.05
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



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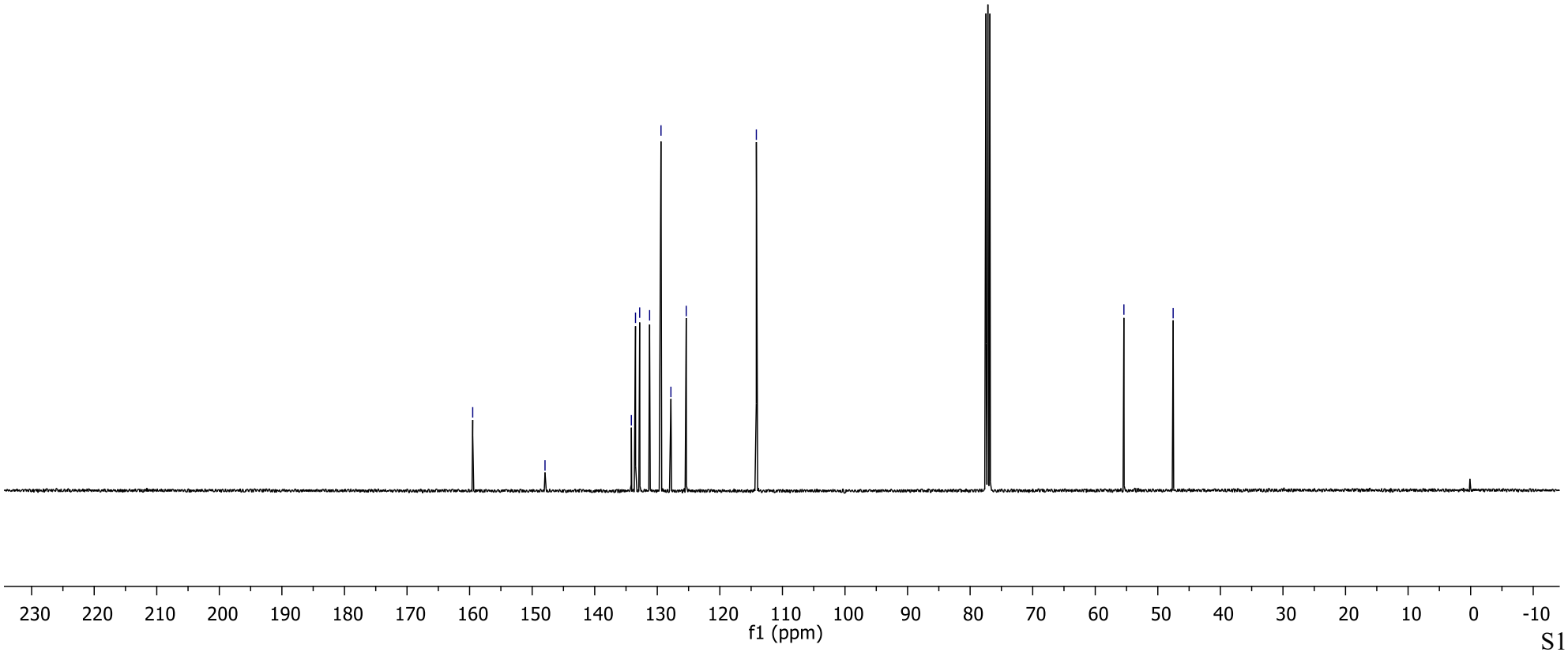
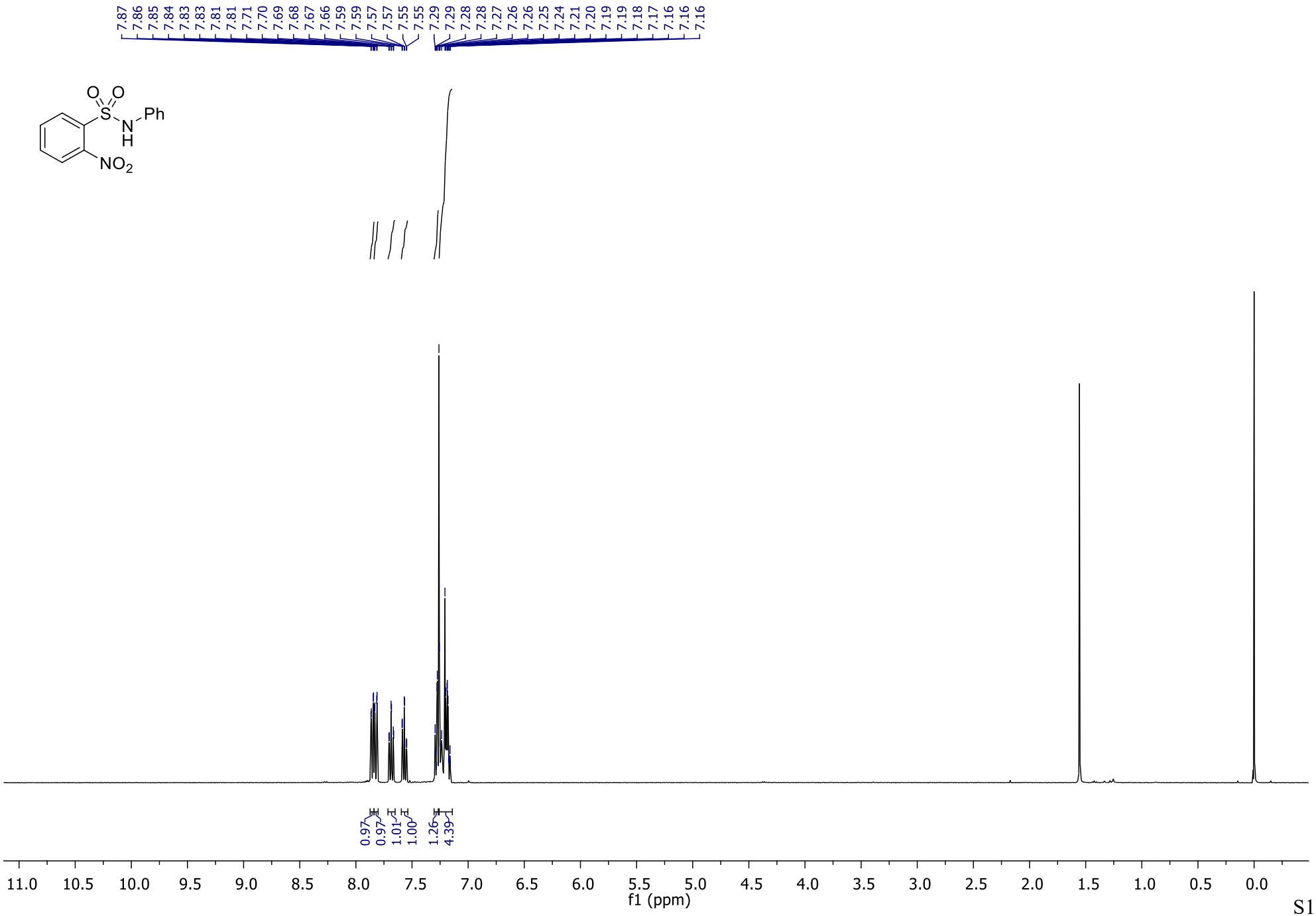
129.41
127.82
125.37
114.17
55.42
47.55

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7.86
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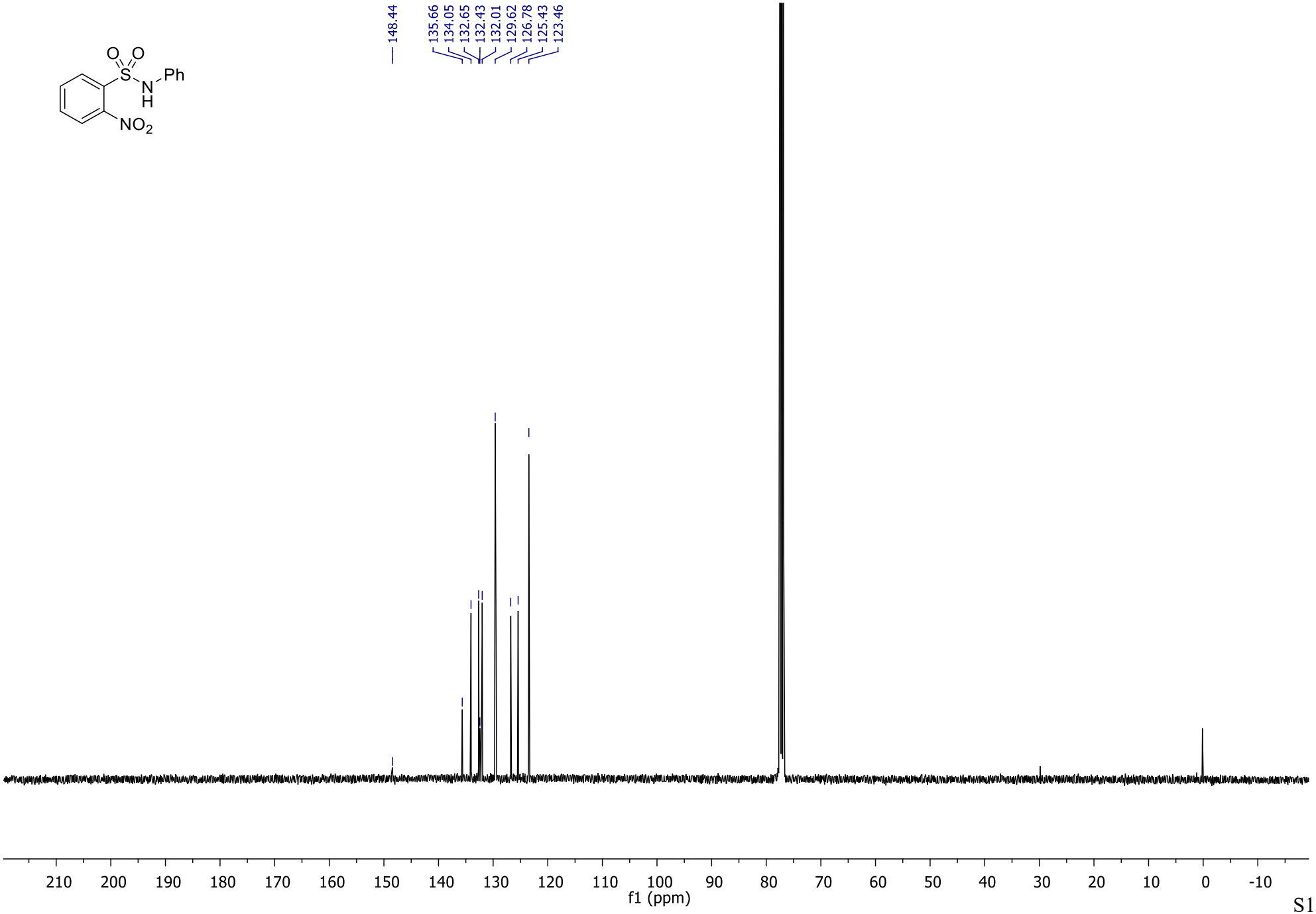
7.83
7.83
7.81
7.81
7.71
7.70
7.69
7.68
7.67
7.66
7.59
7.59
7.57
7.57
7.55
7.55
7.29
7.29
7.28
7.28
7.27
7.26
7.26
7.25
7.24
7.21
7.20
7.19
7.19
7.18
7.17
7.16
7.16
7.16
O
O
S
N
H
Ph
NO2
0.97
0.97
1.01
1.00
1.26
4.39
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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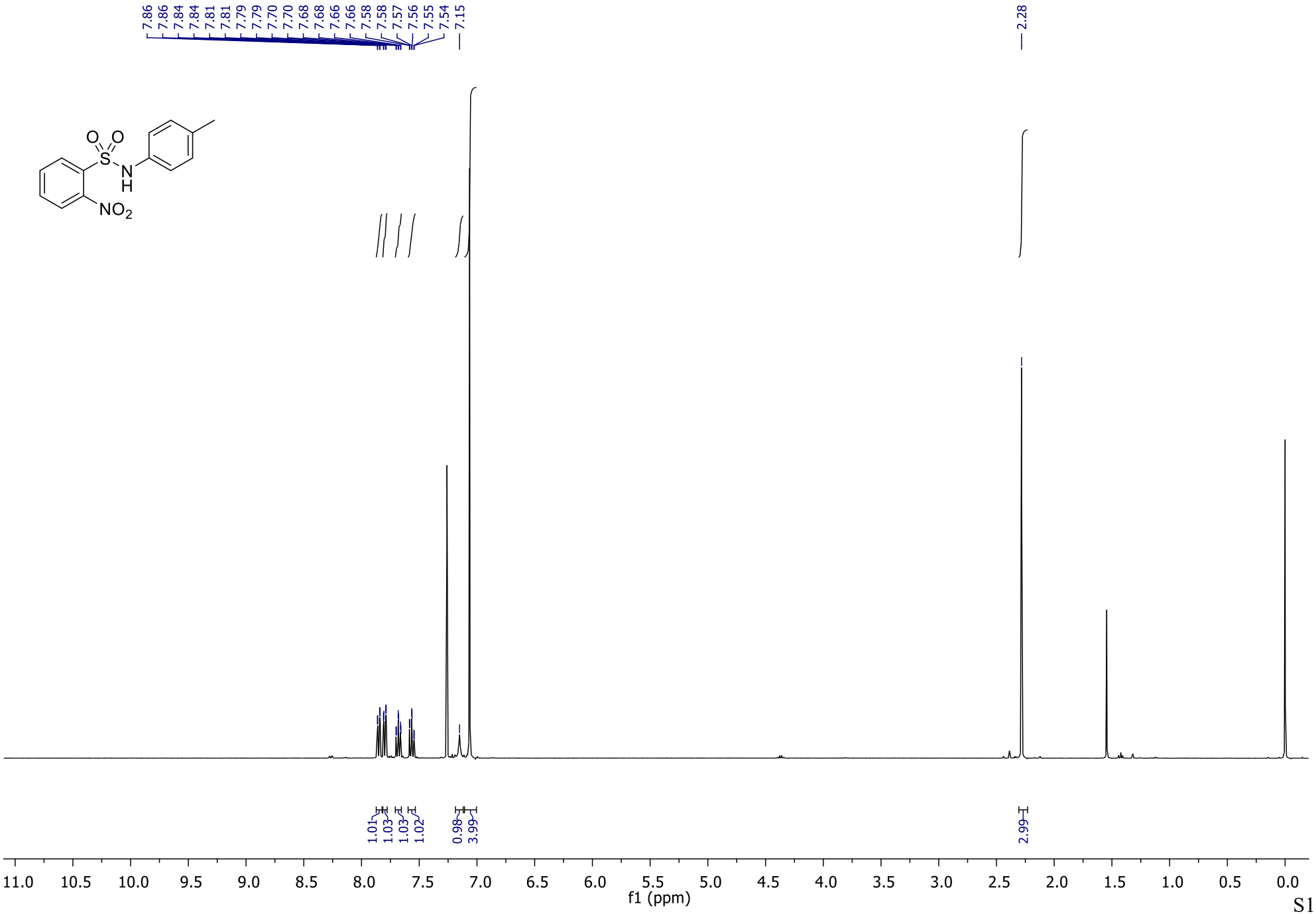
132.01
129.62
126.78
125.43
123.46
O
O
S
N
H
Ph
NO2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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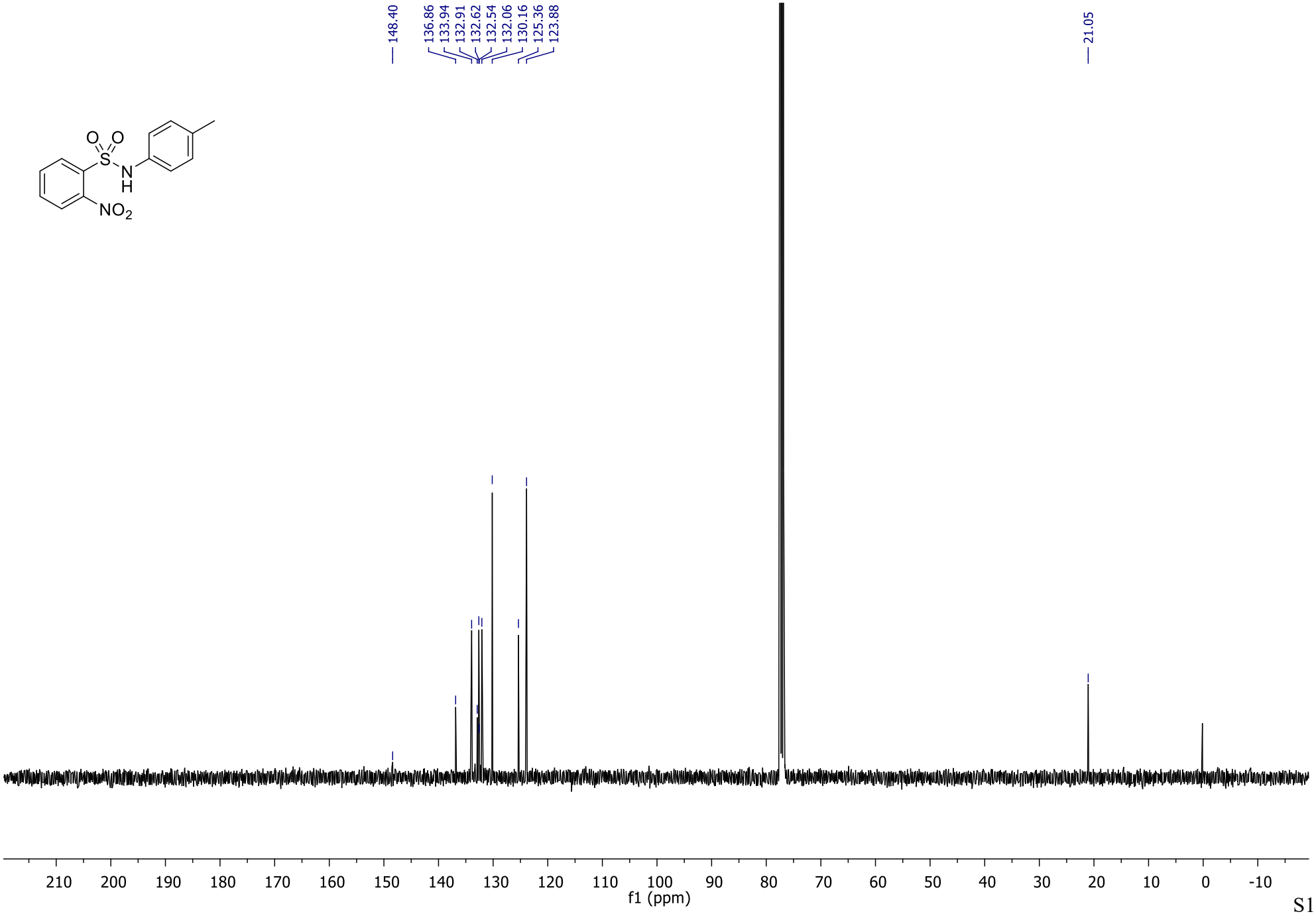
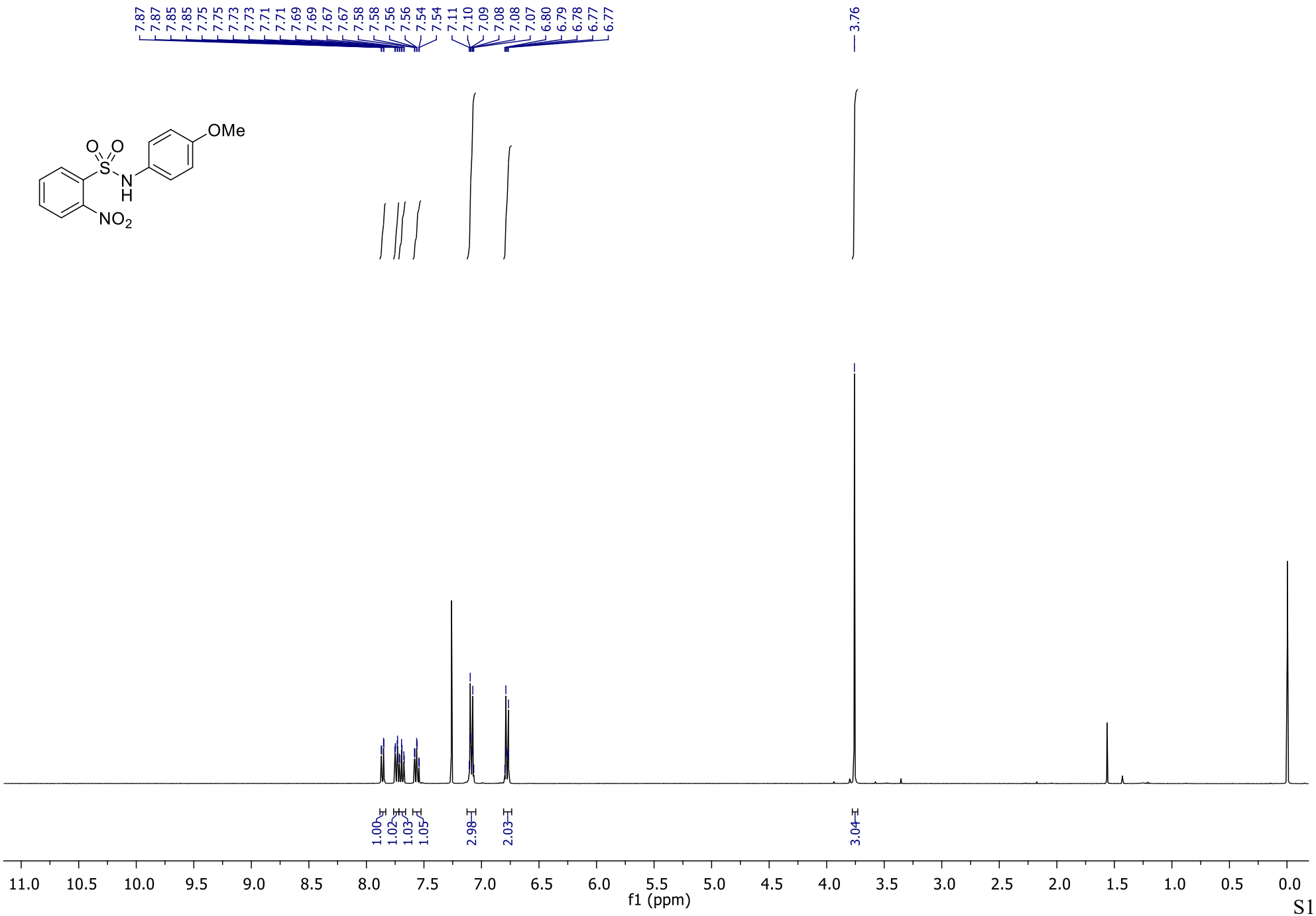
7.86
7.84
7.84
7.81
7.81
7.79
7.79
7.70
7.70
7.68
7.68
7.66
7.66
7.58
7.58
7.57
7.56
7.55
7.54
7.15
2.28
O
O
S
N
H
NO2
1.01
1.03
1.03
1.02
0.98
3.99
2.99
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


148.40
136.86
133.94
132.91
132.62
132.54
132.06
130.16
125.36
123.88
21.05
O
O
S
N
H
NO2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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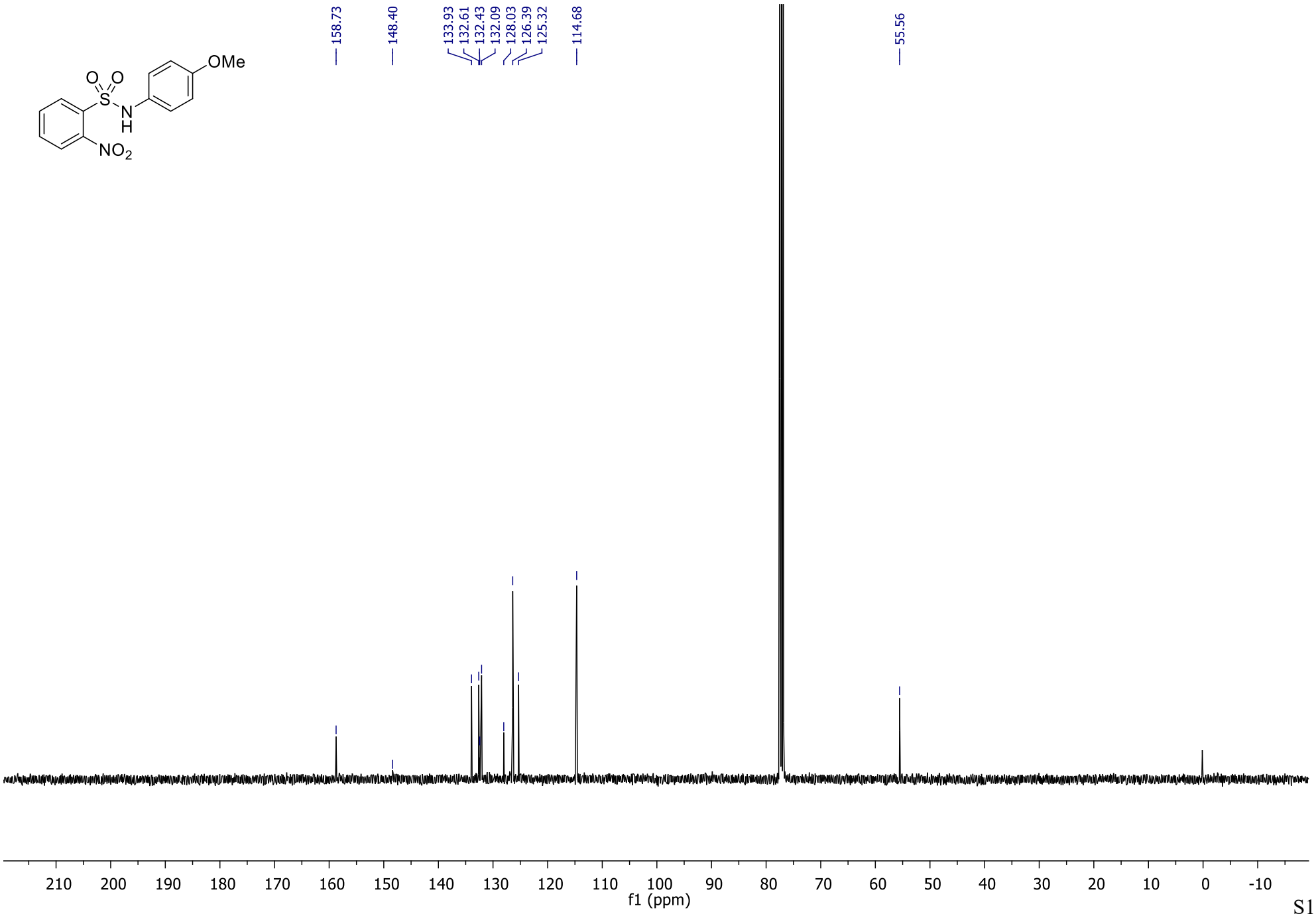
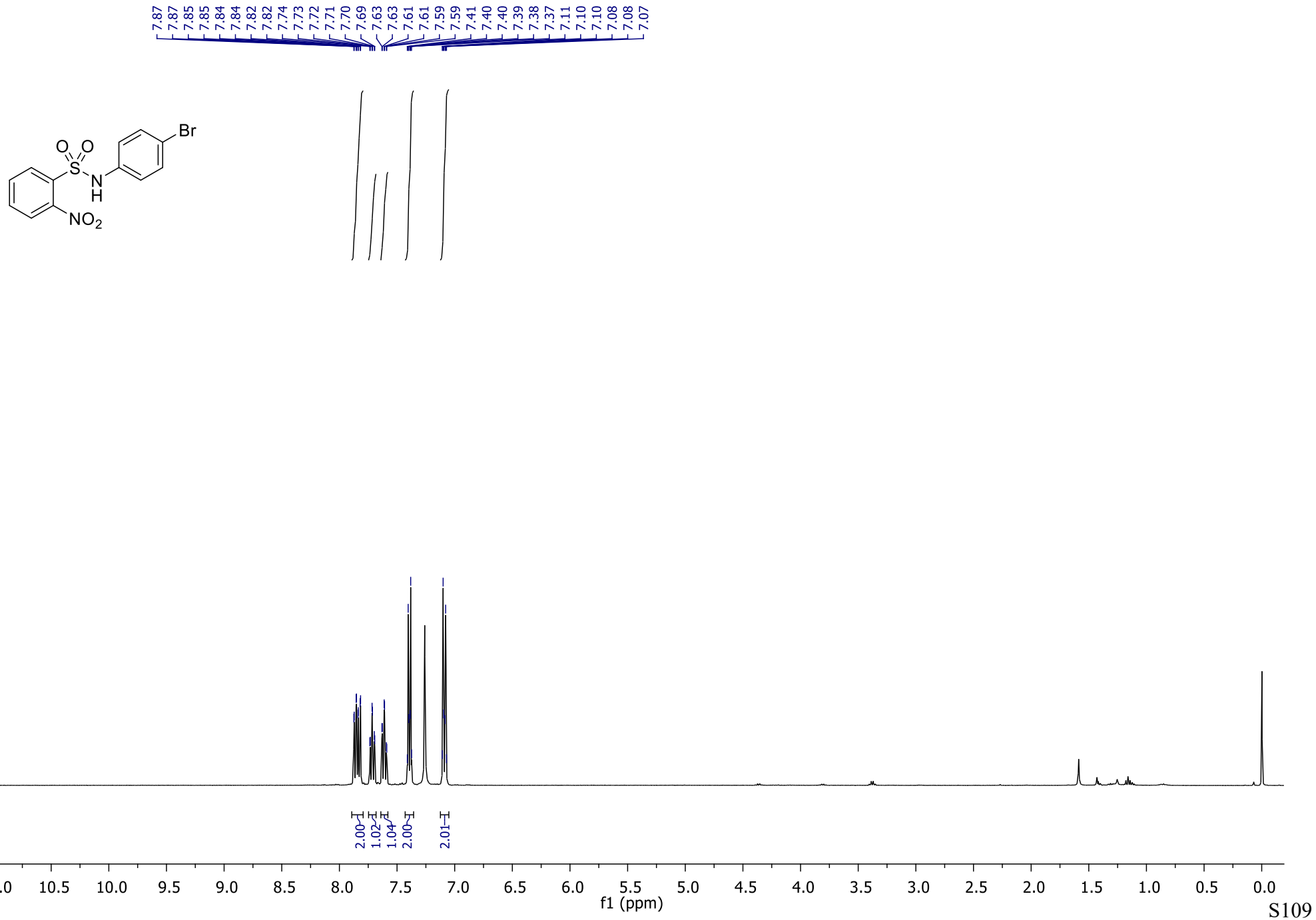
7.87
7.85
7.85
7.75
7.75
7.73
7.73
7.71
7.71
7.69
7.69
7.67
7.67
7.58
7.58
7.56
7.56
7.54
7.54
7.11
7.10
7.09
7.08
7.08
7.07
6.80
6.79
6.78
6.77
6.77
3.76
OMe
O
O
S
N
H
NO2
1.00
1.02
1.03
1.05
2.98
2.03
3.04
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


158.73
148.40
133.93
132.61
132.43
132.09
128.03
126.39
125.32
114.68
55.56
OMe
O
O
S
N
H
NO2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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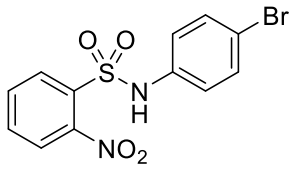
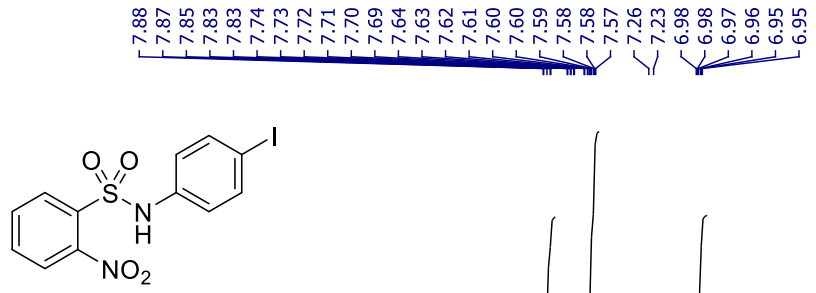
7.87
7.85
7.85
7.84
7.84
7.82
7.82
7.74
7.73
7.72
7.71
7.70
7.69
7.63
7.63
7.61
7.61
7.59
7.59
7.41
7.40
7.40
7.39
7.38
7.37
7.11
7.10
7.10
7.08
7.08
7.07
Br
O
O
S
N
H
NO2
2.00
1.02
1.04
2.00
2.01
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
H
Br
NO2

148.36
134.75
134.32
132.86
132.74
132.09
131.98
125.55
125.00
120.28
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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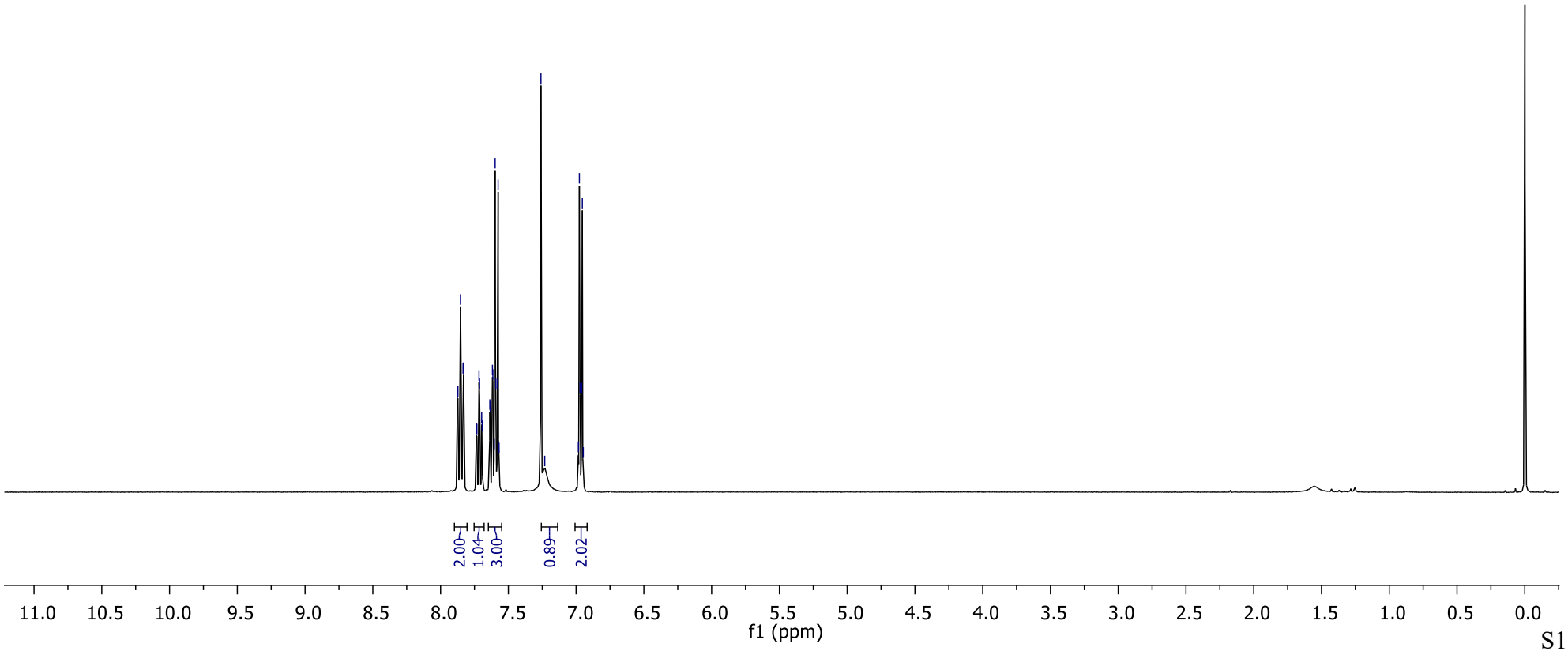
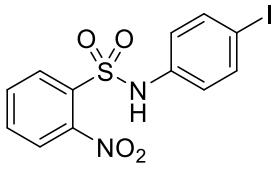
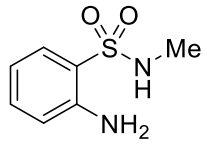
7.83
7.74
7.73
7.72
7.71
7.70
7.69
7.64
7.63
7.62
7.61
7.60
7.60
7.59
7.58
7.58
7.57
7.26
7.23
6.98
6.98
6.97
6.96
6.95
6.95
O
O
S
N
H
NO2
I


2.00
1.04
3.00
0.89
2.02
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
H
I
NO2

148.37
138.71
135.52
134.31
132.88
132.15
132.00
125.57
125.07
91.20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
O
S
N
H
Me
NH2

8a

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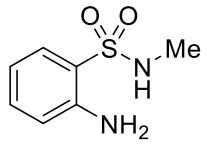
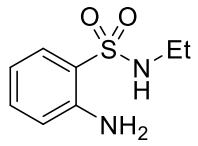
7.33
6.84
6.84
6.82
6.82
6.82
6.80
6.80
6.78
6.78
6.76
6.76
4.85
4.66
2.58
2.57
1.00
1.01
2.02
3.00
3.04
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
Me
H
NH2

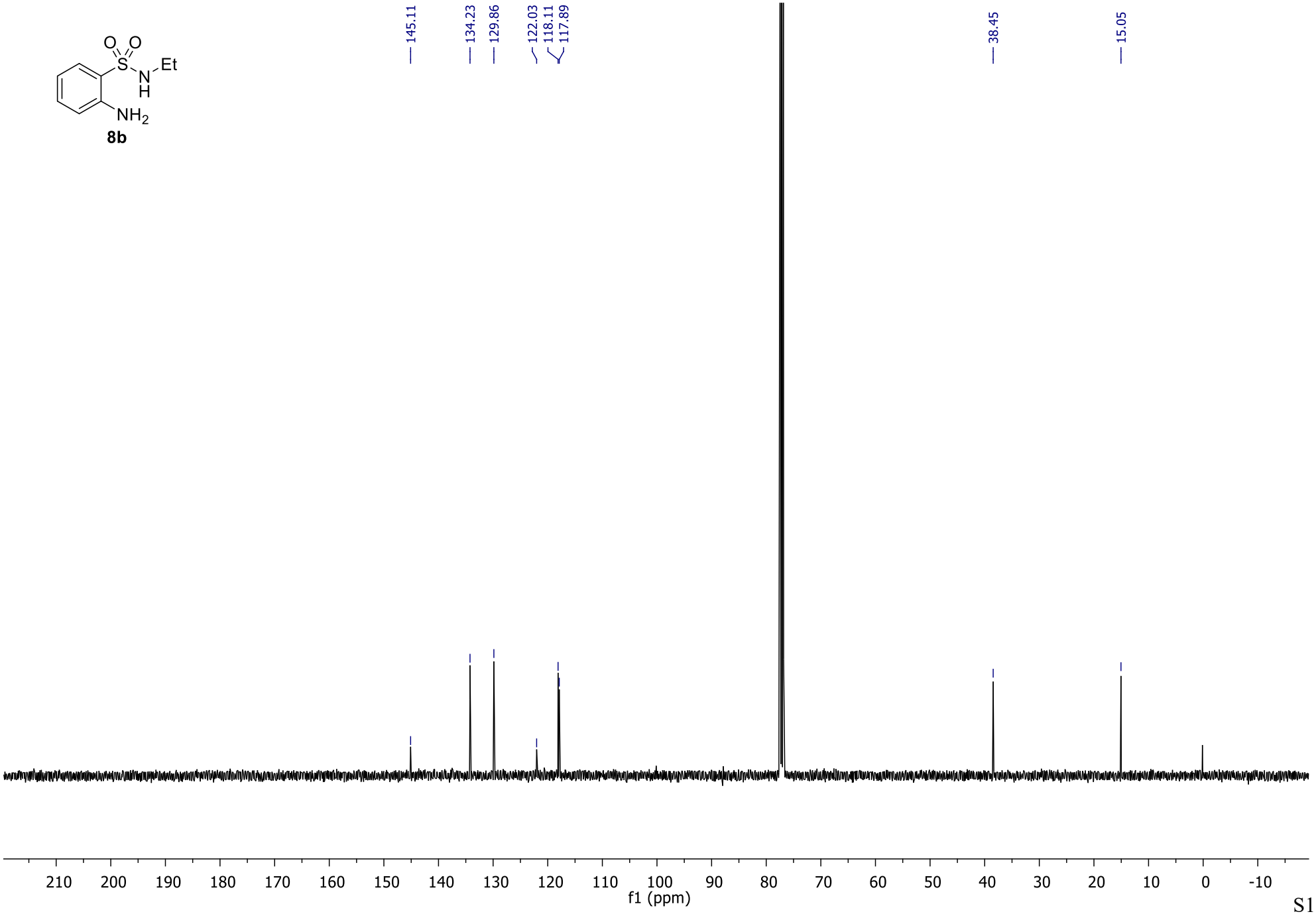
8a

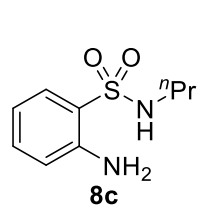
145.23
134.35
130.17
120.68
118.06
117.92
29.54
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
O
S
N
H
Et
NH2

8b

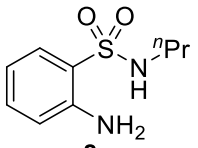
7.73
7.72
7.71
7.70
7.33
7.33
6.83
6.82
6.81
6.80
6.79
6.78
6.77
6.76
6.75
4.82
4.61
2.97
2.96
2.95
2.94
2.93
2.92
2.92
2.90
1.09
1.07
1.05
1.00
1.02
1.03
1.02
1.89
1.11
2.08
3.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
H
Et
NH2
8b
145.11
134.23
129.86
122.03
118.11
117.89
38.45
15.05
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
O
S
N
H
nPr
NH2

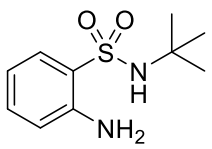
8c

7.70
7.70
7.68
7.68
7.30
7.28
7.26
6.80
6.78
6.77
6.75
4.90
4.88
2.84
2.82
2.81
2.79
1.44
1.42
0.83
1.01
0.99
2.00
3.01
2.11
2.11
3.09
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
H
nPr
NH2

8c

145.12
134.14
129.71
121.73
117.84
117.83
45.05
22.80
11.15
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
O
S
N
H
NH2

8d

7.75
7.74
7.73
7.72
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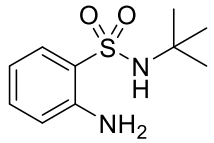
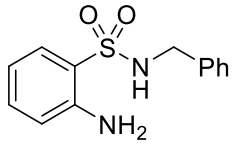
7.27
7.26
6.81
6.81
6.79
6.77
6.77
6.74
6.72
4.85
4.81
1.18
1.00
1.00
2.09
3.01
9.37
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
H
NH2

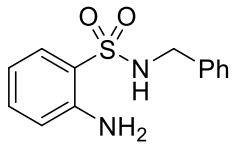
8d

144.87
133.82
129.40
125.28
118.03
117.80
54.75
30.04
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
O
S
N
H
Ph
NH2

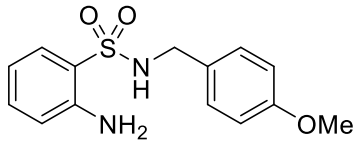
8e

7.75
7.75
7.73
7.73
7.26
7.26
7.20
6.84
6.84
6.82
6.80
6.80
6.78
6.78
6.76
6.76
4.96
4.84
4.06
4.04
0.92
0.98
1.02
2.43
1.89
1.00
0.96
1.06
1.82
1.98
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
H
Ph
NH2

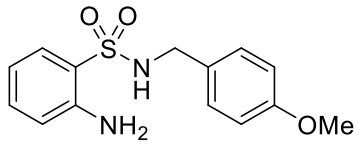
8e

145.16
136.36
134.39
129.94
128.82
128.05
128.02
121.82
118.18
117.93
47.49
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
O
S
N
H
NH2
OMe

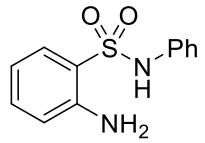
8f

7.75
7.74
7.73
7.73
7.36
7.34
7.34
7.32
7.32
7.10
7.08
7.08
6.84
6.84
6.82
6.80
6.80
6.78
6.76
6.76
4.88
4.87
4.85
4.83
3.99
3.97
3.79
3.77
1.00
1.01
1.99
4.01
3.01
1.99
3.10
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
H
NH2
OMe

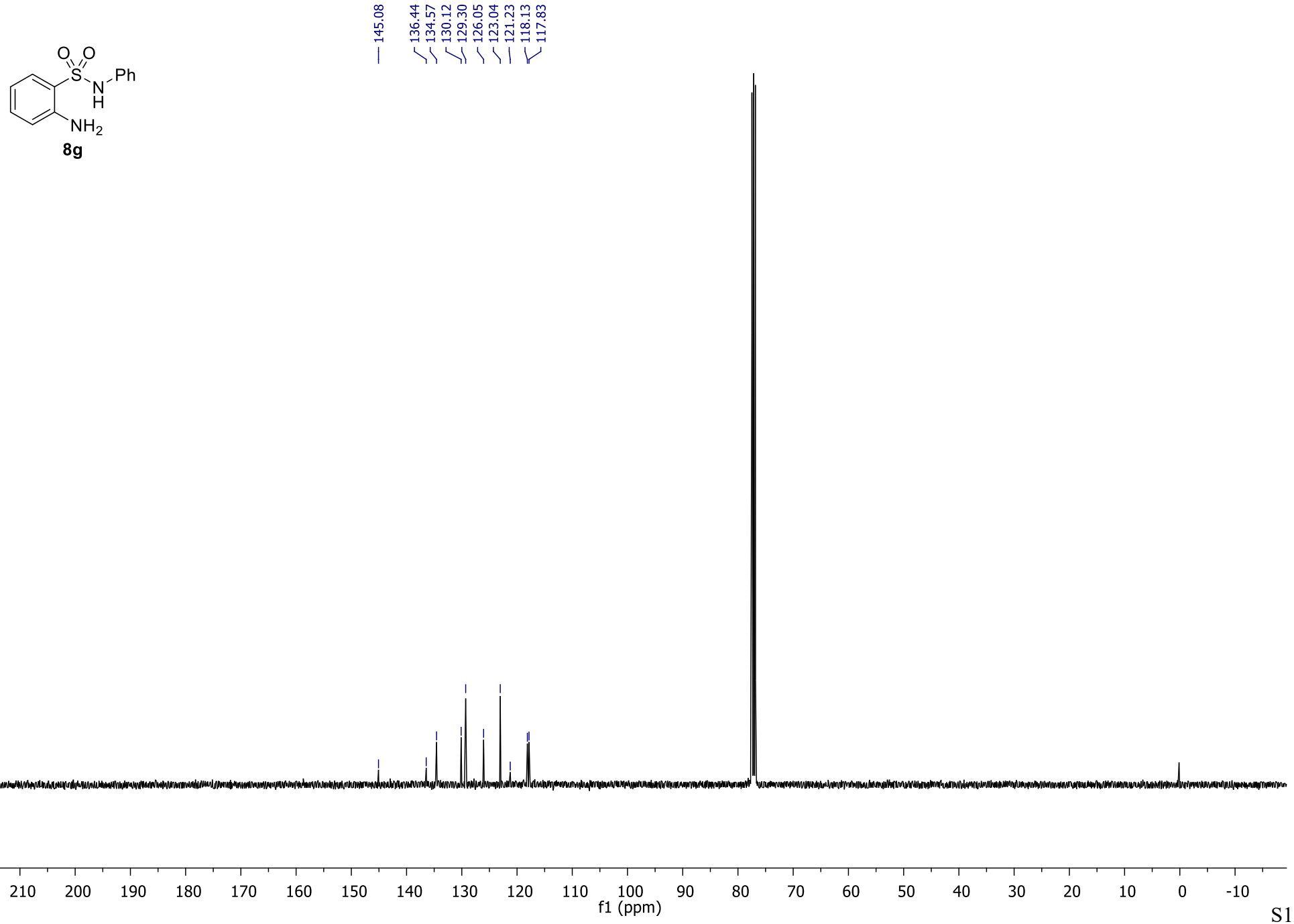
8f

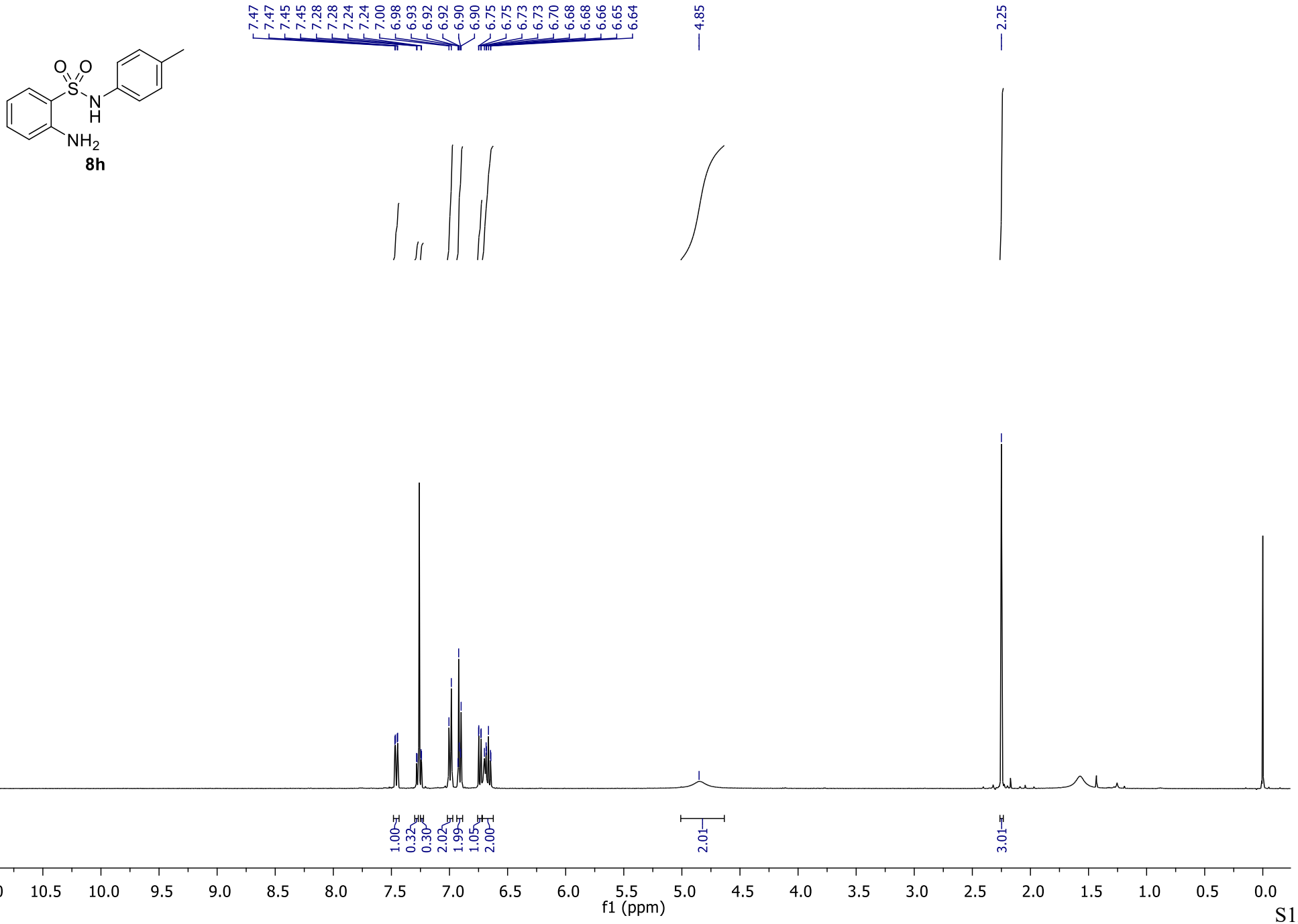
159.44
145.14
134.35
129.96
129.42
128.36
121.82
118.14
117.89
114.19
55.43
47.01
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

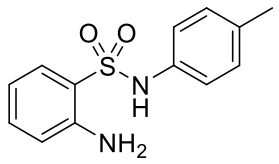

O
O
S
N
Ph
H
NH2

8g

7.50
7.49
7.48
7.47
7.28
7.28
7.26
7.24
7.24
7.22
7.20
7.19
7.18
7.13
7.12
7.12
7.10
7.05
7.05
7.04
7.03
6.77
6.75
6.75
6.73
6.72
6.69
6.68
6.67
6.65
6.65
4.86
0.98
0.37
0.41
1.96
1.05
1.93
1.94
1.00
1.96
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

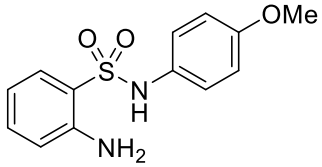

145.08
136.44
134.57
130.12
129.30
126.05
123.04
121.23
118.13
117.83
O
O
S
N
H
Ph
NH2
8g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.47
7.47
7.45
7.45
7.28
7.28
7.24
7.24
7.00
6.98
6.93
6.92
6.92
6.90
6.90
6.75
6.75
6.73
6.73
6.70
6.68
6.68
6.66
6.65
6.64
4.85
2.25
O
O
S
N
H
NH2
8h
1.00
0.32
0.30
2.02
1.99
1.05
2.00
2.01
3.01
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
H
NH2

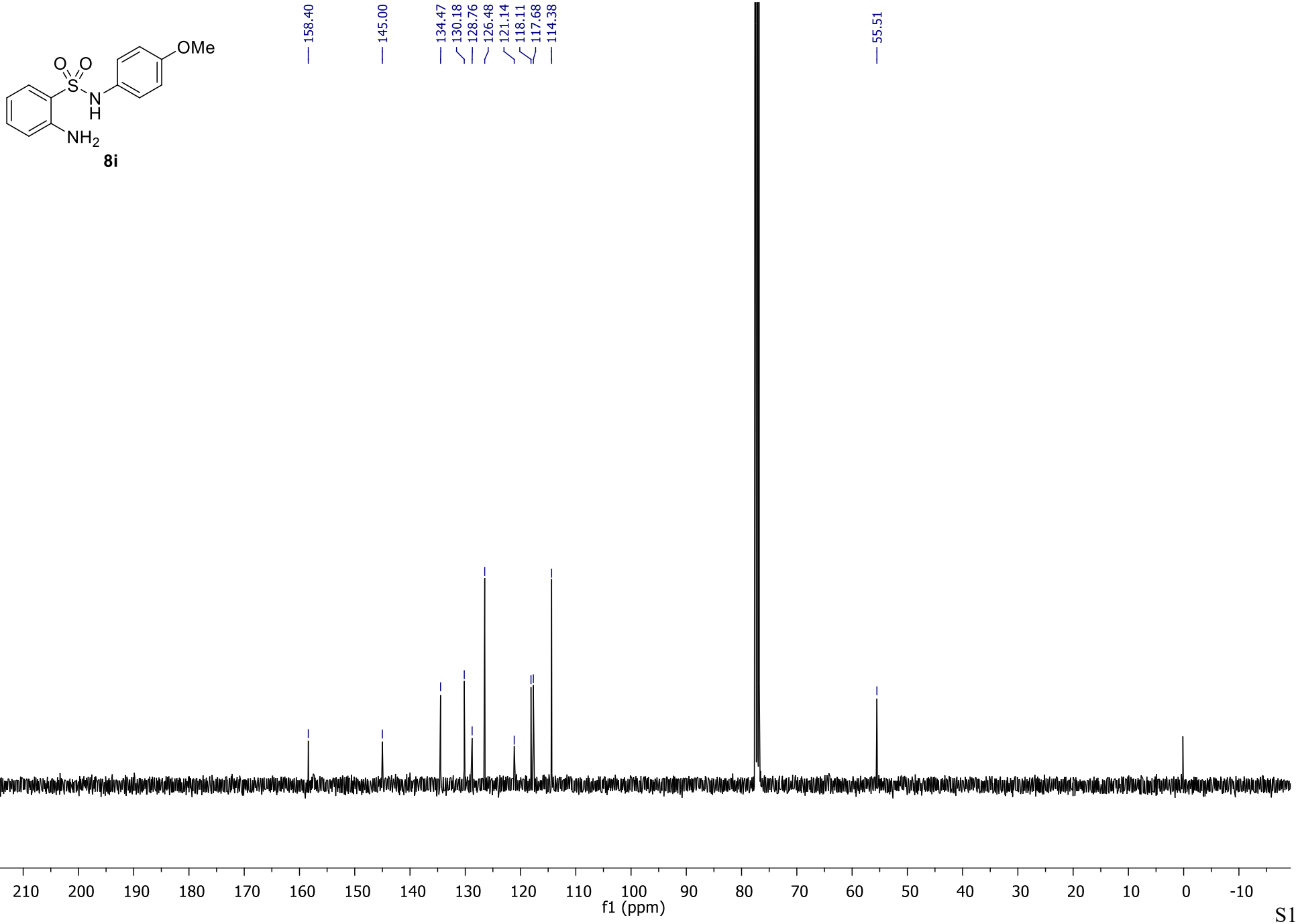
8h

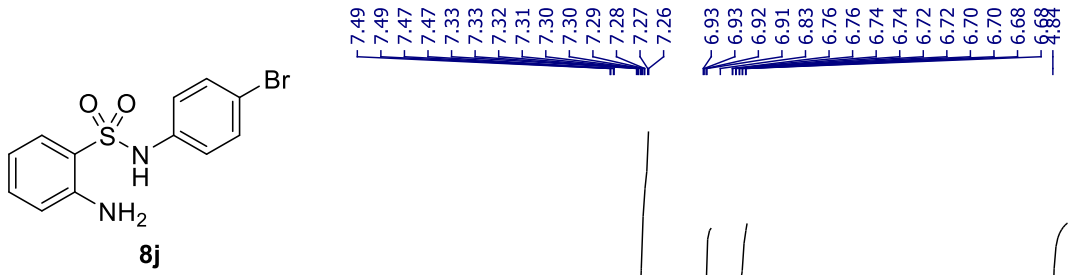
145.06
136.11
134.47
133.66
130.16
129.85
123.64
121.34
118.09
117.77
21.02
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OMe
O
O
S
N
H
NH2

8i

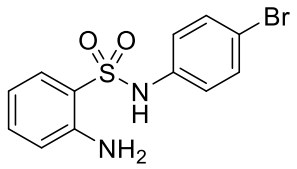
7.41
7.41
7.39
7.39
7.30
7.29
7.27
6.94
6.94
6.93
6.92
6.76
6.74
6.72
6.72
6.71
6.70
6.68
6.68
6.66
6.64
6.64
6.59
4.84
3.73
1.00
0.89
0.26
2.02
3.04
1.06
0.93
2.02
3.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


158.40
145.00
134.47
130.18
128.76
126.48
121.14
118.11
117.68
114.38
55.51
OMe
O
O
S
N
H
NH2
8i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Br
O
O
S
N
H
NH2

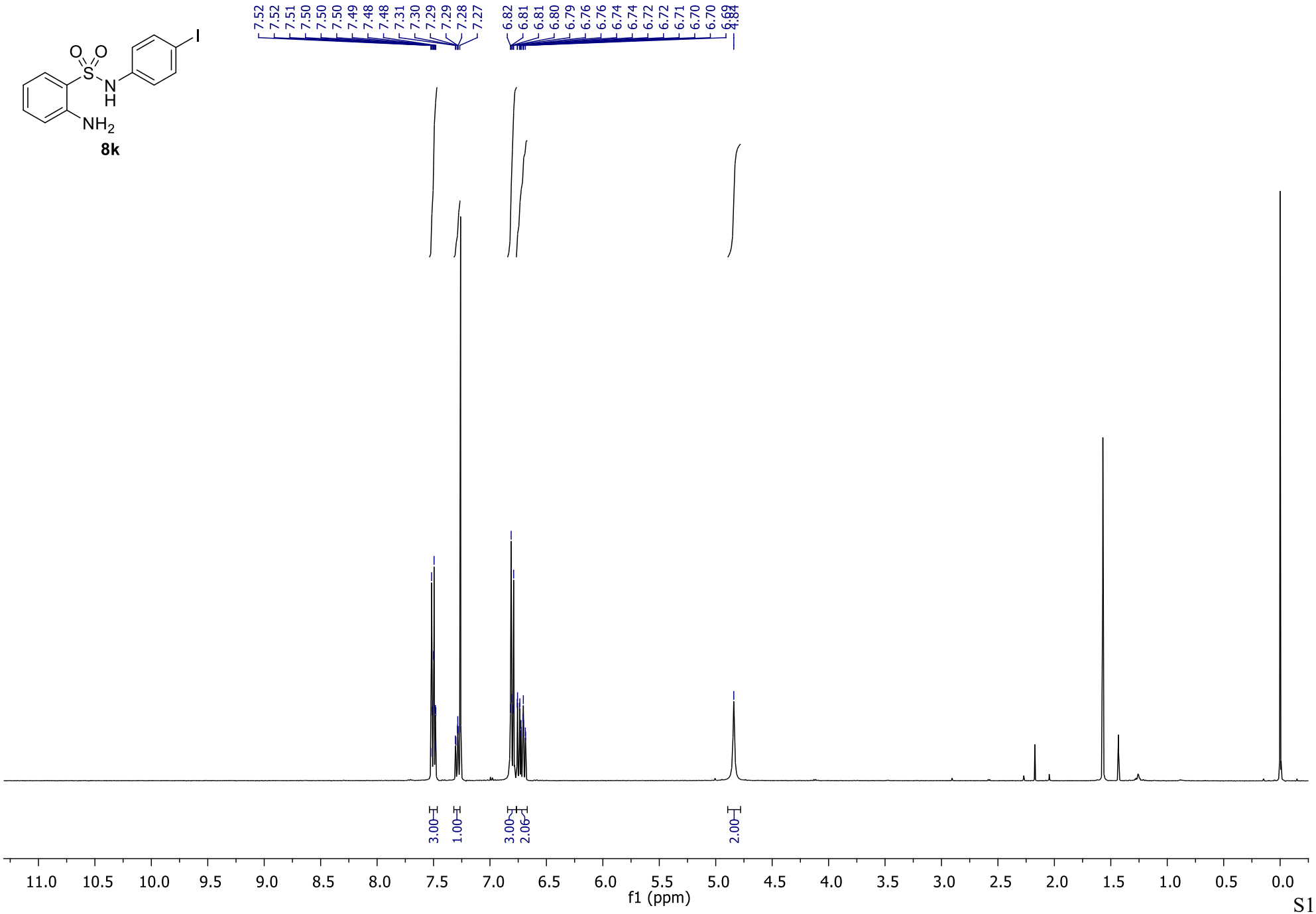
8j

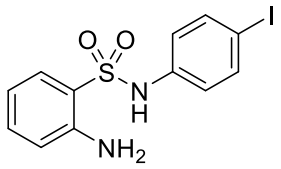
7.49
7.49
7.47
7.47
7.33
7.33
7.32
7.31
7.30
7.30
7.29
7.28
7.27
7.26
6.93
6.93
6.92
6.91
6.83
6.76
6.76
6.74
6.74
6.72
6.72
6.70
6.70
6.68
4.84
1.00
3.13
1.95
1.01
2.01
2.02
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
H
NH2
Br

8j

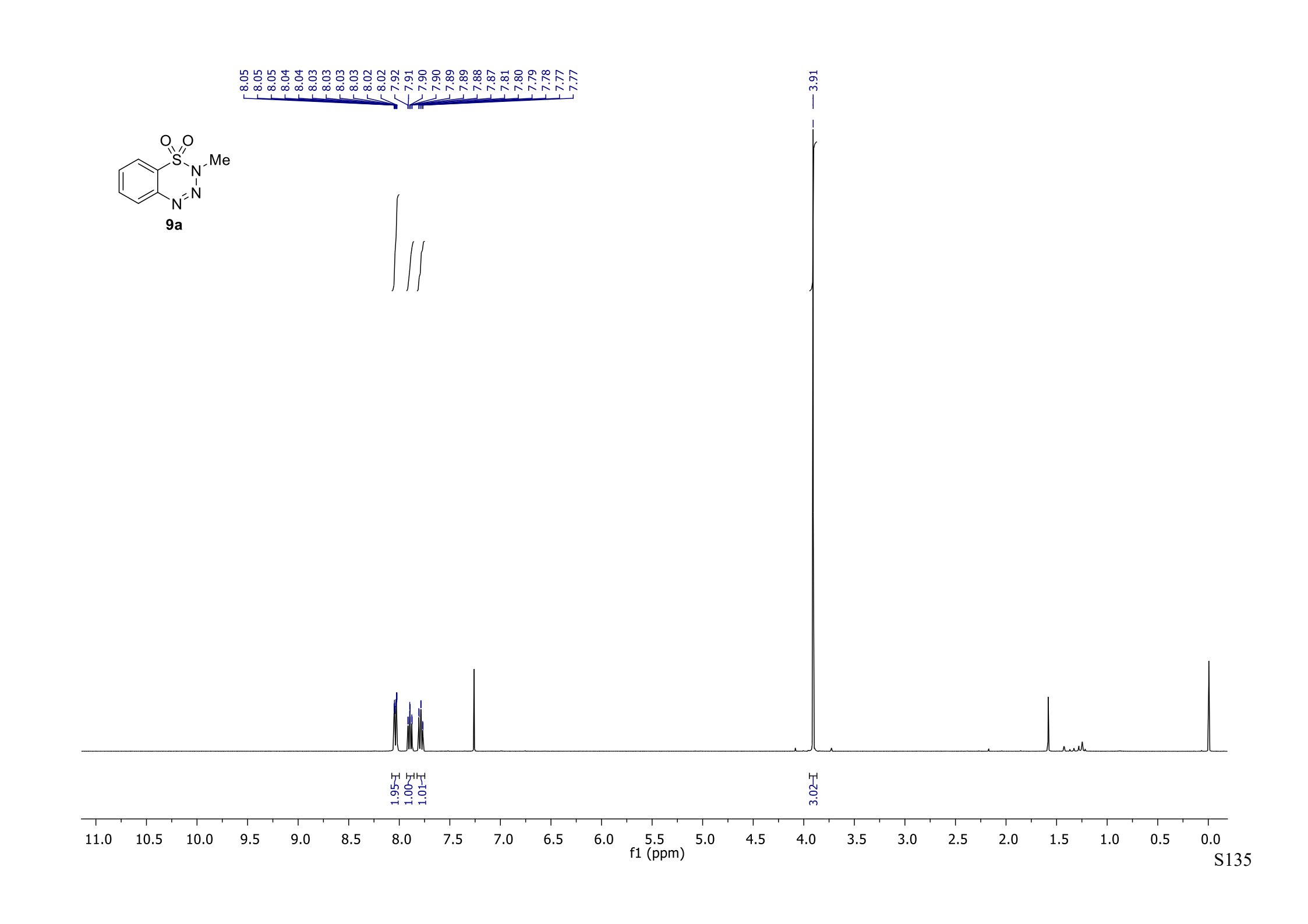
145.02
135.60
134.82
132.40
130.07
124.58
121.00
119.43
118.36
117.96
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

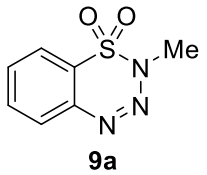

7.52
7.52
7.51
7.50
7.50
7.50
7.49
7.48
7.48
7.31
7.30
7.29
7.29
7.28
7.27
6.82
6.81
6.81
6.80
6.79
6.76
6.76
6.74
6.74
6.72
6.72
6.71
6.70
6.70
6.69
4.84
O
O
S
N
H
NH2
I
8k
3.00
1.00
3.00
2.06
2.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
H
NH2
I

8k

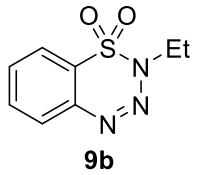
145.02
138.36
136.36
134.82
130.07
124.58
121.03
118.37
117.98
90.19
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.05
8.05
8.05
8.04
8.04
8.03
8.03
8.03
8.03
8.02
8.02
7.92
7.91
7.90
7.90
7.89
7.89
7.88
7.87
7.81
7.80
7.79
7.78
7.77
7.77
3.91
O
O
S
N
Me
N
N
9a
1.95
1.00
1.01
3.02
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
Me
N
N
N

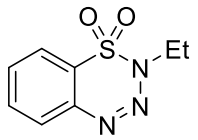
9a

141.79
134.31
132.78
129.48
125.40
120.64
33.97
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
O
S
N
Et
N
N
N

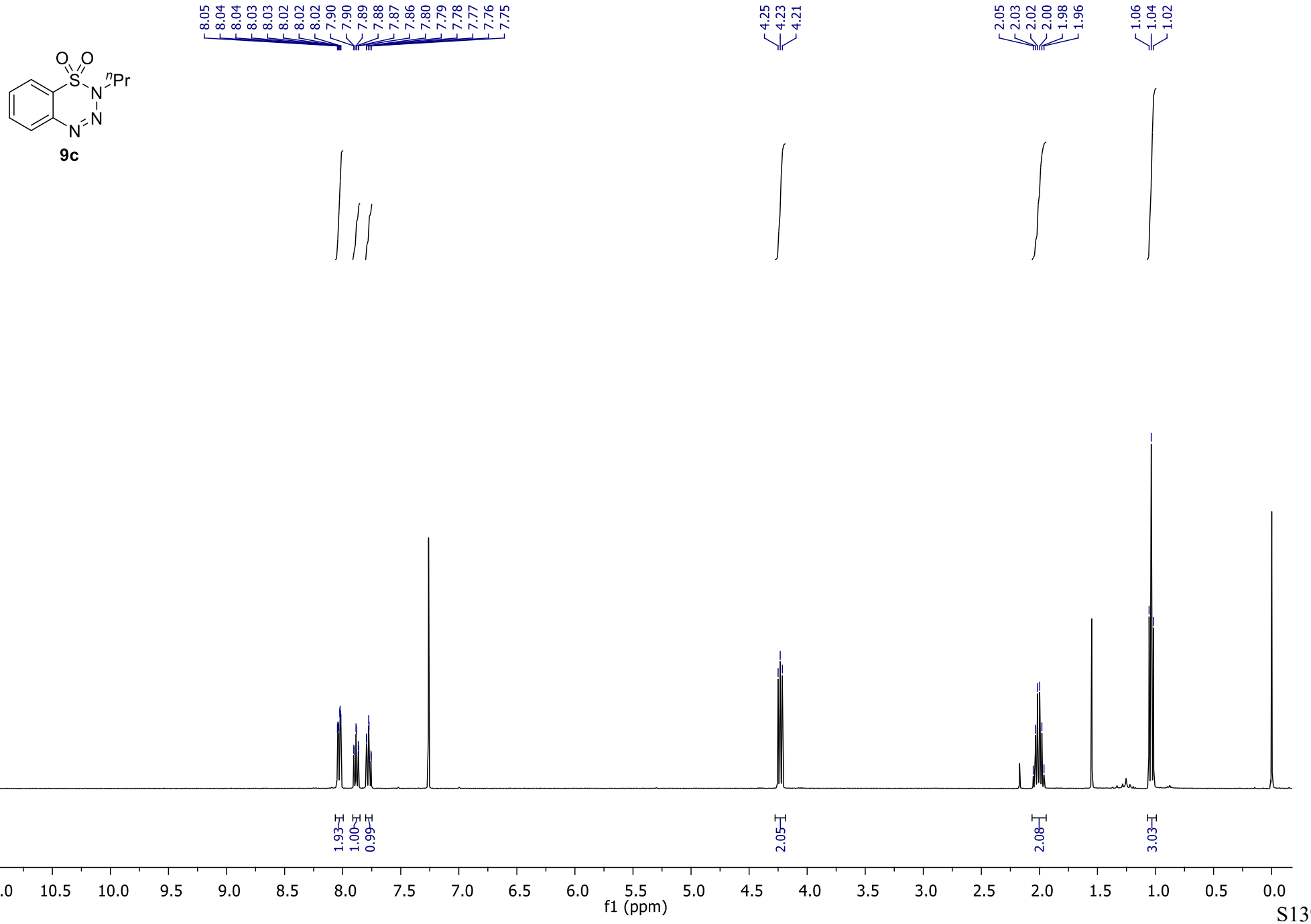
9b

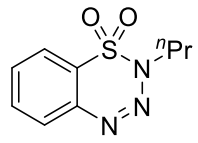
8.04
8.04
8.03
8.02
8.02
8.01
8.01
8.00
7.90
7.90
7.88
7.88
7.86
7.86
7.79
7.79
7.77
7.77
7.75
7.75
4.34
4.33
1.61
1.59
1.57
1.96
1.01
1.00
2.07
3.12
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
Et
N
N

9b

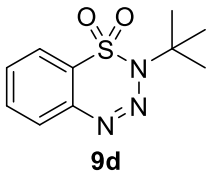
141.79
134.14
132.61
129.32
125.69
120.42
43.72
15.96
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.05
8.04
8.04
8.03
8.03
8.02
8.02
8.02
7.90
7.90
7.89
7.88
7.87
7.86
7.80
7.79
7.78
7.77
7.76
7.75
4.25
4.23
4.21
2.05
2.03
2.02
2.00
1.98
1.96
1.06
1.04
1.02
O
O
S
N
nPr
N
N
9c
1.93
1.00
0.99
2.05
2.08
3.03
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
nPr
N
N

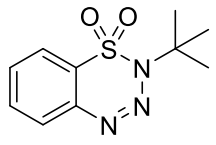
9c

141.82
134.13
132.60
129.34
125.71
120.50
50.03
23.69
11.16
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



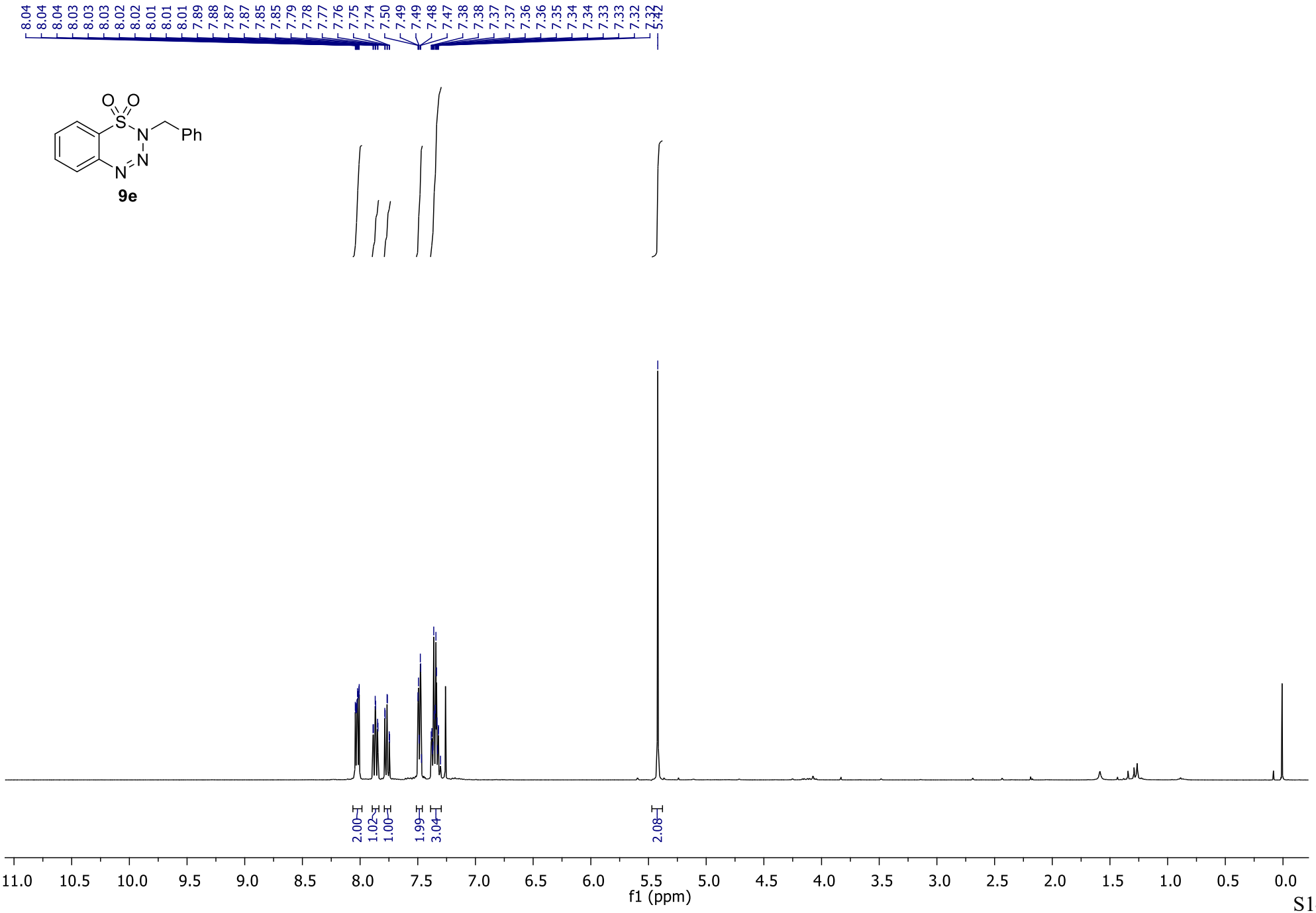
9d

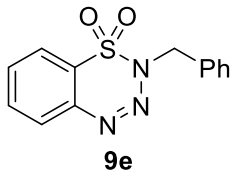
8.02
8.01
7.99
7.97
7.97
7.87
7.87
7.85
7.85
7.83
7.83
7.76
7.76
7.74
7.74
7.72
7.72
1.82
1.94
1.00
1.01
9.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



9d

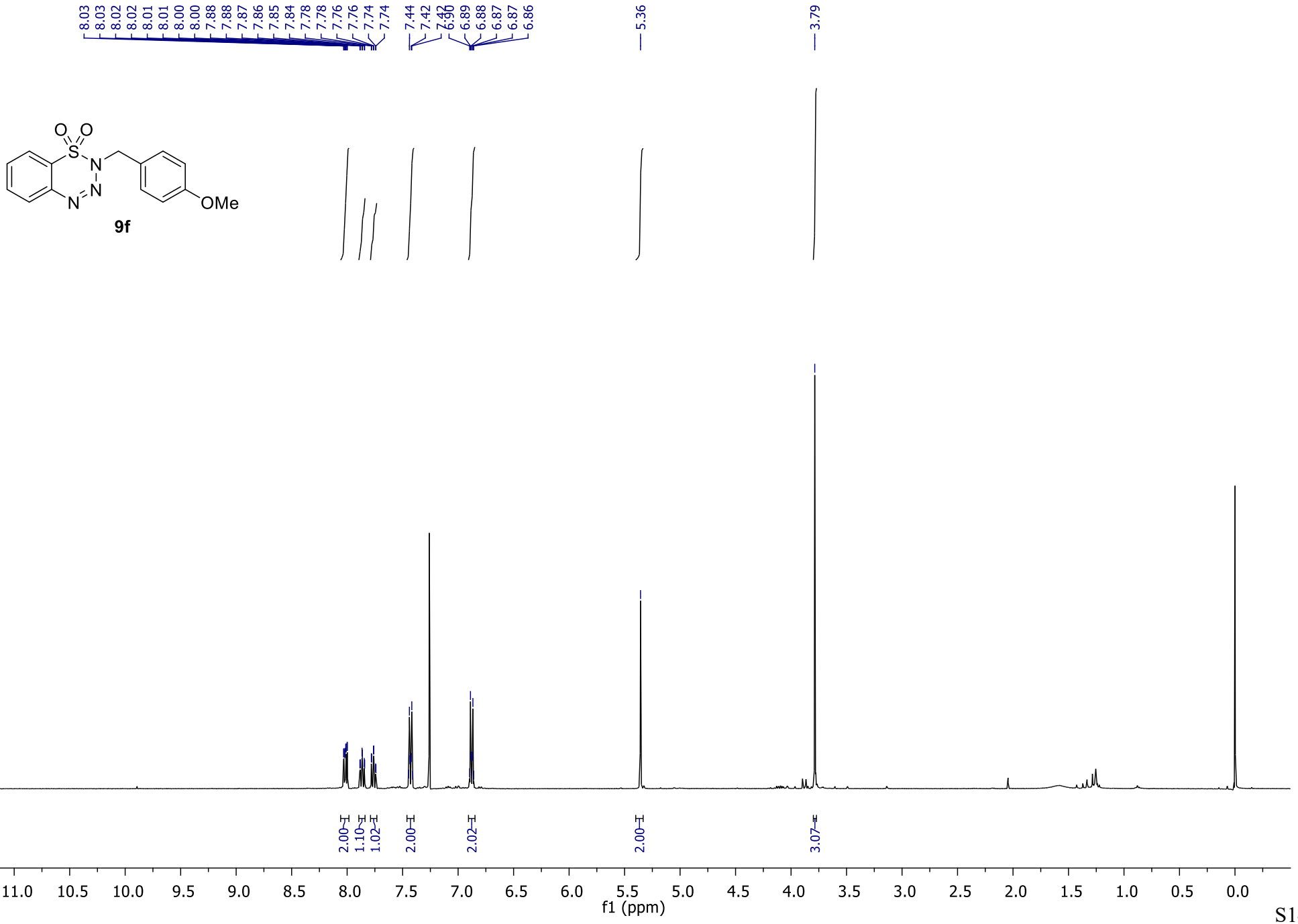
141.16
133.98
132.29
128.57
126.29
120.42
67.88
30.54
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.04 8.04 8.04 8.03 8.03 8.03 8.02 8.02 8.01 8.01 8.01 7.89 7.88 7.87 7.87 7.85 7.85 7.79 7.78 7.77 7.76 7.75 7.74 7.50 7.49 7.49 7.48 7.47 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.34 7.34 7.33 7.33 7.32 7.32 5.42
O
O
S
N
N
N
Ph
9e
2.00
1.02
1.00
1.99
3.04
2.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


O
O
S
N
N
N
Ph

9e

141.76
135.38
134.19
132.75
129.51
128.96
128.90
128.60
126.09
120.59
51.27
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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8.02
8.02
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8.00
8.00
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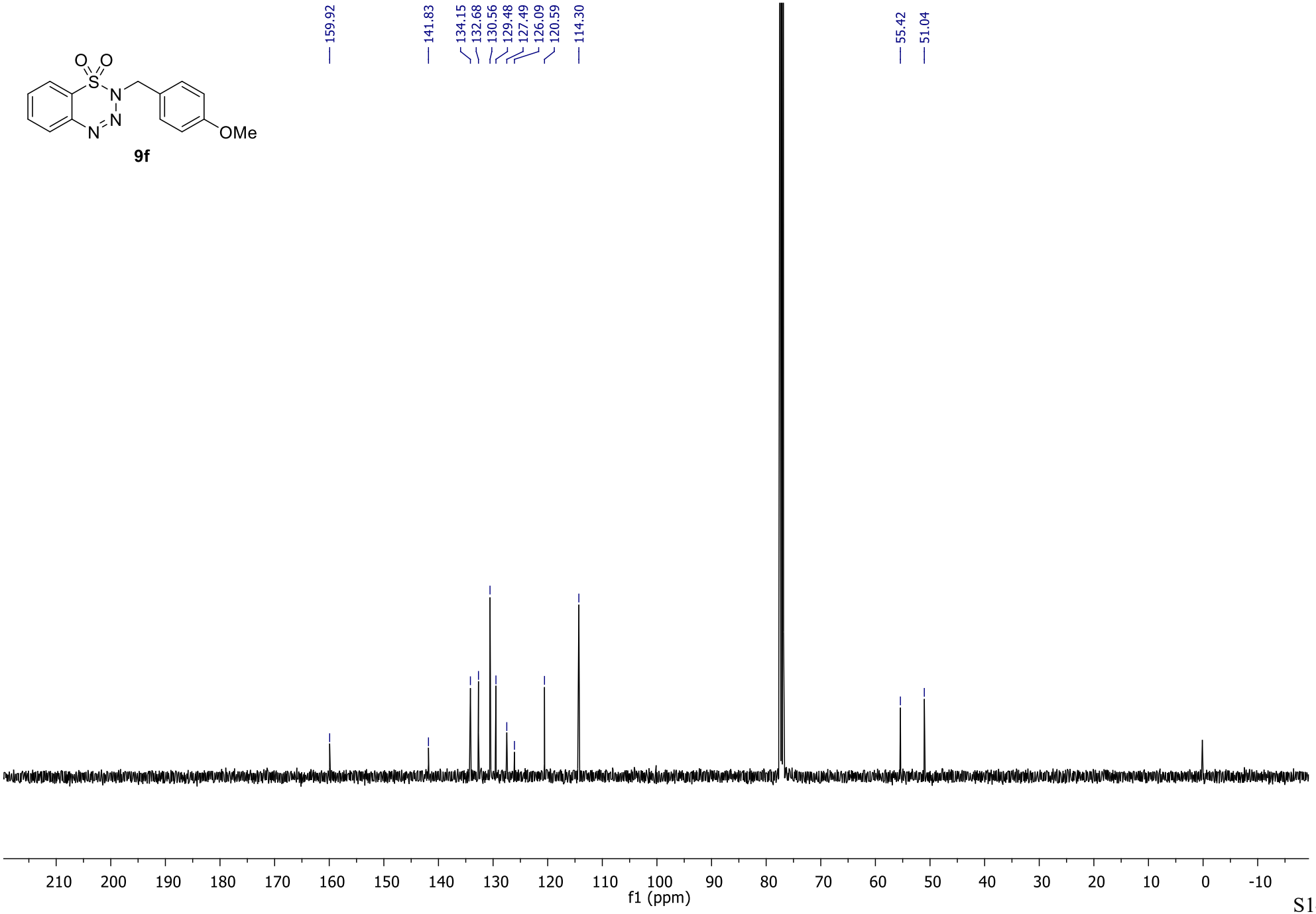
7.88
7.87
7.86
7.85
7.84
7.78
7.78
7.76
7.76
7.74
7.74
7.44
7.42
7.42
6.90
6.89
6.88
6.87
6.87
6.86
5.36
3.79
O
O
S
N
N
N
OMe
9f
2.00
1.10
1.02
2.00
2.02
2.00
3.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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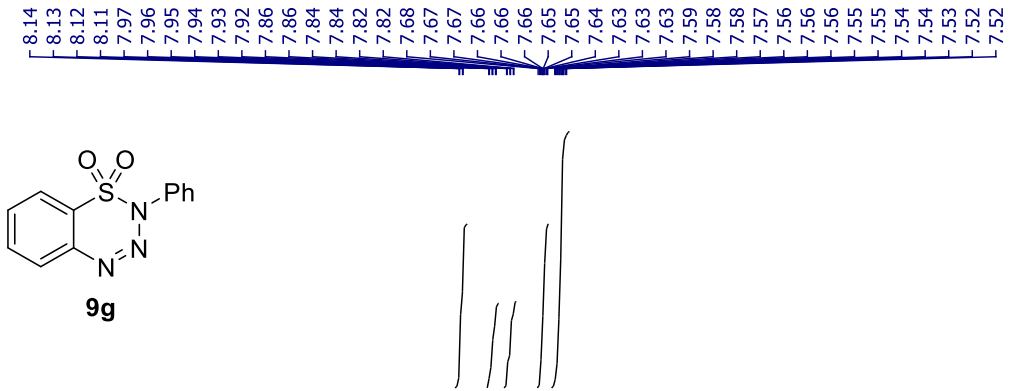
134.15
132.68
130.56
129.48
127.49
126.09
120.59
114.30
55.42
51.04
OMe
9f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.94
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7.92
7.86
7.86
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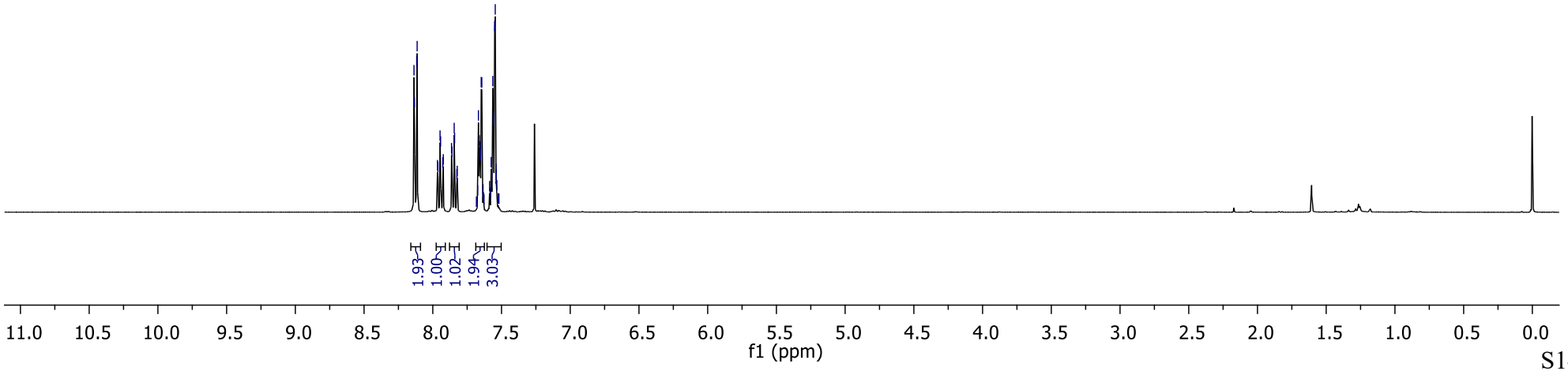
7.84
7.82
7.82
7.68
7.67
7.67
7.66
7.66
7.66
7.65
7.65
7.64
7.63
7.63
7.63
7.59
7.58
7.58
7.57
7.56
7.56
7.56
7.55
7.55
7.54
7.54
7.53
7.52
7.52
O
O
S
N
Ph
N
N
9g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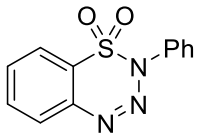
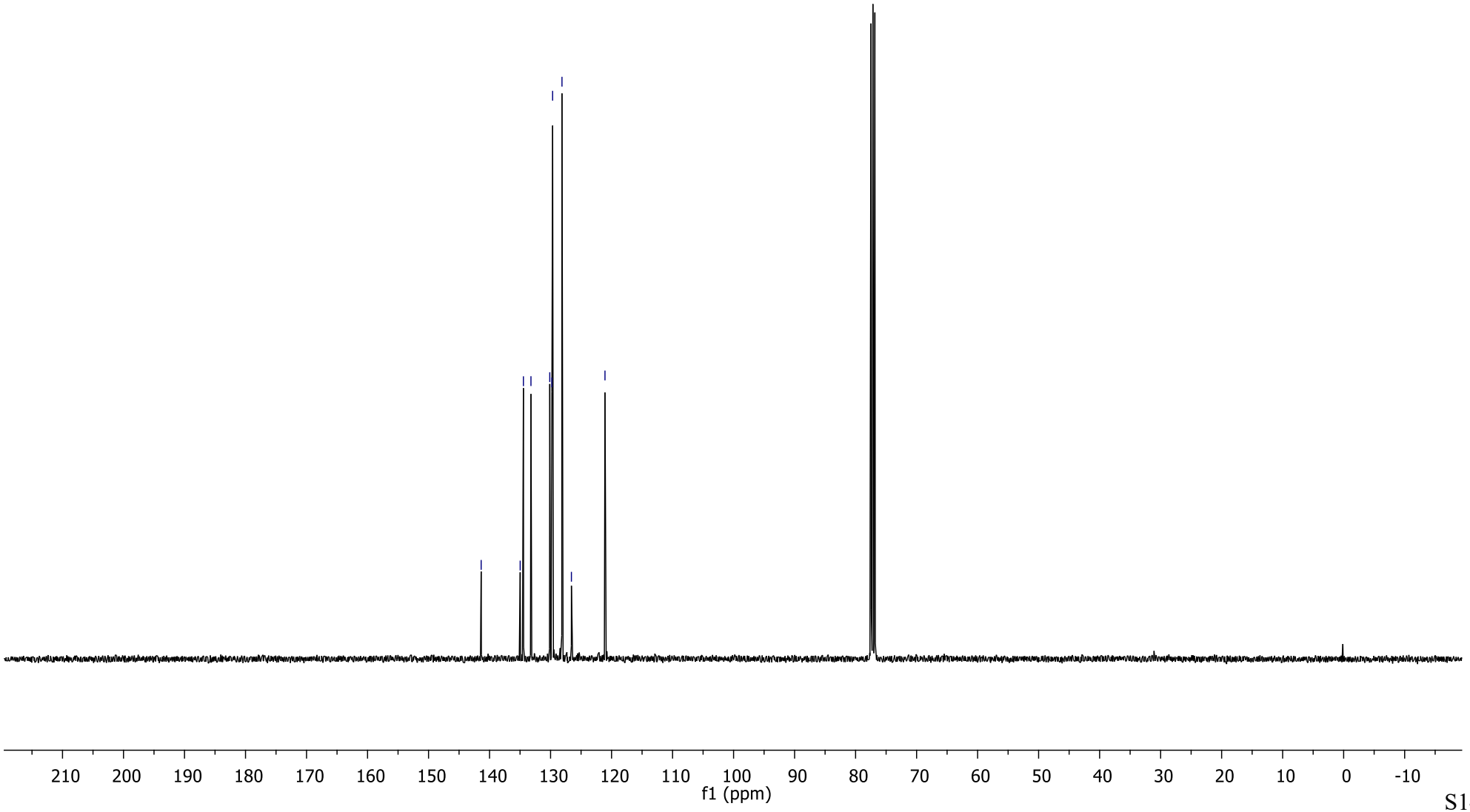
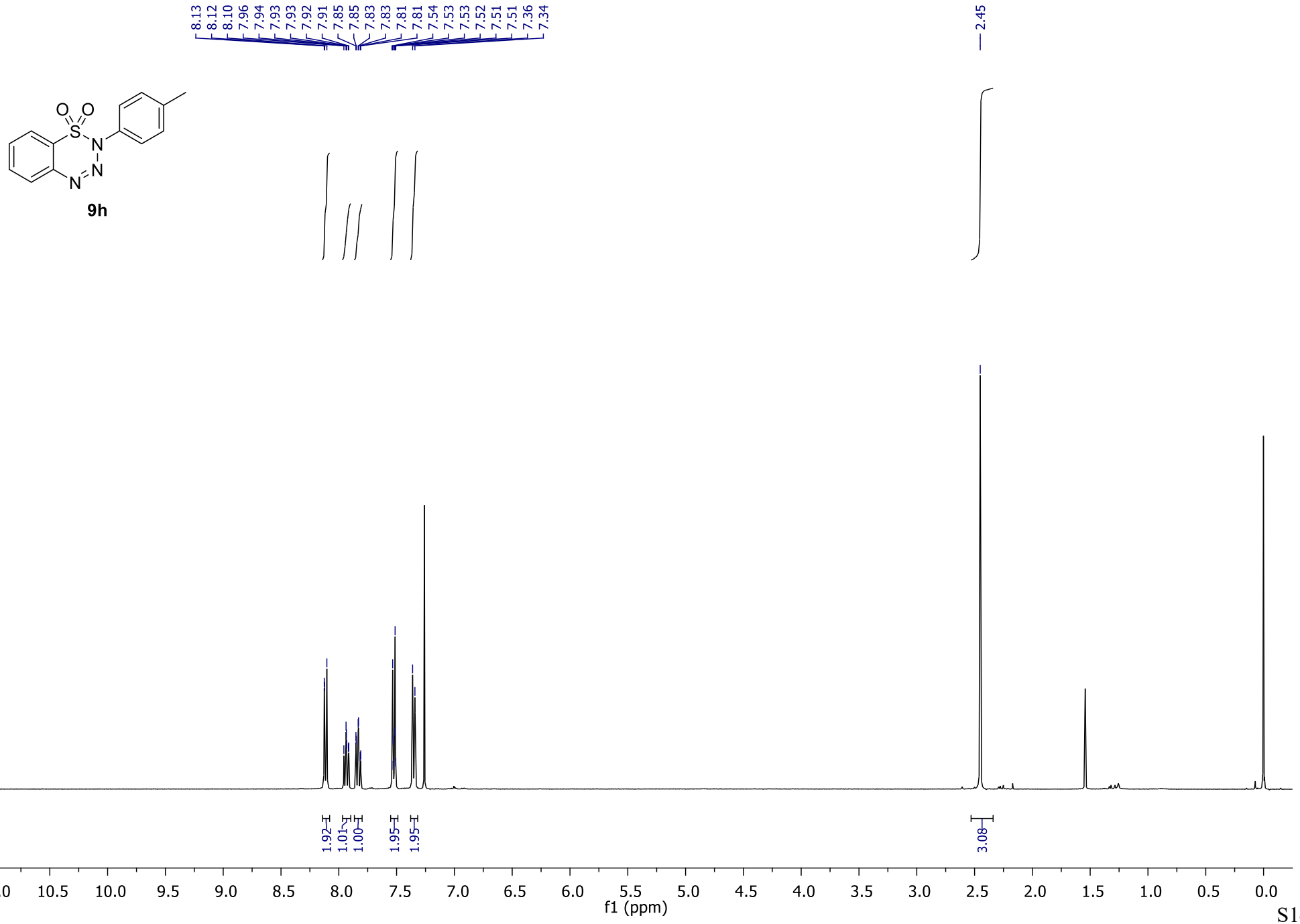
1.00
1.02
1.94
3.03
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



9g

141.38
134.98
134.45
133.21
130.13
129.78
129.66
128.13
126.58
121.08

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7.92
7.91
7.85
7.85
7.83
7.83
7.81
7.81
7.54
7.53
7.53
7.52
7.51
7.51
7.36
7.34
2.45
9h
1.92
1.01
1.00
1.95
1.95
3.08
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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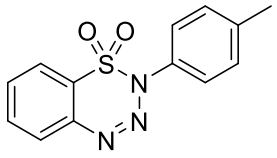
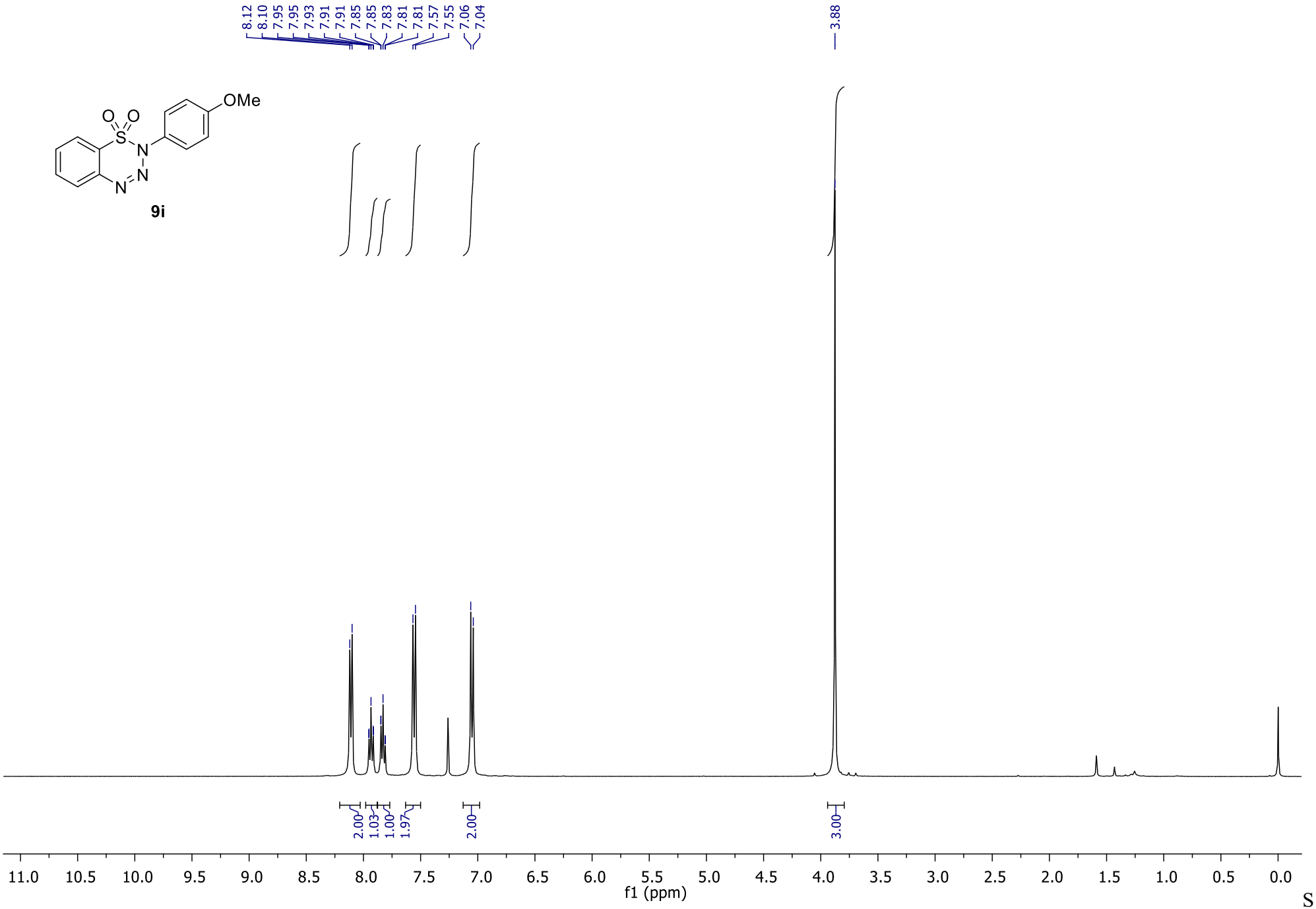
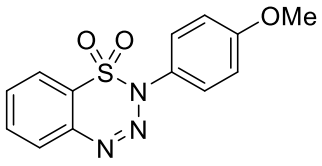
0.0
f1 (ppm)



9h

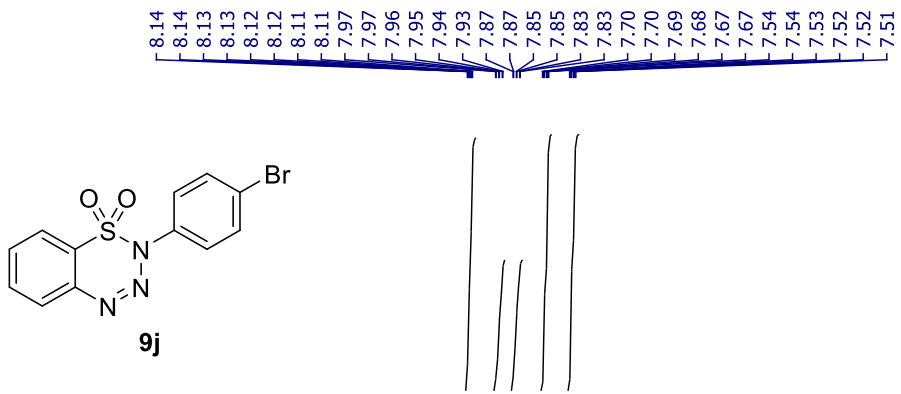
141.49
140.54
134.36
133.09
132.29
130.32
129.75
128.13
126.65
121.12
21.45
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

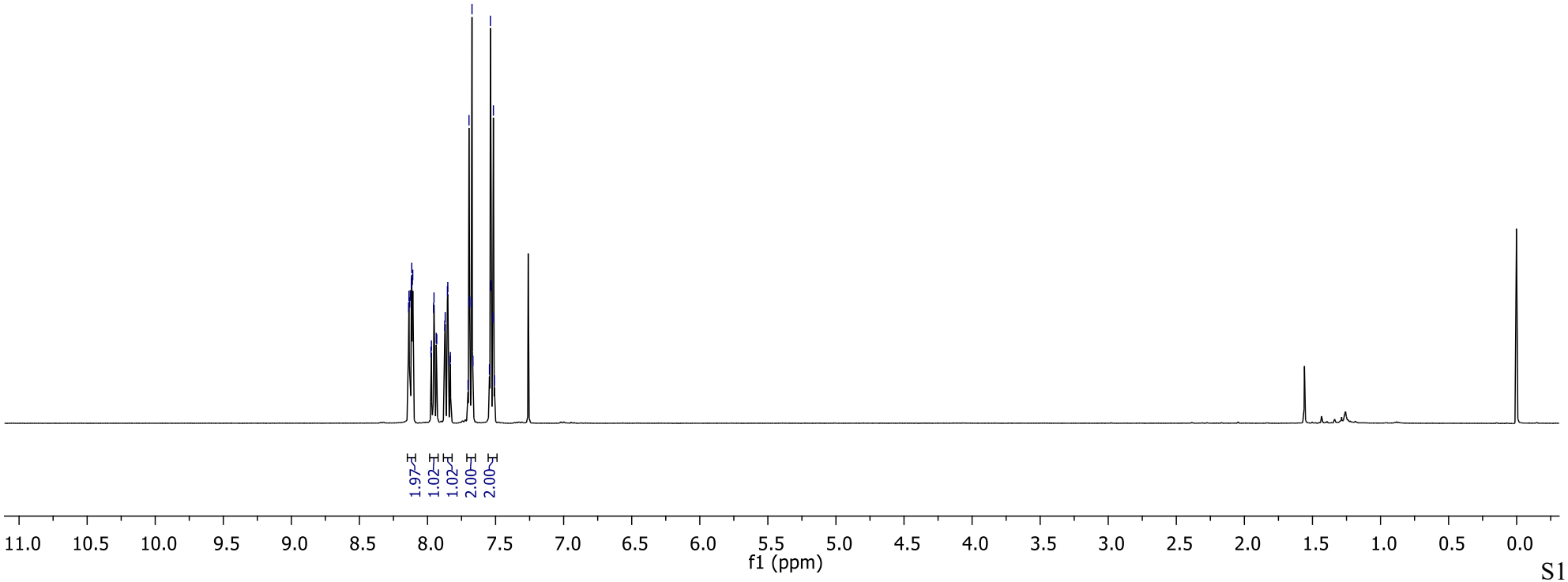

8.12
8.10
7.95
7.95
7.93
7.91
7.91
7.85
7.85
7.83
7.81
7.81
7.57
7.55
7.06
7.04
3.88
OMe
O
O
S
N
N
N
9i
2.00
1.03
1.00
1.97
2.00
3.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


OMe
O
O
S
N
N
N

9i

161.12
141.43
134.38
133.09
130.01
129.73
127.06
126.50
121.15
114.90
55.76
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.14
8.14
8.13
8.13
8.12
8.12
8.11
8.11
7.97
7.97
7.96
7.95
7.94
7.93
7.87
7.87
7.85
7.85
7.83
7.83
7.70
7.70
7.69
7.68
7.67
7.67
7.54
7.54
7.53
7.52
7.52
7.51
Br
O
O
S
N
N
N
9j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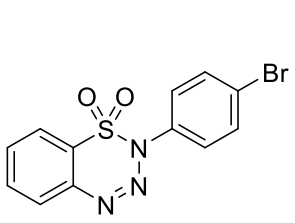
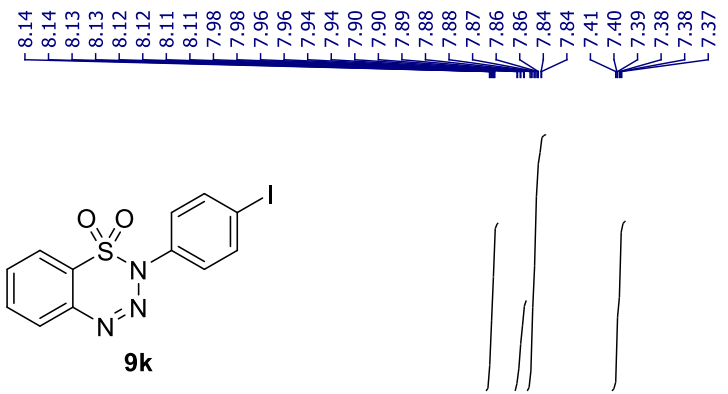
1.02
1.02
2.00
2.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
N
N
Br

9j

141.28
134.59
134.05
133.41
132.90
129.94
129.49
126.61
124.36
121.13
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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8.13
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8.12
8.11
8.11
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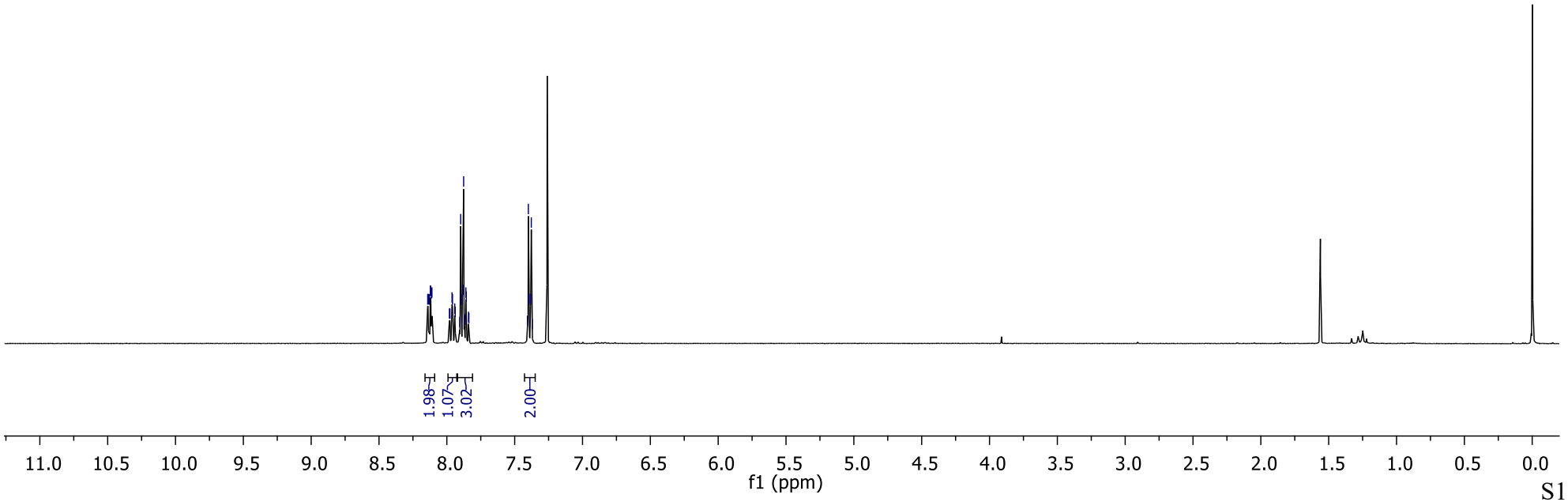
7.98
7.96
7.96
7.94
7.94
7.90
7.90
7.89
7.88
7.88
7.87
7.86
7.86
7.84
7.84
7.41
7.40
7.39
7.38
7.38
7.37
O
O
S
N
N
N
I
9k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1.07
3.02
2.00
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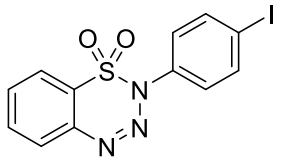
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
S
N
N
N
I

9k

141.29
138.90
134.81
134.59
133.41
129.95
129.56
126.60
121.14
96.00
210
200
190
180
170
160
150
140
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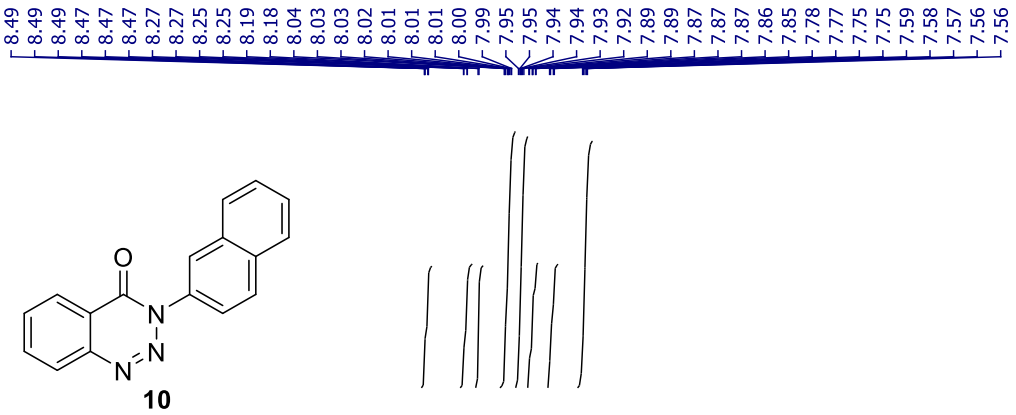
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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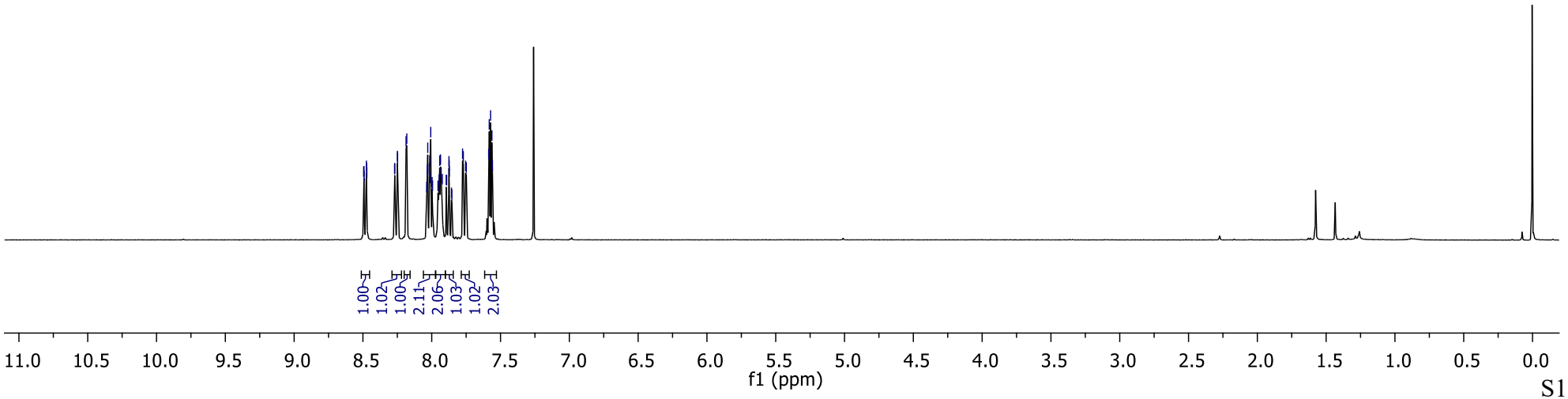
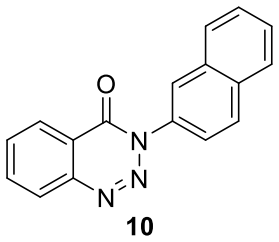
8.47
8.47
8.27
8.27
8.25
8.25
8.19
8.18
8.04
8.03
8.03
8.02
8.01
8.01
8.01
8.00
7.99
7.95
7.95
7.94
7.94
7.93
7.92
7.89
7.89
7.87
7.87
7.87
7.86
7.85
7.78
7.77
7.75
7.75
7.59
7.58
7.57
7.56
7.56
O
N
N
N
10


1.00
1.02
1.00
2.11
2.06
1.03
1.02
2.03
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
N
N
N

10

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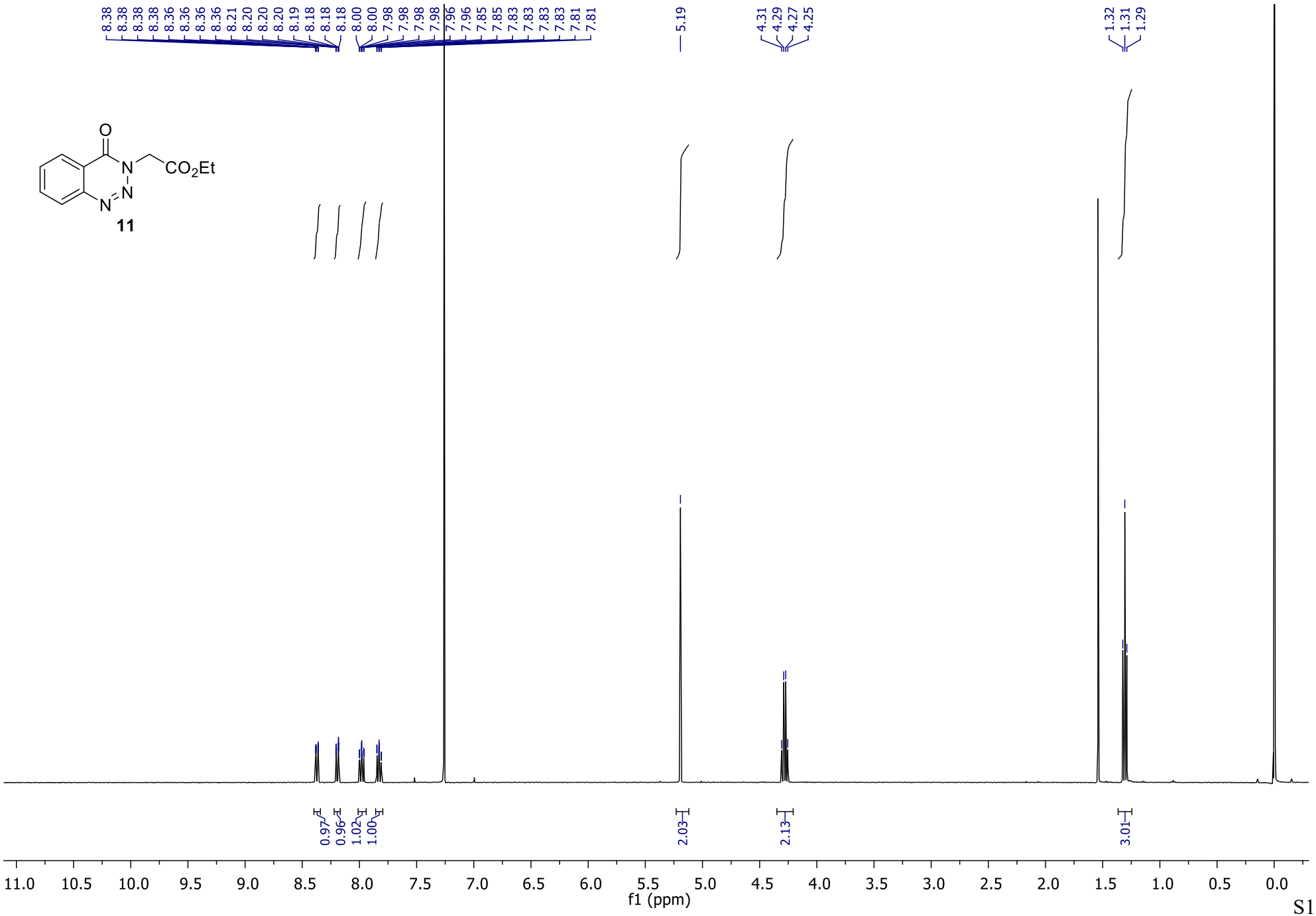
143.87
136.44
135.27
133.33
133.23
132.95
129.05
128.73
128.64
127.94
127.22
126.94
125.82
125.12
123.83
120.61
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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8.38
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8.21
8.20
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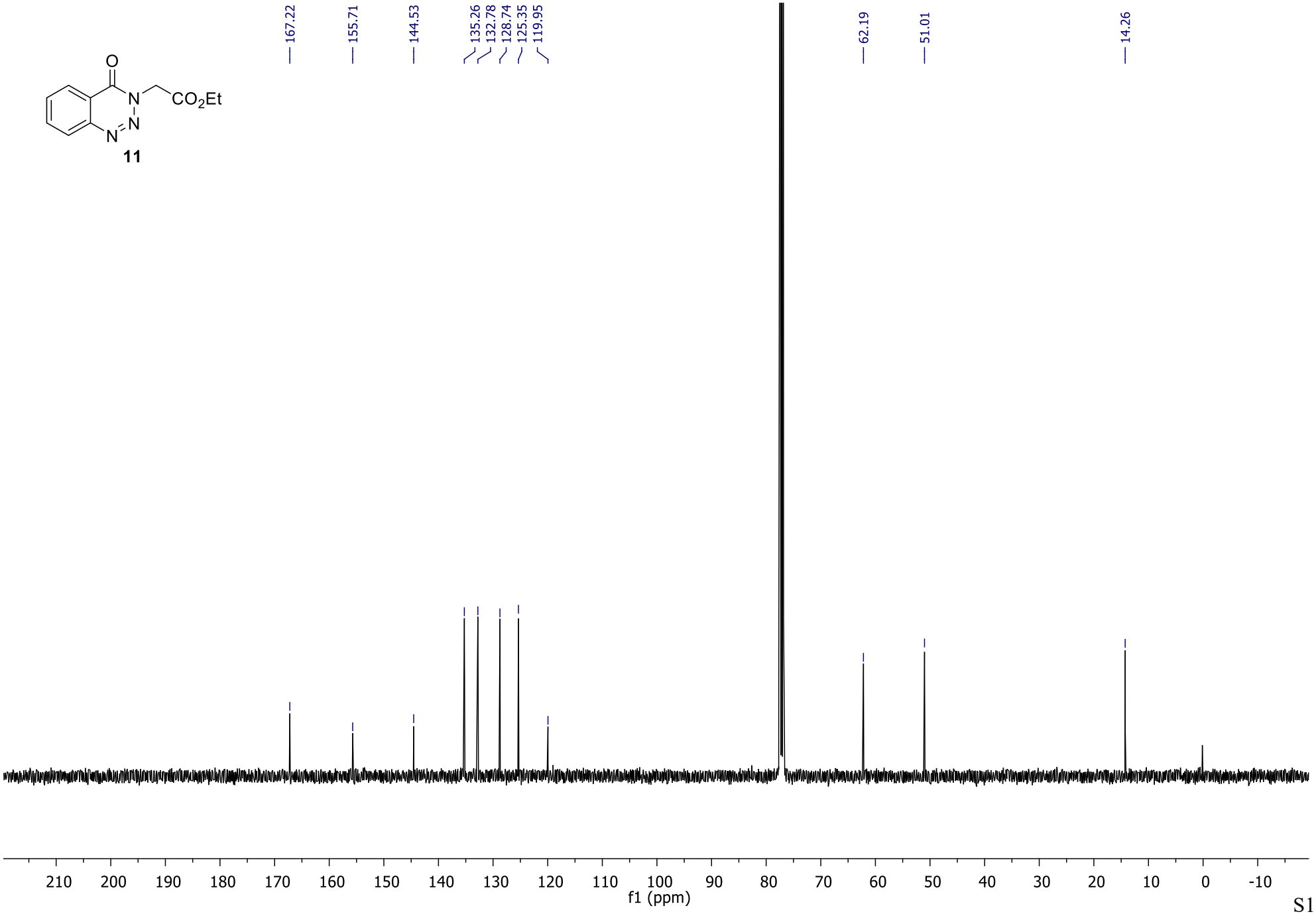
8.20
8.19
8.18
8.18
8.18
8.00
8.00
7.98
7.98
7.98
7.96
7.96
7.85
7.85
7.83
7.83
7.83
7.81
7.81
5.19
4.31
4.29
4.27
4.25
1.32
1.31
1.29
O
N
N
N
CO2Et
11
0.97
0.96
1.02
1.00
2.03
2.13
3.01
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
N
N
N
CO2Et
11
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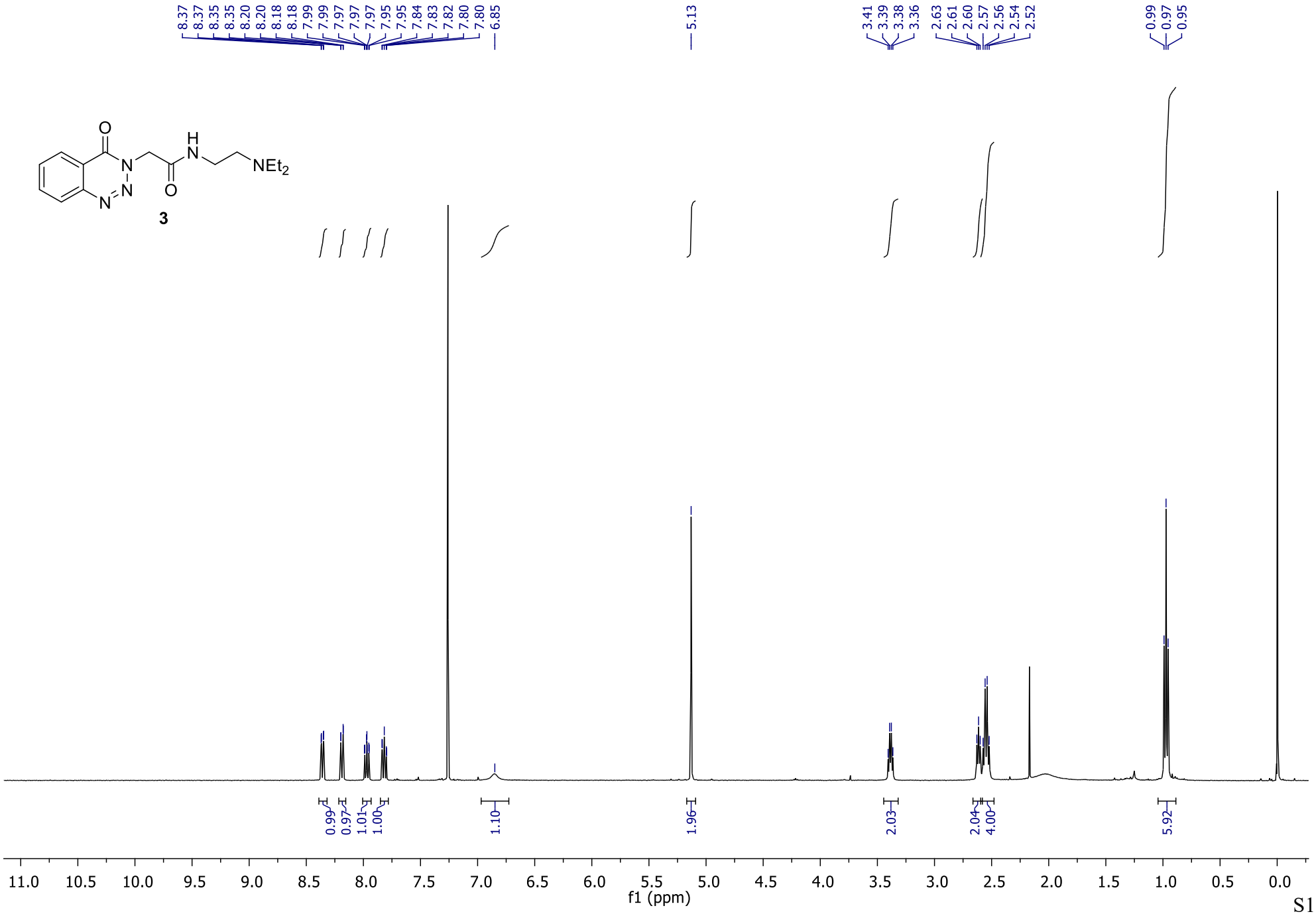
155.71
144.53
135.26
132.78
128.74
125.35
119.95
62.19
51.01
14.26
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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8.35
8.35
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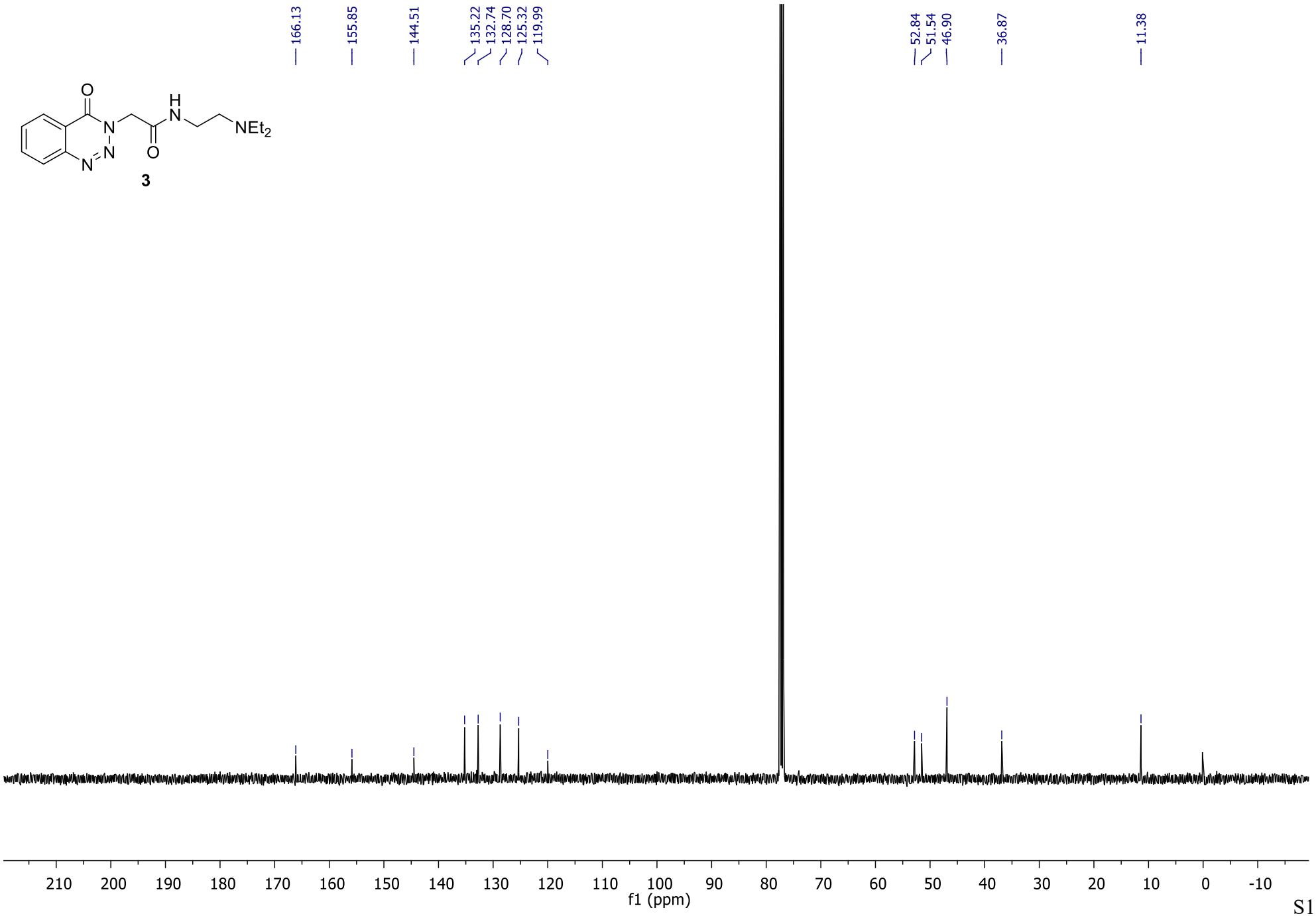
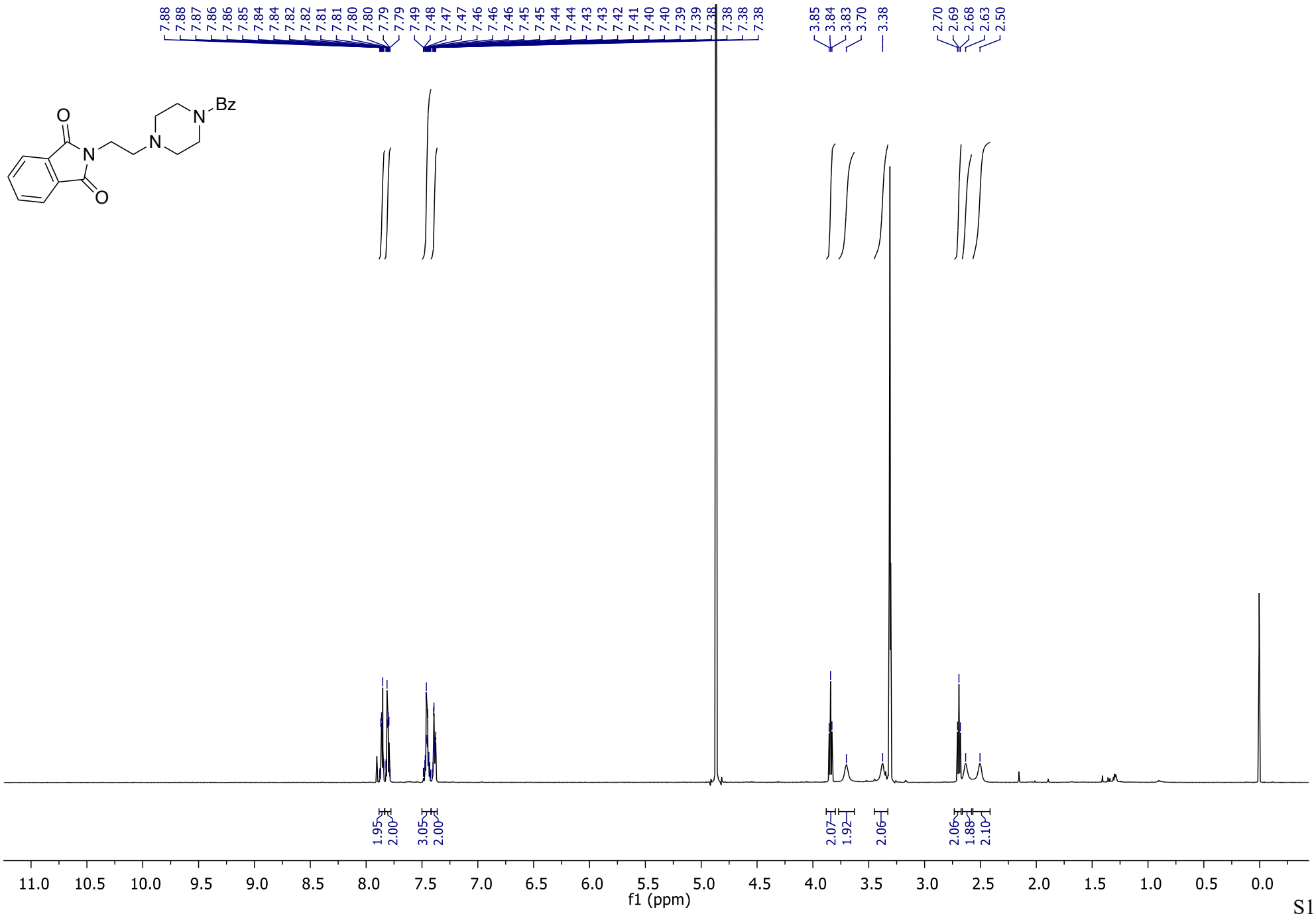
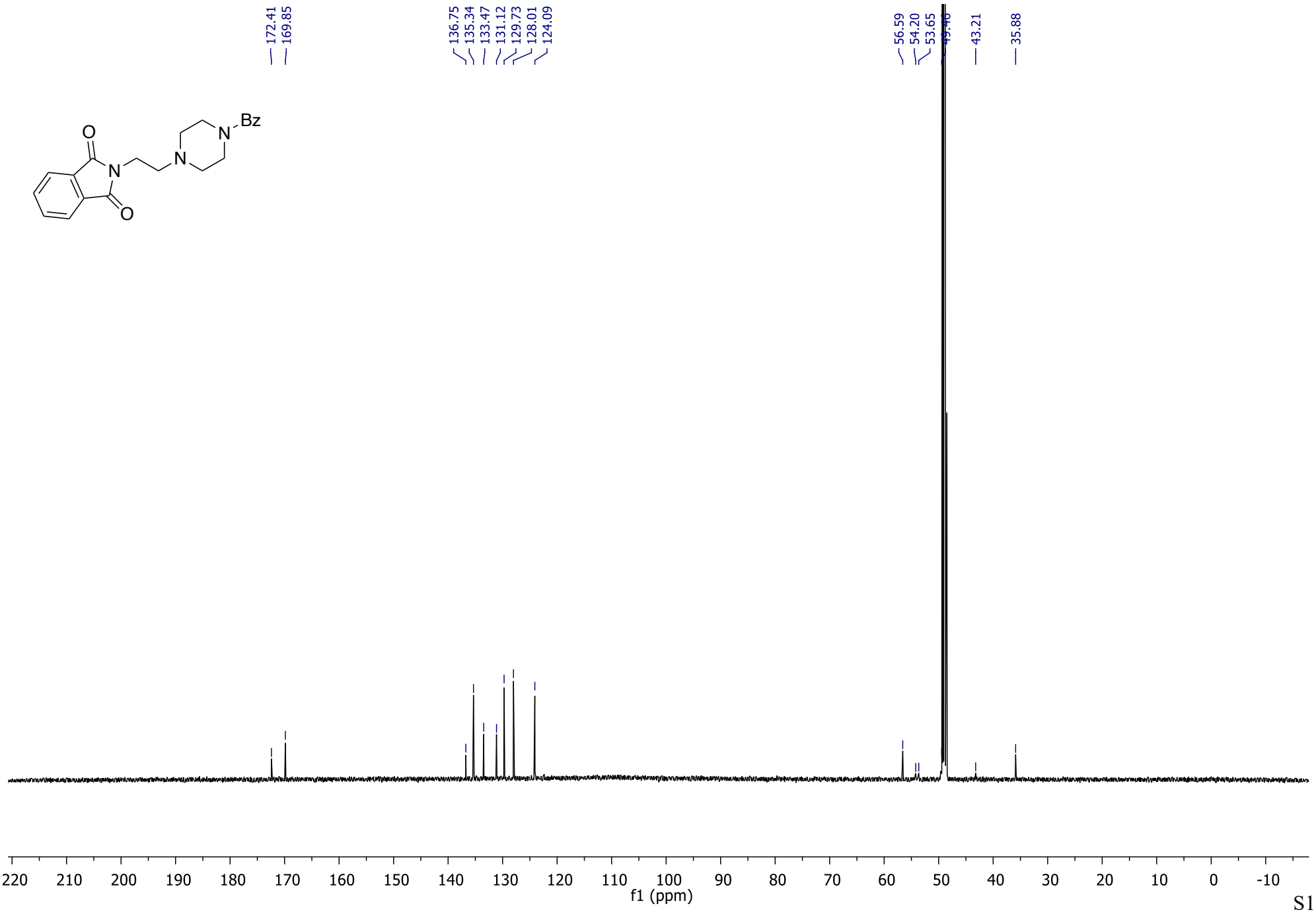
8.20
8.18
8.18
7.99
7.99
7.97
7.97
7.97
7.95
7.95
7.84
7.83
7.82
7.80
7.80
6.85
5.13
3.41
3.39
3.38
3.36
2.63
2.61
2.60
2.57
2.56
2.54
2.52
0.99
0.97
0.95
O
H
N
N
N
N
O
NEt2
3
0.99
0.97
1.01
1.00
1.10
1.96
2.03
2.04
4.00
5.92
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


166.13
155.85
144.51
135.22
132.74
128.70
125.32
119.99
52.84
51.54
46.90
36.87
11.38
O
H
N
N
N
N
O
NEt2
3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.88 7.88 7.87 7.86 7.86 7.85 7.84 7.84 7.82 7.82 7.81 7.81 7.80 7.80 7.79 7.79 7.49 7.48 7.47 7.47 7.46 7.46 7.46 7.45 7.45 7.44 7.44 7.43 7.43 7.42 7.41 7.40 7.40 7.39 7.39 7.38 7.38 7.38 7.38
3.85 3.84 3.83 3.70 3.38
2.70 2.69 2.68 2.63 2.50
O
N
N
N
Bz
O
1.95 2.00 3.05 2.00 2.07 1.92 2.06 2.06 1.88 2.10
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


172.41
169.85
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135.34
133.47
131.12
129.73
128.01
124.09
56.59
54.20
53.65
43.21
35.88
O
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N
N
Bz
O
220
210
200
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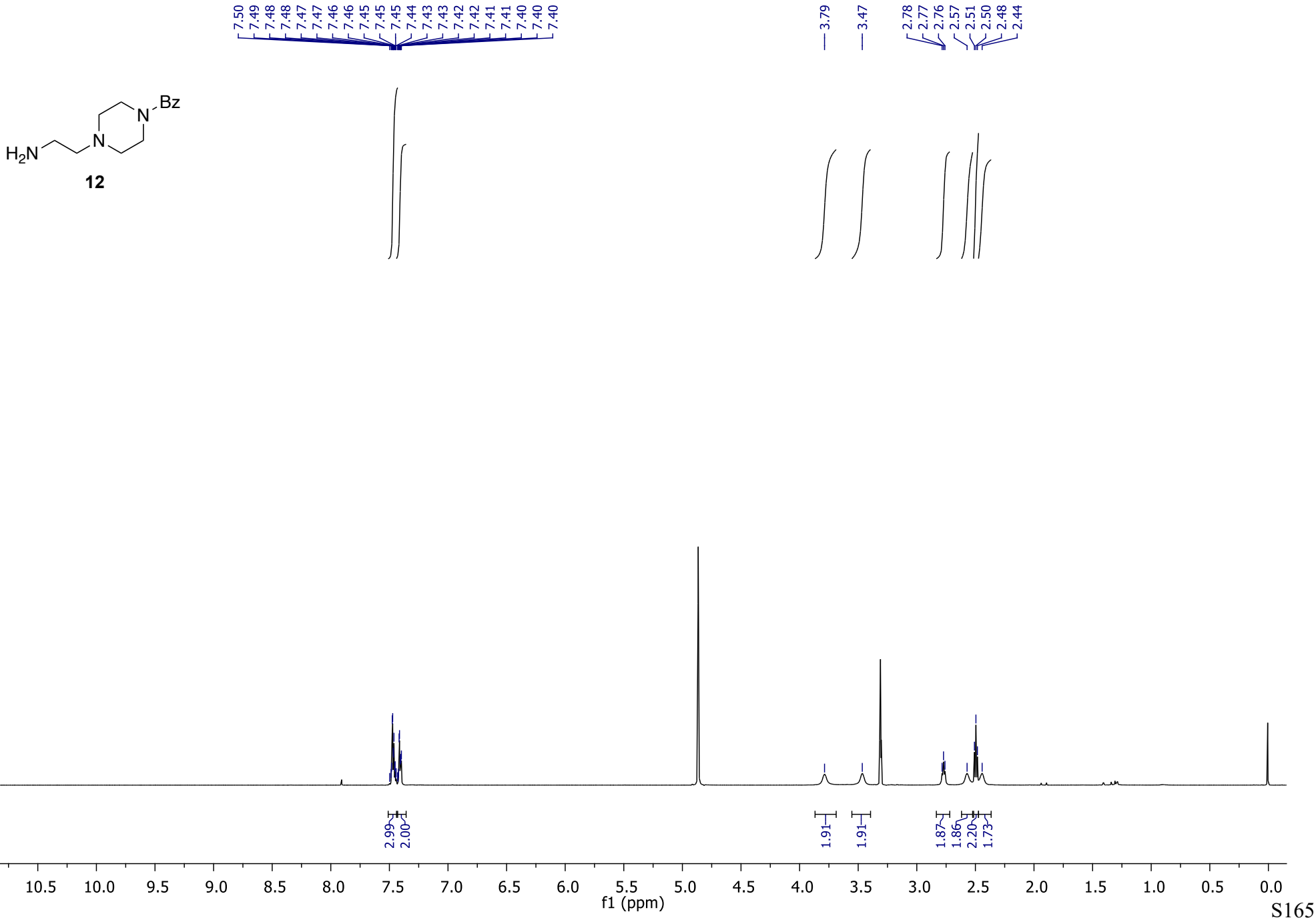
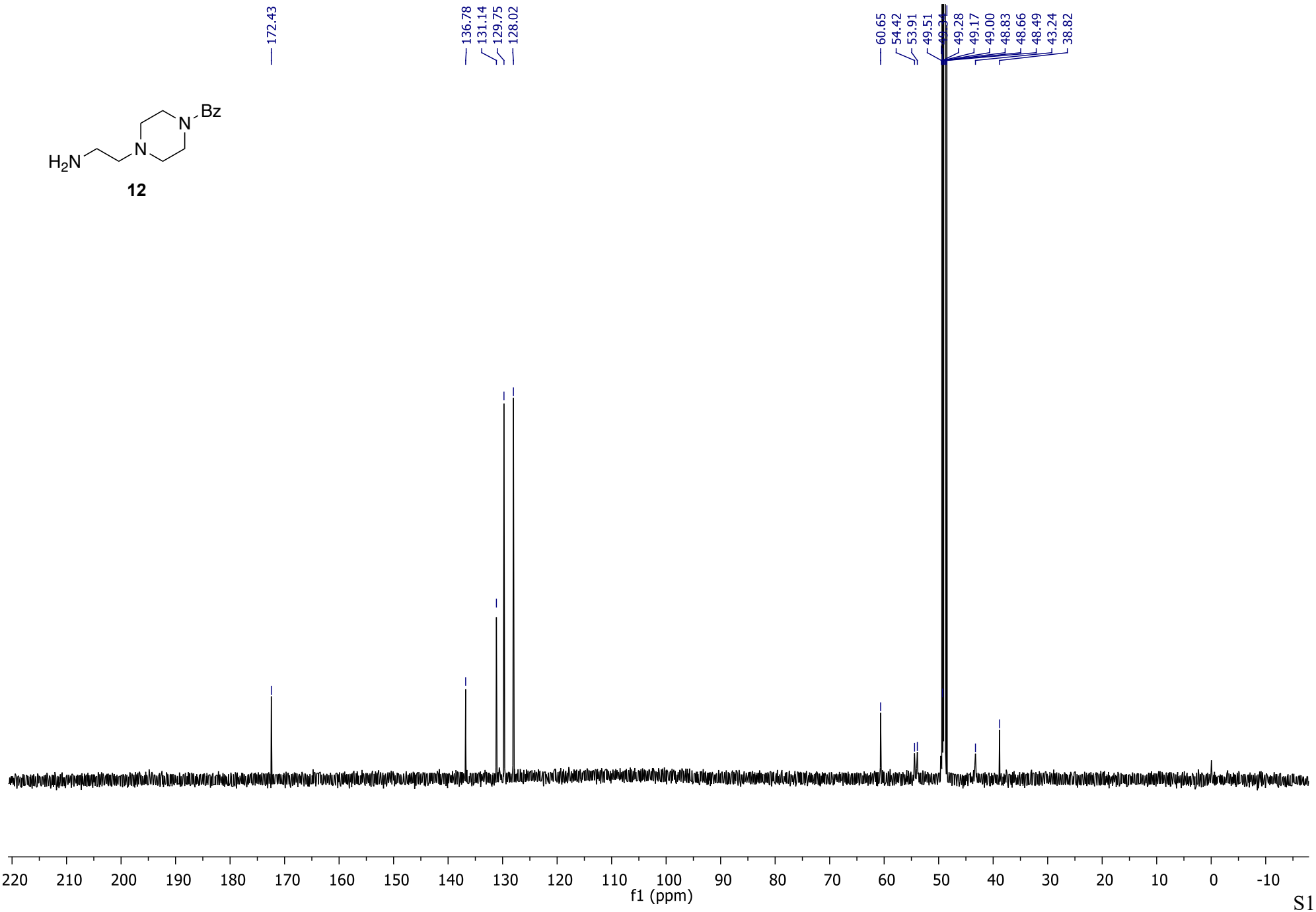
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.50
7.49
7.48
7.48
7.47
7.47
7.46
7.46
7.45
7.45
7.45
7.44
7.43
7.43
7.42
7.42
7.41
7.41
7.40
7.40
7.40
3.79
3.47
2.78
2.77
2.76
2.57
2.51
2.50
2.48
2.44
Bz
N
N
H2N
12
2.99
2.00
1.91
1.91
1.87
1.86
2.20
1.73
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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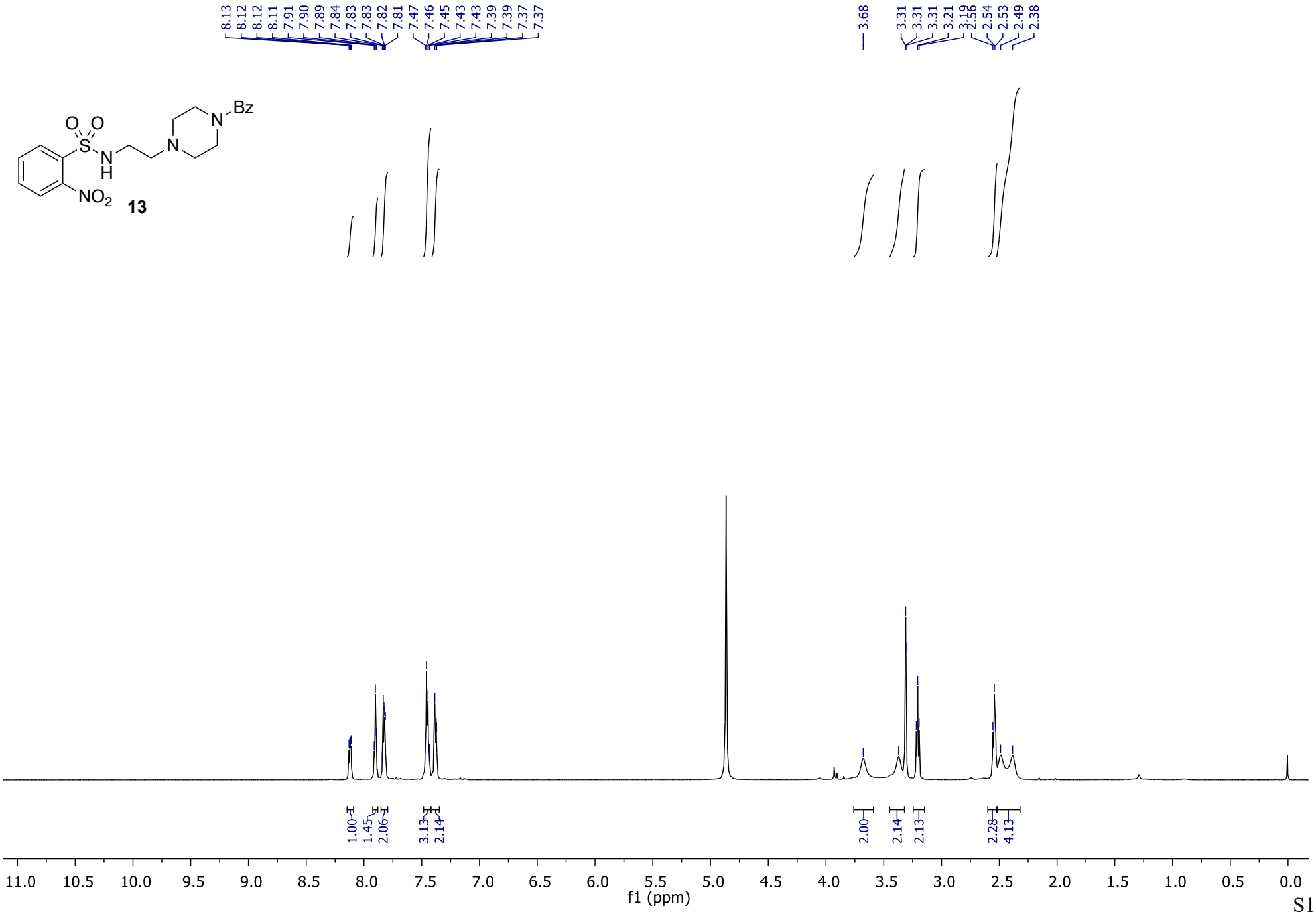
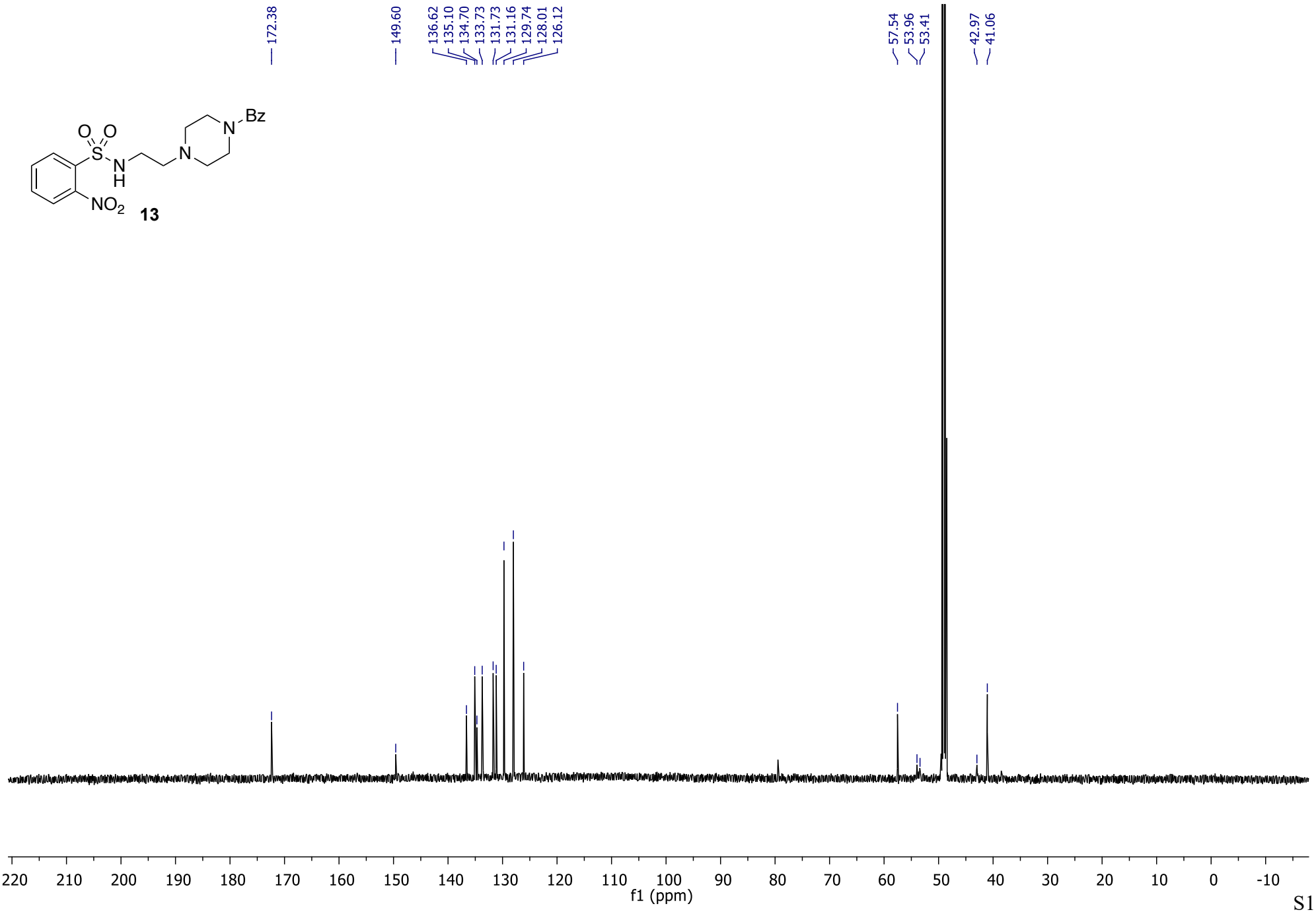
136.78
131.14
129.75
128.02
60.65
54.42
53.91
49.51
49.28
49.17
49.00
48.83
48.66
48.49
43.24
38.82
Bz
N
N
H2N
12
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.13
8.12
8.12
8.11
7.91
7.90
7.89
7.84
7.83
7.83
7.82
7.81
7.47
7.46
7.45
7.43
7.43
7.39
7.39
7.37
7.37
3.68
3.31
3.31
3.31
3.21
3.19
3.16
2.54
2.53
2.49
2.38
O
O
S
N
H
N
N
Bz
NO2
13
1.00
1.45
2.06
3.13
2.14
2.00
2.14
2.13
2.28
4.13
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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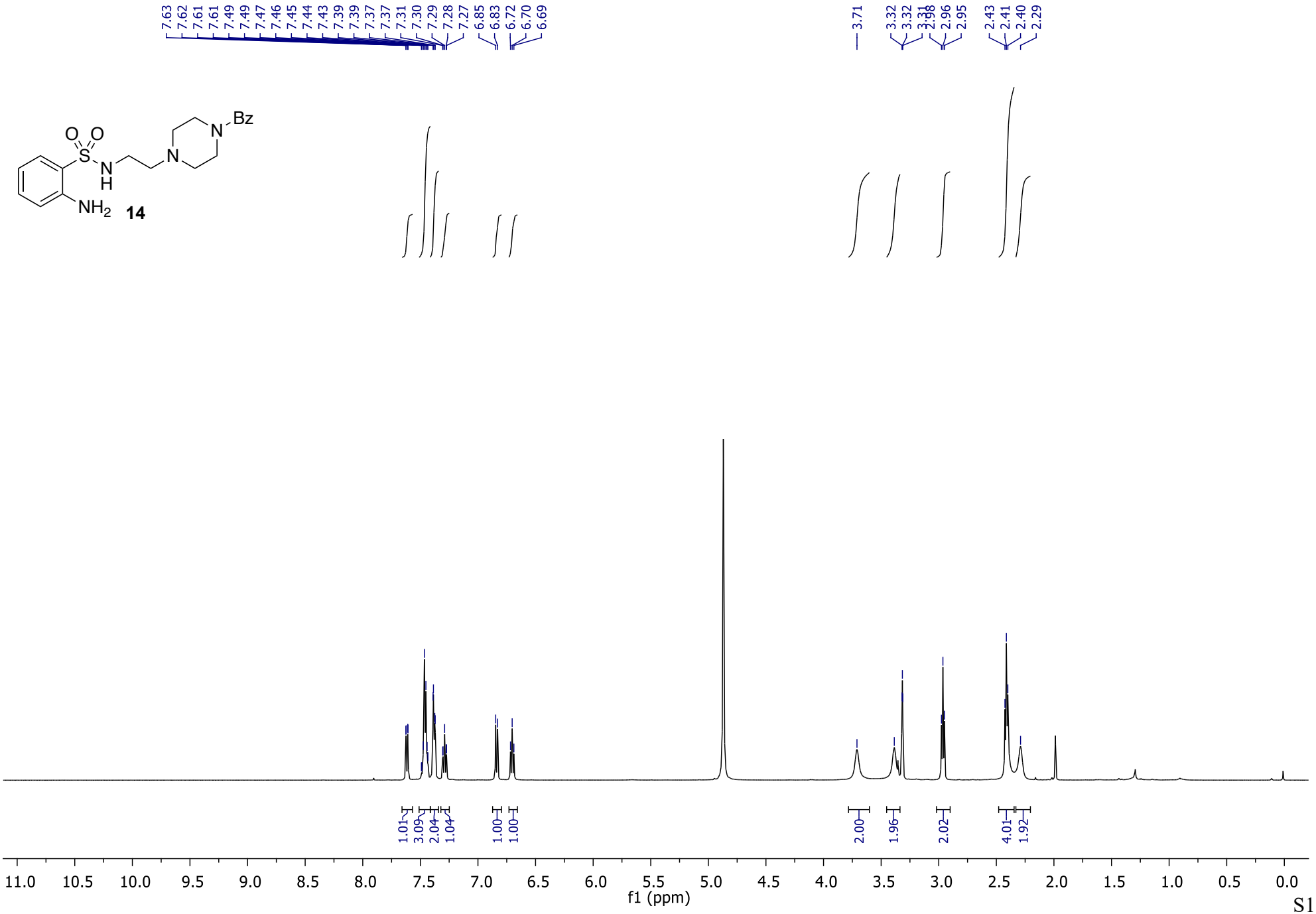
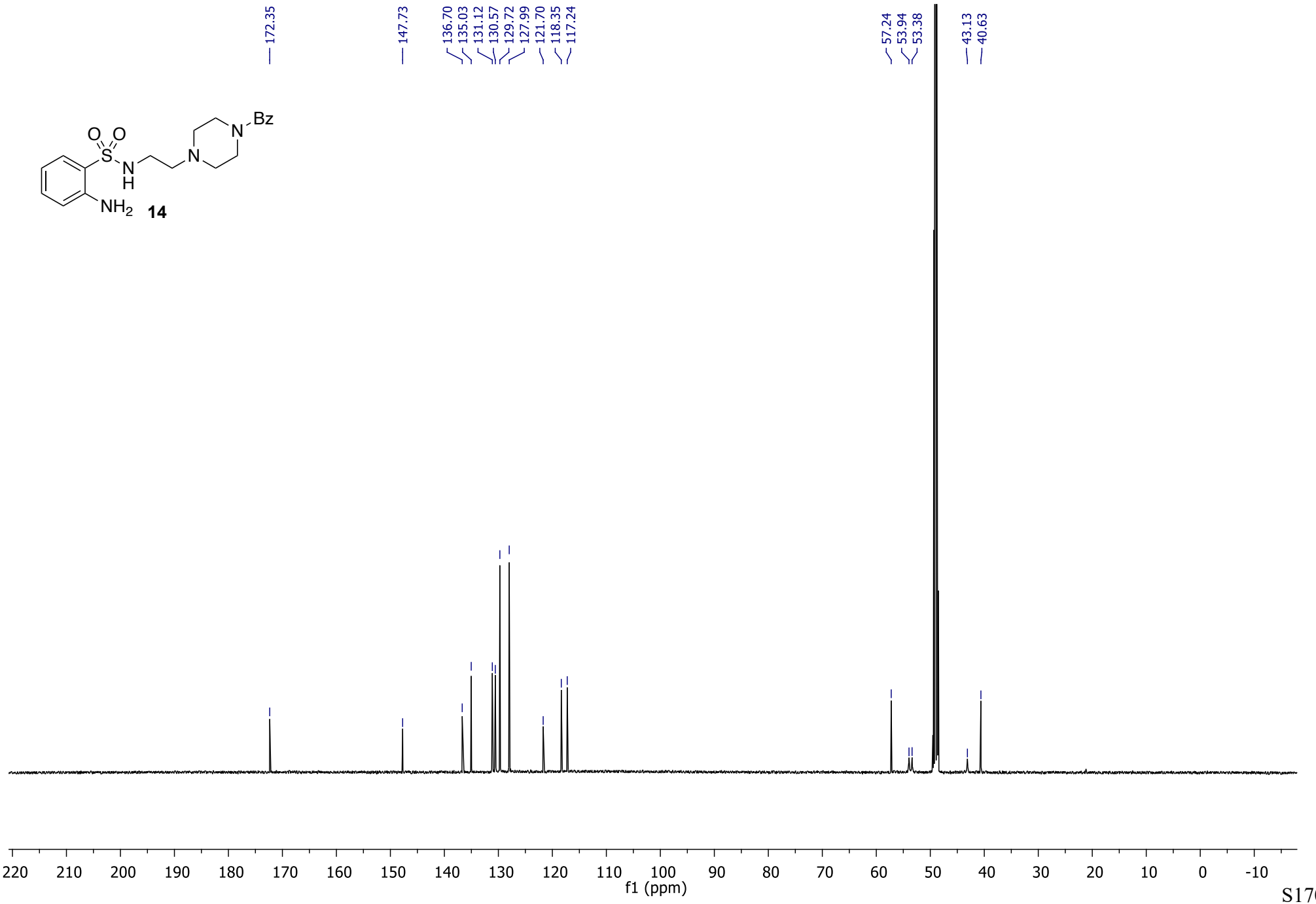
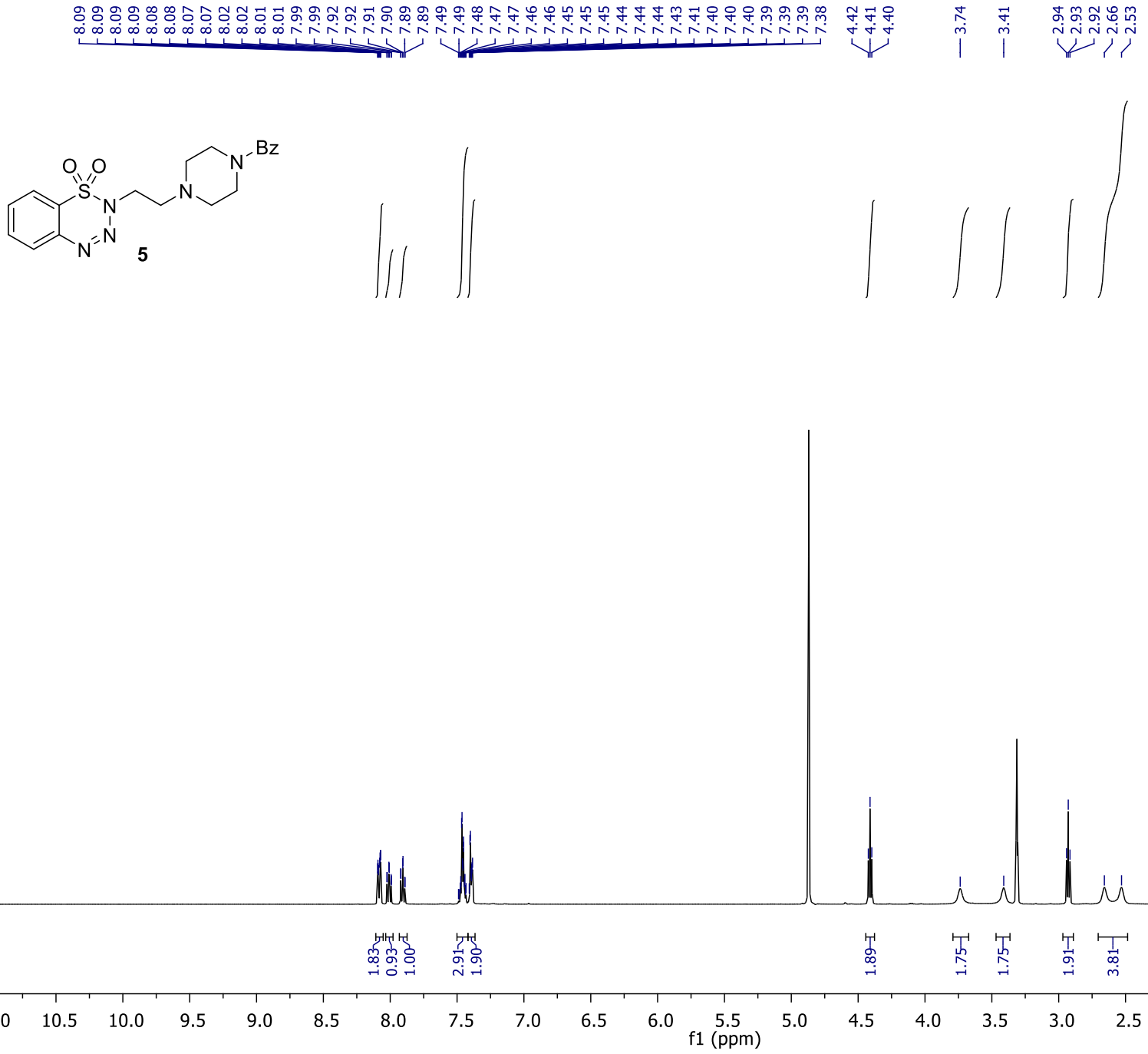
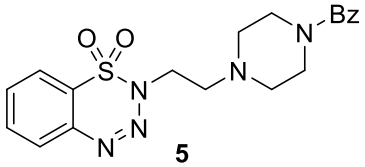
149.60
136.62
135.10
134.70
133.73
131.73
131.16
129.74
128.01
126.12
57.54
53.96
53.41
42.97
41.06
O
O
S
N
H
N
N
Bz
NO2
13
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.63
7.62
7.61
7.61
7.49
7.49
7.47
7.46
7.45
7.44
7.43
7.39
7.39
7.37
7.37
7.31
7.30
7.29
7.28
7.27
6.85
6.83
6.72
6.70
6.69
3.71
3.32
3.32
3.31
2.98
2.96
2.95
2.43
2.41
2.40
2.29
O
O
S
N
H
NH2
N
N
Bz
14
1.01
3.09
2.04
1.04
1.00
1.00
2.00
1.96
2.02
4.01
1.92
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

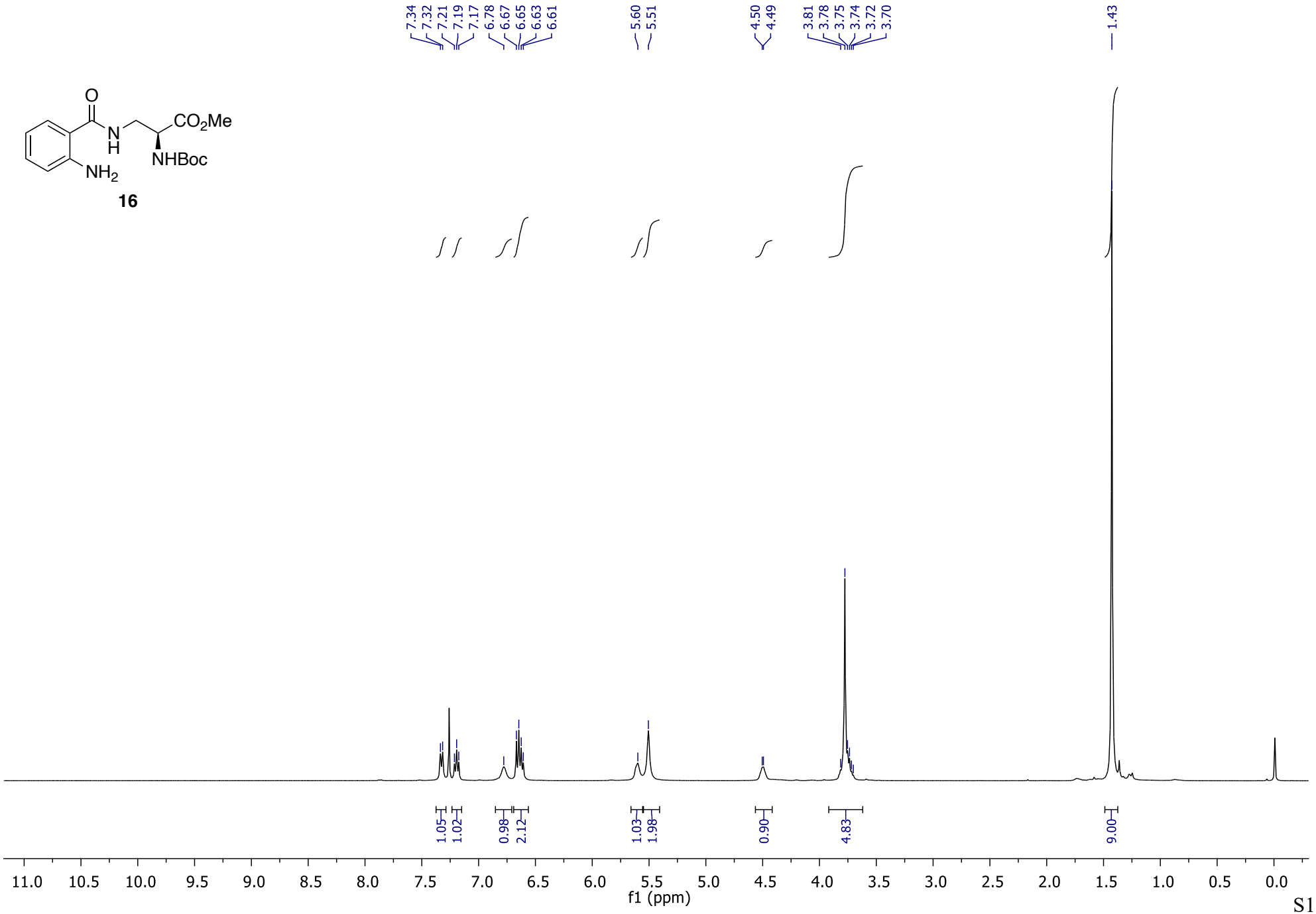

172.35
147.73
136.70
135.03
131.12
130.57
129.72
127.99
121.70
118.35
117.24
57.24
53.94
53.38
43.13
40.63
O
O
S
N
H
NH2
N
N
Bz
14
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

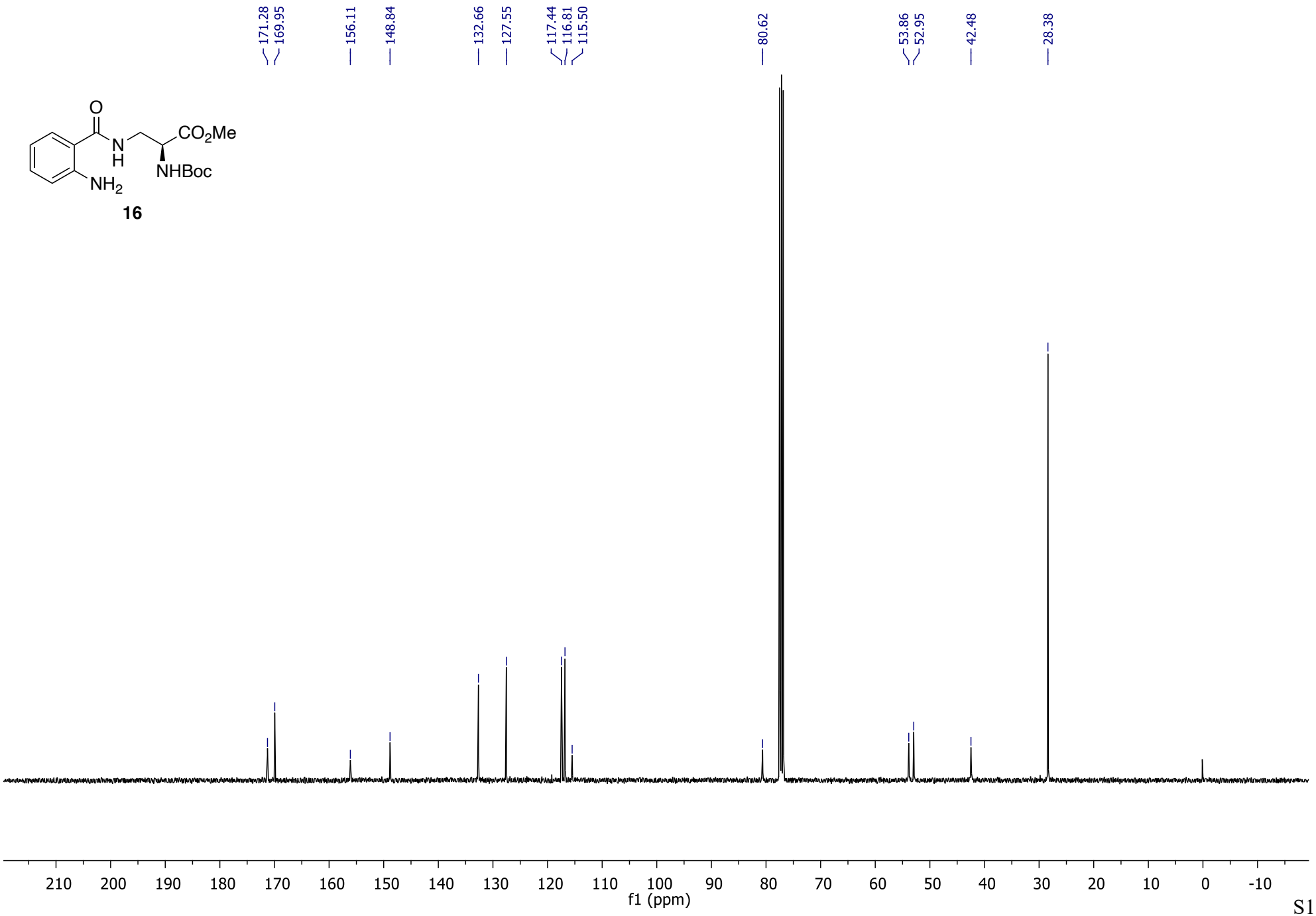

8.09 8.09 8.09 8.09 8.08 8.08 8.07 8.07 8.02 8.02 8.01 8.01 7.99 7.99 7.92 7.92 7.91 7.90 7.89 7.89
7.49 7.49 7.48 7.47 7.47 7.46 7.46 7.45 7.45 7.45 7.44 7.44 7.44 7.43 7.41 7.40 7.40 7.40 7.39 7.39 7.38
4.42 4.41 4.40
3.74
3.41
2.94 2.93 2.92 2.66 2.53
O O
S
N
N
N
N
N
Bz
5
1.83 0.93 1.00 2.91 1.90 1.89 1.75 1.75 1.91 3.81
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

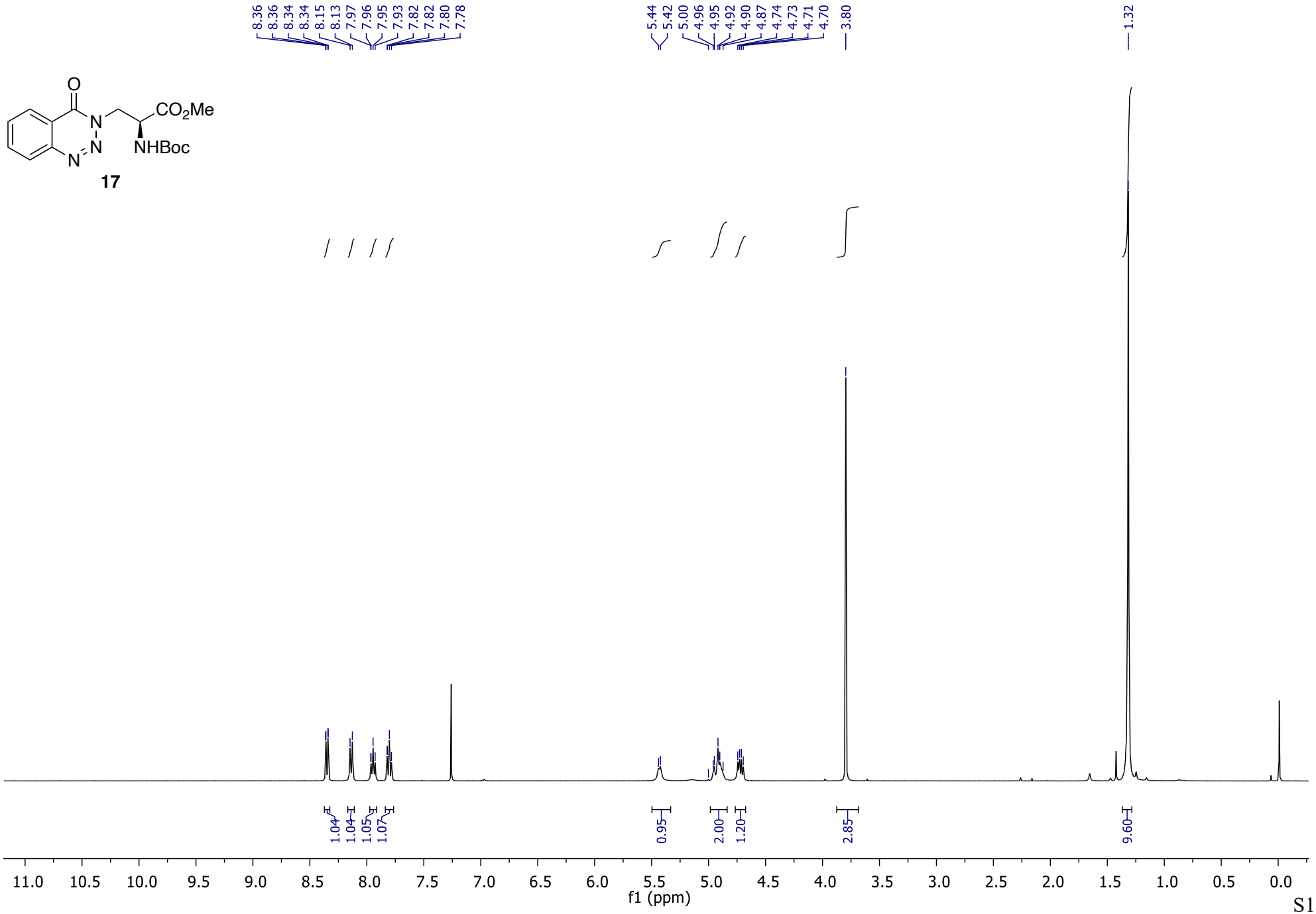

O
O
S
N
N
N
N
N
Bz

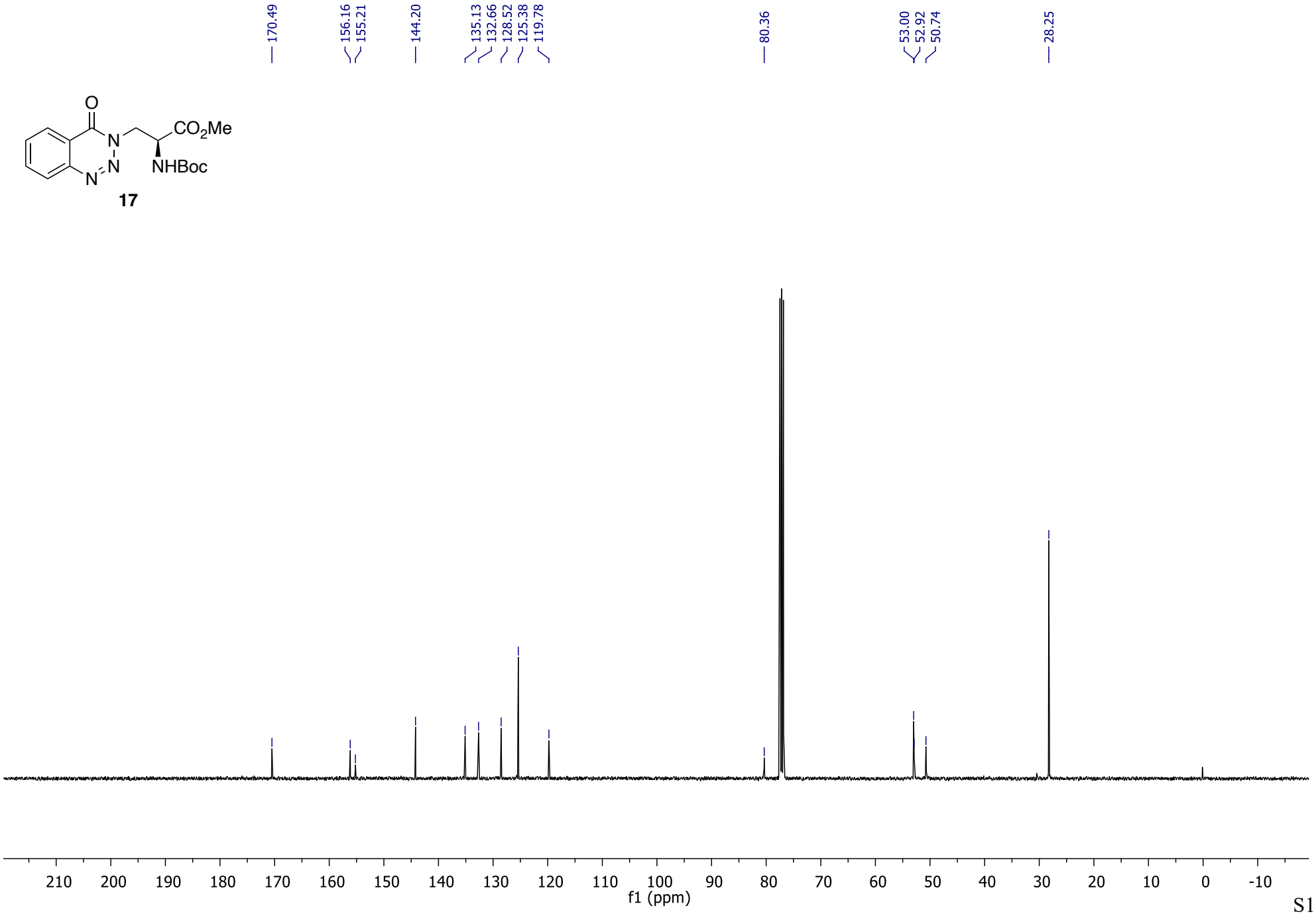
5

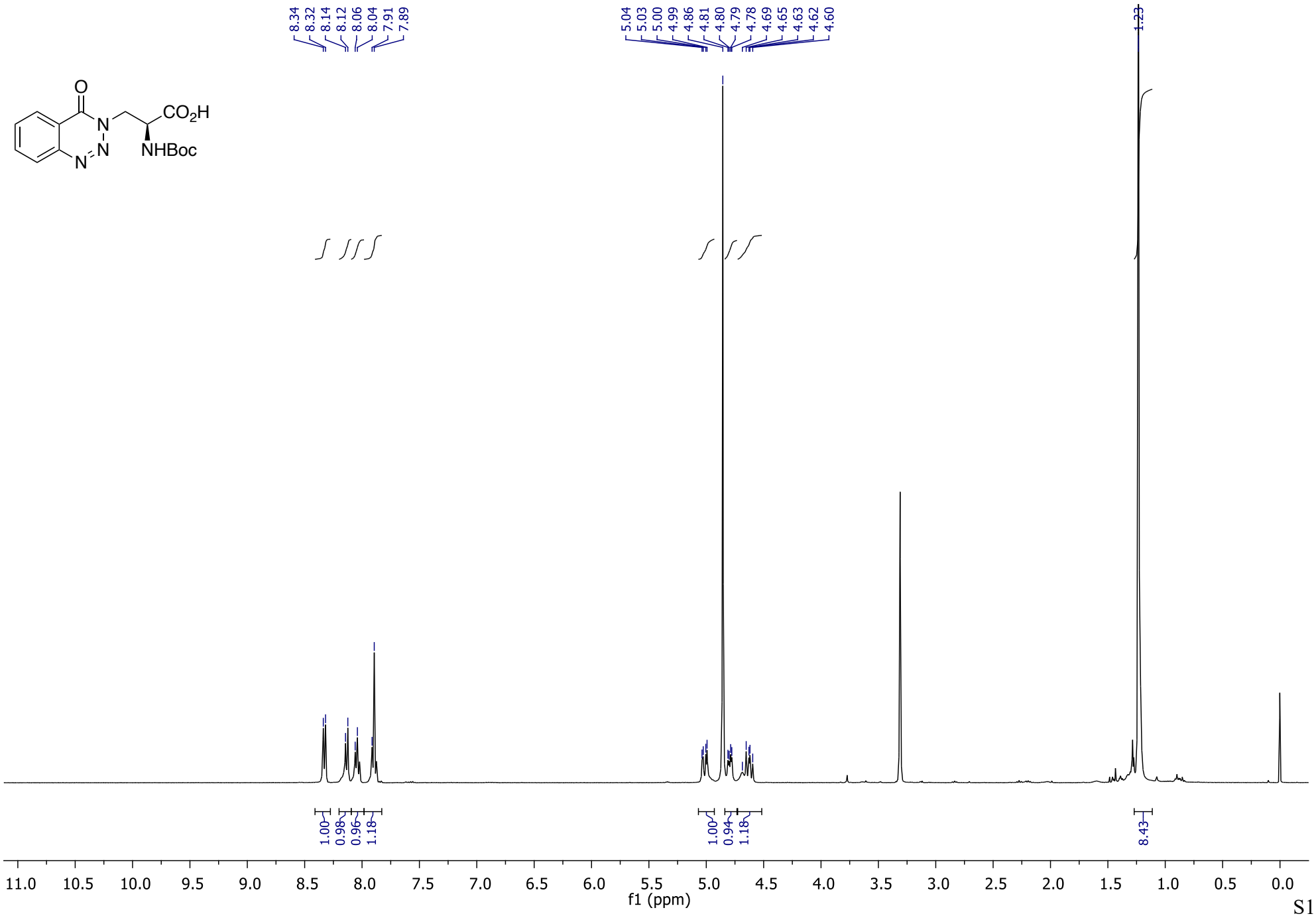
172.43
142.87
135.63
134.39
131.12
130.27
129.73
128.01
121.19
57.97
54.16
46.23
43.23
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

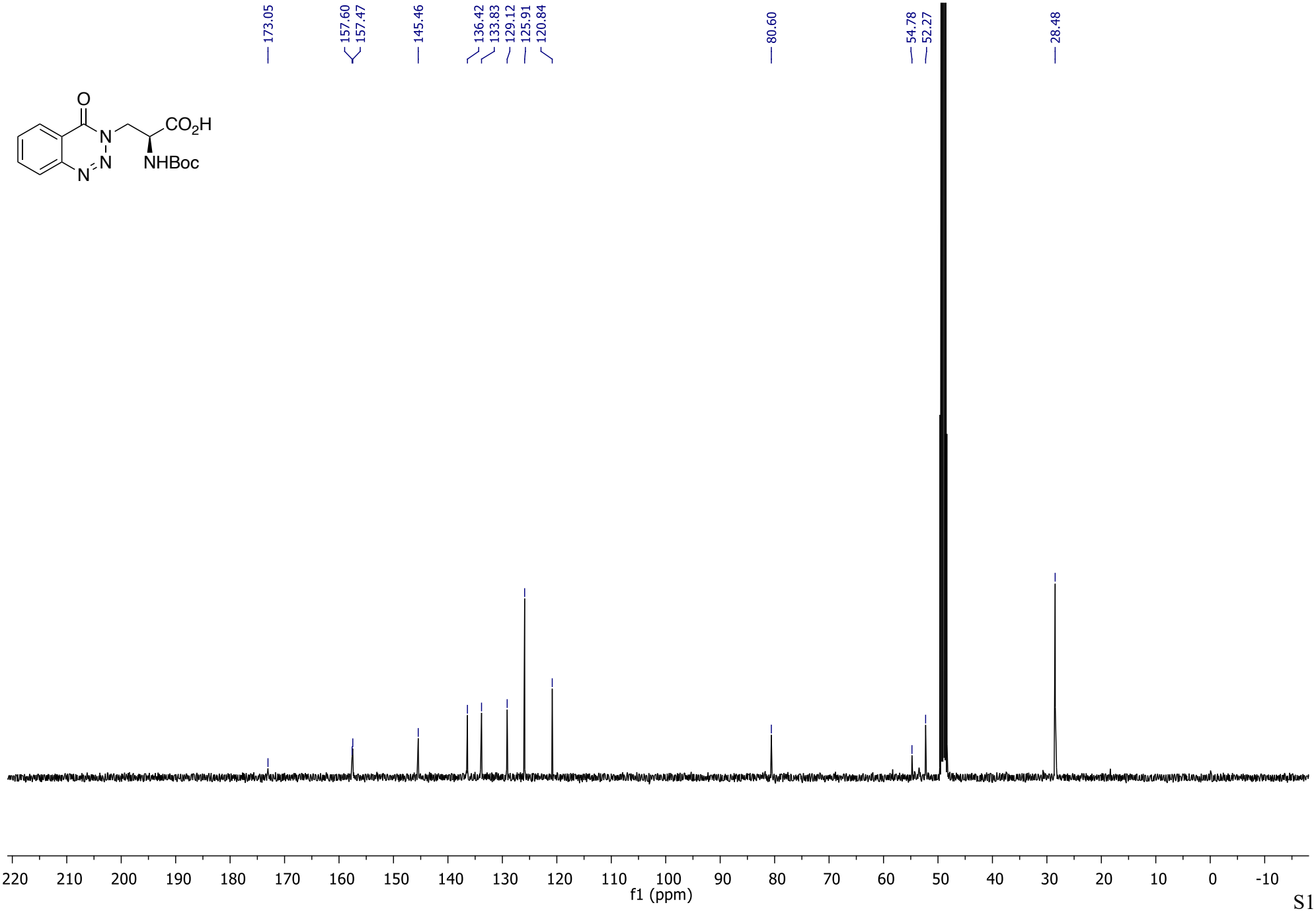

7.34
7.32
7.21
7.19
7.17
6.78
6.67
6.65
6.63
6.61
5.60
5.51
4.50
4.49
3.81
3.78
3.75
3.74
3.72
3.70
1.43
O
N
H
CO2Me
NHBoc
NH2
16
1.05
1.02
0.98
2.12
1.03
1.98
0.90
4.83
9.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

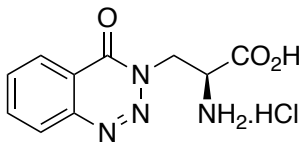

171.28
169.95
156.11
148.84
132.66
127.55
117.44
116.81
115.50
80.62
53.86
52.95
42.48
28.38
O
N
H
CO2Me
NHBoc
NH2
16
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.36
8.36
8.34
8.34
8.15
8.13
7.97
7.96
7.95
7.93
7.82
7.82
7.80
7.78
5.44
5.42
5.00
4.96
4.95
4.92
4.90
4.87
4.74
4.73
4.71
4.70
3.80
1.32
O
N
N
N
CO2Me
NHBoc
17
1.04
1.04
1.05
1.07
0.95
2.00
1.20
2.85
9.60
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


170.49
156.16
155.21
144.20
135.13
132.66
128.52
125.38
119.78
80.36
53.00
52.92
50.74
28.25
O
N
N
N
CO2Me
NHBoc
17
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

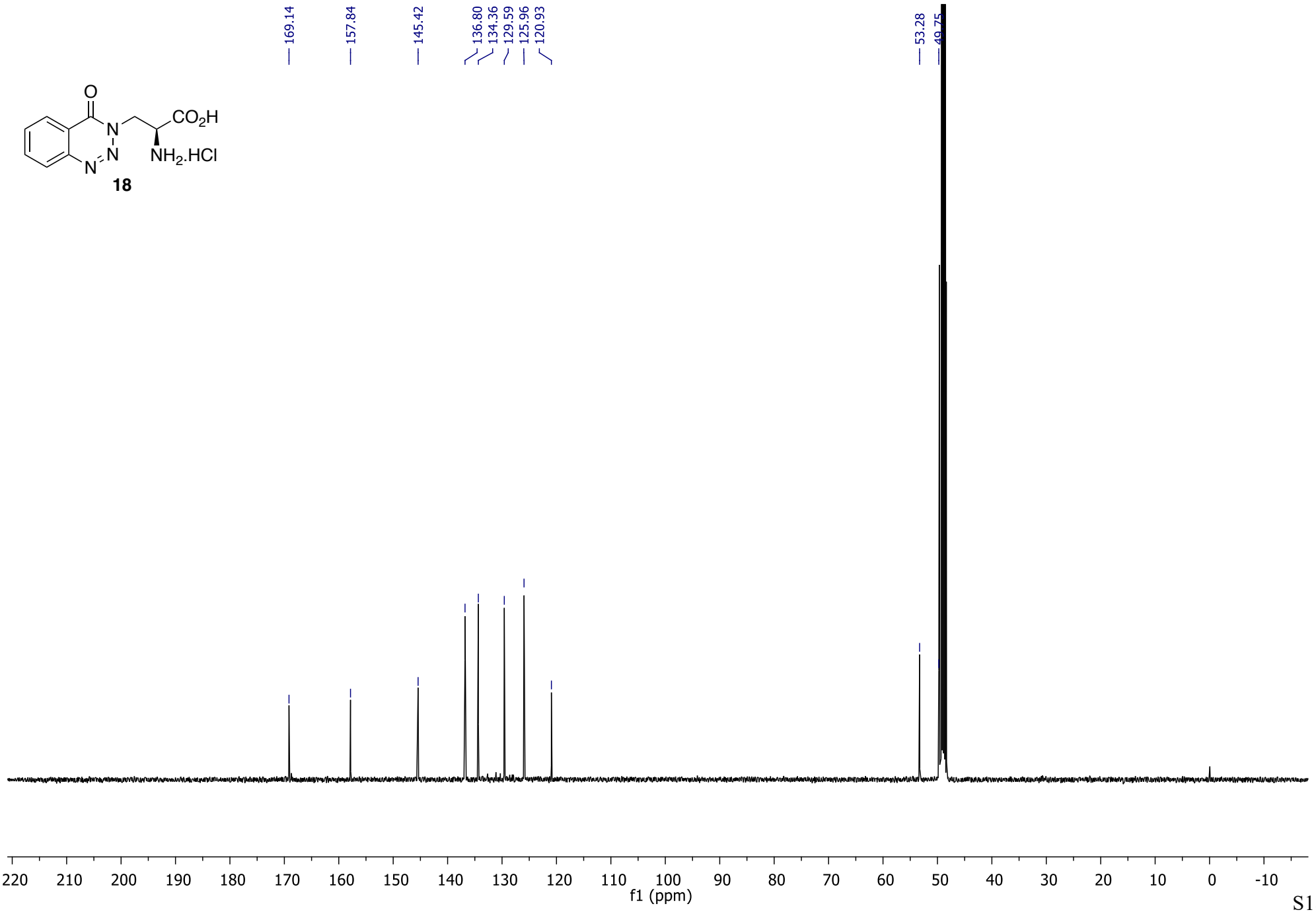

8.34
8.32
8.14
8.12
8.06
8.04
7.91
7.89
5.04
5.03
5.00
4.99
4.86
4.81
4.80
4.79
4.78
4.69
4.65
4.63
4.62
4.60
1.23
O
N
N
N
CO2H
NHBoc
1.00
0.98
0.96
1.18
1.00
0.94
1.18
8.43
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


173.05
157.60
157.47
145.46
136.42
133.83
129.12
125.91
120.84
80.60
54.78
52.27
28.48
O
N
N
N
CO2H
NHBoc
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
N
N
N
CO2H
NH2.HCl

18

8.37
8.36
8.35
8.34
8.22
8.20
8.12
8.12
8.10
8.10
8.08
8.08
7.97
7.96
7.95
7.93
7.93
5.13
5.12
5.10
5.09
4.97
4.95
4.93
4.92
4.64
4.63
4.63
4.61
1.00
1.00
1.00
1.00
1.19
1.36
0.92
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


169.14
157.84
145.42
136.80
134.36
129.59
125.96
120.93
53.28
49.75
O
N
N
N
CO2H
NH2.HCl
18
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)