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Supporting Information

Metal-Free Cascade Reactions for One Pot Tetrahydroquinoxaline Construction through Nitro and Imine Hydrogenation with Water

Yanqi Chen[†], Subin Hao[†], Lingfeng Yin[†], Xinluo Song[†], Zhiyao Liu[†], Mingde Li[†], Li Dang[†,*]

[†]Department of Chemistry and Key Laboratory for Preparation and Application of Ordered Structural Materials of Guangdong Province, Shantou University, Guangdong 515063, P. R. China

Supporting Information Placeholder

Email: ldang@stu.edu.cn

1. General information

All reagents and solvents were purchased from commercial suppliers and used without further purification unless otherwise stated. Analytic thin-layer chromatography (TLC) was carried out with silica gel HF 254-coated plates. Flash column chromatography was performed using the indicated solvent system on silica gel or alumina (300–400 mesh). All compounds were characterized by ^{1}H NMR (400 MHz), ^{13}C NMR (101 MHz), ^{19}F NMR (377 MHz). NMR data were recorded by Bruker 400 MHz instrument.

2. General procedure for the reduction of nitroarenes

Nitroarenes (0.2 mmol), B_2cat_2 (5.0 equiv, 1.0 mmol) were added in a 10 mL tube containing a magnetic stir bar. Then add THF (0.6 ml) and H_2O (36 μl) in a nitrogen-filled glove box and plug with a rubber stopper. The reaction was heated from room temperature to 80 ° C for 1 h. After reaction, the mixture was cooled to room temperature and concentrated under reduced pressure. The residue was purified by silica gel or alumina column chromatography.

3. General procedure for synthesis of dihydroquinoxalinone

2-nitroaniline (0.2 mmol), α-ketoester (0.2mmol), B_2cat_2 (6.0 equiv, 1.2 mmol), MeOH (0.6 ml) and H_2O (36 μl) were added in a 10 mL tube containing a magnetic stir bar. The reaction was heated from room temperature to 80 ° C for 5 h. After reaction, the mixture was cooled to room temperature and concentrated under reduced pressure. The residue was purified by silica gel or alumina column chromatography.

4. General procedure for synthesis of tetrahydroquinoxaline

2-nitroaniline (0.2 mmol), 1,2-dicarbonyl compounds (0.2mmol), B_2cat_2 (8.0 equiv, 1.6 mmol), MeOH (0.6 ml) and H_2O (36 μl) were added in a 10 mL tube containing a magnetic stir bar. The reaction was heated from room temperature to 80 ° C for 7 h. After reaction, the mixture was cooled to room temperature and concentrated under reduced pressure. The residue was purified by silica gel or alumina column chromatography.

5. Reduction of 1,2-difluoro-4,5-dinitrobenzene to 4,5-difluorobenzene-1,2-diamine

1,2-difluoro-4,5-dinitrobenzene (0.2 mmol), B_2cat_2 (9.0 equiv, 1.8 mmol) were added in a 10 mL tube containing a magnetic stir bar. Then add THF (0.6 ml) and H_2O (72 μl) in a nitrogen-filled glove box and plug with a rubber stopper. The reaction was heated from room temperature to 80 ° C for 2 h. After reaction, the mixture was cooled to room temperature and concentrated under reduced pressure. The residue was purified by silica gel or alumina column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a brown solid. ^{1}H NMR (400 MHz, DMSO) δ 6.41 (t, J = 10.5 Hz, 2H), 4.56 (s, 4H). ^{13}C NMR (101 MHz, DMSO) δ 142.74 (d, J = 15.5 Hz), 140.44 (d, J = 15.5 Hz), 131.96 (t, J = 5.1 Hz), 102.46 (s)[1].

Scheme S1. 1,2- Difluoro-4,5-dinitrobenzene reacts with B_2cat_2 to form 4,5-difluorobenzene-1,2-diamine

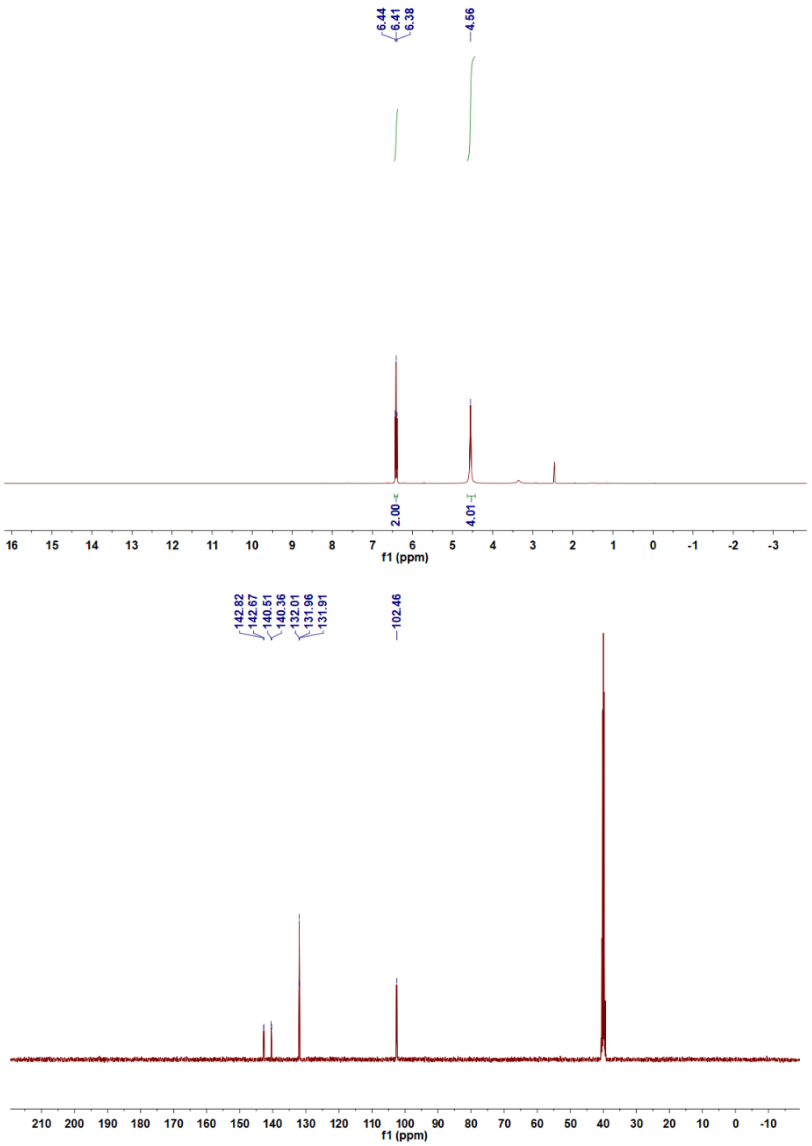


Figure S1. ^{1}H and ^{13}C NMR of reaction between 1,2-difluoro-4,5-dinitrobenzene and B_2cat_2 to form 4,5-difluorobenzene-1,2-diamine.

6. Control experiments

6. 1 Reduction of nitrosobenzene

nitrosobenzene (0.2 mmol), B_2cat_2 (4.0 equiv, 1.0 mmol) were added in a 10 mL tube containing a magnetic stir bar. Then add THF (0.6 ml) and H_2O (36 μl) in a nitrogen-filled glove box and plug with a rubber stopper. The reaction was heated from room temperature to 80 ° C for 30 min. After reaction, the mixture was cooled to room temperature and concentrated under reduced pressure. The yield was measured by ^{1}H NMR using 1,3,5-trimethoxybenzene as an internal standard.

Other reactions were performed according to general procedures and yields were determined by ^{1}H NMR.

Scheme S2. Controlled experiments with nitrosobenzene and Br substituted nitrobenzene with or without water.

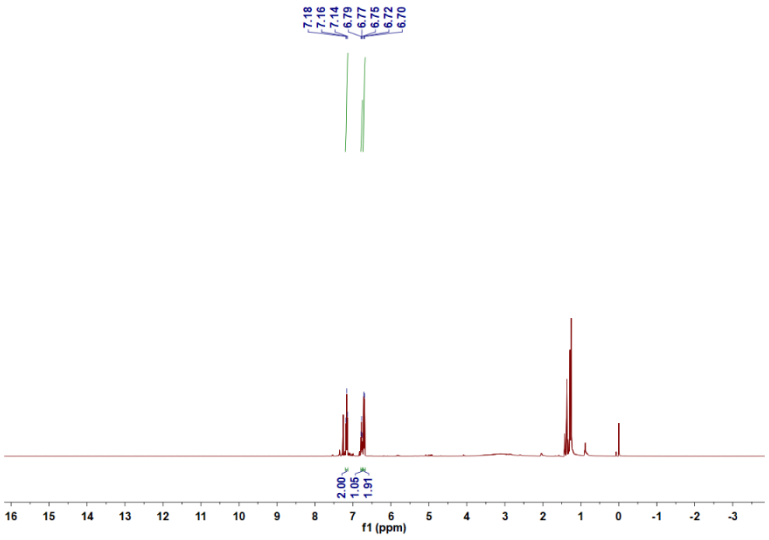


Figure S2. ^{1}H NMR of aniline.

6. 2 Synthesis of tetrahydroquinoxaline

All reactions were carried out at 0.2 mmol of substrate, 0.6 ml of MeOH and 36 μl of H_2O, and the yields were the isolated yields.

NMR spectra is consistent with the one reported in the literature[2].

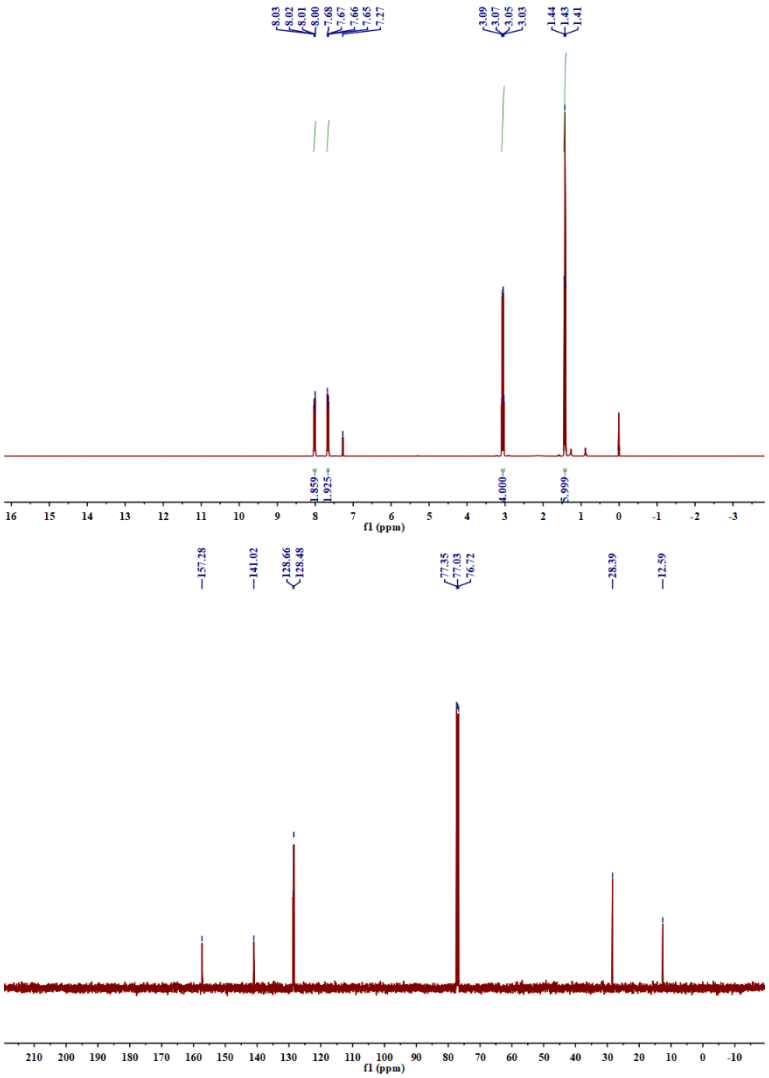


Figure S3. ^{1}H and ^{13}C NMR of **8ii**.

NMR spectra is consistent with reported in the literature[3].

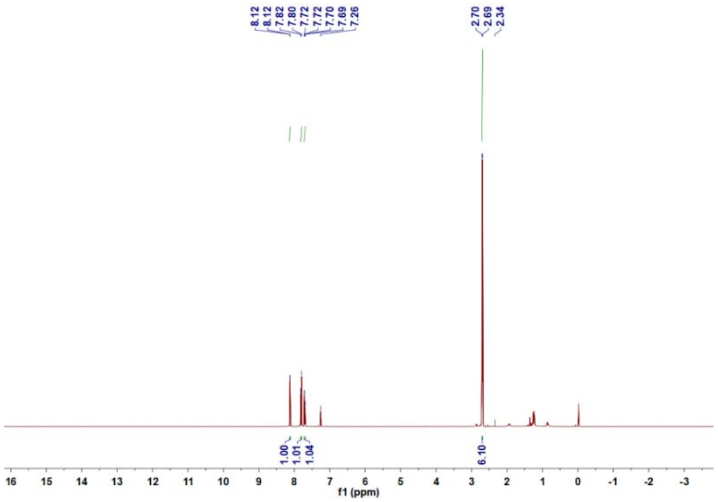


Figure S4. ^{1}H NMR of **9aa**.

7. Characterization data of all products

4-bromoaniline (**2a**)[4]: Purified by column chromatography using hexane/EtOAc = 10:1 as eluent. Obtained as a white solid (31.5 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (d, J = 8.7 Hz, 2H), 6.58 (d, J = 8.7 Hz, 2H), 3.65 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.37 (s), 132.02 (s), 116.72 (s), 110.24 (s).

4-chloroaniline (**2b**)[5]: Purified by column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a white solid (24.4 mg, 96%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (d, J = 8.7 Hz, 2H), 6.62 (d, J = 8.7 Hz, 2H), 3.59 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.95 (s), 129.13 (s), 123.19 (s), 116.24 (s).

4-aminobenzonitrile (**2c**)[4]: Purified by column chromatography using hexane/CH_2Cl_2 = 1:2 as eluent. Obtained as a white solid (21.9 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, J = 8.6 Hz, 2H), 6.66 (d, J = 8.6 Hz, 2H), 4.19 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.39 (s), 132.80 (s), 119.09 (s), 113.43 (s), 99.23 (s).

4-aminobenzoic acid (**2d**)[6]: Purified by column chromatography using hexane/EtOAc = 1:1 as eluent. Obtained as a white solid (25.2 mg, 92%). ^{1}H NMR (400 MHz, DMSO) δ 11.95 (s, 1H), 7.60 (d, J = 8.6 Hz, 2H), 6.53 (d, J = 8.7 Hz, 2H), 5.87 (s, 2H). ^{13}C NMR (101 MHz, DMSO) δ 167.92 (s), 153.58 (s), 131.65 (s), 117.37 (s), 113.01 (s).

4-aminophenyl trifluoromethanesulfonate (**2e**)[7]: Purified by column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a yellow liquid (45.3 mg, 94%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (d, J = 8.9 Hz, 1H), 6.66 (d, J = 9.0 Hz, 1H), 3.71 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.51 (s), 141.57 (s), 122.17 (s), 120.38 (s), 117.19 (s), 115.48 (s). ^{19}F NMR (377 MHz, $CDCl_3$) δ -72.82 (s).

ethyl 4-aminobenzoate (**2f**)[8]: Purified by column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a white solid (32.0 mg, 97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, J = 8.6 Hz, 2H), 6.65 (d, J = 8.6 Hz, 2H), 4.33 (q, J = 7.1 Hz, 2H), 4.08 (s, 2H), 1.37 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.70 (s), 149.72 (s), 130.53 (s), 119.09 (s), 112.75 (s), 59.29 (s), 13.40 (s).

1-(4-aminophenyl)ethan-1-one (**2g**)[4]: Purified by column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a yellow green solid (25.7 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, J = 8.6 Hz, 2H), 7.81 (d, J = 8.6 Hz, 2H), 6.65 (d, J = 8.7 Hz, 2H), 6.65 (d, J = 8.7 Hz, 2H), 4.16 (s, 2H), 2.51 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.41 (s), 151.10 (s), 130.78 (s), 127.96 (s), 113.72 (s), 26.01 (s).

4-nitroaniline (**2h**)[7]: Purified by column chromatography using hexane/EtOAc = 2:1 as eluent. Obtained as a yellow solid (17.1 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 9.1 Hz, 2H), 6.64 (d, J = 9.1 Hz, 2H), 4.41 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.49 (s), 139.18 (s), 126.35 (s), 113.39 (s).

benzene-1,4-diamine (**2i**)[4]: Purified by column chromatography using CH_2Cl_2/MeOH = 40:1 as eluent. Obtained as a brown solid (18.4 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.59 (s, 4H), 3.34 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.61 (s), 116.75 (s).

(4-aminophenyl)(phenyl)methanone (**2j**)[9]: Purified by column chromatography using hexane/EtOAc =3:1 as eluent. Obtained as a white solid (37.8mg, 96%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.70 (m, 1H), 7.50 (dt, J = 33.5, 7.3 Hz, 1H), 6.68 (d, J = 8.5 Hz, 1H), 4.20 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.33 (s), 150.98 (s), 138.88 (s), 132.94 (s), 131.40 (s), 129.52 (s), 128.07 (s), 127.41 (s), 113.64 (s).

3-nitroaniline (**2k**)[10]: Purified by column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a yellow solid (22.4 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (dd, J = 8.1, 1.4 Hz, 1H), 7.51 (t, J = 2.2 Hz, 1H), 7.29 (t, J = 6.5 Hz, 1H), 6.96 (dd, J = 8.0, 1.7 Hz, 1H), 4.01 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.43 (s), 129.91 (s), 120.58 (s), 113.17 (s), 109.04 (s).

[1,1'-biphenyl]-2-amine (**2l**)[11]: Purified by column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a yellow liquid (29.8 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 7.5 Hz, 4H), 7.43 (t, J = 5.5 Hz, 1H), 7.25 – 7.21 (m, 2H), 6.94 – 6.90 (m, 1H), 6.84 – 6.82 (m, 1H), 3.73 (s, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 143.60 (s), 139.65 (s), 130.52 (s), 129.17 (s), 128.88 (s), 128.57 (s), 127.71 (s), 127.23 (s), 118.70 (s), 115.69 (s).

3,4-dimethylaniline (**2m**)[12]: Purified by column chromatography using hexane/EtOAc = 5:1 as eluent. Obtained as a yellow liquid (20.6 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96 (d, J = 7.9 Hz, 1H), 6.56 (s, 1H), 6.50 (d, J = 8.0 Hz, 1H), 3.65 (s, 2H), 2.21 (d, J = 10.4 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.05 (s), 137.41 (s), 130.33 (s), 126.71 (s), 117.04 (s), 112.81 (s), 19.86 (s), 18.77 (s).

3-ethynyl-4-fluoroaniline (**2n**): Purified by column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a green liquid (22.2 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.88 (t, J = 8.9 Hz, 1H), 6.77 (dd, J = 5.6, 2.9 Hz, 1H), 6.67 – 6.60 (m, 1H), 3.55 (s, 2H), 3.26 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.23 (s), 155.82 (s), 142.21 (d, J = 2.5 Hz), 119.30 (s), 117.12 (d, J = 7.3 Hz), 116.10 (s), 115.88 (s), 110.64 (d, J = 16.9 Hz), 81.69 (d, J = 3.4 Hz), 77.29 (d, J = 19.0 Hz).

ethyl 4-amino-3-fluorobenzoate (**2o**)[13]: Purified by column chromatography using hexane/EtOAc = 7:1 as eluent. Obtained as a white solid (32.6 mg, 89%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.64 (m, 2H), 6.74 (t, J = 8.6 Hz, 1H), 4.32 (q, J = 7.1 Hz, 2H), 3.96 (s, 2H), 1.36 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.98 (s), 151.51 (s), 149.13 (s), 139.36 (d, J = 13.1 Hz), 126.79 (d, J = 2.9 Hz), 120.29 (d, J = 6.4 Hz), 116.50 (d, J = 19.9 Hz), 115.27 (d, J = 3.7 Hz), 60.65 (s), 14.33 (s).

ethyl 4-amino-3-methylbenzoate (**2p**)[14]: Purified by column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a white solid (33.7 mg, 94%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.71 (m, 2H), 6.64 (d, J = 8.1 Hz, 1H), 4.33 (q, J = 7.1 Hz, 2H), 2.18 (s, 3H), 1.38 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.93 (s), 149.08 (s), 132.18 (s), 129.26 (s), 121.01 (s), 120.02 (s), 113.69 (s), 60.24 (s), 17.10 (s), 14.43 (s).

N-(4-amino-3-(trifluoromethyl)phenyl)isobutyramide (**2q**)[15]: Purified by column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a white solid (45.8 mg, 93%). ^{1}H NMR (400 MHz, DMSO) δ 9.65 (s, 1H), 7.73 (d, J = 2.4 Hz, 1H), 7.42 (dd, J = 8.8, 2.2 Hz, 1H), 6.79 (d, J = 8.8 Hz, 1H), 5.28 (s, 2H), 2.55 – 2.48 (m, 1H), 1.07 (d, J = 6.8 Hz, 6H).^{13}C NMR (101 MHz, DMSO) δ 175.15 (s), 142.45 (s), 128.88 (s), 126.81 (s), 125.55 (s), 124.10 (s), 117.76 – 116.81 (m), 110.85 (d, J = 29.3 Hz), 110.60 – 110.23 (m), 35.22 (s), 19.94 (s).

4,5-difluoro-2-nitroaniline (**2r**)[16]: Purified by column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a yellow solid (24.7 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (t, J = 9.3 Hz, 1H), 6.65 – 6.59 (m, 1H), 6.13 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.00 (d, J = 14.9 Hz), 154.42 (d, J = 14.5 Hz), 143.09 (s), 142.94 – 142.29 (m), 140.60 (d, J = 14.3 Hz), 114.60 (s), 114.35 (s), 105.67 (s), 105.46 (s).

naphthalen-1-amine (**2s**)[7]: Purified by column chromatography using hexane/EtOAc = 4:1 as eluent. Obtained as a red liquid (25.2 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, J = 5.3, 3.9 Hz, 2H), 7.53 – 7.45 (m, 2H), 7.38 – 7.29 (m, 2H), 6.81 (dd, J = 6.8, 1.3 Hz, 1H), 4.13 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.09 (s), 134.44 (s), 128.57 (s), 126.36 (s), 125.86 (s), 124.87 (s), 123.70 (s), 120.81 (s), 119.00 (s), 109.71 (s).

5-bromonaphthalen-1-amine (**2t**)[17]: Purified by column chromatography using hexane/CH_2Cl_2 = 1:2 as eluent. Obtained as a brown solid (31.5 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, J = 12.3, 7.9 Hz, 2H), 7.74 (d, J = 8.5 Hz, 1H), 7.45 – 7.37 (m, 1H), 7.31 (d, J = 8.2 Hz, 1H), 6.86 (d, J = 7.5 Hz, 1H), 4.20 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.43 (s), 132.97 (s), 130.12 (s), 127.74 (s), 124.84 (d, J = 7.9 Hz), 123.68 (s), 120.73 (s), 118.19 (s), 110.70 (s).

pyren-4-amine (**2u**): Purified by column chromatography using hexane/EtOAc = 5:1 as eluent. Obtained as a yellow green solid (40.0mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (t, J = 6.7 Hz, 2H), 8.03 – 7.93 (m, 5H), 7.85 (d, J = 8.9 Hz, 1H), 7.38 (d, J = 8.2 Hz, 1H), 4.48 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.92 (s), 132.23 (s), 131.68 (s), 127.63 (s), 126.01 (d, J = 5.2 Hz), 125.53 (s), 124.22 (d, J = 19.9 Hz), 123.76 (s), 123.56 (s), 120.17 (s), 116.90 (s), 113.97 (s).

2-chloropyridin-3-amine (**2v**)[5]: Purified by column chromatography using hexane/EtOAc = 3:1 as eluent. Obtained as a white solid (24.2 mg, 94%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (t, J = 2.9 Hz, 1H), 7.05 (d, J = 3.1 Hz, 2H), 3.89 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.68 (s), 138.60 (s), 136.96 (s), 123.34 (s), 122.41 (s).

2-bromopyridin-3-amine (**2w**): Purified by column chromatography using hexane/EtOAc = 4:1 as eluent. Obtained as a white solid (31.1 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (dd, J = 4.4, 1.7 Hz, 1H), 7.04 (ddd, J = 9.6, 7.9, 3.1 Hz, 2H), 3.99 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.43 (s), 139.17 (s), 129.64 (s), 123.62 (s), 121.88 (s).

quinolin-5-amine (**2x**)[7]: Purified by column chromatography using CH_2Cl_2/MeOH = 20:1 as eluent. Obtained as a brown solid (22.2mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (dd, J = 4.2, 1.5 Hz, 1H), 8.21 (d, J = 8.5 Hz, 1H), 7.62 – 7.51 (m, 2H), 7.37 (dd, J = 8.5, 4.2 Hz, 1H), 6.85 (dd, J = 7.3, 0.9 Hz, 1H), 4.21 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.16 (s), 149.08 (s), 142.24 (s), 130.04 (s), 129.55 (s), 120.18 (s), 119.56 (s), 118.76 (s), 110.06 (s).

quinoxalin-6-amine (**2y**)[18]: Purified by column chromatography using CH_2Cl_2/MeOH = 100:1 as eluent. Obtained as an orange solid (23.2 mg, 80%). ^{1}H NMR (400 MHz, DMSO) δ 8.60 (d, J = 1.7 Hz, 1H), 8.44 (d, J = 1.7 Hz, 1H), 7.73 (d, J = 9.0 Hz, 1H), 7.24 (dd, J = 9.0, 2.4 Hz, 1H), 6.91 (d, J = 2.4 Hz, 1H), 6.07 (s, 2H). ^{13}C NMR (101 MHz, DMSO) δ 150.98 (s), 145.39 (d, J = 8.2 Hz), 140.15 (s), 136.99 (s), 130.10 (s), 122.85 (s), 105.49 (s).

1H-indazol-6-amine (**2z**)[19]: Purified by column chromatography using CH_2Cl_2/MeOH = 20:1 as eluent. Obtained as a yellow solid (23.2 mg, 87%). ^{1}H NMR (400 MHz, DMSO) δ 12.26 (s, 1H), 7.72 (s, 1H), 7.35 (d, J = 8.5 Hz, 1H), 6.51 – 6.46 (m, 2H), 5.21 (s, 2H). ^{13}C NMR (101 MHz, DMSO) δ 148.11 (s), 142.54 (s), 133.63 (s), 120.96 (s), 115.98 (s), 112.75 (s), 90.87 (s).

2,3-dihydrobenzofuran-5-amine (**2aa**)[20]: Purified by column chromatography using hexane/EtOAc = 4:1 as eluent. Obtained as a white solid (22.7 mg, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.64 – 6.60 (m, 2H), 6.48 (dd, J = 8.4, 2.4 Hz, 1H), 4.51 (t, J = 8.6 Hz, 2H), 3.34 (s, 2H), 3.14 (t, J = 8.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.21 (s), 139.91 (s), 127.82 (s), 114.68 (s), 112.75 (s), 109.32 (s), 70.91 (s), 30.25 (s).

3-phenyl-3,4-dihydroquinoxalin-2(1H)-one (**5a**)[21]: Purified by column chromatography using CH_2Cl_2/MeOH = 100:1 as eluent. Obtained as a white solid (36.3 mg, 81%). ^{1}H NMR (400 MHz, DMSO) δ 10.43 (s, 1H), 7.34 – 7.24 (m, 5H), 6.76 (dd, J = 16.8, 7.0 Hz, 3H), 6.67 (s, 1H), 6.62 – 6.57 (m, 1H), 4.92 (s, 1H). ^{13}C NMR (101 MHz, DMSO) δ 166.31 (s), 140.73 (s), 134.25 (s), 128.73 (s), 128.02 (s), 127.33 (s), 125.78 (s), 123.44 (s), 118.08 (s), 115.23 (s), 113.74 (s), 59.79 (s).

3-(p-tolyl)-3,4-dihydroquinoxalin-2(1H)-one (**5b**)[21]: Purified by column chromatography using CH_2Cl_2/MeOH = 150:1 as eluent. Obtained as a yellow solid (41.0 mg, 86%). ^{1}H NMR (400 MHz, DMSO) δ 7.22 (d, J = 7.9 Hz, 2H), 7.08 (d, J = 7.9 Hz, 2H), 6.84 (t, J = 7.6 Hz, 1H), 6.74 (dd, J = 13.0, 7.8 Hz, 2H), 6.66 (t, J = 7.2 Hz, 1H), 4.89 (s, 1H), 2.26 (s, 3H).^{13}C NMR (101 MHz, DMSO) δ 168.08 (s), 137.50 (s), 136.81 (s), 133.86 (s), 128.72 (s), 126.57 (s), 125.01 (s), 123.63 (s), 118.14 (s), 114.92 (s), 113.45 (s), 59.90 (s), 19.69 (s).

3-(4-chlorophenyl)-3,4-dihydroquinoxalin-2(1H)-one (**5c**)[21]: Purified by column chromatography using CH_2Cl_2/MeOH = 100:1 as eluent. Obtained as a yellow solid (40.9 mg, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H), 7.37 (d, J = 8.1 Hz, 2H), 7.31 (d, J = 7.2 Hz, 2H), 6.94 (t, J = 7.4 Hz, 1H), 6.79 – 6.72 (m, 3H), 5.06 (s, 1H), 4.27 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.57 (s), 137.26 (s), 134.43 (s), 132.67 (s), 128.96 (s), 128.63 (s), 124.64 (s), 124.25 (s), 119.69 (s), 115.58 (s), 113.88 (s), 60.11 (s).

3-methyl-3,4-dihydroquinoxalin-2(1H)-one (**5d**)[21]: Purified by column chromatography using CH_2Cl_2/MeOH = 100:1 as eluent. Obtained as a white solid (22.7 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.40 (s, 1H), 6.88 (t, J = 7.3 Hz, 1H), 6.74 (ddd, J = 27.6, 17.5, 7.2 Hz, 4H), 4.02 (dd, J = 12.5, 6.0 Hz, 1H), 1.46 (d, J = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.96 (s), 133.46 (s), 125.68 (s), 123.78 (s), 119.56 (s), 115.61 (s), 114.06 (s), 51.89 (s), 17.93 (s).

3-(trifluoromethyl)-3,4-dihydroquinoxalin-2(1H)-one (**5e**)[22]: Purified by column chromatography using CH_2Cl_2/MeOH = 100:1 as eluent. Obtained as a white solid (35.9 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.46 (s, 1H), 6.99 – 6.94 (m, 1H), 6.83 (d, J = 3.4 Hz, 2H), 6.76 (d, J = 7.7 Hz, 1H), 4.56 (q, J = 7.6 Hz, 1H), 4.42 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.84 (s), 130.22 (s), 124.65 (s), 123.65 (s), 122.05 (s), 120.28 (s), 115.90 (s), 113.90 (s), 58.44 (s), 58.14 (s).

3-butyl-3,4-dihydroquinoxalin-2(1H)-one (**5f**)[23]: Purified by column chromatography using CH_2Cl_2/MeOH = 100:1 as eluent. Obtained as a yellow solid (39.6 mg, 97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.04 (s, 1H), 6.89 (dd, J = 9.8, 4.0 Hz, 1H), 6.78 – 6.73 (m, 2H), 6.68 (d, J = 7.6 Hz, 1H), 4.06 – 3.87 (m, 2H), 1.84 (ddd, J = 14.9, 9.8, 5.2 Hz, 1H), 1.77 – 1.68 (m, 1H), 1.46 – 1.32 (m, 4H), 0.91 (t, J = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.25 (s), 133.00 (s), 125.30 (s), 123.81 (s), 119.30 (s), 115.38 (s), 114.05 (s), 56.41 (s), 31.57 (s), 27.45 (s), 22.47 (s), 13.96 (s).

6,7-dimethyl-3-phenyl-3,4-dihydroquinoxalin-2(1H)-one (**5g**)[21]: Purified by column chromatography using CH_2Cl_2/MeOH = 60:1 as eluent. Obtained as a white solid (43.9 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (s, 1H), 7.41 (d, J = 6.2 Hz, 2H), 7.32 (d, J = 7.2 Hz, 2H), 6.51 (s, 2H), 5.03 (s, 1H), 4.13 (s, 1H), 2.15 (d, J = 5.7 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.07 (s), 139.20 (s), 132.13 (s), 130.56 (s), 128.78 (s), 128.35 (s), 127.45 (s), 127.15 (s), 122.52 (s), 116.67 (s), 115.28 (s), 60.89 (s), 19.35 (s), 18.88 (s).

6,7-difluoro-3-phenyl-3,4-dihydroquinoxalin-2(1H)-one (**5h**)[21]: Purified by column chromatography using CH_2Cl_2/MeOH = 70:1 as eluent. Obtained as a yellow solid (43.9 mg, 87%). ^{1}H NMR (400 MHz, DMSO) δ 10.52 (s, 1H), 7.28 (d, J = 14.6 Hz, 5H), 6.82 (s, 1H), 6.71 (dt, J = 15.5, 7.8 Hz, 2H), 4.93 (s, 1H). ^{13}C NMR (101 MHz, DMSO) δ 166.06 (s), 146.60 (d, J = 13.4 Hz), 144.24 (d, J = 13.3 Hz), 143.26 (d, J = 13.7 Hz), 140.94 (d, J = 13.8 Hz), 140.08 (s), 131.13 (d, J = 7.6 Hz), 128.86 (s), 128.24 (s), 127.36 (s), 121.98 (d, J = 6.8 Hz), 104.08 (s), 103.86 (s), 102.06 (s), 101.85 (s), 59.25 (s).

6,7-dichloro-3-phenyl-3,4-dihydroquinoxalin-2(1H)-one (**5i**)[21]: Purified by column chromatography using CH_2Cl_2/MeOH = 100:1 as eluent. Obtained as a yellow solid (41.6 mg, 71%). ^{1}H NMR (400 MHz, DMSO) δ 10.65 (s, 1H), 7.28 (dd, J = 13.3, 9.1 Hz, 5H), 7.06 (s, 1H), 6.86 (d, J = 18.1 Hz, 2H), 4.99 (s, 1H). ^{13}C NMR (101 MHz, DMSO) δ 165.82 (s), 140.16 (s), 134.55 (s), 128.94 (s), 128.33 (s), 127.28 (s), 126.04 (s), 124.56 (s), 118.53 (s), 115.89 (s), 114.04 (s), 59.13 (s).

7-methyl-3-phenyl-3,4-dihydroquinoxalin-2(1H)-one and **6-methyl-3-phenyl-3,4-dihydroquinoxalin-2(1H)-one** (**5j**)[24]: Purified by column chromatography using CH_2Cl_2/MeOH = 150:1 as eluent. Obtained as a white solid (45.3 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 7.37 (dd, J = 33.7, 6.1 Hz, 5H), 6.74 – 6.52 (m, 3H), 5.05 (d, J = 6.3 Hz, 1H), 4.21 (d, J = 18.3 Hz, 1H), 2.25 (d, J = 3.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.17 (s), 166.72 (s), 139.06 (d, J = 13.9 Hz), 133.89 (s), 132.75 (s), 130.53 (s), 129.11 (s), 128.80 (s), 128.41 (s), 127.16 (d, J = 4.8 Hz), 124.75 (s), 124.51 (s), 122.33 (s), 119.94 (s), 116.05 (s), 115.28 (s), 114.41 (s), 113.80 (s), 60.81 (d, J = 13.5 Hz), 21.01 (s), 20.57 (s).

5-methyl-3-phenyl-3,4-dihydroquinoxalin-2(1H)-one (**5k**): Purified by column chromatography using CH_2Cl_2/MeOH = 150:1 as eluent. Obtained as a yellow solid (40.5 mg, 85%). ^{1}H NMR (400 MHz, DMSO) δ 10.36 (s, 1H), 7.24 (d, J = 17.9 Hz, 5H), 6.66 (d, J = 6.9 Hz, 1H), 6.57 (d, J = 7.2 Hz, 1H), 6.49 (t, J = 7.2 Hz, 1H), 6.13 (s, 1H), 4.92 (s, 1H), 2.13 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 166.01 (s), 140.94 (s), 131.73 (s), 128.74 (s), 127.90 (s), 126.66 (s), 125.36 (s), 124.96 (s), 121.63 (s), 117.80 (s), 113.40 (s), 59.63 (s), 17.54 (s).

1,3-diphenyl-3,4-dihydroquinoxalin-2(1H)-one (**5l**): Purified by column chromatography using CH_2Cl_2/MeOH = 100:1 as eluent. Obtained as a white solid (37.9 mg, 63%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.42 (m, 5H), 7.39 – 7.31 (m, 3H), 7.25 (s, 1H), 6.94 (t, J = 7.1 Hz, 1H), 6.80 (d, J = 7.8 Hz, 1H), 6.67 (t, J = 8.3 Hz, 1H), 6.33 (d, J = 8.1 Hz, 1H), 5.22 (s, 1H), 4.51 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.71 (s), 138.86 (s), 137.49 (s), 134.03 (s), 129.81 (s), 129.52 (s), 128.88 (d, J = 16.6 Hz), 128.37 (d, J = 9.2 Hz), 127.04 (s), 123.91 (s), 119.31 (s), 116.85 (s), 114.34 (s), 61.13 (s).

1-methyl-3-phenyl-3,4-dihydroquinoxalin-2(1H)-one (**5m**)[25]: Purified by column chromatography using CH_2Cl_2/MeOH = 100:1 as eluent. Obtained as a white solid (36.2 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (ddd, J = 16.1, 10.2, 4.6 Hz, 5H), 6.96 (dd, J = 14.9, 7.6 Hz, 2H), 6.89 – 6.83 (m, 1H), 6.74 (d, J = 8.8 Hz, 1H), 5.05 (s, 1H), 3.38 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 166.04 (s), 139.11 (s), 134.49 (s), 128.71 (s), 128.33 (d, J = 8.4 Hz), 127.13 (s), 123.77 (s), 119.54 (s), 114.79 (s), 114.02 (s), 60.83 (s), 29.22 (s).

3-butyl-6,7-difluoro-3,4-dihydroquinoxalin-2(1H)-one (**5n**): Purified by column chromatography using CH_2Cl_2/MeOH = 70:1 as eluent. Obtained as a yellow solid (41.0 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.56 (s, 1H), 6.68 – 6.48 (m, 2H), 3.99 – 3.82 (m, 2H), 1.86 – 1.66 (m, 2H), 1.40 (dd, J = 18.3, 7.9 Hz, 4H), 0.92 (t, J = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.20 (s), 147.57 (d, J = 13.8 Hz), 145.03 (dd, J = 26.3, 13.5 Hz), 142.53 (d, J = 13.6 Hz), 129.19 (s), 121.15 (s), 104.73 (s), 104.51 (s), 103.05 (s), 102.83 (s), 56.06 (s), 31.40 (s), 27.37 (s), 22.42 (s), 13.90 (s).

2,3-dimethyl-1,2,3,4-tetrahydroquinoxaline (**8a**)[26]: Purified by column chromatography using hexane/EtOAc = 10:1 as eluent. Obtained as white solid (26.6 mg, 82%). *cis*/*trans* = 67/33 (separable).

***cis* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.60 (dt, J = 7.2, 3.6 Hz, 2H), 6.54 – 6.50 (m, 2H), 3.51 (q, J = 5.8 Hz, 2H), 1.15 (d, J = 6.4 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.63 (s), 118.58 (s), 114.44 (s), 49.06 (s), 17.20 (s).

***trans* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.60 (d, J = 2.9 Hz, 1H), 6.54 – 6.50 (m, 1H), 3.52 (s, 1H), 3.04 (s, 1H), 1.20 – 1.18 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.50 (s), 118.58 (s), 113.94 (s), 52.06 (s), 18.99 (s).

2,3,5-trimethyl-1,2,3,4-tetrahydroquinoxaline (**8b**)[27]: Purified by column chromatography using hexane/EtOAc = 15:1 as eluent. Obtained as green liquid (33.8 mg, 96%). *cis*/*trans* = 71/29 (separable).

***cis* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.53 (s, 2H), 6.42 (dd, J = 6.6, 2.5 Hz, 1H), 3.53 (ddd, J = 28.3, 6.5, 2.7 Hz, 2H), 2.12 (s, 3H), 1.16 (dd, J = 11.1, 6.5 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.13 (s), 130.68 (s), 121.70 (s), 120.19 (s), 117.77 (s), 112.60 (s), 49.33 (s), 48.81 (s), 17.54 (s), 17.20 (s), 17.08 (d, J = 21.1 Hz).

***trans* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.58 – 6.48 (m, 2H), 6.43 (dd, J = 6.5, 2.2 Hz, 1H), 3.10 – 2.99 (m, 2H), 2.11 (s, 3H), 1.21 (dd, J = 15.8, 6.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.95 (s), 131.50 (s), 121.29 (s), 120.26 (s), 117.81 (s), 112.15 (s), 52.34 (s), 51.79 (s), 19.07 (d, J = 16.5 Hz), 16.93 (s).

2,3,6-trimethyl-1,2,3,4-tetrahydroquinoxaline (**8c**)[26]: Purified by column chromatography using hexane/EtOAc = 15:1 as eluent. Obtained as white solid (32.8 mg, 93%). *cis*/*trans* = 70/30 (separable).

***cis* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.46 – 6.32 (m, 3H), 3.52 – 3.45 (m, 2H), 2.19 (s, 3H), 1.13 (d, J = 6.4 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.64 (s), 130.00 (s), 128.23 (s), 119.00 (s), 115.17 (s), 114.76 (s), 49.15 (s), 20.66 (s), 17.10 (s).
***trans* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.44 (d, J = 6.8 Hz, 2H), 6.35 (s, 1H), 3.08 (t, J = 39.6 Hz, 4H), 2.19 (s, 3H), 1.18 (d, J = 5.7 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.53 (s), 130.93 (s), 128.22 (s), 118.92 (s), 115.55 – 114.81 (m), 114.46 (d, J = 43.7 Hz), 52.22 (s), 20.68 (s), 19.02 (d, J = 5.4 Hz).

2,3,5,7-tetramethyl-1,2,3,4-tetrahydroquinoxaline (**8d**): Purified by column chromatography using hexane/EtOAc = 8:1 as eluent. Obtained as white solid (33.1 mg, 87%). *cis*/*trans* = 69/31 (separable).
***cis* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.37 (s, 1H), 6.27 (s, 1H), 3.52 (dd, J = 19.8, 6.3 Hz, 2H), 2.21 (s, 3H), 2.11 (s, 3H), 1.16 (dd, J = 11.7, 6.5 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.28 (s), 128.15 (s), 127.27 (s), 122.04 (s), 120.83 (s), 113.24 (s), 49.42 (s), 48.96 (s), 20.62 (s), 17.50 (s), 17.17 (s), 17.05 (d, J = 21.6 Hz).
***trans* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.34 (s, 1H), 6.26 (s, 1H), 2.98 (d, J = 30.5 Hz, 2H), 2.15 (d, J = 20.0 Hz, 3H), 2.09 (s, 3H), 1.19 (dd, J = 17.2, 5.8 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.14 (s), 128.98 (s), 127.33 (s), 121.59 (s), 120.78 (s), 112.75 (s), 52.43 (s), 51.98 (s), 20.57 (s), 19.08 (d, J = 7.1 Hz), 16.85 (s).

6-(tert-butyl)-2,3-dimethyl-1,2,3,4-tetrahydroquinoxaline (**8e**)[28]: Purified by column chromatography using hexane/EtOAc = 20:1 as eluent. Obtained as white solid (36.2 mg, 83%). *cis*/*trans* = 80/20 (separable).
***cis* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.63 (d, J = 8.0 Hz, 1H), 6.56 (d, J = 1.8 Hz, 1H), 6.48 (d, J = 8.1 Hz, 1H), 3.49 (dd, J = 9.4, 6.1 Hz, 2H), 1.26 (s, 9H), 1.14 (dd, J = 6.4, 3.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.92 (s), 132.15 (s), 115.54 (s), 114.41 (s), 112.03 (s), 49.28 (d, J = 6.0 Hz), 33.91 (s), 31.58 (s), 17.21 (d, J = 20.3 Hz), 17.07 – 16.64 (m).
***trans* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.61 (d, J = 17.6 Hz, 2H), 6.49 (d, J = 7.3 Hz, 1H), 3.03 (s, 2H), 1.26 (s, 9H), 1.18 (d, J = 5.6 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.01 (s), 132.92 (s), 130.89 (s), 115.57 (s), 113.97 (s), 111.53 (s), 52.19 (d, J = 10.8 Hz), 33.91 (s), 31.54 (s), 18.94 (s).

6-chloro-2,3-dimethyl-1,2,3,4-tetrahydroquinoxaline (**8f**)[26]: Purified by column chromatography using hexane/EtOAc = 20:1 as eluent. Obtained as white solid (37.4 mg, 95%). *cis*/*trans* = 83/17 (separable).
***cis* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.52 (dd, J = 8.2, 2.2 Hz, 1H), 6.46 (d, J = 2.2 Hz, 1H), 6.39 (d, J = 8.2 Hz, 1H), 3.47 (dt, J = 9.6, 3.1 Hz, 2H), 1.14 – 1.11 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.75 (s), 131.06 (s), 122.99 (s), 117.78 (s), 114.90 (s), 113.67 (s), 48.87 (d, J = 3.5 Hz), 17.08 (s).
***trans* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.52 (dd, J = 8.2, 2.1 Hz, 1H), 6.46 (d, J = 2.2 Hz, 1H), 6.40 (d, J = 8.2 Hz, 1H), 3.54 (s, 2H), 3.00 (tq, J = 13.2, 6.5 Hz, 2H), 1.17 (d, J = 5.8 Hz, 6H). ^{13}C NMR (101 MHz,

$CDCl_3$) δ 134.49 (s), 131.87 (s), 122.98 (s), 117.76 (s), 114.41 (s), 113.23 (s), 51.85 (d, J = 6.5 Hz), 18.93 (d, J = 3.5 Hz).

methyl 2,3-dimethyl-1,2,3,4-tetrahydroquinoxaline-6-carboxylate (**8g**)[28]: Purified by column chromatography using hexane/EtOAc = 20:1 as eluent. Obtained as white solid (41.4 mg, 94%). *cis*/*trans* = 77/23 (inseparable).

Mixture of cis and trans isomer of 8g (inseparable): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.29 (m, 1H), 7.18 (dd, J = 4.2, 1.8 Hz, 1H), 6.41 (dd, J = 8.2, 4.1 Hz, 1H), 3.81 (s, 3H), 3.50 (ddd, J = 41.0, 6.5, 2.9 Hz, 2H), 3.14 – 3.02 (m, 1H), 3.00 – 2.85 (m, 1H), 1.17 (d, J = 6.2 Hz, 2H), 1.11 (t, J = 6.3 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.75 (s), 138.37 (s), 137.77 (s), 132.41 (s), 131.60 (s), 121.80 (d, J = 6.4 Hz), 119.23 (s), 115.40 (s), 114.96 (s), 112.59 (s), 112.19 (s), 52.40 (s), 51.60 (d, J = 12.1 Hz), 49.39 (s), 48.64 (s), 19.11 (d, J = 16.7 Hz), 17.49 (s), 17.20 (s).

6,7-difluoro-2,3-dimethyl-1,2,3,4-tetrahydroquinoxaline (**8h**)[28]: Purified by column chromatography using hexane/EtOAc = 15:1 as eluent. Obtained as white solid (38.4 mg, 97%). *cis*/*trans* = 83/17 (separable).

***cis* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.30 (t, J = 9.6 Hz, 2H), 3.45 (dd, J = 11.6, 5.8 Hz, 4H), 1.12 (d, J = 6.3 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.32 (d, J = 15.7 Hz), 141.96 (d, J = 15.6 Hz), 128.32 (t, J = 5.0 Hz), 102.77 (dd, J = 13.4, 8.4 Hz), 48.87 (s), 16.93 (s).

***trans* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.29 (t, J = 9.6 Hz, 1H), 3.02 – 2.91 (m, 1H), 1.16 (d, J = 5.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.29 (d, J = 15.7 Hz), 141.93 (d, J = 15.4 Hz), 129.14 (s), 102.34 (dd, J = 13.3, 8.5 Hz), 51.86 (s), 18.82 (s).

2,3-diethyl-1,2,3,4-tetrahydroquinoxaline (**8i**)[26]: Purified by column chromatography using hexane/EtOAc = 8:1 as eluent. Obtained as white solid (34.3 mg, 90%). *cis*/*trans* = 0/100.

***trans* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.59 (dd, J = 5.6, 3.5 Hz, 2H), 6.52 (dd, J = 5.5, 3.6 Hz, 2H), 3.28 (t, J = 6.2 Hz, 2H), 1.48 (p, J = 7.2 Hz, 4H), 1.00 (t, J = 7.5 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.80 (s), 118.51 (s), 114.38 (s), 54.61 (s), 22.96 (s), 10.46 (s).

2,3-diphenyl-1,2,3,4-tetrahydroquinoxaline (**8j**)[28]: Purified by column chromatography using hexane/EtOAc = 30:1 as eluent. Obtained as yellow solid (43.5 mg, 76%). *cis*/*trans* = 0/100.

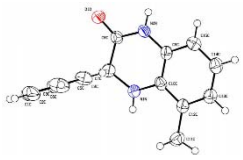
***trans* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.12 (m, 6H), 6.93 – 6.89 (m, 4H), 6.74 (dd, J = 5.6, 3.5 Hz, 2H), 6.66 (dd, J = 5.6, 3.5 Hz, 2H), 4.77 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.59 (s), 133.11 (s), 127.92 (s), 127.69 (s), 127.31 (s), 118.93 (s), 114.19 (s), 77.38 (s), 77.07 (s), 76.75 (s), 59.49 (s).

2-methyl-1,2,3,4-tetrahydroquinoxaline (**8k**)[26]: Purified by column chromatography using hexane/EtOAc = 5:1 as eluent. Obtained as yellow solid (16.8 mg, 57%). *cis*/*trans* = 0/100. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.60 (dt, J = 7.2, 3.6 Hz, 2H), 6.56 – 6.50 (m, 2H), 3.53 (dd, J = 14.4, 6.2 Hz, 1H), 3.34 (dd, J = 10.7, 2.9 Hz, 1H), 3.06 (dd, J = 10.7, 8.2 Hz, 1H), 1.21 (d, J = 6.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.40 (s), 133.03 (s), 118.83 (s), 114.59 (d, J = 6.2 Hz), 48.20 (s), 45.75 (s), 19.81 (s).

2-phenyl-1,2,3,4-tetrahydroquinoxaline (**8l**)[26]: Purified by column chromatography using hexane/EtOAc = 5:1 as eluent. Obtained as white solid (25.6 mg, 61%). *cis*/*trans* = 0/100. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (dt, J = 14.5, 7.0 Hz, 5H), 6.69 – 6.59 (m, 4H), 4.52 (dd, J = 8.3, 2.7 Hz, 1H), 3.49 (dd, J = 11.1, 2.8 Hz, 1H), 3.34 (dd, J = 10.9, 8.6 Hz, 1H), 1.64 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 128.73 (s), 128.06 (s), 127.04 (s), 120.08 (s), 115.69 (s), 114.70 (s), 54.60 (s).

dibenzo[a,c]phenazine (**8m**)[29]: Purified by column chromatography using hexane/EtOAc = 5:1 as eluent. Obtained as yellow solid (49.9 mg, 89%).
***trans* isomer**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.40 (d, J = 7.8 Hz, 2H), 8.55 (d, J = 7.9 Hz, 2H), 8.37 –8.30 (m, 2H), 7.87 – 7.72 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.42 (s), 142.17 (s), 132.05 (s), 130.28(s), 129.71 (s), 129.44 (s), 127.90 (s), 126.27 (s), 122.89 (s).

8. X-ray results of the product

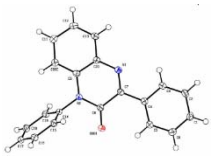
≡ 

CCDC:2292058

5k

Chemical formula	$C_{15}H_{14}N_2O$
Formula weight	238.28
Space group	$P2_1$
Z	2
a/Å	8.1113 (5)
b/Å	6.7331 (3)

c/Å	11.6092 (7)
α/°	90.00
β/°	105.805 (7)
γ/°	90.00 (2)
Volume/Å^3	610.06 (6)
ρ_{calc}g/cm^3	1.297
μ/mm^{-1}	0.658
Temperature/K	100.00 (10)

≡ 

CCDC:2292057

5l

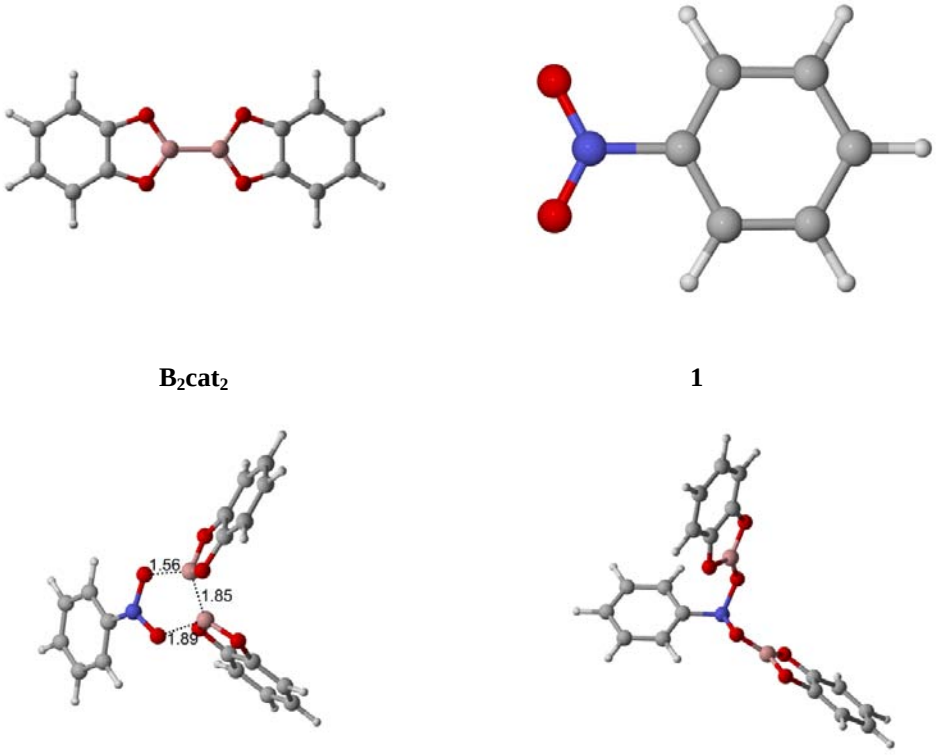
Chemical formula	$C_{20}H_{16}N_2O$
Formula weight	300.35
Space group	P-1
Z	2
a/Å	5.69230 (10)
b/Å	11.2384 (3)
c/Å	11.8487 (3)
α/°	109.053 (2)
β/°	93.530 (2)
γ/°	92.661 (2)
Volume/Å^3	713.32 (3)
ρ_{calc}g/cm^3	1.398
μ/mm^{-1}	0.689
Temperature/K	99.99 (10)

9. Computational Results

9.1 Computational Details

All the calculations were carried out via density functional theory (DFT) calculation using Gaussian 16 with the M06-2X functional. Geometric structures of all species in this work were optimized in gas phase. In addition, free energy corrections were considered at a concentration of 1 M and a temperature of 298.15 K. Frequency calculation were performed to determine all the stationary points (no imaginary frequency) and transition state structures (only one imaginary frequency). The 6-311G(d) basis set was used for all atoms. In addition, the intrinsic reaction coordinate (IRC) calculation was applied to confirm the connection of each transition state to its corresponding appropriate intermediates, reactants, or products. The solvent effect of Tetrahydrofuran was evaluated through the SMD method, in which a better basis system was used. We employed 6-311++G(d,p) basis sets for all atoms.

Most of the computational work was based on previous work by our group[30].



B_2cat_2 **1**

TS1 **INT1**

Figure S5. Optimized geometries with partial structural parameters (distances in Å) for the species involved in the process of this study.

9.2 Cartesian coordinates of the optimized structures

B_2cat_2

E = -812.762271516 a.u.

0 1

C	-4.93808600	-1.13508800	1.30603700
C	-3.54259900	-1.15173600	1.32422800
C	-2.91395400	0.07607000	1.34361100
C	-3.62572000	1.26884500	1.34503600
C	-5.00475300	1.29876400	1.32717500
C	-5.65284500	0.06283200	1.30746900
H	-5.47717800	-2.07459600	1.29030100
H	-2.97436100	-2.07297000	1.32334700
H	-5.54563600	2.23630800	1.32852200
H	-6.73568400	0.03458400	1.29295200
O	-1.57247200	0.35971700	1.36378000
O	-2.73925800	2.31484100	1.36612200
B	-1.48045300	1.74037300	1.37738500
C	2.10848600	3.07483900	1.43618400
C	3.48752500	3.04525000	1.45401500
C	4.13531900	4.28133900	1.47376200
C	3.42026500	5.47908300	1.47526100
C	2.02477400	5.49539300	1.45709800
C	1.39642200	4.26743600	1.43767400
H	4.02863200	2.10783600	1.45261500
H	5.21815100	4.30985200	1.48825800
H	3.95912800	6.41872300	1.49102800
H	1.45631500	6.41649100	1.45803100
O	1.22228500	2.02862100	1.41507100
O	0.05501300	3.98345500	1.41752100
B	-0.03665700	2.60276500	1.40386200

1

E = -436.673286117 a.u.

0 1

N	0.04506300	2.37139900	-0.04455600
C	0.54390100	3.06769500	1.16131200
C	-0.37754700	3.58380700	2.05915600
C	1.91334000	3.17697200	1.34677400

C	0.09881700	4.23602800	3.18885900
H	-1.43528700	3.46994800	1.86460600
C	2.37333300	3.83214600	2.48157800
H	2.58759600	2.75535000	0.61378900
C	1.46923700	4.35956700	3.39911800
H	-0.60174300	4.64799000	3.90504100
H	3.43913800	3.93023000	2.64848600
H	1.83459300	4.86979000	4.28279800
O	0.86838700	1.92909400	-0.81379900
O	-1.15443100	2.28873300	-0.18462900
C	0.40644400	3.41781100	6.66469200
C	-0.58752700	1.21477500	7.00310600
C	1.29672200	3.16175400	7.69565700
H	0.41934300	4.35113300	6.11768000
C	0.31064700	0.98285000	8.03345700
H	-1.32250800	0.47687700	6.71161800
C	1.25067100	1.94999100	8.38091000
H	2.02868500	3.91291300	7.96658500
H	0.27707100	0.04050700	8.56661800
H	1.94632100	1.76054000	9.18976900

TS1

E = -1249.39954539 a.u.

0 1

C	-4.70171200	-0.51167600	0.27951500
C	-3.61403600	-0.73597000	1.12670300
C	-3.17378500	0.33679700	1.87581800
C	-3.78464300	1.59247500	1.79761400
C	-4.85376600	1.82317700	0.95394000
C	-5.30800300	0.74132900	0.19601100
H	-5.07873000	-1.32733600	-0.32596900
H	-3.12730800	-1.70056600	1.19850500
H	-5.31458800	2.80127600	0.89791500
H	-6.14981900	0.88093000	-0.47197500
O	-2.13623800	0.39112100	2.75102200
O	-3.16773200	2.45856800	2.63580800
B	-2.09279500	1.72646900	3.23022500
C	1.63399500	2.75267900	2.55605600
C	3.00331900	2.58542500	2.52521400
C	3.69246400	3.25770400	1.51394500
C	3.02476500	4.05430000	0.58319200
C	1.63840000	4.21418400	0.62164400
C	0.96714700	3.54950600	1.62752900
H	3.50670100	1.96048100	3.25192400
H	4.76930500	3.15615100	1.45056800
H	3.59344000	4.55935300	-0.18842200
H	1.10607800	4.82633600	-0.09512800
O	0.72099000	2.22122400	3.42328200
O	-0.37189100	3.52868900	1.89601600
B	-0.52575000	2.68912500	2.99090200
N	-1.43355900	2.69994800	5.27719000
O	-2.11268800	1.71536500	4.79362800
O	-1.24664900	3.63186600	4.46100200
C	-0.51516700	2.42962700	6.32499800

INT1

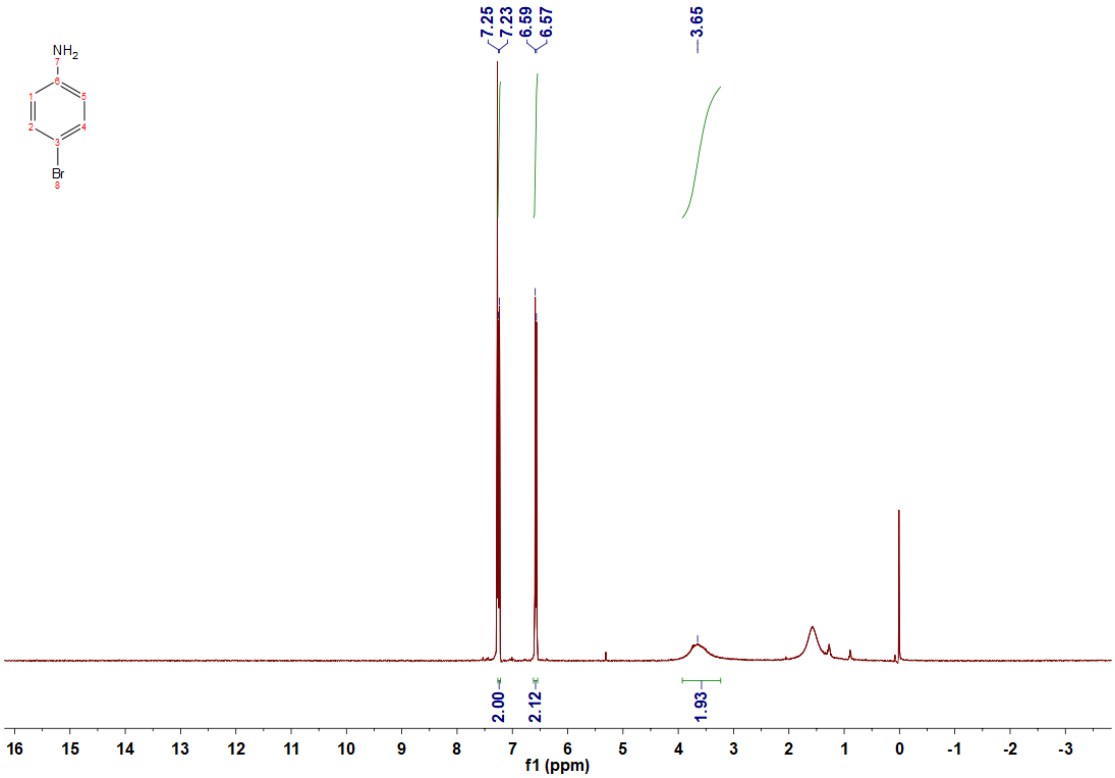
E = -1249.53865266 a.u.

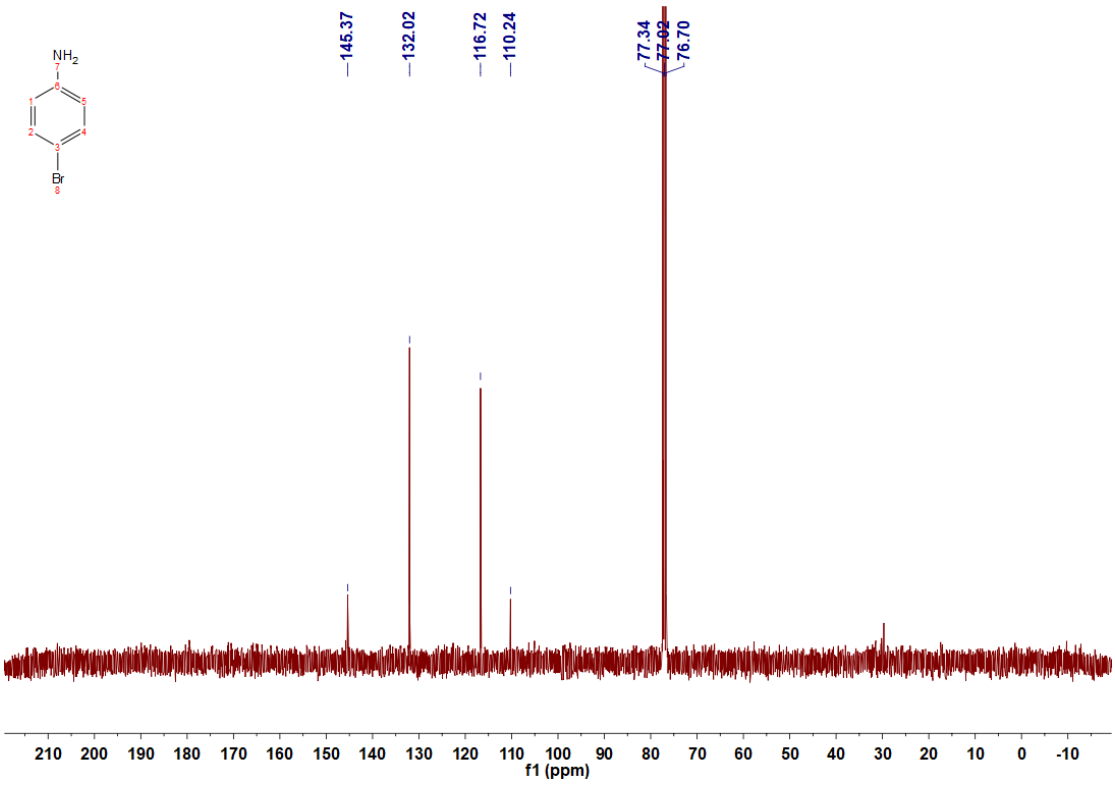
0 1

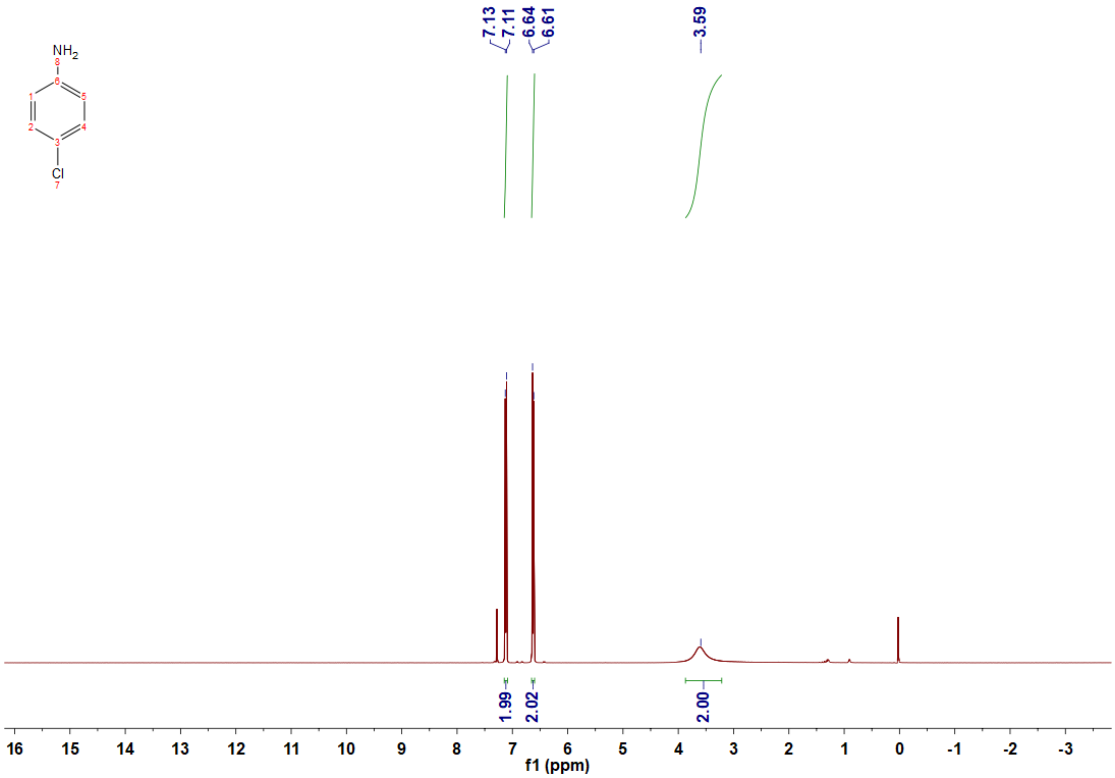
C	-5.00865500	-2.81678700	-2.84629800
C	-3.68420600	-3.09477200	-2.49399500
C	-3.06372900	-2.18372800	-1.66899100
C	-3.71475800	-1.04453300	-1.20528500
C	-5.01809400	-0.75934300	-1.54485100
C	-5.65988300	-1.67651900	-2.38292200
H	-5.53729700	-3.50526800	-3.49447400
H	-3.16466100	-3.97656600	-2.84660300
H	-5.51013500	0.13170100	-1.17655900
H	-6.68624200	-1.49323400	-2.67714200
O	-1.78151600	-2.20518600	-1.17081200
O	-2.85620100	-0.32558700	-0.40549100
B	-1.69218500	-1.05907500	-0.40760800
C	3.18965000	0.83055200	-0.71379000
C	4.41782600	0.21279500	-0.78421900
C	5.39290500	0.84925100	-1.55848400
C	5.12826300	2.04515500	-2.22095500
C	3.87603000	2.66233000	-2.14076500
C	2.92489700	2.02582700	-1.37524400
H	4.60729100	-0.71678300	-0.26304200
H	6.37494700	0.39981700	-1.64332900
H	5.90810100	2.50972500	-2.81227400
H	3.65532300	3.59165900	-2.65014100
O	2.06170400	0.43111700	-0.03469900
O	1.62668400	2.40399700	-1.12432300
B	1.13177400	1.41199400	-0.30251000
N	-0.61864800	0.43470700	0.98854700
O	-0.52997300	-0.75447200	0.24372100
O	-0.15741800	1.47308100	0.15626400
C	0.19058800	0.31988000	2.17484600

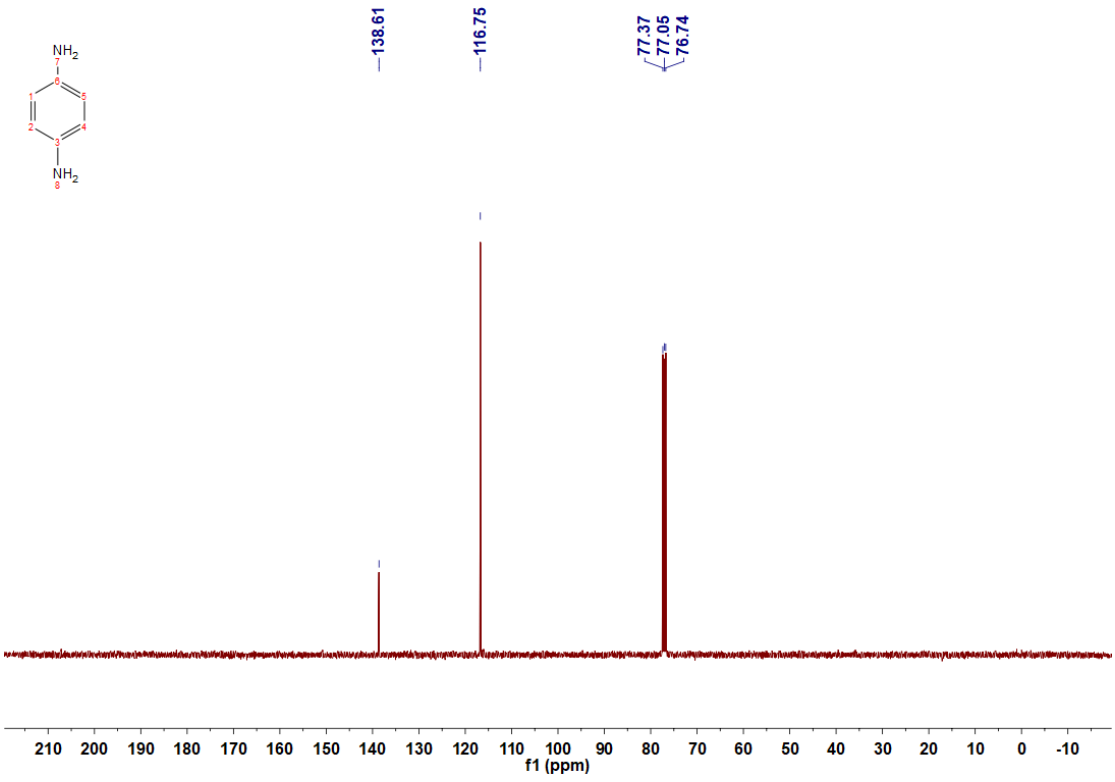
C	0.50068400	1.49551500	2.85541200	H	0.32575700	-1.82070200	2.13748900
C	0.56372400	-0.91815300	2.68196900	C	1.59110900	0.19177500	4.56713300
C	1.20646600	1.42411500	4.04815600	H	1.45146800	2.33841600	4.57612200
H	0.18115200	2.44939800	2.45406300	H	1.56287000	-1.93639300	4.27662800
C	1.26458500	-0.97186700	3.88200400	H	2.13988700	0.14014300	5.50000200

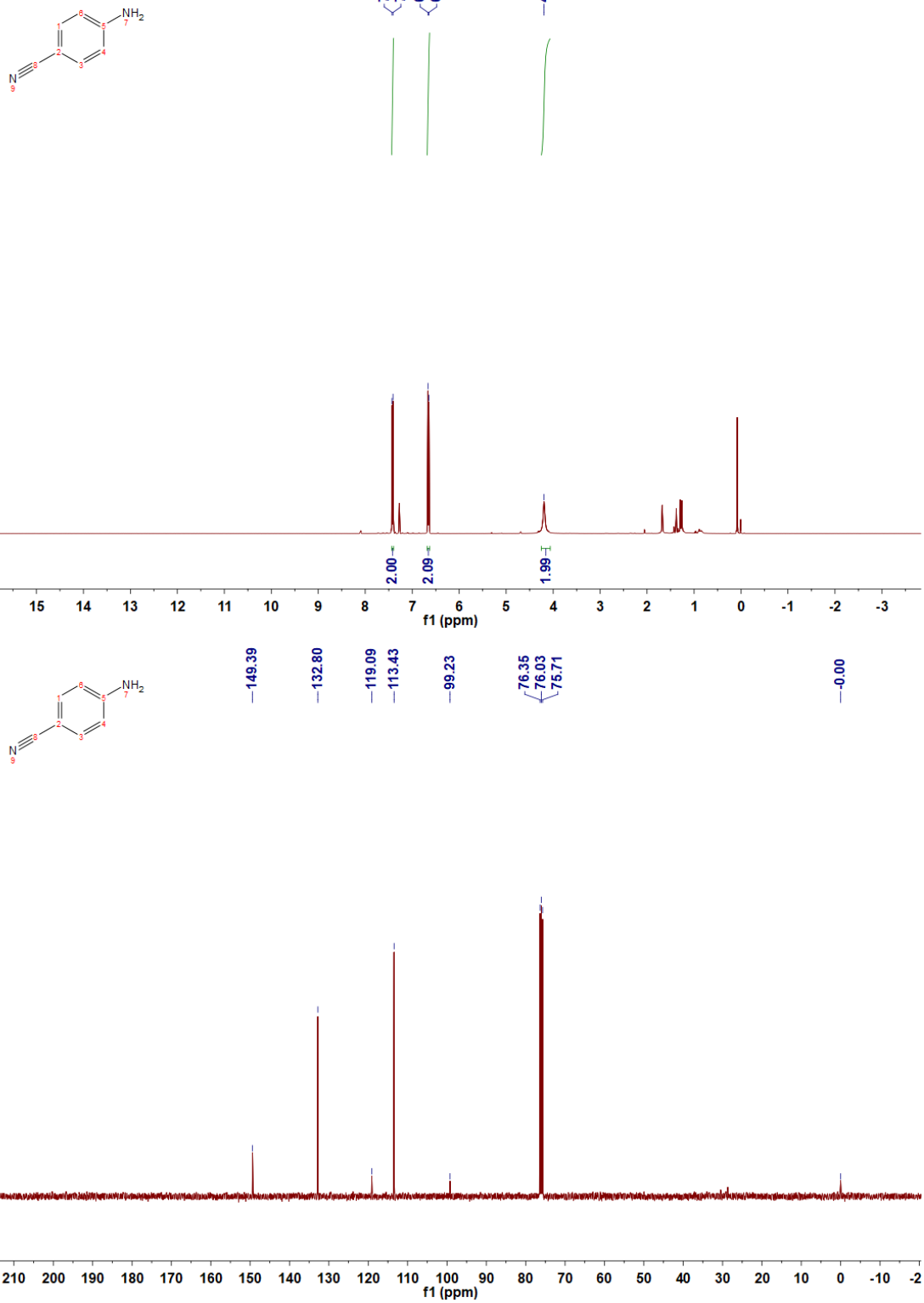
10. ^{1}H 、 ^{13}C and ^{19}FNMR spectra of the products

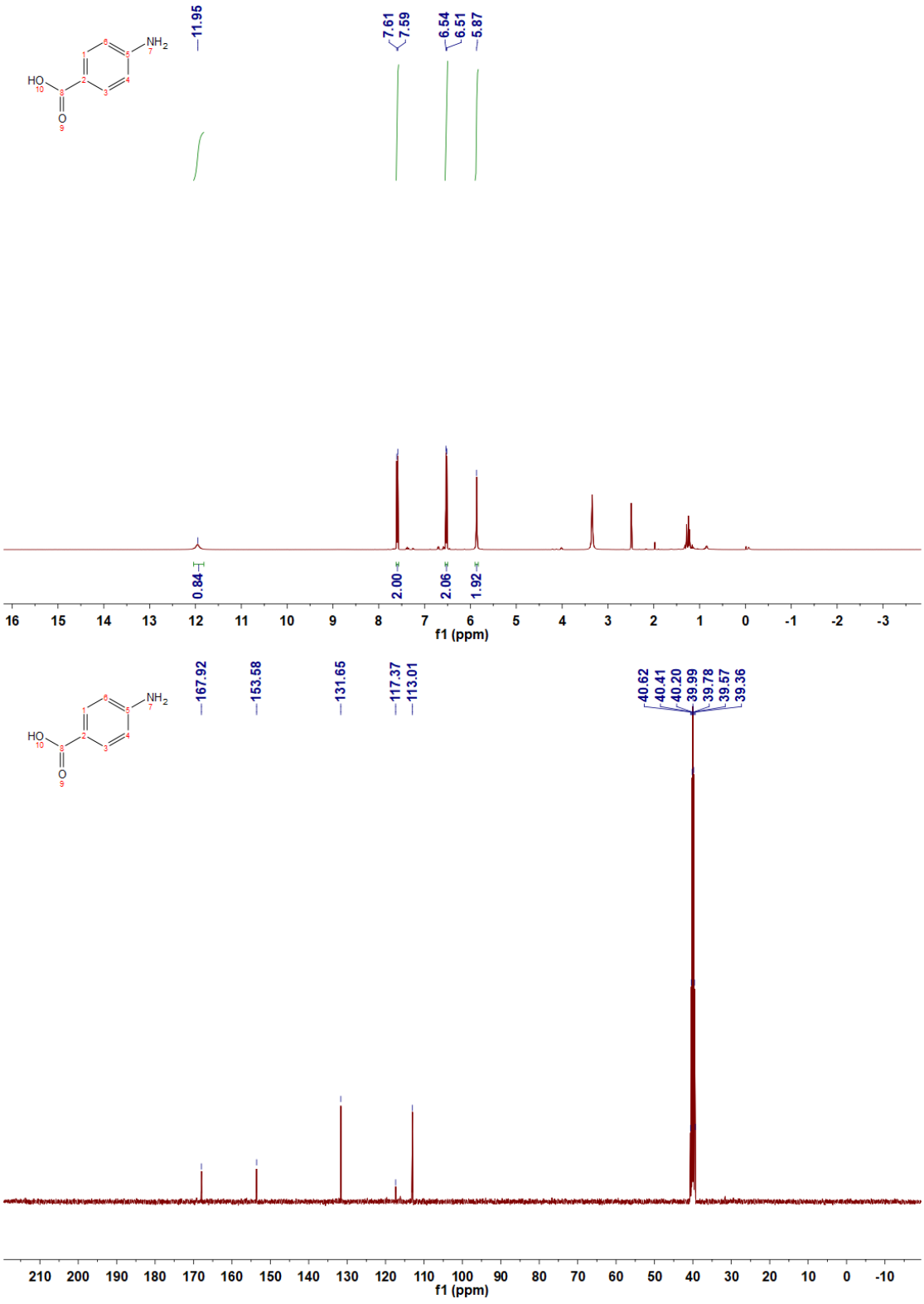

NH2
Br
7.25
7.23
6.59
6.57
3.65
2.00
2.12
1.93
f1 (ppm)

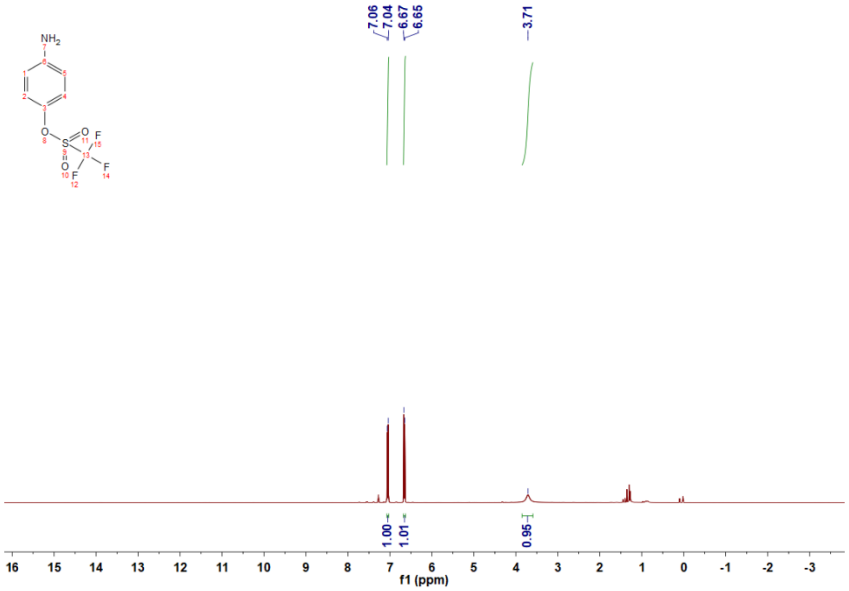

NH2
Br
145.37
132.02
116.72
110.24
77.34
77.02
76.70
f1 (ppm)

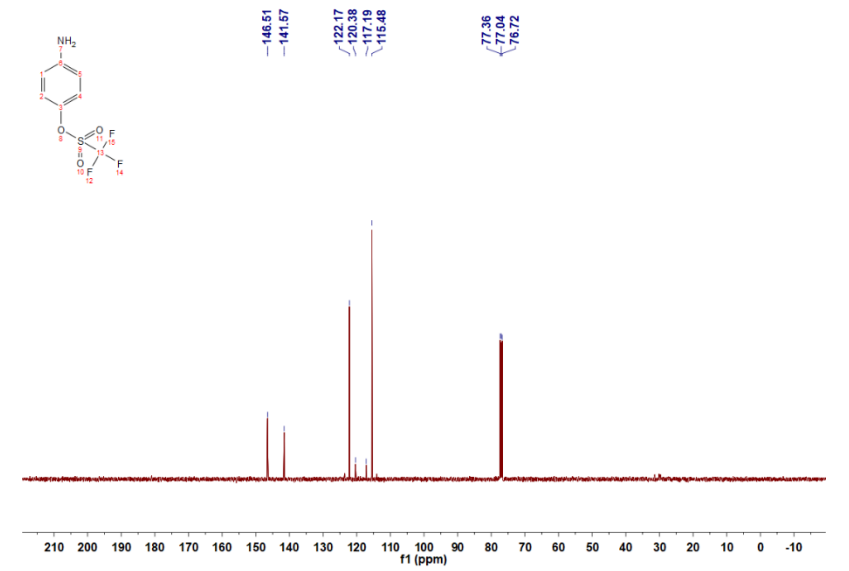

NH2
Cl
7.13
7.11
6.64
6.61
3.59
1.99
2.02
2.00
f1 (ppm)


NH2
NH2
138.61
116.75
77.37
77.05
76.74
f1 (ppm)


7.43
7.41
6.67
6.64
4.19
2.00
2.09
1.99
f1 (ppm)
149.39
132.80
119.09
113.43
99.23
76.35
76.03
75.71
0.00
f1 (ppm)


11.95
7.61
7.59
6.54
6.51
5.87
0.84
2.00
2.06
1.92
f1 (ppm)
167.92
153.58
131.65
117.37
113.01
40.62
40.41
40.20
39.99
39.78
39.57
39.36
f1 (ppm)


7.06
7.04
6.67
6.65
3.71
1.00
1.01
0.95
f1 (ppm)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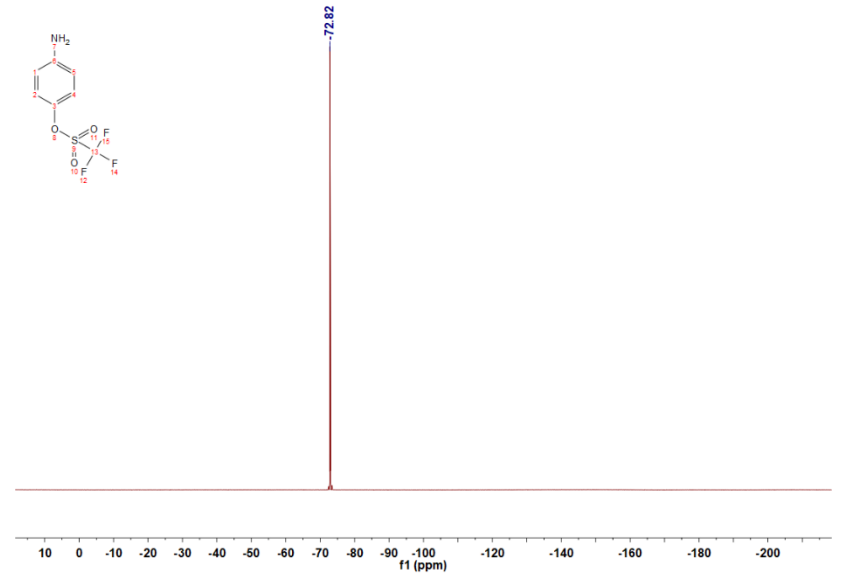
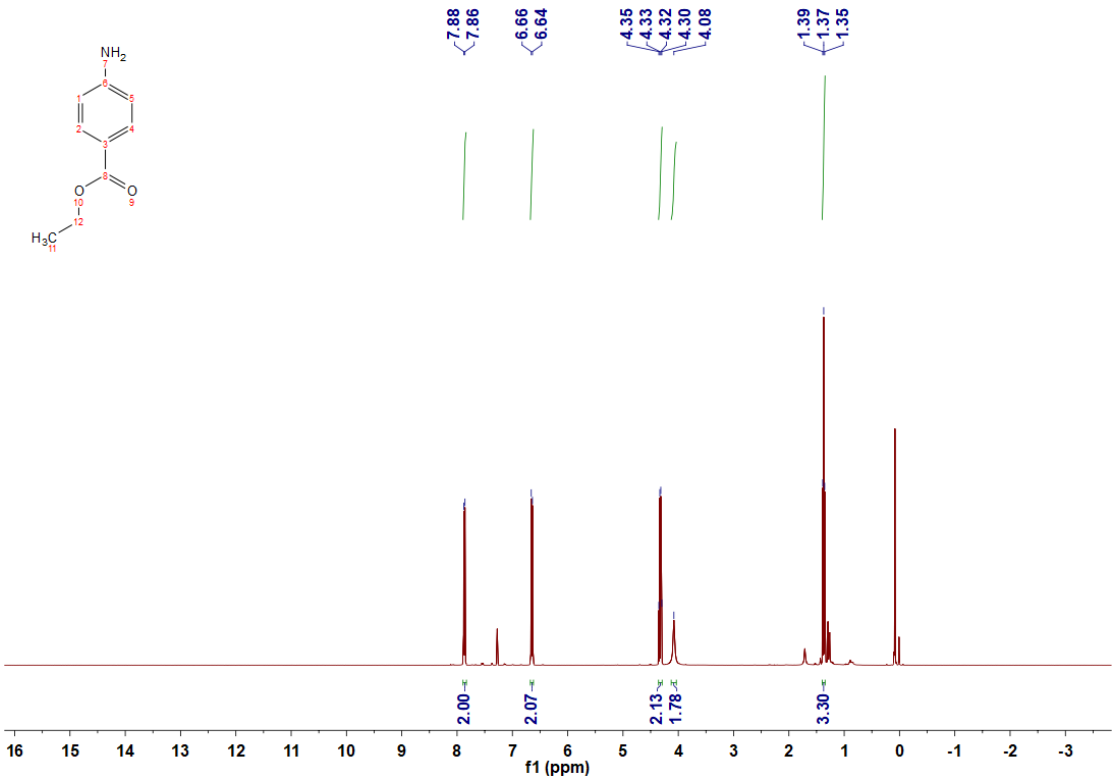
141.57
122.17
120.38
117.19
115.48
77.36
77.04
76.72
f1 (ppm)


-72.82
f1 (ppm)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6.66
6.64
4.35
4.33
4.32
4.30
4.08
1.39
1.37
1.35
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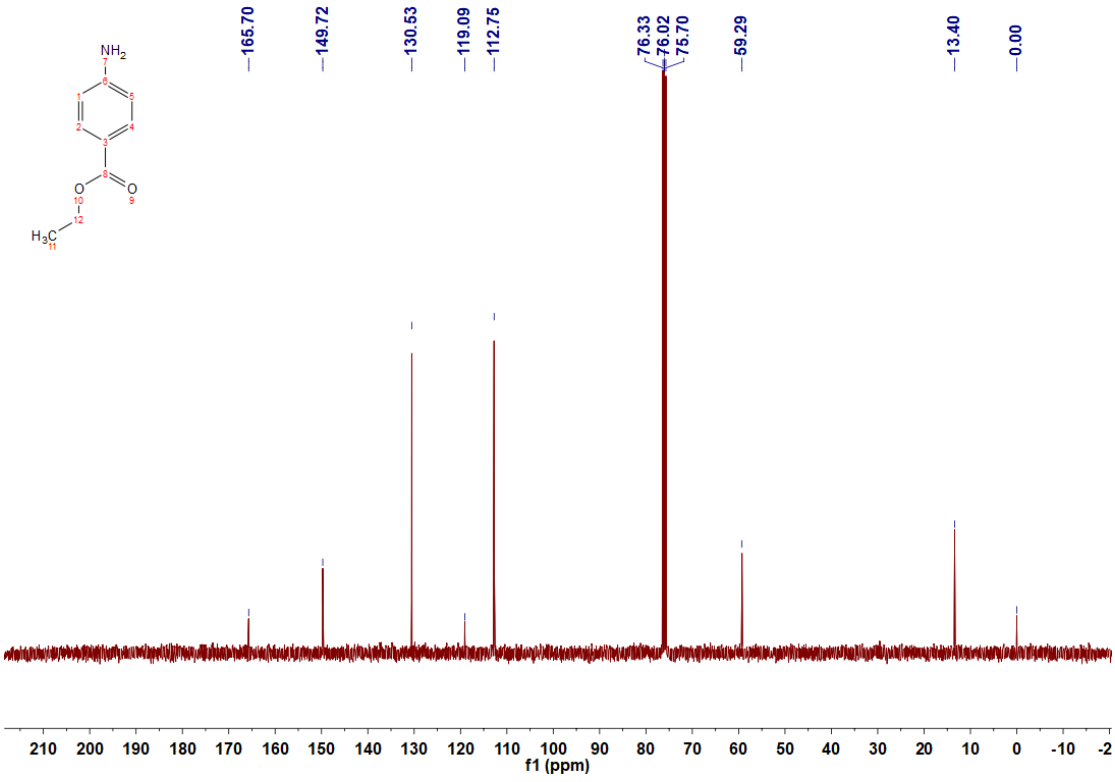
2.07
2.13
1.78
3.30
f1 (ppm)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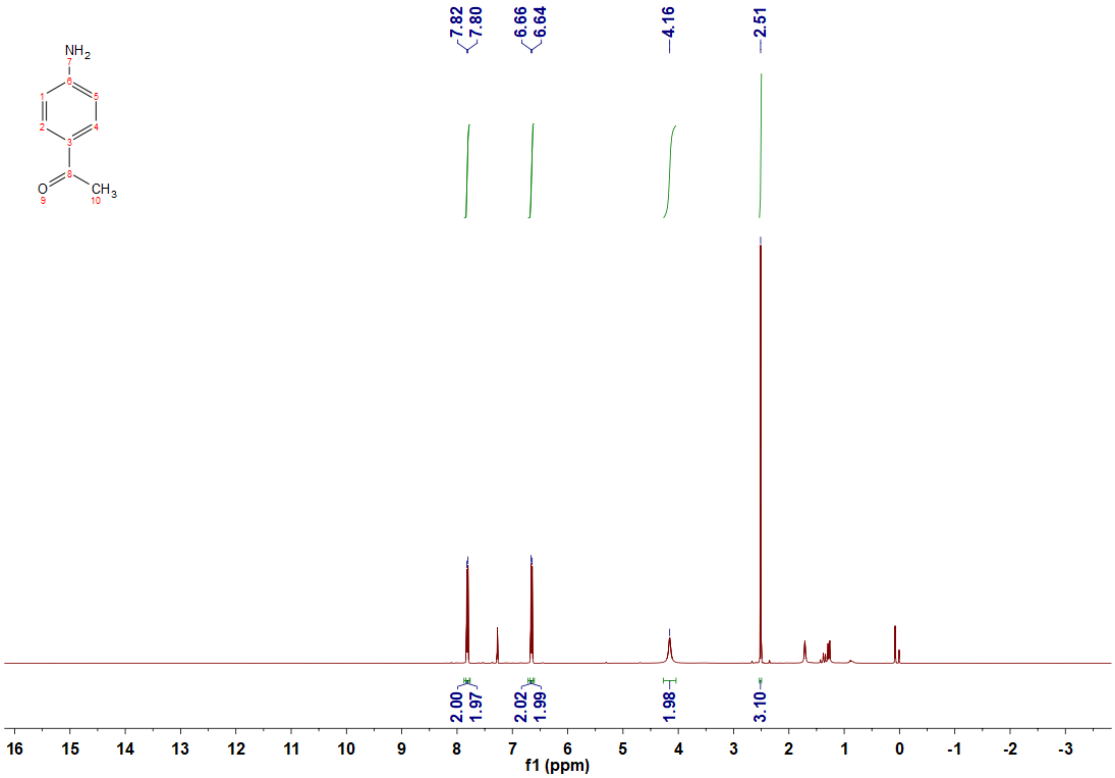
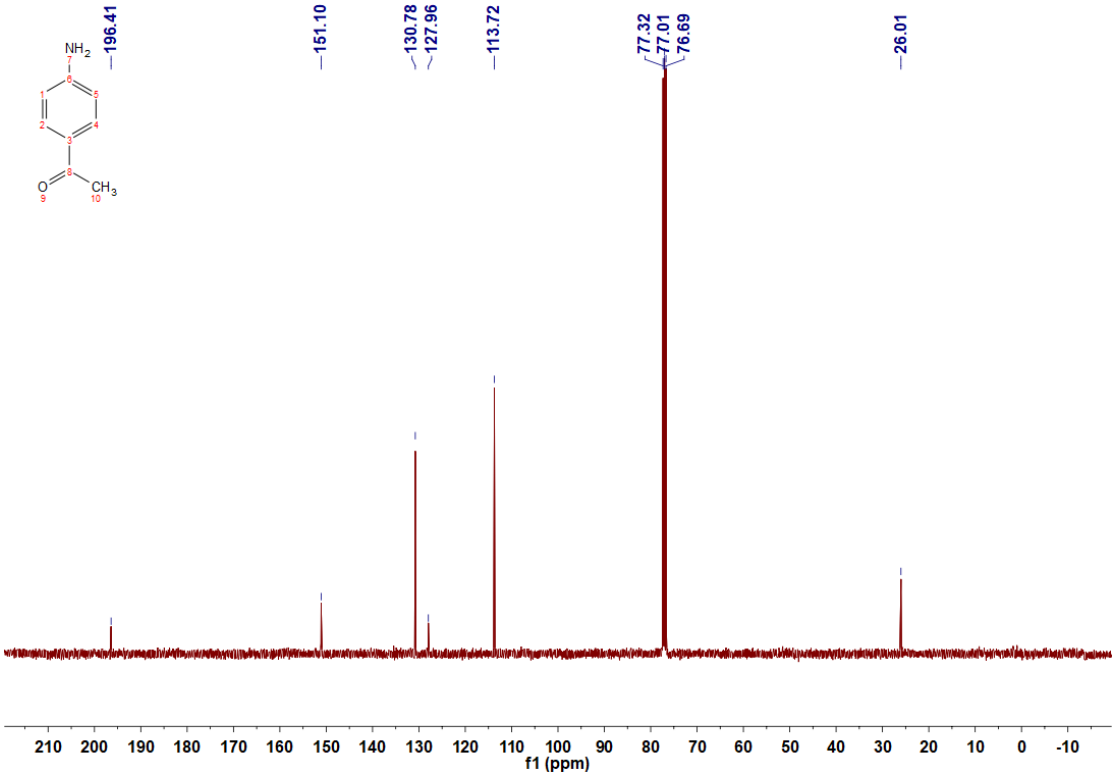
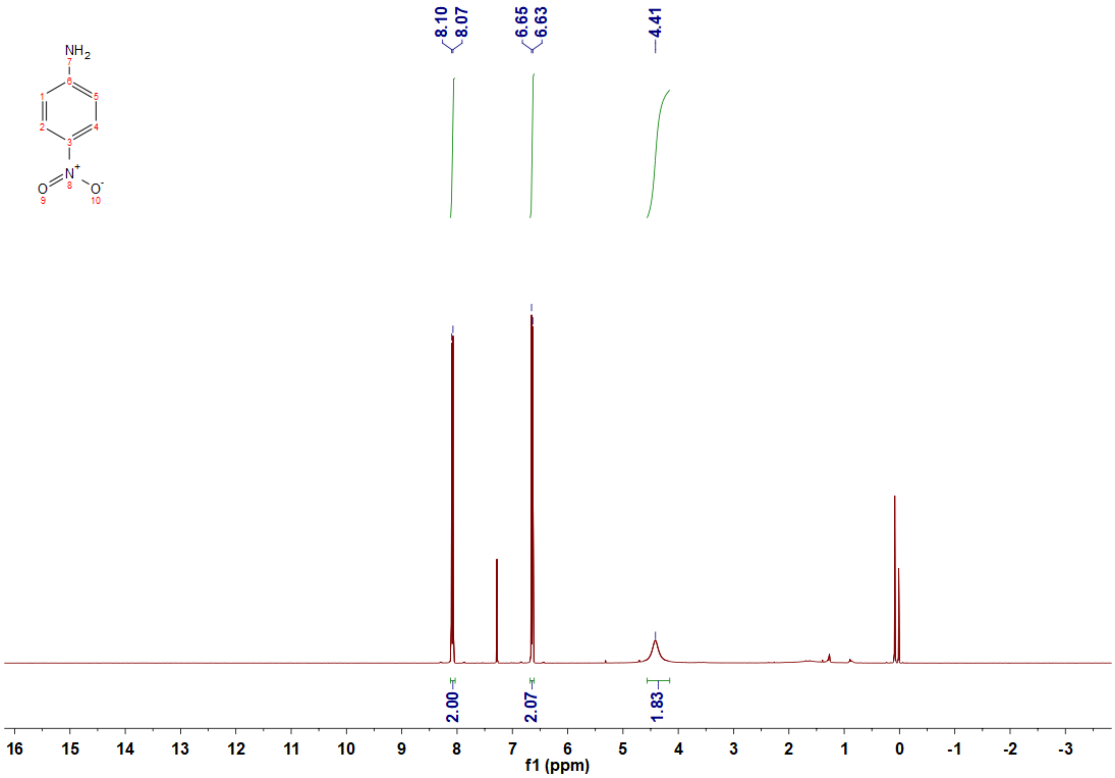
149.72
130.53
119.09
112.75
76.33
76.02
75.70
59.29
13.40
0.00
f1 (ppm)


7.82
7.80
6.66
6.64
4.16
2.51
2.00
1.97
2.02
1.99
1.98
3.10
f1 (ppm)


196.41
151.10
130.78
127.96
113.72
77.32
77.01
76.69
26.01
f1 (ppm)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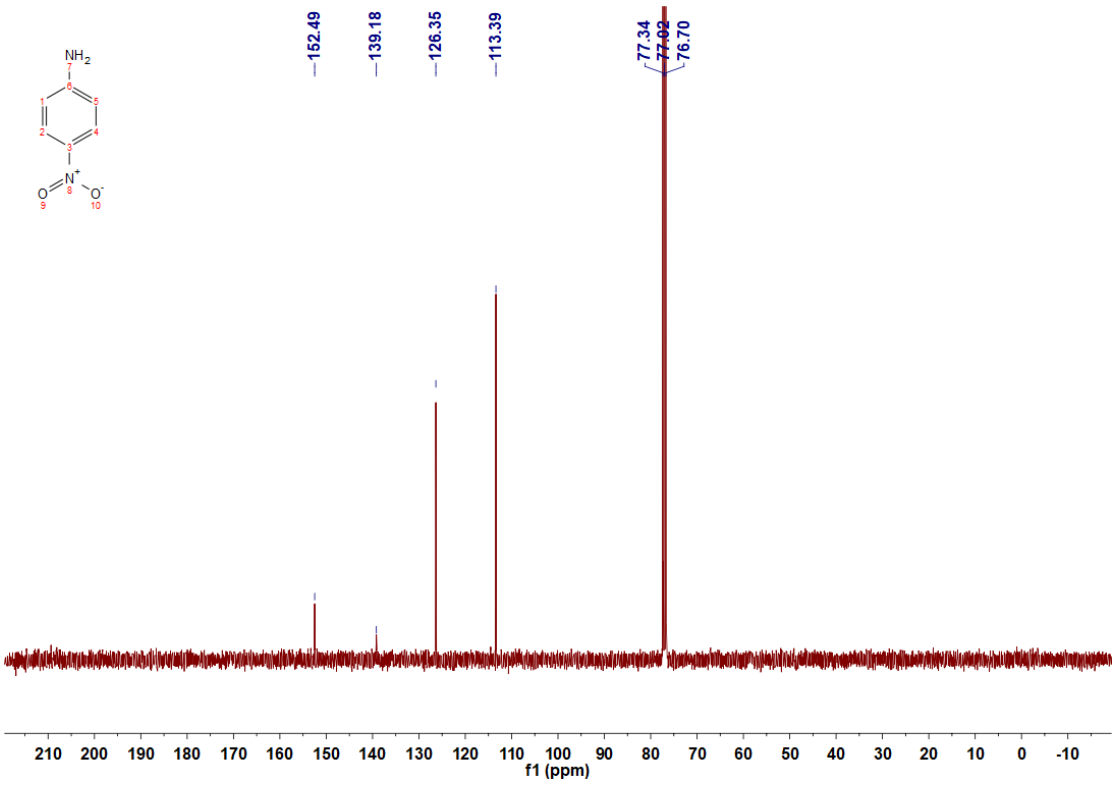
8.07
6.65
6.63
4.41
2.00
2.07
1.83
f1 (ppm)


NH2
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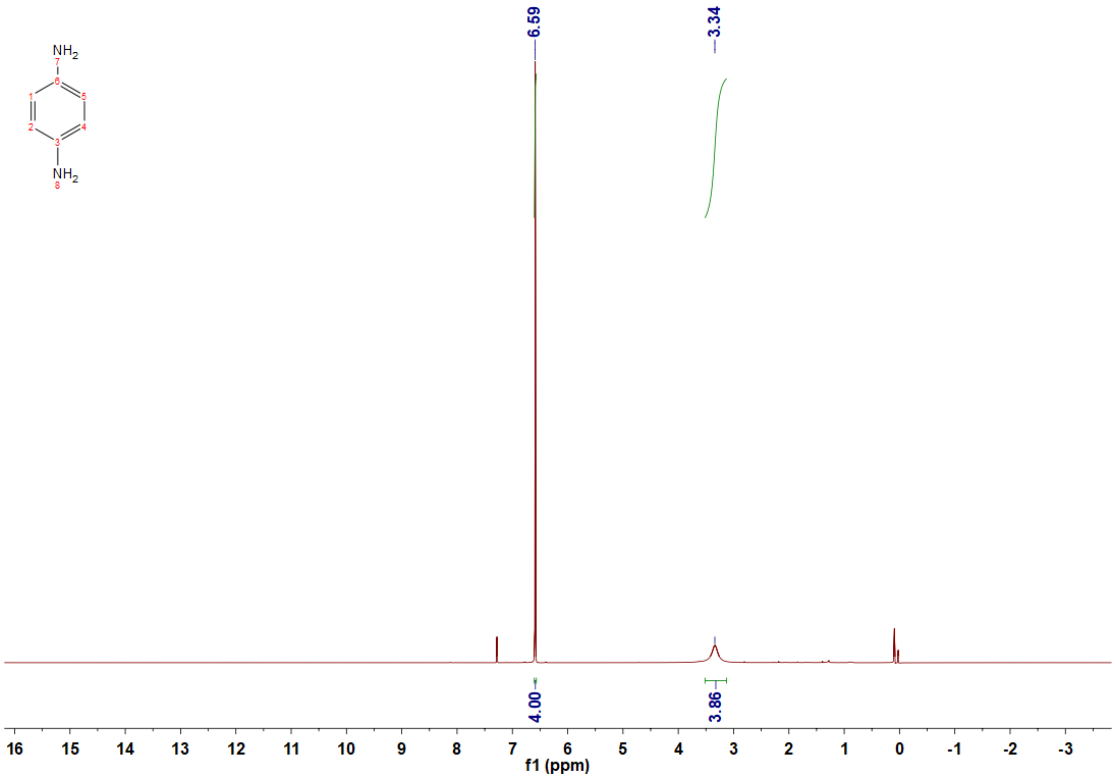
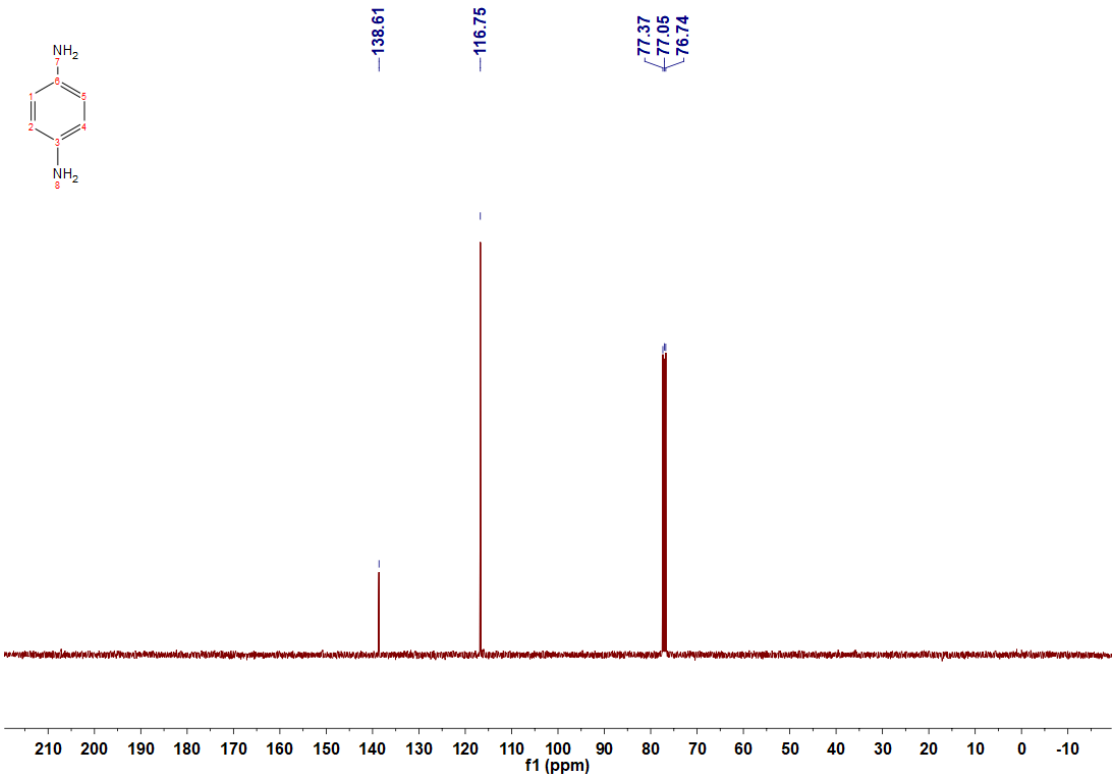
126.35
113.39
77.34
77.02
76.70
f1 (ppm)


NH2
NH2
6.59
3.34
4.00
3.86
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


NH2
NH2
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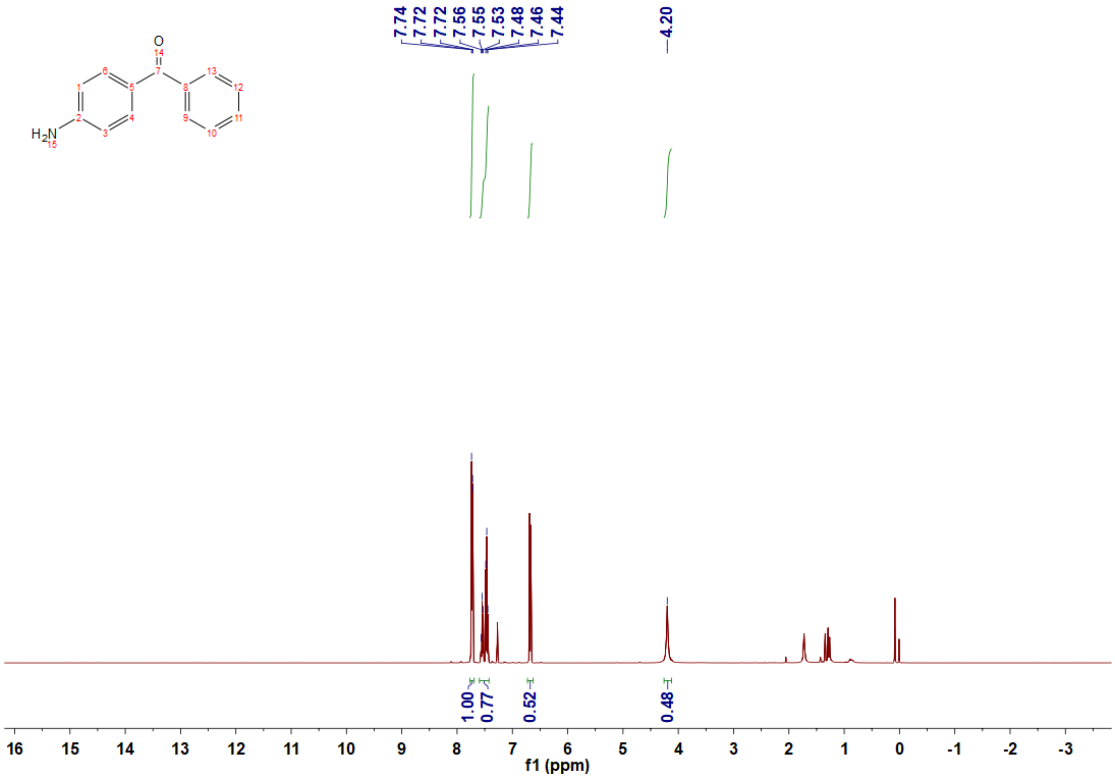
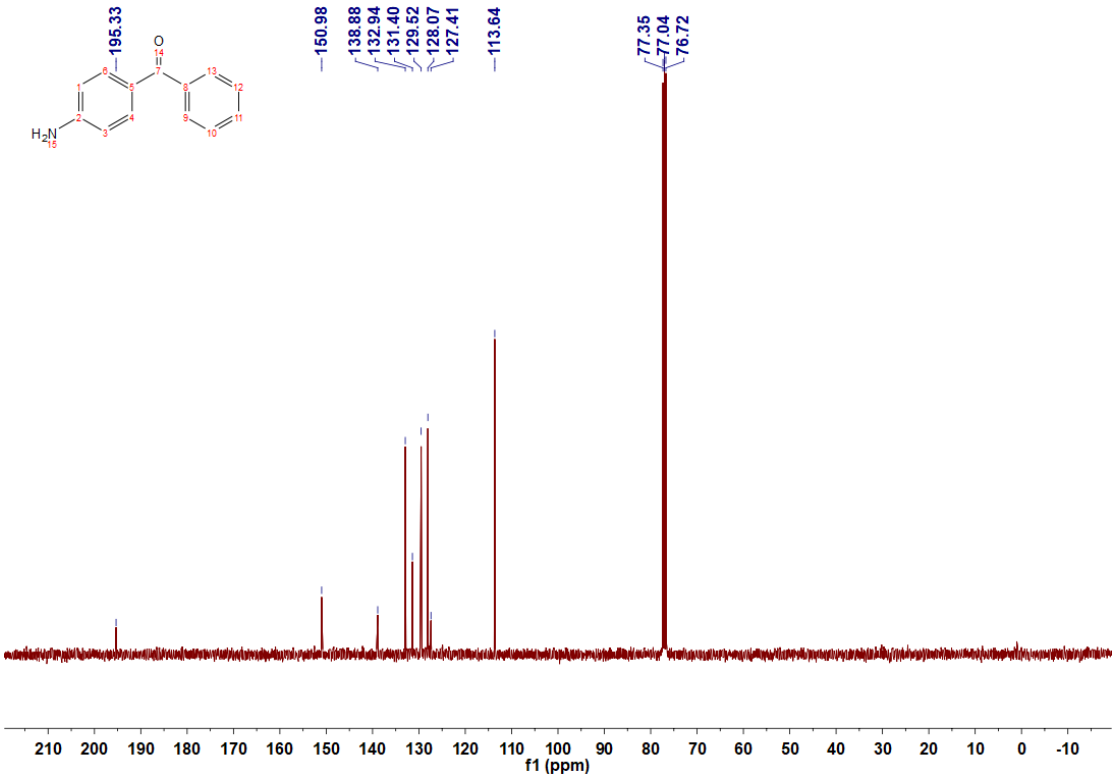
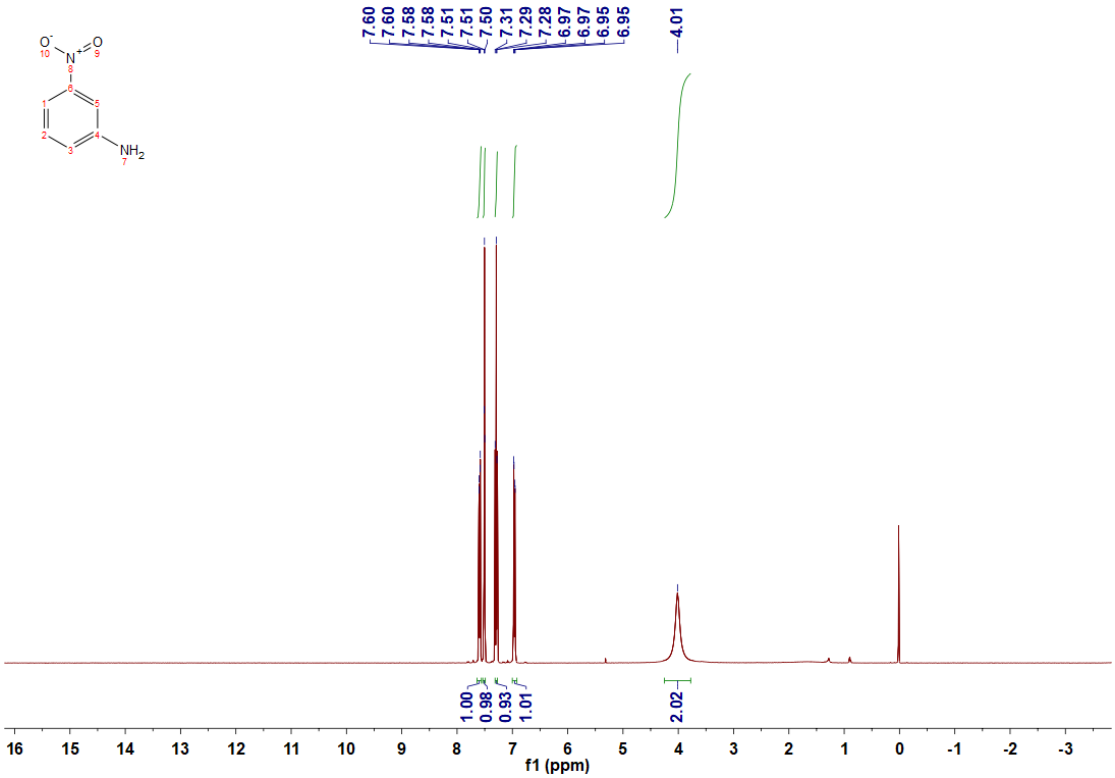
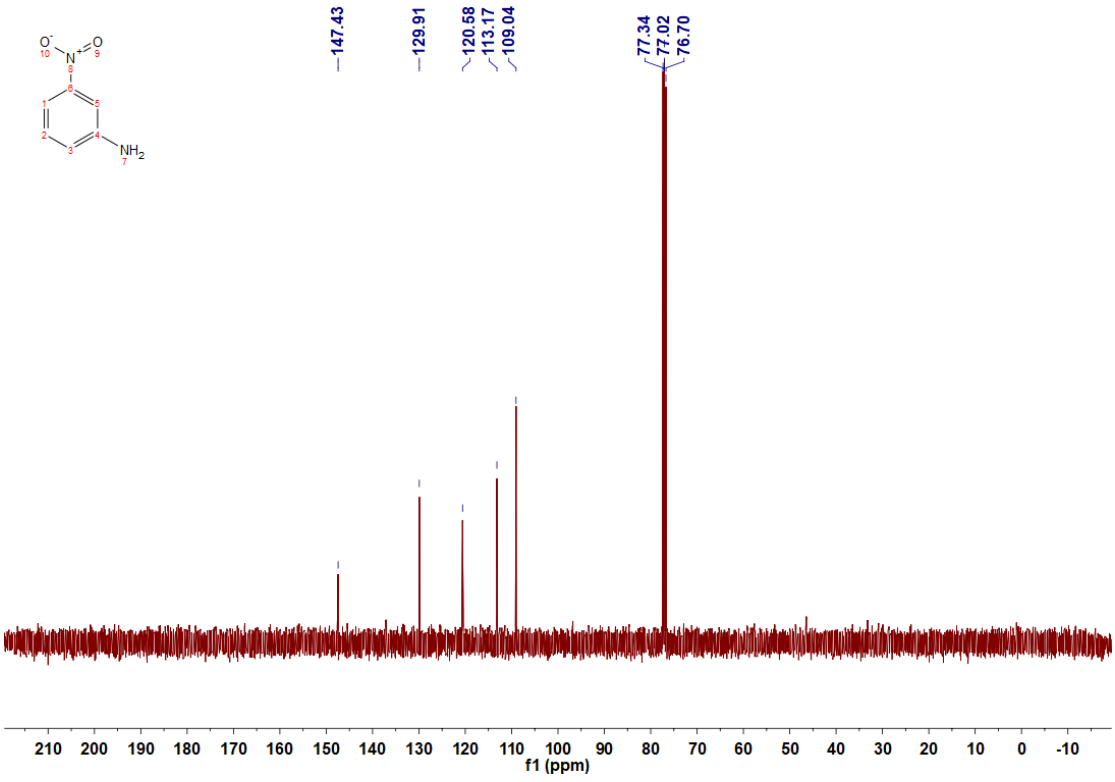
116.75
77.37
77.05
76.74
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.74
7.72
7.72
7.56
7.55
7.53
7.48
7.46
7.44
4.20
1.00
0.77
0.52
0.48
f1 (ppm)


195.33
150.98
138.88
132.94
131.40
129.52
128.07
127.41
113.64
77.35
77.04
76.72
f1 (ppm)


7.60
7.60
7.58
7.58
7.51
7.51
7.50
7.31
7.29
7.28
6.97
6.97
6.95
6.95
4.01
1.00
0.98
0.93
1.01
2.02
f1 (ppm)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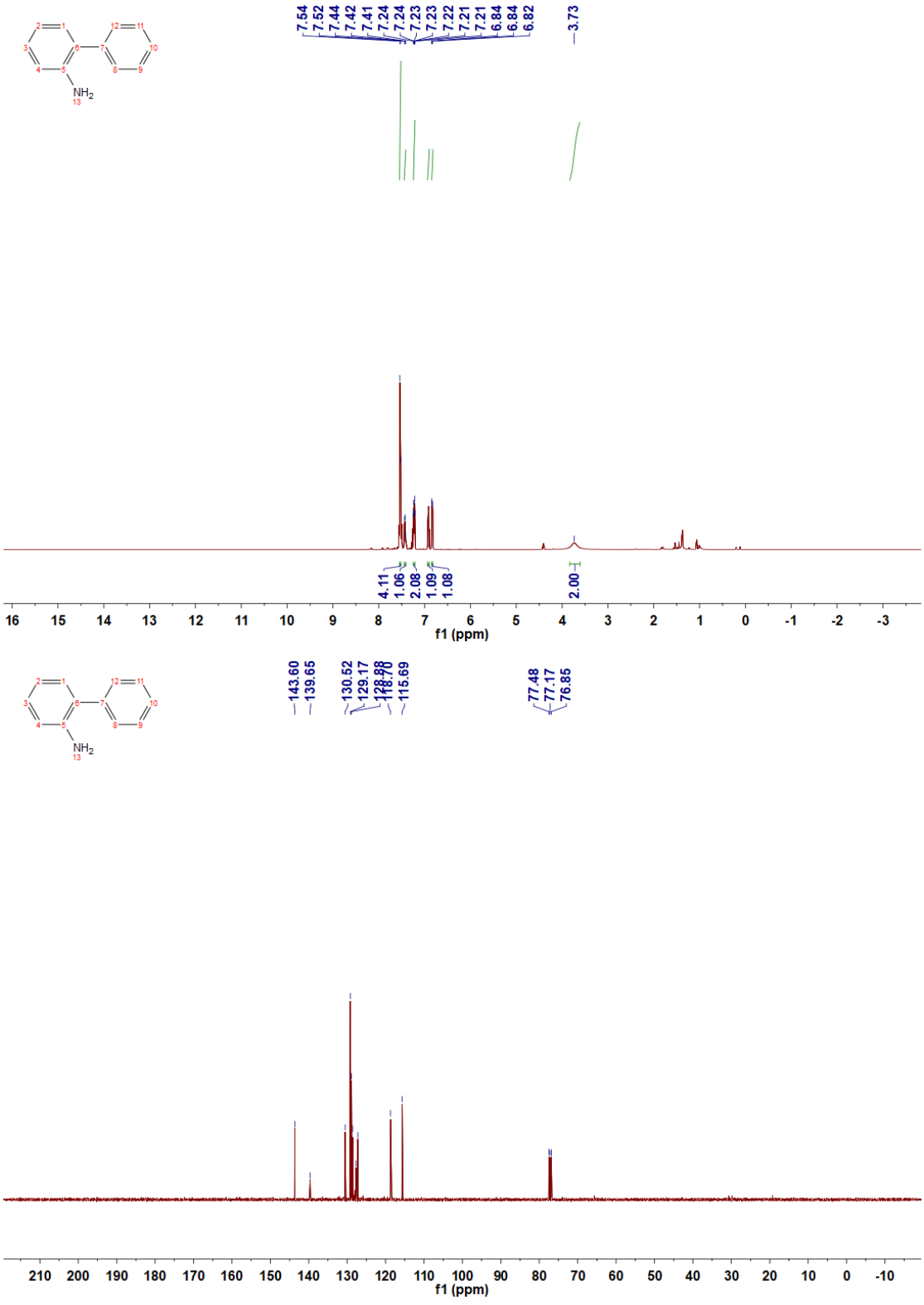
129.91
120.58
113.17
109.04
77.34
77.02
76.70
f1 (ppm)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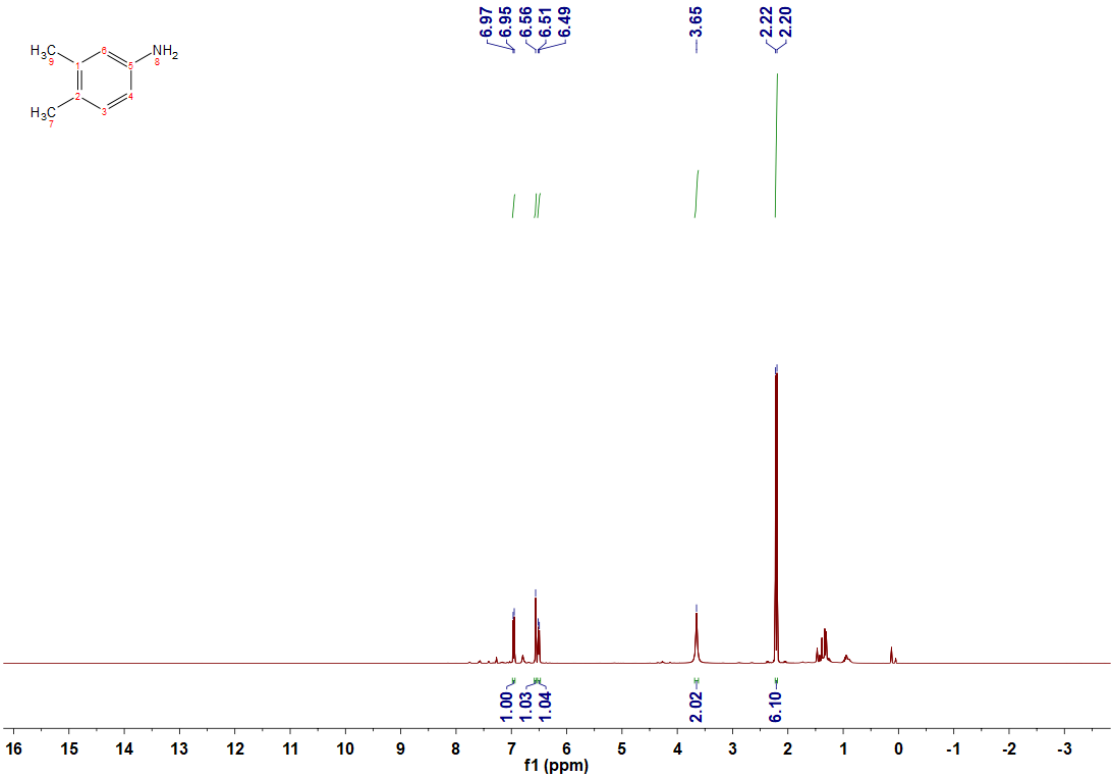
7.52
7.44
7.42
7.41
7.24
7.24
7.23
7.23
7.22
7.21
7.21
6.84
6.84
6.82
3.73
4.11
1.06
2.08
1.09
1.08
2.00
f1 (ppm)
143.60
139.66
130.52
129.17
115.69
77.48
77.17
76.85
f1 (ppm)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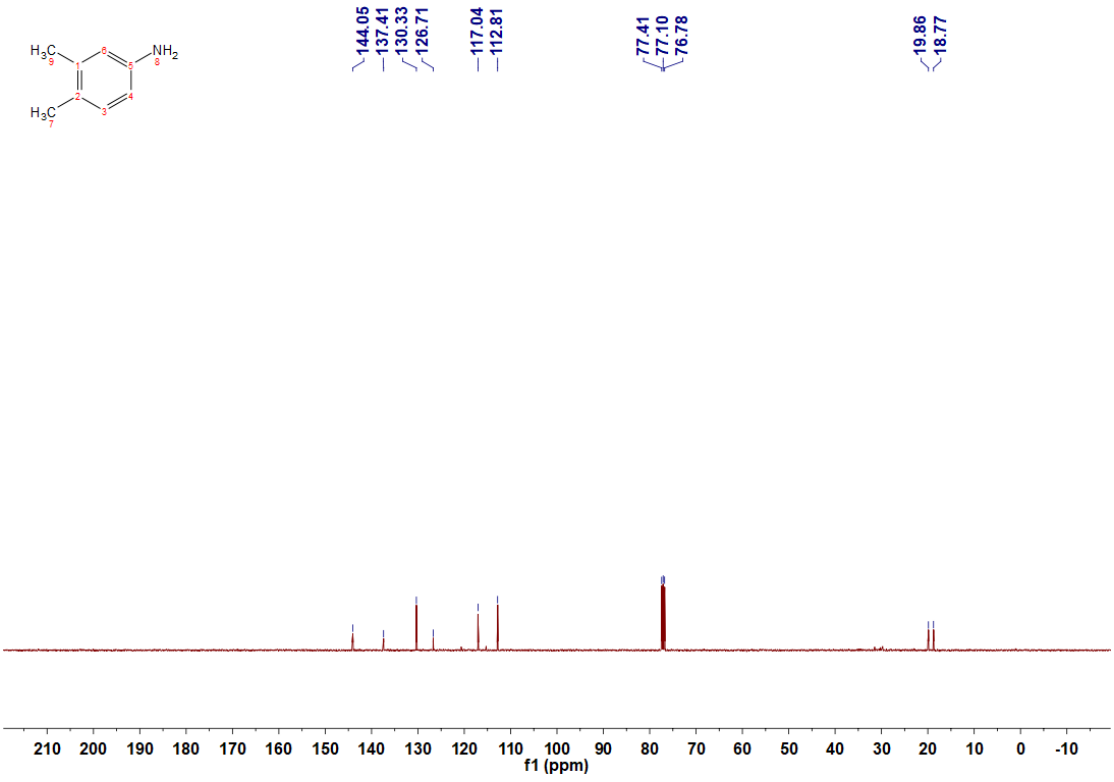
6.95
6.56
6.51
6.49
3.65
2.22
2.20
1.00
1.03
1.04
2.02
6.10
f1 (ppm)


144.05
137.41
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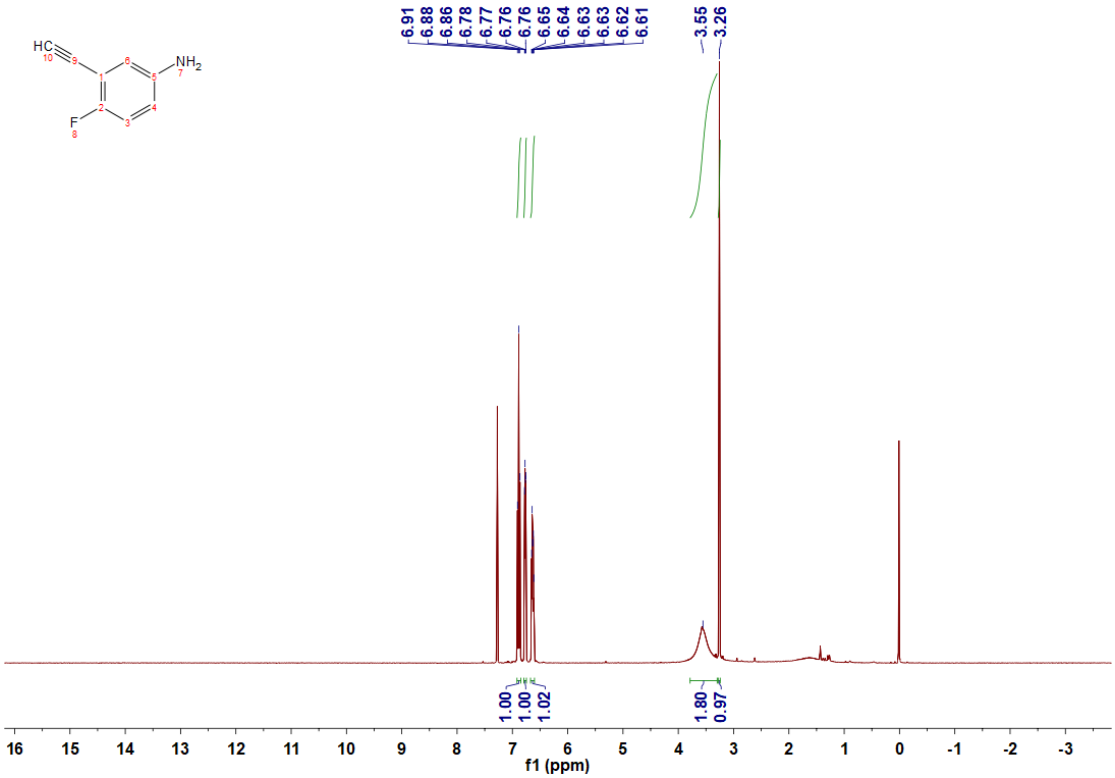
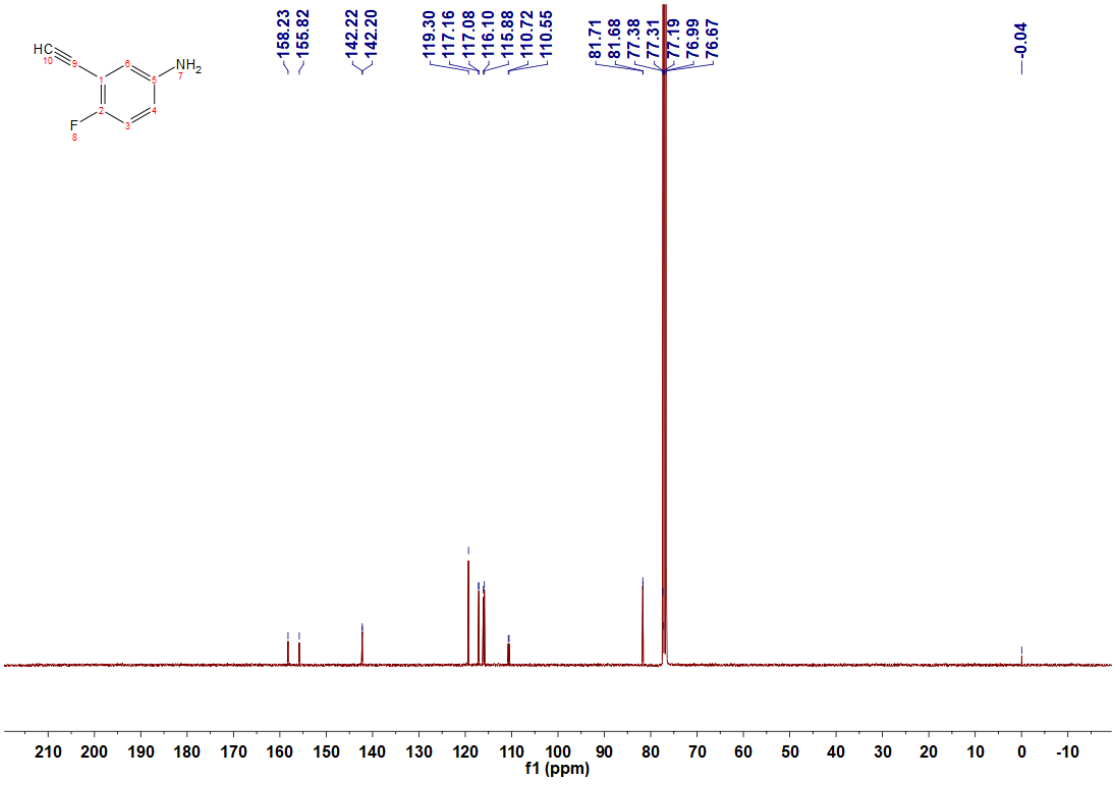
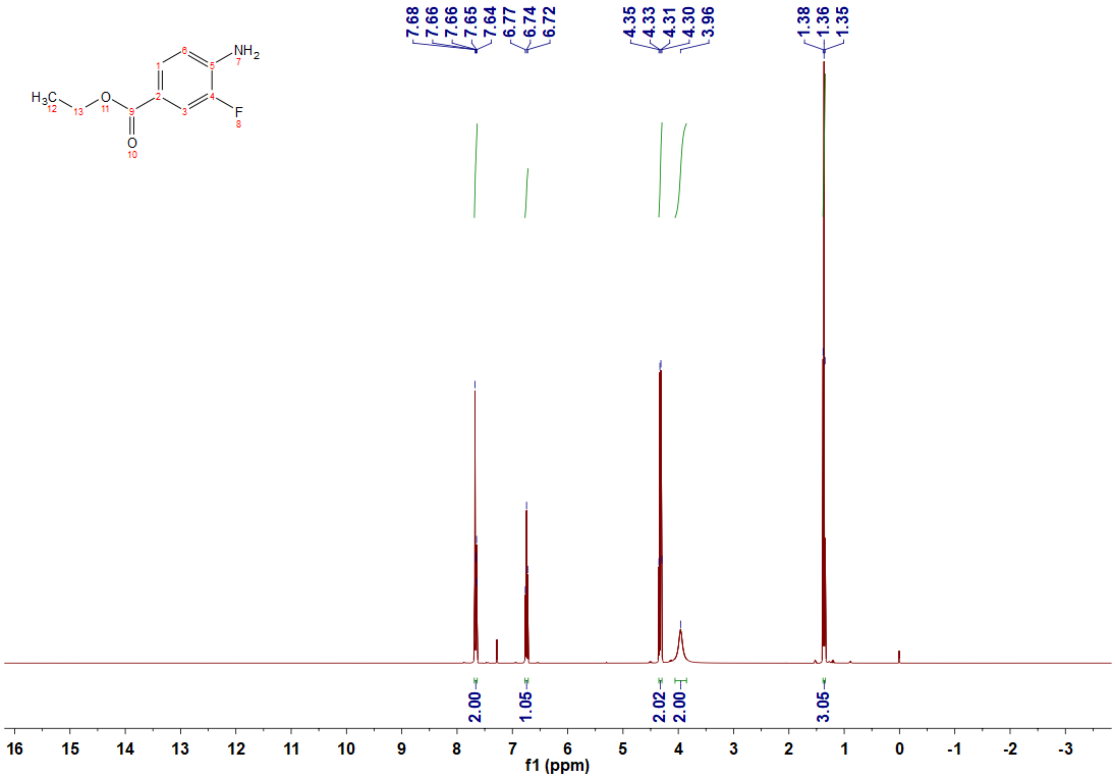
126.71
117.04
112.81
77.41
77.10
76.78
19.86
18.77
f1 (ppm)


6.91
6.88
6.86
6.78
6.77
6.76
6.76
6.65
6.64
6.63
6.63
6.62
6.61
3.55
3.26
1.00
1.00
1.02
1.80
0.97
f1 (ppm)


158.23
155.82
142.22
142.20
119.30
117.16
117.08
116.10
115.88
110.72
110.55
81.71
81.68
77.38
77.31
77.19
76.99
76.67
-0.04
f1 (ppm)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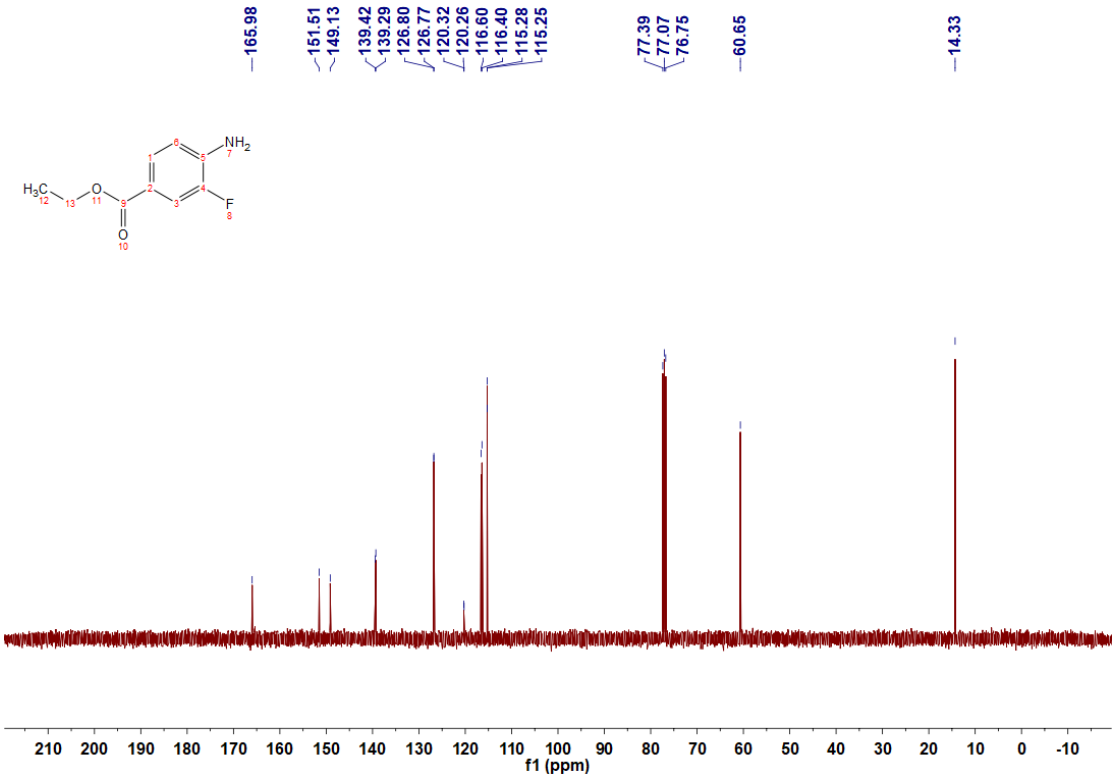
7.66
7.66
7.65
7.64
6.77
6.74
6.72
4.35
4.33
4.31
4.30
3.96
1.38
1.36
1.35
2.00
1.05
2.02
2.00
3.05
f1 (ppm)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151.51
149.13
139.42
139.29
126.80
126.77
120.32
120.26
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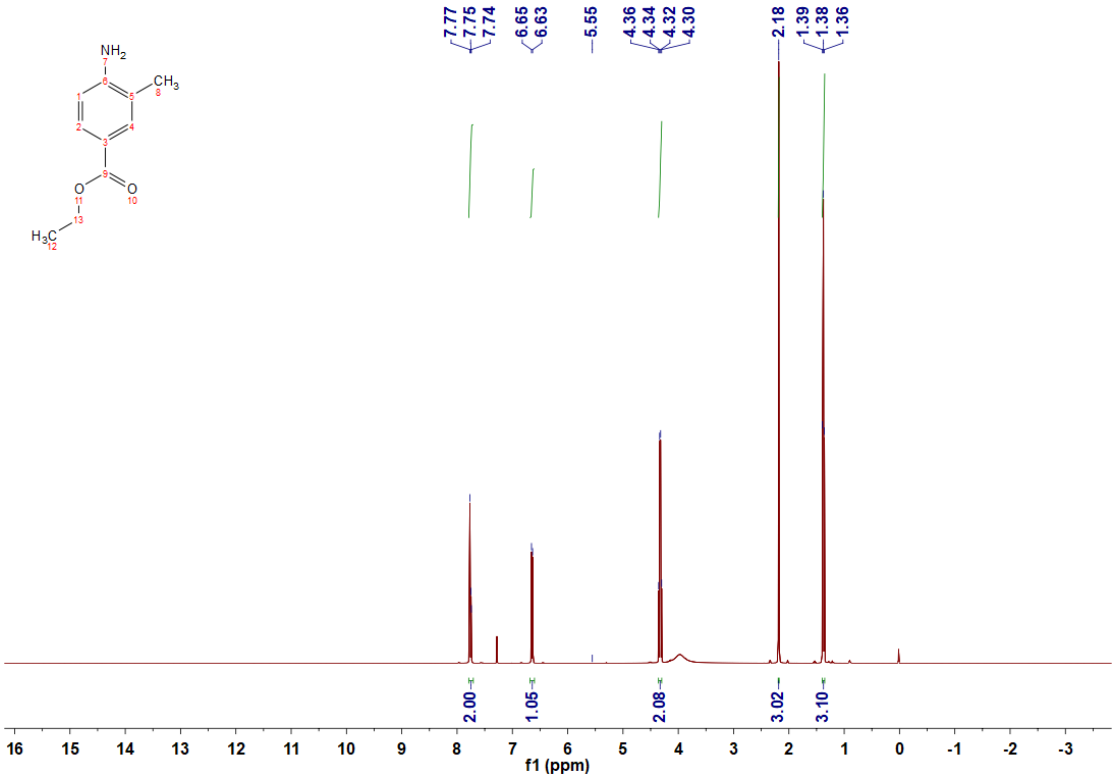
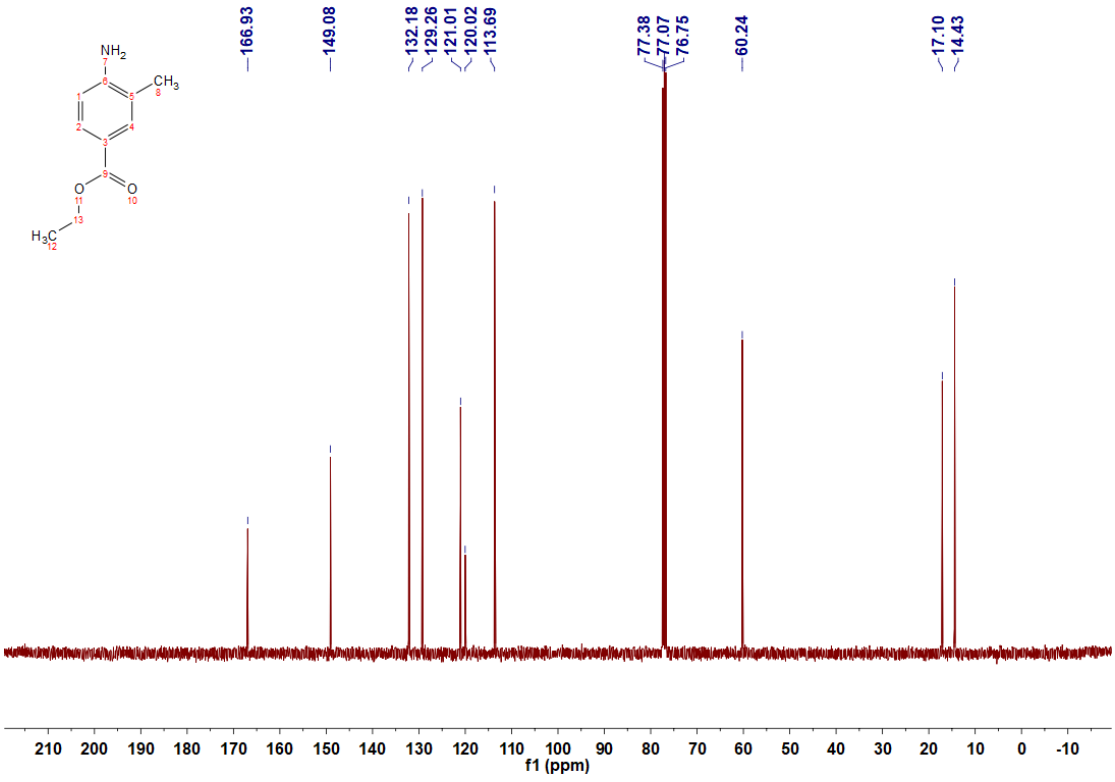
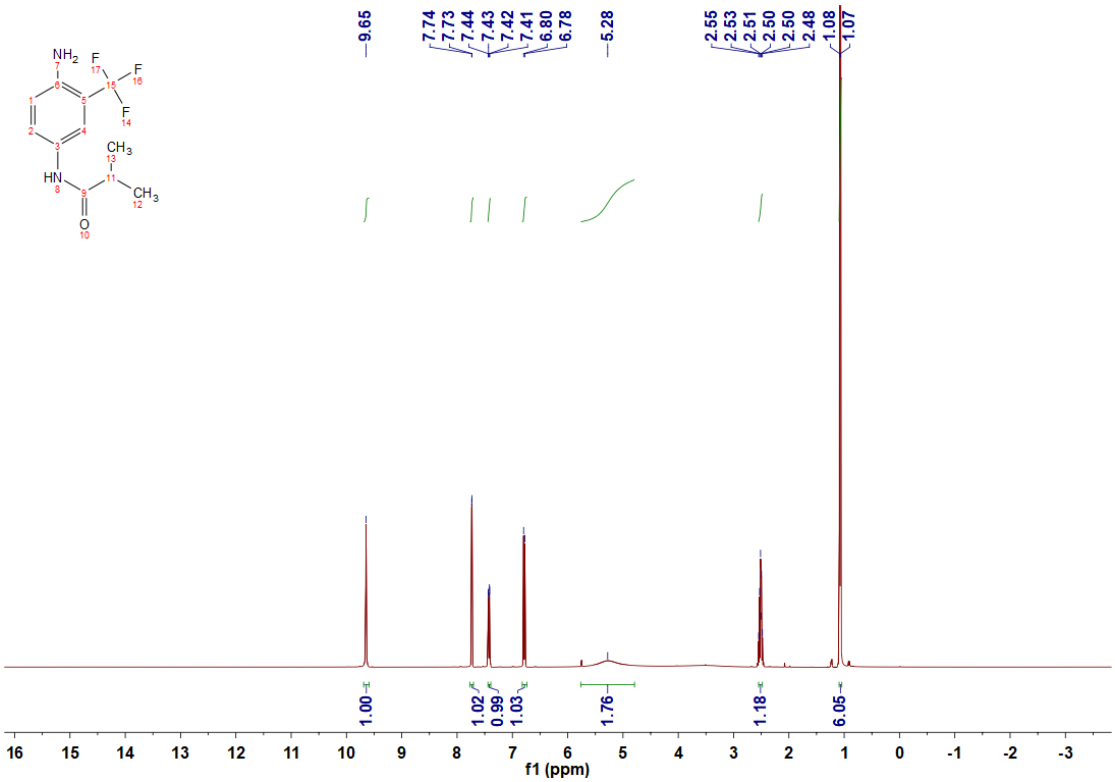
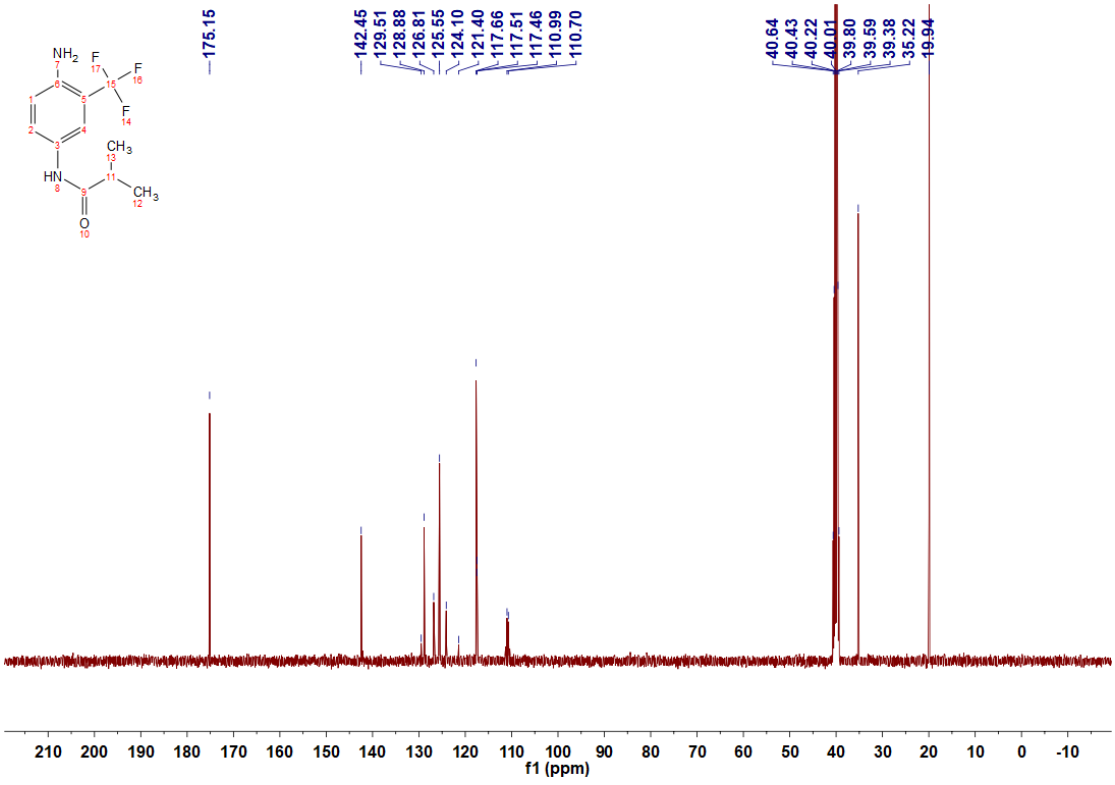
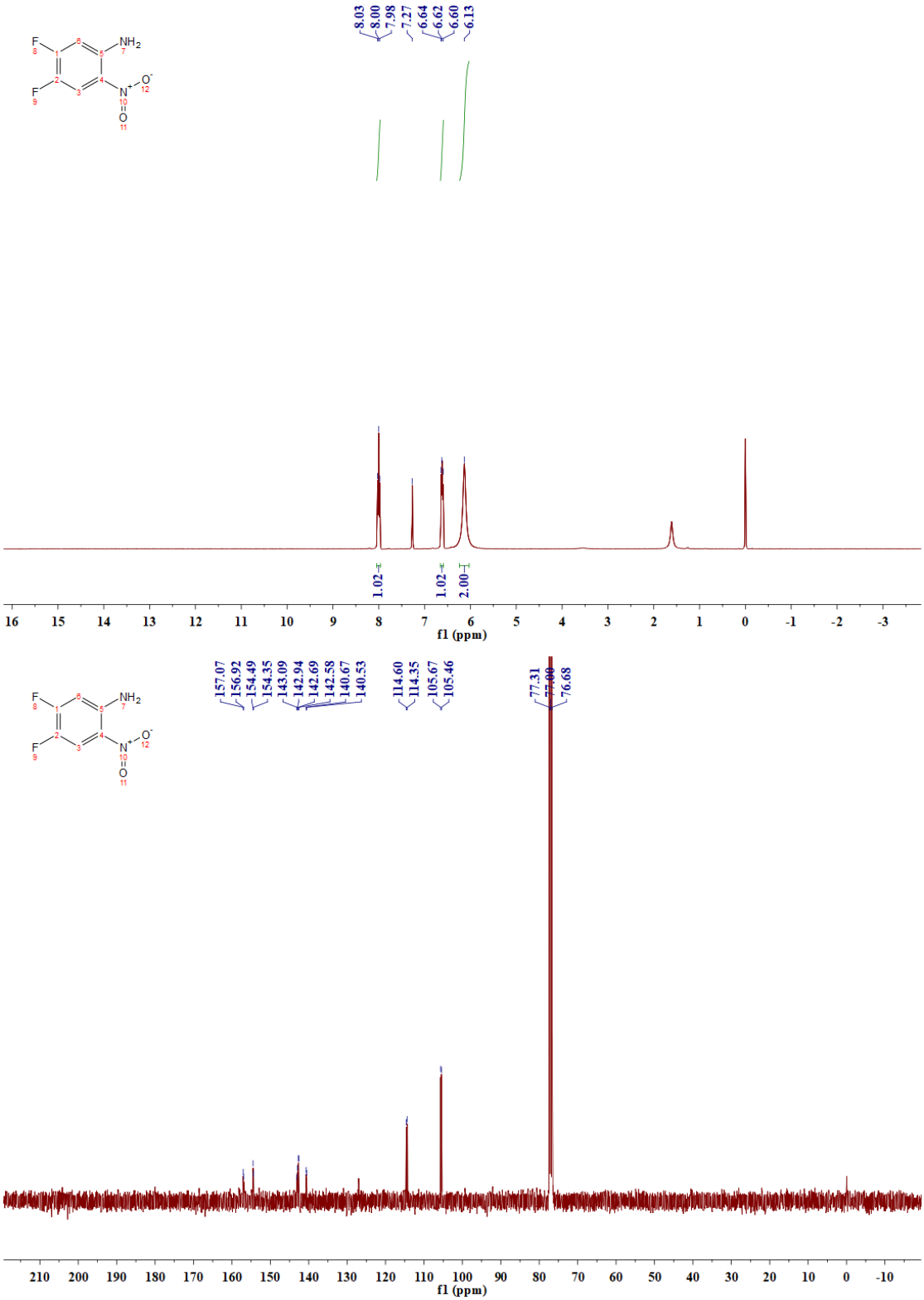
116.40
115.28
115.25
77.39
77.07
76.75
60.65
14.33
f1 (ppm)

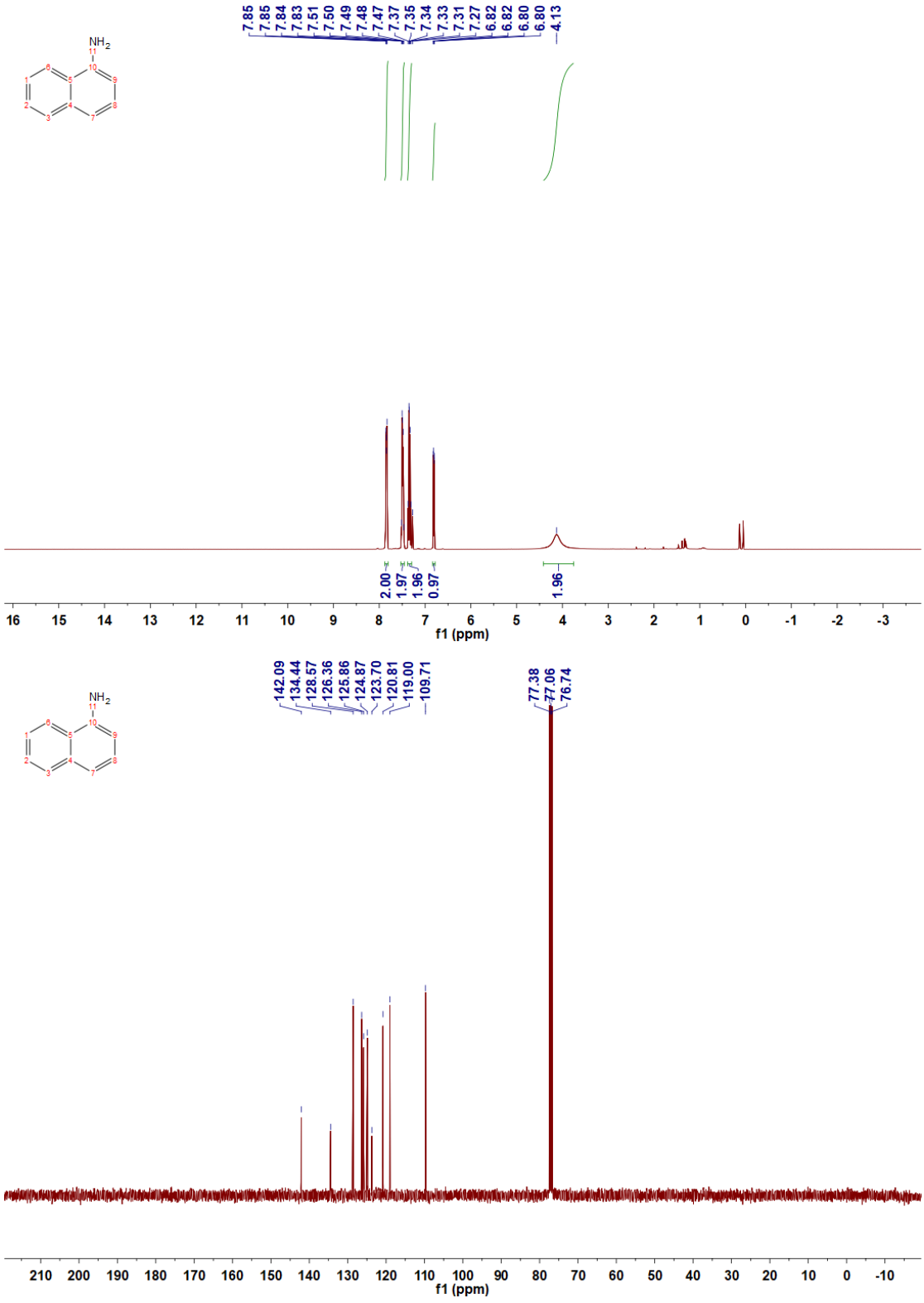

7.77
7.75
7.74
6.65
6.63
5.55
4.36
4.34
4.32
4.30
2.18
1.39
1.38
1.36
2.00
1.05
2.08
3.02
3.10
f1 (ppm)

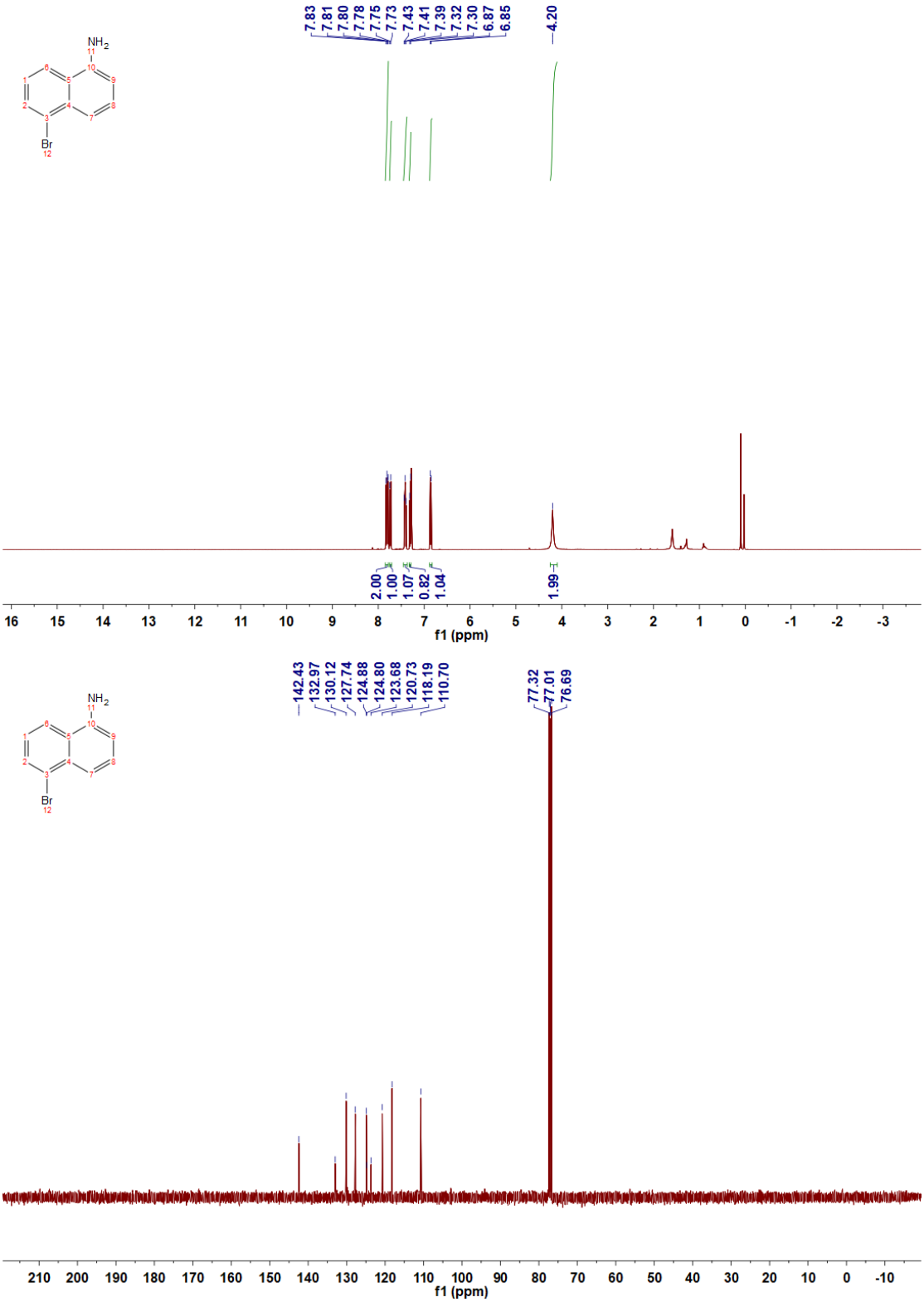

166.93
149.08
132.18
129.26
121.01
120.02
113.69
77.38
77.07
76.75
60.24
17.10
14.43
f1 (ppm)


9.65
7.74
7.73
7.44
7.43
7.42
7.41
6.80
6.78
5.28
2.55
2.53
2.51
2.50
2.50
2.48
1.08
1.07
1.00
1.02
0.99
1.03
1.76
1.18
6.05
f1 (ppm)


175.15
142.45
129.51
128.88
126.81
125.55
124.10
121.40
117.66
117.51
117.46
110.99
110.70
40.64
40.43
40.22
40.01
39.80
39.59
39.38
35.22
19.94
f1 (ppm)


8.03
8.00
7.98
7.27
6.64
6.62
6.60
6.13
1.02
1.02
2.00
f1 (ppm)
157.07
156.92
154.49
154.35
143.09
142.94
142.69
142.58
140.67
140.53
114.60
114.35
105.67
105.46
77.31
77.00
76.68
f1 (ppm)


7.85
7.85
7.84
7.83
7.51
7.50
7.49
7.48
7.47
7.37
7.35
7.34
7.33
7.31
7.27
6.82
6.82
6.80
6.80
4.13
NH2
2.00
1.97
1.96
0.97
1.96
f1 (ppm)
142.09
134.44
128.57
126.36
125.86
124.87
123.70
120.81
119.00
109.71
77.38
77.06
76.74
NH2
f1 (ppm)


NH2
Br
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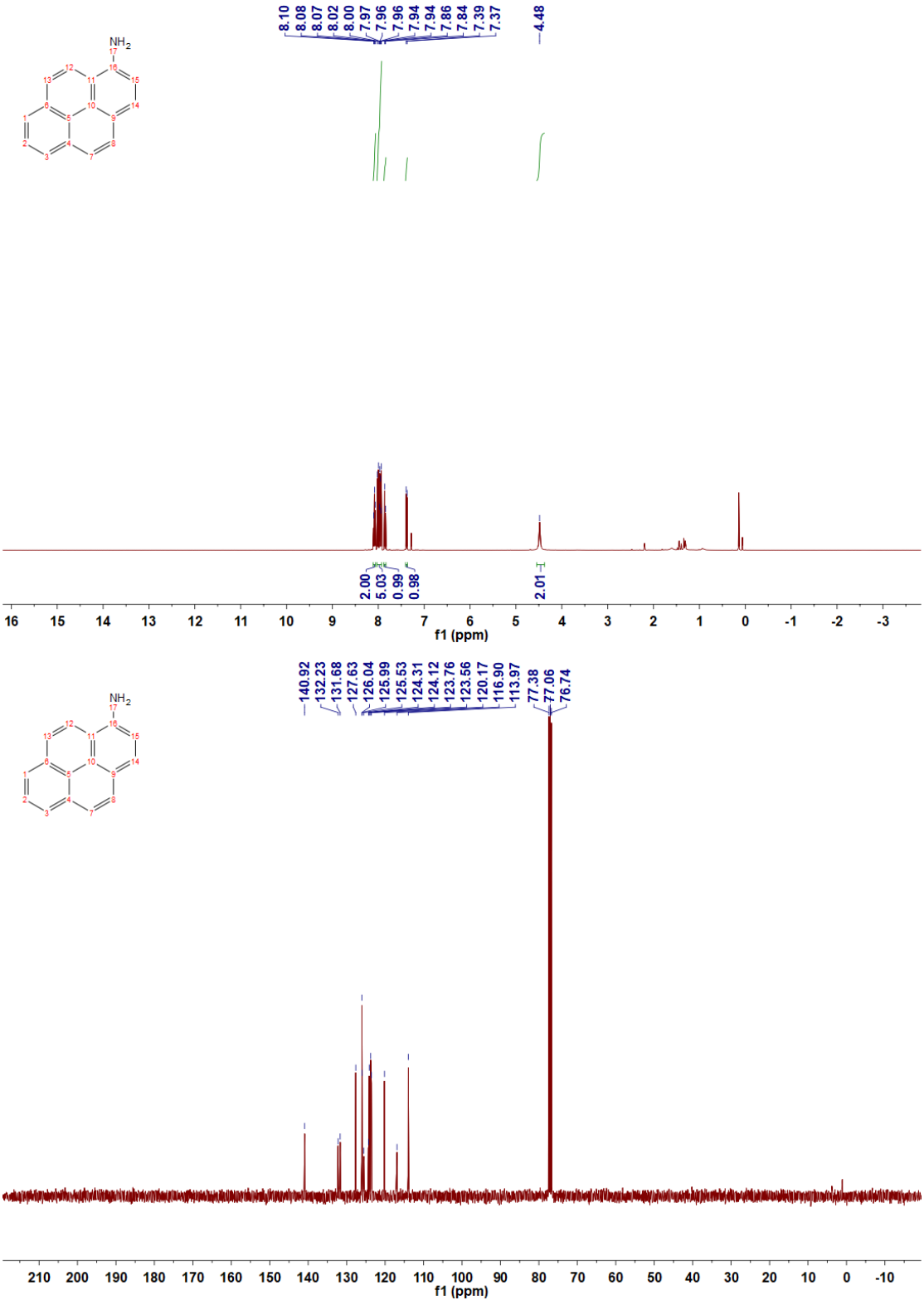
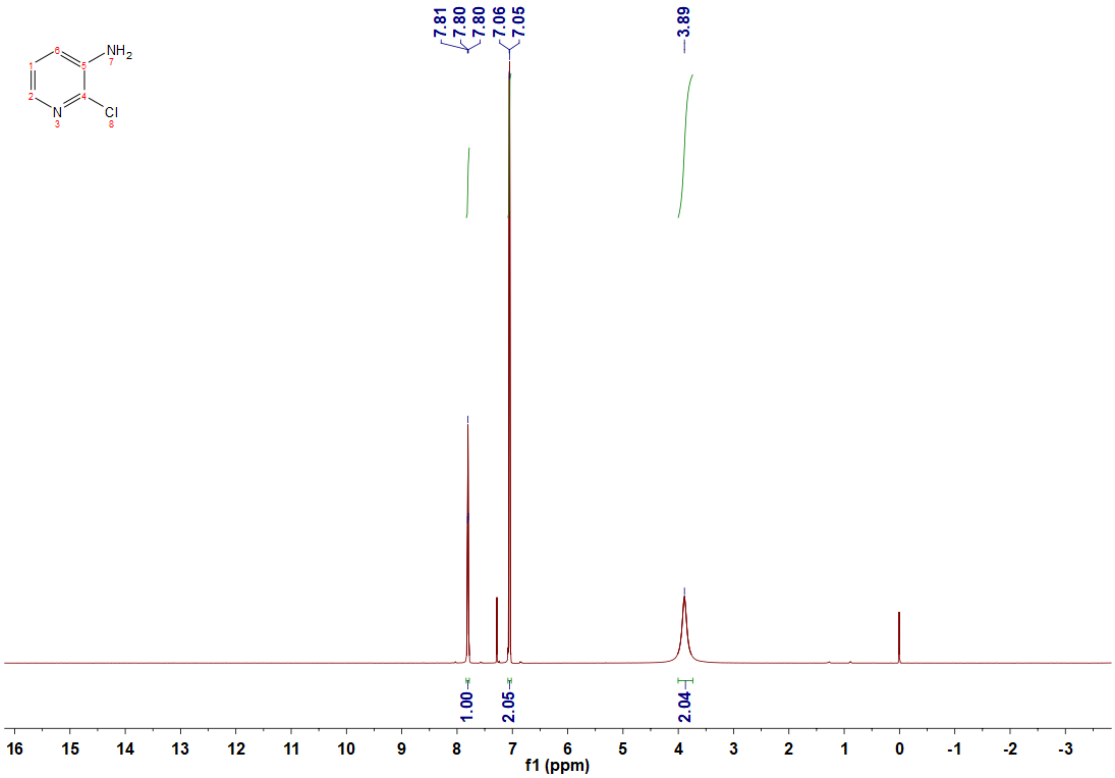
7.81
7.80
7.78
7.75
7.73
7.43
7.41
7.39
7.32
7.30
6.87
6.85
4.20
2.00
1.00
1.07
0.82
1.04
1.99
f1 (ppm)
142.43
132.97
130.12
127.74
124.88
124.80
123.68
120.73
118.19
110.70
77.32
77.01
76.69
f1 (ppm)


NH2
8.10
8.08
8.07
8.02
8.00
7.97
7.96
7.96
7.94
7.94
7.86
7.84
7.39
7.37
4.48
2.00
5.03
0.99
0.98
2.01
f1 (ppm)
NH2
140.92
132.23
131.68
127.63
126.04
125.99
125.53
124.31
124.12
123.76
123.56
120.17
116.90
113.97
77.38
77.06
76.74
f1 (ppm)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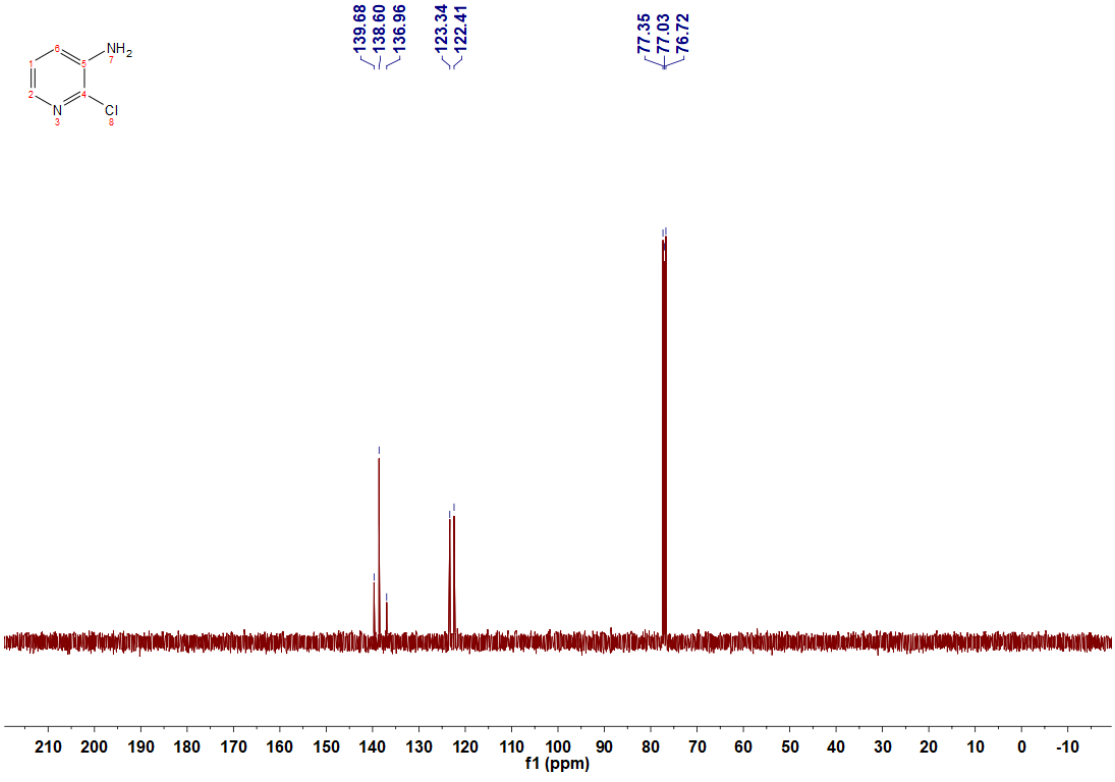
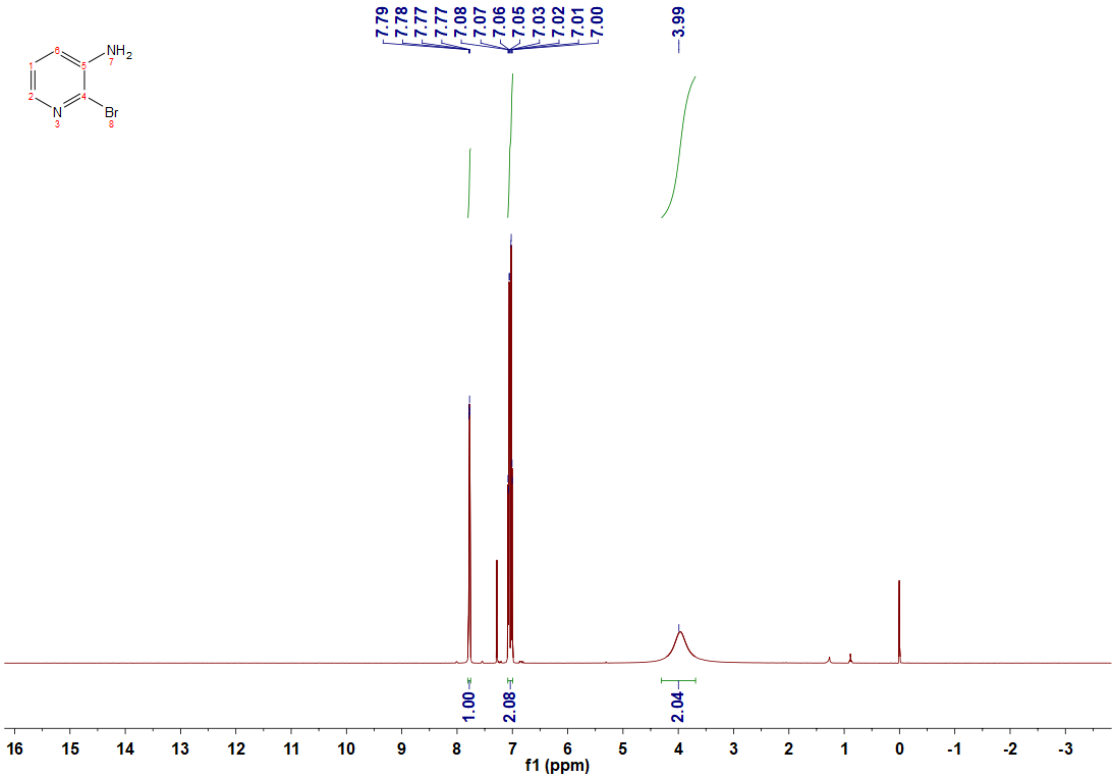
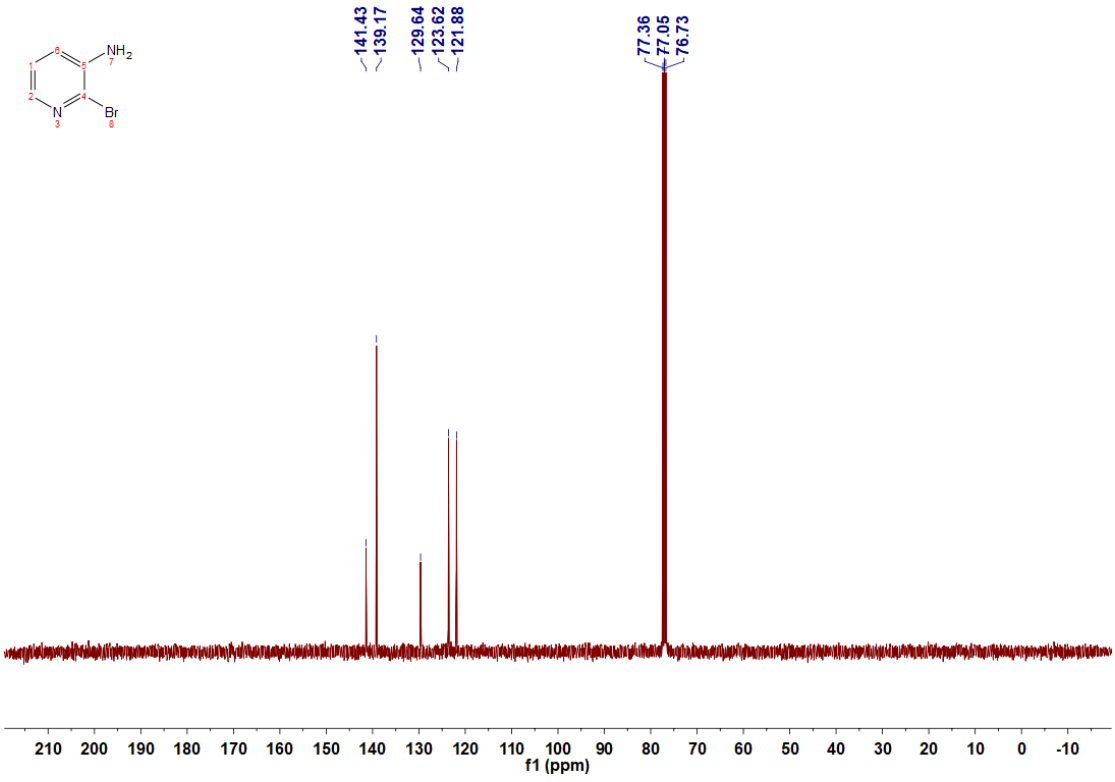
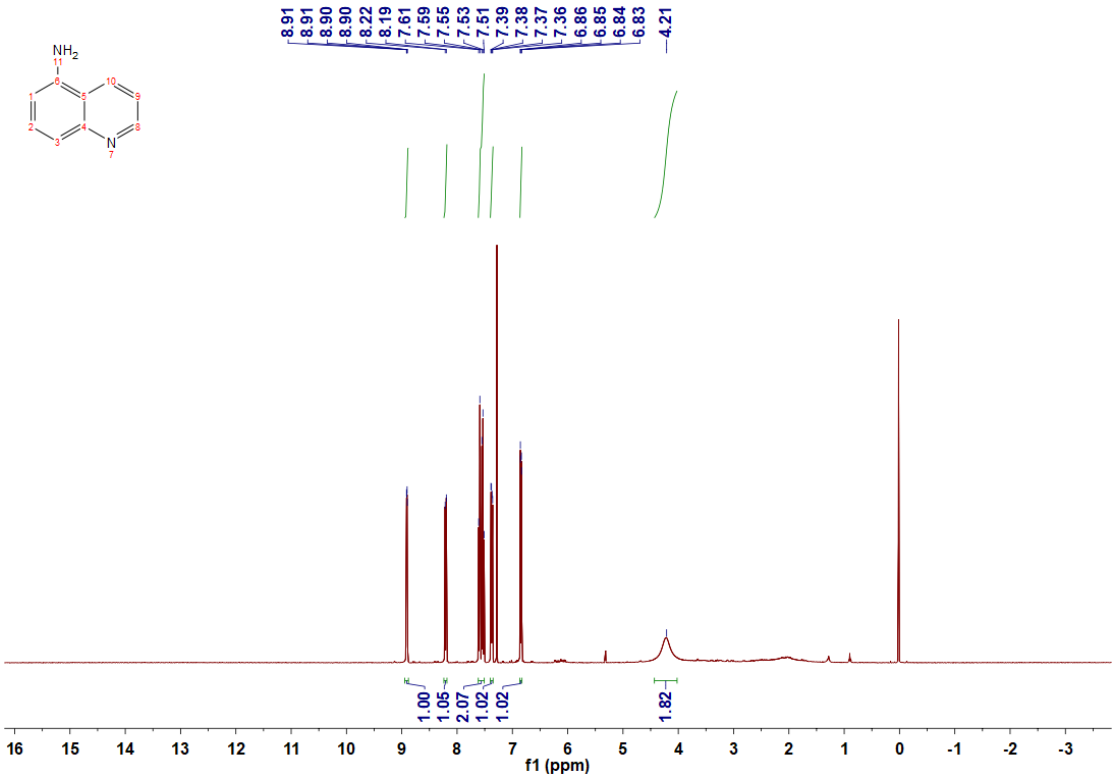
7.80
7.80
7.06
7.05
3.89
1.00
2.05
2.04
f1 (ppm)


139.68
138.60
136.96
123.34
122.41
77.35
77.03
76.72
f1 (ppm)


7.79
7.78
7.77
7.77
7.08
7.07
7.06
7.05
7.03
7.02
7.01
7.00
3.99
NH2
Br
1.00
2.08
2.04
f1 (ppm)


141.43
139.17
129.64
123.62
121.88
77.36
77.05
76.73
NH2
Br
f1 (ppm)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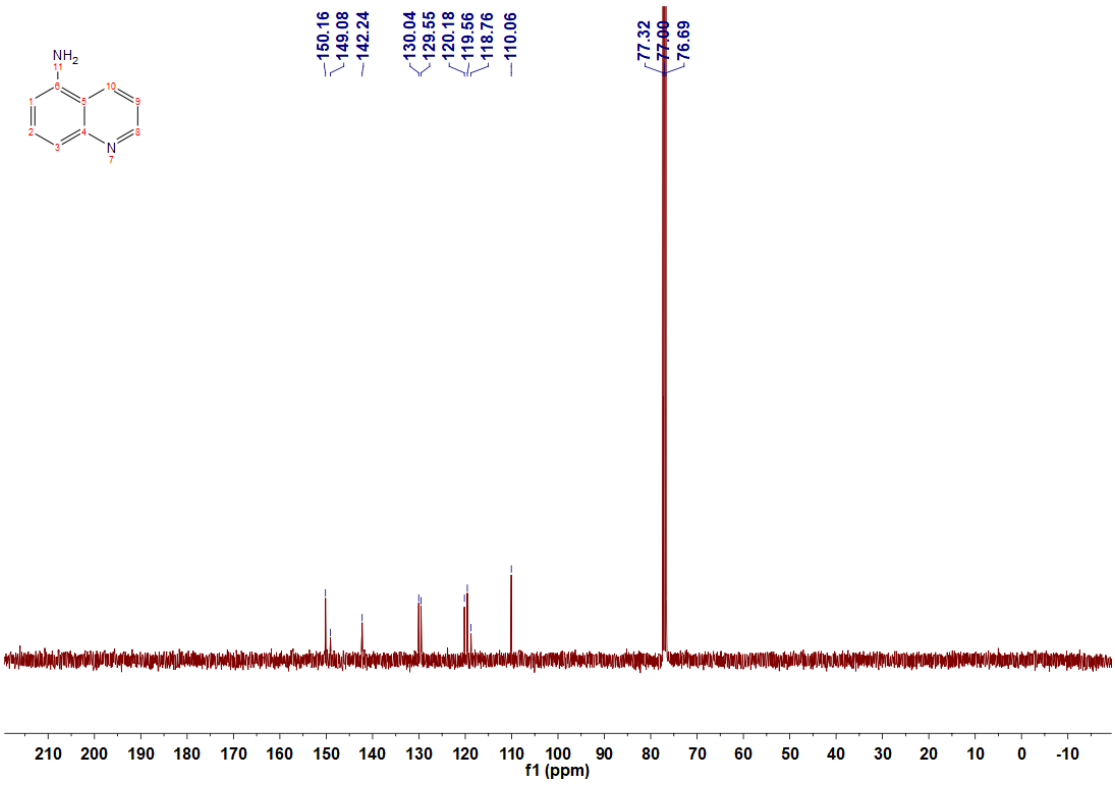
8.91
8.90
8.90
8.22
8.19
7.61
7.59
7.55
7.53
7.51
7.39
7.38
7.37
7.36
6.86
6.85
6.84
6.83
4.21
1.00
1.05
2.07
1.02
1.02
1.82
f1 (ppm)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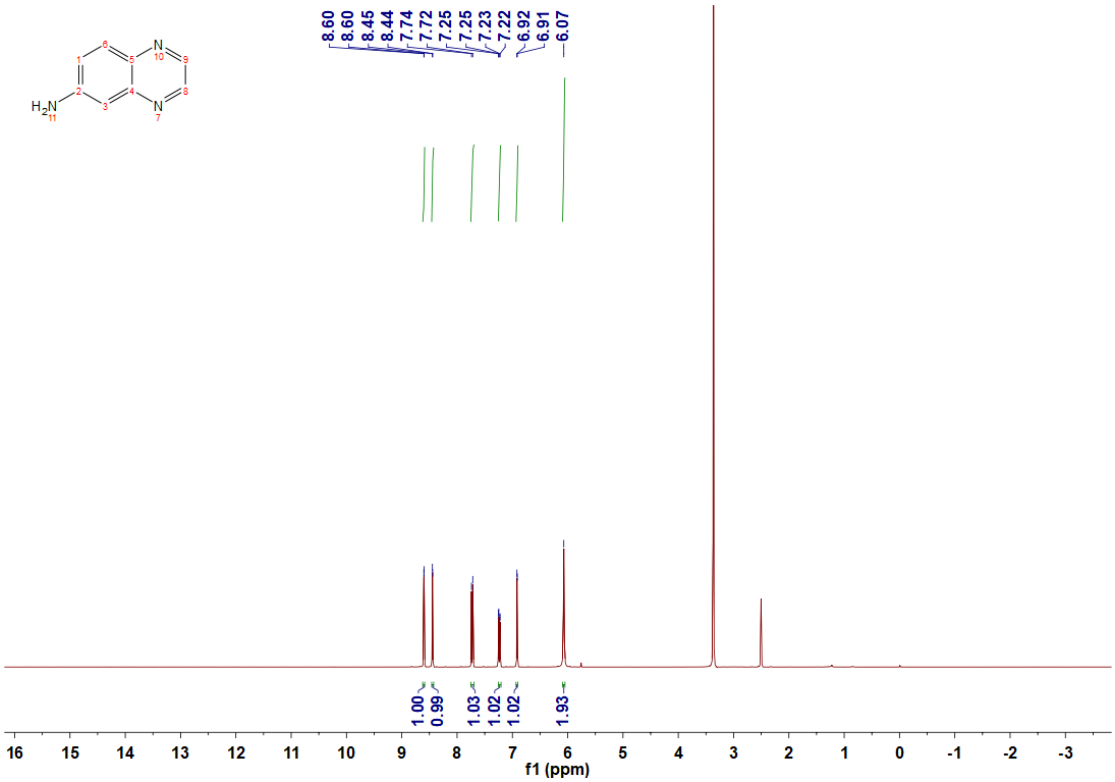
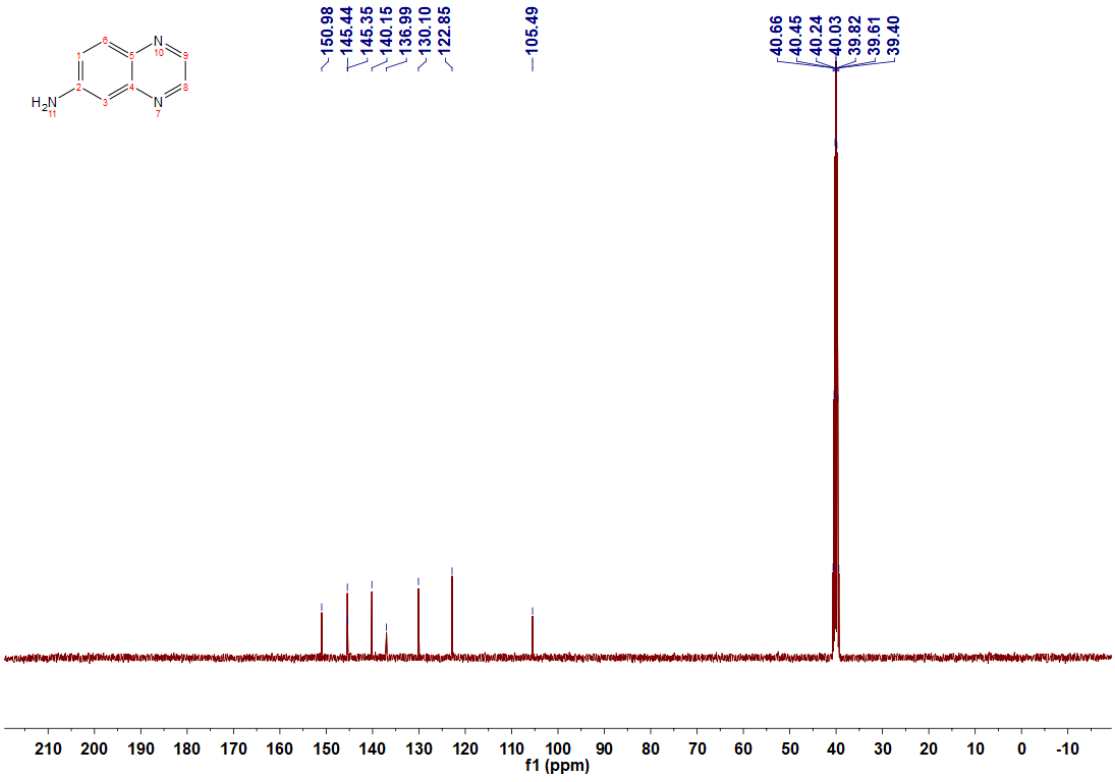
142.24
130.04
129.55
120.18
119.56
118.76
110.06
77.32
77.00
76.69
f1 (ppm)


8.60
8.60
8.45
8.44
7.74
7.72
7.25
7.25
7.23
7.22
6.92
6.91
6.07
1.00
0.99
1.03
1.02
1.02
1.93
f1 (ppm)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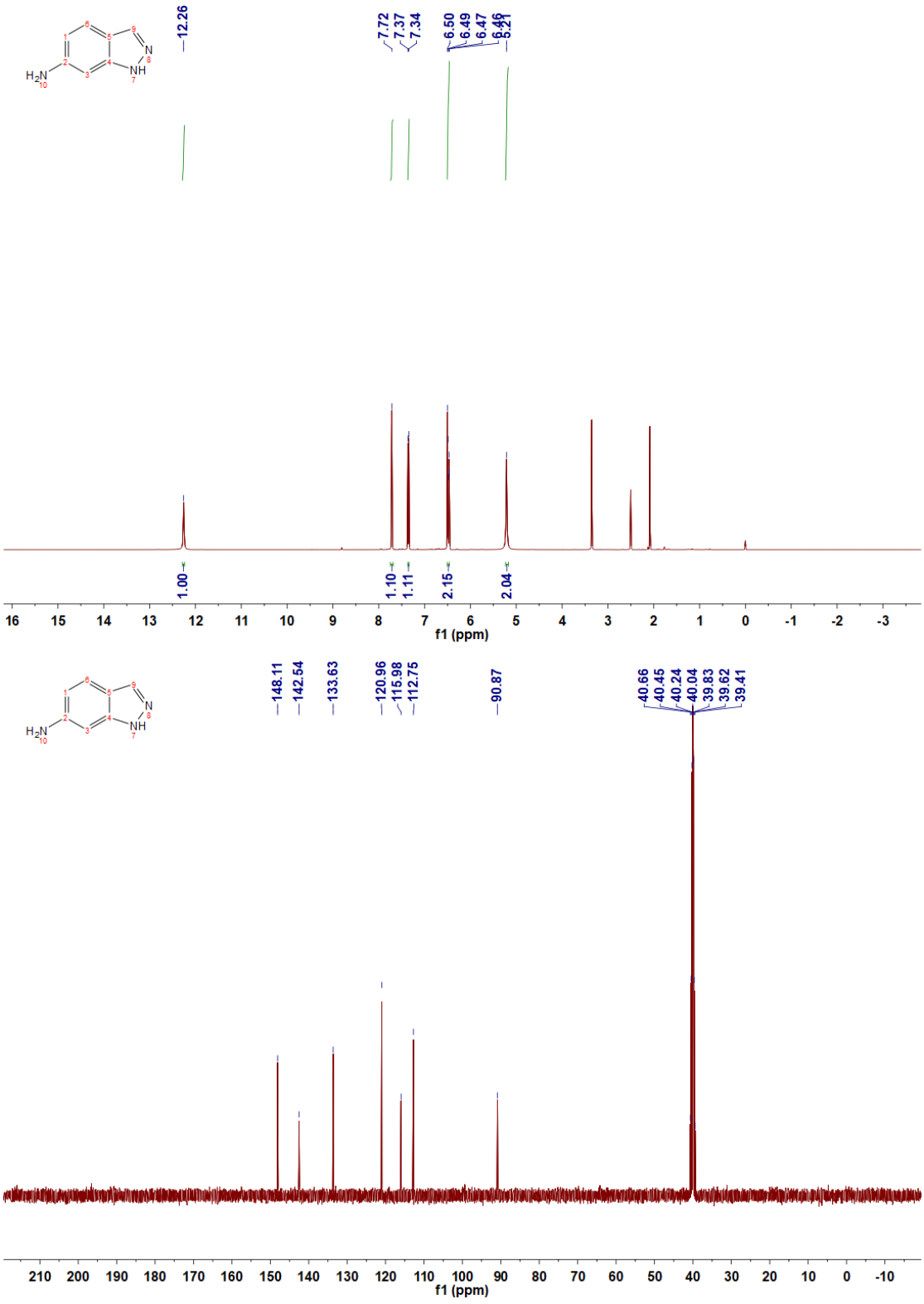
130.10
122.85
105.49
40.66
40.45
40.24
40.03
39.82
39.61
39.40
f1 (ppm)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7.34
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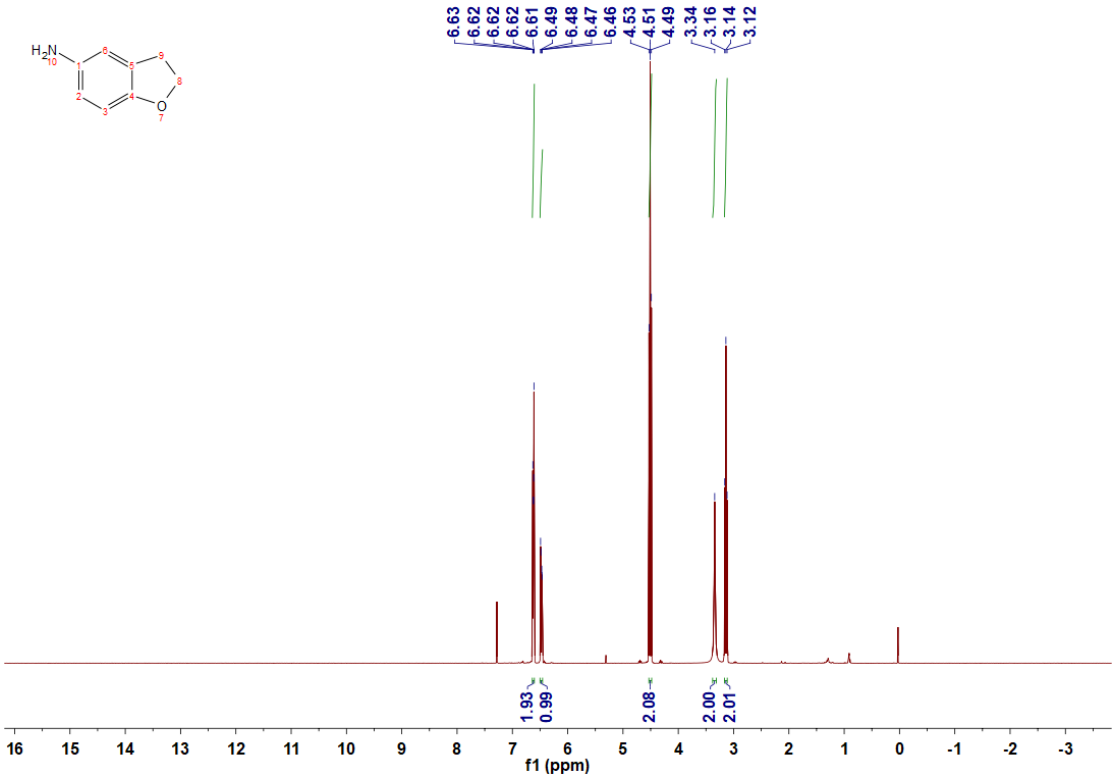
6.49
6.47
6.46
6.21
1.00
1.10
1.11
2.15
2.04
f1 (ppm)
148.11
142.54
133.63
120.96
115.98
112.75
90.87
40.66
40.45
40.24
40.04
39.83
39.62
39.41
f1 (ppm)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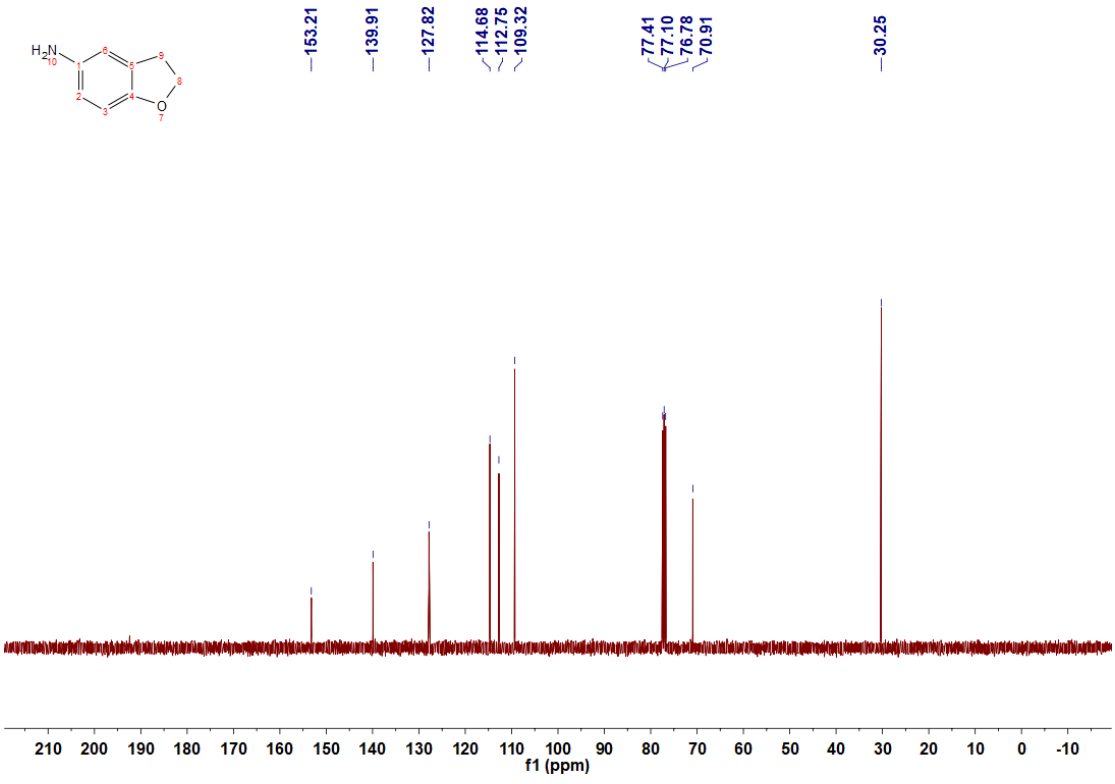
6.62
6.62
6.62
6.61
6.49
6.48
6.47
6.46
4.53
4.51
4.49
3.34
3.16
3.14
3.12
1.93
0.99
2.08
2.00
2.01
f1 (ppm)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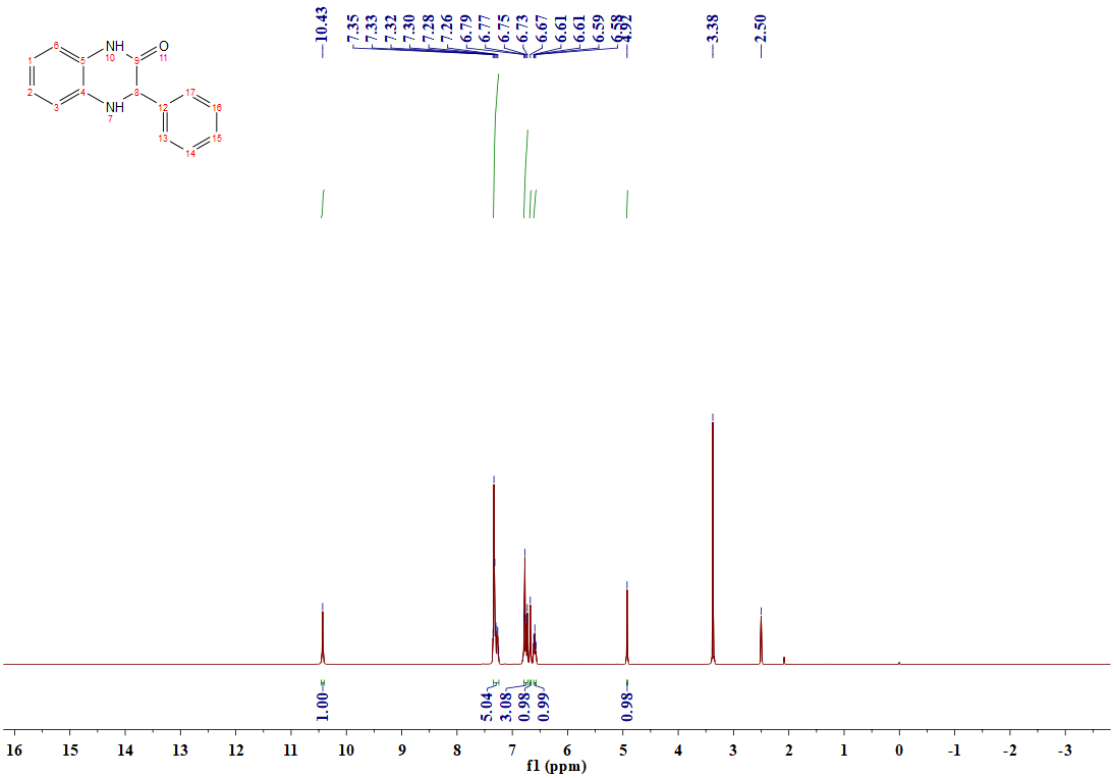
114.68
112.75
109.32
77.41
77.10
76.78
70.91
30.25
f1 (ppm)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7.35
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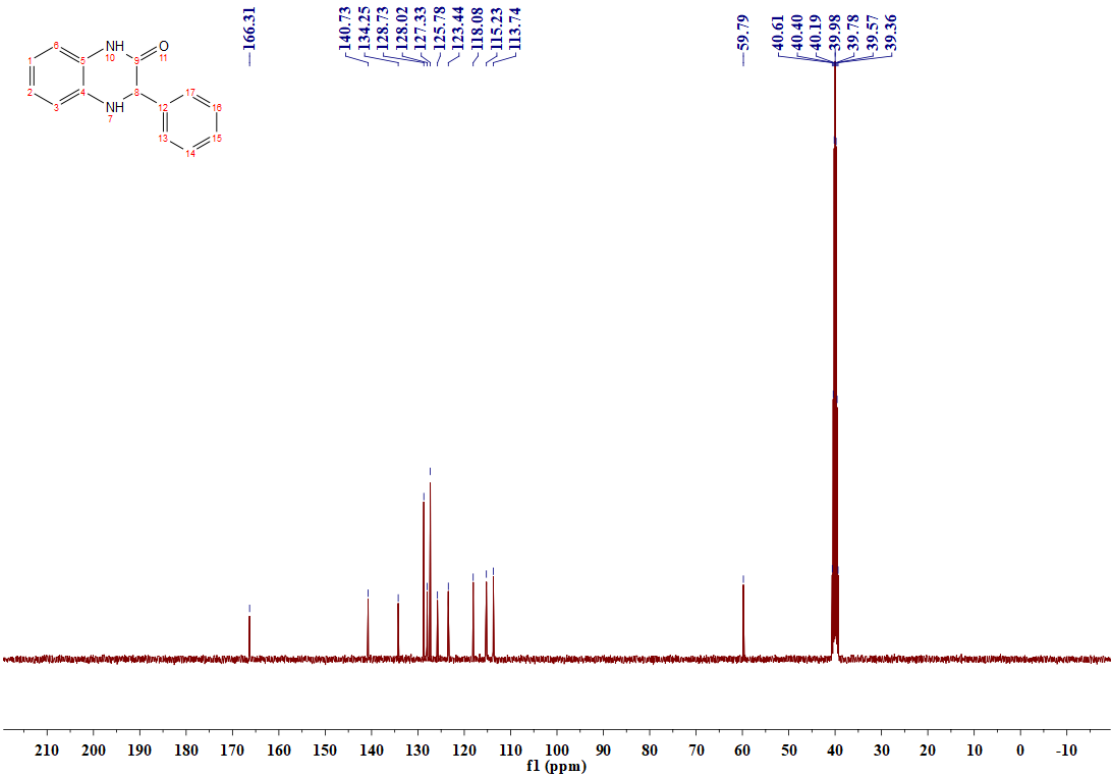
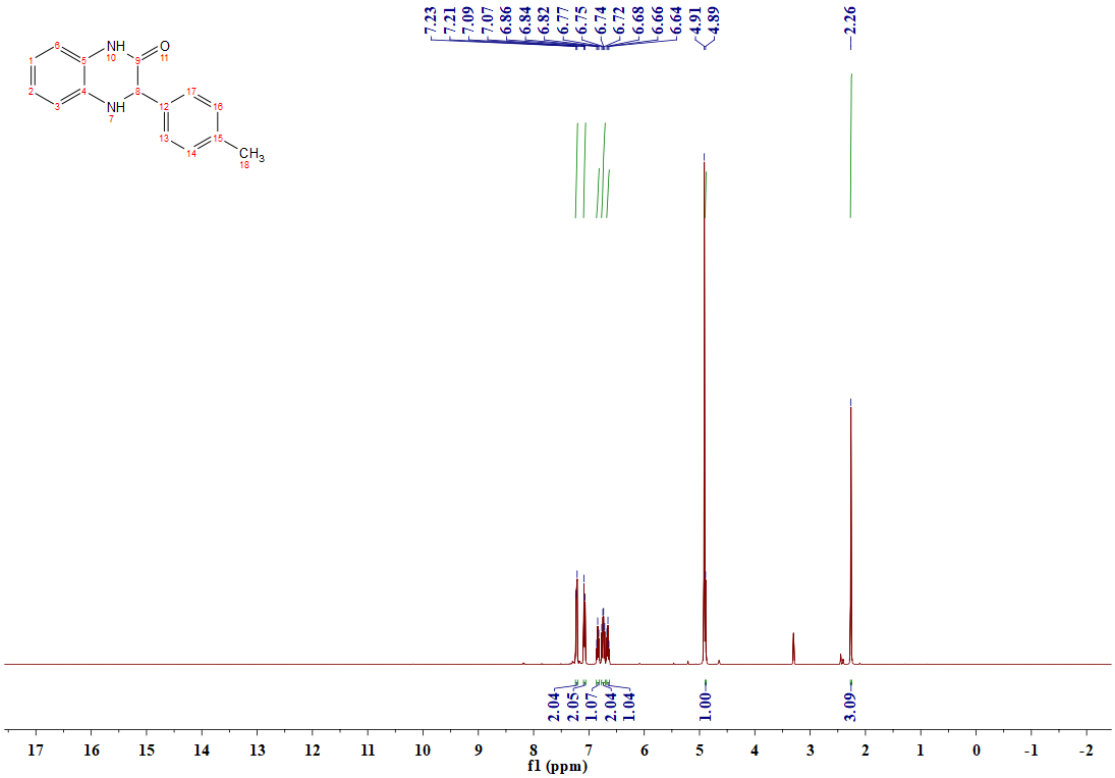
7.32
7.30
7.28
7.26
6.79
6.77
6.75
6.73
6.67
6.61
6.61
6.59
6.58
4.92
3.38
2.50
1.00
5.04
3.08
0.98
0.99
0.98
f1 (ppm)


166.31
140.73
134.25
128.73
128.02
127.33
125.78
123.44
118.08
115.23
113.74
59.79
40.61
40.40
40.19
39.98
39.78
39.57
39.36
f1 (ppm)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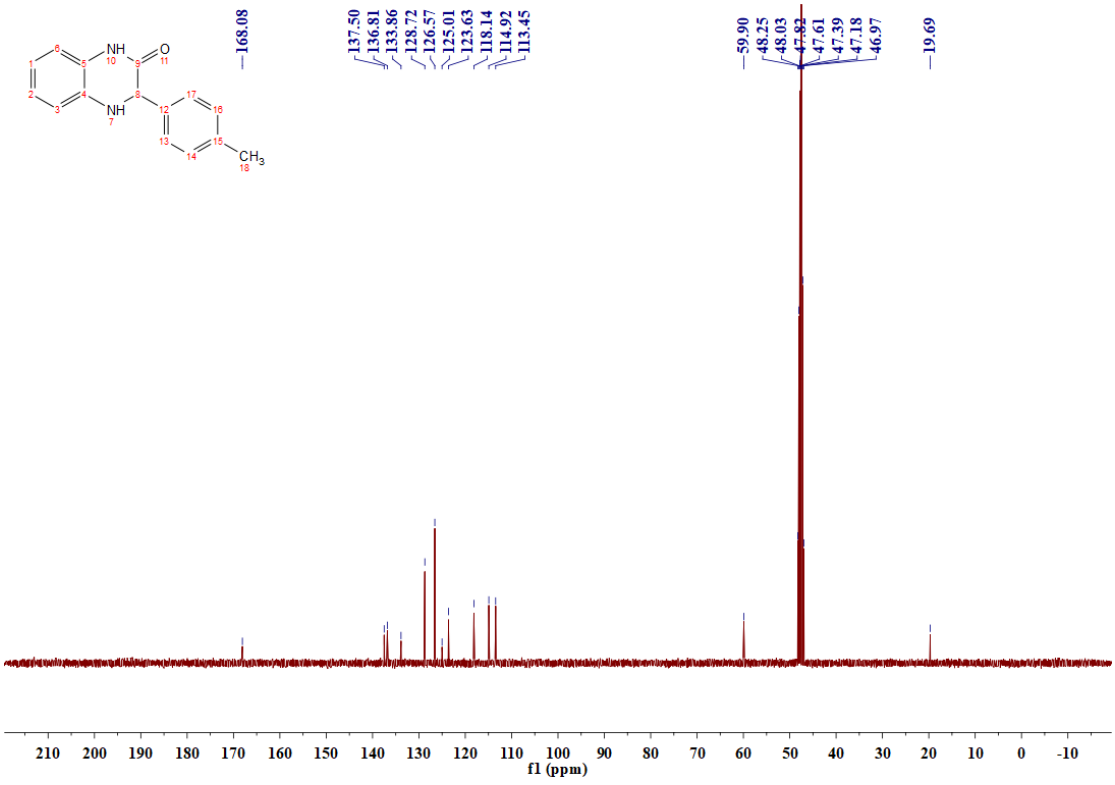
7.09
7.07
6.86
6.84
6.82
6.77
6.75
6.74
6.72
6.68
6.66
6.64
4.91
4.89
2.26
2.04
2.05
1.07
2.04
1.04
1.00
3.09
f1 (ppm)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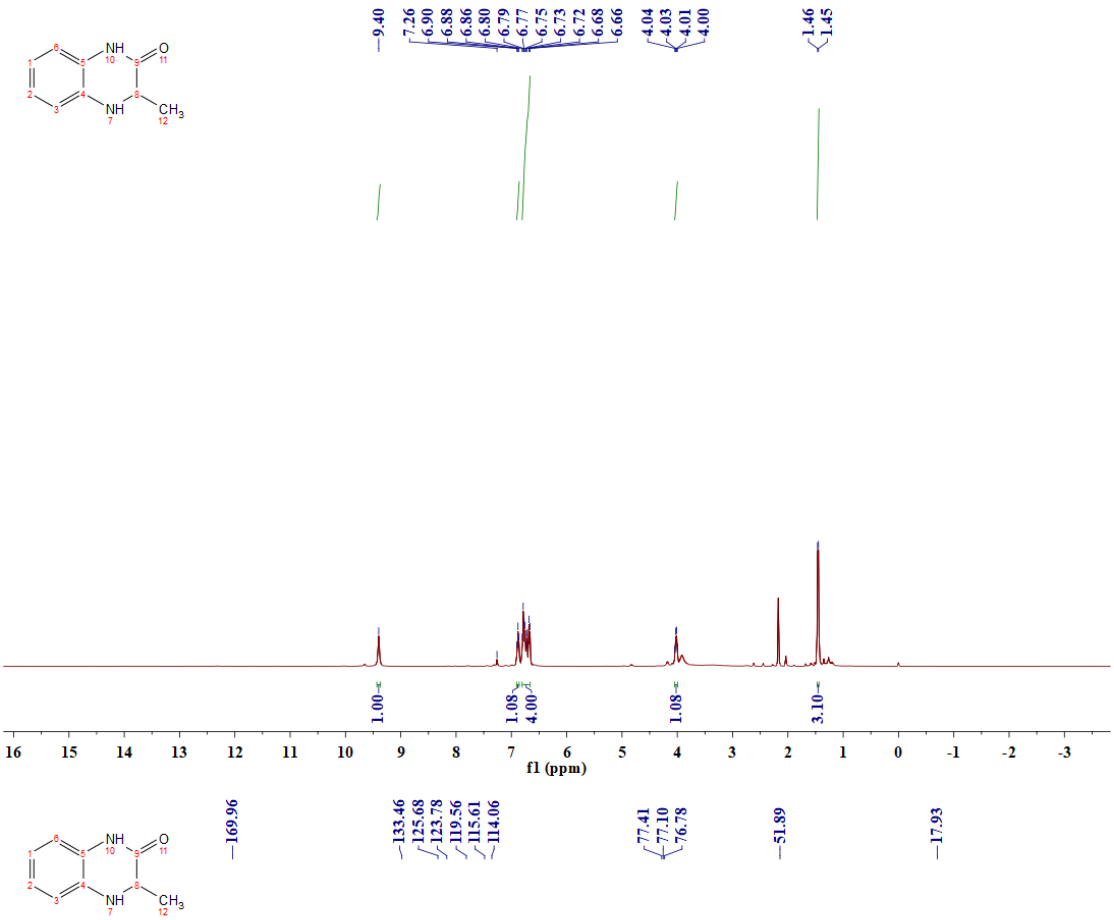
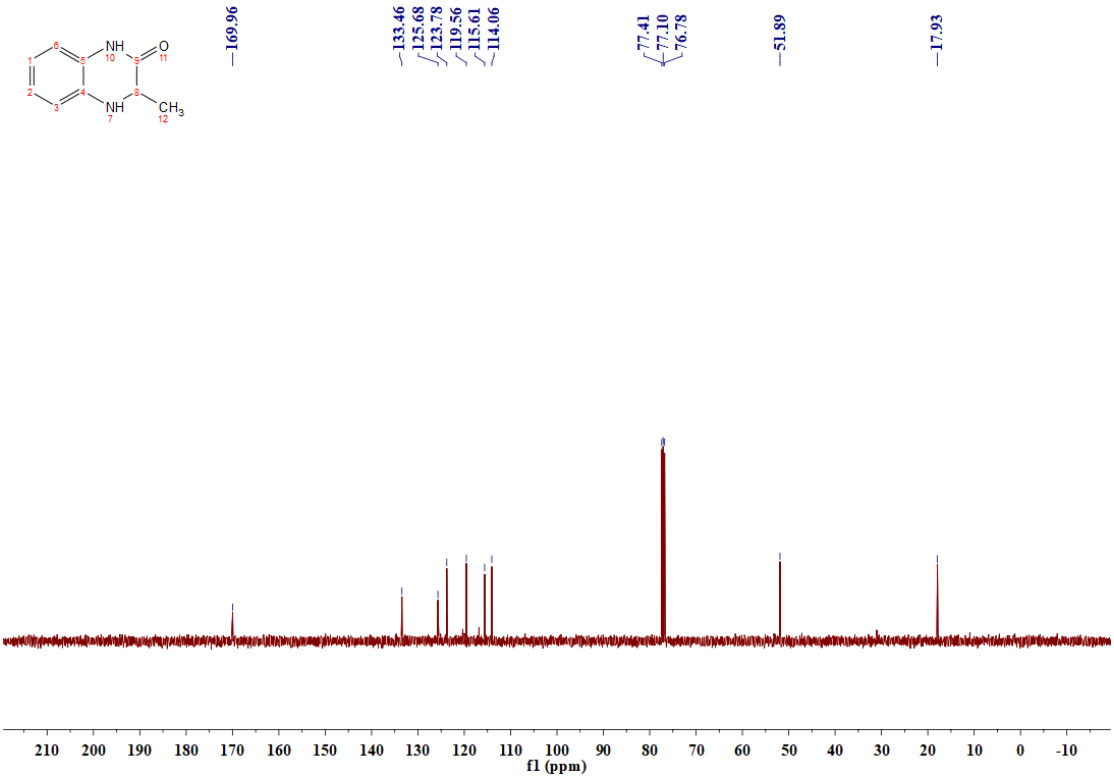
137.50
136.81
133.86
128.72
126.57
125.01
123.63
118.14
114.92
113.45
59.90
48.25
48.03
47.82
47.61
47.39
47.18
46.97
19.69
f1 (ppm)


8.71
7.38
7.36
7.32
7.30
6.94
6.79
6.75
6.74
6.72
5.06
4.27
0.95
2.05
2.04
1.04
3.04
1.00
0.99
f1 (ppm)
166.57
137.26
134.43
132.67
128.96
128.63
124.64
124.25
119.69
115.58
113.88
60.11
f1 (ppm)


9.40
7.26
6.90
6.88
6.86
6.80
6.79
6.77
6.75
6.73
6.72
6.68
6.66
4.04
4.03
4.01
4.00
1.46
1.45
1.00
1.08
4.00
1.08
3.10
f1 (ppm)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133.46
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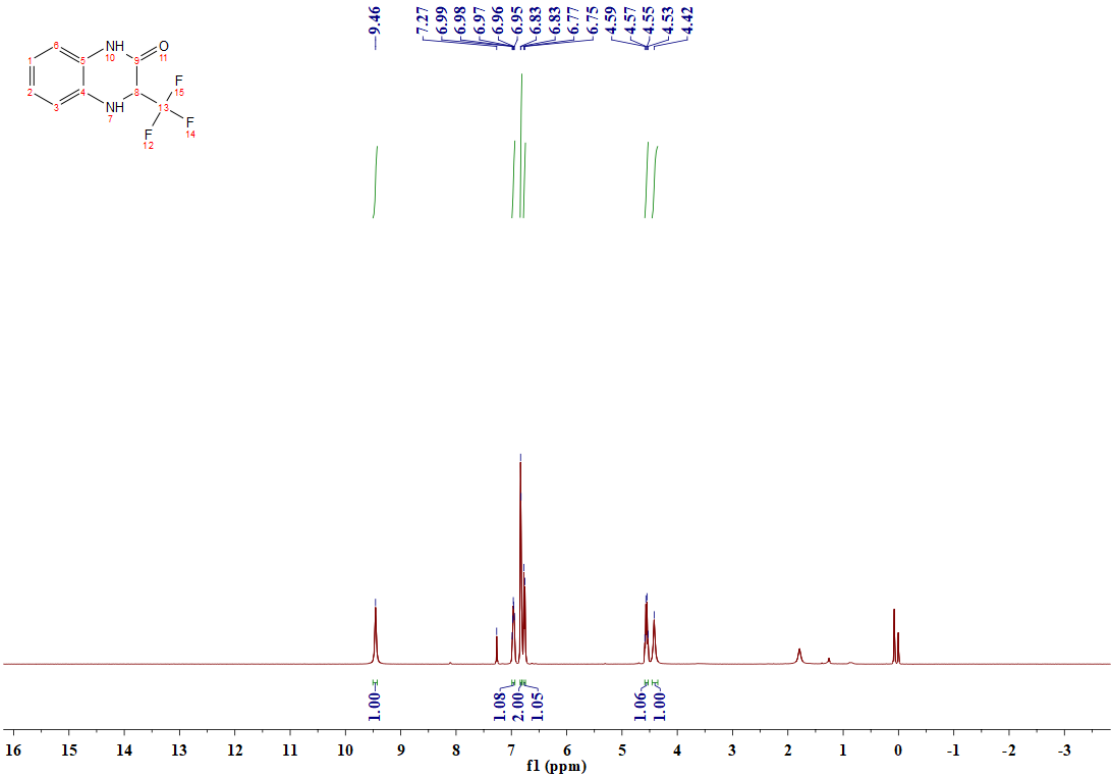
119.56
115.61
114.06
77.41
77.10
76.78
51.89
17.93
f1 (ppm)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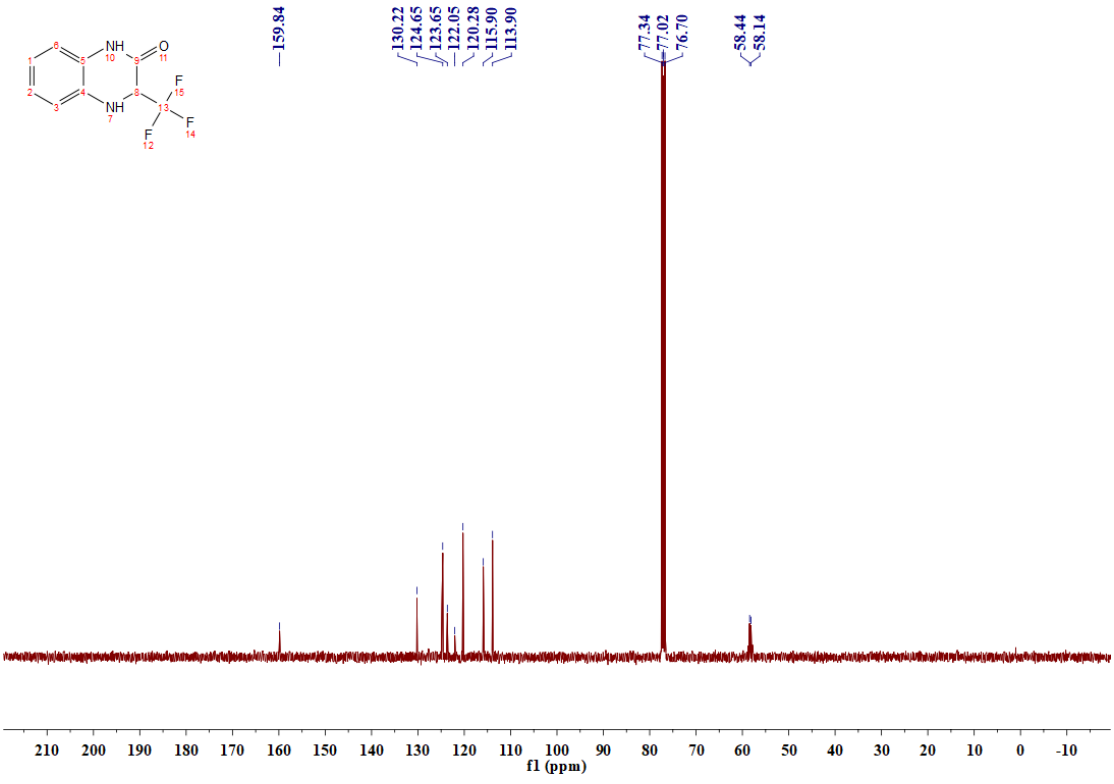
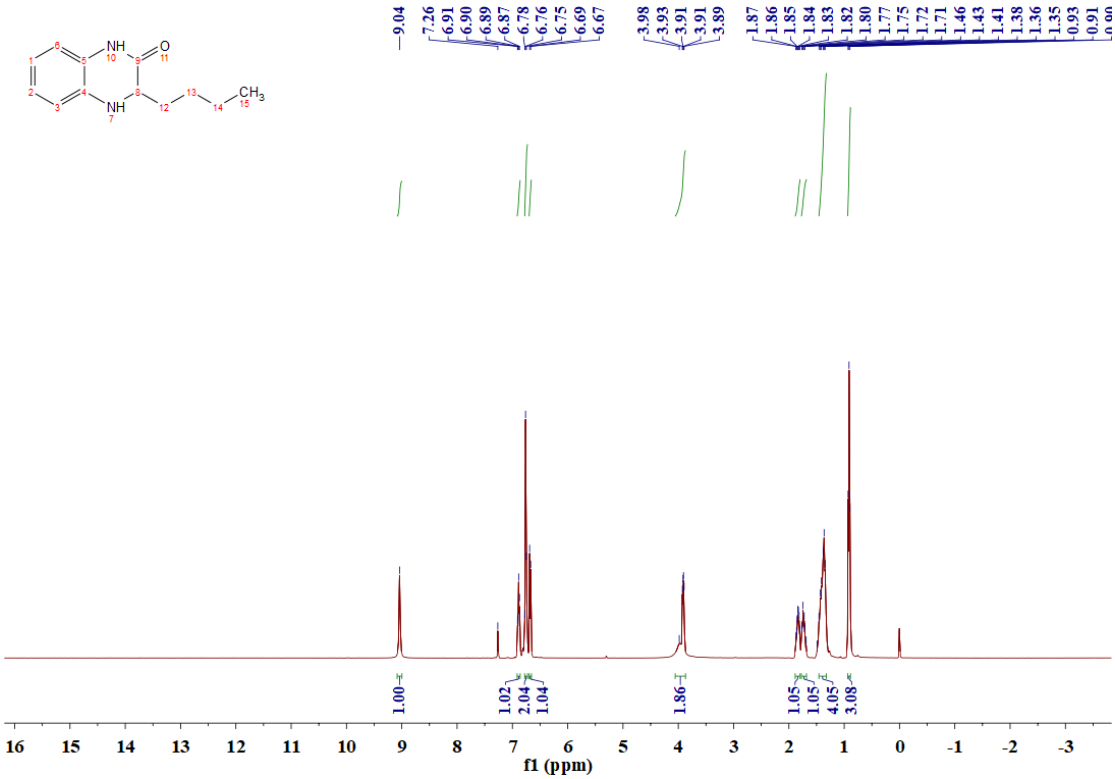
7.27
6.99
6.98
6.97
6.96
6.95
6.83
6.83
6.77
6.75
4.59
4.57
4.55
4.53
4.42
1.00
1.08
2.00
1.05
1.06
1.00
f1 (ppm)


159.84
130.22
124.65
123.65
122.05
120.28
115.90
113.90
77.34
77.02
76.70
58.44
58.14
f1 (ppm)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6.90
6.89
6.87
6.78
6.76
6.75
6.69
6.67
3.98
3.93
3.91
3.91
3.89
1.87
1.86
1.85
1.84
1.83
1.82
1.80
1.77
1.75
1.72
1.71
1.46
1.43
1.41
1.38
1.36
1.35
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0.91
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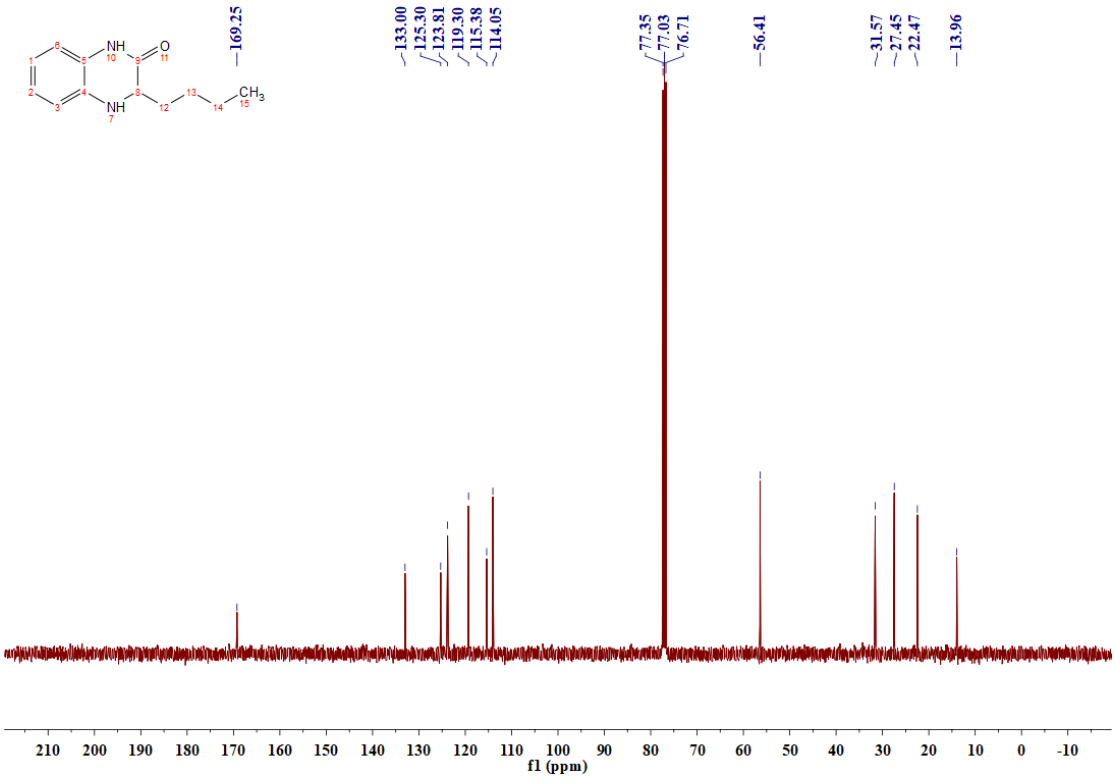
1.02
2.04
1.04
1.86
1.05
1.05
4.05
3.08
f1 (ppm)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123.81
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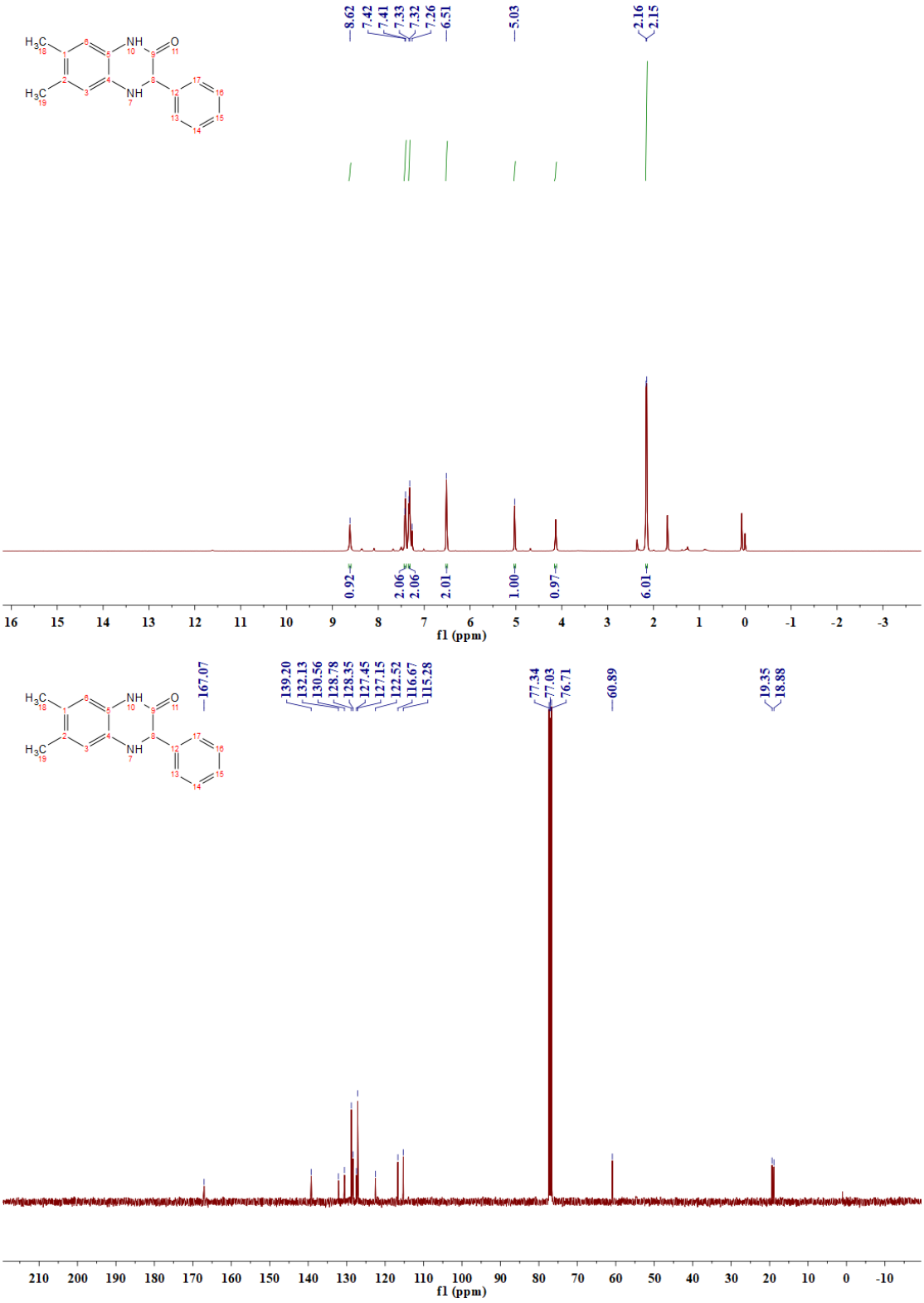
115.38
114.05
77.35
77.03
76.71
56.41
31.57
27.45
22.47
13.96
f1 (ppm)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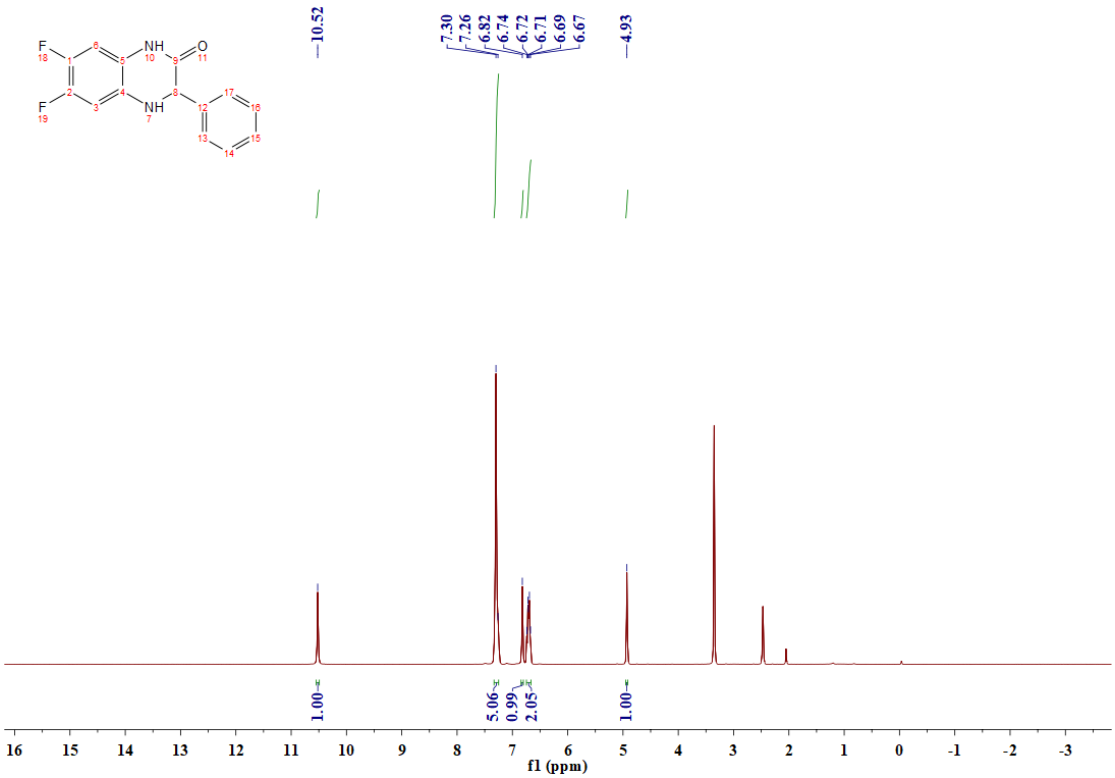
7.42
7.41
7.33
7.32
7.26
6.51
5.03
2.16
2.15
0.92
2.06
2.06
2.01
1.00
0.97
6.01
f1 (ppm)
167.07
139.20
132.13
130.56
128.78
128.35
127.45
127.15
122.52
116.67
115.28
77.34
77.03
76.71
60.89
19.35
18.88
f1 (ppm)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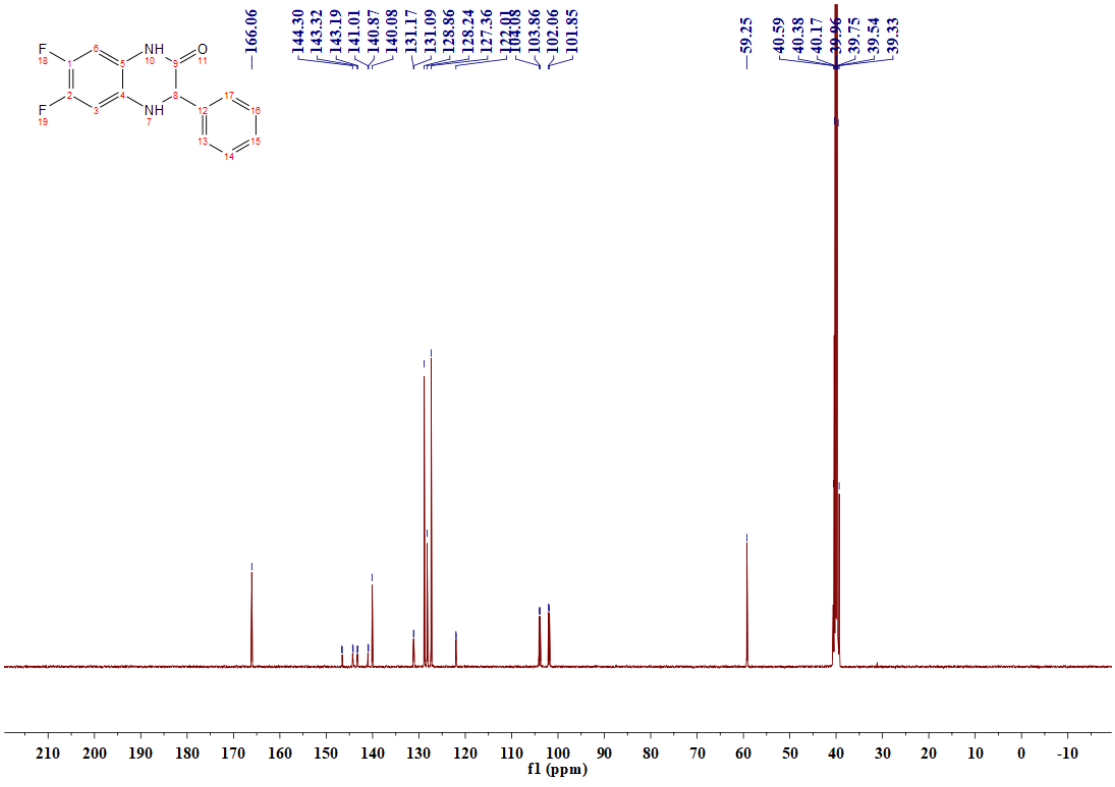
7.26
6.82
6.74
6.72
6.71
6.69
6.67
4.93
1.00
5.06
0.99
2.05
1.00
f1 (ppm)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143.32
143.19
141.01
140.87
140.08
131.17
131.09
128.86
128.24
127.36
122.01
104.08
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102.06
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59.25
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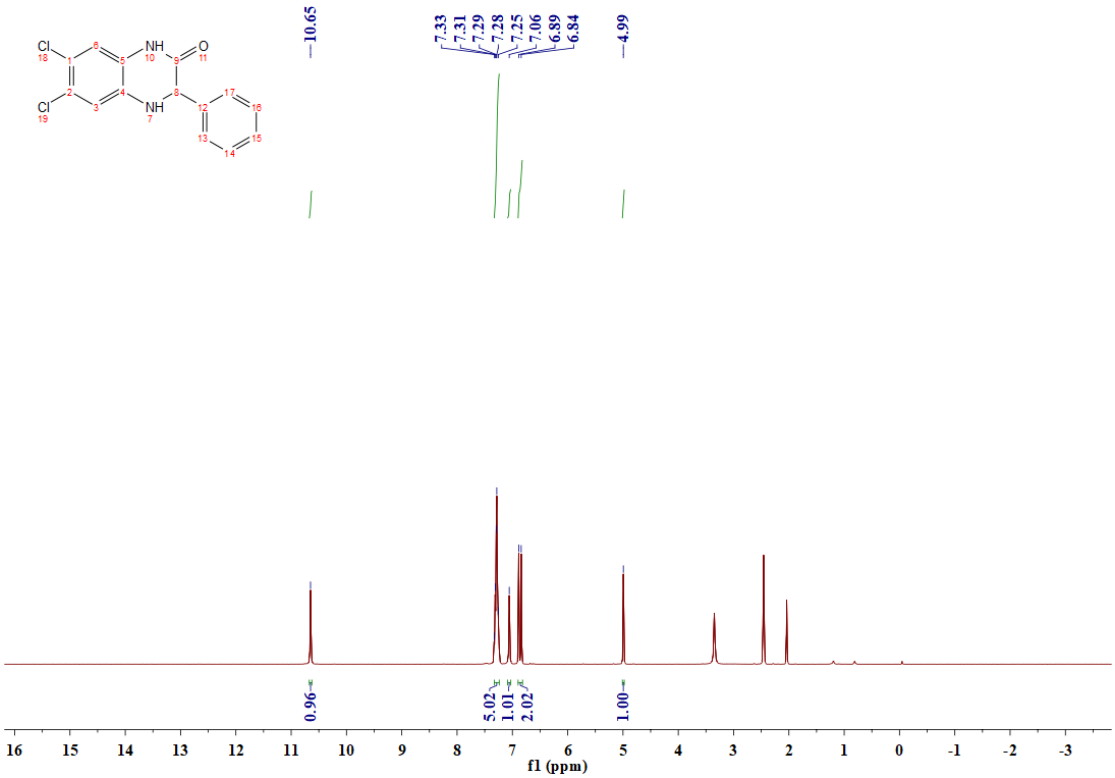
40.38
40.17
39.96
39.75
39.54
39.33
f1 (ppm)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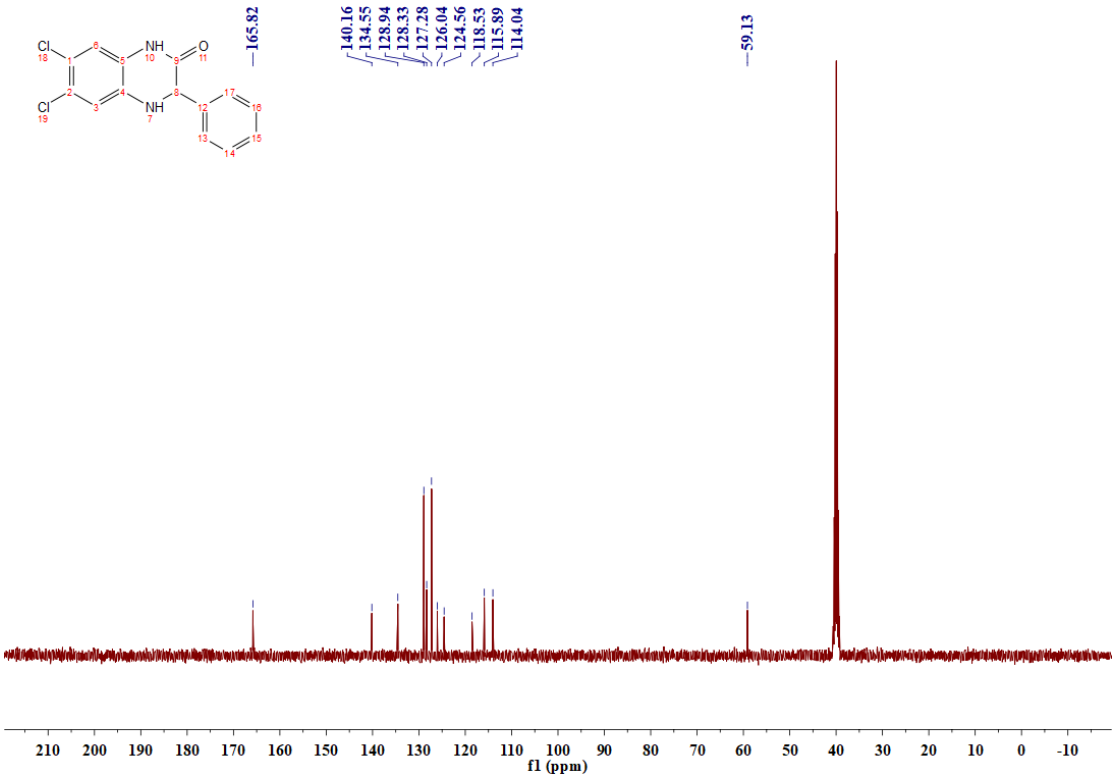
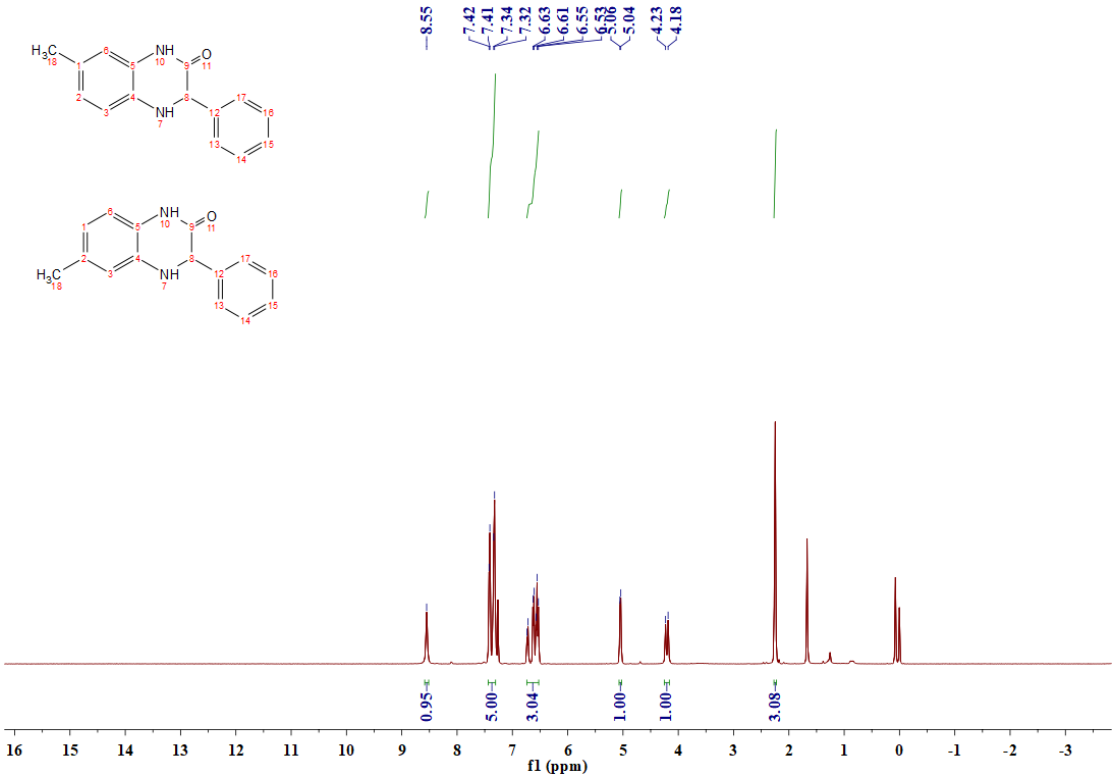
7.29
7.28
7.25
7.06
6.89
6.84
4.99
0.96
5.02
1.01
2.02
1.00
f1 (ppm)


165.82
140.16
134.55
129.94
128.33
127.28
126.04
124.56
118.53
115.89
114.04
59.13
f1 (ppm)


8.55
7.42
7.41
7.34
7.32
6.63
6.61
6.55
6.53
5.06
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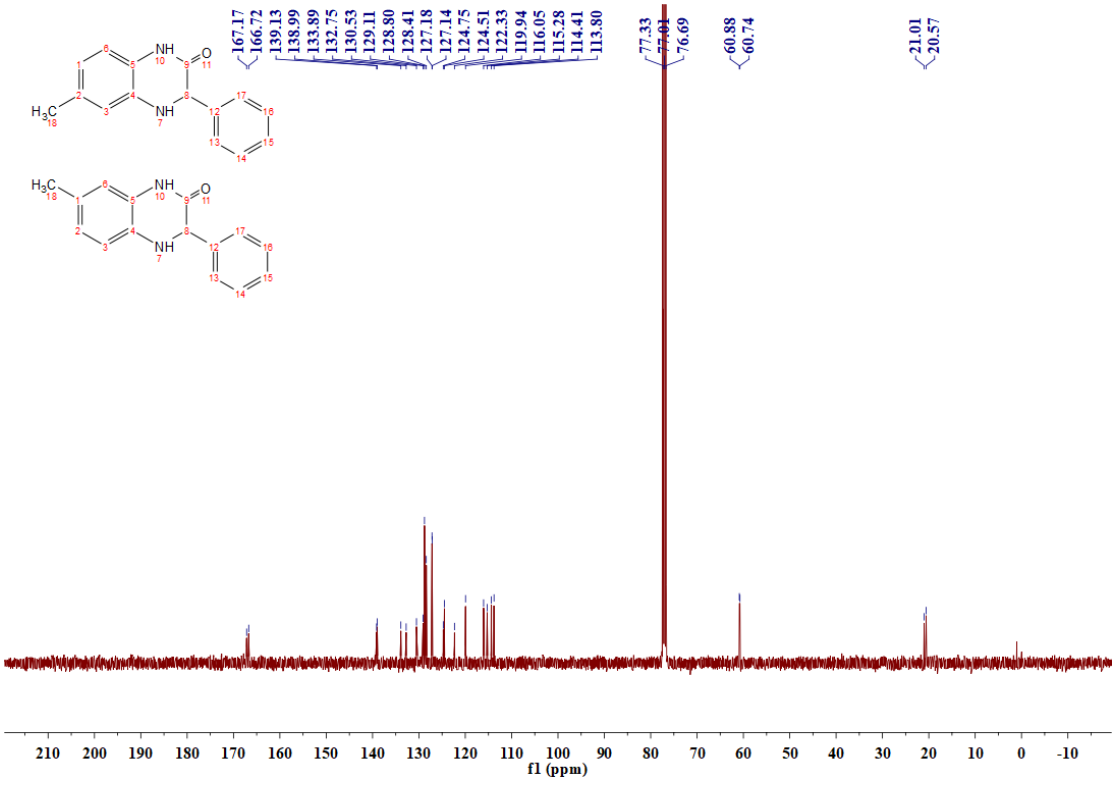
4.23
4.18
0.95
5.00
3.04
1.00
1.00
3.08
f1 (ppm)


167.17
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133.89
132.75
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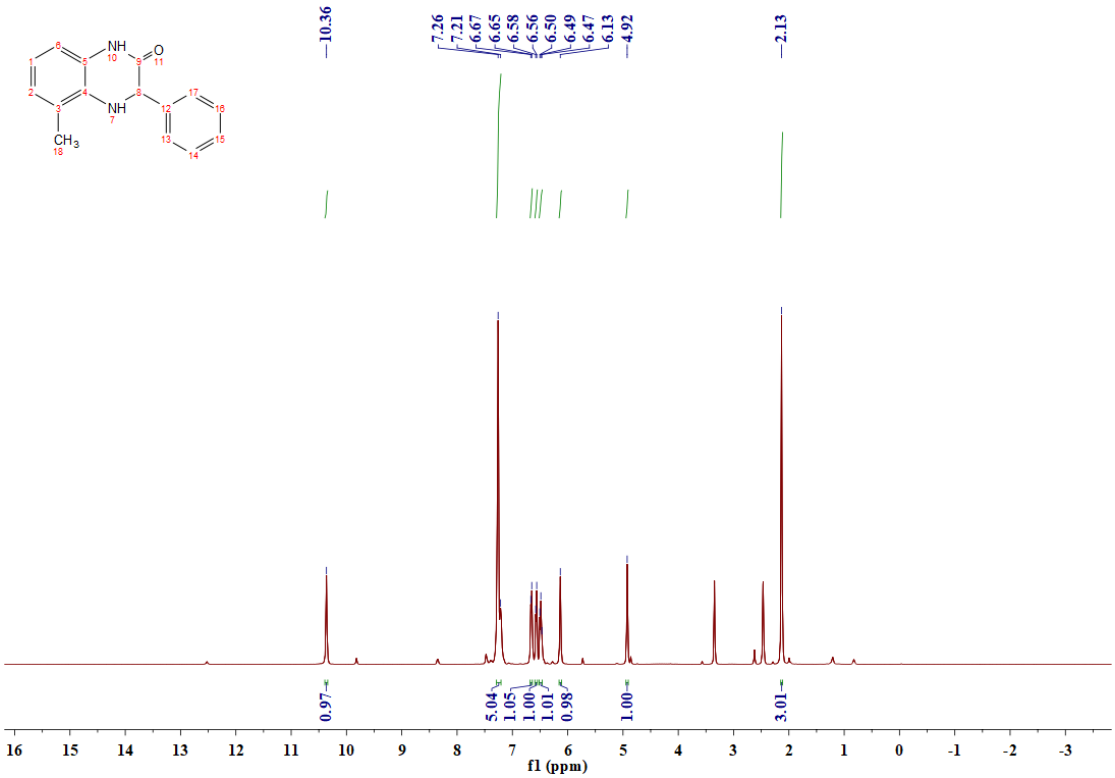
129.11
128.80
128.41
127.18
127.14
124.75
124.51
122.33
119.94
116.05
115.28
114.41
113.80
77.33
77.01
76.69
60.88
60.74
21.01
20.57
f1 (ppm)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6.50
6.49
6.47
6.13
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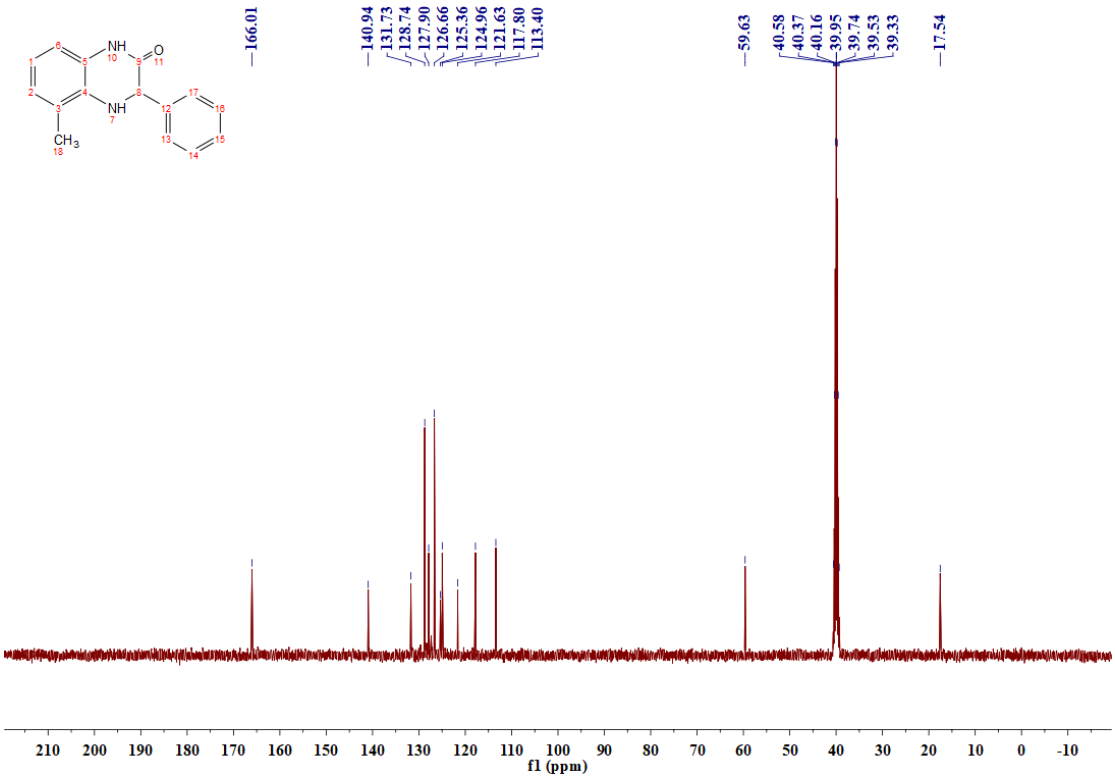
2.13
0.97
5.04
1.05
1.00
1.01
0.98
1.00
3.01
f1 (ppm)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121.63
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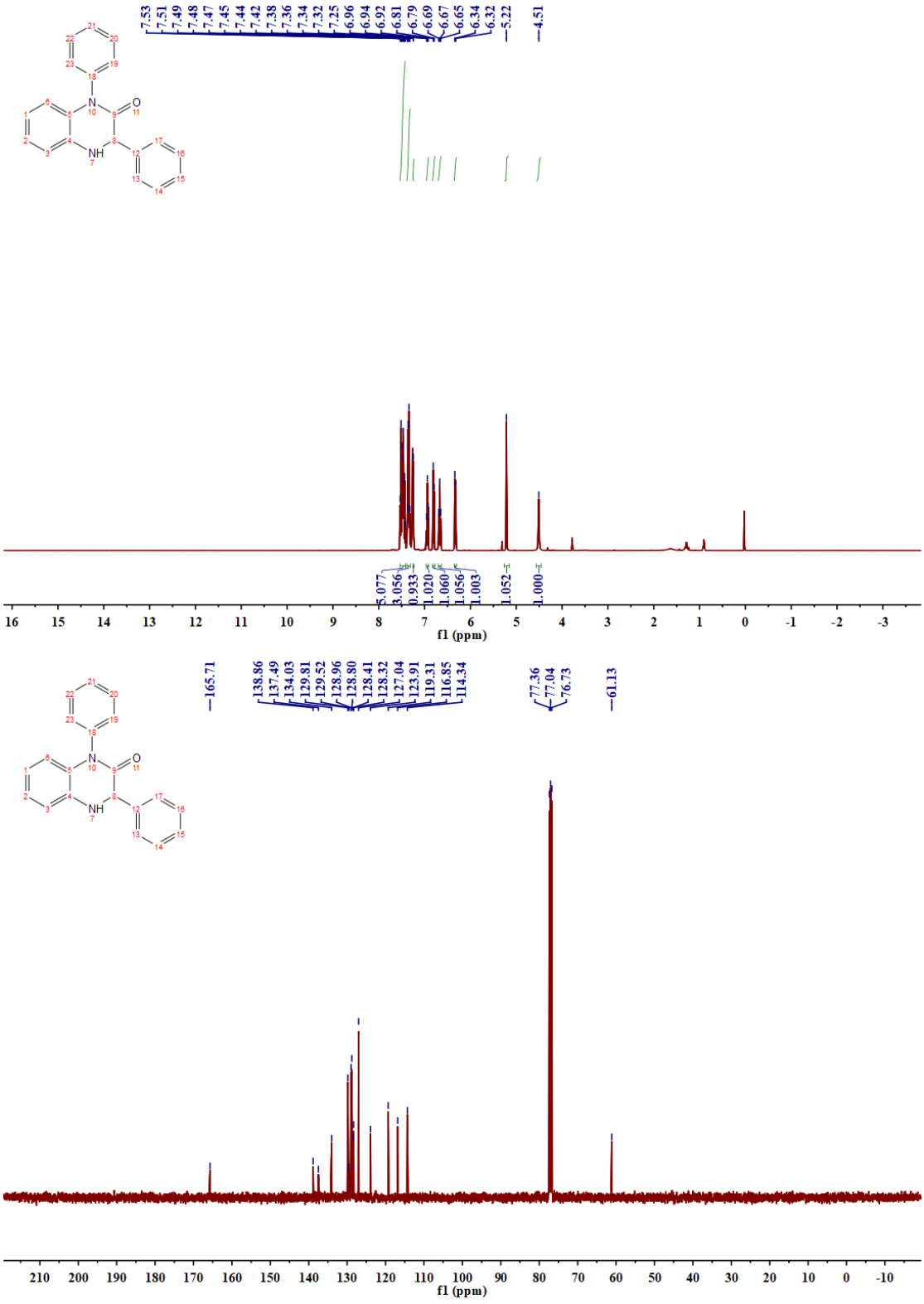
40.16
39.95
39.74
39.53
39.33
17.54
f1 (ppm)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7.47
7.45
7.44
7.42
7.38
7.36
7.34
7.32
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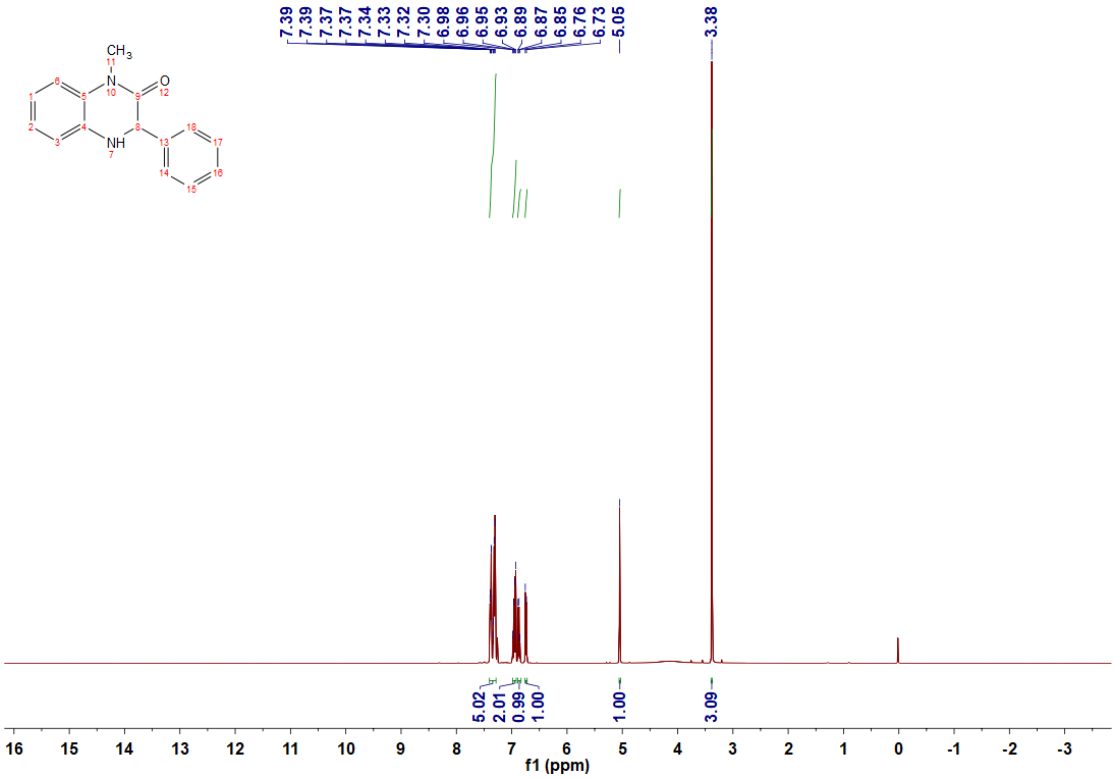
6.96
6.94
6.92
6.81
6.79
6.69
6.67
6.65
6.34
6.32
5.22
4.51
5.077
3.056
0.933
1.020
1.060
1.056
1.003
1.052
1.000
f1 (ppm)
165.71
138.86
137.49
134.03
129.81
129.52
128.96
128.80
128.41
128.32
127.04
123.91
119.31
116.85
114.34
77.36
77.04
76.73
61.13
f1 (ppm)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7.39
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7.34
7.33
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7.30
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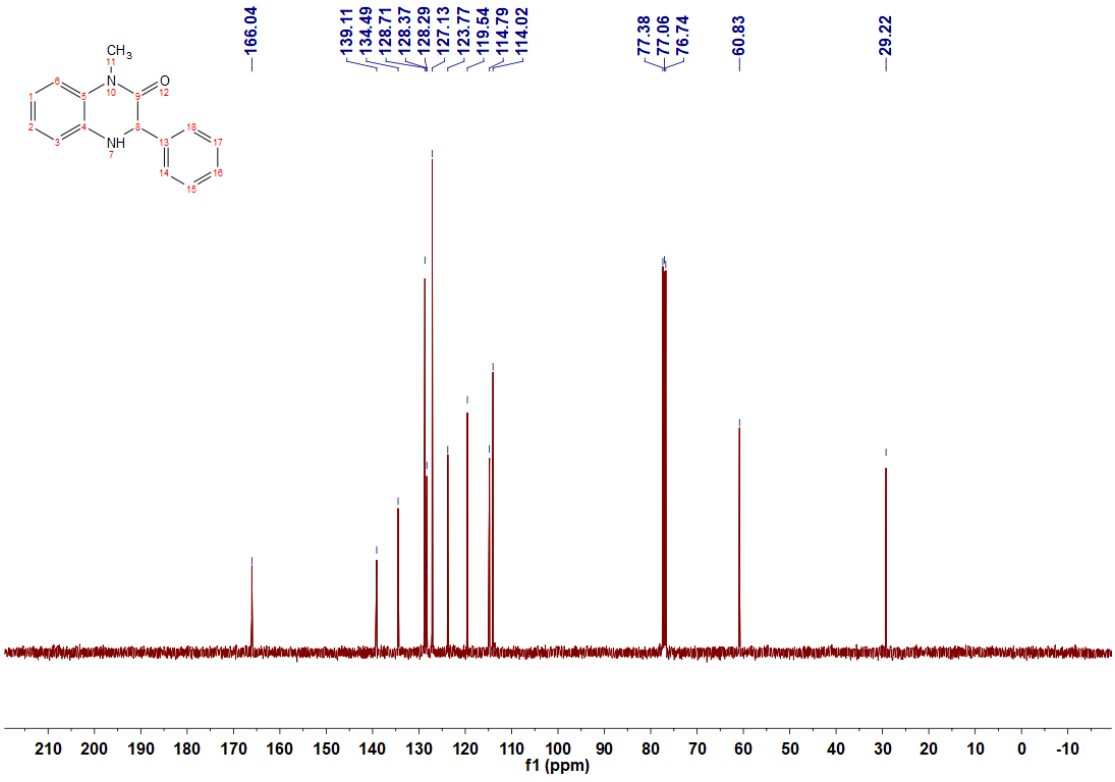
6.96
6.95
6.93
6.89
6.87
6.85
6.76
6.73
5.05
3.38
5.02
2.01
0.99
1.00
1.00
3.09
f1 (ppm)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128.37
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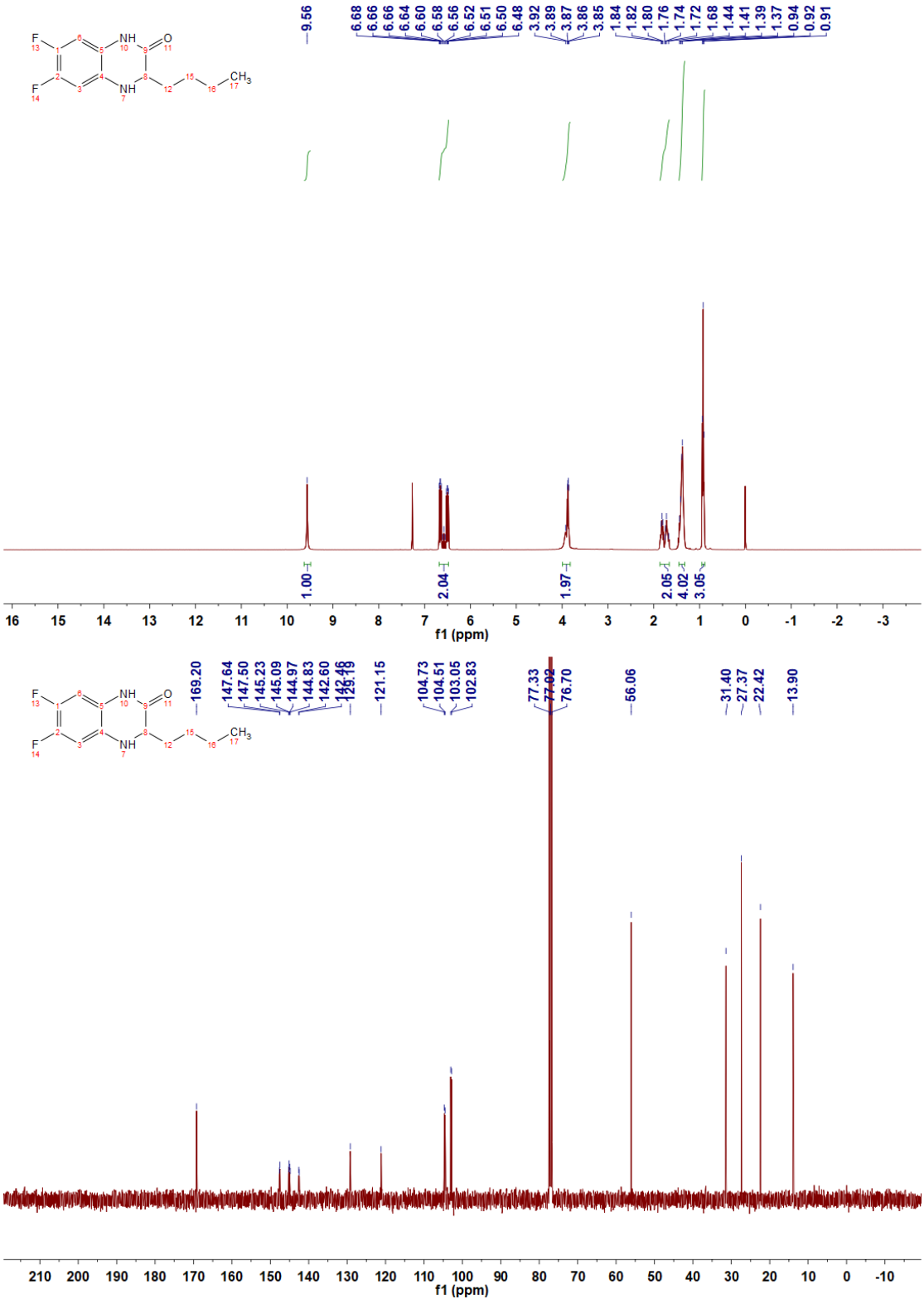
114.79
114.02
77.38
77.06
76.74
60.83
29.22
f1 (ppm)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6.60
6.58
6.56
6.52
6.51
6.50
6.48
3.92
3.89
3.87
3.86
3.85
1.84
1.82
1.80
1.76
1.74
1.72
1.68
1.44
1.41
1.39
1.37
0.94
0.92
0.91
1.00
2.04
1.97
2.05
4.02
3.05
f1 (ppm)
169.20
147.64
147.50
145.23
145.09
144.97
144.83
142.60
121.15
104.73
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103.05
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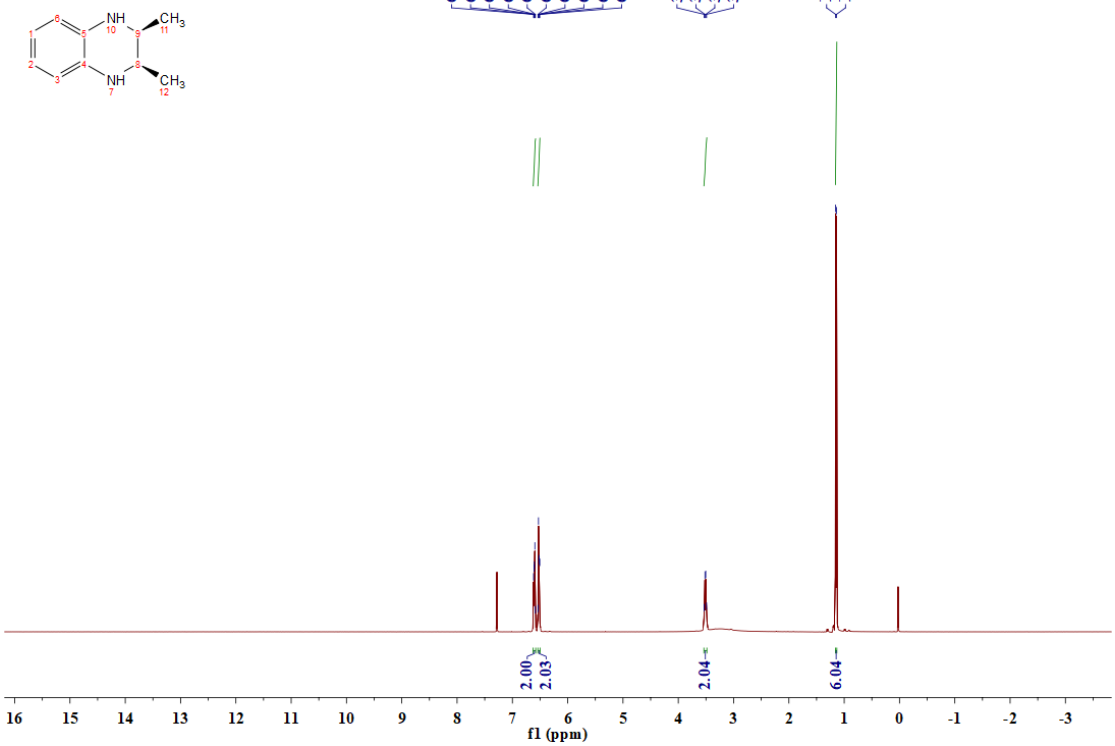
77.33
77.02
76.70
56.06
31.40
27.37
22.42
13.90
f1 (ppm)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6.54
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6.51
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3.53
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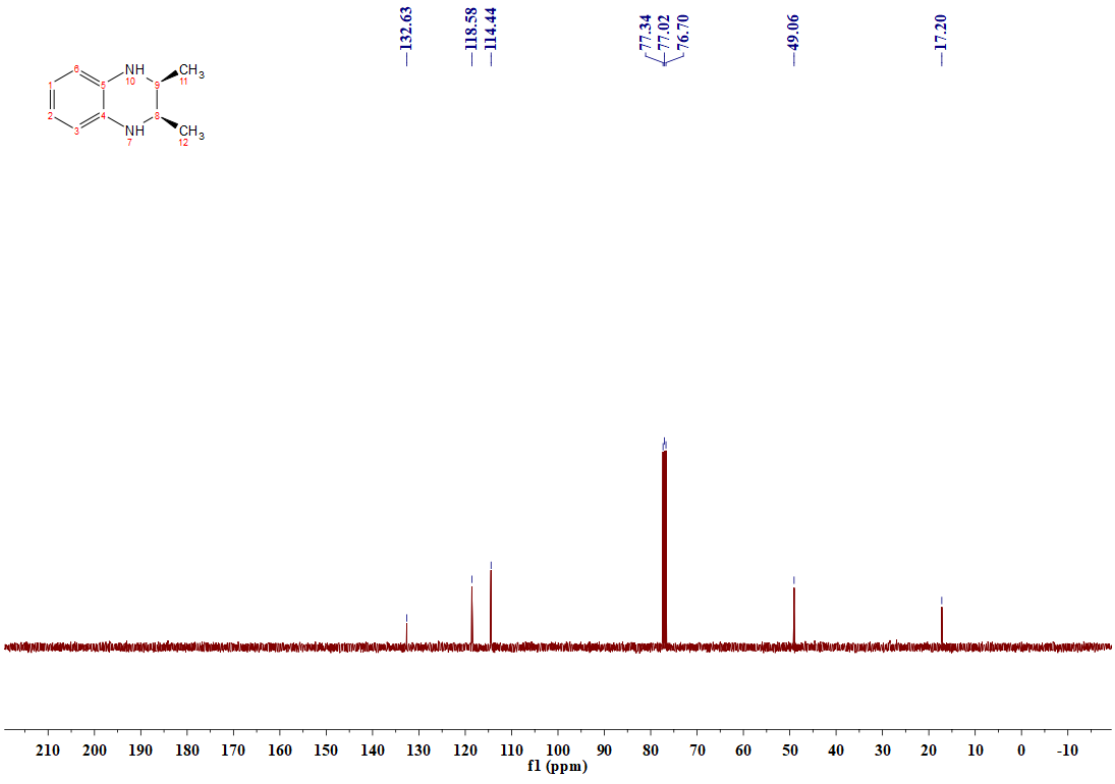
3.50
3.49
1.16
1.14
2.00
2.03
2.04
6.04
f1 (ppm)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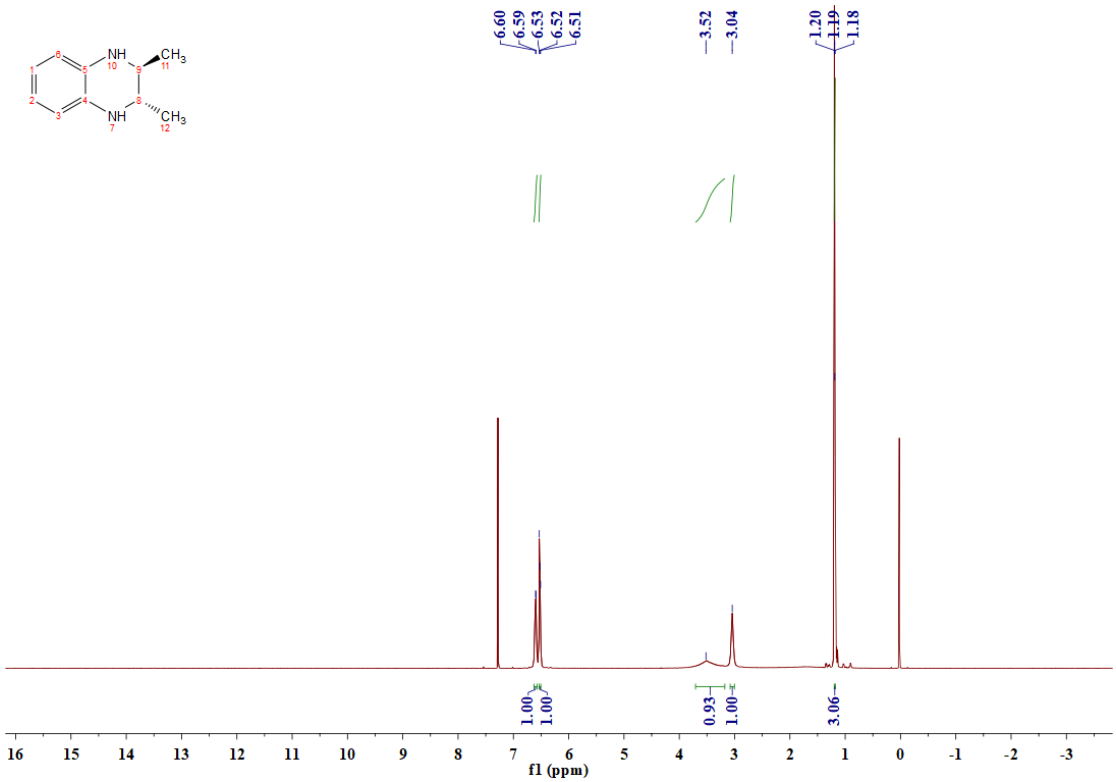
77.02
76.70
49.06
17.20
f1 (ppm)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6.59
6.53
6.52
6.51
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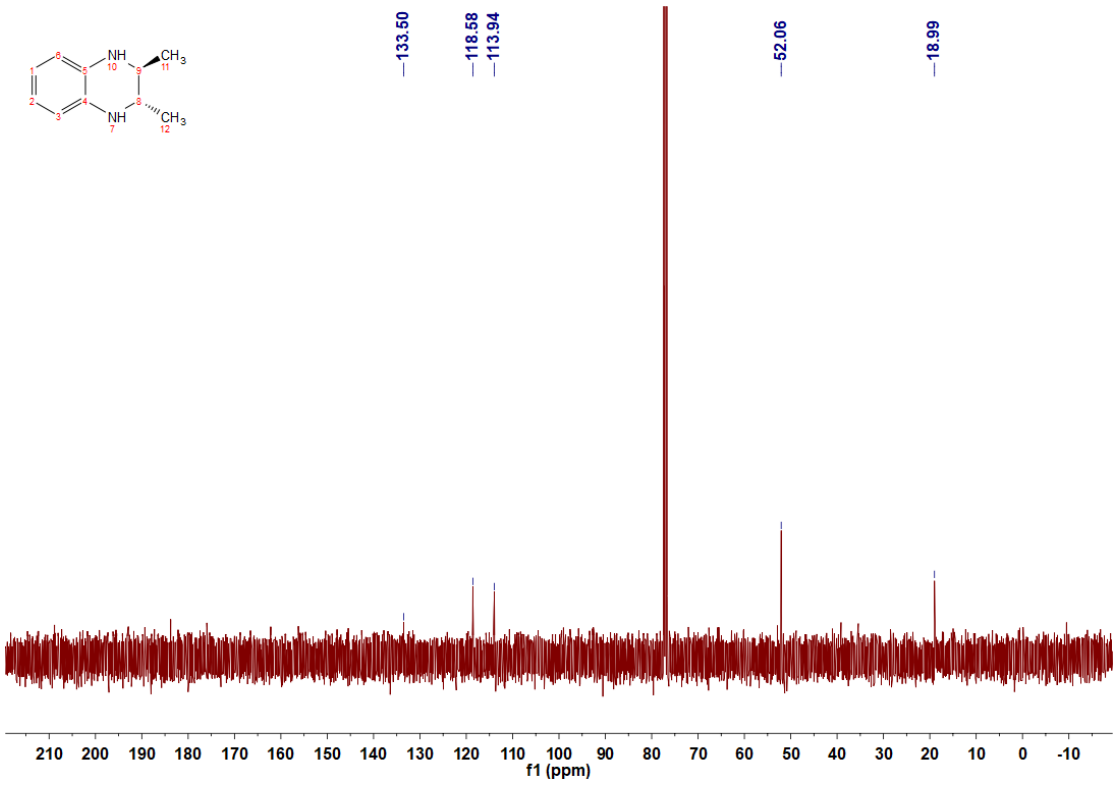
1.20
1.19
1.18
1.00
1.00
0.93
1.00
3.06
f1 (ppm)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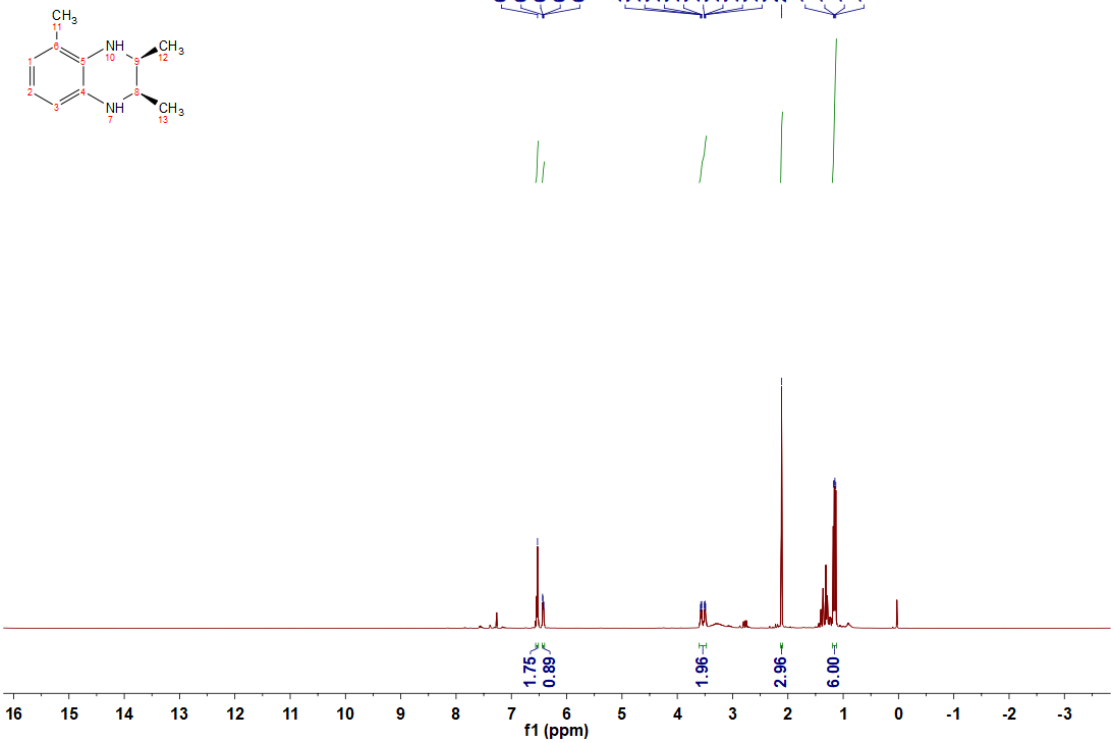
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6.41
3.58
3.57
3.57
3.56
3.51
3.50
3.49
3.49
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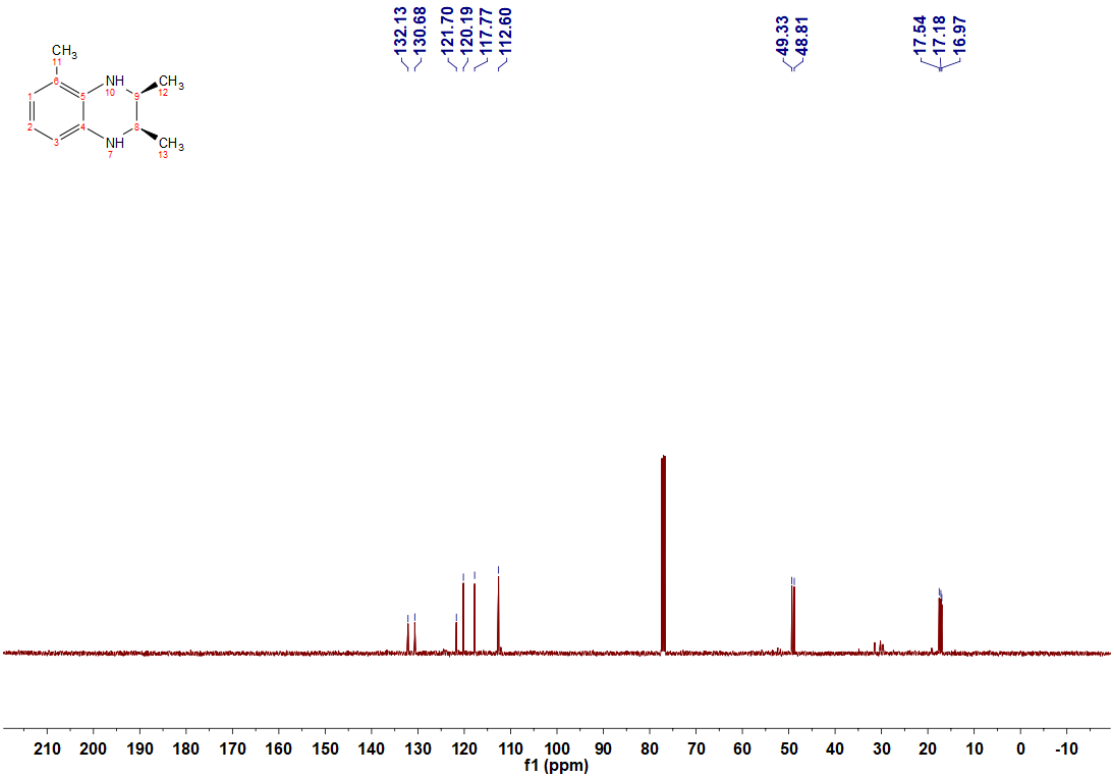
1.16
1.15
1.13
1.75
0.89
1.96
2.96
6.00
f1 (ppm)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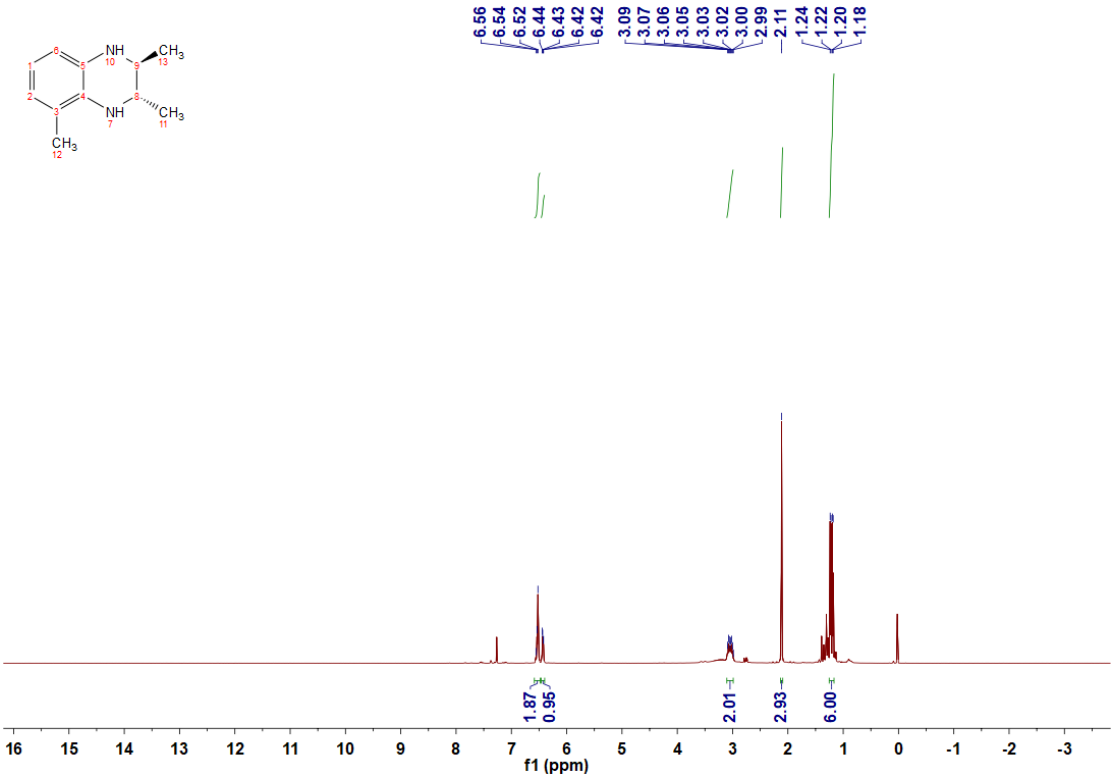
117.77
112.60
49.33
48.81
17.54
17.18
16.97
f1 (ppm)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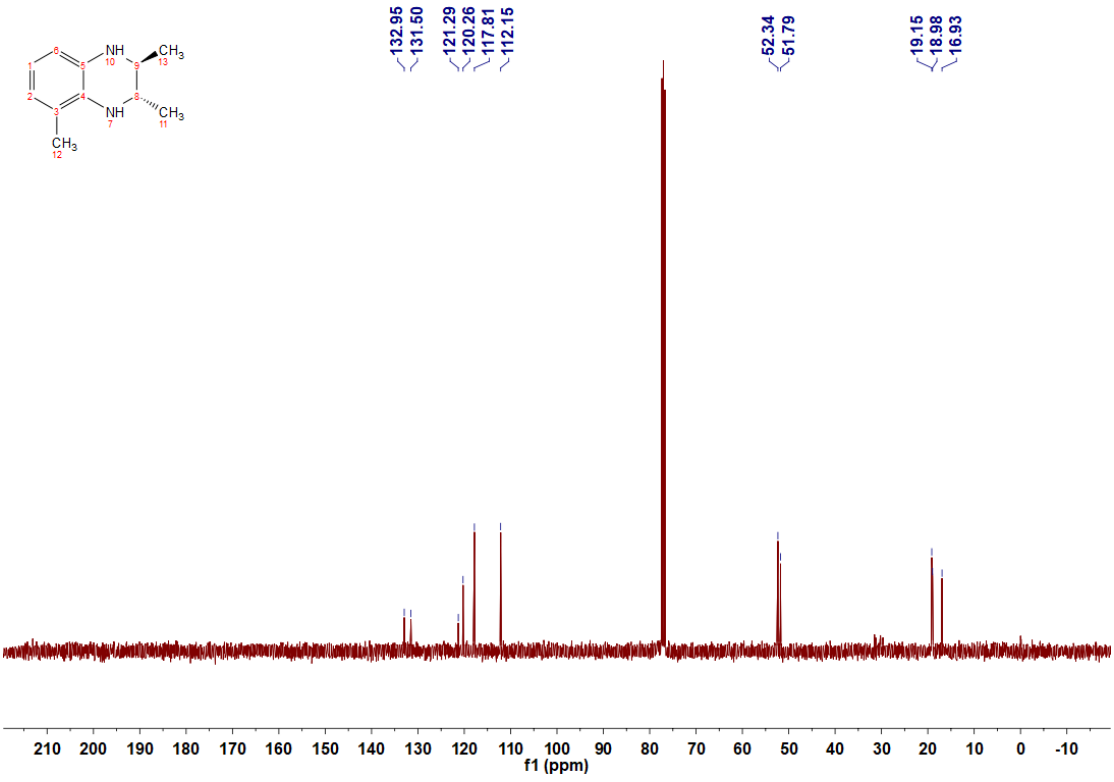
6.42
6.42
3.09
3.07
3.06
3.05
3.03
3.02
3.00
2.99
2.11
1.24
1.22
1.20
1.18
1.87
0.95
2.01
2.93
6.00
f1 (ppm)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51.79
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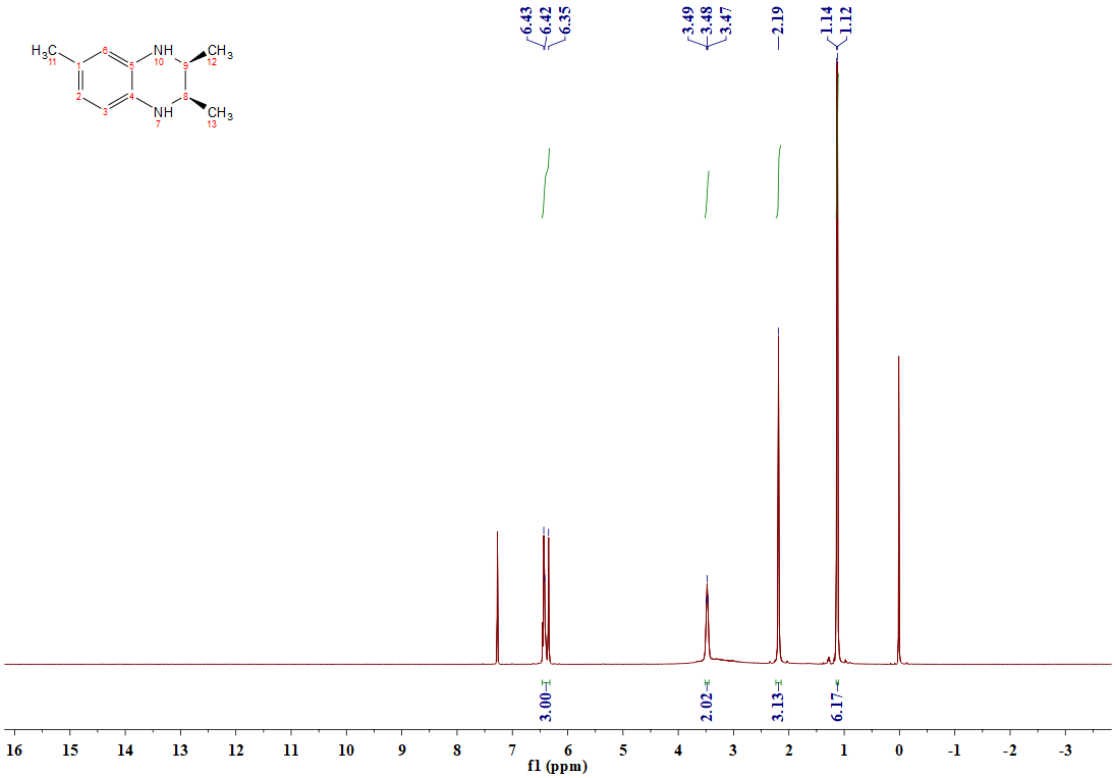
18.98
16.93
f1 (ppm)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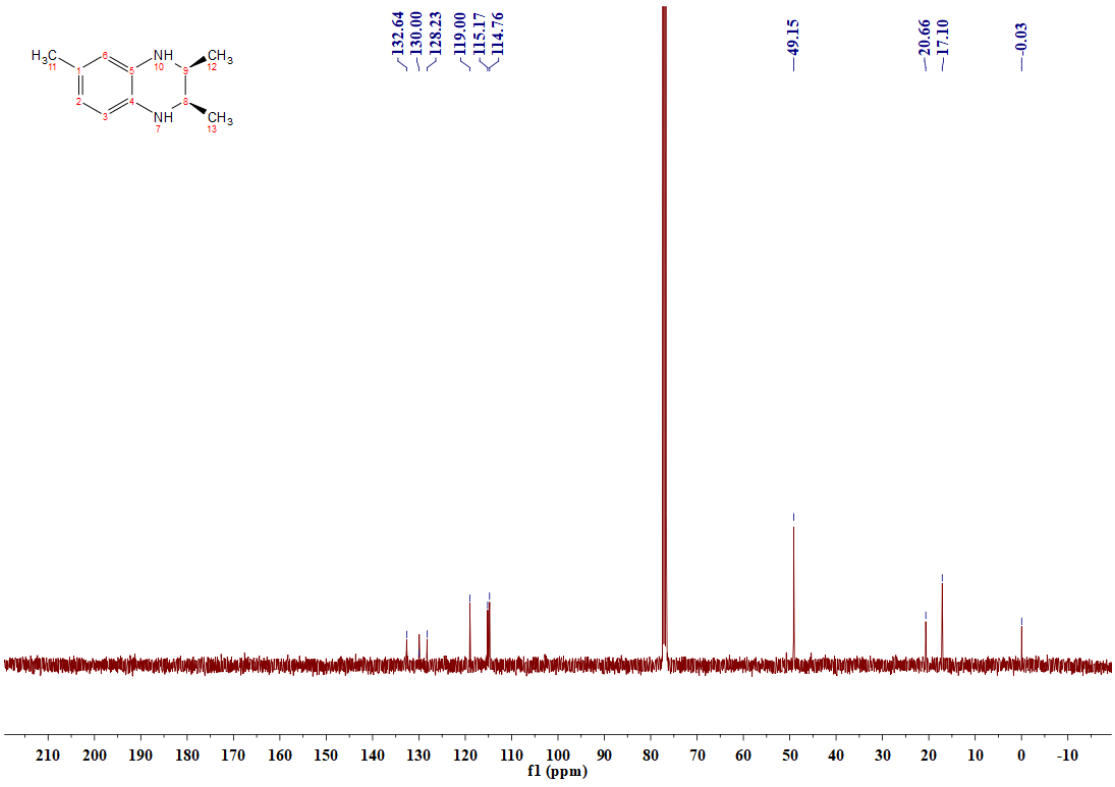
1.14
1.12
3.00
2.02
3.13
6.17
f1 (ppm)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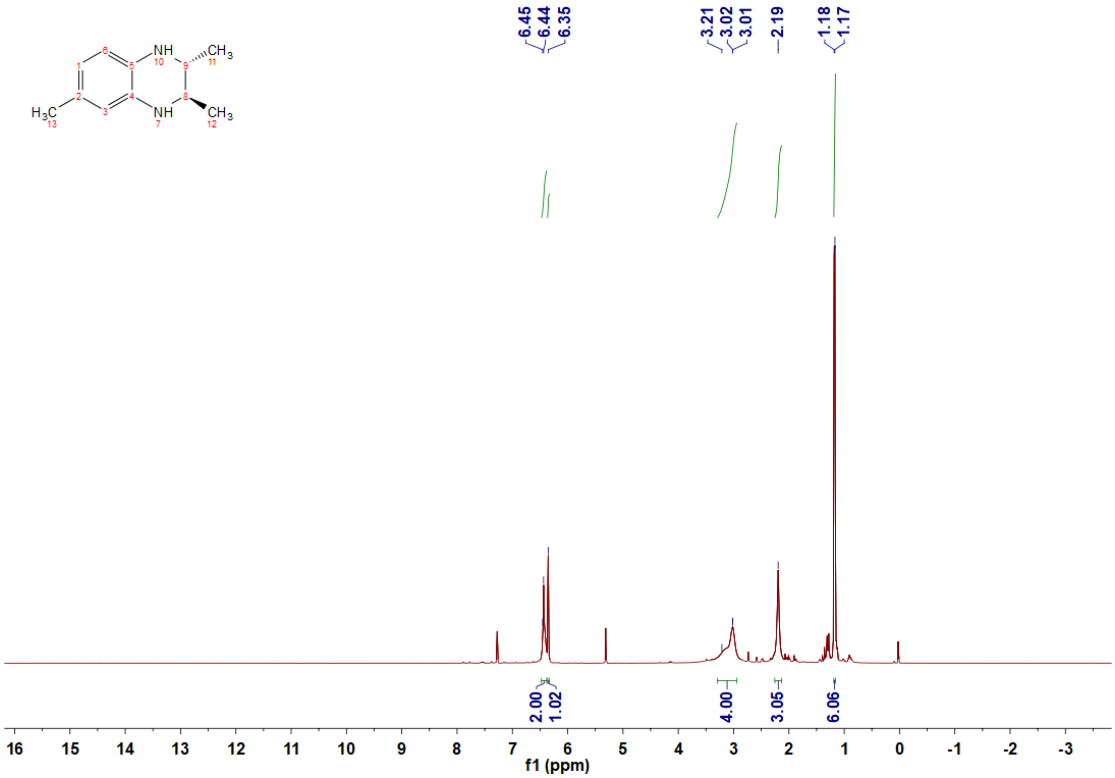
114.76
49.15
20.66
17.10
-0.03
f1 (ppm)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2.19
1.18
1.17
2.00
1.02
4.00
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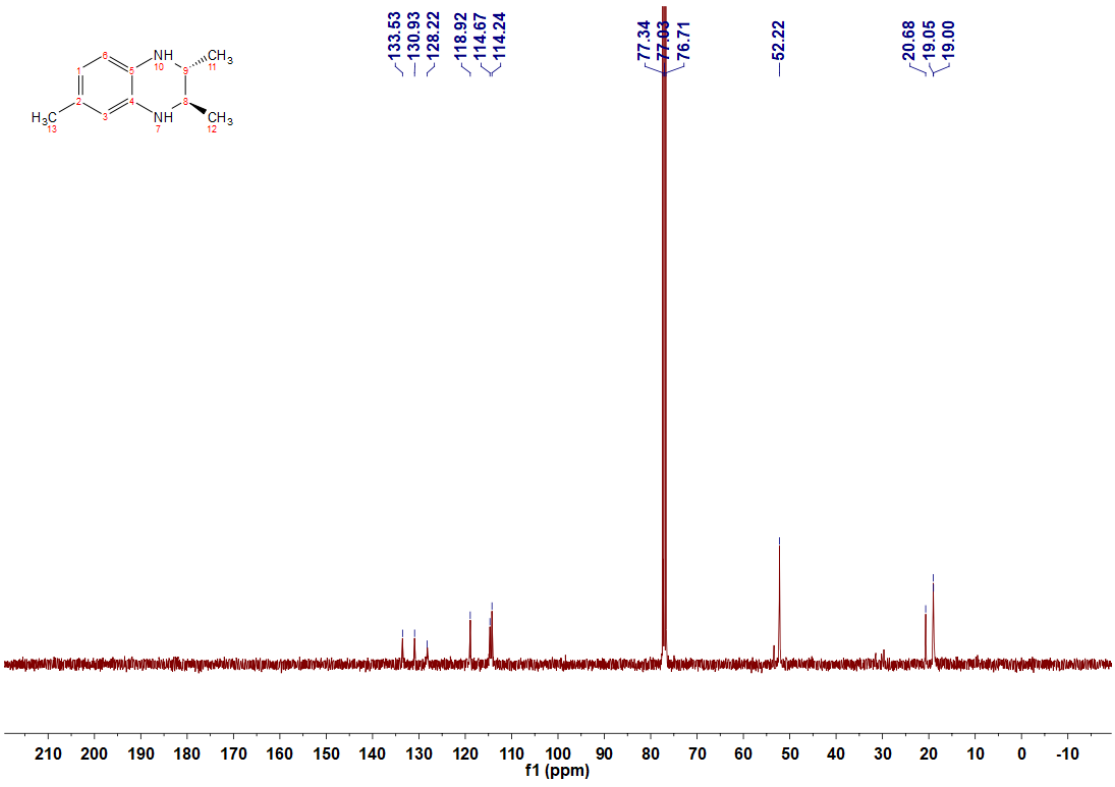
6.06
f1 (ppm)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130.93
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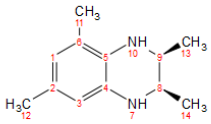
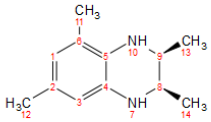
118.92
114.67
114.24
77.34
77.03
76.71
52.22
20.68
19.05
19.00
f1 (ppm)



6.37
6.27
3.56
3.54
3.51
3.49
2.21
2.11
1.19
1.17
1.16
1.14
0.93
0.93
1.99
2.96
2.95
6.00
f1 (ppm)



132.28
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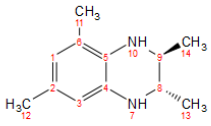
120.83
113.24
49.42
48.96
20.62
17.50
17.16
16.94
f1 (ppm)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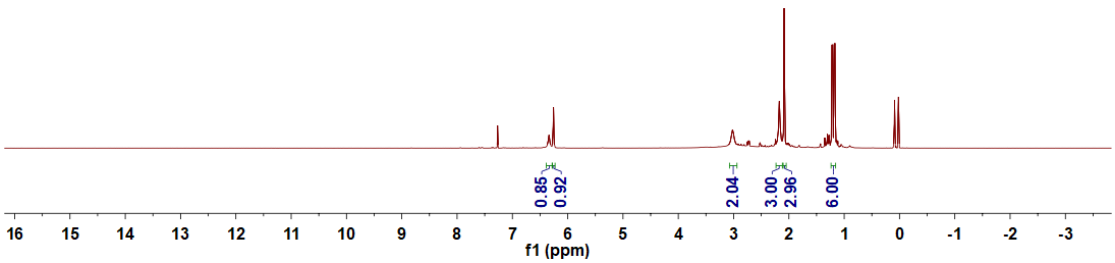
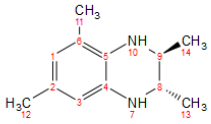
NH
10
CH3
14
H3C
12
NH
7
CH3
13


0.85
0.92
2.04
3.00
2.96
6.00
f1 (ppm)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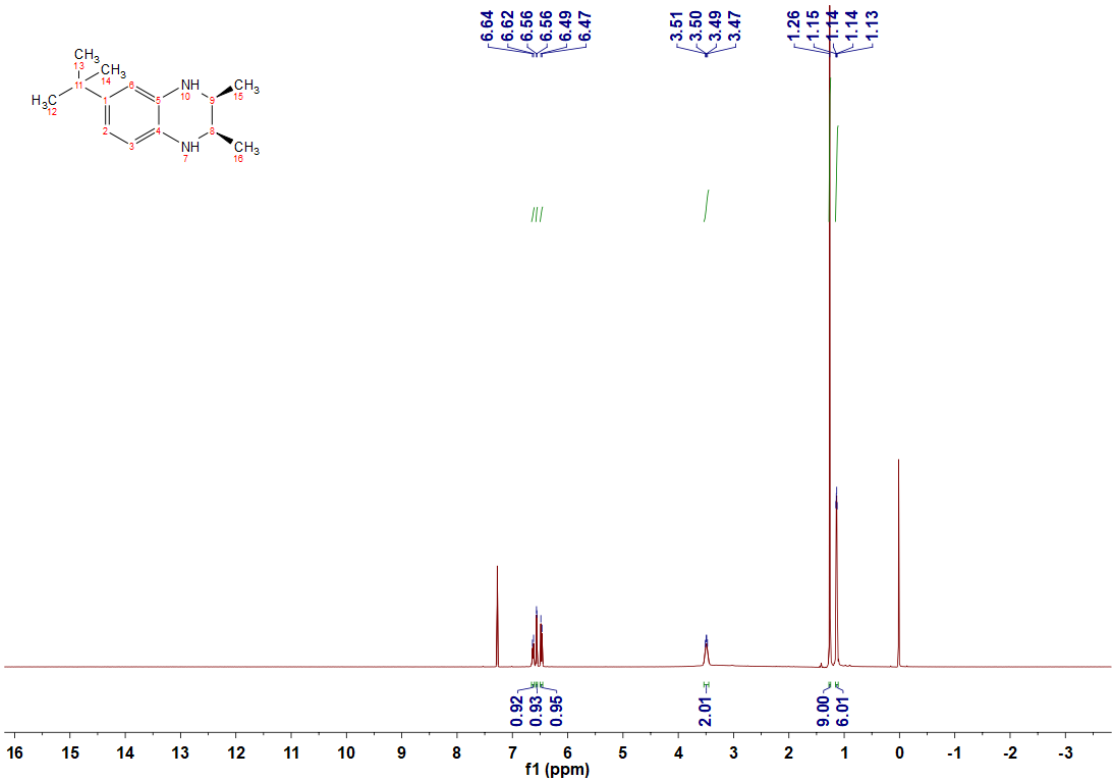
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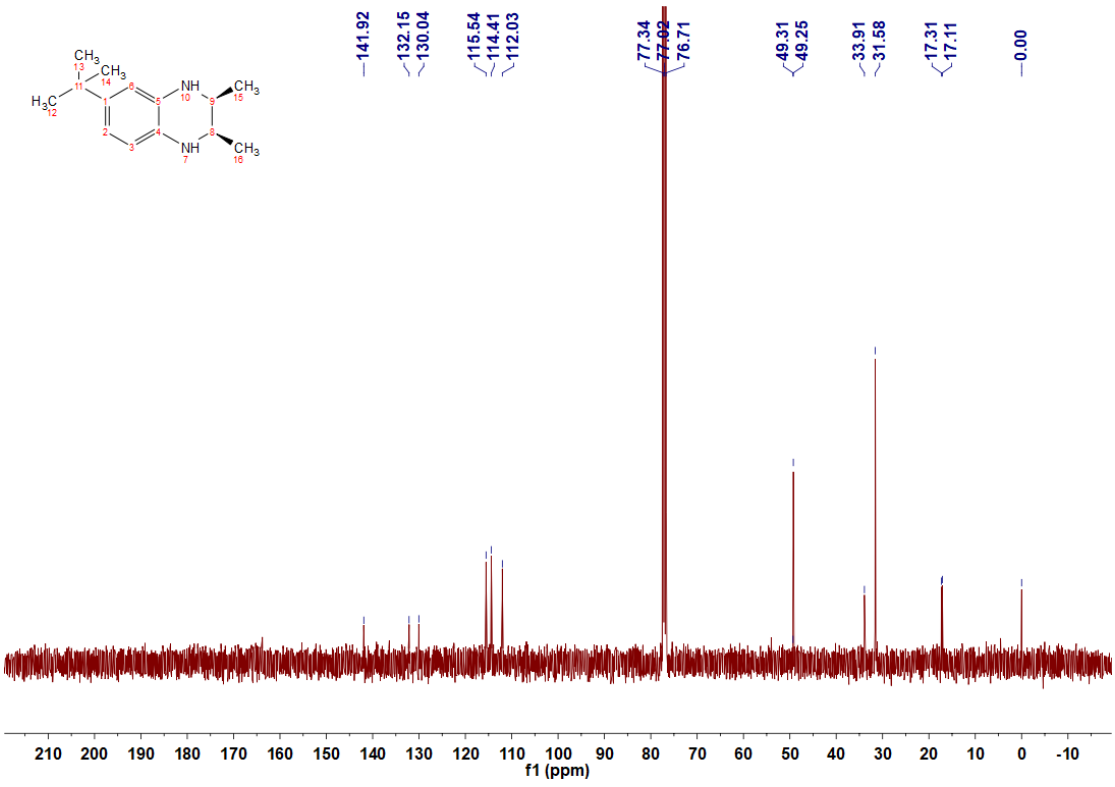
f1 (ppm)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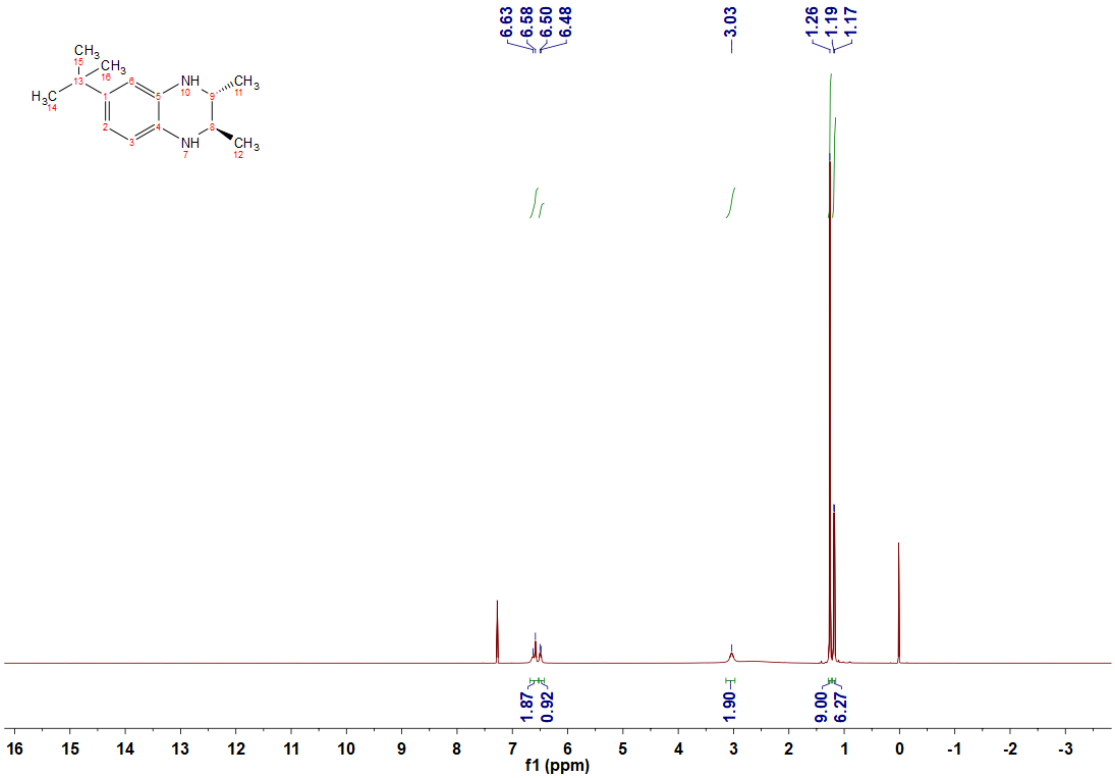
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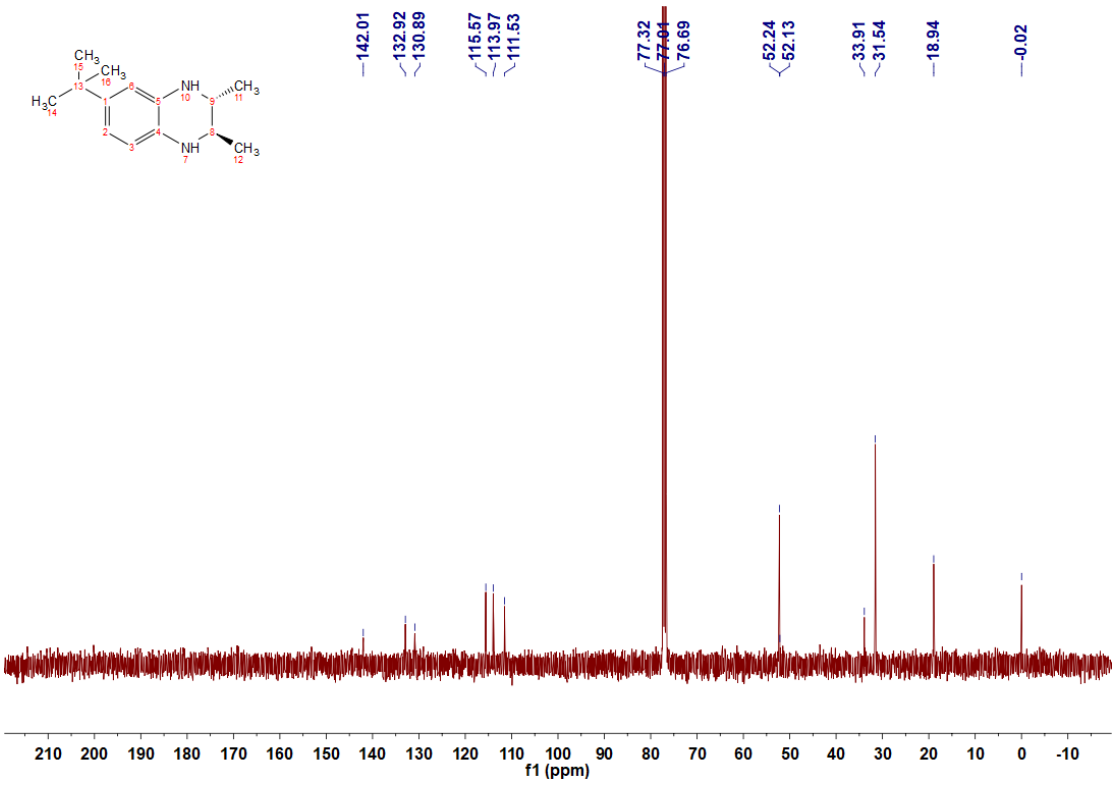
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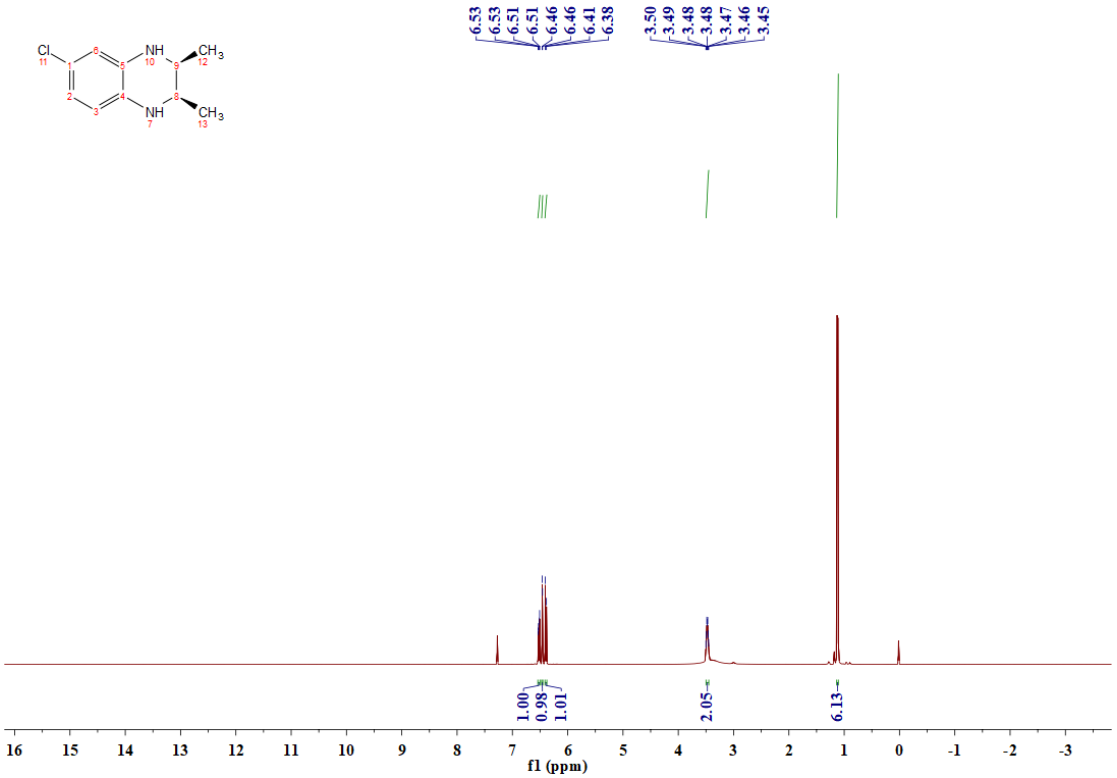
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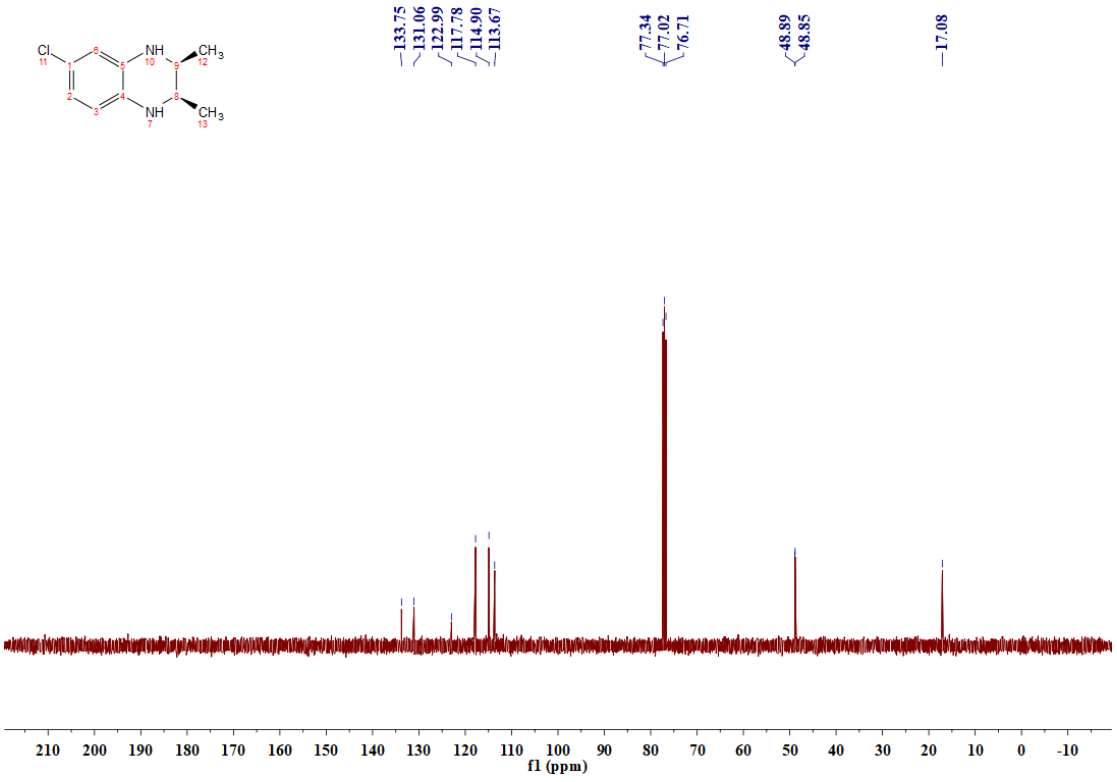
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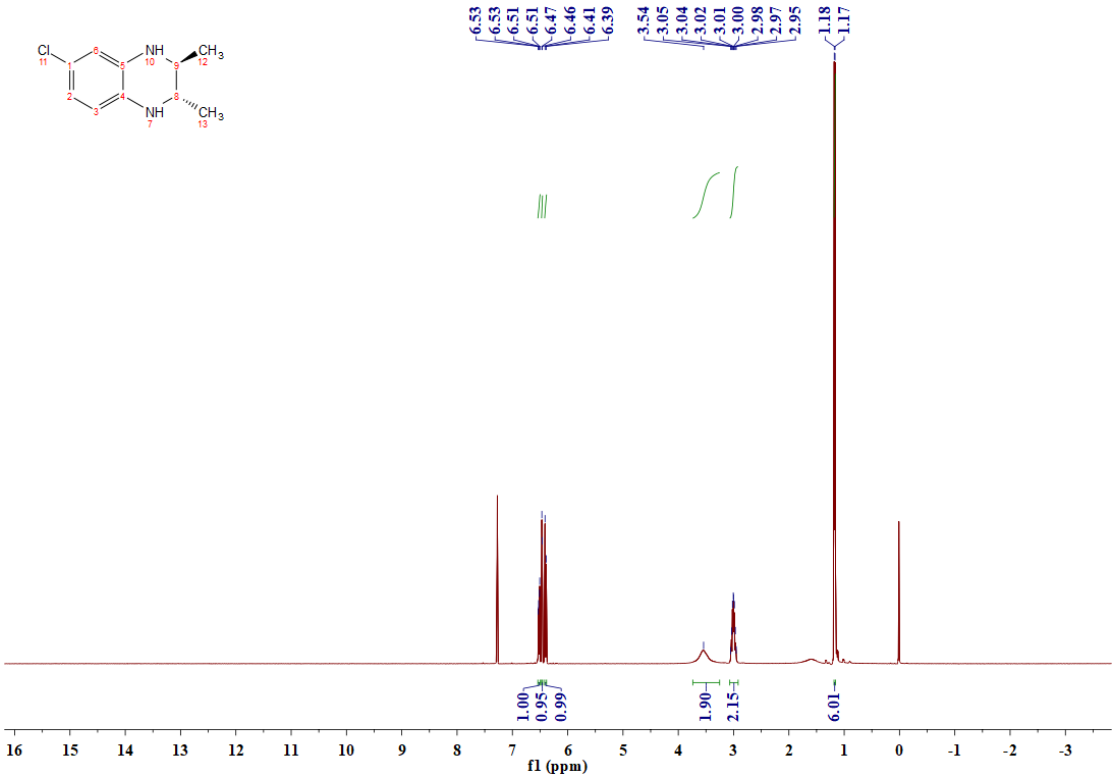
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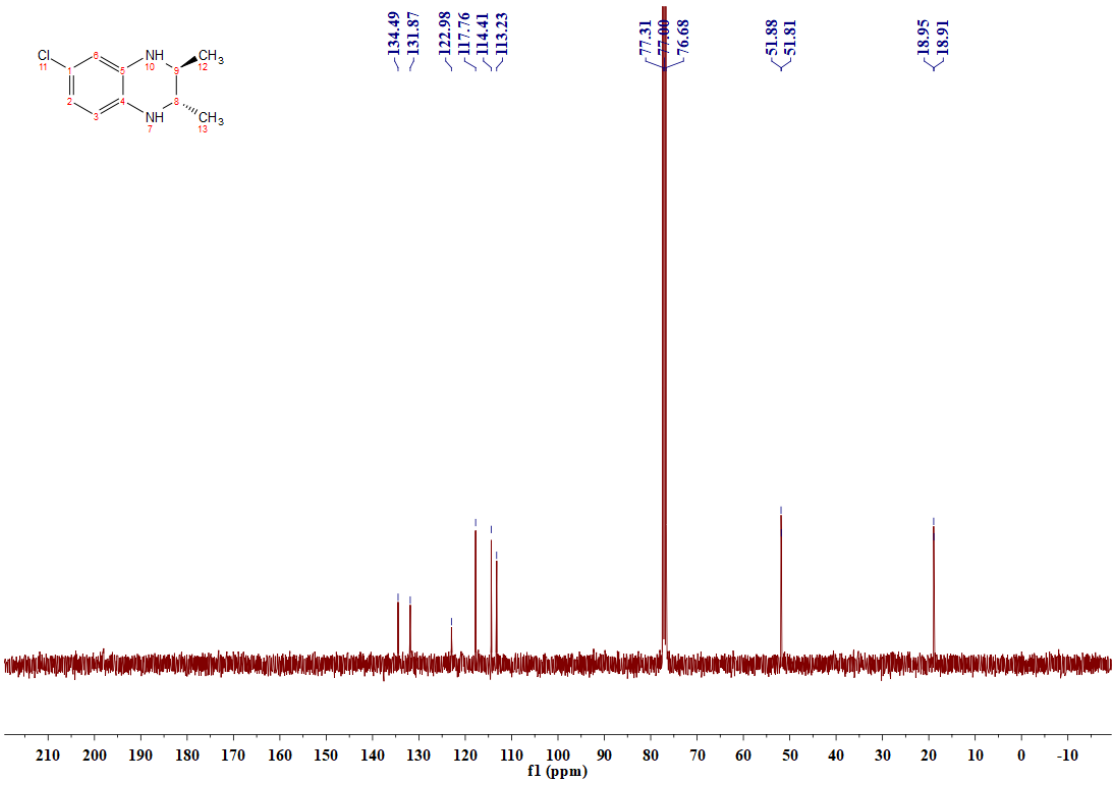
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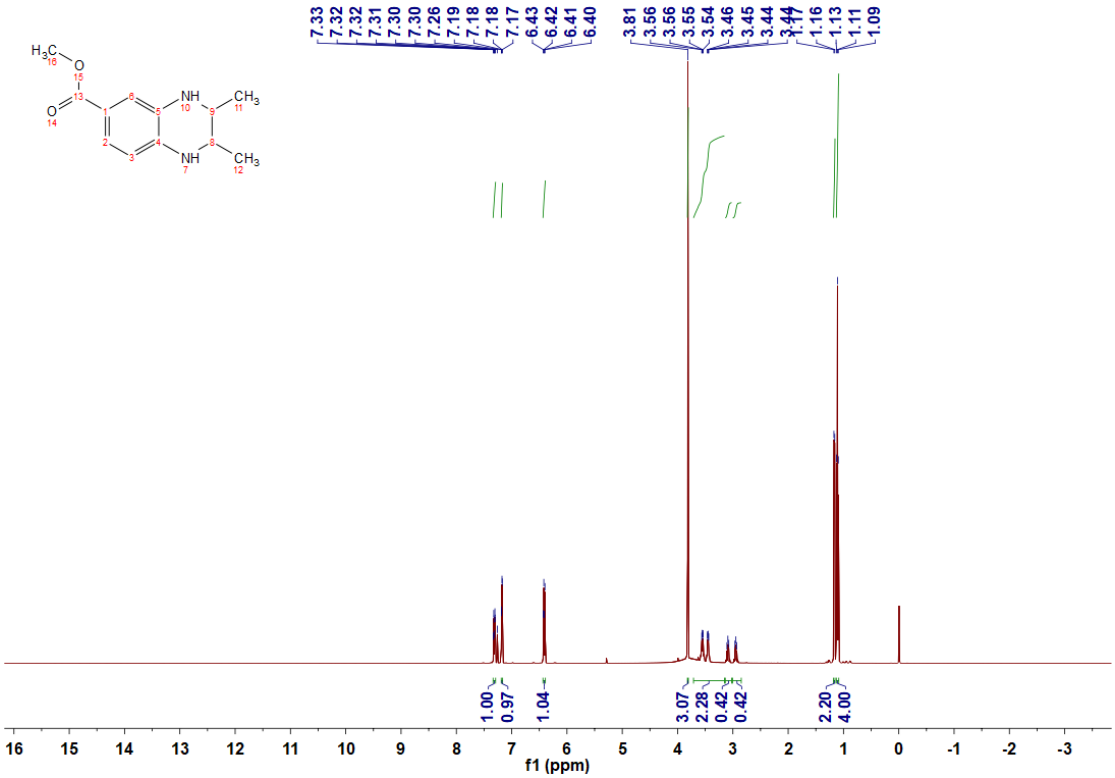
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3.44
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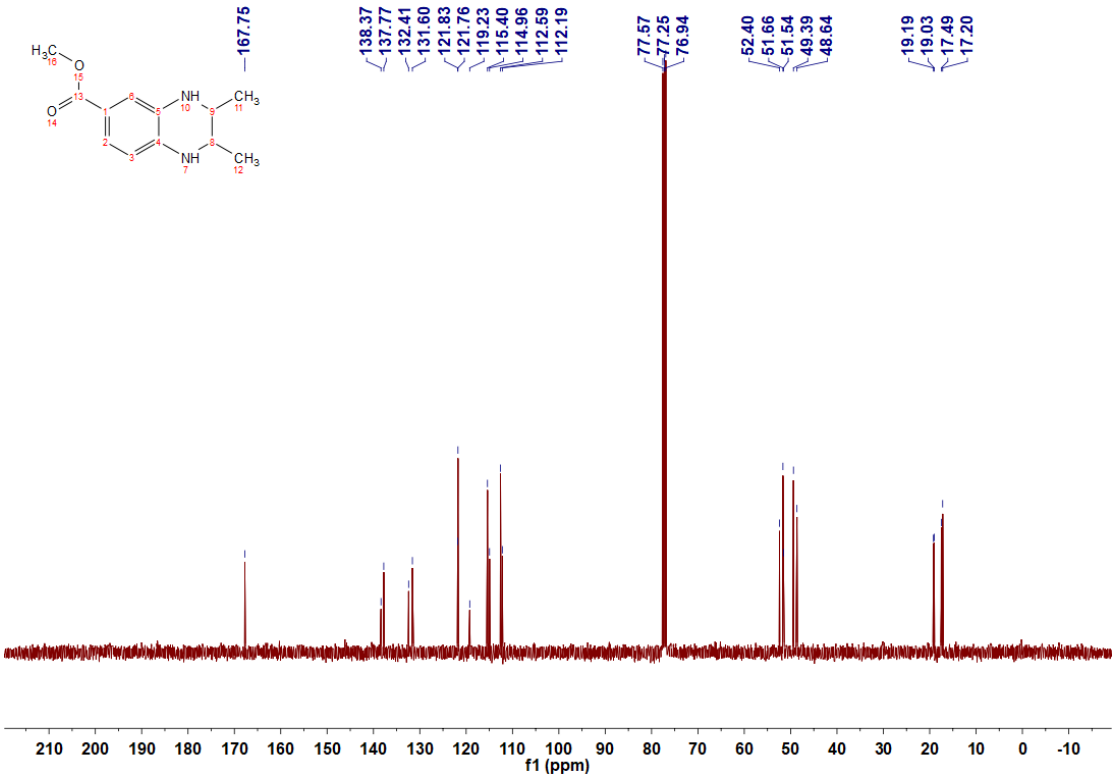
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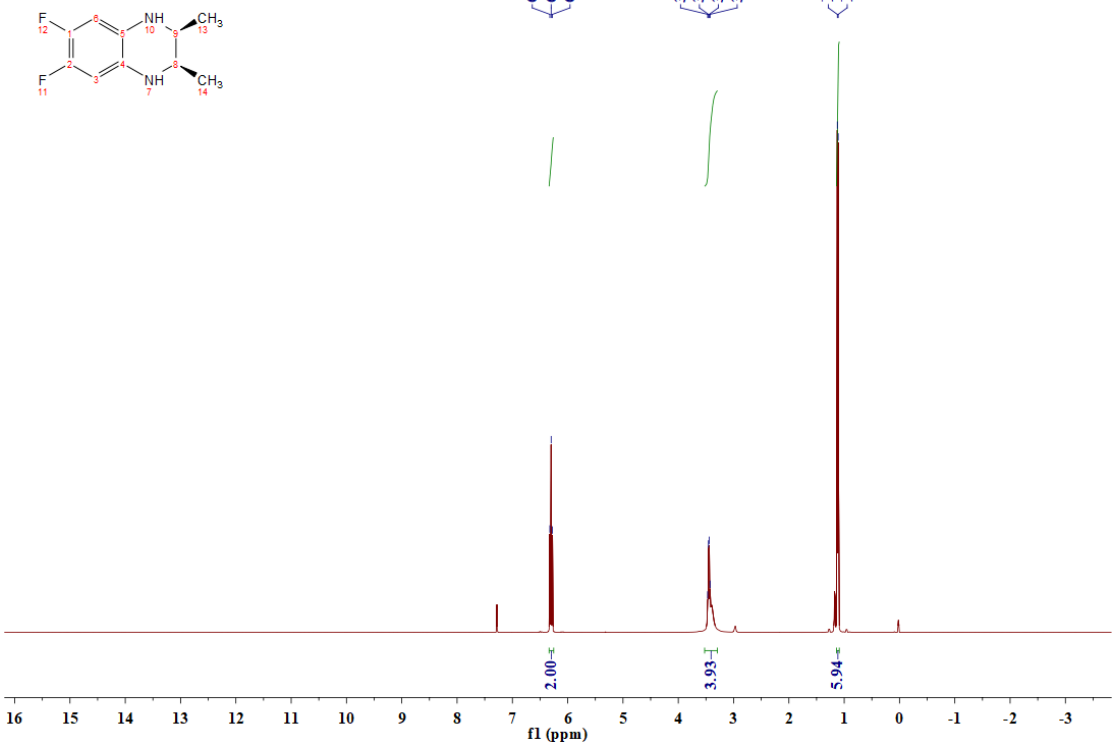
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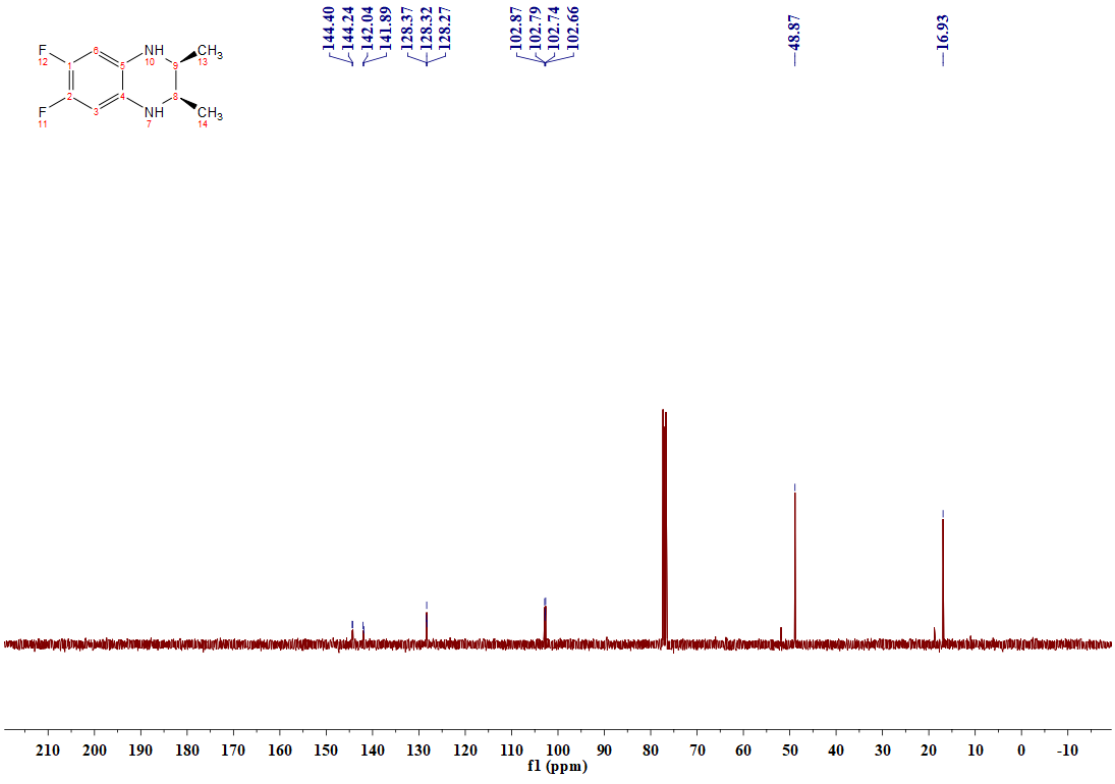
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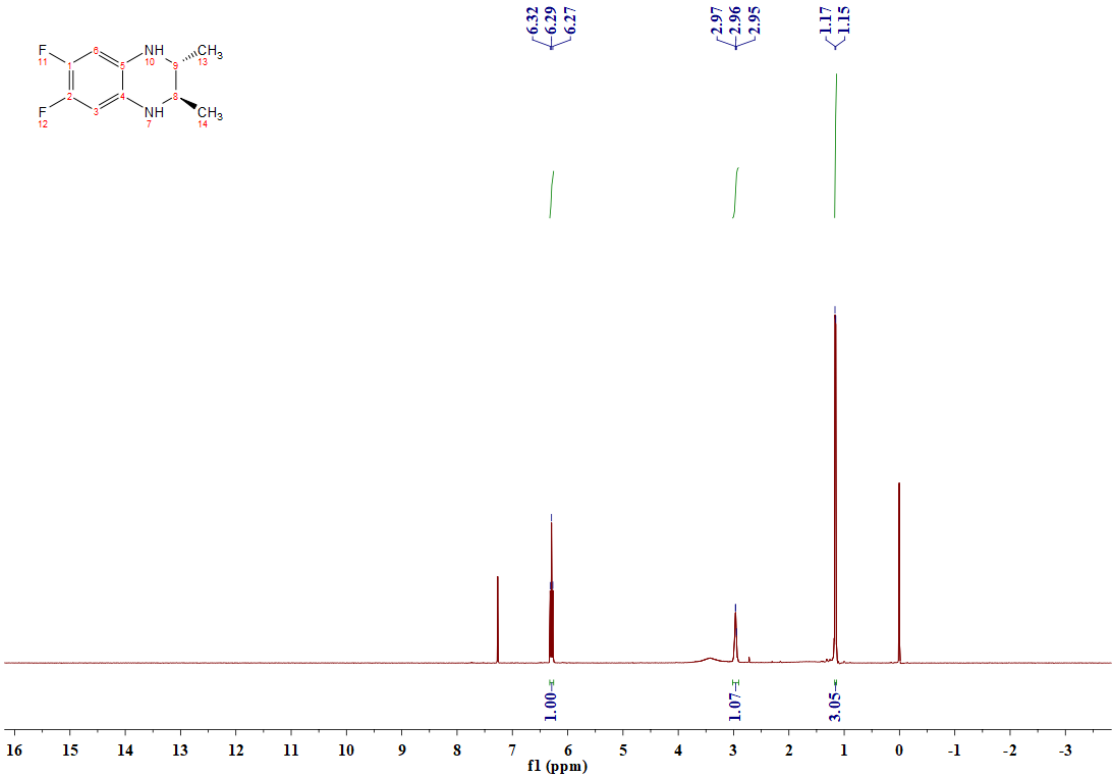
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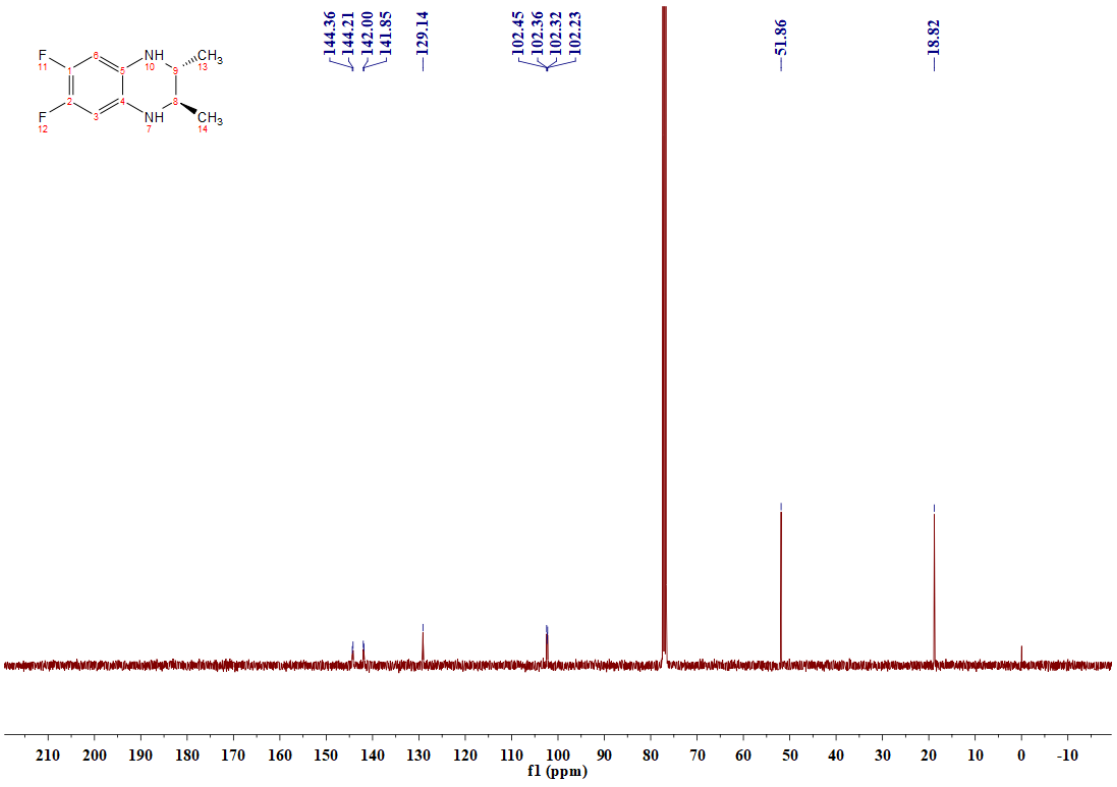
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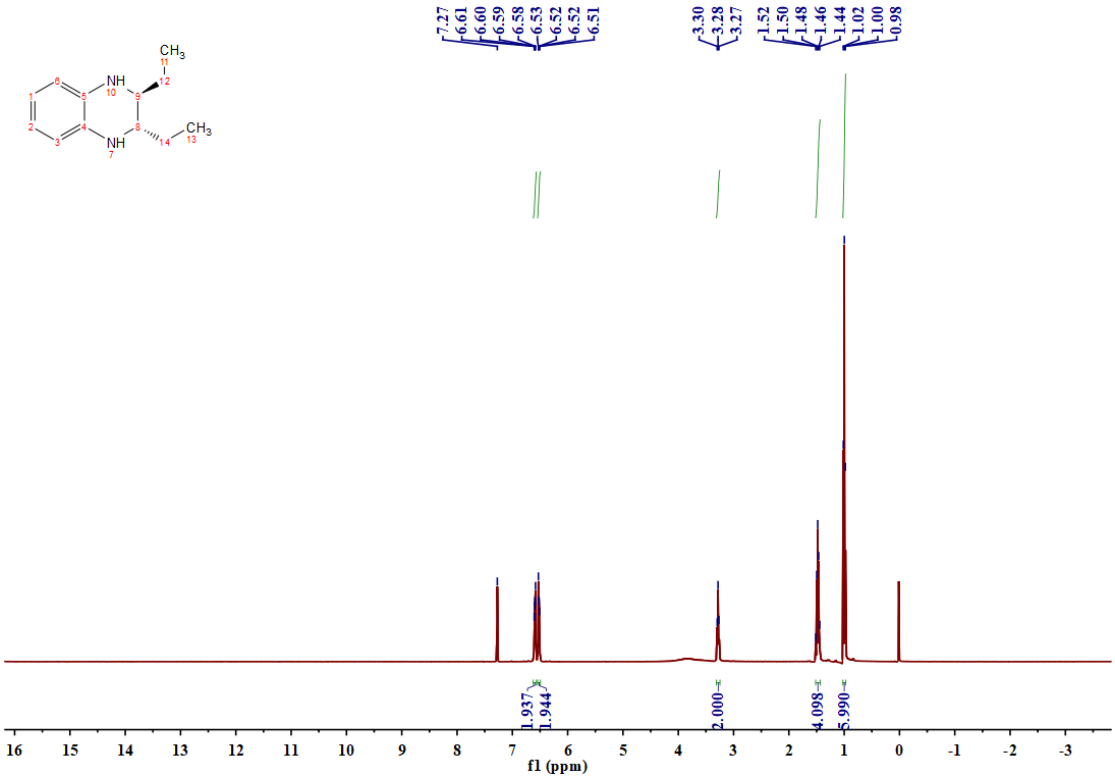
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1.50
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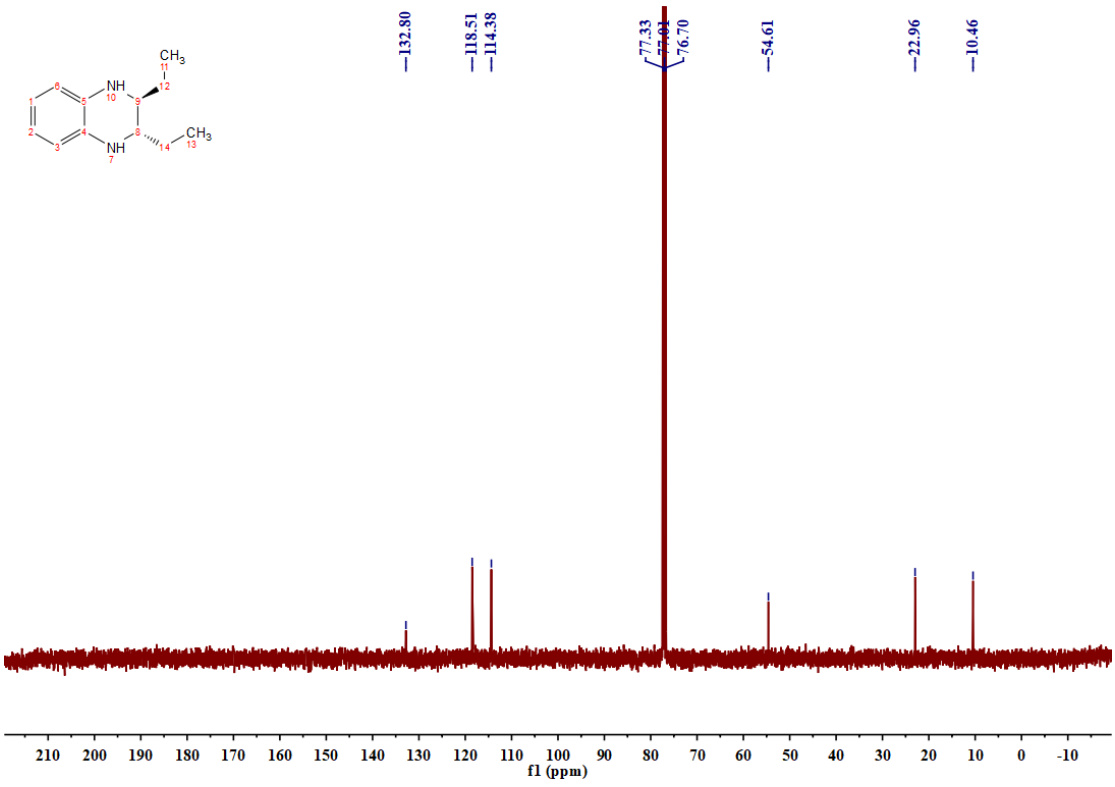
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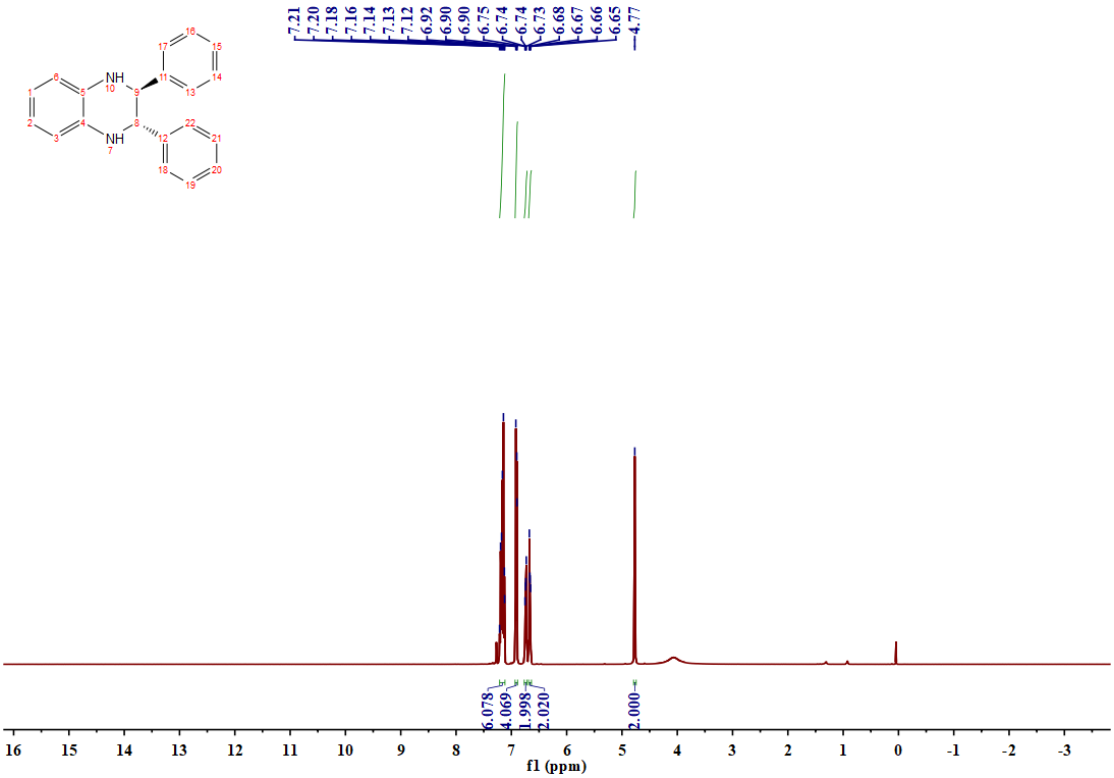
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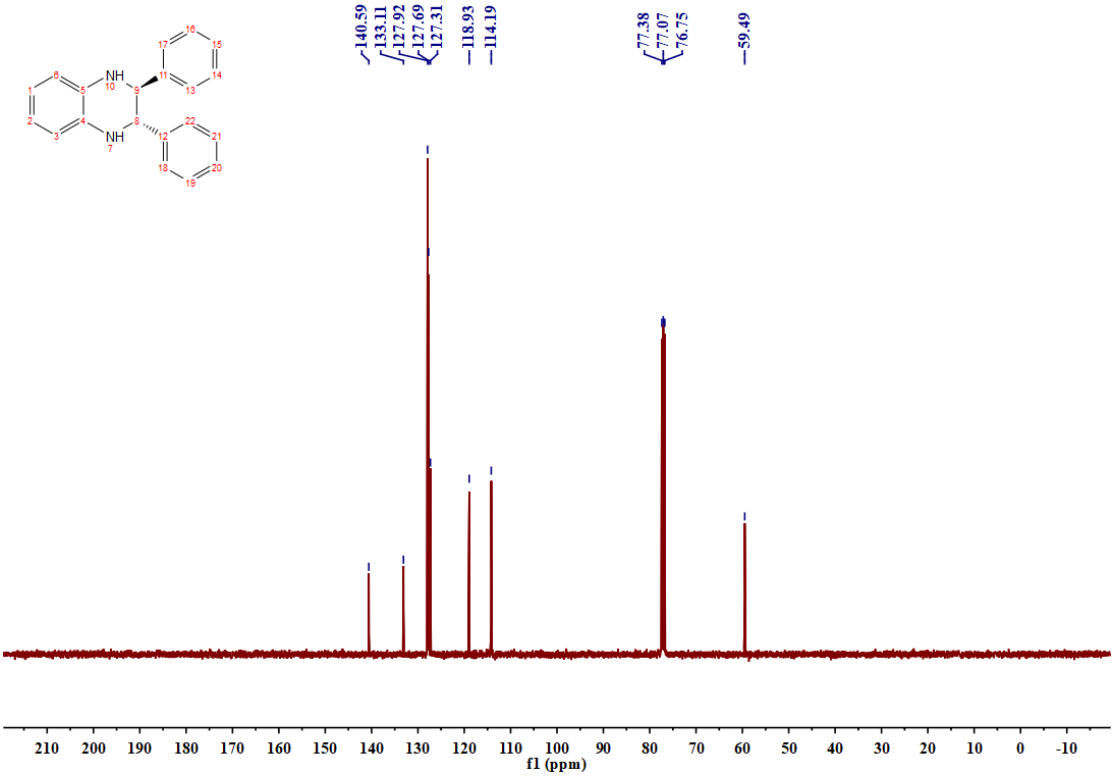
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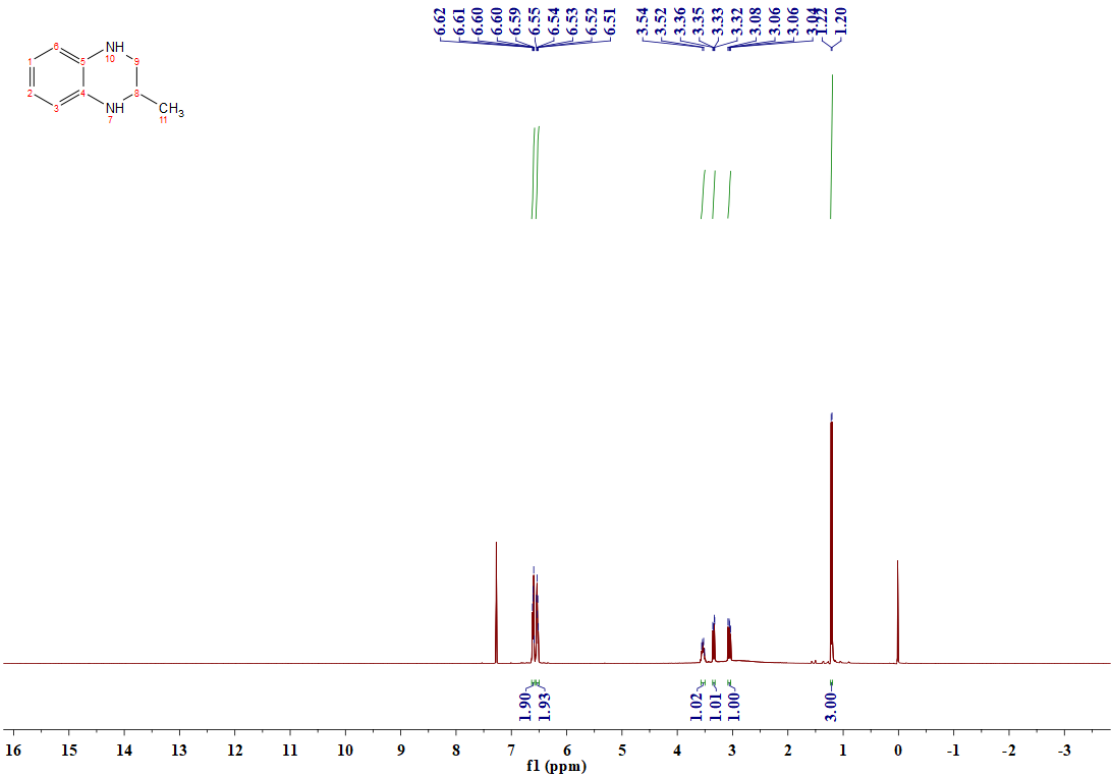
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3.36
3.35
3.33
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1.90
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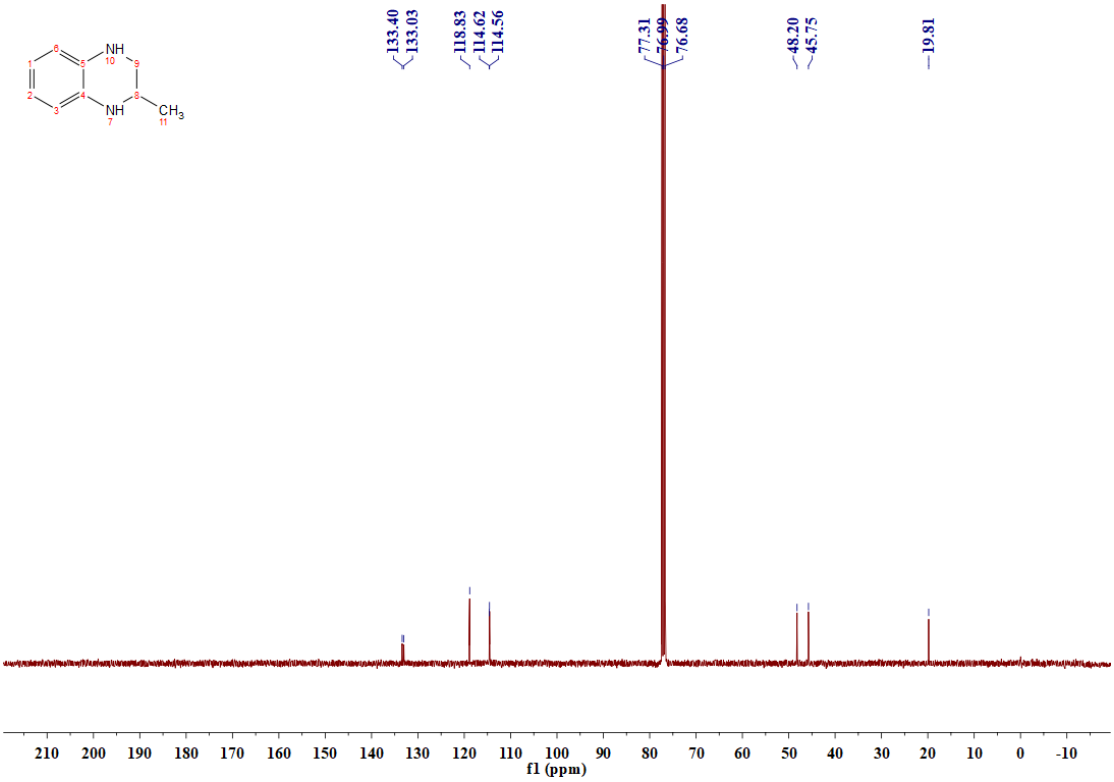
1.01
1.00
3.00
f1 (ppm)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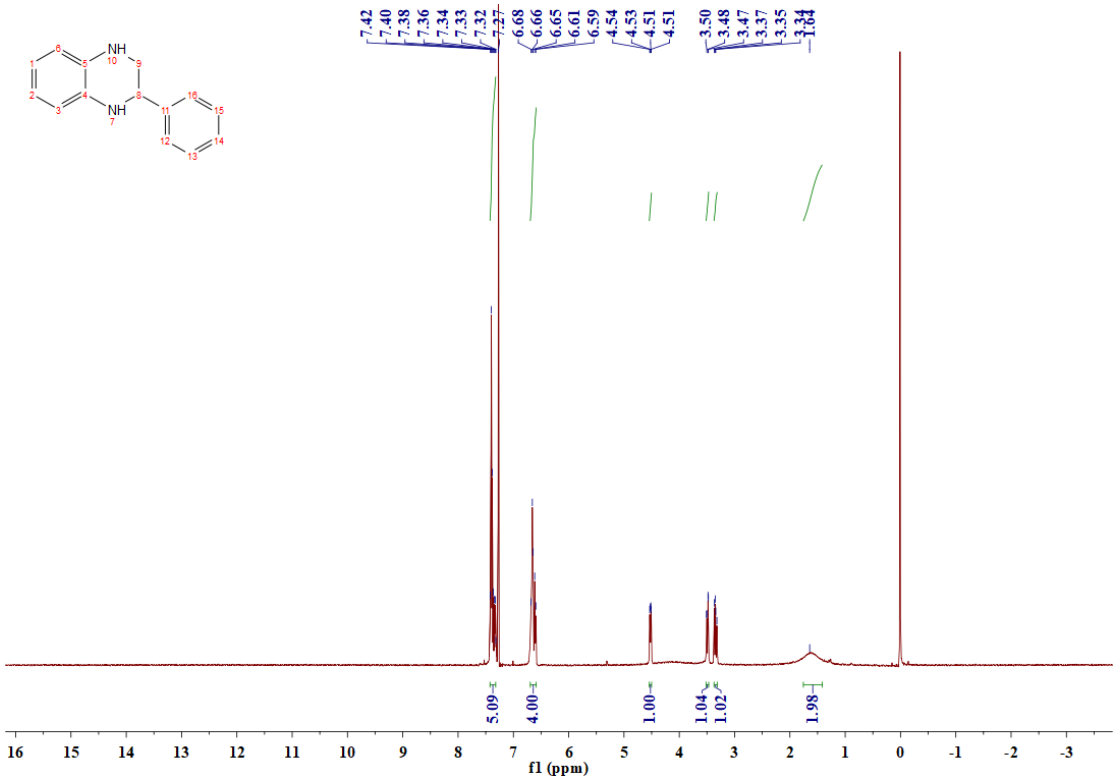
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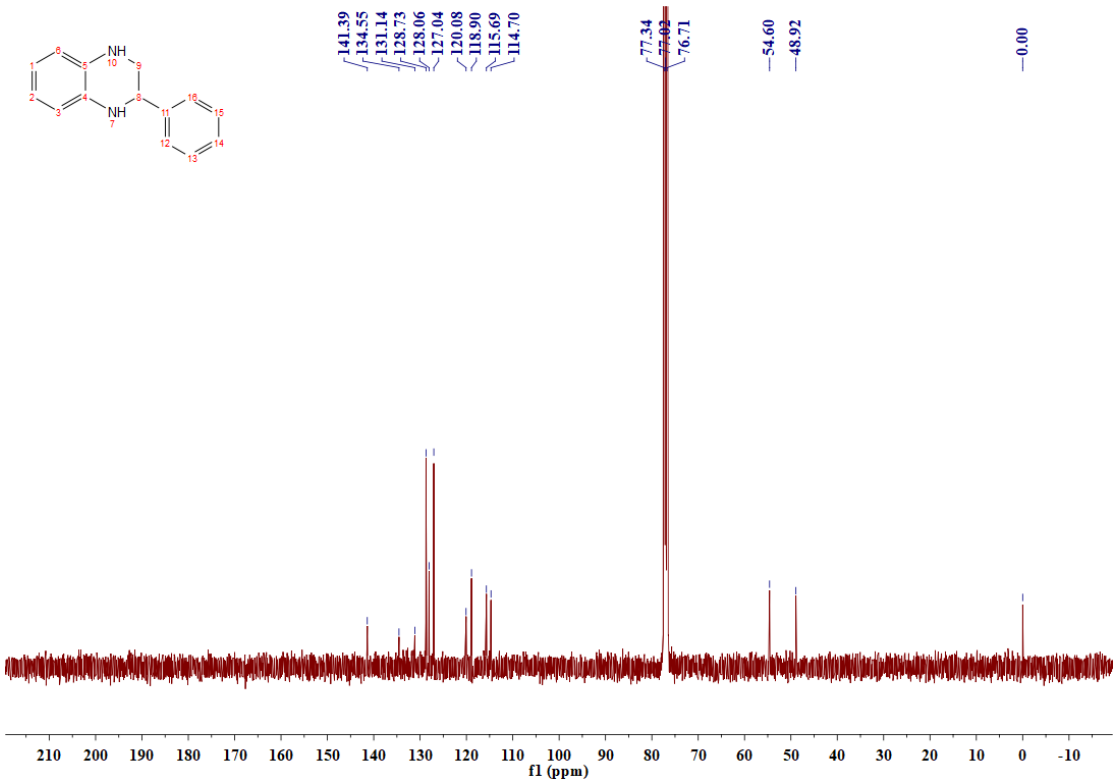
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76.71
54.60
48.92
0.00
f1 (ppm)


9.41
9.39
8.56
8.54
8.34
8.33
8.32
7.87
7.86
7.85
7.81
7.80
7.78
7.76
7.74
7.73
7.27
2.00
2.04
2.05
6.08
f1 (ppm)
142.42
142.17
132.05
130.28
129.71
129.44
127.90
126.27
122.89
f1 (ppm)

11. References

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