Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Cobalt-catalyzed alkylation of methyl-substituted N-heteroarenes with primary Alcohols: direct access to functionalized N-heteroaromatics

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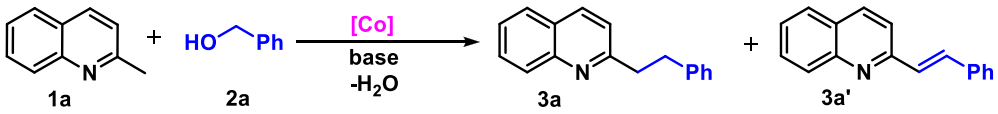
Content

1. General Consideration

Reagent information. All the catalytic reaction were carried out under argon atmosphere. Glass apparatus were oven dried prior to use. Solvents were dried according to literature procedures. All the commercial reagents and metal precursors were purchased from Sigma-Aldrich, Alfa-Aesar, Spectrochem, Avra, SD-fine chemical and Arora Matthey, India. 1-Benzyl-2-phenyl-1H-benzimidazole and complex **A** were synthesized by following the literature report.[1] For column chromatography, 100-200 mesh silica gel (from SDFCL) was used. Column chromatography was performed by using a gradient of hexane/ethyl acetate as mobile phase, based on Merck aluminium TLC plate (silica gel 60 F254).

Analytical information. All the ^{1}H (400 and 500 MHz) and ^{13}C (100 MHz) spectra were recorded at 298 K by using $CDCl_3$, and DMSO-D_6 in JEOL Spectrometer. NMR experiments were reported in parts per million (ppm) and coupling constant (*J*) was reported in hertz (Hz) units. All ^{1}H and ^{13}C spectra were measured relative to the signals for residual deuterated chloroform solvent (7.25 ppm for ^{1}H NMR and 77.10 ppm ^{13}C NMR spectra) unless otherwise stated. ESI-MS were recorded on a Waters Micromass Quattro Micro triple-quadrupole mass spectrometer. All the GC analysis were performed using Perkein Elmer Clarus 600 and Agilent 7890 B Gas Chromatograph, whereas GC-MS were measured using Agilent 7890 A Gas Chromatograph equipped with Agilent 5890 triple-quadrupole mass system.

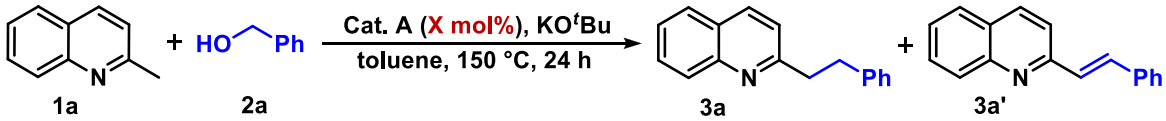
2. Optimization Details



An oven dried 9 mL pressure tube was taken inside the argon filled glove box and charged with a magnetic stir bar, base, catalyst, 2-methylquinoline **1a**, benzyl alcohol **2a** and solvent. Then pressure tube was closed tightly, removed from the glove box and placed in a preheated oil bath with specified temperature. After the reaction it was allowed to cool at room temperature and the solution was quenched with brine and was extracted with ethyl acetate (4×10mL). 20 µL reaction mixture was syringed out and directly subjected to GC analysis to determine conversion as well as selectivity. The organic layer was combined and then dried over Na_2SO_4. After evaporation of

solvent under reduced pressure, the residue was purified by column chromatography on silica gel using petroleum ether-ethyl acetate to afford the pure product.

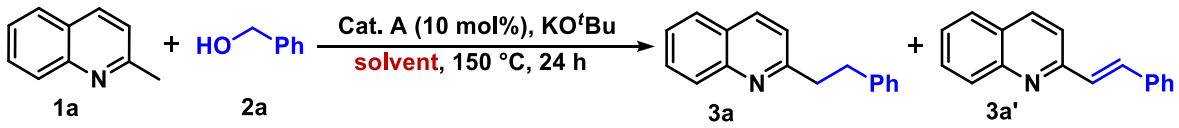
Table S1: Screening of Catalyst **A** Loading[a]



Entry	**Catalyst A (x mol%)**	Conversion (%)[b]	**3a:3a′**[b]	Yield of **3a** (%)
1	-	2	48:52	1
2	5	76	97:3	74
3	10	99	88:12	87

[a]Reaction conditions: 2-Methyl quinoline **1a** (0.6 mmol), benzyl alcohol **2a** (0.3 mmol), cat. **A** (10 mol%), and KO^{t}Bu (0.45 mmol), in toluene (2 mL), at 150°C (oil bath temperature), for 24 h. [b]Conversion and selectivity was determined by GC using *n*-dodecane as internal standard.

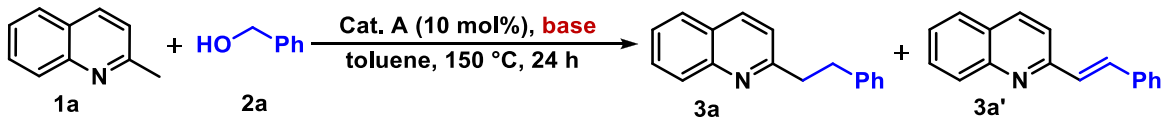
Table S2: Screening of Solvent[a]



Entry	**Solvent**	Conversion (%)[b]	**3a:3a′**[b]	Yield of **3a** (%)
1	Dioxane	2	86:14	2
2	*m*-xylene	38	97:3	37
3	*p*-xylene	21	85:15	18
4	Toluene	99	88:12	87

[a]Reaction conditions: 2-Methyl quinoline **1a** (0.6 mmol), benzyl alcohol **2a** (0.3 mmol), cat. **A** (10 mol%), and KO^{t}Bu (0.45 mmol), solvent (2 mL), at 150°C (oil bath temperature), for 24 h. [b]Conversion and selectivity was determined by GC using *n*-dodecane as internal standard.

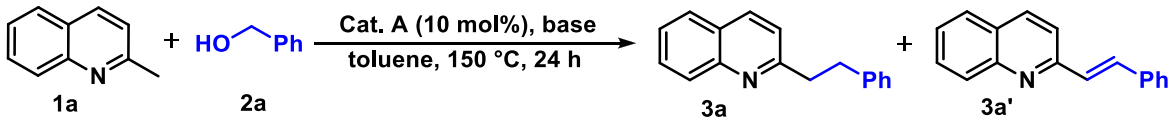
Table S3: Screening of Base[a]



Entry	**Base (1.5 equiv.)**	Conversion (%)[b]	**3a:3a′**[b]	Yield of **3a** (%)
1	NaOH	5	90:10	5
2	KOH	48	66:34	31
3	KO^{t}Bu	99	88:12	87
4	CsOH	6	53:47	32
5	Cs_2CO_3	0	0	0
6	NaOMe	15	23:77	35

[a]Reaction conditions: 2-Methyl quinoline **1a** (0.6 mmol), benzyl alcohol **2a** (0.3 mmol), cat. **A** (10 mol%), and Base (0.45 mmol), in toluene (2 mL), at 150°C (oil bath temperature), for 24 h. [b]Conversion and selectivity was determined by GC using *n*-dodecane as internal standard.

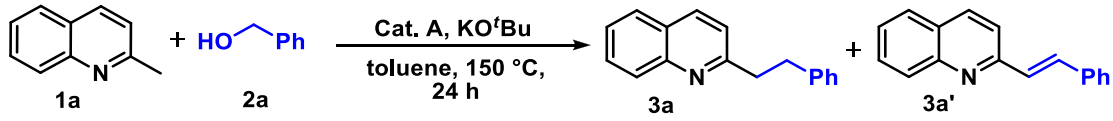
Table S4: Screening of Base Loading[a]



Entry	**KO^{t}Bu (equiv.)**	Conversion (%)[b]	**3a:3a′**[b]	Yield of **3a** (%)
1	-	3	33:67	1
2	1	77	61:39	47
3	1.5	99	88:12	87
4	2	99	95:5	94

[a]Reaction conditions: 2-Methyl quinoline **1a** (0.6 mmol), benzyl alcohol **2a** (0.3 mmol), cat. **A** (10 mol%), and KO^{t}Bu (mmol), in toluene (2 mL), at 150°C (oil bath temperature), for 24 h. [b]Conversion and selectivity was determined by GC using *n*-dodecane as internal standard.

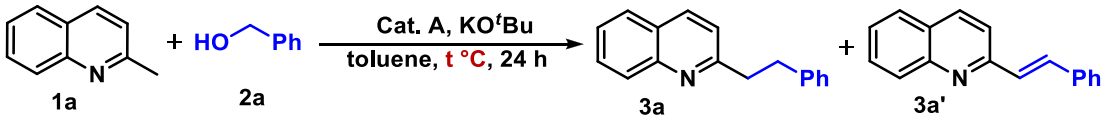
Table S5: Screening the amount of **1a** and **2a**[a]



Entry	**1a (mmol)**	**2a (mmol)**	Conversion (%)[b]	**3a:3a′** (%)[b]	Yield of **3a** (%)
1	1	1	63	60:40	38
2	1	2	87	71:29	62
3	2	1	99	88:12	87

[a]Reaction conditions: 2-Methyl quinoline **1a** (mmol), benzyl alcohol **2a** (mmol), cat. **A** (10 mol%), and KO^{t}Bu (0.45 mmol), in toluene (2 mL), at 150°C (oil bath temperature), for 24 h. [b]Conversion and selectivity was determined by GC using *n*-dodecane as internal standard.

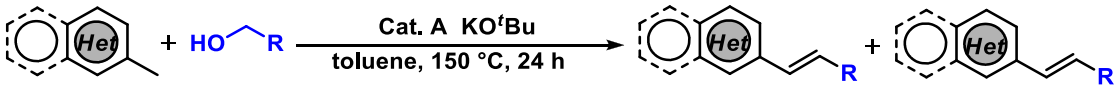
Table S6: Screening of Reaction Temperature[a]



Entry	**Temperature (°C)**	Conversion (%)[b]	**3a:3a′** (%)[b]	Yield of **3a** (%)
1	120	6	30:70	18
2	140	63	90:10	57
3	150	99	88:12	87

[a]Reaction conditions: 2-Methyl quinoline **1a** (0.6 mmol), benzyl alcohol **2a** (0.3 mmol), cat. **A** (10 mol%), and KO^{t}Bu (0.45 mmol), in toluene (2 mL), at T °C (oil bath temperature), for 24 h. [b]Conversion and selectivity was determined by GC using *n*-dodecane as internal standard.

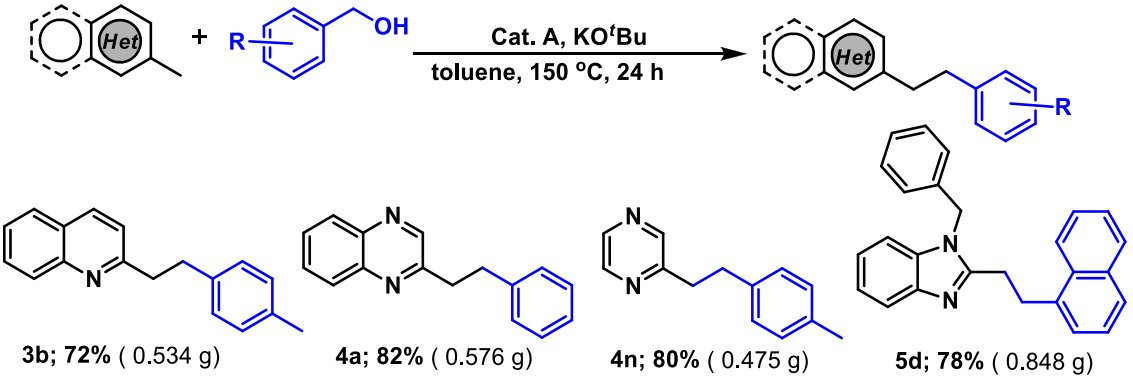
3. General Procedure for Alkylation of Methyl Substituted N-Heteroarenes



An oven dried 9 mL pressure tube was taken inside the argon filled glove box and charged with a magnetic stir bar, KO^{t}Bu (0.45 mmol), Co(NNN) complex **A** (10 mol%) methyl substituted N-heteroarenes **1a** (0.6 mmol), Benzyl alcohol **2a** (0.3 mmol), in toluene (2 mL)., Then pressure tube was closed tightly, removed from the glove box and placed in a preheated oil bath at 150 °C (oil bath temperature). After 24 h the reaction was allowed to cool at room temperature and was quenched with brine and extracted with ethyl acetate (4×10mL). 20 µL reaction mixture was syringed out and directly subjected to GC analysis to determine conversion as well as selectivity. The organic layer was combined and then dried over Na_2SO_4. After evaporation of solvent under reduced pressure, the residue was purified by column chromatography on silica gel using petroleum ether-ethyl acetate to afford the desired product.

4. Procedure for Preparative Scale Synthesis

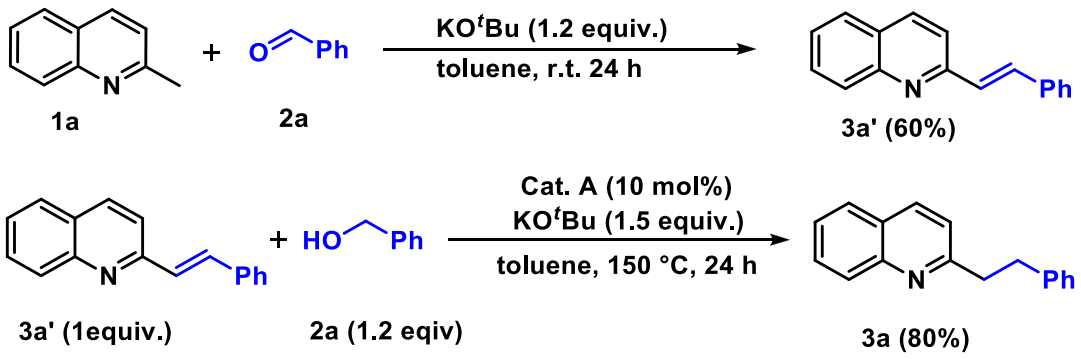
An oven dried 15 mL pressure tube, equipped with a magnetic stir-bar, was taken inside the argon filled glove box. After that methyl substituted N-heteroarenes (6 mmol), alcohol (3 mmol), complex **A** (10 mol%), KO^{t}Bu (1.5 equiv.) and toluene (10 mL) were added into the tube and sealed it. Then the tube was placed in a preheated oil bath at 150 °C (oil bath temperature) for 24 h. Then, it was cooled to room temperature and extracted with ethyl acetate. Finally, alkylated N-heteroarene derivatives were purified by column chromatography using hexane/ethyl acetate as eluent to afford the corresponding pure product.



5. Controlled Experiment

5.1. Synthesis of 2-Styrylquinoline and Intermediate Determination

These controlled experiments were performed to find out mechanistic insight for alkylation of methyl substituted N-heteroarenes.

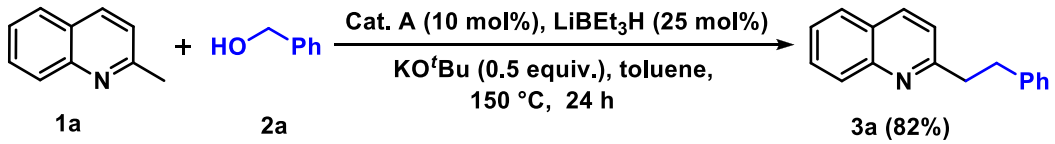


A mixture of 2-Methylquinoline **1a** (1mmol) and KO^{t}Bu (1.2mmol) in THF were taken in a 100 mL round bottom flask equipped with a magnetic pellet. Next benzaldehyde (1.2mmol) was added

slowly, then reaction mixture was stirred for 12 h under argon atmosphere at room temperature. After completion of the reaction, mixture was quenched with water and organic part was extracted with dicholoromethane (3×15 mL), dried over Na_2SO_4. Solvent was evaporated in reduced pressure and purified by column chromatography using hexane/ethyl acetate as eluent to afford the corresponding pure product. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 8.10-8.07 (m, 2H), 7.75 (d, $J_{H,H}$ = 8.16 Hz, 1H), 7.71-7.69 (m, 1H), 7.67-7.62 (m, 4H), 7.49-7.45 (m, 1H), 7.42-7.37 (m, 3H), 7.33-7.29 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 156.08, 148.34, 136.60, 136.44, 134.52, 129.84, 129.28, 129.10, 128.88, 128.72, 127.59, 127.43, 127.35, 126.26, 119.34.

Next, reaction of 2-styrylquinoline with benzyl alcohol under standard reaction conditions leads to the formation of desired alkylated quinoline product.

5.2. Alkylation of N-heteroarenes in Presence of Superhydride



1a **2a** **3a (82%)**

An oven dried 9 mL pressure tube, equipped with a magnetic stir-bar, was taken inside the argon filled glove box. Next, Complex **A** (10 mol%) and 2 mL toluene were taken then $LiBEt_3H$ (1M in THF, 25 mol%) solution was added dropwise under stirring condition. During this addition we observed that a gradual colour change from light yellow to dark pink. After stirring for 15 minutes, 2-methylquinoline (0.6 mmol) **1a**, benzyl alcohol **2a** (0.3 mmol), KO^{t}Bu (0.45 mmol), were added to the mixture. Then pressure tube was closed tightly, removed from the glove box and placed in a preheated oil bath at 150 °C (oil bath temperature). After 24 h the reaction was allowed to cool at room temperature and 4 mL of ethyl acetate was added and 20 µL reaction mixture was syringed out and directly subjected to GC. Yield of 2-phenethylquinoline was 82% by using *n*-dodecane as internal standard (78% isolated).

5.3. Time Dependent Product Distribution Plot

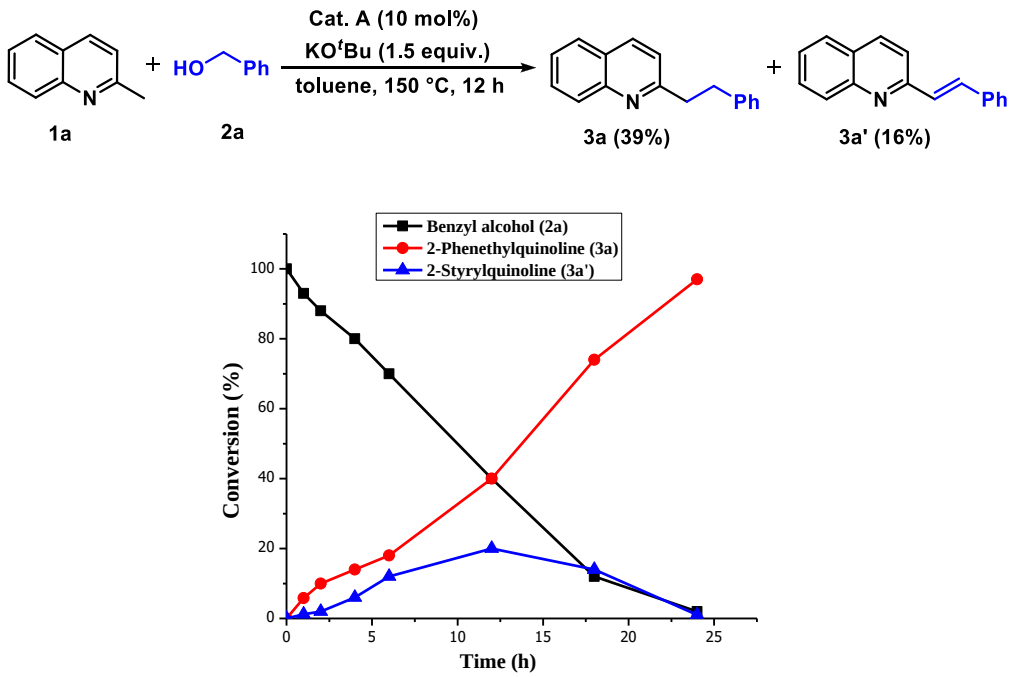


Fig. S1 Time course monitoring of the reaction of 2-methylquinoline with benzyl alcohol.

6. Plausible Reaction Pathway

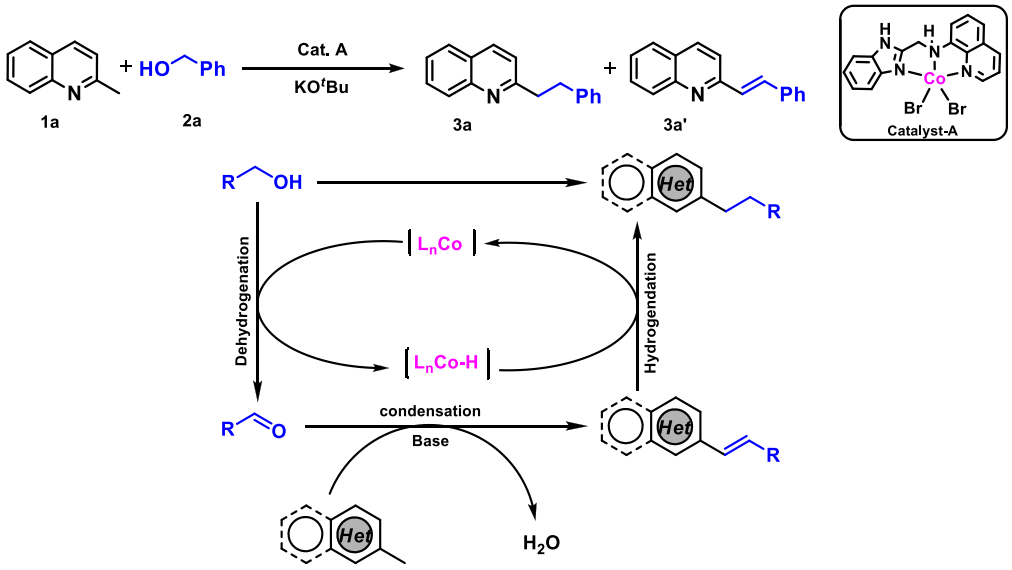
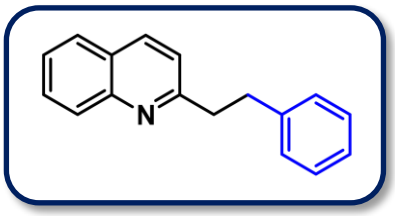


Fig. S2 Plausible reaction pathway for cat. **A** catalyzed alkylation of methyl substituted N-heteroarenes with alcohols.

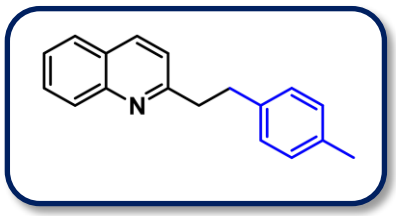
6. Characterization of Products

2-Phenethylquinoline (3a)[2]: Isolated as a pale yellow liquid, 56 mg, 81% yield.



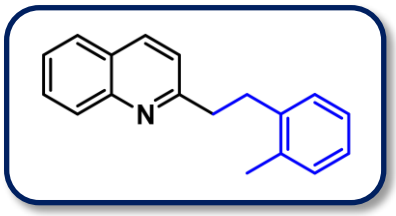
^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.08 (d, $J_{H,H}$ = 8.50 Hz, 1H), 8.04 (d, $J_{H,H}$ = 8.40 Hz, 1H), 7.77 (d, $J_{H,H}$ = 8.05 Hz, 1H), 7.71-7.68 (m, 1H), 7.49 (t, $J_{H,H}$ = 7.05 Hz, 1H), 7.29-7.21 (m, 5H), 7.19 (t, $J_{H,H}$ = 6.95 Hz, 1H), 3.31-3.28 (m, 2H), 3.17-3.14 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 161.91, 148.04, 141.61, 136.31, 129.50, 128.96, 128.61, 128.49, 127.63, 126.89, 126.09, 125.86, 121.66, 41.10, 35.87. **GC-MS (M^+)**: 233.1.

2-(4-methylphenethyl)quinoline (3b)[2]: Isolated as a pale yellow liquid, 64 mg, 87% yield.



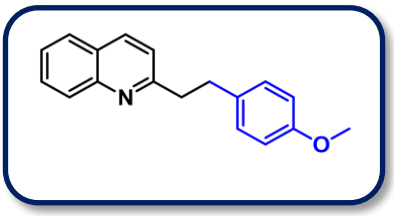
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.07-8.02 (m, 2H), 7.77 (d, $J_{H,H}$ = 8.24 Hz, 1H), 7.71-7.66 (m, 1H), 7.50-7.46 (m, 1H), 7.25-7.24 (m, 1H), 7.14 (d, $J_{H,H}$ = 7.96 Hz, 2H), 7.08 (d, $J_{H,H}$ = 7.96 Hz, 2H), 3.28-3.24 (m, 2H), 3.12-3.08 (m, 2H), 2.31 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 162.04, 148.05, 138.51, 136.31, 135.54, 129.48, 129.17, 128.94, 128.47, 127.62, 126.88, 125.87, 121.68, 41.25, 35.65, 21.12. **GC-MS (M^+)**: 233.1.

2-(2-methylphenethyl)quinoline (3c)[3]: Isolated as a pale yellow liquid, 65 mg, 88% yield.



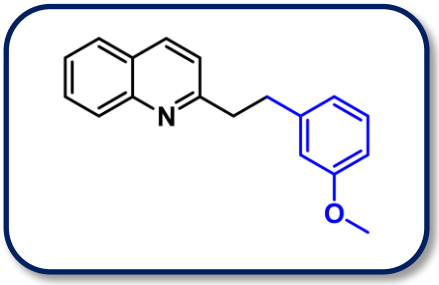
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.13 (d, $J_{H,H}$ = 8.56 Hz, 1H), 8.03 (d, $J_{H,H}$ = 8.44 Hz, 1H), 7.78 (d, $J_{H,H}$ = 8.20 Hz, 1H), 7.73-7.69 (m, 1H), 7.52-7.48 (m, 1H), 7.24-7.20 (m, 2H), 7.17-7.14 (m, 3H), 3.30-3.26 (m, 2H), 3.19-3.15 (m, 2H), 2.37 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 162.28, 148.28, 139.67, 136.34, 136.14, 130.36, 129.54, 129.04, 128.99, 127.68, 126.93, 126.31, 126.19, 125.94, 121.65, 40.07, 33.40, 19.53. **GC-MS (M^+)**: 247.3.

2-(4-methoxyphenethyl)quinoline (3d)[4]: Isolated as a pale yellow liquid, 60 mg, 78% yield.



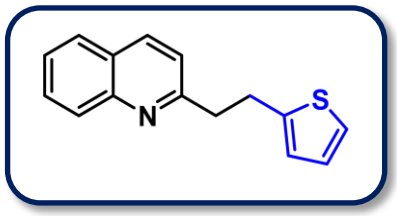
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.06 (d, $J_{H,H}$ = 8.52 Hz, 1H), 8.02 (d, $J_{H,H}$ = 8.52 Hz, 1H), 7.76 (d, $J_{H,H}$ = 8.52 Hz, 1H), 7.68 (d, $J_{H,H}$ = 7.08 Hz, 1H), 7.48 (d, $J_{H,H}$ = 7.12 Hz, 1H), 7.20 (d, $J_{H,H}$ = 8.48 Hz, 1H), 7.14 (d, $J_{H,H}$ = 8.52 Hz, 2H), 6.81 (d, $J_{H,H}$ = 8.60 Hz, 2H), 3.76 (s, 3H), 3.27-3.23 (m, 2H), 3.11-3.07 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 161.82, 158.07, 148.11, 136.26, 133.72, 129.50, 129.46, 128.84, 127.60, 126.80, 125.79, 121.69, 114.07, 55.38, 41.44, 35.29. **GC-MS (M^+)**: 263.3.

2-(3-methoxyphenethyl)quinoline (3e)[3]: Isolated as a pale yellow liquid, 58 mg, 74% yield.



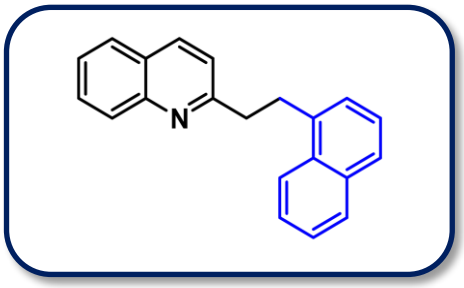
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.08 (d, $J_{H,H}$ = 8.45 Hz, 1H), 8.03 (d, $J_{H,H}$ = 8.40 Hz, 1H), 7.77 (d, $J_{H,H}$ = 8.10 Hz, 1H), 7.69 (t, $J_{H,H}$ = 7.10 Hz, $J_{H,H}$ = 8.25 Hz, 1H), 7.50-7.47 (m, 1H), 7.24-7.18 (m, 2H), 6.85 (d, $J_{H,H}$ = 7.50 Hz, 1H), 6.82-6.80 (m, 1H), 6.75-6.73 (m, 1H), 3.76 (s, 3H), 3.31-3.28 (m, 2H), 3.16-3.13 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 161.85, 159.72, 148.11, 143.26, 136.29, 129.48, 129.44, 128.97, 127.61, 126.91, 125.88, 121.64, 121.00, 114.24, 111.63, 55.20, 40.94, 36.02. **GC-MS (M^+)**: 263.13.

2-(2-(thiophen-2-yl)ethyl)quinoline (3f)[4]: Isolated as a light brown liquid, 17 mg, 24% yield.



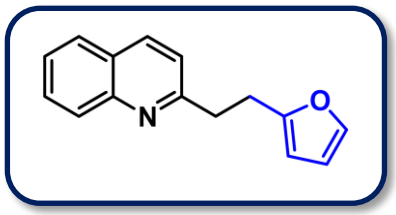
^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.08 (d, $J_{H,H}$ = 8.60 Hz, 1H), 8.05 (d, $J_{H,H}$ = 8.45 Hz, 1H), 7.76 (d, $J_{H,H}$ = 8.10 Hz, 1H), 7.70 (t, $J_{H,H}$ = 7.25 Hz, 1H), 7.49 (t, $J_{H,H}$ = 7.90 Hz, 1H), 7.25 (t, $J_{H,H}$ = 4.40 Hz, 1H), 7.11 (d, $J_{H,H}$ = 5.10 Hz, 1H), 6.90 (dd, $J_{H,H}$ = 4.95 Hz, $J_{H,H}$ = 5.00 Hz, 1H), 6.82 (d, $J_{H,H}$ = 3.00 Hz, 1H), 3.41-3.33 (m, 4H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 158.61, 145.49, 141.75, 133.93, 127.06, 126.37, 125.11, 124.42, 124.29, 123.47, 122.15, 120.83, 119.03, 38.54, 27.41. **GC-MS (M^+)**: 239.0.

2-(2-(naphthalen-1-yl)ethyl)quinoline (3g)[3]: Isolated as a light brown solid, 73 mg, 86% yield.



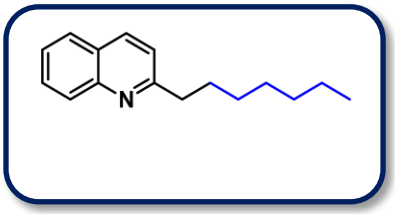
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.18 (d, $J_{H,H}$ = 8.24 Hz, 1H), 8.11 (d, $J_{H,H}$ = 8.48 Hz, 1H), 8.02 (d, $J_{H,H}$ = 8.40 Hz, 1H), 7.86 (d, $J_{H,H}$ = 7.80 Hz, 1H), 7.78 (d, $J_{H,H}$ = 8.04 Hz, 1H), 7.73-7.69 (m, 2H), 7.54-7.46 (m, 3H), 7.38-7.33 (m, 2H), 7.20 (d, $J_{H,H}$ = 8.28 Hz, 1H), 3.64-3.60 (m, 2H), 3.44-3.40 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 162.09, 148.20, 137.72, 136.38, 133.96, 131.96, 129.57, 129.03, 128.91, 127.66, 126.92, 126.22, 126.22, 126.02, 125.91, 125.66, 125.60, 123.97, 121.74, 40.38, 33.37. **GC-MS (M^+)**: 283.1.

2-(2-(furan-2-yl)ethyl)quinoline (3h)[2]: Isolated as a pale yellow liquid, 21 mg, 34% yield.



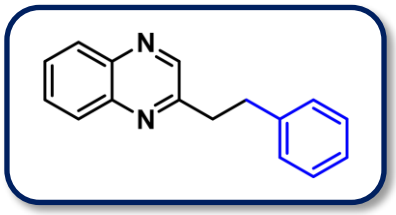
^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.06-8.02 (m, 1H), 7.76 (d, $J_{H,H}$ = 8.10 Hz, 1H), 7.68 (d, $J_{H,H}$ = 7.05 Hz, 1H), 7.49-7.46 (m, 1H), 7.32-7.30 (m, 1H), 7.25-7.21 (m, 1H), 6.27-6.24 (m, 1H), 6.00-5.98 (m, 1H), 3.34-3.30 (m, 2H), 3.21-3.17 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 161.33, 155.22, 148.06, 141.05, 136.35, 129.50, 128.98, 127.60, 126.92, 125.93, 121.42, 110.24, 105.47, 37.65, 28.23. **GC-MS (M^+)**: 223.1.

2-heptylquinoline (3i)[4]: Isolated as a pale yellow liquid, 38 mg, 50% yield.



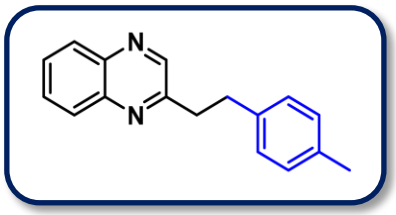
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.03 (d, $J_{H,H}$ = 8.30 Hz, 2H), 75 (d, $J_{H,H}$ = 8.15 Hz, 1H), 7.66 (t, $J_{H,H}$ = 8.20 Hz, $J_{H,H}$ = 7.00 Hz, 1H), 7.45 (t, $J_{H,H}$ = 7.00 Hz, $J_{H,H}$ = 7.05 Hz, 1H), 7.26 (t, $J_{H,H}$ = 8.40 Hz, $J_{H,H}$ = 7.25 Hz, 1H), 2.95 (t, $J_{H,H}$ = 7.85 Hz, $J_{H,H}$ = 7.80 Hz, 2H), 1.83-1.76 (m, 2H), 1.41-1.32 (m, 4H), 1.27-1.25 (m, 4H), 0.88-0.85 (m, 3H).**^{13}C NMR (100 MHz, $CDCl_3$):** δ = 163.14, 147.99, 136.24, 129.37, 128.90, 127.54, 126.79, 125.69, 121.44, 39.47, 31.86, 30.18, 29.63, 29.29, 22.73, 14.16. **GC-MS (M^+)**: 227.1.

2-phenethylquinoxaline (4a)[5]: Isolated as a pale yellow liquid, 62 mg, 89% yield.



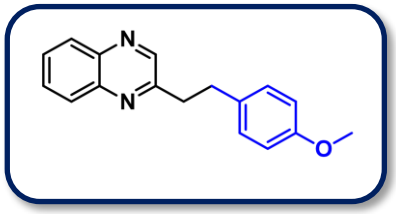
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.58 (s, 1H), 8.06-8.03 (m, 2H), 7.71-7.62 (m, 2H), 7.26-7.14 (m, 5H), 3.30-3.26 (m, 2H), 3.16-3.12 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 156.49, 145.89, 142.31, 141.35, 140.86, 130.03, 129.31, 129.13, 128.99, 128.64, 128.56, 126.37, 38.16, 35.30. **GC-MS (M^+)**: 234.1.

2-(4-methylphenethyl)quinoxaline (4b)[4]: Isolated as a pale yellow liquid, 65 mg, 88% yield.



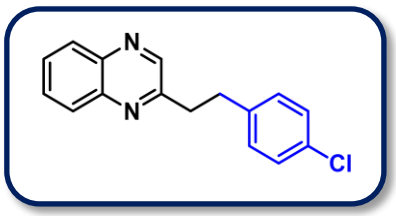
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.60 (s, 1H), 8.07-8.05 (m, 2H), 7.76-7.68 (m, 2H), 7.12-7.06 (m, 4H), 3.32-3.28 (m, 2H), 3.15-3.11 (m, 2H), 2.30 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 156.67, 145.94, 142.33, 141.32, 137.71, 135.87, 130.08, 129.32, 129.28, 129.17, 128.97, 128.43, 96.52, 38.39, 35.02, 21.12. **GC-MS (M^+)**: 248.1.

2-(4-methoxyphenethyl)quinoxaline (4c)[5]: Isolated as a pale yellow liquid, 67mg, 85% yield.



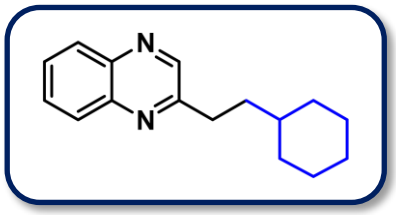
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.59 (s, 1H), 8.05 (d, $J_{H,H}$ = 8.72 Hz, 2H), 7.76-7.68 (m, 2H), 7.12 (d, $J_{H,H}$ = 8.60 Hz, 2H), 6.81-6.80 (m, 2H), 3.76 (s, 3H), 3.30-3.27 (m, 2H), 3.13-3.09 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 158.25, 156.80, 145.94, 142.42, 141.34, 132.83, 130.06, 129.49, 129.29, 129.15, 128.97, 114.02, 95.94, 55.32, 38.61, 34.75. **GC-MS (M^+)**: 264.1.

2-(4-chlorophenethyl)quinoxaline(4d)[4]: Isolated as a pale yellow liquid, 62 mg, 78% yield.



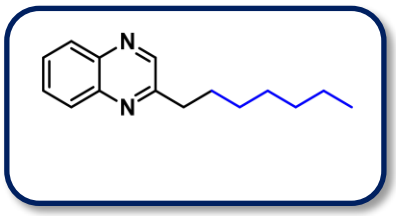
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.61 (s, 1H), 8.06 (t, $J_{H,H}$ = 8.00 Hz, $J_{H,H}$= 8.40 Hz, 2H), 7.76-7.69 (m, 2H), 7.25-7.22 (m, 2H), 7.15-7.13 (m, 2H), 3.31-3.28 (m, 2H), 3.17-3.14 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 156.05, 145.76, 142.34, 141.43, 139.29, 132.13, 130.13, 129.90, 129.34, 129.25, 128.98, 128.73, 37.90, 34.50. **GC-MS (M^+)**: 268.07.

2-(2-cyclohexylethyl)quinoxaline (4e)[5]: Isolated as a colourless liquid, 54 mg, 80% yield.



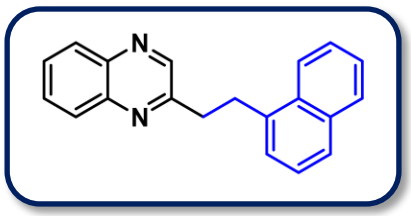
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.69 (s, 1H), 8.04-7.98 (m, 2H), 7.71-7.63 (m, 2H), 3.00-2.96 (m, 2H), 1.79-1.76 (m, 2H), 1.70-1.66 (m, 4H), 1.64-1.60 (m, 1H), 1.37-1.27 (m, 1H), 1.21-1.11 (m, 3H), 0.99-0.89 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 158.10, 145.91, 142.40, 141.23, 129.92, 129.22, 128.90, 37.69, 37.18, 34.09, 33.08, 26.64, 26.34. **GC-MS (M^+)**: 240.1.

2-heptylquinoxaline (4f)[4]: Isolated as a colourless liquid, 57 mg, 82% yield.



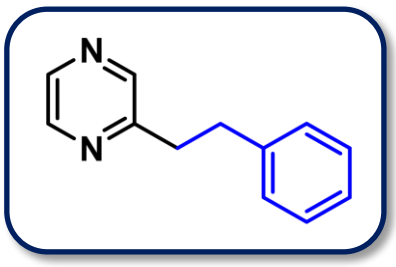
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.67 (s, 1H), 8.01-7.96 (m, 2H), 7.67-7.59 (m, 2H), 2.93 (t, $J_{H,H}$ = 7.68 Hz, 2H), 1.81-1.73 (m, 2H), 1.38-1.26 (m, 4H), 1.24-1.18 (m, 4H), 0.82-0.78 (m, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 157.72, 145.86, 142.23, 141.22, 129.90, 129.20, 128.89, 36.57, 31.76, 29.61, 29.46, 29.14, 22.92, 14.12. **GC-MS (M^+)**: 228.1.

2-(2-(naphthalen-1-yl)ethyl)quinoxaline (4g)[5]: Isolated as a pale yellow solid, 70 mg, 86% yield.



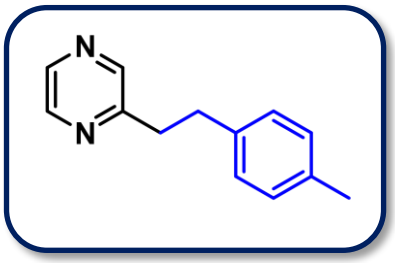
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.59 (s, 1H), 8.16-8.07 (m, 3H), 7.87 (d, $J_{H,H}$ = 6.40 Hz, 1H), 7.79-7.71 (m, 3H), 7.55-7.47 (m, 2H), 7.37-7.30 (m, 2H), 3.67-3.64 (m, 2H), 3.48-3.45 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 156.68, 145.80, 142.41, 141.33, 136.91, 134.11, 131.78, 130.14, 129.24, 129.03, 127.26, 126.33, 126.18, 125.71, 125.64, 129.62, 37.31, 32.51. **GC-MS (M^+)**: 284.1.

2-phenethylpyrazine (4h)[6]: Isolated as a pale yellow liquid, 49 mg, 88% yield.



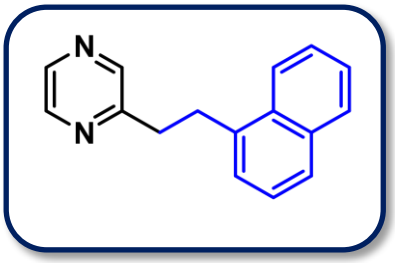
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.49 (t, $J_{H,H}$ = 2.24 Hz, 1H), 8.38 (d, $J_{H,H}$ = 2.60 Hz, 1H), 8.33 (t, $J_{H,H}$ = 1.12 Hz, 1H), 7.27-7.24 (m, 2H), 7.19-7.14 (m, 3H), 3.13-3.03 (m, 4H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 156.82, 144.77, 144.19, 142.41, 140.83, 128.58, 128.49, 126.31, 37.30, 35.45. **GC-MS (M^+)**: 284.1.

2-(4-methylphenethyl)pyrazine (4i)[6]: Isolated as a pale yellow liquid, 54 mg, 90% yield.



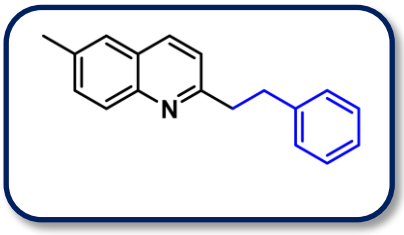
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.52-8.50 (m, 1H), 8.40-8.38 (m, 1H), 8.35-8.33 (m, 1H), 7.08-7.04 (m, 4H), 3.11-3.08 (m, 2H), 3.04-3.01 (m, 2H), 2.30 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 156.98, 144.77, 144.18, 142.33, 137.79, 135.73, 129.27, 128.36, 37.69, 35.37, 21.03. **GC-MS (M^+)**: 298.1.

2-(2-(naphthalen-1-yl)ethyl)pyrazine (4j)[6]: Isolated as a pale yellow solid, 60 mg, 86% yield.



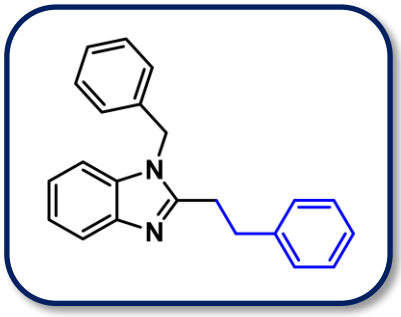
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.55 (s, 1H), 8.42-8.39 (m, 1H), 8.34 (s, 1H), 8.10 (d, $J_{H,H}$ = 8.30 Hz, 1H), 7.86 (d, $J_{H,H}$ = 8.00 Hz, 1H), 7.73 (d, $J_{H,H}$ = 8.15 Hz, 1H), 7.54-7.47 (m, 2H), 7.36 (t, $J_{H,H}$ = 7.55 Hz, 1H), 7.28-7.25 (m, 1H), 3.55-3.51 (m, 2H), 3.26-3.23 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 157.23, 144.74, 144.26, 142.48, 137.15, 136.95, 134.23, 131.79, 129.01, 127.20, 126.24, 126.15, 125.68, 125.61, 123.60, 36.53, 32.79. **GC-MS (M^+)**: 234.1.

6-methyl-2-phenethylquinoline (4k)[2]: Isolated as a light brown liquid, 36 mg, 56% yield.



^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.97-7.93 (m, 2H), 7.53-7.50 (m, 2H), 7.29-7.22 (m, 4H), 7.20-7.16 (m, 2H), 3.28-3.24 (m, 2H), 3.16-3.12 (m, 4H), 2.51 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 160.94, 146.53, 141.67, 135.74, 135.66, 131.74, 128.62, 128.56, 128.47, 126.95, 126.53, 126.06, 121.59, 41.13, 36.16, 21.81. **GC-MS (M^+)**: 247.1.

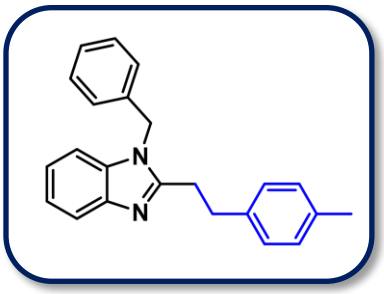
1-benzyl-2-phenethyl-1H-benzoimidazole (5a)[6]: Isolated as a pale yellow solid, 79 mg, 84% yield.



^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.83 (d, $J_{H,H}$ = 7.95 Hz, 1H), 7.29-7.25 (m, 6H), 7.22-7.20 (m, 3H), 7.17 (d, $J_{H,H}$ = 7.05 Hz, 2H), 6.99-6.97 (m, 2H), 5.16 (s, 3H), 3.20-3.17 (m, 2H), 3.13-3.10 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 154.67, 142.72, 140.92, 136.06, 135.45, 129.13, 128.71,

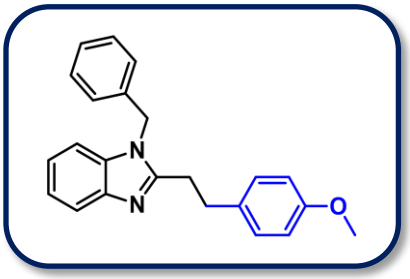
128.53, 128.02, 126.51, 126.25, 122.59, 122.27, 119.43, 109.82, 46.92, 34.12, 29.80. **GC-MS (M^+)**: 312.1.

1-benzyl-2-(4-methylphenethyl)-1H-benzoimidazole (5b)[7]: Isolated as a light brown solid, 84 mg, 86% yield.



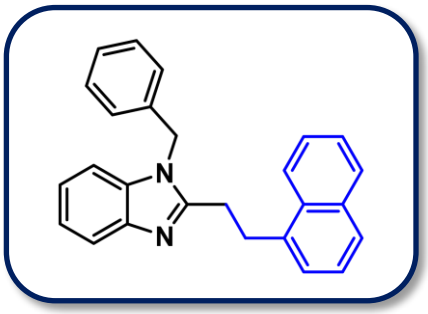
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.79 (d, $J_{H,H}$ = 7.92 Hz, 1H), 7.27-7.23 (m, 5H), 7.20-7.19 (m, 2H), 7.07-7.02 (m, 4H), 6.98-6.96 (m, 2H), 5.18 (s, 3H), 3.12-3.06 (m, 4H), 2.30 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 154.75, 142.65, 137.81, 136.03, 135.98, 135.40, 129.34, 129.08, 128.36, 127.98, 126.24, 122.52, 122.22, 119.39, 109.62, 46.83, 33.67, 29.93, 21.13. **GC-MS (M^+)**: 326.1.

1-benzyl-2-(4-methoxyphenethyl)-1H-benzoimidazole(5c)[7]: Isolated as a pale yellow solid, 90 mg, 88% yield.



^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.79 (d, $J_{H,H}$ = 7.84 Hz, 1H), 7.27-7.23 (m, 4H), 7.20-7.19 (m, 2H), 7.05 (d, $J_{H,H}$ = 8.56 Hz, 2H), 6.97-6.95 (m, 2H), 6.80-6.78 (m, 2H), 5.16 (s, 2H), 3.75 (s, 3H), 3.10-3.05 (m, 4H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 158.23, 154.75, 142.81, 136.05, 135.40, 132.94, 129.46, 129.08, 127.98, 126.23, 122.51, 122.21, 119.38, 114.05, 109.64, 55.34, 47.03, 33.28, 30.24. **GC-MS (M^+)**: 342.1.

1-benzyl-2-(2-(naphthalen-1-yl)ethyl)-1H-benzoimidazole (5d)[7]:



Isolated as a pale yellow solid, 97 mg, 90% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.93 (d, $J_{H,H}$ = 8.08 Hz, 1H), 7.85 (d, $J_{H,H}$ = 7.72 Hz, 2H), 7.72 (d, $J_{H,H}$ = 8.16 Hz, 1H), 7.48-7.41 (m, 2H), 7.37-7.33 (m, 1H), 7.31-7.19 (m, 7H), 6.91-6.88 (m, 2H), 5.06 (s, 2H), 3.66-3.62 (m, 2H), 3.25-3.21 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 155.09, 142.85, 137.00, 136.05, 135.52, 133.97, 131.70, 129.06, 128.95, 127.96, 127.30, 126.38, 126.24, 126.13, 125.73, 123.52, 122.56, 122.25, 119.47, 109.59, 46.70, 31.27, 29.12. **GC-MS (M^+)**: 362.1.

7. References:

1. (a) G.-L. Gao, C. Yang and W. Xia, *Chem. Commun.*, 2017, **53**, 1041-1044; (b) S. Shee, K. Ganguli, K. Jana, S. Kundu, *Chem. Commun.*, 2018, **54**, 6883-6886.
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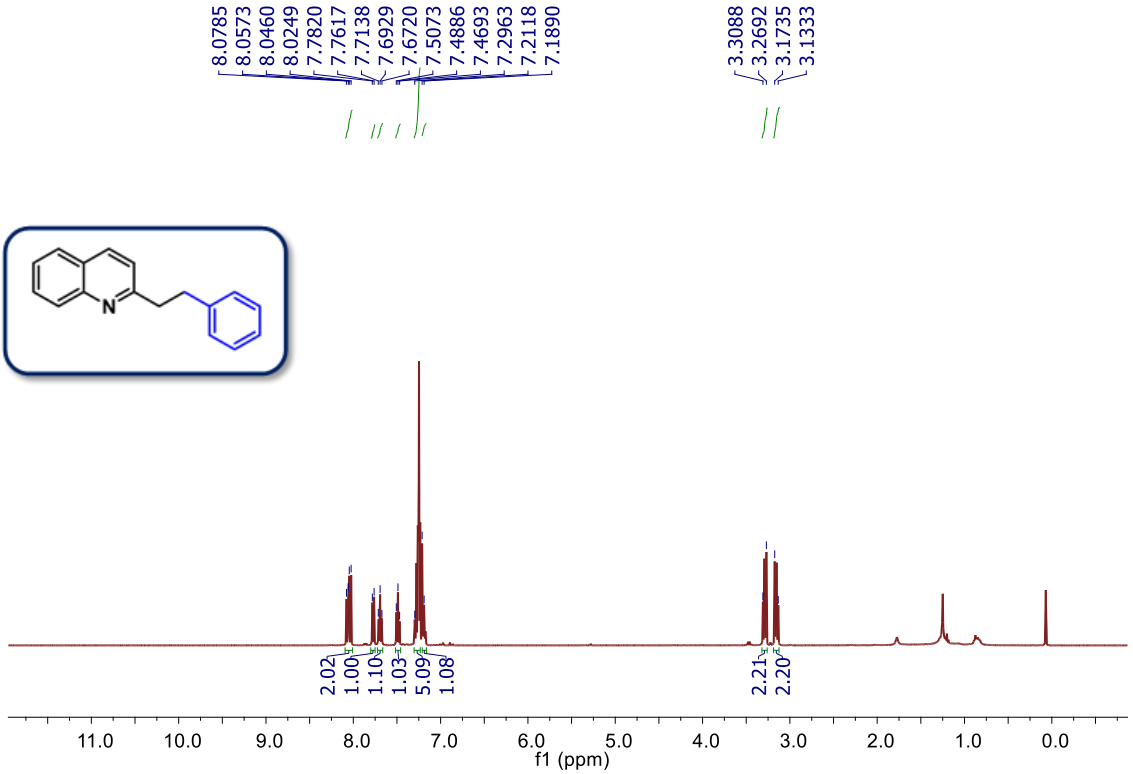
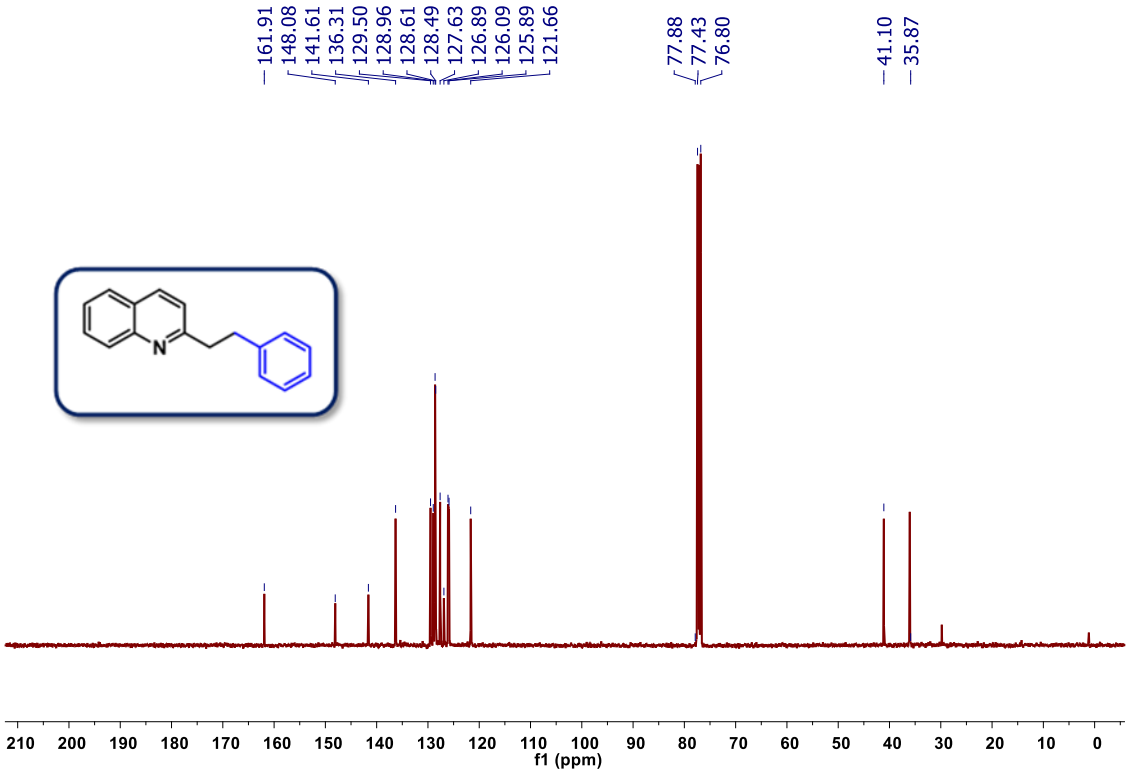
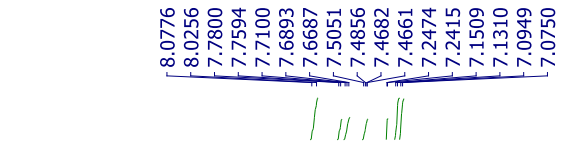
7. M. K. Barman, S. Waiba and B. Maji, *Angew. Chem. Int. Ed.*, 2018, **57**, 9126-9130.

8. NMR Spectra



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7.6687
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7.4682
7.4661
7.2474
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7.1310
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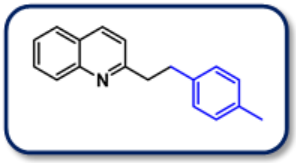
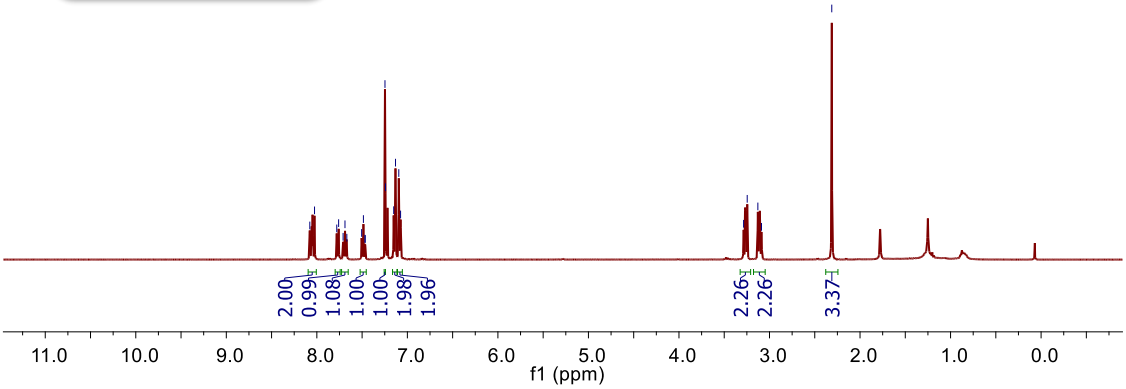
3.0883
2.3122

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2.26
2.26
3.37
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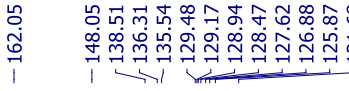
f1 (ppm)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129.48
129.17
128.94
128.47
127.62
126.88
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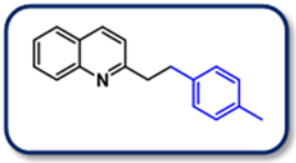
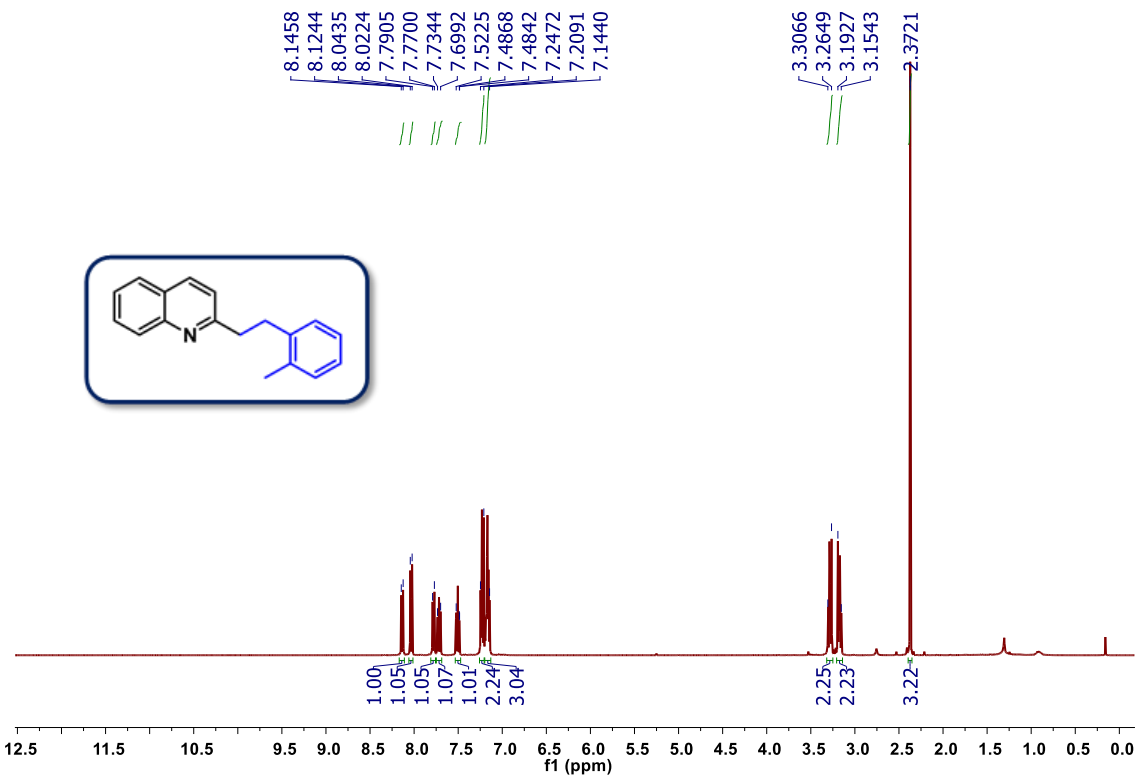
121.68
77.44
77.12
76.80
41.25
35.65
21.12



190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.7344
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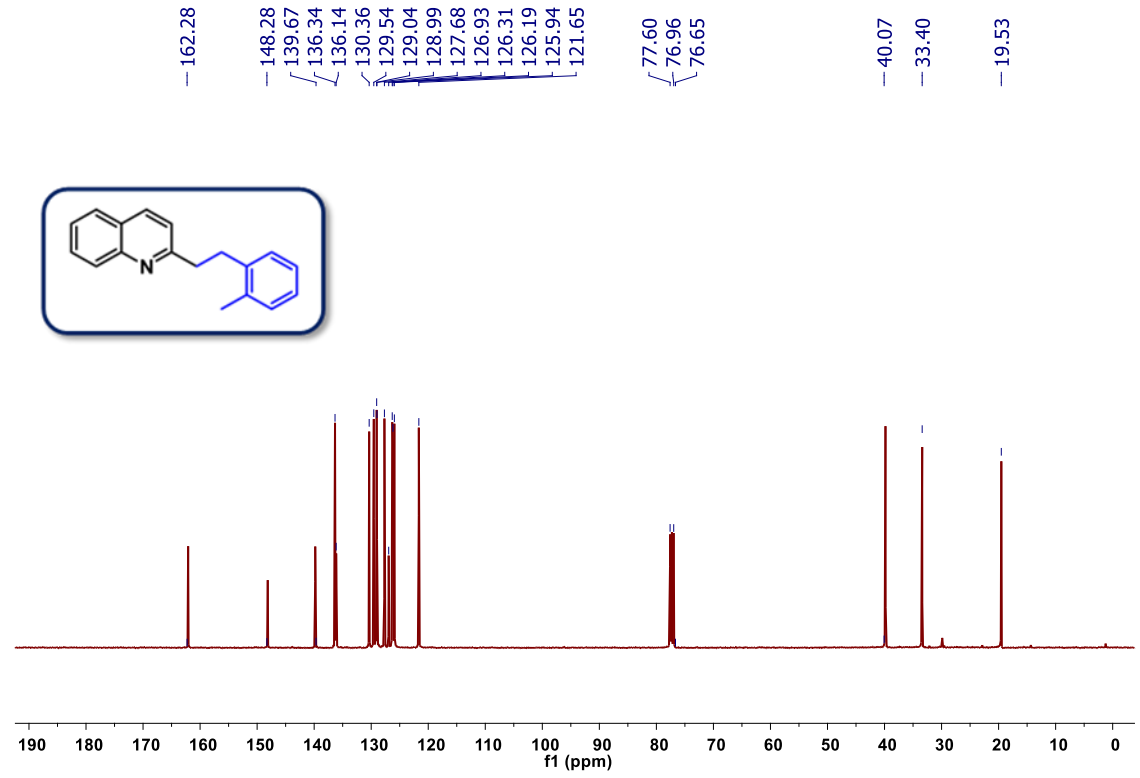
7.5225
7.4868
7.4842
7.2472
7.2091
7.1440
3.3066
3.2649
3.1927
3.1543
2.3721
1.00
1.05
1.05
1.07
1.01
2.24
3.04
2.25
2.23
3.22
f1 (ppm)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129.04
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127.68
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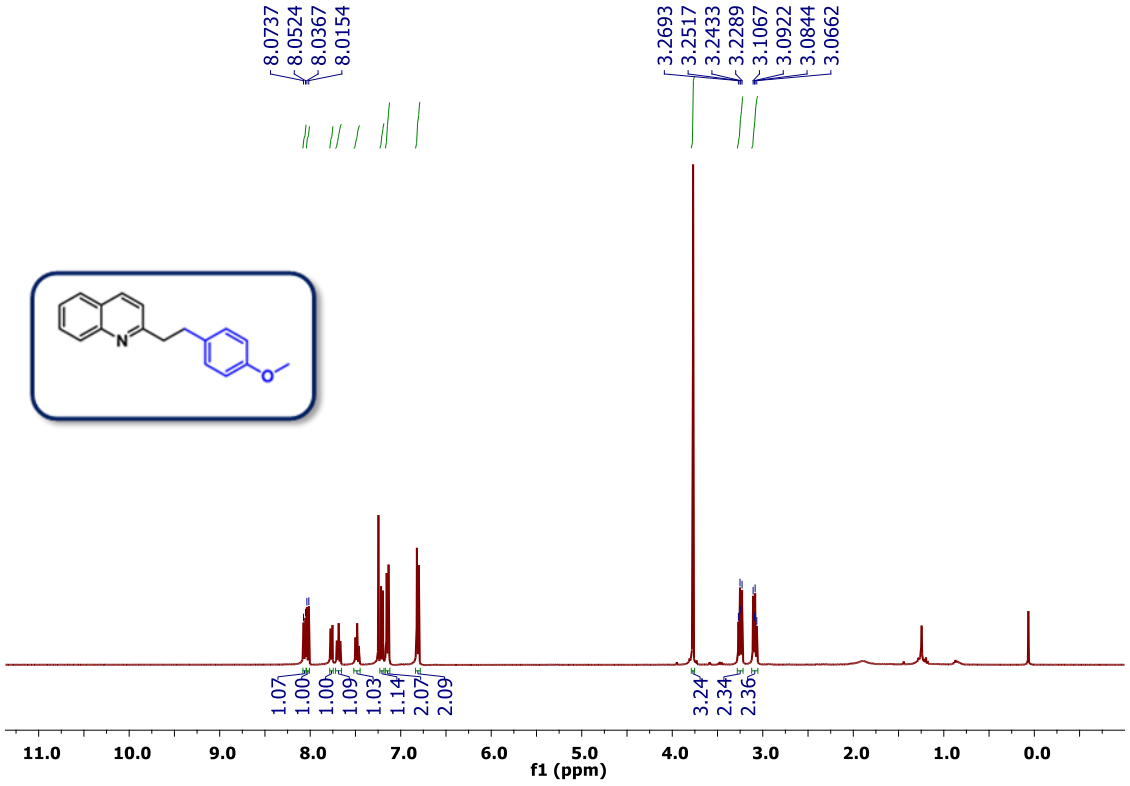
125.94
121.65
77.60
76.96
76.65
40.07
33.40
19.53
f1 (ppm)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8.0524
8.0367
8.0154
3.2693
3.2517
3.2433
3.2289
3.1067
3.0922
3.0844
3.0662
1.07
1.00
1.00
1.09
1.03
1.14
2.07
2.09
3.24
2.34
2.36
11.0
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9.0
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7.0
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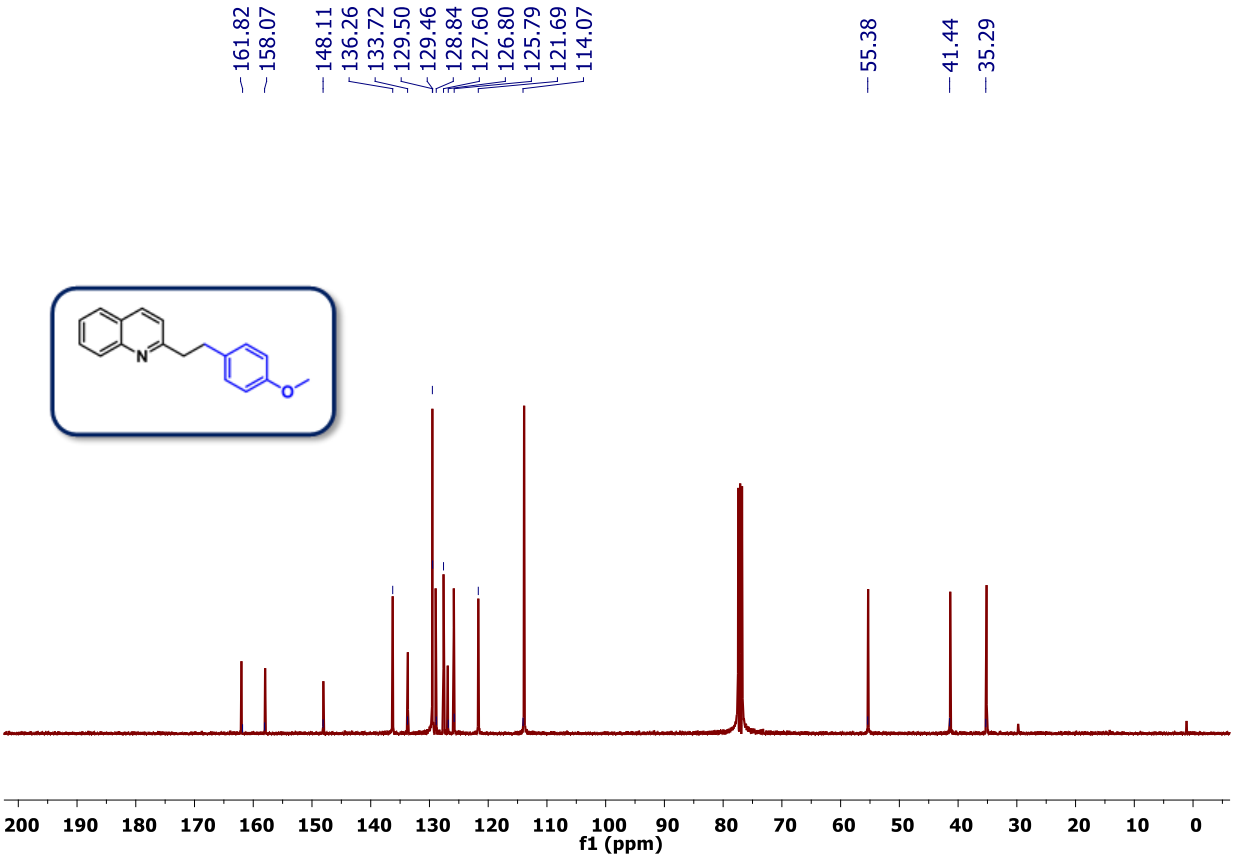
f1 (ppm)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136.26
133.72
129.50
129.46
128.84
127.60
126.80
125.79
121.69
114.07
55.38
41.44
35.29
200
190
180
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110
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90
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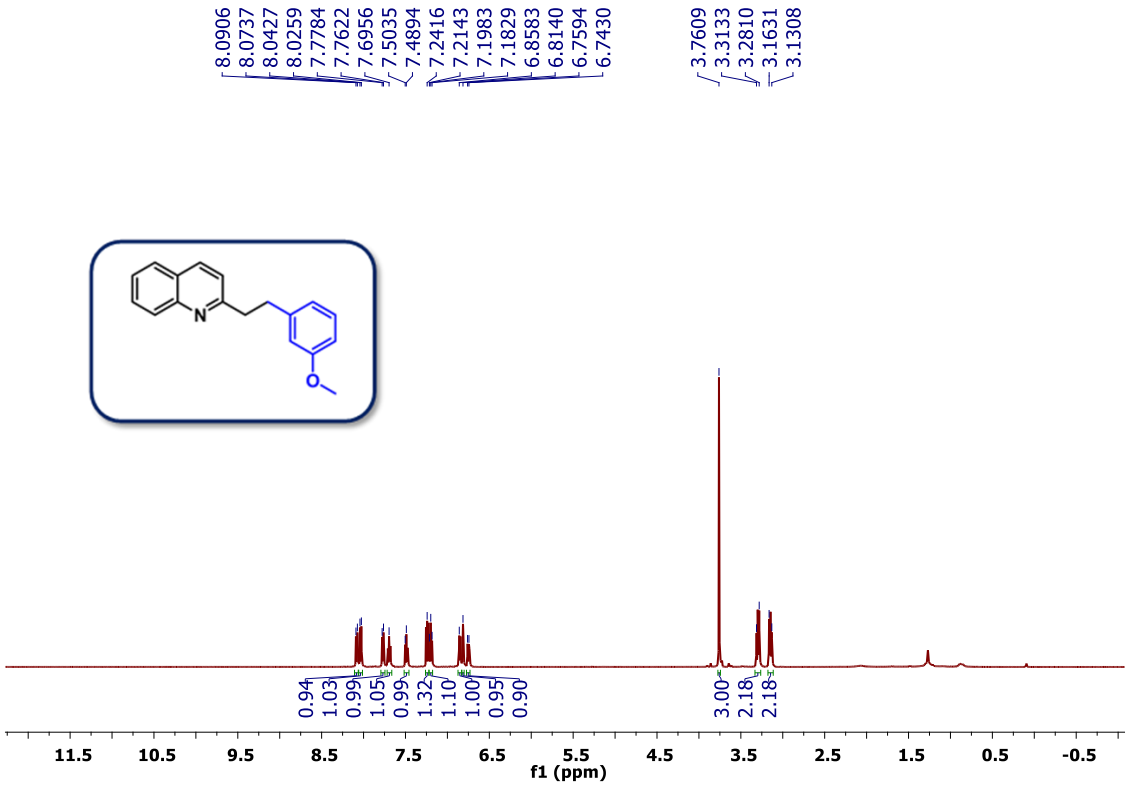
f1 (ppm)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7.7622
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7.5035
7.4894
7.2416
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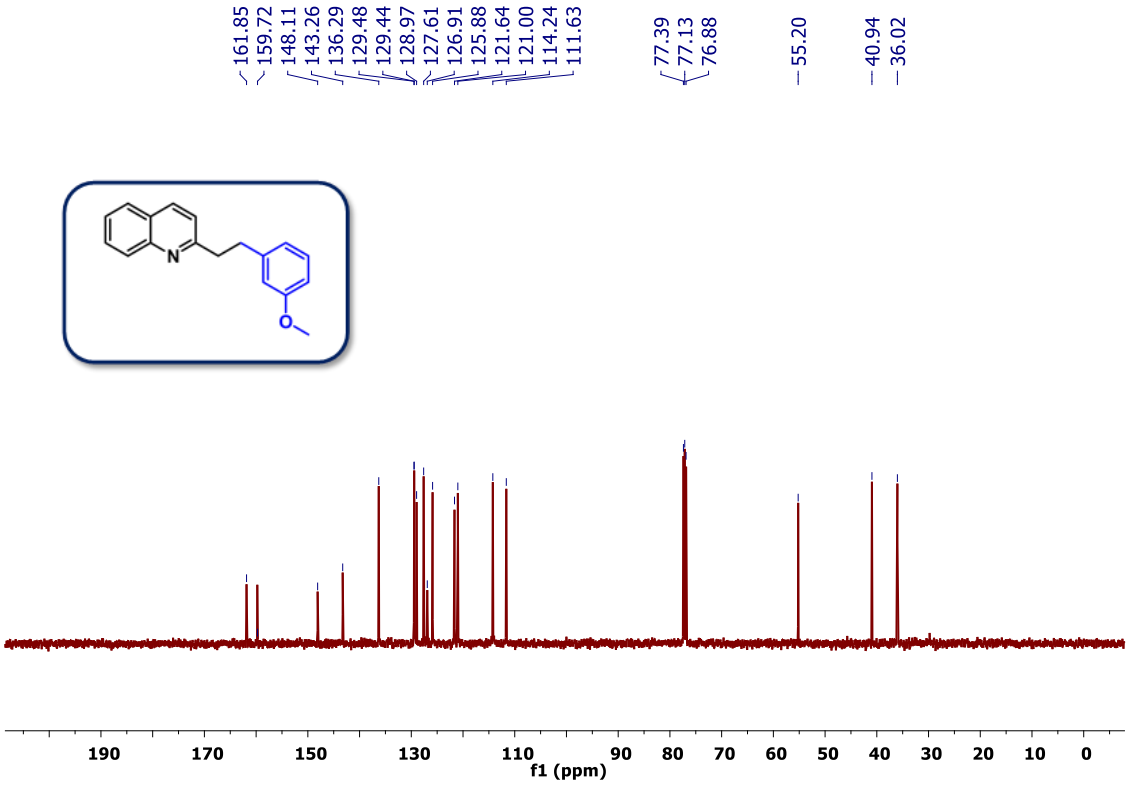
7.1983
7.1829
6.8583
6.8140
6.7594
6.7430
3.7609
3.3133
3.2810
3.1631
3.1308
0.94
1.03
0.99
1.05
0.99
1.32
1.10
1.00
0.95
0.90
3.00
2.18
2.18
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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159.72
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143.26
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129.48
129.44
128.97
127.61
126.91
125.88
121.64
121.00
114.24
111.63
77.39
77.13
76.88
55.20
40.94
36.02
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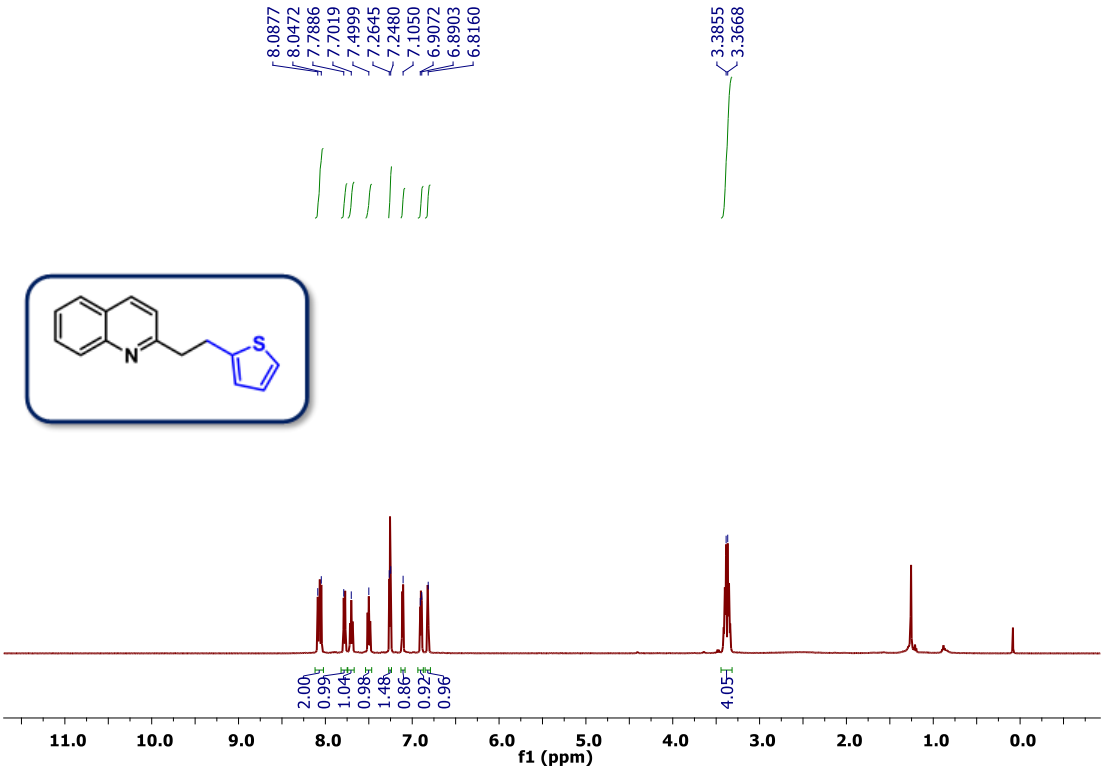
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.9072
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3.3668
N
S
2.00
0.99
1.04
0.98
1.48
0.86
0.92
0.96
4.05
11.0
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9.0
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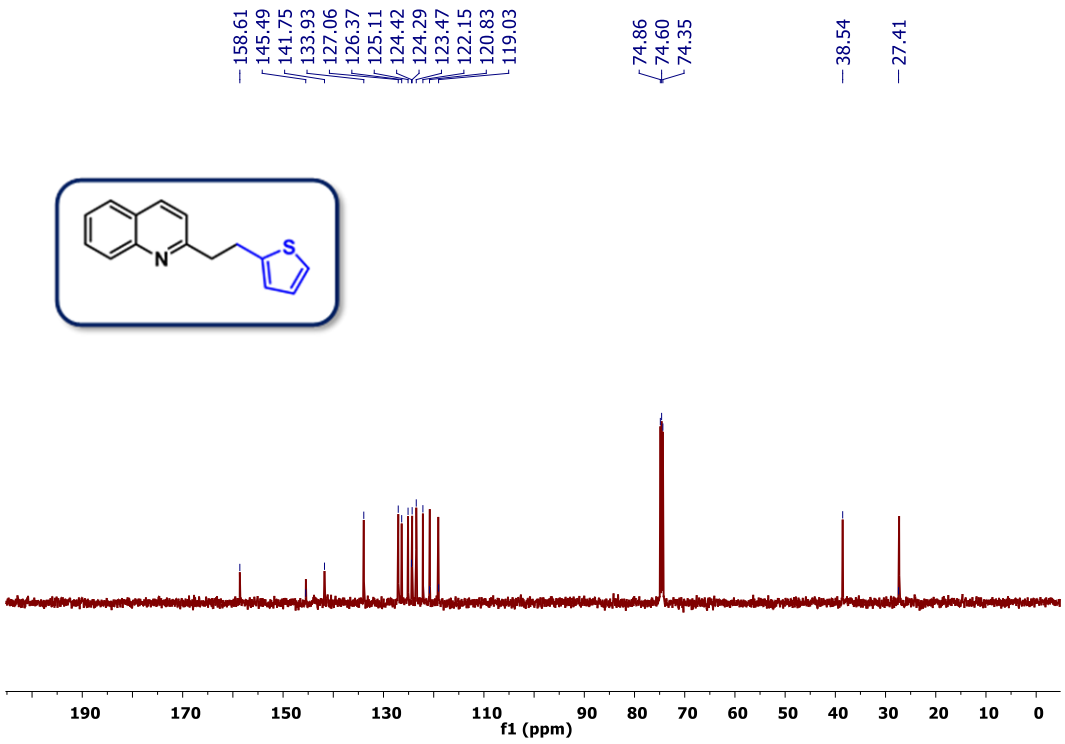
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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126.37
125.11
124.42
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123.47
122.15
120.83
119.03
74.86
74.60
74.35
38.54
27.41
N
S
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170
150
130
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90
80
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50
40
30
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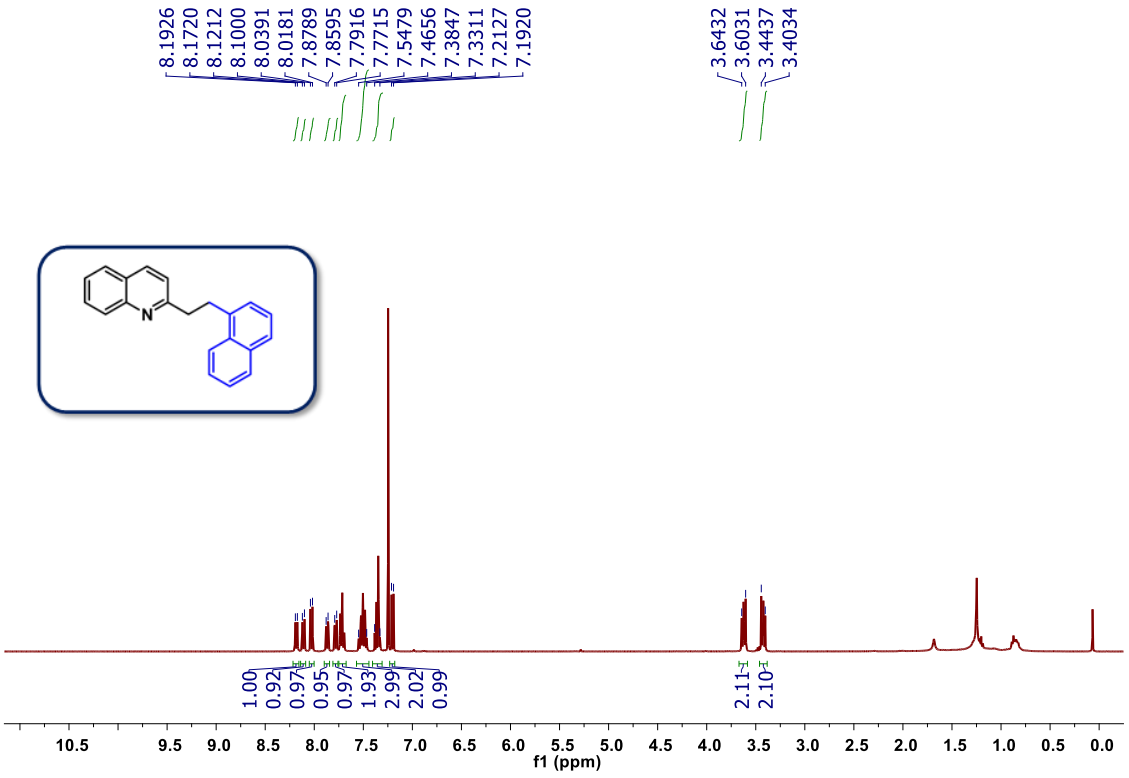
10
0
f1 (ppm)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8.0181
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7.3847
7.3311
7.2127
7.1920
3.6432
3.6031
3.4437
3.4034
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0.92
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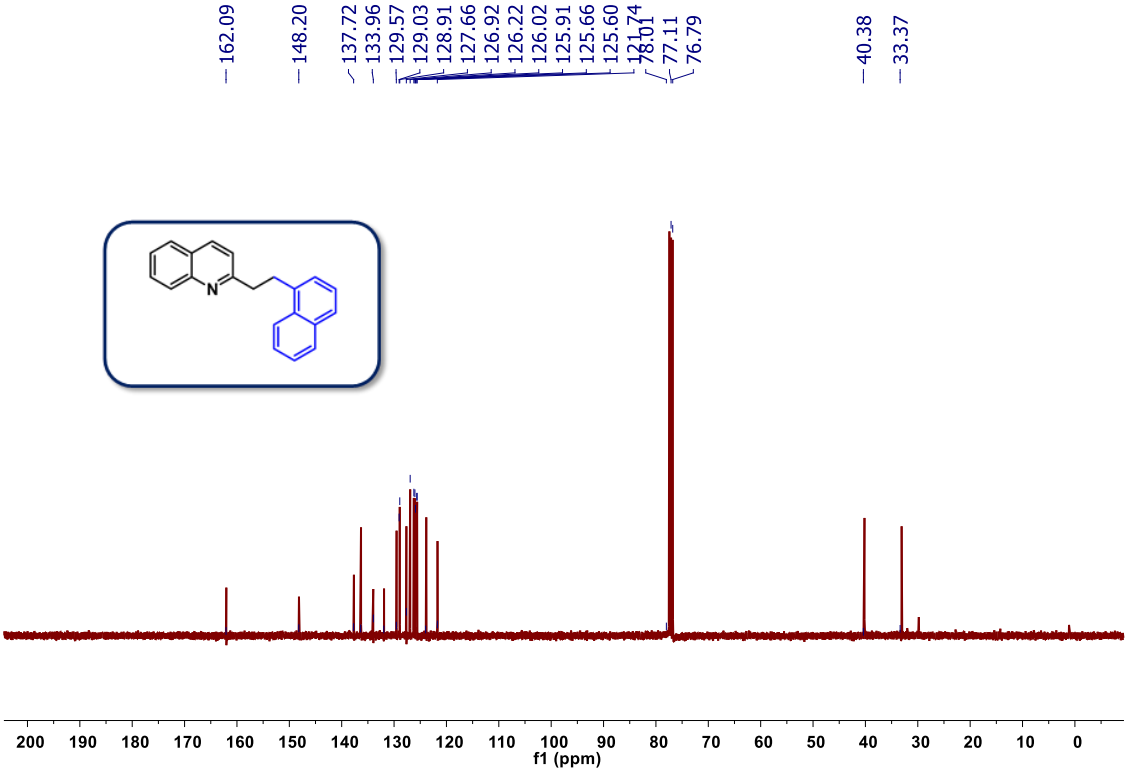
0.95
0.97
1.93
2.99
2.02
0.99
2.11
2.10
f1 (ppm)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129.03
128.91
127.66
126.92
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126.02
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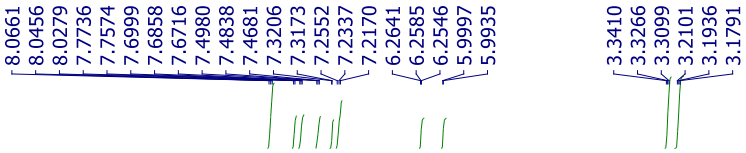
125.60
121.74
78.01
77.11
76.79
40.38
33.37
f1 (ppm)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7.7574
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7.4681
7.3206
7.3173
7.2552
7.2337
7.2170
6.2641
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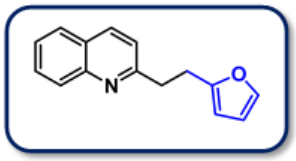
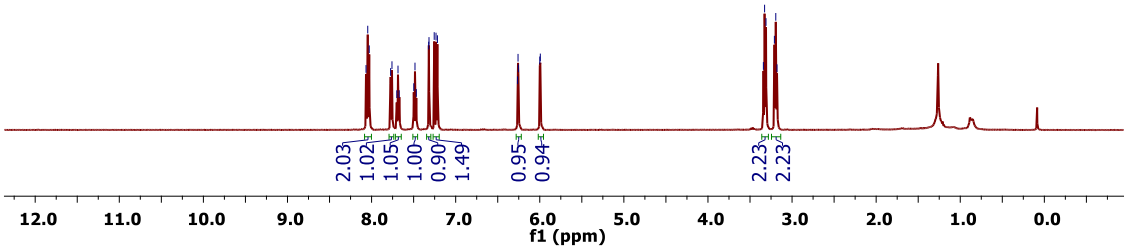
5.9997
5.9935
3.3410
3.3266
3.3099
3.2101
3.1936
3.1791

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1.49
0.95
0.94
2.23
2.23
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


161.33
155.22
148.06
141.05
136.35
129.50
128.98
127.60
126.92
125.93
121.42
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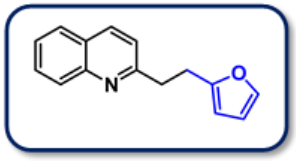
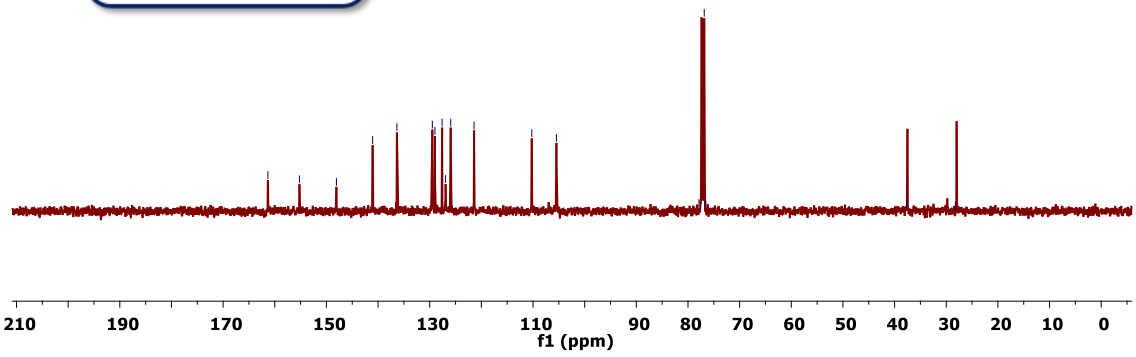
105.47
77.87
76.86
76.54
37.65
28.23

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130
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90
80
70
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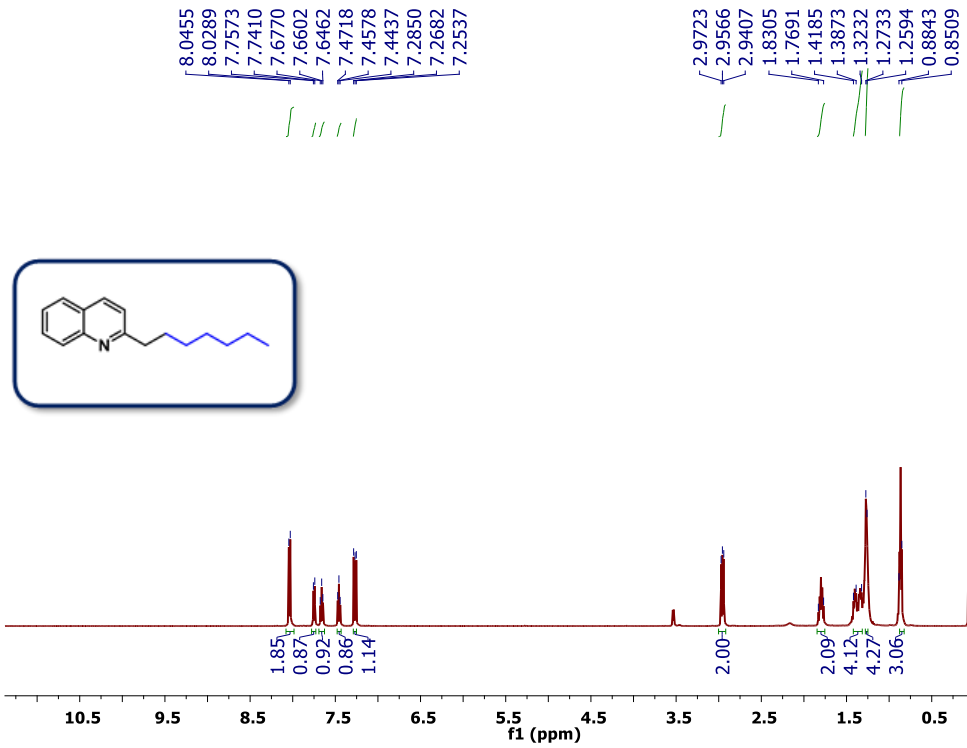
50
40
30
20
10
0
f1 (ppm)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7.2682
7.2537
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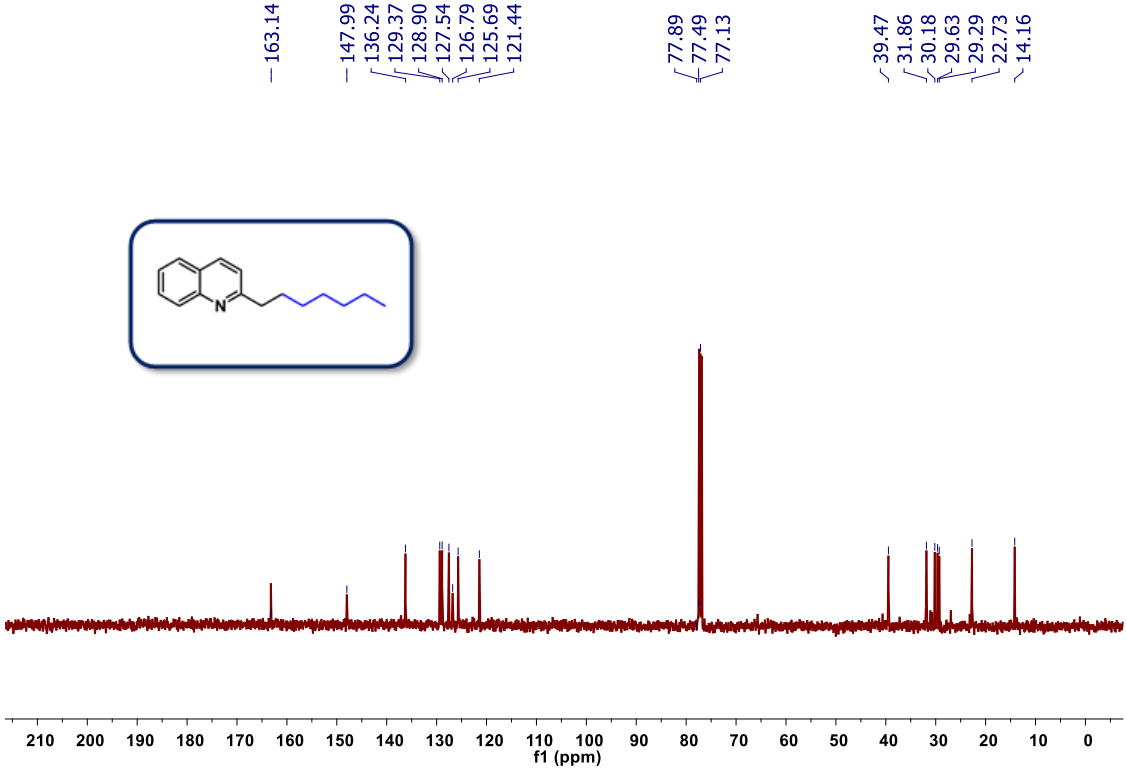
2.9566
2.9407
1.8305
1.7691
1.4185
1.3873
1.3232
1.2733
1.2594
0.8843
0.8509
1.85
0.87
0.92
0.86
1.14
2.00
2.09
4.12
4.27
3.06
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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128.90
127.54
126.79
125.69
121.44
77.89
77.49
77.13
39.47
31.86
30.18
29.63
29.29
22.73
14.16
210
200
190
180
170
160
150
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130
120
110
100
90
80
70
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50
40
30
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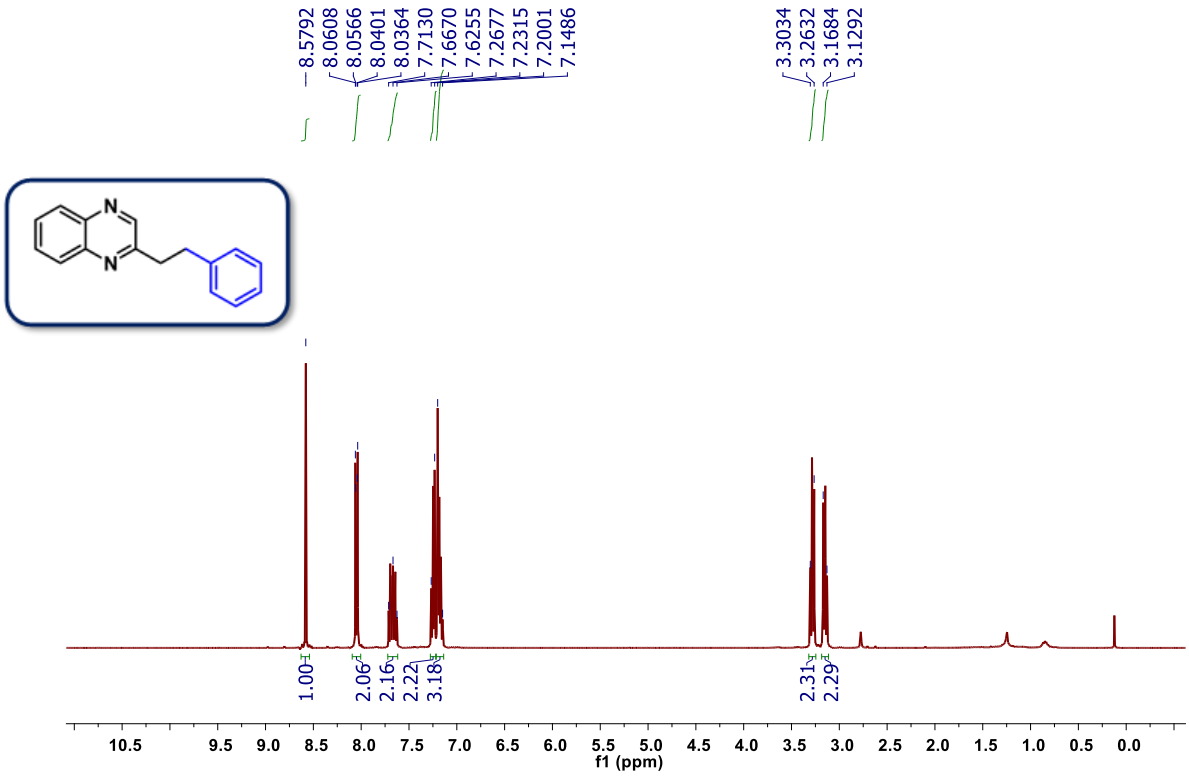
10
0
f1 (ppm)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7.6670
7.6255
7.2677
7.2315
7.2001
7.1486
3.3034
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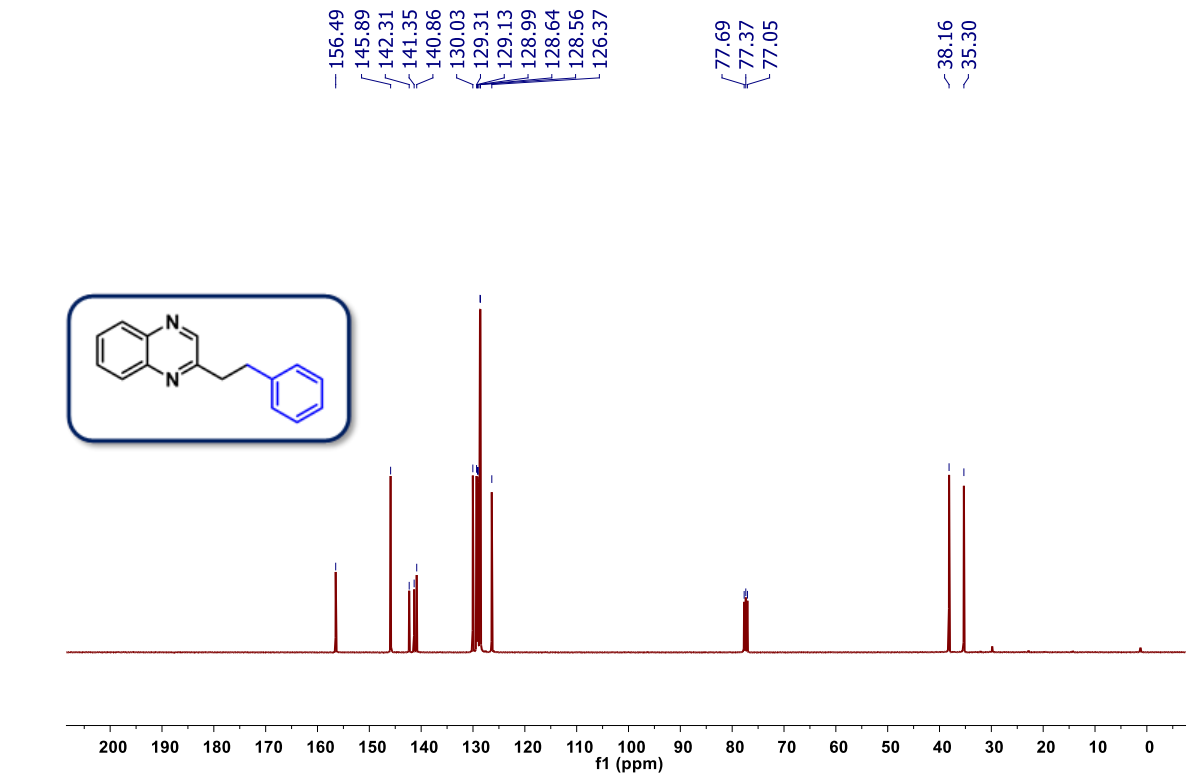
3.1292
1.00
2.06
2.16
2.22
3.18
2.31
2.29
f1 (ppm)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129.13
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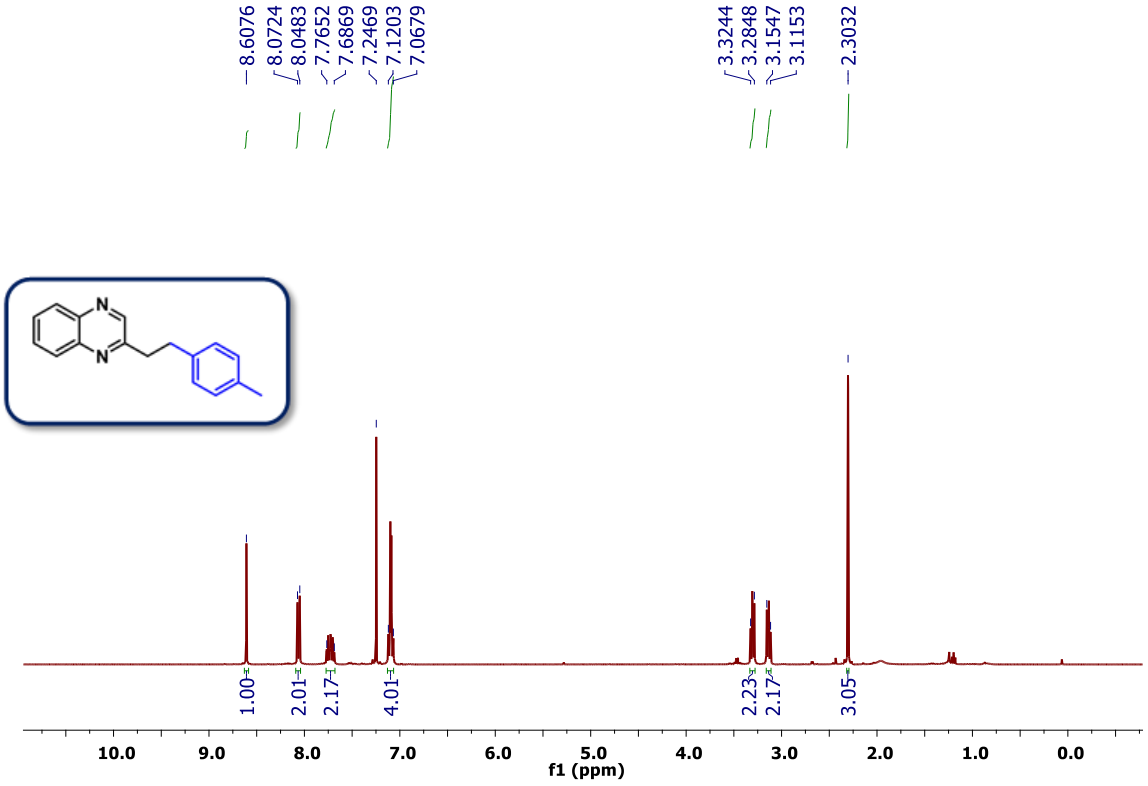
126.37
77.69
77.37
77.05
38.16
35.30
f1 (ppm)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3.1547
3.1153
2.3032
1.00
2.01
2.17
4.01
2.23
2.17
3.05
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5.0
4.0
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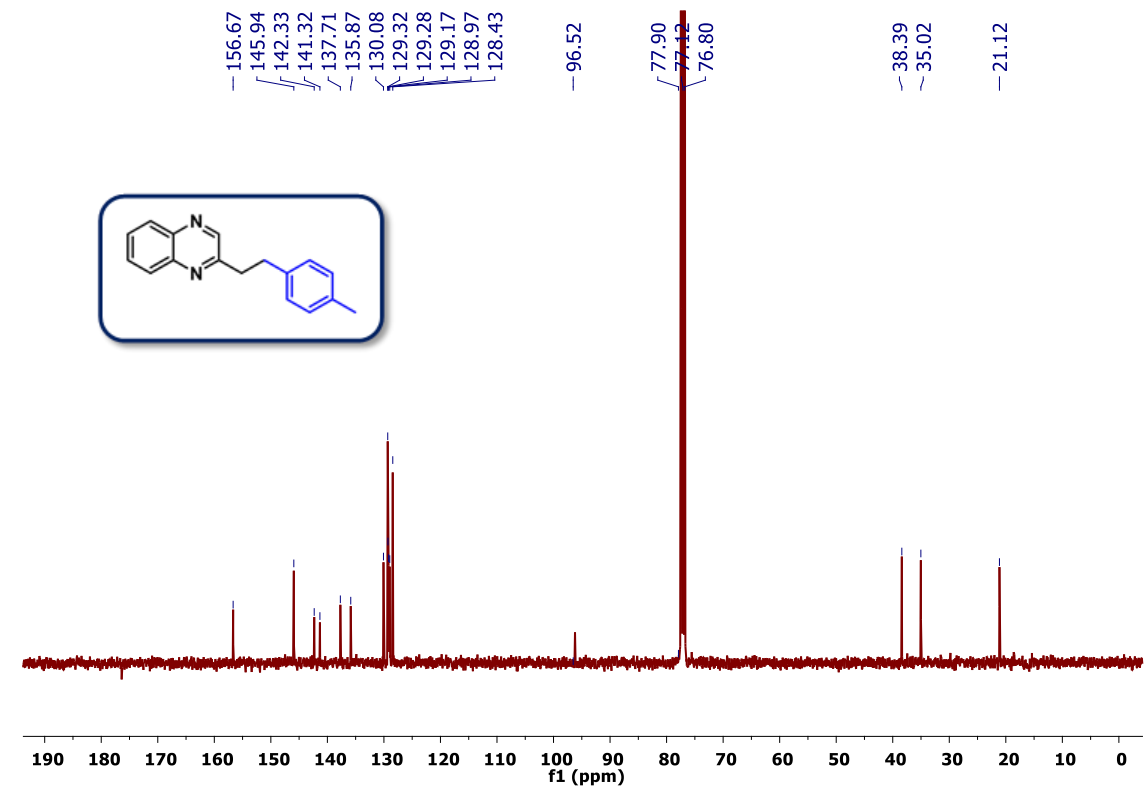
2.0
1.0
0.0
f1 (ppm)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128.97
128.43
96.52
77.90
77.12
76.80
38.39
35.02
21.12
190
180
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130
120
110
100
90
80
70
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50
40
30
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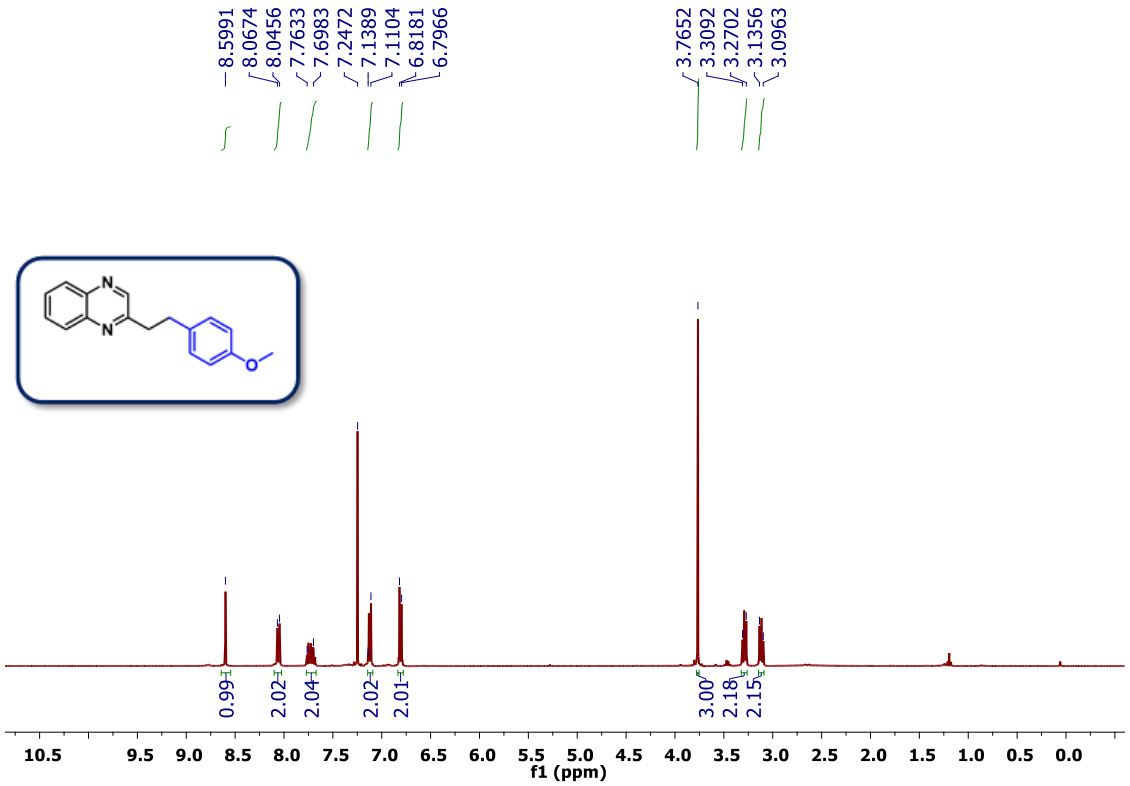
10
0
f1 (ppm)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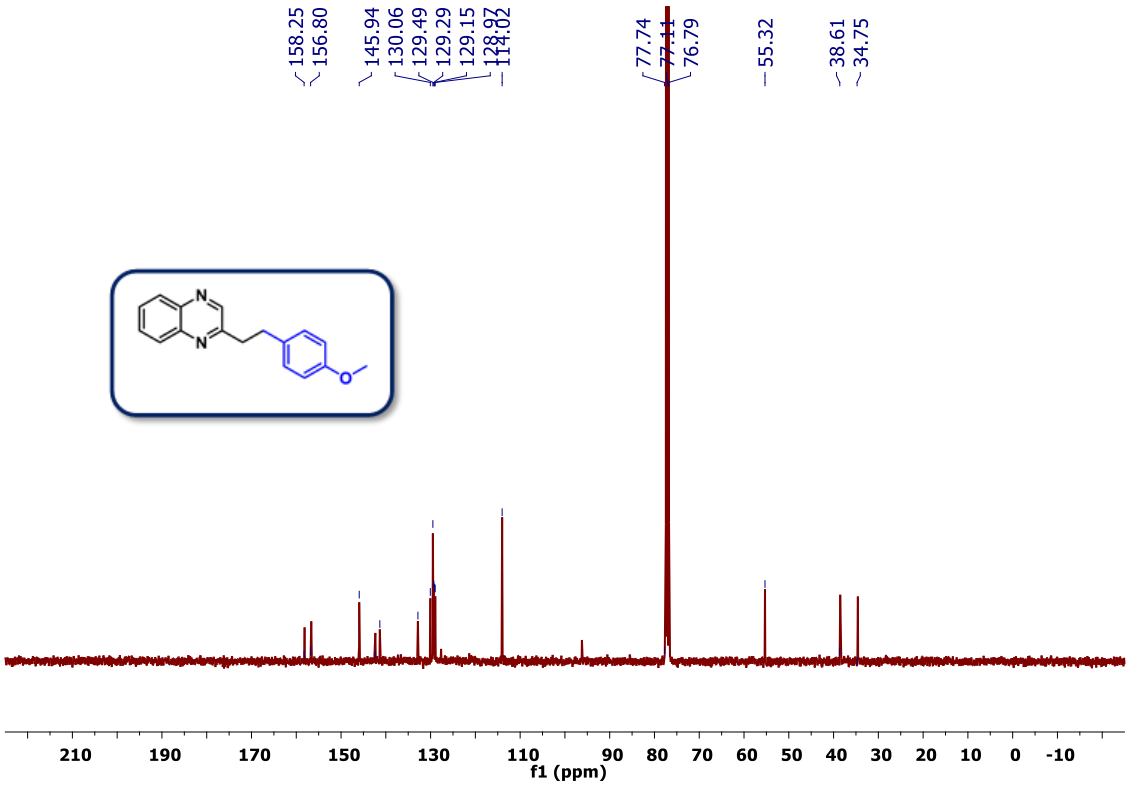
3.3092
3.2702
3.1356
3.0963
0.99
2.02
2.04
2.02
2.01
3.00
2.18
2.15
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.15
128.97
114.02
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76.79
55.32
38.61
34.75
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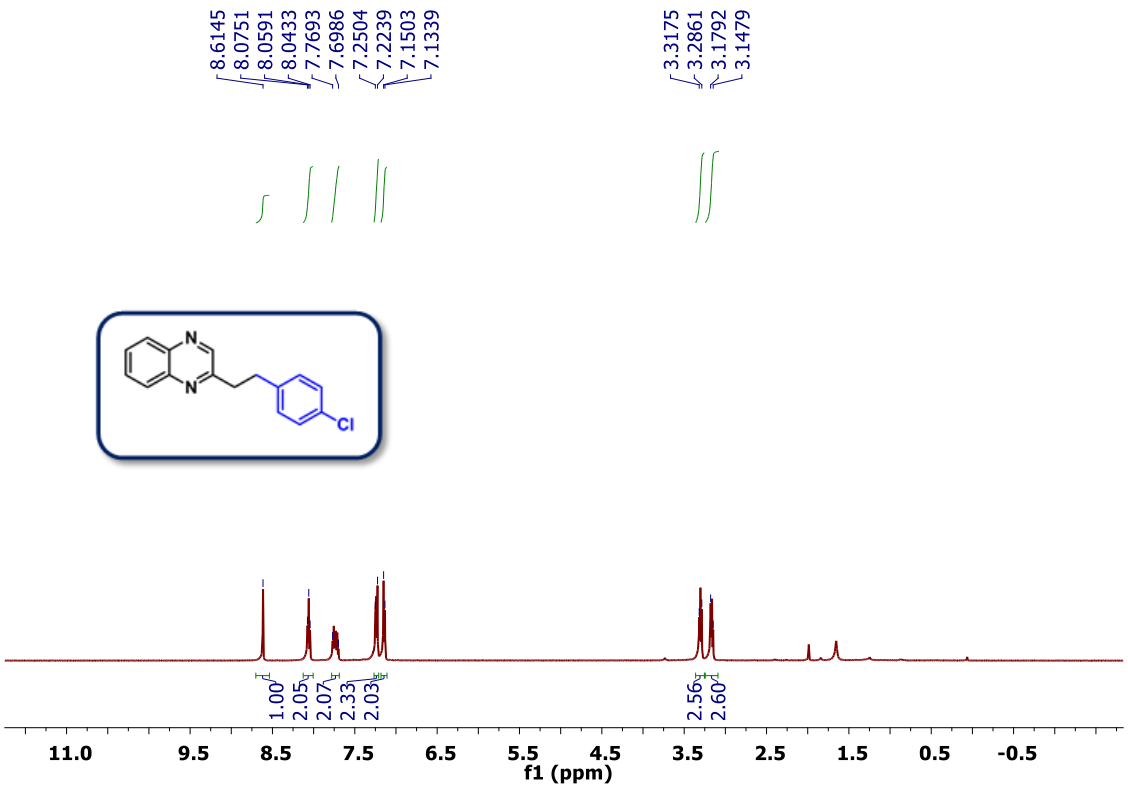
f1 (ppm)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3.2861
3.1792
3.1479
Cl
1.00
2.05
2.07
2.33
2.03
2.56
2.60
11.0
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6.5
5.5
4.5
3.5
2.5
1.5
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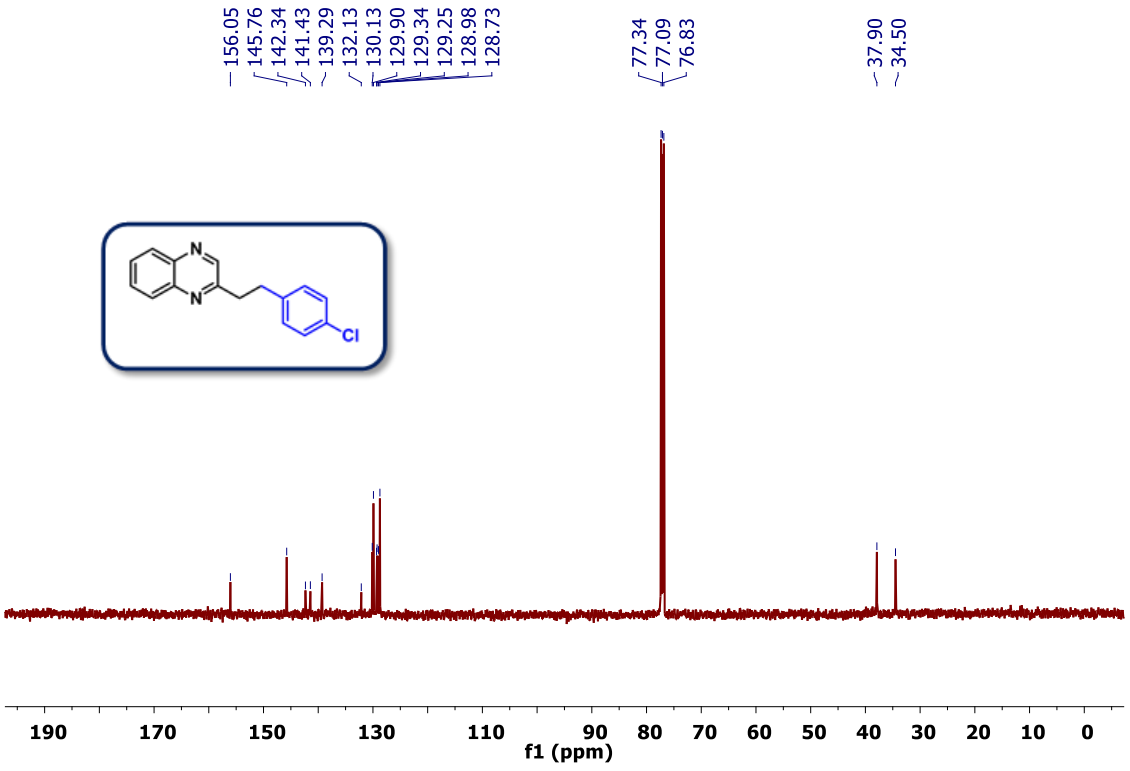
-0.5
f1 (ppm)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128.98
128.73
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77.09
76.83
37.90
34.50
Cl
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170
150
130
110
90
80
70
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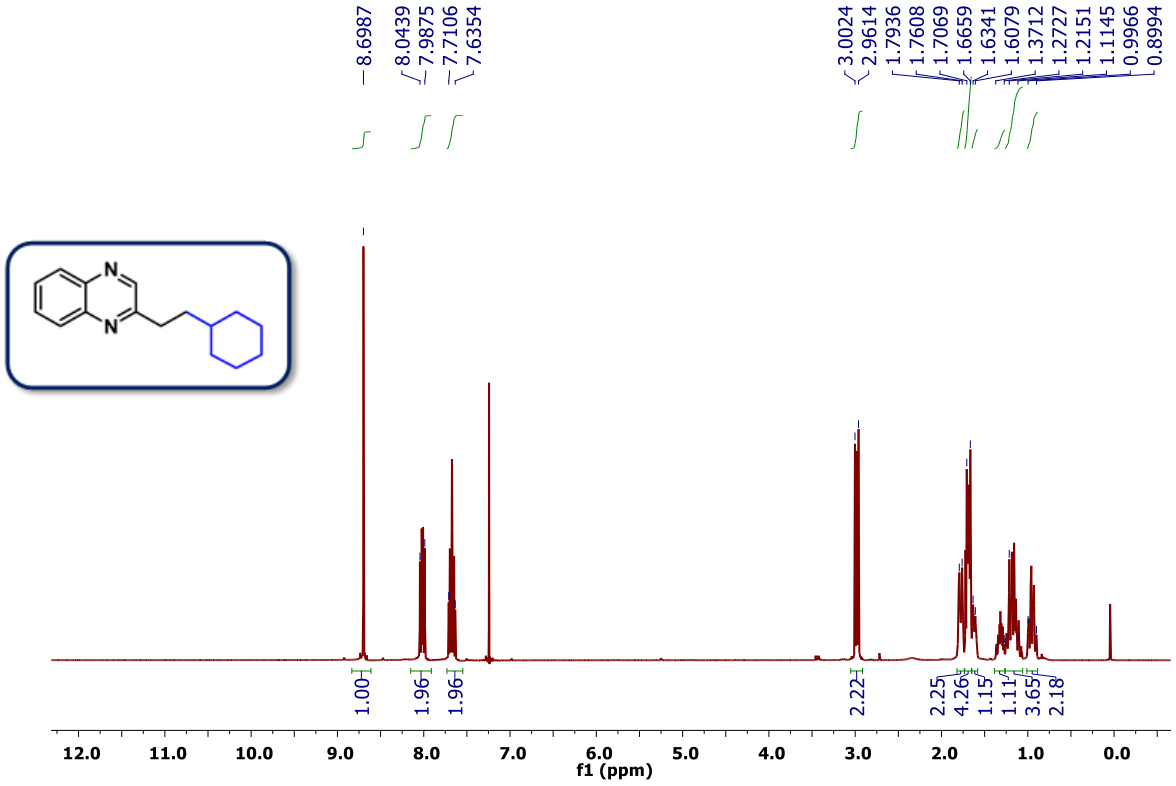
50
40
30
20
10
0
f1 (ppm)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1.6341
1.6079
1.3712
1.2727
1.2151
1.1145
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0.8994
1.00
1.96
1.96
2.22
2.25
4.26
1.15
1.11
3.65
2.18
12.0
11.0
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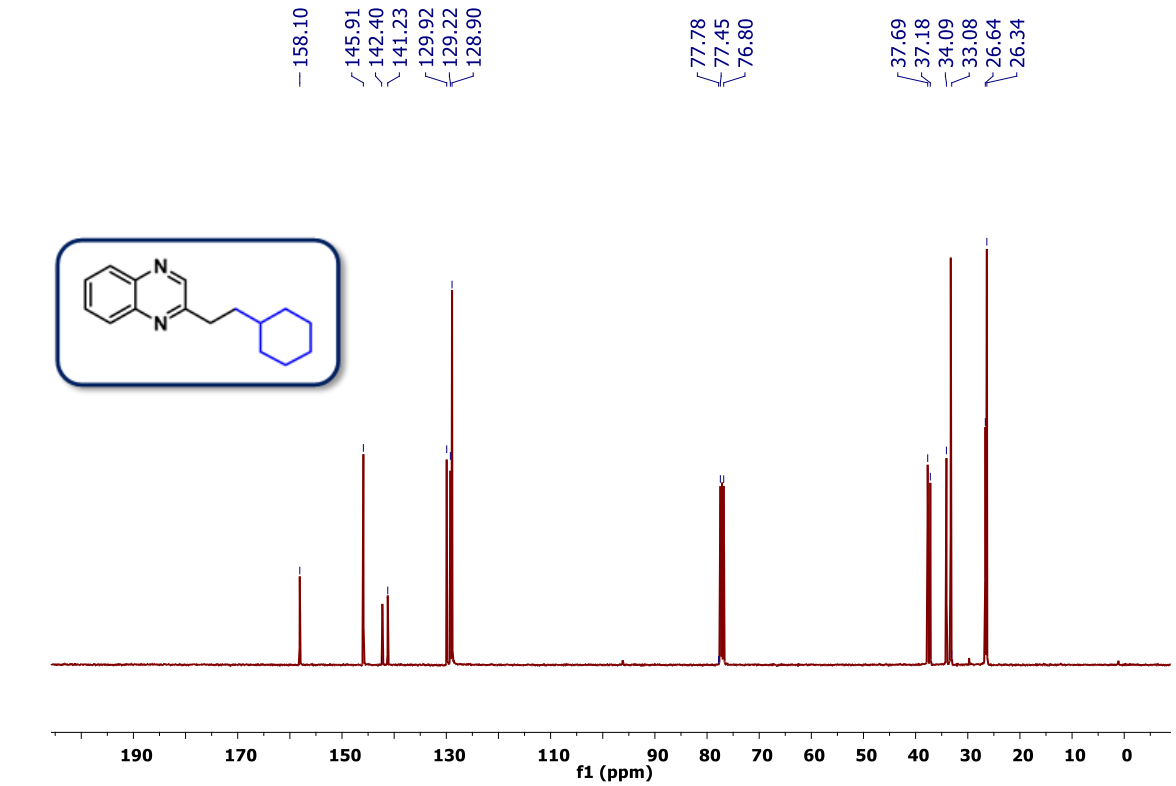
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141.23
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129.22
128.90
77.78
77.45
76.80
37.69
37.18
34.09
33.08
26.64
26.34
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130
110
90
80
70
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50
40
30
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10
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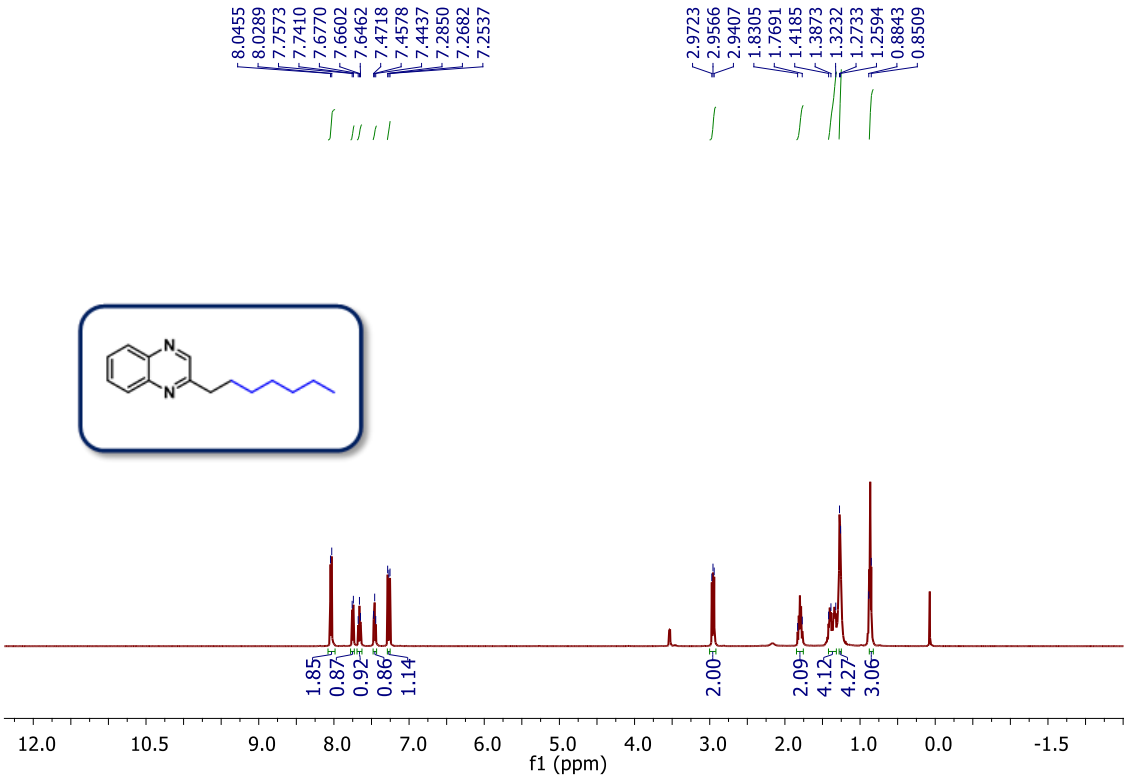
f1 (ppm)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7.6602
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7.4578
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7.2682
7.2537
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2.9566
2.9407
1.8305
1.7691
1.4185
1.3873
1.3232
1.2733
1.2594
0.8843
0.8509
1.85
0.87
0.92
0.86
1.14
2.00
2.09
4.12
4.27
3.06
12.0
10.5
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4.0
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2.0
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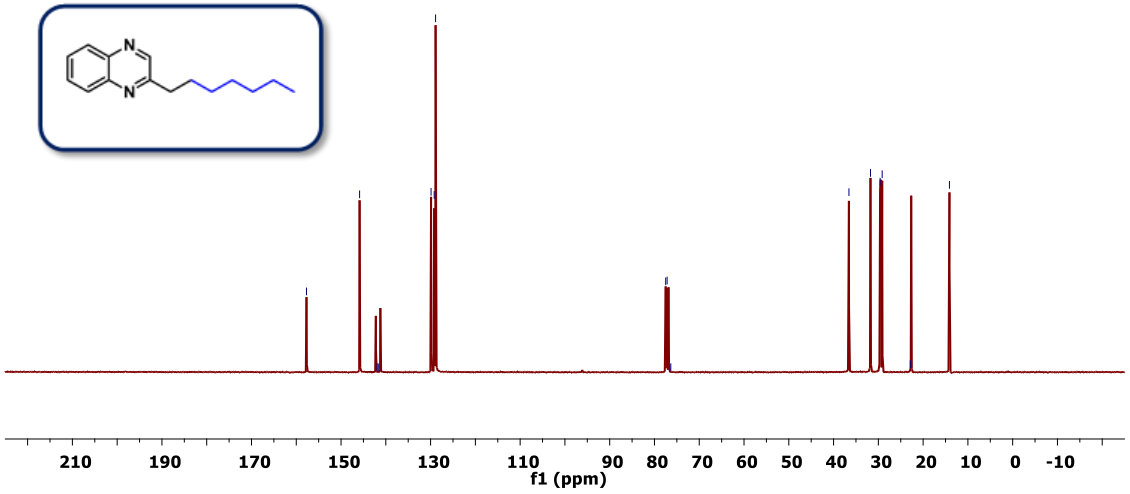
f1 (ppm)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77.49
77.18
76.35
36.57
31.76
29.61
29.14
22.86
14.12
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150
130
110
90
80
70
60
50
40
30
20
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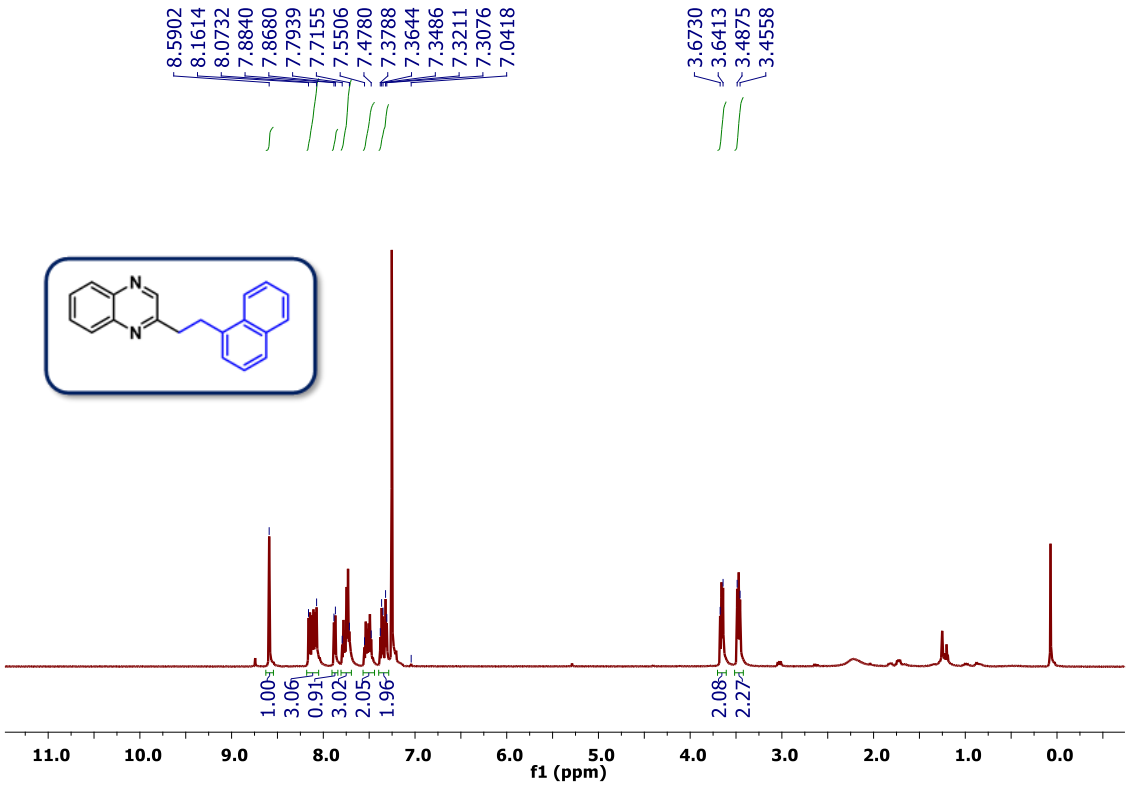
-10
f1 (ppm)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7.7155
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7.4780
7.3788
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7.3486
7.3211
7.3076
7.0418
3.6730
3.6413
3.4875
3.4558
1.00
3.06
0.91
3.02
2.05
1.96
2.08
2.27
11.0
10.0
9.0
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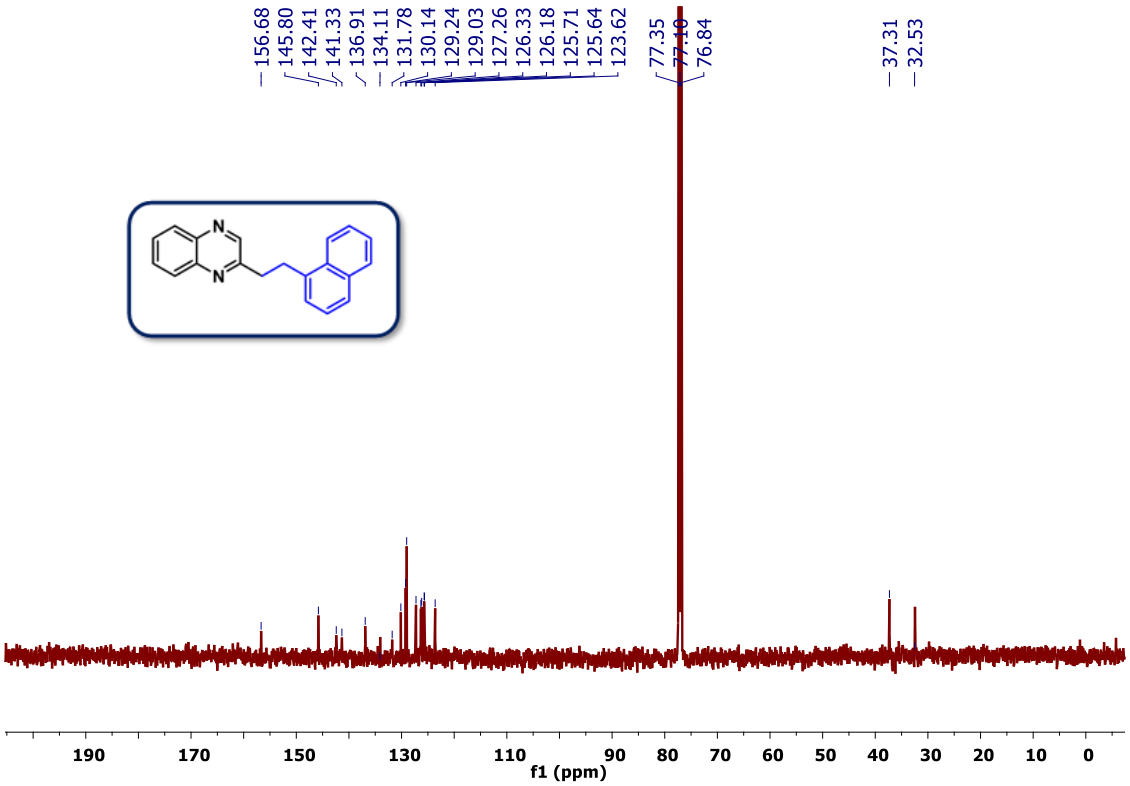
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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134.11
131.78
130.14
129.24
129.03
127.26
126.33
126.18
125.71
125.64
123.62
77.35
77.10
76.84
37.31
32.53
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170
150
130
110
90
80
70
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50
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30
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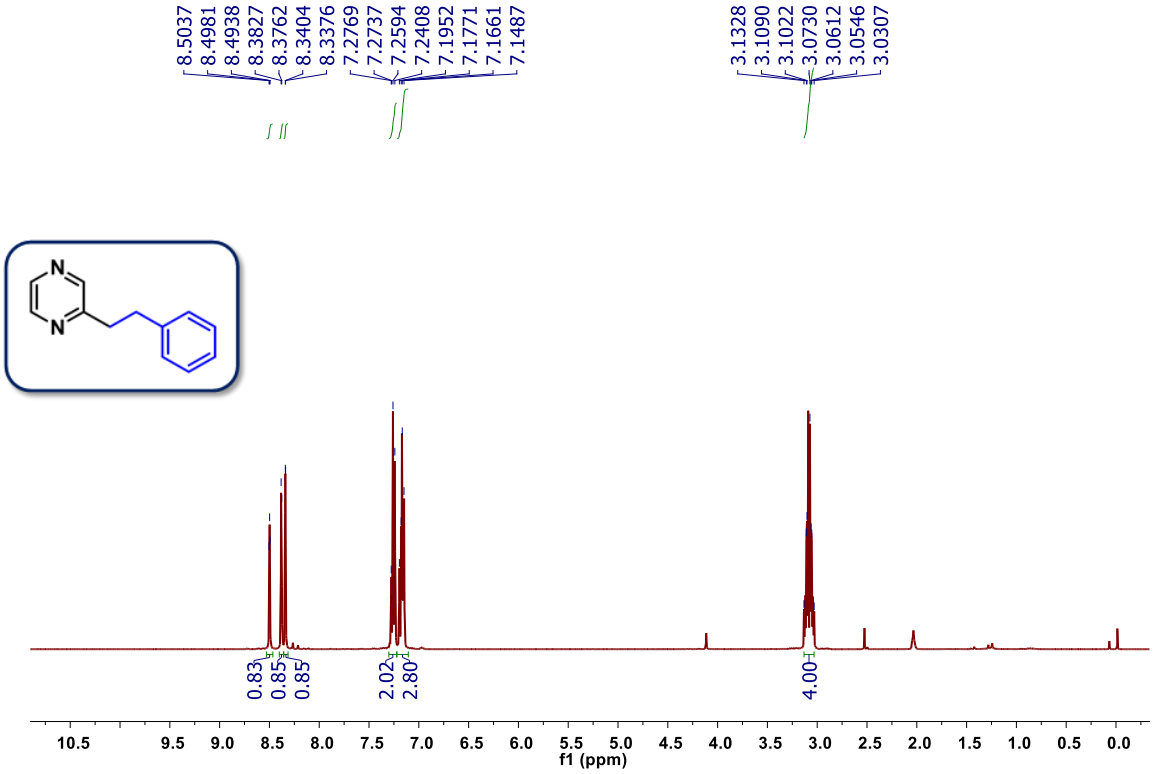
f1 (ppm)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8.3376
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7.2408
7.1952
7.1771
7.1661
7.1487
3.1328
3.1090
3.1022
3.0730
3.0612
3.0546
3.0307
0.83
0.85
0.85
2.02
2.80
4.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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2.5
2.0
1.5
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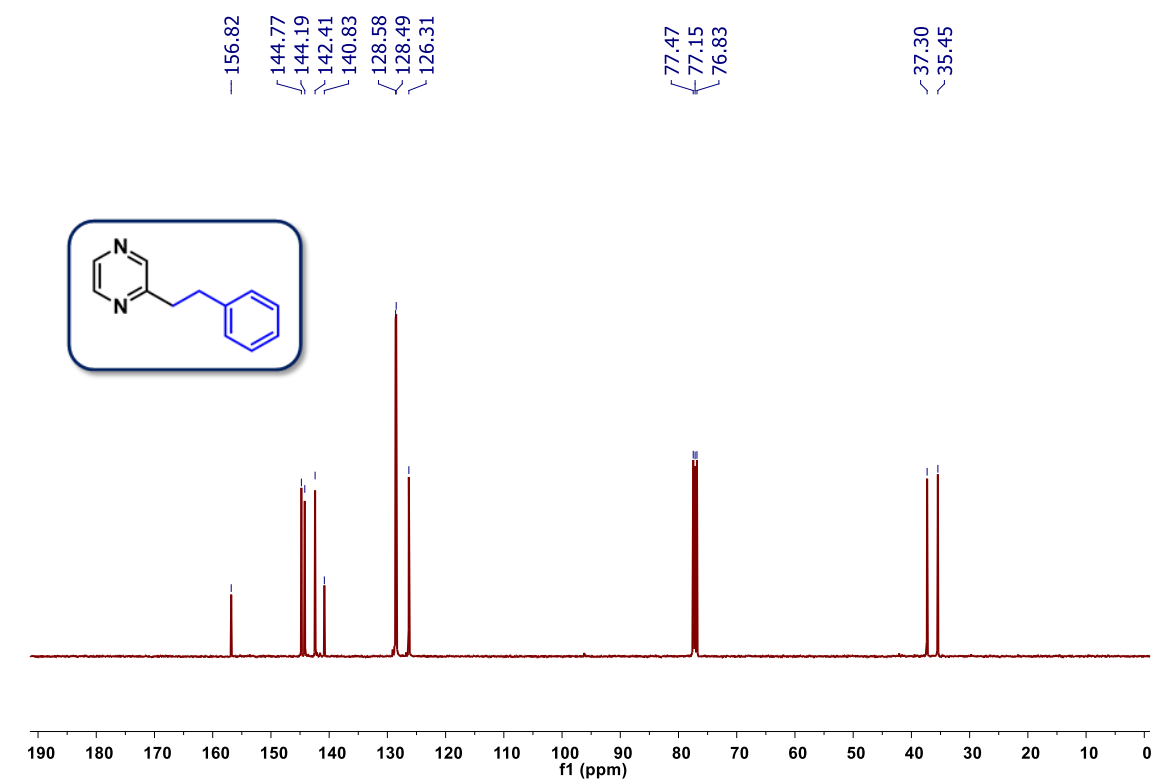
0.0
f1 (ppm)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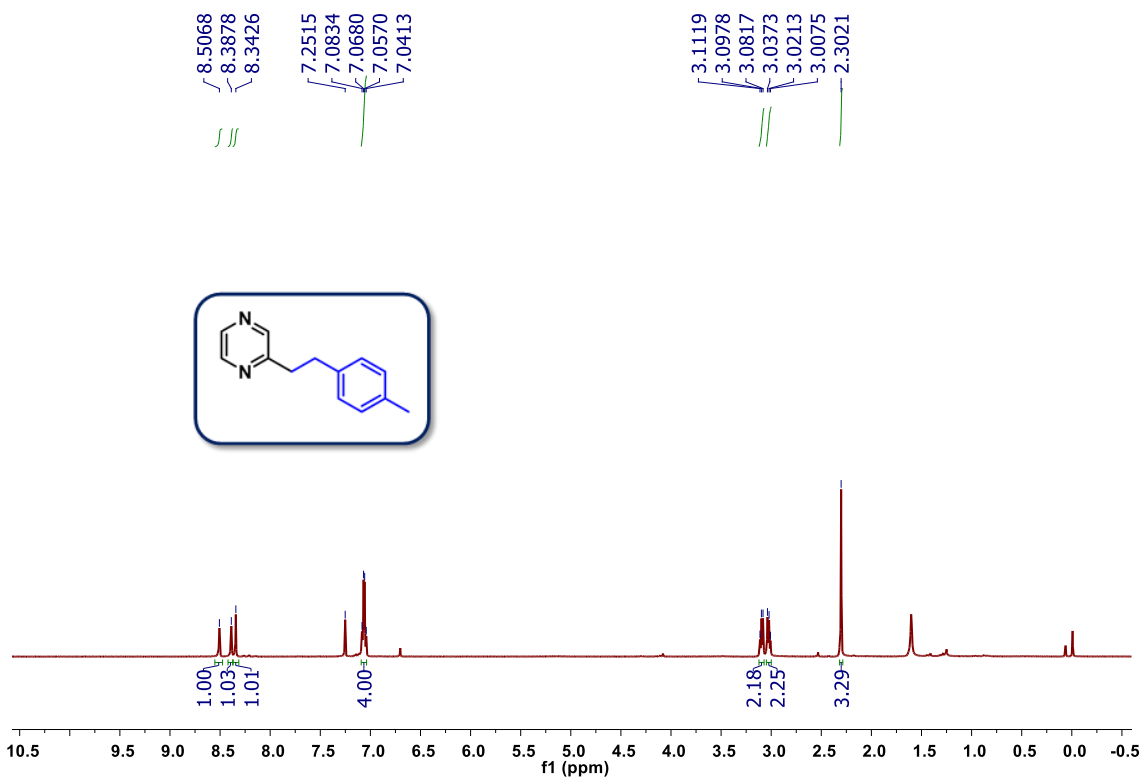
144.19
142.41
140.83
128.58
128.49
126.31
77.47
77.15
76.83
37.30
35.45
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.3878
8.3426
7.2515
7.0834
7.0680
7.0570
7.0413
3.1119
3.0978
3.0817
3.0373
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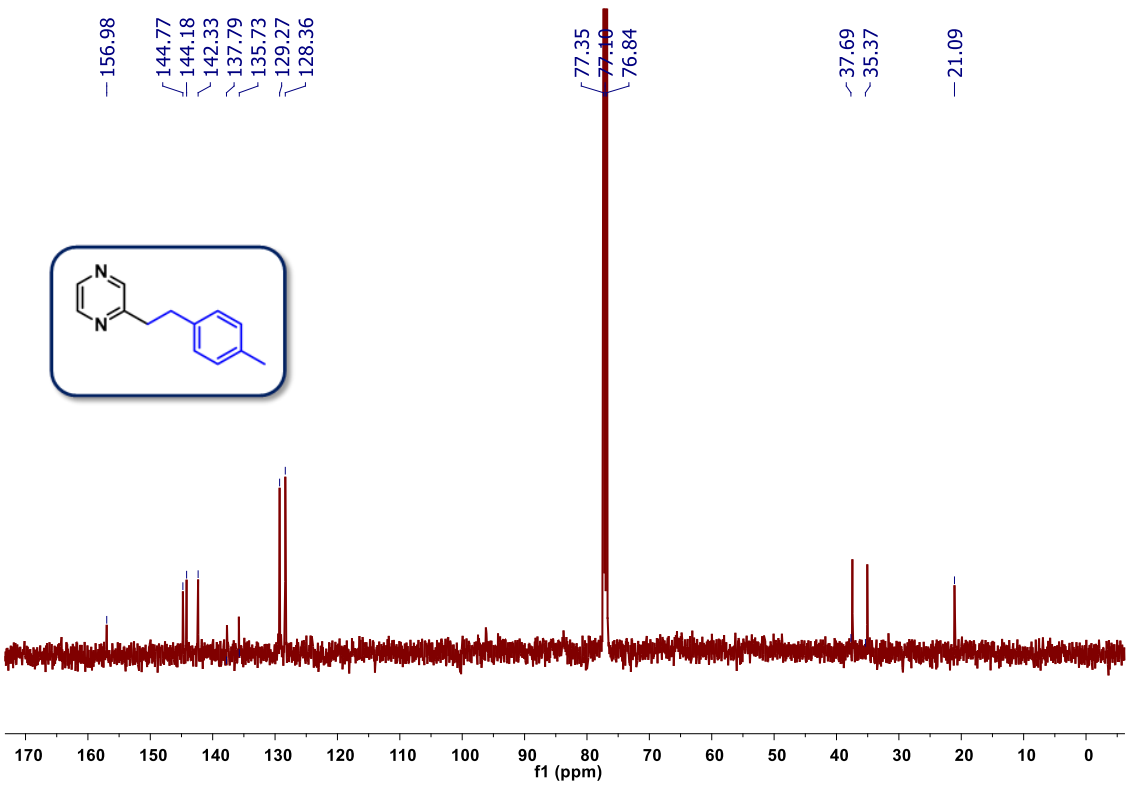
2.3021
1.00
1.03
1.01
4.00
2.18
2.25
3.29
f1 (ppm)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128.36
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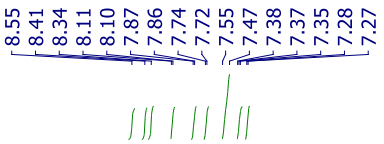
77.10
76.84
37.69
35.37
21.09
f1 (ppm)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8.11
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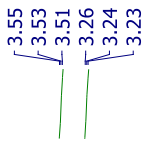
7.74
7.72
7.55
7.47
7.38
7.37
7.35
7.28
7.27


3.55
3.53
3.51
3.26
3.24
3.23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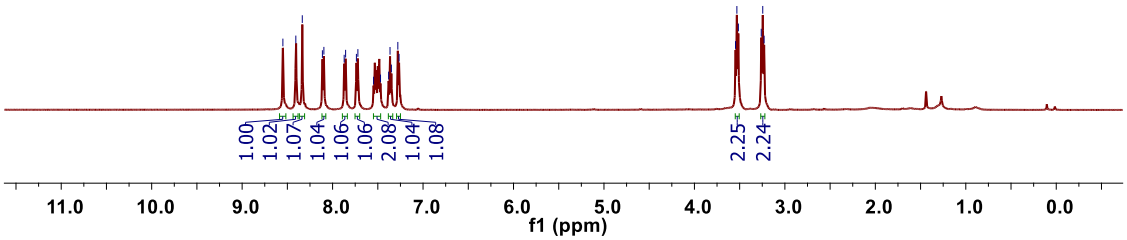
N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1.02
1.07
1.04
1.05
1.05
2.08
1.04
1.08
2.25
2.24
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


157.23
144.74
144.26
142.48
137.15
136.95
134.23
131.79
129.01
127.20
126.24
126.15
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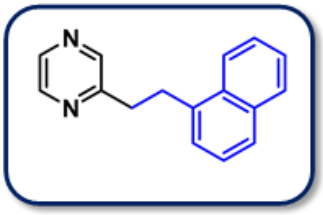
125.61
123.60
77.42
77.17
76.91
36.53
32.79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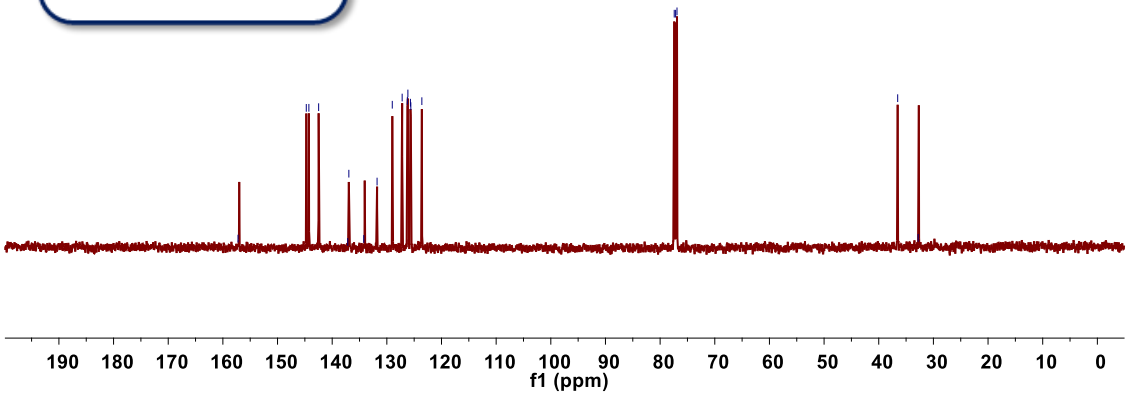
190
180
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100
90
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70
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50
40
30
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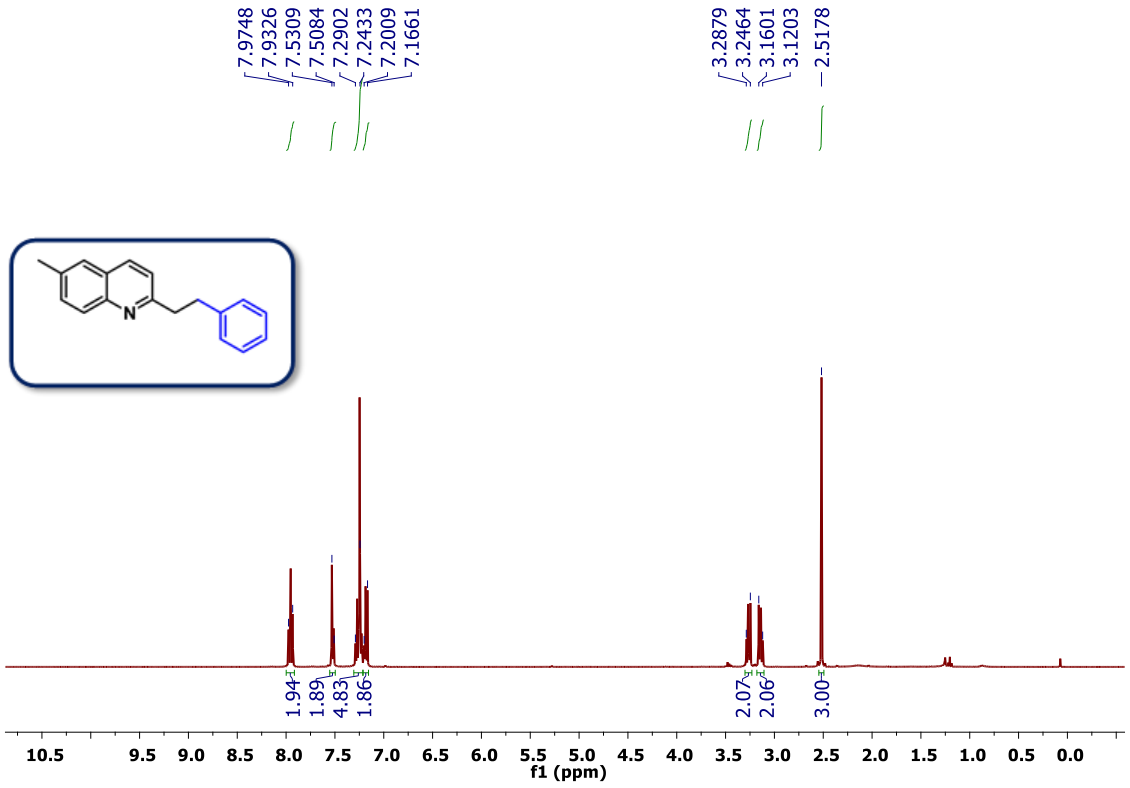
10
0
f1 (ppm)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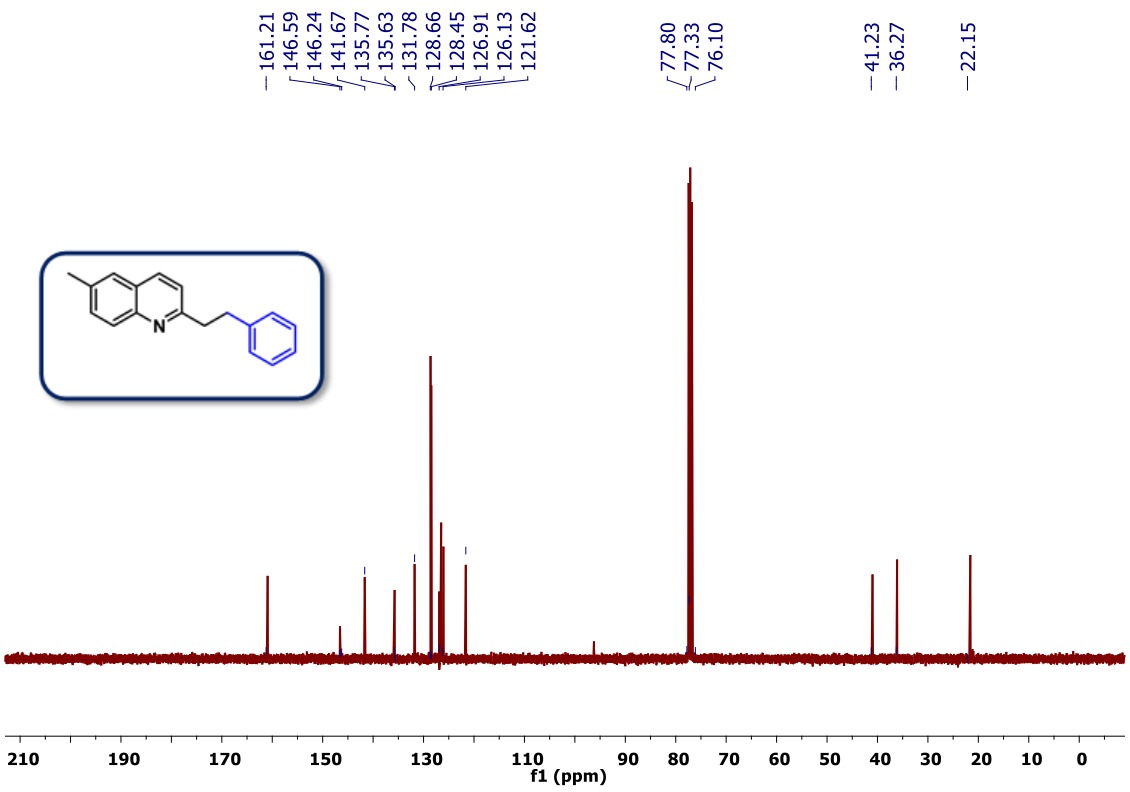
1.89
4.83
1.86
2.07
2.08
3.00
f1 (ppm)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135.63
131.78
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126.13
121.62
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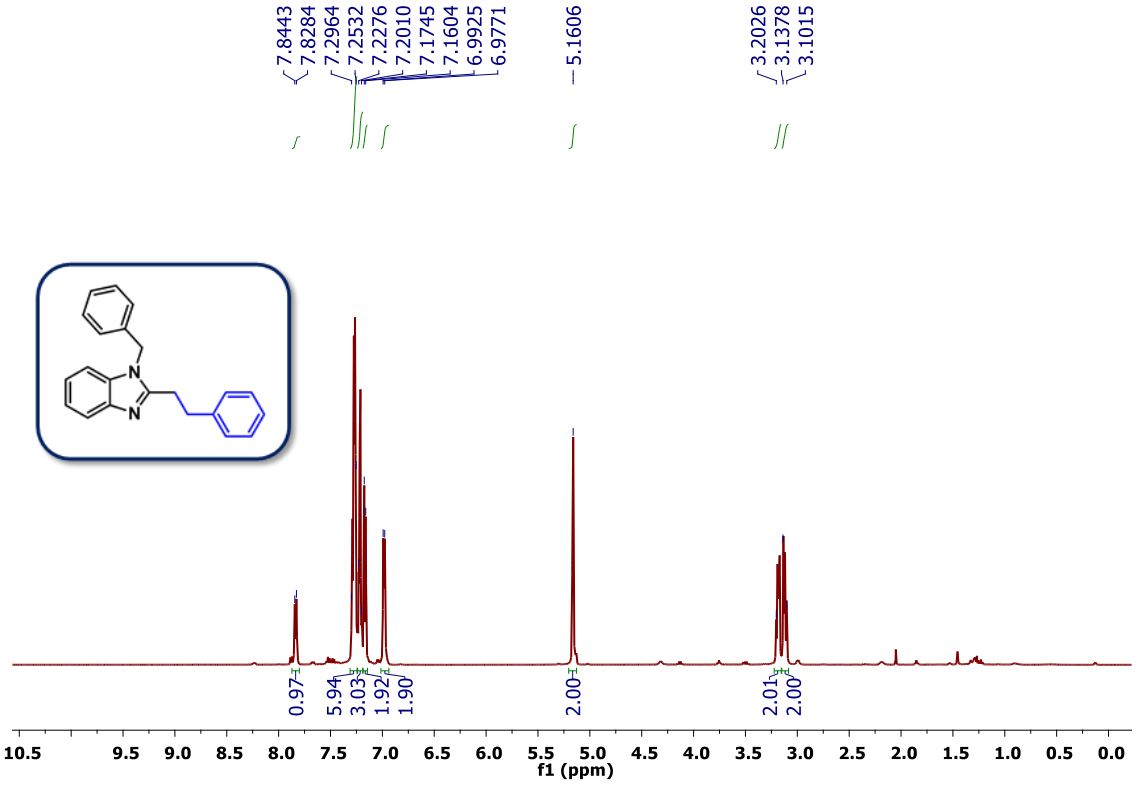
76.10
41.23
36.27
22.15
f1 (ppm)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7.2010
7.1745
7.1604
6.9925
6.9771
5.1606
3.2026
3.1378
3.1015
0.97
5.94
3.03
1.92
1.90
2.00
2.01
2.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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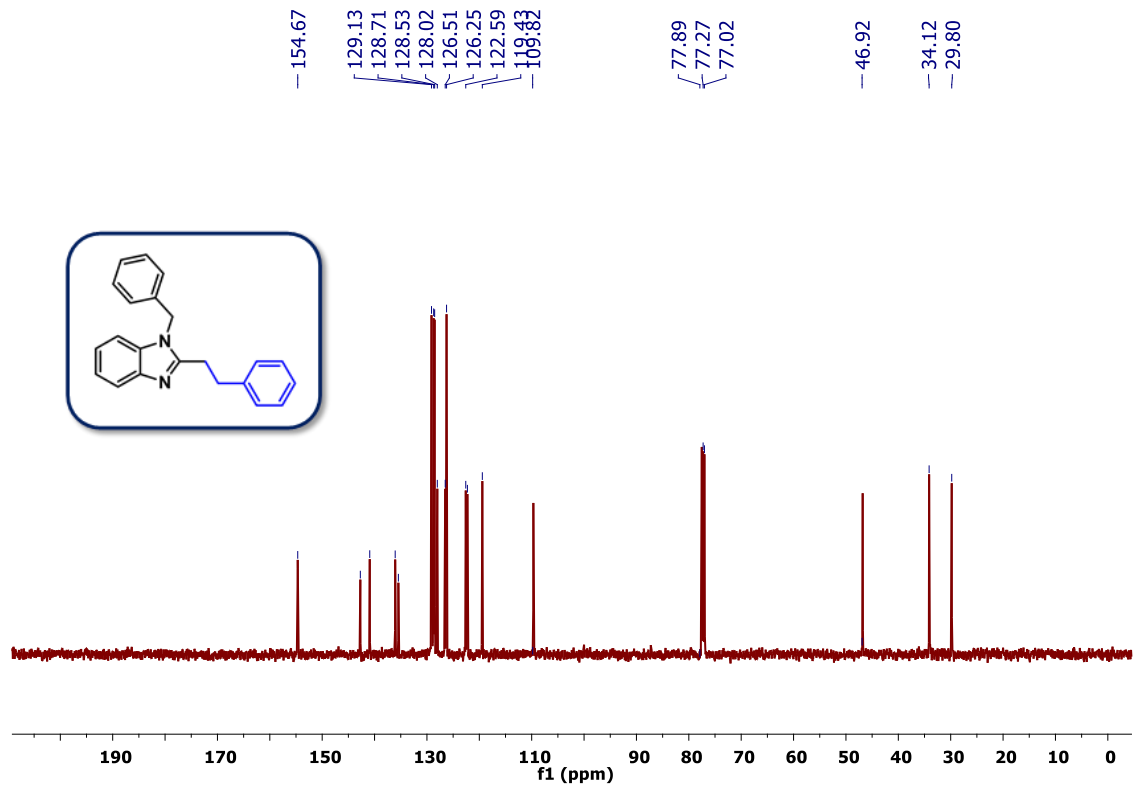
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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126.51
126.25
122.59
119.43
109.82
77.89
77.27
77.02
46.92
34.12
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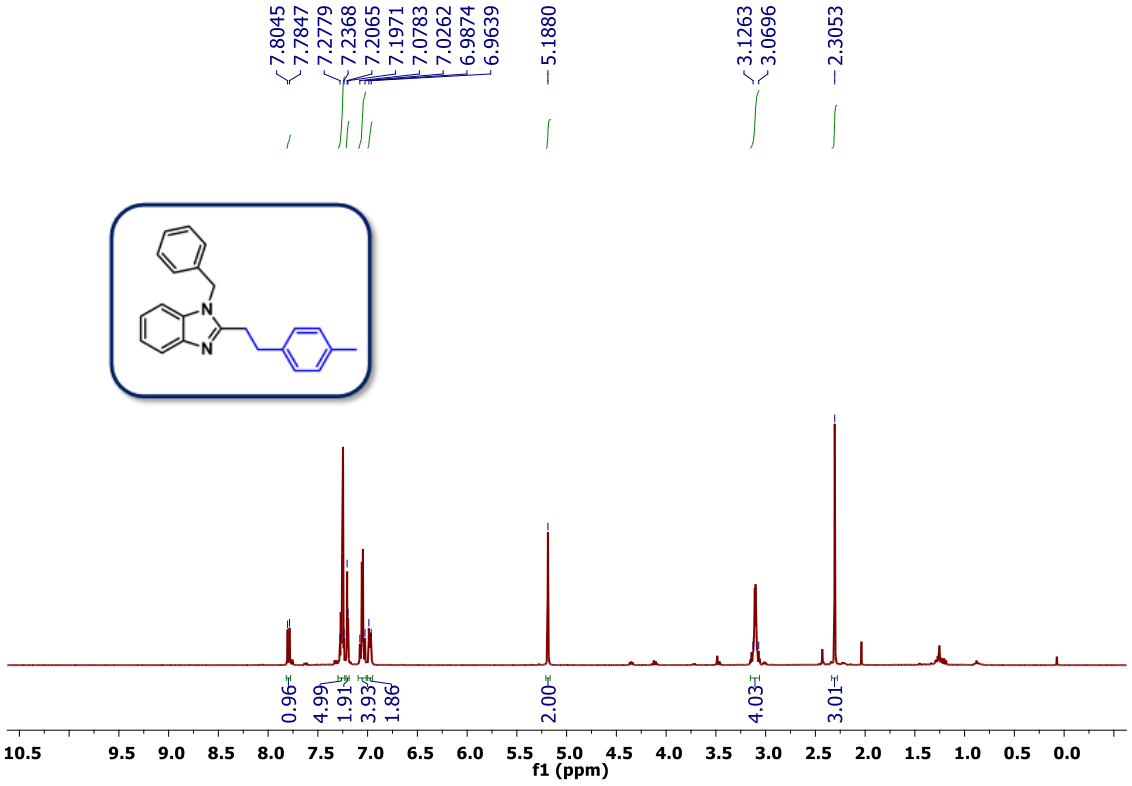
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.0262
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6.9639
5.1880
3.1263
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1.91
3.93
1.86
2.00
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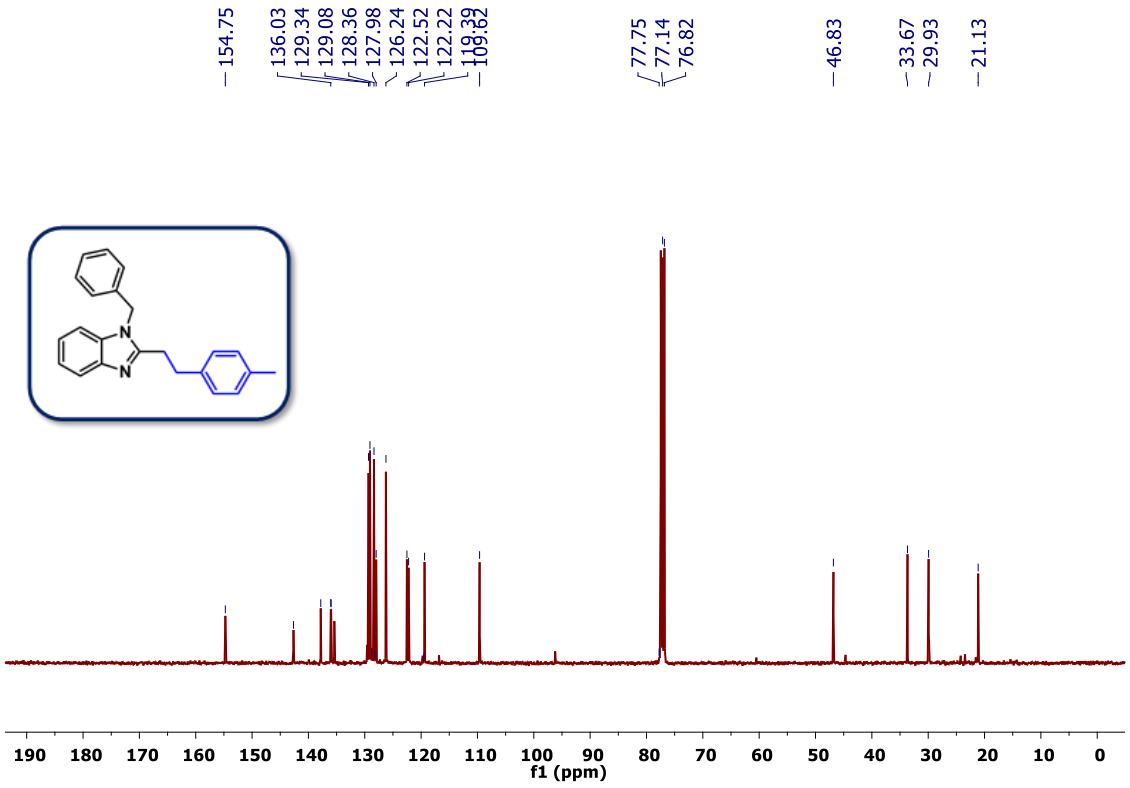
3.01
f1 (ppm)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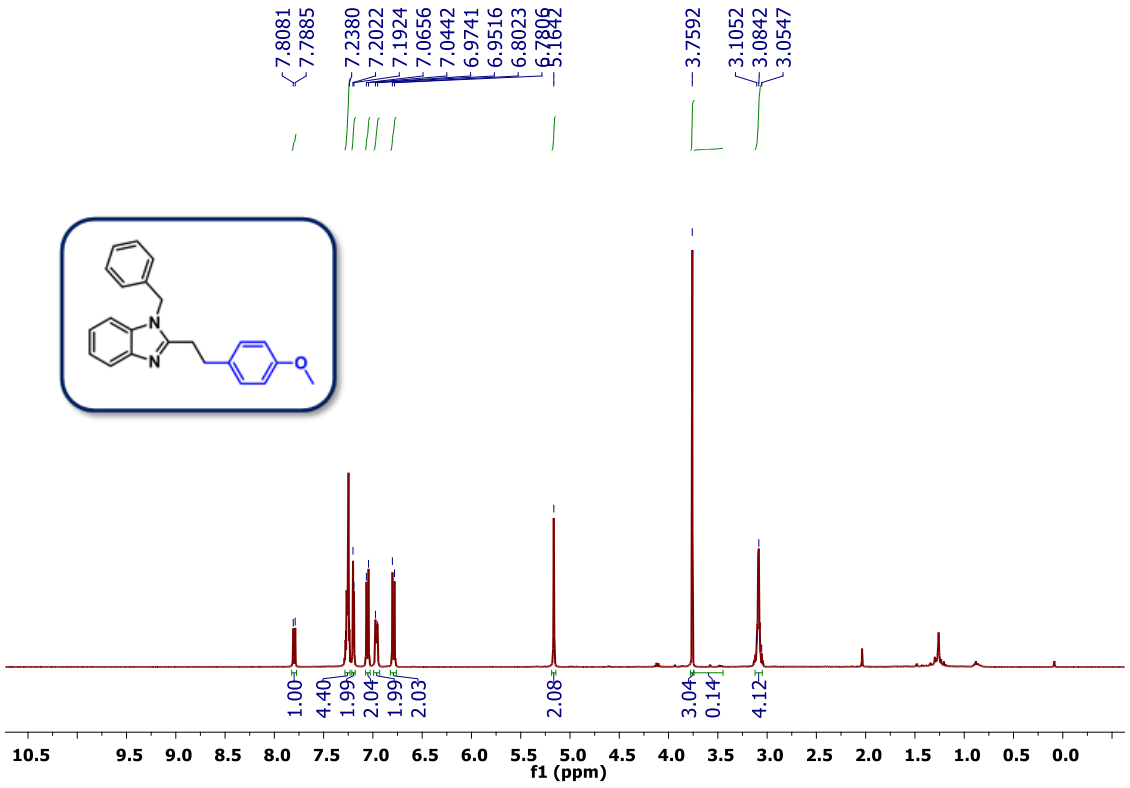
76.82
46.83
33.67
29.93
21.13
f1 (ppm)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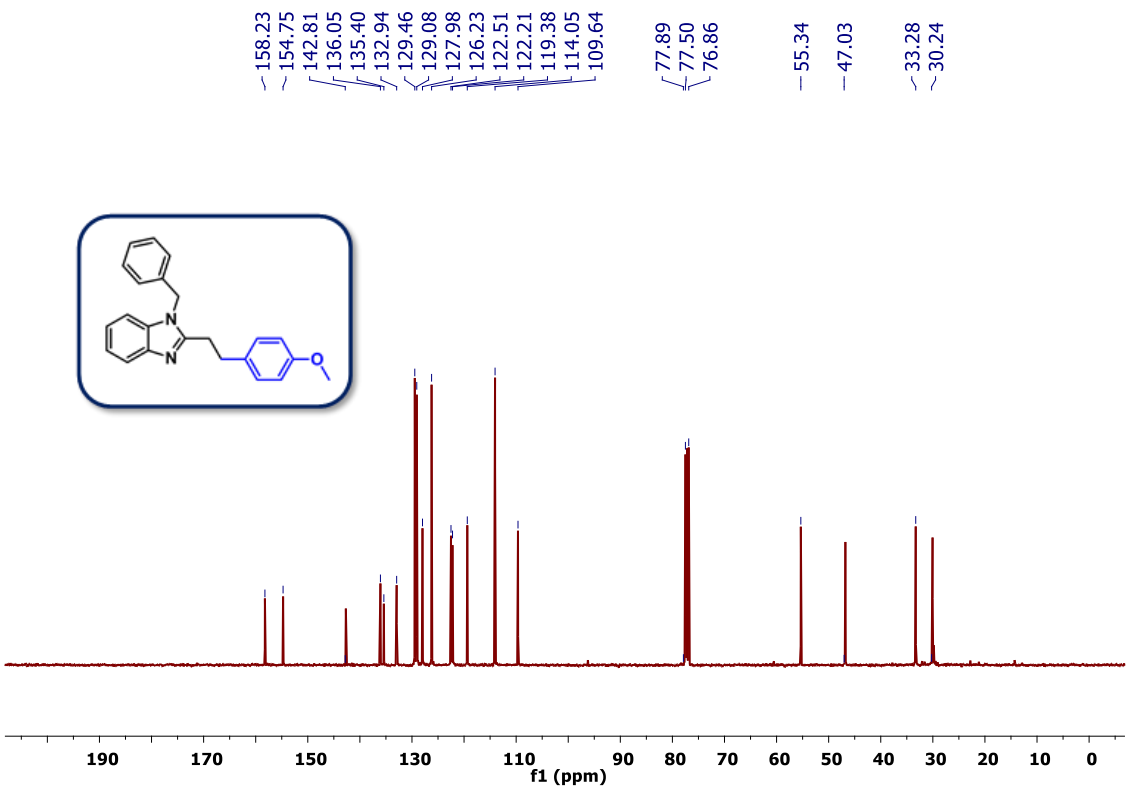
5.1642
3.7592
3.1052
3.0842
3.0547
1.00
4.40
1.99
2.04
1.99
2.03
2.08
3.04
0.14
4.12
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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136.05
135.40
132.94
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129.08
127.98
126.23
122.51
122.21
119.38
114.05
109.64
77.89
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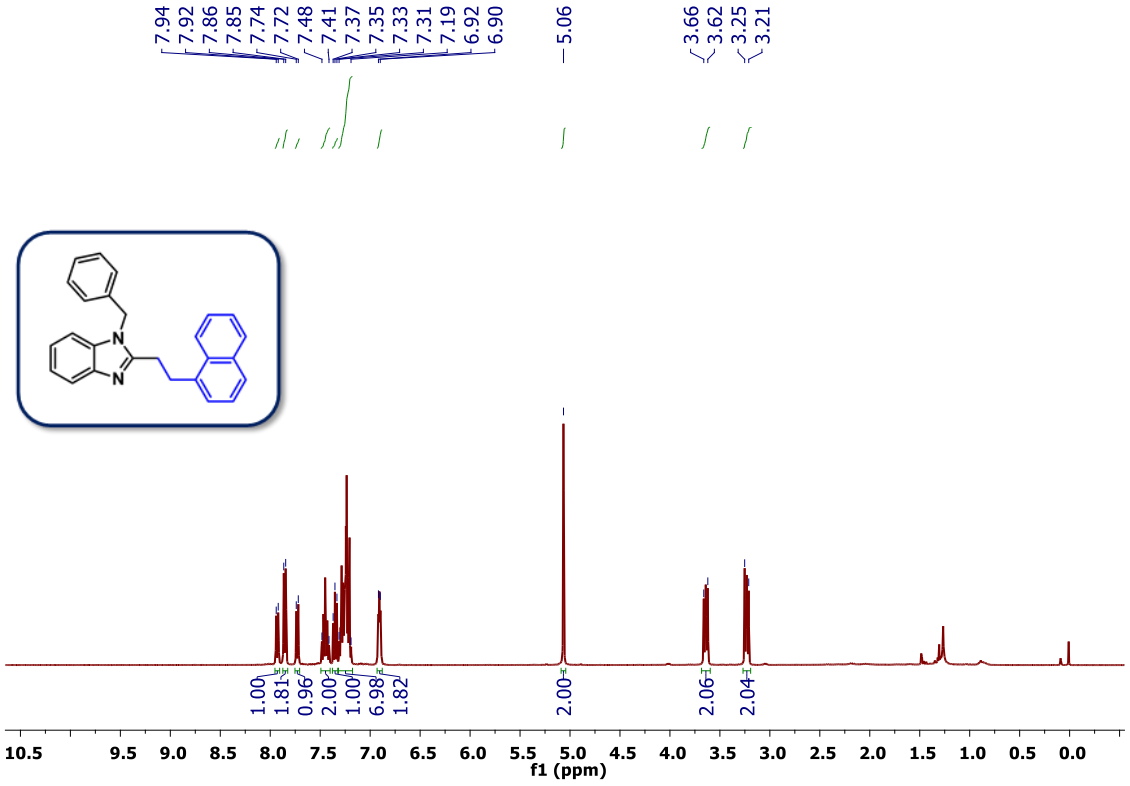
76.86
55.34
47.03
33.28
30.24
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.33
7.31
7.19
6.92
6.90
5.06
3.66
3.62
3.25
3.21
1.00
1.81
0.96
2.00
1.00
6.98
1.82
2.00
2.06
2.04
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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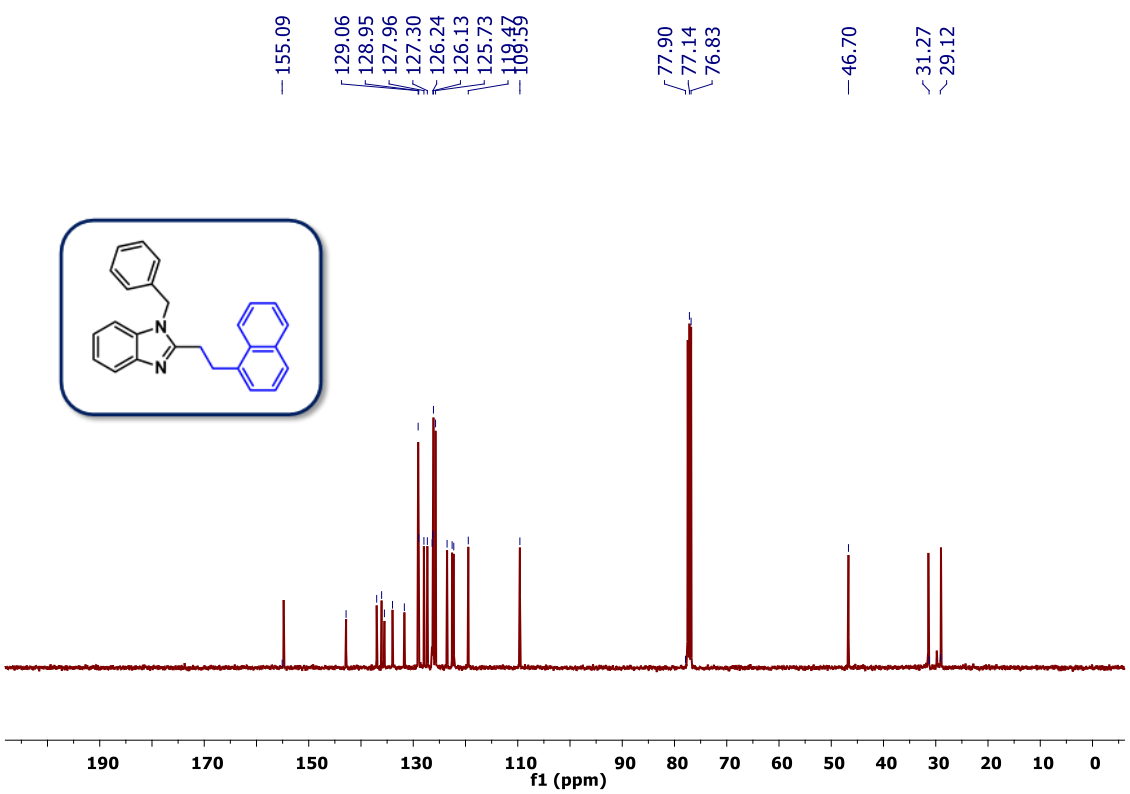
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77.90
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31.27
29.12
190
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150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)