Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Tandem synthesis of quinazolinone scaffolds from 2-aminobenzonitriles using aliphatic alcohol-water system

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Contents

1. General procedures and materials

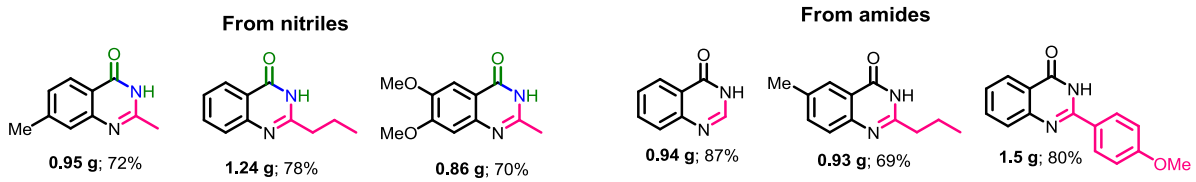
All the experiments were carried out under inert atmosphere using either standard Schlenk line techniques or argon filled Glove box. Glass apparatus were oven-dried overnight at 100 °C before use. Solvents were dried according to standard literature methods and deoxygenated with inert gas prior to use. Complexes **1a-6** were synthesized according to our previous work.[1, 2] All 2-aminobenzonitriles, few 2-aminobenzamides and other commercially available reagents were purchased from Sigma-Aldrich, Alfa-Aesar, TCI-India, SDFCL, Avra and Spectrochem. Rest of the 2-aminobenzamides were prepared from 2-aminobenzoic acids according to previous literature report.[3] $RuCl_3.nH_2O$ (39% Ru on metal basis) was purchased from Arora-matthey, India. ^1H, ^{13}C and ^{31}P spectra were recorded on JEOL 400 and 500 MHz Spectrometer. All ^1H and proton decoupled ^{13}C NMR spectra were reported in ppm relative to residual DMSO peak (2.5 ppm) and deuterated DMSO (39.5 ppm) respectively. ESI-MS were recorded on a Waters Micromass Quattro Micro triple-quadrupole mass spectrometer.

2. General synthesis procedures

2A. Coupling of 2-aminobenzamides with methanol and other long chain alcohols: To a pressure tube, magnetic stir-bar, Cat. **2** (0.5-2 mol%), Cs_2CO_3 (0.5 equiv.), 2-aminobenzamide derivatives (0.5 mmol) and methanol or other long chain alcohols (1.5 mL) were added under argon atmosphere. Then, the tube was sealed and dipped in a preheated oil-bath at 150 °C for specified time. After completion of the reaction, the tube was allowed to cool to room temperature and the reaction mixture was concentrated under reduced pressure. Finally, the desired product was purified through silica gel column chromatography using hexane/ethyl acetate as the eluent.

2B. Coupling of 2-aminobenzonitriles with methanol and other long chain alcohols: To a pressure tube, magnetic stir-bar, Cat. **2** (1-2 mol%), Cs_2CO_3 (1 equiv.), 2-aminobenzonitrile derivatives (0.5 mmol), water (0.18 mL) and methanol or other long chain alcohols (1.5 mL) were added under argon atmosphere. Then, the tube was sealed and dipped in a preheated oil-bath at 150 °C for specified time. After completion of the reaction, the tube was allowed to cool to room temperature and the reaction mixture was concentrated under reduced pressure. Finally, the desired product was purified through silica gel column chromatography using hexane/ethyl acetate as the eluent.

3. Procedure for preparative scale synthesis:



Scheme S1: Preparative scale synthesis of quinazolinones

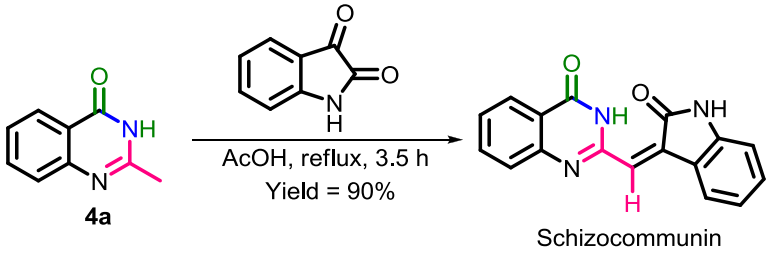
3A. Synthesis of quinazolinones from 2-aminobenzonitriles: To a pressure tube, magnetic stir-bar, Cat. **2** (1 mol%), Cs_2CO_3 (1 equiv.), 2-aminobenzonitrile derivatives (1.0 g), water (20 equiv.) and ethanol or 1-butanol (25 mL) were added under argon atmosphere. Then, the tube was sealed and dipped in a preheated oil-bath at 150 °C for specified time. After completion of the reaction, the tube was allowed to cool to room temperature and the reaction mixture was concentrated under reduced pressure. Finally, the desired product was purified through silica gel column chromatography using hexane/ethyl acetate as the eluent.

3B. Synthesis of quinazolinones from 2-aminobenzamides: To a pressure tube, magnetic stir-bar, Cat. **2** (0.5 mol%), Cs_2CO_3 (0.5 equiv.), 2-aminobenzamide derivatives (1.0 g) and methanol or 1-butanol (25 mL) were added under argon atmosphere. Then, the tube was sealed and dipped in a preheated oil-bath at 150 °C for specified time. After completion of the reaction, the tube was allowed to cool to room temperature and the reaction mixture was concentrated under reduced pressure. Finally, the desired product was purified through silica gel column chromatography using hexane/ethyl acetate as the eluent.

3C. Synthesis of 2-(4-methoxyphenyl)quinazolin-4(3H)-one under neat condition: To a pressure tube, magnetic stir-bar, Cat. **2** (1 mol%), KO^{t}Bu (1.5 equiv.), 2-aminobenzamide (1.0 g) and 4-methoxybenzyl alcohols (1 mL) were added under argon atmosphere. Then, the tube was sealed and dipped in a preheated oil-bath at 150 °C for 26 hour. After completion of the reaction, the tube was allowed to cool to room temperature and the reaction mixture was concentrated under reduced pressure. Finally, the desired product was purified through silica gel column chromatography using hexane/ethyl acetate as the eluent.

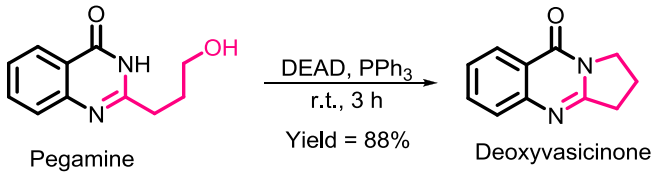
Procedure for natural product synthesis:

3D. Synthesis of 2-methylquinazolin-4(3H)-one (4a): To a pressure tube, magnetic stir-bar, Cat. **2** (1 mol%), Cs_2CO_3 (1 equiv.), 2-aminobenzonitrile (1 g), water (3 mL) and ethanol (25 mL) were added under argon atmosphere. Then, the tube was sealed and dipped in a preheated oil-bath at 150 °C for specified time. After completion of the reaction, the tube was allowed to cool to room temperature and the reaction mixture was concentrated under reduced pressure. Finally, the desired product was purified through silica gel column chromatography using hexane/ethyl acetate as the eluent.



3E. Synthesis of Schizocommunin: Schizocommunin was prepared from previously synthesized compound 2-methylquinazolin-4(3H)-one according to previous literature report.[4]

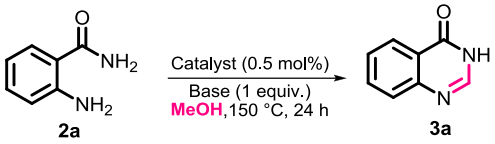
3F. Synthesis of Pegamine: In a Schlenk flask, magnetic stir-bar, Cat. **2** (1 mol%), KO^{t}Bu (1.5 equiv.), 2-aminobenzamide (1.0 g), butane-1,4-diol (1.1 equiv.) and *p*-xylene (30 mL) were added under argon condition. Then the flask was sealed and dipped in a preheated oil-bath at 150 °C for specified time. After completion of the reaction, the flask was allowed to cool to room temperature and the reaction mixture was concentrated under reduced pressure. Finally, the desired product was purified through silica gel column chromatography using hexane/ethyl acetate as the eluent.

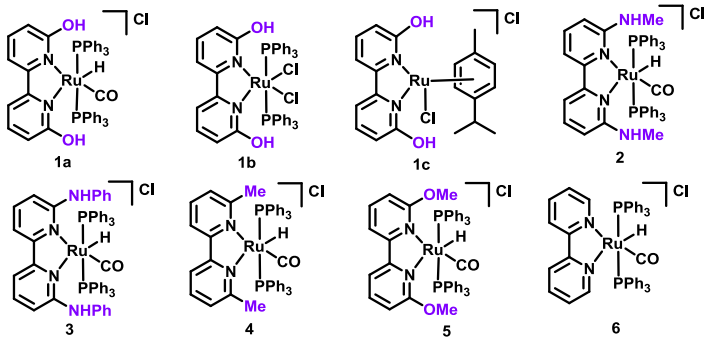


3G. Synthesis of Deoxyvasicinone: Deoxyvasicinone was prepared from previously synthesized compound pegamine according to previous literature report.[5]

4. Optimization data for the coupling of 2-aminobenzamide with methanol

Table S1: Optimization table





Entry	Catalyst	Base (equiv.)	Yield of **3a** (%)
1	**1a**	NaOMe (1)	76
2	**1b**	NaOMe (1)	23
3	**1c**	NaOMe (1)	19
4	**2**	NaOMe (1)	91
5	**3**	NaOMe (1)	72
6	**4**	NaOMe (1)	78
7	**5**	NaOMe (1)	76
8	**6**	NaOMe (1)	58
9	**2**	Cs_2CO_3 (1)	99
10	**2**	KO^{t}Bu (1)	85
11	**2**	NaO^{t}Bu (1)	80
12	**2**	LiO^{t}Bu (1)	58
13	**2**	Cs_2CO_3 (0.8)	95
14	**2**	Cs_2CO_3 (0.5)	93
15[b]	**2**	**Cs_2CO_3 (0.5)**	**>99**
16[c]	**2**	Cs_2CO_3 (0.5)	78
17[c,d]	**2**	Cs_2CO_3 (0.5)	74
18[c,e]	**2**	Cs_2CO_3 (0.5)	70

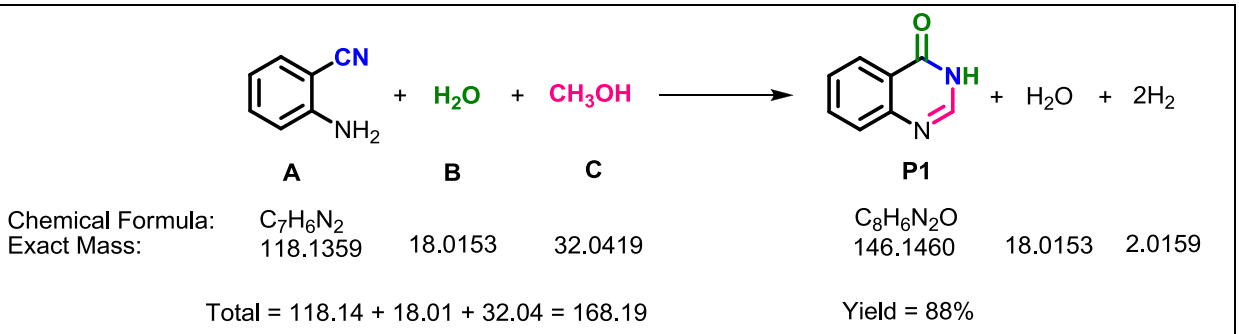
[a] Reaction conditions: 2-aminobenzamide (0.5 mmol), Catalyst (0.5 mol%), base (0.5 mmol), MeOH (1.5 mL), 150 °C (oil bath temperature), 24 h, closed argon atmosphere; yield was

determined by ^{1}H NMR using 1,3,5-trimeyhoxybenzene as internal standard. [b] 26 h. [c] 140 °C. [d] Toluene : MeOH (v/v=1:1). [e] *p*-Xylene : MeOH (v/v=1:1).

5. Determination of green chemistry metrics

To a pressure tube, magnetic stir-bar, Cat. **2** (1 mol%), Cs_2CO_3 (8.46 mmol), 2-aminobenzonitrile (1 g), water (3.05 mL) and methanol (25 mL) were added under argon atmosphere. Then, the tube was sealed and dipped in a preheated oil-bath at 150 °C for specified time. After completion of the reaction, the tube was allowed to cool to room temperature and the reaction mixture is used for the determination of green chemistry metrics[6-9] and the details are mentioned in the table below.

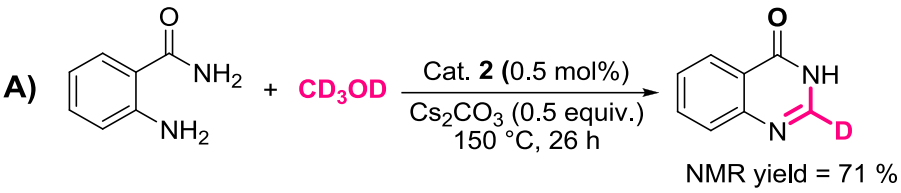
Table S2: Data for green chemistry metrics



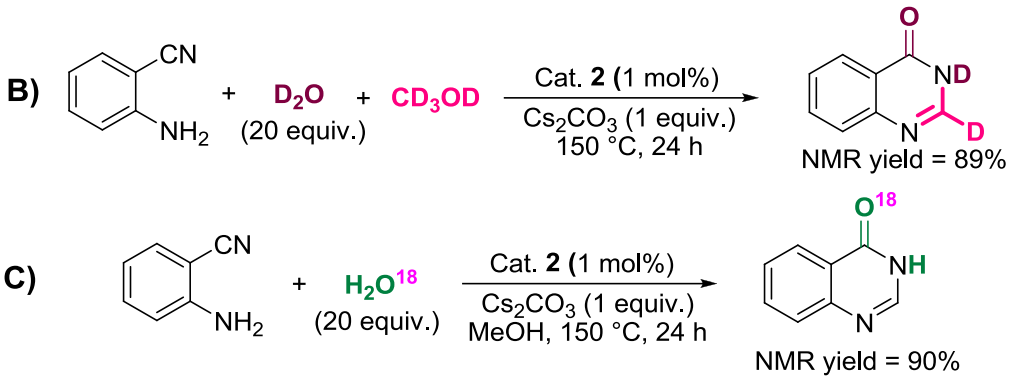
	Chemicals	Wt. (g)	Formula Wt.
Reactant **A**	2-Aminobenzonitrile	1.00	118.14
Reactant **B**	Water	3.05	18.01
Reactant **C**	Methanol	19.8	32.04
Base	Cs_2CO_3	2.76	325.82
Recycle solvent	-	18.2	-
Auxiliary	-	-	-
By-product	Hydrogen	0.034	2.01
Product	Quinazolin-4(3H)-one	1.09	146.15

- ✓ **E factor** = [{(1 + 3.05 + 19.8 + 2.76 + 0.034) - (18.2 + 1.09)}g/1.09 g] = 7.354 g/1.09 g = **6.7 kg waste/1 kg product**
- ✓ **Atom economy** = (146.15/168.19) x 100 = **87%**
- ✓ **Atom efficiency** = 88 x (100/100) = **88%**
- ✓ **Carbon efficiency** = (8/8) x 100 = **100%**
- ✓ **Reaction mass efficiency** = [1.09 / (1+ 0.152 + 0.271)] x 100 = **76%**

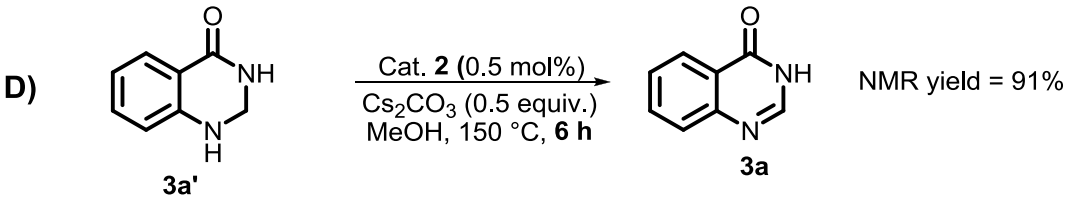
6. Procedure for kinetic experiments



The experiment was carried out following the general procedure **2A** by replacing only methanol with methanol-d_4. After the reaction, 1,3,5-trimethoxybenzene was added to the reaction mixture as internal standard and the solvent was evaporated under reduced pressure. Then, crude mixture was analyzed by using ^{1}H NMR and ESI-MS analysis. The reaction was performed twice and average data was reported.



Both of the reactions (B & C) were carried out following general procedure **2B** (D_2O and methanol-d_4 were used in the case of B and in case of C, H_2O^{18} was used in place of standard reagents). After the reaction, 1,3,5-trimethoxybenzene was added to the reaction mixture as internal standard and the solvent was evaporated under reduced pressure. Then, crude mixture was analyzed by using ^{1}H NMR and ESI-MS analysis. All the reactions were repeated multiple times and average data was reported.



The experiment was carried out following the general procedure **2A** where only 2,3-dihydroquinazolin-4(1H)-one (**3a**') in place of 2-aminobenzamide. After the reaction, 1,3,5-

trimethoxybenzene was added to the reaction mixture as internal standard and the solvent was evaporated under reduced pressure. Then, crude mixture was analyzed by using ^{1}H NMR and ESI-MS analysis. All the reactions were repeated multiple times and average data was reported.

7. Kinetic Isotope Effect (KIE) studies

Kinetic isotope effect of the synthesis of quinazolin-4-(3H)-one (**3a**) from 2-aminobenzamide was studied from the standard reactions which were carried out both in methanol and methanol-d_4 for different time periods. After obtaining the average yield of **3a** at different time interval, ln(a/a-x) vs time (hour) was plotted and k_H/k_D was calculated accordingly.

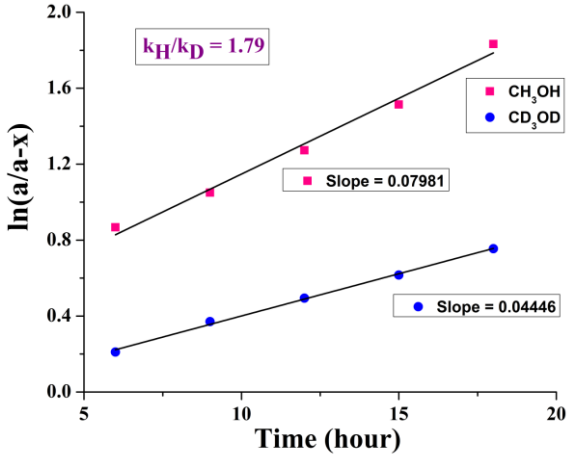


Fig. S1: Determination of Kinetic Isotopic Effect for synthesis of **3a** from 2-aminobenzamide

8. Characterization of the Products:

Quinazolin-4(3H)-one (3a, 5a)[10]: White solid (70 mg, 96% isolated yield for **3a** and 67 mg, 91% isolated yield for **5a**); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.24 (brs, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 8.09 (s, 1H), 7.79 (t, *J* = 7.1 Hz, 1H), 7.65 (d, *J* = 8 Hz, 1H), 7.51 (t, *J* = 8 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): 160.78, 148.82, 145.48, 134.34, 127.27, 126.77, 125.87, 122.66.

6-Methylquinazolin-4(3H)-one (3b)[10]: Light yellow solid (75 mg, 94% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): 8.02 (s, 1H), 7.90 (s, 1H), 7.62 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.55 (d, *J* = 8.2 Hz, 1H), 2.43 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 163.10, 160.93, 146.79, 144.88, 136.37, 135.54, 127.03, 125.23, 122.39, 20.85.

6,7-Dimethoxyquinazolin-4(3H)-one (3c, **5c)**[10]: Gray solid (98 mg, 95% isolated yield for **3c** and 94 mg, 91% isolated yield for **5c**); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.06 (brs, 1H), 7.98 (s, 1H), 7.43 (s, 1H), 7.12 (s, 1H), 3.90 (s, 3H), 3.86 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 160.04, 154.43, 148.52, 144.85, 143.82, 115.58, 107.99, 104.88, 55.90, 55.67.

6,7,8-Trimethoxyquinazolin-4(3H)-one (3d)[11]: Pale brown solid (78 mg, 66% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.17 (brs, 1H), 7.99 (s, 1H), 7.32 (s, 1H), 3.93 (s, 3H), 3.88 (s, 3H), 3.86 (s, 3H).**^{13}C NMR** (100 MHz, DMSO-d_6): 160.15, 152.21, 147.77, 147.12, 142.90, 138.51, 118.74, 101.20, 61.88, 60.89, 55.92.

6-Fluoroquinazolin-4(3H)-one (3e)[10]: White solid (76 mg, 92% isolated yield); **^{1}H NMR** (500 MHz, DMSO-d_6): δ = 12.31 (brs, 1H), 8.06 (s, 1H), 7.73 (dd, *J* = 8.6, 2.9 Hz, 1H), 7.71-7.68 (m, 1H), 7.64 (td, *J* = 8.6, 3, 1H). **^{13}C NMR** (125 MHz, DMSO-d_6): 161.0, 160.19, 159.05, 145.21 (d, *J* = 93.7 Hz), 130.02 (d, *J* = 8.2 Hz), 123.88 (d, *J* = 8.2 Hz), 122.68 (d, *J* = 23.9 Hz), 110.45 (d, *J* = 23.1 Hz).

6-Chloroquinazolin-4(3H)-one (3f, **5e)**[10]: White solid (63 mg, 70% isolated yield for **3f** and 83 mg, 92% isolated yield for **5e**); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.44 (brs, 1H), 8.12 (s, 1H), 8.04 (d, *J* = 2.4 Hz, 1H), 7.82 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.68 (d, *J* = 8.8 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): 159.81, 147.45, 145.95, 134.42, 131.01, 129.48, 124.82, 123.86.

6-Bromoquinazolin-4(3H)-one (3g)[10]: White solid (101 mg, 90% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.38 (brs, 1H), 8.14 (d, *J* = 1.9 Hz, 1H), 8.11 (s, 1H), 7.89 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.57 (d, *J* = 8.7 Hz, 1H). **^{13}C NMR** (125 MHz, DMSO-d_6): 159.65, 147.68, 146.01, 137.07, 129.56, 127.94, 124.20, 119.18.

6-Bromo-8-methylquinazolin-4(3H)-one (3h)[12]: White solid (72 mg, 60% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.39 (brs, 1H), 8.14 (s, 1H), 7.95 (d, J=1.7 Hz, 1H), 7.89 (s, 1H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 160.16, 145.55, 144.14, 138.68, 137.72, 125.24, 123.80, 121.53, 20.38; **ESI-MS** calculated for $C_9H_8BrN_2O$; 238.9820, found: 238.9833 ($[M+H]^+$).

Benzo[g]quinazolin-4(3H)-one (3i)[13]: White solid (85 mg, 86% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.07 (brs, 1H), 8.82 (s, 1H), 8.22 (s, 1H), 8.19 (d, *J* =8.4 Hz, 1H), 8.07 (d, *J* = 6.4 Hz, 2H), 7.64 (t, *J* = 7.1 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-

d_6): 161.25, 144.58, 144.19, 136.03, 130.90, 129.20, 128.45, 127.79, 127.26, 126.31, 124.72, 121.61.

2H-Benzo[e][1,2,4]thiadiazine 1,1-dioxide (3j)[10]: White solid (50 mg, 55% isolated yield); **^{1}H NMR** (500 MHz, DMSO-d_6): δ = 7.98 (s, 1H), 7.81 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.65 (t, *J* = 8.4 Hz, 1H), 7.44 (t , *J* = 7.4 Hz, 1H), 7.31 (d, *J* = 8.2 Hz, 1H). **^{13}C NMR** (125 MHz, DMSO-d_6): 147.71, 134.72, 133.14, 126.71, 123.71, 122.56, 117.58.

2-Methylquinazolin-4(3H)-one (4a, **5f)**[14]**:** White solid (76 mg, 94% isolated yield for **4a** and 76 mg, 95% isolated yield for **5f**); ^{1}H NMR (400 MHz, DMSO-d_6): δ = 12.18 (brs, 1H), 8.05 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.74-7.70 (m, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 1H), 2.33 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 161.78, 154.27, 149.02, 134.22, 126.61, 125.81, 125.70, 120.69, 21.47.

2-Propylquinazolin-4(3H)-one (4b, **5g)**[15]: White solid (87 mg, 92% isolated yield of **4b** and 91 mg, 96% isolated yield for **5g**); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.15 (brs, 1H), 8.07 (d, *J* = 7.9 Hz, 1H), 7.75 (t, *J* =7.2 Hz, 1H), 7.58 (d, *J* = 7.1 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 2.56 (t, *J* =7.4 Hz, 2H), 1.78-1.69 (m, 2H), 0.92 (t, *J* =7.4 Hz, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6): 161.85, 157.32, 148.93, 134.21, 126.77, 125.87, 125.67, 120.78, 36.35, 20.20, 13.47.

2-Pentylquinazolin-4(3H)-one (4c, **5h)**[15]: White solid (101 mg, 93% isolated yield for **4c** and 102 mg, 94% isolated yield for **5h**); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.15 (brs, 1H), 8.06 (d, *J* = 7.9 Hz, 1H), 7.74 (t, *J* = 8.3 Hz, 1H), 7.57(d, *J* = 8.1 Hz, 1H), 7.43 (t, *J* = 7.2 Hz, 1H), 2.57 (t, *J* = 7.5 Hz, 2H), 1.73-1.66 (m, 2H), 1.29-1.25 (m, 4H), 0.83 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 161.70, 157.40, 148.74, 134.17, 126.58, 125.80, 125.54, 120.55, 34.29, 30.59, 26.38, 21.68, 13.67.

6-Fluoro-2-pentylquinazolin-4(3H)-one (4d): White solid (101 mg, 86% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.29 (brs, 1H), 7.74-7.72 (m, 1H), 7.66-7.64 (m, 2H), 2.58 (t, *J* = 7.5 Hz, 2H), 1.74-1.67 (m, 2H), 1.31 (m, 4H), 0.86 (t, *J* = 6.6 Hz, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 161.02 (d, J = 47 Hz) , 158.35, 159.93, 145.81, 129.52 (d, *J* =7.9 Hz), 122.56 (d, *J* =23.6 Hz), 121.91 (d, *J* =8.1 Hz), 110.20 (d, *J* = 23.2 Hz), 34.38, 30.77, 26.45, 21.85, 13.79; **ESI-MS**: calculated for $C_{13}H_{16}FN_2O$; 235.1247, found: 235.1241 ($[M+H]^+$).

6-Chloro-2-propylquinazolin-4(3H)-one (4e, **5o)**[16]: White solid (98 mg, 88% isolated yield for **4e** and 89 mg, 84% isolated yield for **5o**); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.35 (brs, 1H), 7.97 (d, *J*= 2.4 Hz, 1H), 7.75 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.59 (d, *J* = 8.7, Hz, 1H), 2.56 (t, *J* = 7.4 Hz, 2H), 1.77-1.67 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 160.88, 158.00, 147.59, 134.30, 130.11, 128.99, 124.66, 122.02, 36.33, 20.12, 13.46.

6-Bromo-2-methylquinazolin-4(3H)-one (4f)[14]: White solid (108 mg, 89% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.36 (brs, 1H), 8.11(d, *J* = 2.3 Hz, 1H), 7.88 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.50 (d, *J* = 8 Hz, 1H), 2.33 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6):160.61, 155.13, 147.85, 137.06, 128.94, 127.78, 122.25, 118.16, 21.49.

6-Methyl-2-propylquinazolin-4(3H)-one (4g)[16]: White solid (81 mg, 80% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.05 (brs, 1H), 7.86 (s, 1H), 7.57 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.48 (d, *J* = 8.4, Hz, 1H), 2.55 (t, *J* = 7.5 Hz, 2H), 2.41 (s, 3H), 1.77-1.68 (m, 2H), 0.92 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 161.76, 156.36, 146.95, 135.50, 135.44, 126.66, 125.03, 120.53, 36.28, 20.74, 20.21, 13.49.

2-Pentylbenzo[g]quinazolin-4(3H)-one (4h): White solid (101 mg, 76% isolated yield); **^{1}H NMR** (400MHz, DMSO-d_6): δ = 11.97 (brs, 1H), 8.78 (s, 1H), 8.17-8.15 (m, 2H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.64 (t, *J* = 7.04 Hz, 1H), 7.55 (t, *J*= 7.2 Hz, 1H), 2.61 (t, *J*= 7.7 Hz, 2H), 1.80-1.73 (m, 2H), 1.34-1.32 (m, 4H), 0.88 (t, *J* = 6.6 Hz, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 162.24, 156.50, 144.35, 136.22, 130.54, 129.17, 128.33, 127.68, 127.03, 125.95, 123.93, 120.11, 34.58, 30.78, 26.27, 21.86, 13.85; **ESI-MS** calculated for $C_{17}H_{19}N_2O$; 267.1497, found: 267.1496 ($[M+H]^+$).

3-Methyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide (4i)[17]: White solid (53 mg, 54% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 7.78 (d, *J* = 8.0 Hz, 1H), 7.66 (t, *J*= 7.3 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 1H), 7.30 (d, *J* = 8.3 Hz, 1H), 2.30 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 157.24, 135.19, 133.01, 126.14, 123.43, 121.01, 117.21, 22.60.

7-Methylquinazolin-4(3H)-one (5b)[10]: White solid (71 mg, 88% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.14 (brs, 1H), 8.05 (s, 1H), 8.00 (d, *J* = 8.1 Hz, 1H), 7.46 (s, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 2.44 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 160.64, 148.88, 145.43, 144.83, 128.16, 126.87, 125.70, 120.21, 21.32.

7-Chloroquinazolin-4(3H)-one (5d)[10]: White solid (85 mg, 94% isolated yield**)**; **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 8.11 (s, 1H), 8.08 (d, *J* = 8.6 Hz, 1H), 7.67 (d, *J* = 1.9 Hz, 1H), 7.52 (dd, *J* = 8.6, 2.0 Hz, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): 160.31, 149.88, 146.99, 139.04, 128.04, 127.13, 126.40, 121.48.

2,7-Dimethylquinazolin-4(3H)-one (5i)[18]: White solid (74 mg, 85% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.08 (brs, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.36 (s, 1H), 7.26 (d, *J* = 8.1 Hz 1H), 2.42 (s, 3H), 2.32 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 161.61, 154.27, 149.12, 144.70, 127.29, 126.23, 125.55, 118.24, 21.44, 21.37.

7-Methyl-2-propylquinazolin-4(3H)-one (5j)[19]: White solid (88 mg, 87% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.05 (brs, 1H), 7.95 (d, *J* = 8.1 Hz, 1H), 7.39 (s, 1H), 7.26 (d, *J* = 8.2, Hz, 1H), 2.55 (t, *J* = 7.5 Hz, 2H), 2.42 (s, 3H), 1.77-1.68 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6):161.73, 157.32, 149.08, 144.69, 127.32, 126.48, 125.54, 118.39, 36.32, 21.33, 20.20, 13.47.

6,7-Dimethoxy-2-methylquinazolin-4(3H)-one (5k)[14]: White solid (88 mg, 80% isolated yield); **^{1}H NMR** (500 MHz, DMSO-d_6): δ = 12.02 (brs, 1H), 7.38 (s,1H), 7.04 (s, 1H), 3.87 (s, 3H), 3.84 (s, 3H), 2.30 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 161.11 154.46, 152.52, 147.94 145.10, 113.42, 107.50, 104.84, 55.84, 55.61, 21.20.

6,7-Dimethoxy-2-pentylquinazolin-4(3H)-one (5l): White solid (124 mg, 90% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.00 (brs, 1H), 7.39 (s, 1H), 7.07 (s, 1H), 3.88 (s, 3H), 3.84 (s, 3H), 2.55 (t, *J* = 7.6 Hz, 2H), 1.74-1.66 (m, 2H), 1.33-1.26 (m, 4H), 0.87 (t, *J* = 6.5 Hz, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 161.21, 155.89, 154.50, 147.99, 145.08, 113.55, 107.68, 104.82, 55.86, 55.62, 34.30, 30.75, 26.54, 21.83, 13.84. **ESI-MS** calculated for $C_{15}H_{20}N_2O_3$; 277.1552, found: 277.1556 ($[M+H]^+$).

7-Chloro-2-methylquinazolin-4(3H)-one (5m)[14]: White solid (72 mg, 74% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.33 (brs, 1H), 8.05 (d, *J* = 8.6 Hz, 1H), 7.60 (d, *J* = 1.6 Hz, 1H), 7.47 (dd, *J* = 8.6, 1.8 Hz, 1H), 2.34 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 161.11, 156.06, 150.09, 138.88, 127.80, 126.16, 125.72, 119.47, 21.50.

7-Chloro-2-propylquinazolin-4(3H)-one (5n)[20]: White solid (94 mg, 84% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.29 (brs, 1H), 8.05 (d, *J* = 8.8 Hz, 1H), 7.61 (s, 1H), 7.46 (d,

J = 8.5 Hz, 1H), 2.56 (t, *J*= 7.5 Hz, 2H), 1.77-1.68 (m, 2H), 0.92 (t, *J* =7.4 Hz, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6): 161.22, 159.07, 150.05, 138.89, 127.79, 126.20, 125.93, 119.61, 36.37, 20.17, 13.46.

Pegamine[5]: White solid (0.99 g, 66% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.15 (brs, 1H), 8.07 (d, *J* = 8.1 Hz, 1H), 7.76 (t, *J* = 7.5 Hz, 1H), 7.58 (d, *J* = 8.3 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 4.56 (brs, 1H), 3.47 (t, *J* = 6.3 Hz, 2H), 2.65 (t, *J* = 7.6 Hz, 2H), 1.91-1.84 (m, 2H). **^{13}C NMR** (100 MHz, DMSO-d_6): 161.78, 157.48, 148.91, 134.24, 126.75, 125.87, 125.66, 120.78, 60.07, 31.28, 29.82. **ESI-MS**: calculated for $C_{11}H_{13}N_2O_2$; 205.0977, found: 205.0976 ($[M+H]^+$).

Deoxyvasicinone[5]: White solid (0.794 g, 88% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 8.08 (d, *J* = 8.1 Hz, 1H),7.74 (t, *J* = 8.1 Hz, 1H), 7.56 (d, *J* = 8.2 Hz, 1H), 7.44 (t, *J* = 7.9 Hz, 1H), 4.02 (t, *J* = 7.4 Hz, 2H), 3.04 (t, *J* = 8 Hz, 2H), 2.18-2.10 (m, 2H). **^{13}C NMR** (100 MHz, DMSO-d_6): 160.24, 159.91, 148.99, 133.94, 126.57, 125.77, 125.62, 120.06, 46.25, 31.79, 18.86.

Schizocommunin[4]: Orange powder (1.84 g, 90% isolated yield); **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 14.39 (s, 1H), 11.48 (brs, 1H), 8.17 (dd, *J* = 6.4, 0.7 Hz, 1H), 7.93 (d, *J* = 6 Hz, 1H), 7.90-7.86 (m, 1H), 7.78 (d, *J* = 6.4 Hz, 1H), 7.60 (t, *J* = 6.2 Hz, 1H), 7.56 (s, 1H), 7.36 (t, *J* = 6.1 Hz, 1H), 7.08 (t, *J* = 6 Hz, 1H), 6.92 (d, *J* = 6.2 Hz, 1H). **ESI-MS**: calculated for $C_{17}H_{12}N_3O_2$; 290.0930, found: 290.0923 ($[M+H]^+$).

2,3-Dihydroquinazolin-4(1H)-one (3a'): White solid; **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 7.89 (s, 1H), 7.63 (d, *J* = 7.5 Hz, 1H), 7.24 (t, *J* = 7.4 Hz, 1H), 6.75-6.68 (m, 2H), 6.54(s, 1H), 4.45 (s, 2H). **^{13}C NMR** (100 MHz, DMSO-d_6): 164.33, 149.60, 133.07, 127.74, 117.47, 116.08, 114.70, 53.96. **ESI-MS**: calculated for $C_8H_9N_2O$; 149.0715, found: 149.0710 ($[M+H]^+$).

3a-D (White solid): **^{1}H NMR** (400 MHz, DMSO-d_6): δ = 12.24 (brs, 1H), 8.13-8.09 (m, 1H), 7.80 (t, *J* = 7.7 Hz, 1H), 7.65 (d, *J* = 8.2 Hz, 1H), 7.53-7.50 (m, 1H). **^{13}C NMR** (100 MHz, DMSO-d_6): 160.77, 148.77, 134.32, 127.23, 126.74, 126.63, 125.85, 122.65.

9. Computational Studies: All calculations were performed using the Gaussian 09 package.[21] Full geometry optimization followed by frequency calculations on the stationary points were carried out to ascertain the nature of the stationary points as minima or first order saddle point. Hybrid functional, B3LYP was used with the LANL2DZ basis set[22] for Ru and 6-31G** basis set[23-25] for non-metal elements. The transition states (TS) were further confirmed by performing

intrinsic reaction coordinate (IRC) calculation using same method. Solvent effect was incorporated using the polarizable continuum model (PCM) with methanol as solvent.[26]

9A. *Inner-sphere* Pathway:

Between two possible pathways of methanol activation in this system, *Inner-sphere* pathway is shown in Fig. **S1**. In the *inner-sphere* pathway, initially by the treatment of base and methanol, complex **2** would transform to methoxy-bounded species **I1_in** which further would undergo PPh_3 dissociation to create the vacant space for the β-H elimination. As, there was no available vacant site *cis* to methoxy group of **I2_in**, this penta-coordinated species **I2_in** would further convert to intermediate **I3_in** via pseudo-rotation process having high activation barrier (**TS1_in**). Afterward, **I3_in** would undergo β-hydride elimination through a four-member transition state (**TS2_in**) to produce the metal-hydride species **I4_in**.

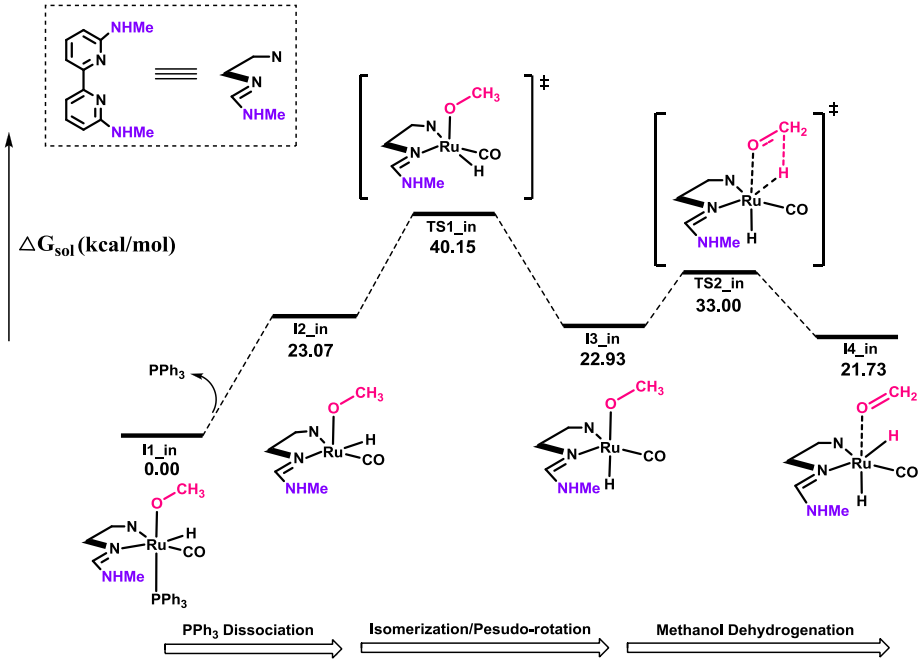


Fig. S2: Calculated Gibbs free energies (kcal/mol) for the methanol dehydrogenation following *inner-sphere* pathway (hybrid functional, M06-2X was used with the LANL2DZ basis set for Ru and the 6-31G** basis set for non-metal elements).

9B. *Outer-sphere* Pathway:

On the other hand, in the *outer-sphere* mechanism the base-mediated activation of the complex **2** would generate the intermediate **I1_out** which would further undergo the dissociation of one PPh_3

to produce the penta-coordinated species **I2_out** (Fig. **S2**). Afterwards, methanol would be dehydrogenated via the concerted *outer-sphere* manner (**TS1_out**). In this process hydroxyl hydrogen of methanol would transfer to the nitrogen atom of the imine side arm of the ligand and hydrogen of C-H bond of methanol to the electrophilic Ru-centre to produce the dihydride intermediate **I3_out**. For the dehydrogenation of methanol among the two plausible routes, the overall energy barrier was higher for the *inner-sphere* (40.15 Kcal/mol, Fig. **S1**) compared to *outer-sphere* pathway (24.86 Kcal/mol, Fig. **S2**). This suggested that the *outer-sphere* pathway was the more preferred one for this system. Further the energy barrier for liberation of hydrogen molecule from **I3_out** was calculated following outer-sphere pathway and the result revealed that elimination of hydrogen step is more energy demanding compared to methanol dehydrogenation step.

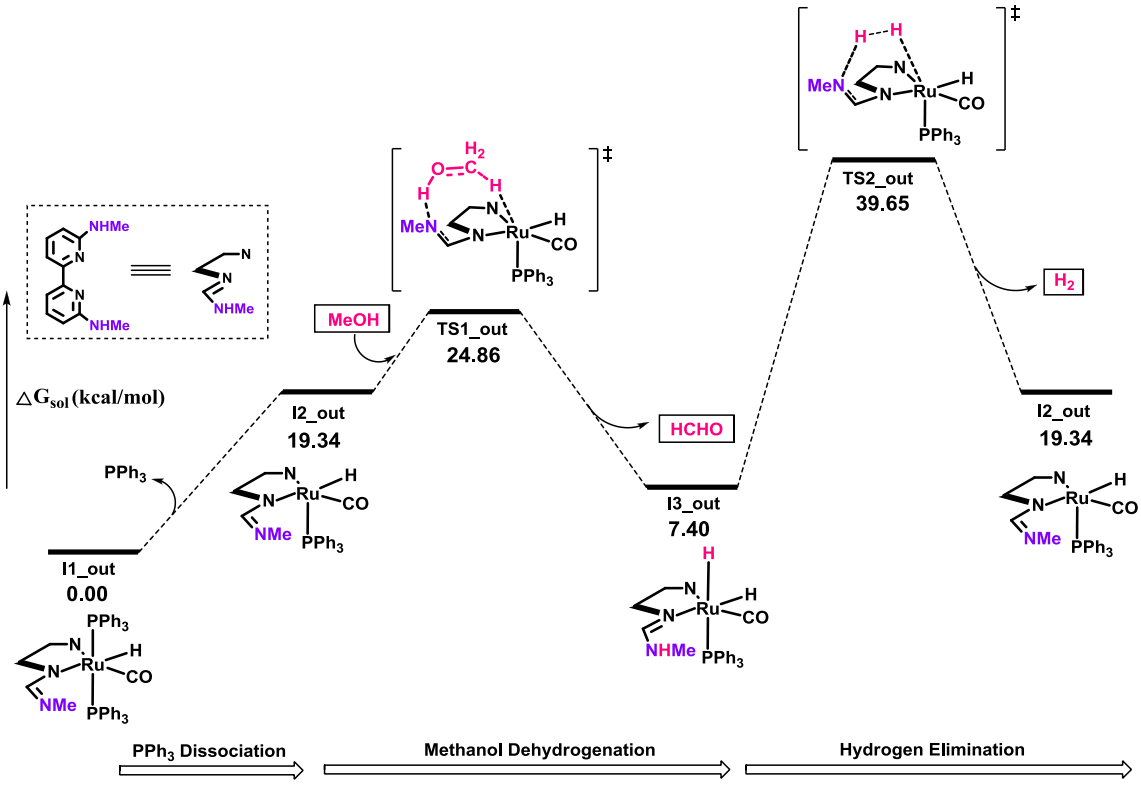


Fig. S3: Calculated Gibbs free energies (kcal/mol) for the methanol dehydrogenation and liberation of hydrogen following *outer-sphere* pathway (hybrid functional, M06-2X was used with the LANL2DZ basis set for Ru and the 6-31G** basis set for non-metal elements).

10. References

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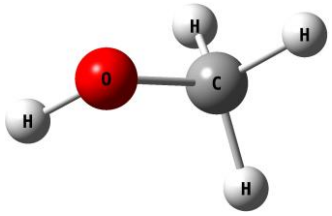
11. Cartesian Coordinates and Statistical Thermodynamic Analysis

Methanol



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Total Thermal Free Energy	:-115.63375

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H	1.02879700	-0.54401800	-0.89140400
H	1.02879700	-0.54401400	0.89140600
O	-0.74457300	0.12225300	0.00000000
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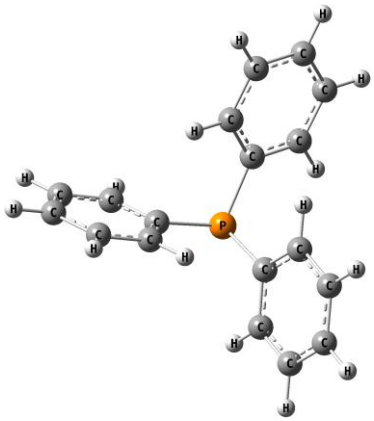
PPh_3



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Total Thermal Free Energy	:-1035.73532

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C	-3.12825900	-0.99718600	1.27565900
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C	-3.97545300	0.47571700	-0.43244600
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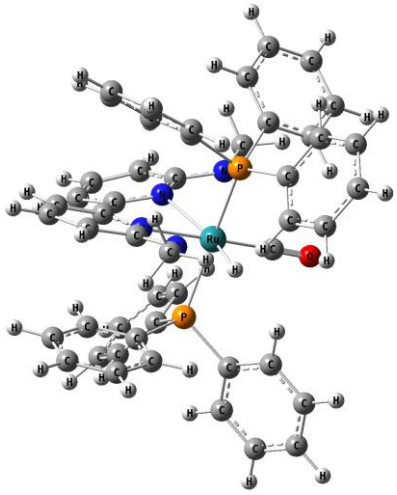
I1_out



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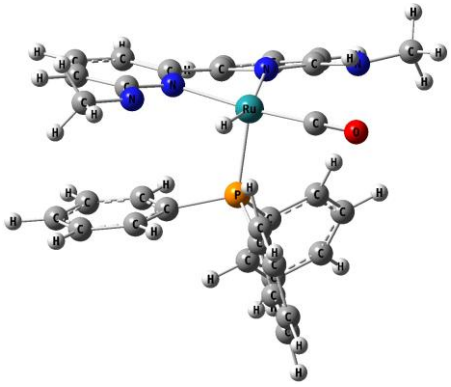
C	-4.18449700	-2.20789800	-2.54997100
C	-0.35260400	-2.83311900	-2.83351300
C	-3.82804500	-1.52807700	-3.71148900
C	-4.62087400	-2.60091700	3.45139500
C	-3.33317700	-2.93777000	3.04020200
C	-3.80362700	-1.71806300	-1.30314000
C	-0.41910000	-2.21793600	-1.51989100
C	2.62480100	-1.61767300	4.52064800
C	0.06754900	-2.12509200	-3.92097700
C	2.62653400	-4.23057600	-0.56923100
C	3.98062200	-1.48136700	4.80075900
C	-5.23569200	-1.45784700	2.94510700
C	-2.64948300	-2.13128400	2.13264700
C	-3.08131500	-0.35582000	-3.62686000
C	2.94255700	-4.13158600	-1.92091500
C	2.12527000	-1.24514500	3.27490000
C	2.50029600	-3.08075400	0.20601900
C	-3.05893500	-0.54034400	-1.21131400
C	-4.55948300	-0.64896000	2.03718600
C	-3.26058700	-0.97630900	1.63232600
C	4.83891400	-0.97278700	3.82841500
C	0.46266800	-0.77744700	-3.79187700

C	-2.68884000	0.12757600	-2.38288700
C	3.13274800	-2.87759400	-2.49780900
C	2.98164400	-0.74148100	2.29002000
C	2.70325200	-1.82144800	-0.36359800
C	4.34427800	-0.60675700	2.58127100
C	0.41521500	-0.22620400	-2.52275100
C	3.01315200	-1.72870300	-1.72467700
C	0.04575400	1.03290400	2.12652500
C	0.72556000	1.21797700	-2.31976600
C	-3.13430500	1.70410500	0.64501600
C	-3.77066600	2.43870900	-0.35762300
C	3.48105400	0.96647900	0.03662400
C	1.44722200	1.96903200	-3.24633400
C	-2.95196800	2.30185700	1.90363400
C	4.70954300	0.69231900	-0.57717600
C	-4.18765500	3.74874600	-0.12028900
C	3.12075200	2.29721400	0.27146100
C	0.31262800	3.10022300	-1.01020200
C	-3.37718900	3.60440100	2.14132000
C	1.56450200	3.33996700	-3.03544900
C	-3.98850400	4.33758900	1.12370900
C	5.55049700	1.73163900	-0.96310200
C	3.96673100	3.33497800	-0.11079200
C	0.96784600	3.93277600	-1.93686900
C	5.17856500	3.05459800	-0.73438700
C	-0.42278400	5.00129200	0.36520900
H	-0.57339000	-4.84816000	-0.85444600
H	-1.76965400	-4.46335400	0.39301700
H	-2.17075300	-4.23027800	-1.31453100
H	-4.75411400	-3.13022000	-2.61088500
H	-0.65940200	-3.86575500	-2.93999200
H	-4.12035300	-1.91847600	-4.68150900
H	-5.14824200	-3.23092000	4.16110300
H	-2.85616800	-3.83418500	3.42574800
H	1.94735400	-2.00783500	5.27363900
H	-4.05990600	-2.27015800	-0.40437700
H	2.46719200	-5.20437300	-0.11518500
H	0.08909900	-2.59944200	-4.89928700
H	4.36817000	-1.76681600	5.77367800
H	-6.24236400	-1.19491900	3.25582400
H	3.02771200	-5.02869500	-2.52685400
H	2.22652500	-3.16461200	1.25399900
H	1.06535600	-1.34702100	3.06241300
H	-1.66099500	-2.40022900	1.76663400
H	-2.77467600	0.16711800	-4.52704900
H	-0.07738800	-1.15119600	1.34377400
H	5.89755200	-0.85842700	4.04090700
H	-5.04387100	0.23984000	1.64146400
H	0.73493500	-0.18601400	-4.65560700
H	3.35104000	-2.78890300	-3.55755600
H	-2.06492500	1.01635500	-2.32072900
H	5.02411900	-0.20595600	1.83591600

H	3.13081500	-0.75491100	-2.19266900
H	-3.95163300	1.98996700	-1.32816100
H	1.90527200	1.49314000	-4.10329500
H	5.00769600	-0.33673400	-0.75485600
H	-2.47645800	1.74161000	2.70441900
H	2.17227900	2.52072900	0.75578600
H	-4.67852700	4.30396300	-0.91340200
H	-0.88532000	2.96065600	0.59721300
H	-3.23181200	4.04606200	3.12265800
H	2.11749900	3.95170900	-3.74180200
H	6.49846800	1.50759900	-1.44214600
H	-4.31460000	5.35677800	1.30566400
H	3.67011200	4.36344000	0.07212000
H	-0.93799700	5.13076800	1.31741900
H	1.02594900	5.00156000	-1.77515400
H	0.53927000	5.52183700	0.42488000
H	-1.02762700	5.46969300	-0.42423000
H	5.83454600	3.86380800	-1.03930500
N	-0.87751400	-2.77943500	-0.43483400
N	0.01575800	-0.90051000	-1.43080100
N	0.22520300	1.77321300	-1.19955700
N	-0.22495900	3.58593400	0.15030800
O	0.07364200	1.56288400	3.15388200
P	-2.37719400	0.03699000	0.38644700
P	2.31406600	-0.32634100	0.62231000
Ru	0.00935300	0.14346300	0.50227600

I2_out

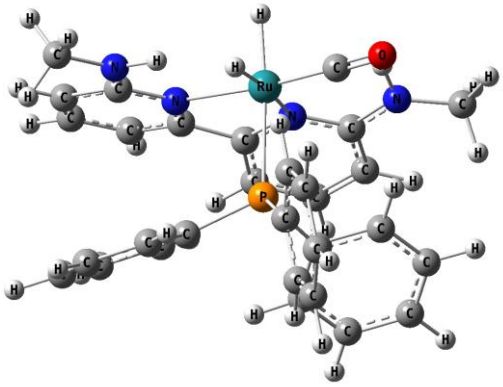


SCF Done	: -1927.518681
SCF Done for solvent	: -1927.54172
Zero-point correction	: 0.53616
Total Electronic Energy	: -1926.98252
Total Thermal Energy	: -1926.94766
Total Thermal Free Energy	: -1927.05056

Atom	X	Y	Z
C	-3.56176900	-2.70848500	-1.93024100
C	-1.63714800	-3.98178700	-0.34496200
C	-1.41748000	-2.69726600	-0.99992400
C	-3.19951900	3.63111500	-1.52616900
C	-0.65884800	-4.57550500	0.38702200
C	-3.94872300	-1.25391300	1.35842200
C	-3.35739800	4.60565300	-0.54549700
C	-3.41574800	-2.19224900	2.23572100
C	-2.36778600	2.53796800	-1.30001500
C	-3.12855600	-0.28047000	0.79256900
C	-2.68144300	4.48386600	0.66570900
C	0.59347100	-3.93786500	0.56231900
C	-2.05975400	-2.15329800	2.55878000
C	-1.69179700	2.40458800	-0.08253100
C	-1.77446500	-0.23013500	1.12276500
C	-1.85414600	3.38994200	0.89817800
C	0.77142300	-2.70746500	-0.03552600
C	-1.24140600	-1.17807400	2.00542500
C	0.61852000	1.53488700	-2.28471400
C	2.06898700	-1.98725600	0.11098700
C	0.54064400	1.46280000	1.50645900
C	3.01240900	-2.34594200	1.07337300
C	0.21757000	1.51836200	2.86855300
C	1.81697700	1.85405500	1.09201900
C	3.47362400	-0.32790800	-0.72885200
C	4.22824900	-1.67192200	1.09627500
C	1.15768500	1.95625400	3.79622000
C	2.75659100	2.28789500	2.02379900
C	4.48966300	-0.66882000	0.18035700
C	2.42965000	2.33878300	3.37527900
C	4.89511300	1.35113200	-1.84341400
H	-4.10226300	-2.86494900	-0.98014000
H	-4.18797900	-2.06843800	-2.55809200
H	-3.50235400	-3.69082800	-2.42783000
H	-2.59864500	-4.46435100	-0.46724900
H	-3.71868200	3.72133700	-2.47476200
H	-5.00157100	-1.28662400	1.09686200
H	-0.83426600	-5.54543500	0.84549600
H	-4.00167500	5.46037700	-0.72599000
H	-4.05350400	-2.96000700	2.66252800
H	-3.54213800	0.42970800	0.08304400
H	-2.24295900	1.78170400	-2.06818800
H	-1.19091600	0.03198900	-2.03135900
H	-2.79562600	5.24341600	1.43239700
H	1.39315400	-4.42895200	1.09862400
H	-1.63402900	-2.89757800	3.22402600
H	-1.32744400	3.31159800	1.84359400
H	-0.17935800	-1.17131500	2.23842000
H	2.79681900	-3.12379000	1.79240900
H	-0.76767400	1.20713800	3.20399300

H	2.07905900	1.81267200	0.03864600
H	2.94409700	0.71700300	-2.36608100
H	4.98183400	-1.93823900	1.83115700
H	0.89815500	1.99260200	4.84944000
H	3.74645700	2.58394300	1.69023700
H	4.76803800	2.09323000	-2.63126800
H	5.43930500	-0.14995600	0.17026100
H	5.22010100	1.87672600	-0.93904300
H	5.68852000	0.65272200	-2.14162200
H	3.16336200	2.67495900	4.10122200
N	-2.27254100	-2.08447300	-1.75629700
N	-0.17160900	-2.09193000	-0.78438900
N	2.28961100	-0.96524100	-0.73956100
N	3.62771200	0.69451400	-1.62412500
O	0.82796300	2.55062800	-2.79407200
P	-0.66348100	0.91348600	0.23243800
Ru	0.25297600	-0.10753900	-1.49373700

I3_out



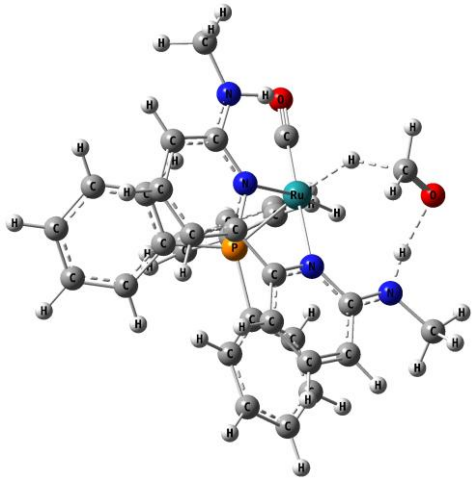
SCF Done	: -1928.74940
SCF Done for solvent	: -1928.77092
Zero-point correction	: 0.555411
Total Electronic Energy	: -1928.19399
Total Thermal Energy	: -1928.15826
Total Thermal Free Energy	: -1928.26255

Atom	X	Y	Z
C	-4.66571300	0.90614100	-1.89354000
C	-4.28068500	-1.44288700	-0.25903200
C	-3.19867000	-0.79750300	-0.90317400
C	1.05164600	4.73610000	-1.28268600
C	-4.02532300	-2.56476000	0.49759800
C	-3.13828400	2.35430200	2.09581100
C	1.56252300	5.43587000	-0.19542300
C	-3.57794000	1.24150900	2.80660600

C	0.67993800	3.39876600	-1.14302900
C	-1.93757800	2.31081900	1.39062200
C	1.70358200	4.80032600	1.03873300
C	-2.71597700	-3.02139600	0.64910900
C	-2.80882700	0.08003100	2.80882100
C	0.81818000	2.75807000	0.08924300
C	-1.15457600	1.15108800	1.38917300
C	1.33380100	3.46867200	1.18027700
C	-1.69832100	-2.30939200	0.02352600
C	-1.61197100	0.03482800	2.10234600
C	1.26291100	0.39960900	-2.72763900
C	-0.26904700	-2.67434100	0.23093800
C	1.67450400	0.35056100	1.30284000
C	0.13233400	-3.43097700	1.32837400
C	1.58260800	-0.04110300	2.63990100
C	2.91455200	0.24533900	0.65467400
C	1.90168600	-2.52046500	-0.56692500
C	1.49269300	-3.70380300	1.47550400
C	2.69746200	-0.54742400	3.30905300
C	4.03117100	-0.22994400	1.33234300
C	2.39049200	-3.27539100	0.52150200
C	3.92295400	-0.64141700	2.66060100
C	4.11787700	-2.40742700	-1.63696900
H	-5.09126100	1.27407900	-0.95124300
H	-4.53011400	1.75639700	-2.56167700
H	-5.38670000	0.22088200	-2.35681200
H	-5.28732300	-1.06478900	-0.38102100
H	0.94486900	5.22540500	-2.24558700
H	-3.73058700	3.26414200	2.08900400
H	-4.84482700	-3.09153200	0.97685500
H	-2.54710200	0.64443300	-2.13774100
H	1.85552400	6.47532100	-0.30628200
H	-4.51431300	1.27749200	3.35434300
H	-1.61001200	3.18396400	0.83404600
H	0.28132100	2.84290200	-1.98669900
H	-0.88183300	0.96341200	-2.45433000
H	2.10488900	5.34369500	1.88854800
H	-2.49771900	-3.91248300	1.22172700
H	-3.14457200	-0.80011000	3.34888900
H	1.44956600	2.97116900	2.14011000
H	-1.02953900	-0.88177000	2.10281200
H	-0.58370200	-3.76295500	2.06831400
H	0.64559700	0.06205600	3.17650500
H	3.00222800	0.53980300	-0.38943000
H	2.24826700	-1.67167600	-2.35141900
H	1.84524200	-4.26076900	2.33799200
H	2.60569500	-0.85147900	4.34731700
H	4.99074500	-0.27324600	0.82521800
H	4.53523800	-1.92001500	-2.51800400
H	3.44839000	-3.48660400	0.61011500
H	4.65572000	-2.03770500	-0.75619600
H	4.29063600	-3.48880500	-1.72021300

H	4.79281200	-1.02144300	3.18737200
N	-3.38504100	0.28208300	-1.68759500
N	-1.93114700	-1.24004300	-0.75677100
N	0.60330300	-2.18290700	-0.66321400
N	2.71808700	-2.07846200	-1.55483800
O	2.15489000	0.81797600	-3.34151600
P	0.29283600	1.00374700	0.26342100
Ru	-0.14242900	-0.27071700	-1.78113200
H	-0.54635000	-1.05573600	-3.12001800

TS1_out



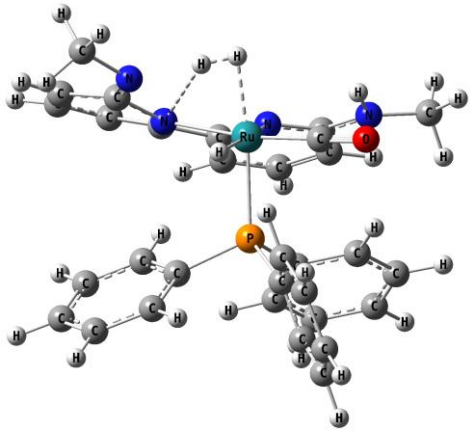
SCF Done	:-2043.19421
SCF Done for solvent	:-2043.21802
Zero-point correction	:0.585502
Total Electronic Energy	:-2042.60871
Total Thermal Energy	:-2042.57093
Total Thermal Free Energy	:-2042.67974

Atom	X	Y	Z
C	-4.42905800	-1.91037100	-1.11778800
C	-2.93442800	-2.70548900	1.15151900
C	-2.30171000	-2.09579700	0.03297400
C	-1.20143400	4.35922900	-2.24156200
C	-2.16288300	-3.17903800	2.18297600
C	-4.05109500	1.00261600	1.37310800
C	-0.91567700	5.48207100	-1.47246000
C	-3.99998200	0.37451900	2.61556400
C	-0.94668700	3.08370900	-1.74262400
C	-2.87648400	1.28566400	0.68348700
C	-0.37586800	5.32678500	-0.19766800
C	-0.77327500	-3.04204000	2.13931200
C	-2.76879800	0.01338900	3.15357700
C	-0.40994300	2.91871100	-0.46111600

C	-1.63380600	0.94555300	1.22818900
C	-0.12539800	4.05468100	0.30532900
C	-0.21573600	-2.38150800	1.05290100
C	-1.59252900	0.28336200	2.45911500
C	0.98937200	0.62101100	-2.56864500
C	1.26524700	-2.21528600	0.94266700
C	1.23674700	1.47215500	1.39989800
C	2.13175300	-2.58394200	1.97001400
C	1.07834000	1.95652800	2.70489600
C	2.52564500	1.18978400	0.93586200
C	3.04167800	-1.67425300	-0.45495700
C	3.50249700	-2.49917800	1.74073800
C	2.18457200	2.12754700	3.53183800
C	3.63117500	1.36105200	1.76428300
C	3.97992600	-2.07500700	0.51599500
C	3.46171800	1.82232500	3.06613400
C	4.79311400	-1.18965600	-2.11872600
H	-4.95016900	-1.32342500	-0.35138800
H	-4.76150500	-1.57389000	-2.10007000
H	-4.71738200	-2.96524300	-1.00251300
H	-4.01030500	-2.81490600	1.16731600
H	-1.61732800	4.47041100	-3.23771000
H	-5.00734300	1.27896700	0.93943400
H	-2.63370100	-3.67169000	3.02850300
H	-2.53110400	-1.69907400	-1.99216300
H	-1.10674100	6.47564000	-1.86571200
H	-4.91613900	0.15986300	3.15678300
H	-2.92662700	1.76942000	-0.28801400
H	-1.16581300	2.21121900	-2.34935100
H	-1.16482000	0.14286600	-2.02573300
H	-0.14353500	6.19841400	0.40599300
H	-0.15790300	-3.45355300	2.92633200
H	-2.71936300	-0.49966800	4.10936900
H	0.30594900	3.94960500	1.29539500
H	-0.64134500	-0.03558100	2.87534800
H	1.76067500	-2.92947400	2.92424400
H	0.08752500	2.20102700	3.07681400
H	2.65892400	0.83836700	-0.08453400
H	2.68129100	-1.13180700	-2.35138400
H	4.19988200	-2.78530400	2.52187300
H	2.04847700	2.50154700	4.54169900
H	4.62331800	1.12656700	1.39059900
H	4.82784100	-0.76837600	-3.12310500
H	5.04164400	-2.03520000	0.30873900
H	5.42097800	-0.56625800	-1.47312700
H	5.22034900	-2.20110400	-2.14672300
H	4.32152500	1.95070400	3.71625600
N	-3.00178300	-1.70627500	-1.04542600
N	-0.95779100	-1.89636700	0.03579800
N	1.72004700	-1.72052400	-0.21926400
N	3.42280400	-1.17544000	-1.66465000
O	1.52682300	1.30617500	-3.32814600

P	-0.13291700	1.21852400	0.20003200
Ru	0.11524900	-0.48030400	-1.39154500
H	0.05667200	-1.65405100	-2.67822500
C	-0.87846100	-2.57272200	-3.22846500
H	-0.76967700	-3.29969900	-2.39791800
H	-0.19382100	-2.80252500	-4.06596800
O	-2.00829200	-2.06323100	-3.47772400

TS2_out



SCF Done : -1928.69807
SCF Done for solvent : -1928.71576
Zero-point correction : 0.550431
Total Electronic Energy : -1928.14764
Total Thermal Energy : -1928.11252
Total Thermal Free Energy : -1928.215

Atom	X	Y	Z
C	-4.60591600	1.63251100	-2.42141600
C	-4.67657900	0.11436100	-0.00134700
C	-3.50852700	0.26927300	-0.83739100
C	2.55961600	4.02418500	-1.59255100
C	-4.69752900	-0.85064700	0.96671400
C	-1.19547100	3.55186700	2.66768300
C	3.60433200	4.30914900	-0.72022100
C	-2.04648900	2.75382800	3.42483700
C	1.69561500	2.96247200	-1.32930600
C	-0.34171500	2.97765200	1.72845900
C	3.78468900	3.53239000	0.42294100
C	-3.58606200	-1.69863700	1.16219400
C	-2.04115000	1.37298200	3.24233400
C	1.87371800	2.17554800	-0.18934500
C	-0.32883900	1.59260300	1.54010900
C	2.92500200	2.47280800	0.68801400
C	-2.45045300	-1.42750300	0.42086400

C	-1.19074400	0.79764900	2.30594900
C	0.95060000	0.14828500	-2.66170800
C	-1.23802900	-2.28664500	0.49900400
C	1.81641700	-0.35957300	1.06662000
C	-0.98319500	-3.12702800	1.57897600
C	1.72966500	-0.71767900	2.41239000
C	2.84571300	-0.89971000	0.28257700
C	0.66565500	-3.00931900	-0.61609200
C	0.15407200	-3.93118400	1.53238200
C	2.64859000	-1.61280200	2.96302300
C	3.77195100	-1.77352100	0.83923600
C	0.98297400	-3.90138100	0.42761300
C	3.66975300	-2.13933400	2.18140500
C	2.54380500	-3.78289300	-2.01057600
H	-4.91685200	2.45197800	-1.75529900
H	-4.39811700	2.07358500	-3.39940500
H	-5.47211700	0.96045600	-2.53490700
H	-5.53841400	0.74633000	-0.17798000
H	2.41257900	4.62529100	-2.48403700
H	-1.19599300	4.62886200	2.80127000
H	-5.59165000	-0.99020500	1.56873500
H	-2.21033700	0.14947300	-2.74079500
H	4.27816600	5.13428700	-0.92854700
H	-2.71563400	3.20466000	4.15075700
H	0.30771100	3.61537200	1.13796300
H	0.87617800	2.74768600	-2.00708300
H	-0.81127000	1.47404200	-1.85706400
H	4.59689100	3.75138700	1.10876400
H	-3.63631400	-2.55075500	1.82672100
H	-2.70800600	0.73875500	3.81771100
H	3.07088600	1.87182400	1.58147600
H	-1.20299100	-0.27866800	2.17458200
H	-1.64204700	-3.13436600	2.43774800
H	0.95727900	-0.29040700	3.04322800
H	2.92590100	-0.62753300	-0.76744700
H	1.02082300	-2.38016800	-2.49026200
H	0.39172000	-4.58661900	2.36462300
H	2.56867200	-1.88454300	4.01093600
H	4.58119500	-2.16148400	0.22765000
H	2.98623700	-3.49787800	-2.96523600
H	1.86593500	-4.52506100	0.37192600
H	3.31526500	-3.68843900	-1.23820600
H	2.23611600	-4.83590400	-2.06604300
H	4.39127100	-2.82465100	2.61518500
N	-3.42199800	0.95715200	-1.94772400
N	-2.36874400	-0.40843800	-0.45105400
N	-0.40740100	-2.20618800	-0.55755500
N	1.44245800	-2.89559300	-1.73108600
O	1.86733100	0.22209300	-3.35982600
P	0.68931700	0.82728300	0.21784100
Ru	-0.52490400	-0.01920900	-1.55003500
H	-1.62471100	-0.40490000	-3.04271100

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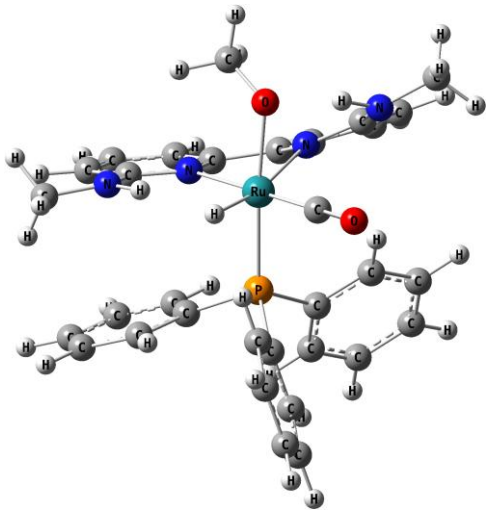

SCF Done	:-2043.24329
SCF Done for solvent	:-2043.26483
Zero-point correction	:0.591047
Total Electronic Energy	:-2042.65224
Total Thermal Energy	:-2042.61425
Total Thermal Free Energy	:-2042.722

Atom	X	Y	Z
C	2.20585300	3.75662600	-2.11565100
C	0.65268500	4.13085900	0.29358800
C	0.46637800	3.00975800	-0.54939100
C	3.38629800	-3.08388400	-2.31198100
C	-0.07774600	4.20560900	1.45818500
C	4.11961000	1.89903200	0.45400500
C	4.05263900	-3.92367100	-1.42653500
C	3.80878600	2.63726500	1.59426100
C	2.46385200	-2.15344200	-1.83613100
C	3.30398100	0.84201300	0.05984700
C	3.79724100	-3.83075300	-0.05993200
C	-0.98303300	3.19455000	1.78642400
C	2.67603500	2.31390300	2.33547600
C	2.20468200	-2.05119600	-0.46610900
C	2.16732000	0.50672000	0.80316800
C	2.88090300	-2.90015500	0.41720600
C	-1.12024700	2.12682800	0.90895100
C	1.85733400	1.26005100	1.94003700
C	-0.71066400	-1.61068200	-2.16968400
C	-2.15070200	1.06786200	1.12249500
C	0.30721300	-1.56849900	1.64505400
C	-2.93647200	0.96273900	2.26583800
C	0.92913200	-1.59986300	2.89939000
C	-0.93397300	-2.19683700	1.49216200

C	-3.42588900	-0.51033700	-0.02515300
C	-3.98041800	0.03362100	2.24425900
C	0.31300900	-2.22765500	3.97861200
C	-1.54954300	-2.82353500	2.57188100
C	-4.26681200	-0.68595300	1.09869000
C	-0.93051600	-2.83460100	3.81804000
C	-4.80742400	-1.83857500	-1.52958200
H	3.00303200	3.80003200	-1.36149200
H	2.63045300	3.38033500	-3.04626000
H	1.83818400	4.77329600	-2.29839700
H	1.35719100	4.90564500	0.02006600
H	3.57403000	-3.15507600	-3.37852300
H	5.00313800	2.14265100	-0.12840000
H	0.04682100	5.05768500	2.11962700
H	0.98256400	2.00215000	-2.20978300
H	4.76519400	-4.65291700	-1.79895900
H	4.44624900	3.46023200	1.90181000
H	3.55310100	0.26980700	-0.83010400
H	1.93779900	-1.50383600	-2.52831800
H	0.62623200	0.20384000	-2.40773000
H	4.30951300	-4.48740300	0.63619000
H	-1.58529000	3.25903500	2.68256800
H	2.41575400	2.89171600	3.21711100
H	2.68265000	-2.84604000	1.48288500
H	0.96695600	1.02935700	2.51715600
H	-2.75749200	1.57390900	3.14033500
H	1.89719700	-1.12640400	3.03679700
H	-1.42082500	-2.18972200	0.52054500
H	-3.14263300	-0.52522200	-1.99629300
H	-4.60367500	-0.09254100	3.12459000
H	0.80523100	-2.24064000	4.94606700
H	-2.51865500	-3.29324200	2.43634500
H	-4.77647300	-2.14083600	-2.57632300
H	-5.12016000	-1.35114300	1.05091900
H	-4.84990300	-2.74749600	-0.91866900
H	-5.73212600	-1.26810400	-1.35928400
H	-1.41290700	-3.31686400	4.66242900
N	1.14200000	2.87272300	-1.71116500
N	-0.40676800	2.03417800	-0.23189600
N	-2.33415900	0.26934900	0.06946100
N	-3.61824900	-1.07578900	-1.23921600
O	-0.80417400	-2.63348700	-2.68909000
P	1.02044600	-0.77391800	0.14252700
Ru	-0.55373000	0.03569500	-1.36765300
O	-2.06024800	0.64216200	-2.74104900
C	-2.48354200	1.95761500	-2.62793000
H	-1.66814300	2.68507400	-2.80022100
H	-3.26673400	2.17806000	-3.37236400
H	-2.90905500	2.19774300	-1.63162500

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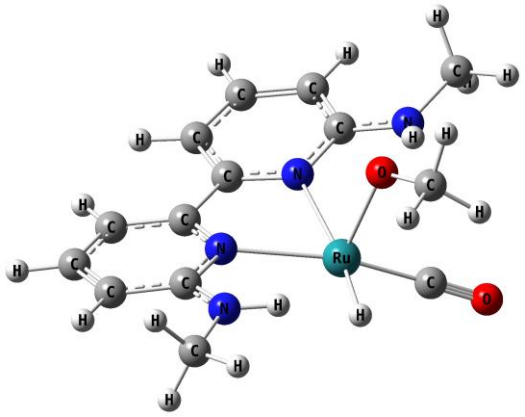

SCF Done	:-1007.20513
SCF Done for solvent	:-1007.22478
Zero-point correction	:0.311414
Total Electronic Energy	:-1006.89372
Total Thermal Energy	:-1006.87208
Total Thermal Free Energy	:-1006.94507

Atom	X	Y	Z
C	-4.48158300	-1.76730100	0.43250500
C	-3.90332600	1.04881100	0.12086800
C	-2.87630900	0.07760000	0.17341400
C	-3.54939000	2.36591500	-0.06974500
C	-2.20562100	2.72797800	-0.18196100
C	-1.24702100	1.72704700	-0.10603400
C	1.33608400	-2.08465600	-1.32218300
C	0.21645000	2.03348200	-0.10830400
C	0.71249700	3.33223800	-0.11966700
C	2.34365100	1.12394300	0.18382900
C	2.09547900	3.50115500	-0.01961700
C	2.92538400	2.41251700	0.14993700
C	4.44090900	0.03335900	0.78929600
H	-5.05615100	-1.55749300	-0.47890000
H	-4.41370600	-2.84797700	0.55341600
H	-5.03175200	-1.36403300	1.29037400
H	-4.93977200	0.75530100	0.22423100
H	-4.32080500	3.12774200	-0.12586700
H	-2.35019200	-1.85803000	0.27214600
H	-0.78757200	-2.38482900	-0.65779400
H	-1.92659600	3.76309800	-0.31928600
H	0.05961100	4.19126600	-0.18631800
H	2.45175100	-0.76235300	0.81055900
H	2.51836700	4.50084600	-0.04042500
H	4.77861200	-0.98554100	0.97851900
H	3.99271700	2.53700400	0.28136600
H	5.04301900	0.43797800	-0.03115400
H	4.63305900	0.63620200	1.68852900
N	-3.14412600	-1.23162500	0.36781600

N	-1.57898900	0.42563100	0.04035200
N	1.02334700	0.96717300	-0.02967400
N	3.04403900	-0.00871200	0.42898900
O	2.11445800	-2.73889500	-1.86804700
Ru	0.08353900	-1.06481000	-0.46730700
O	0.86756800	-1.55553600	1.31875800
C	0.84116800	-2.89859500	1.68346700
H	1.27204300	-3.00131100	2.69091600
H	-0.18060800	-3.30836000	1.71622700
H	1.42594300	-3.54061900	1.00204600

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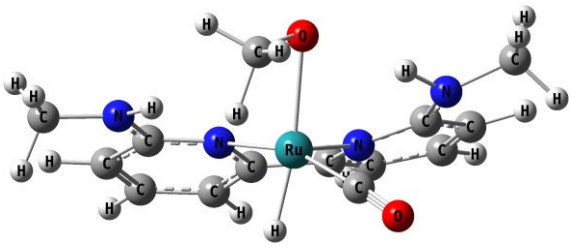
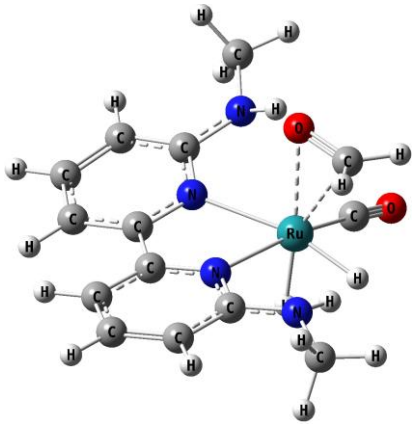


SCF Done	:-1007.20511
SCF Done for solvent	:-1007.22481
Zero-point correction	:0.311292
Total Electronic Energy	:-1006.89382
Total Thermal Energy	:-1006.87214
Total Thermal Free Energy	:-1006.94526

Atom	X	Y	Z
C	-4.48353500	-1.76467000	0.41179500
C	-3.90032700	1.05416300	0.13215600
C	-2.87561900	0.07949600	0.16117900
C	-3.54404500	2.37344700	-0.03758400
C	-2.20006800	2.73350800	-0.15371000
C	-1.24385100	1.72872800	-0.10340700
C	1.35542900	-2.08138400	-1.30782200
C	0.22034700	2.03180200	-0.11170700
C	0.72136800	3.32855000	-0.13616900
C	2.34396900	1.11753200	0.19018800
C	2.10506500	3.49316600	-0.03769300
C	2.93094900	2.40331100	0.14415800
C	4.43516200	0.02062400	0.80909900
H	-5.07133300	-1.53853600	-0.48704800
H	-4.41713800	-2.84739200	0.51383400
H	-5.01937800	-1.37393000	1.28451900
H	-4.93678300	0.76163900	0.23820200
H	-4.31357900	3.13851100	-0.07303800
H	-2.35285600	-1.85882500	0.23270300

H	-0.78767400	-2.38213000	-0.68587800
H	-1.91898400	3.77059500	-0.27048300
H	0.07202300	4.18931400	-0.21477800
H	2.44142600	-0.76628600	0.82727700
H	2.53184000	4.49091300	-0.07035600
H	4.76363100	-0.99770600	1.01655300
H	3.99887700	2.52466300	0.27403200
H	5.04161800	0.40566700	-0.01760100
H	4.63143000	0.63721500	1.69796800
N	-3.14578000	-1.23197600	0.33429900
N	-1.57830300	0.42608800	0.02502000
N	1.02381000	0.96350300	-0.02508400
N	3.03830200	-0.01559700	0.44883000
O	2.15799000	-2.72209300	-1.83420400
Ru	0.08377000	-1.06450100	-0.47706000
O	0.83644100	-1.55369000	1.32267800
C	0.79549300	-2.89546200	1.69011700
H	1.21454000	-2.99917100	2.70243200
H	-0.22974200	-3.29743400	1.71264900
H	1.38254100	-3.54381000	1.01680400

I4_in

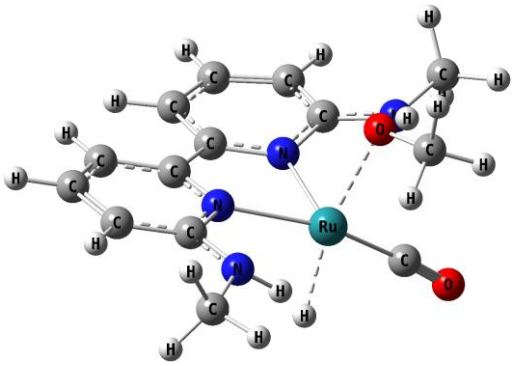


SCF Done	:-1007.21067
SCF Done for solvent	:-1007.22657
Zero-point correction	:0.30945
Total Electronic Energy	:-1006.90123
Total Thermal Energy	:-1006.88009
Total Thermal Free Energy	:-1006.95097

Atom	X	Y	Z
C	-4.60571100	-1.45986500	0.05181600
C	-3.76535100	1.28592900	0.15063500
C	-2.82853600	0.23192900	0.09382300
C	-3.30287800	2.58173700	0.07077200
C	-1.93819000	2.82844400	-0.06204600

C	-1.06961000	1.74334300	-0.09754800
C	1.33028200	-2.30355400	-0.98875200
C	0.40789500	1.93765800	-0.17212300
C	0.99274700	3.19292200	-0.30952800
C	2.47830900	0.91557000	0.12675900
C	2.38352100	3.27707000	-0.25956900
C	3.14384600	2.15105000	-0.01510000
C	4.52641200	-0.25847100	0.78125100
H	-5.09150200	-1.06356300	-0.85012900
H	-4.65570800	-2.54809300	0.02091100
H	-5.17170900	-1.12325000	0.92671100
H	-4.82182100	1.07300800	0.24747000
H	-4.00350200	3.40979800	0.10956100
H	-2.50799400	-1.72364900	-0.16699300
H	-0.23952700	-0.84240900	-1.87342500
H	-1.56944800	3.84265500	-0.11774900
H	0.39739900	4.08325600	-0.45479000
H	2.51657900	-0.92818400	0.87934000
H	2.87039100	4.23968800	-0.38014100
H	4.80500600	-1.28021800	1.03789500
H	4.22011600	2.21126600	0.08237300
H	5.13441500	0.04770300	-0.07557600
H	4.76700100	0.39507300	1.63148000
N	-3.21833500	-1.06984700	0.15121900
N	-1.50663900	0.47160100	-0.00824900
N	1.14724700	0.82714800	-0.04074000
N	3.12322300	-0.24128300	0.43874700
O	2.09819300	-3.03896100	-1.43241700
Ru	0.05972000	-1.13412700	-0.36034100
O	0.55716300	-1.36255900	1.83193700
C	-0.27513000	-2.26808000	1.54805400
H	-1.33825300	-2.13068300	1.79363100
H	-0.92016300	-2.29199300	-0.83744600
H	0.05406700	-3.30405400	1.38819000

TS1_in

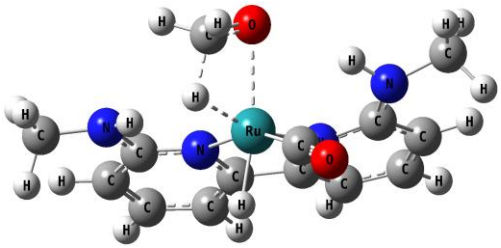


SCF Done	:-1007.17454
SCF Done for solvent	:-1007.19553
Zero-point correction	:0.30848
Total Electronic Energy	:-1006.86606
Total Thermal Energy	:-1006.84472
Total Thermal Free Energy	:-1006.91652

Atom	X	Y	Z
C	-4.53973400	-1.75920300	0.00633700
C	-3.88107400	1.03413200	0.21970300
C	-2.88552400	0.04486400	0.10735500
C	-3.49776700	2.36085400	0.18719400
C	-2.15591400	2.70072600	0.03860700
C	-1.22441100	1.67115100	-0.04403500
C	1.47696400	-1.91973900	-1.24406600
C	0.23573800	1.91739700	-0.13531600
C	0.78342200	3.19076900	-0.19683200
C	2.34887400	0.93567900	0.11787200
C	2.17302600	3.31595200	-0.17320200
C	2.96447300	2.20279100	0.01038400
C	4.41460700	-0.17035900	0.76893600
H	-5.07257800	-1.35699600	-0.86634900
H	-4.52556600	-2.84652800	-0.06468900
H	-5.09653000	-1.49095900	0.90903800
H	-4.92239900	0.75613300	0.31506500
H	-4.24846900	3.14023300	0.26965400
H	-2.47105700	-1.84500300	-0.37769100
H	-0.77320100	-1.40401700	-1.81994000
H	-1.85153100	3.73753300	0.00561700
H	0.15189600	4.06587200	-0.25930900
H	2.37489700	-0.84607100	0.96240000
H	2.63005000	4.29708100	-0.25224900
H	4.72107500	-1.17862100	1.04681600
H	4.03877800	2.28812300	0.10967400
H	5.00940700	0.13320300	-0.09844700
H	4.64533500	0.50690400	1.60362700

N	-3.17464600	-1.28868100	0.09719500
N	-1.58525300	0.37649600	0.01222100
N	1.01563900	0.81456700	-0.10227700
N	3.00830000	-0.19845500	0.44069100
O	2.31424400	-2.42869200	-1.84396400
Ru	0.08111600	-1.01954100	-0.39956800
O	0.82333700	-1.27980400	1.55929100
C	0.54495700	-2.59112600	1.88576600
H	0.35903000	-2.70637300	2.96500300
H	-0.38211100	-2.95705700	1.38159900
H	1.34910000	-3.29648800	1.60152100

TS2_in



SCF Done	:-1007.18695
SCF Done for solvent	:-1007.20627
Zero-point correction	:0.307315
Total Electronic Energy	:-1006.87963
Total Thermal Energy	:-1006.85869
Total Thermal Free Energy	:-1006.92958

Atom	X	Y	Z
C	4.58309400	-1.47361500	-0.21207400
C	3.77575800	1.28164200	-0.08929800
C	2.82672900	0.24005800	-0.15573100
C	3.32663400	2.56925800	0.11658700
C	1.96193200	2.82121900	0.23603300
C	1.08261200	1.75120300	0.11752800
C	-1.40121300	-1.99048100	1.27108500
C	-0.39251700	1.94372900	0.13285600
C	-0.98623700	3.19875100	0.09599400
C	-2.44287200	0.87733200	-0.19542000
C	-2.37446600	3.26816100	-0.02032900
C	-3.11555000	2.11747700	-0.19292200
C	-4.43951900	-0.33404600	-0.92495800
H	5.05651400	-1.16614000	0.73032200
H	4.62345700	-2.56042800	-0.28272300
H	5.16562700	-1.06359800	-1.04341800
H	4.83262500	1.06528300	-0.17342700
H	4.03933200	3.38396800	0.19517400
H	2.49130700	-1.72748000	-0.02771900
H	0.35505600	-0.70490600	1.82669600

H	1.60247000	3.82357100	0.42176900
H	-0.39298600	4.10179100	0.12757000
H	-2.43266200	-1.01177100	-0.85426800
H	-2.86992500	4.23378200	-0.02769600
H	-4.69731300	-1.36762500	-1.15347200
H	-4.18383600	2.15862200	-0.35993300
H	-5.10424100	0.00856000	-0.12605100
H	-4.62097100	0.27837700	-1.81895700
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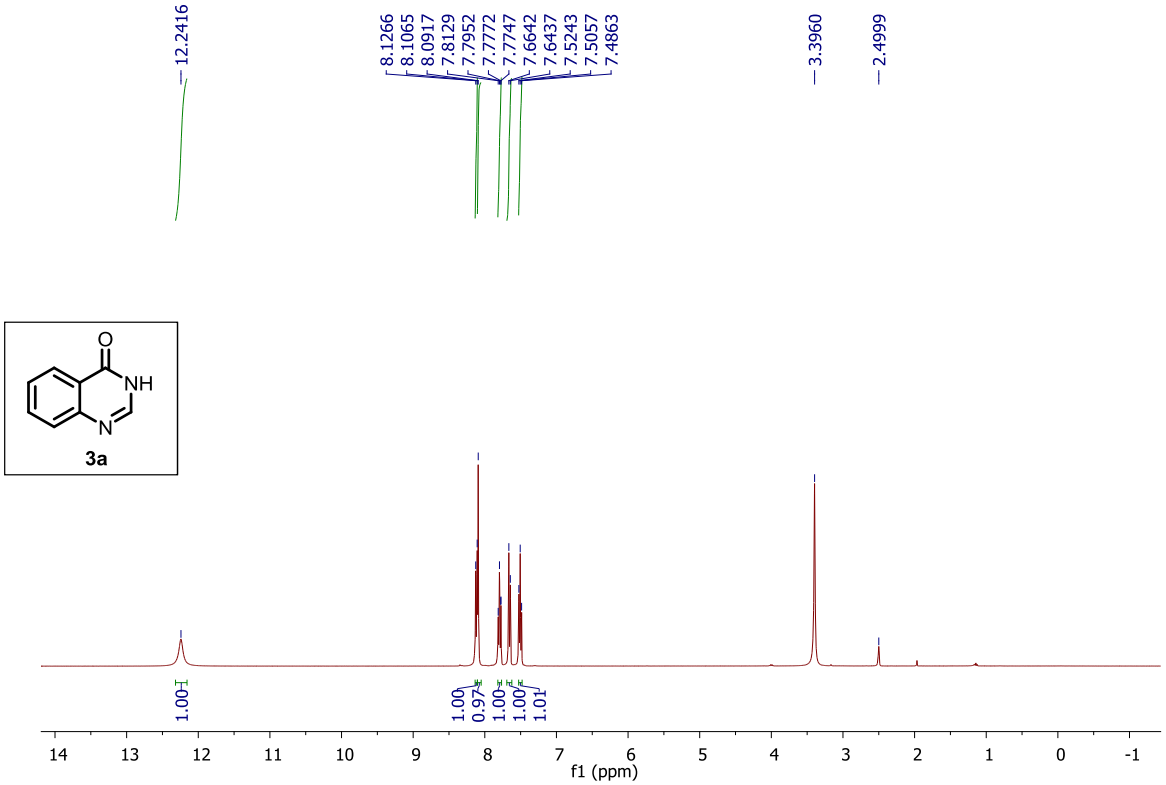
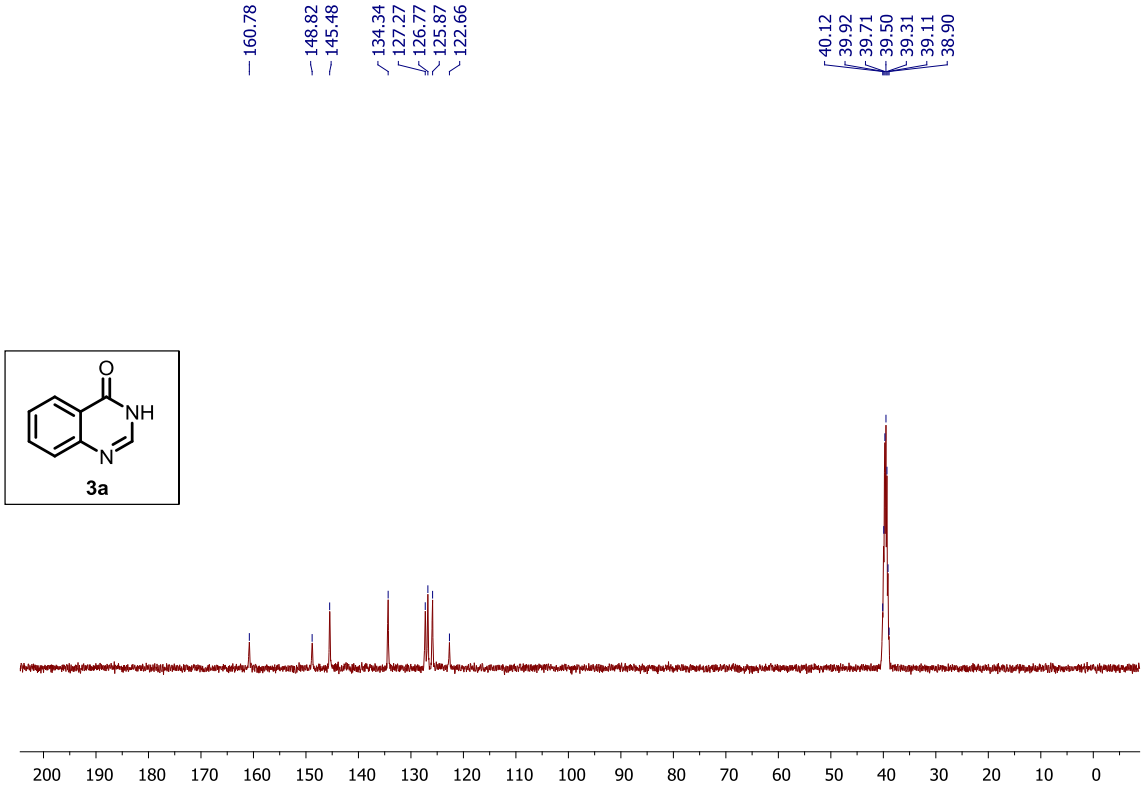
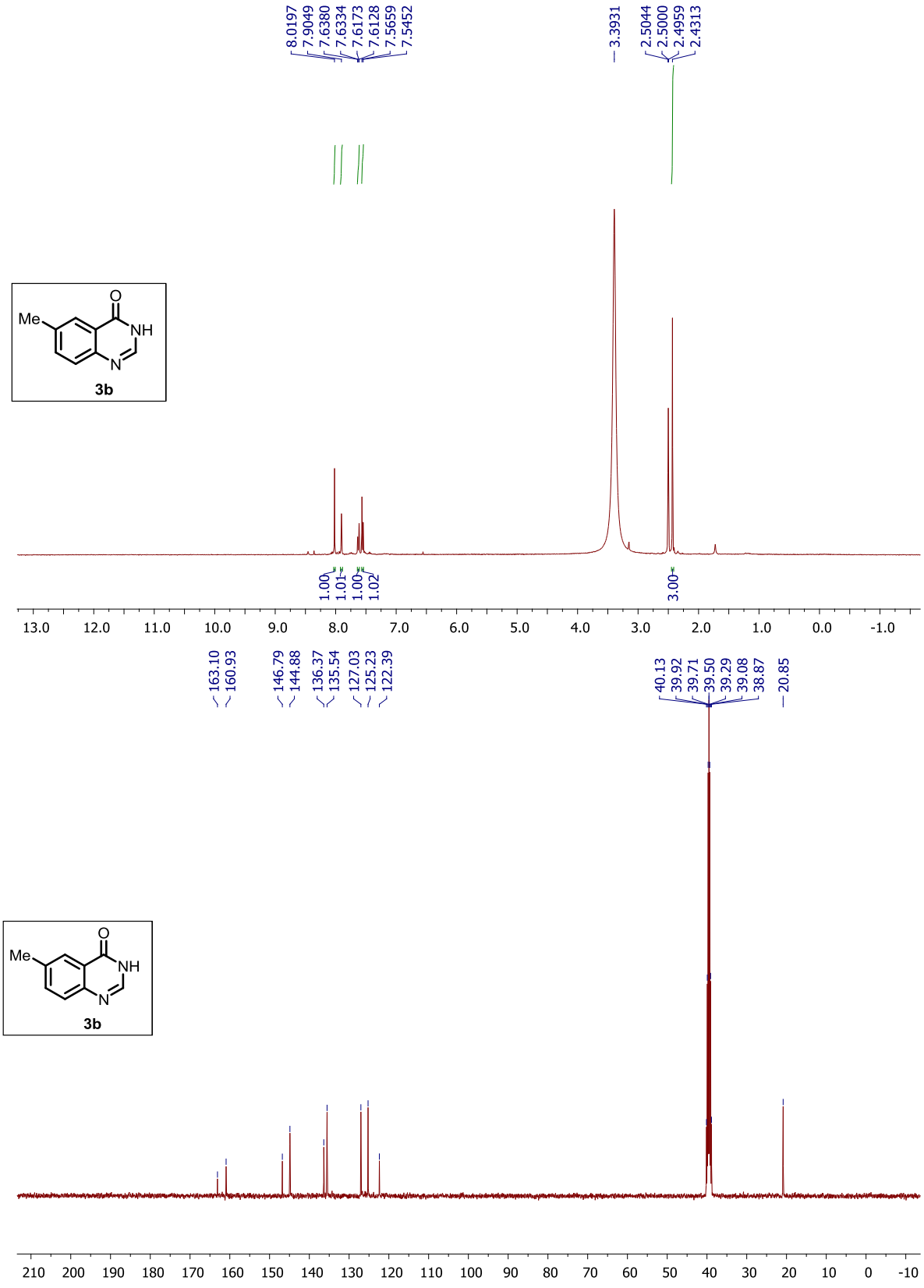
N	1.50673100	0.48773400	-0.08054500
N	-1.12592400	0.81499000	0.09384600
N	-3.06105700	-0.29588800	-0.49136900
O	-2.17102100	-2.54011100	1.93019600
Ru	-0.11044800	-1.04994600	0.35447200
O	-0.43508900	-1.79937800	-1.72249400
C	0.31090000	-2.76195800	-1.26001800
H	1.31896100	-2.87641300	-1.69690300
H	0.74548500	-2.59866000	0.02119600
H	-0.16221000	-3.74088700	-1.06991700

12. Copies of ^{1}H and ^{13}C NMR Spectra of the Products



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2.5000
2.4959
2.4313
Me
NH
N
O
3b
1.00
1.01
1.00
1.02
3.00
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
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160.93
146.79
144.88
136.37
135.54
127.03
125.23
122.39
40.13
39.92
39.71
39.50
39.29
39.08
38.87
20.85
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NH
N
O
3b
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200
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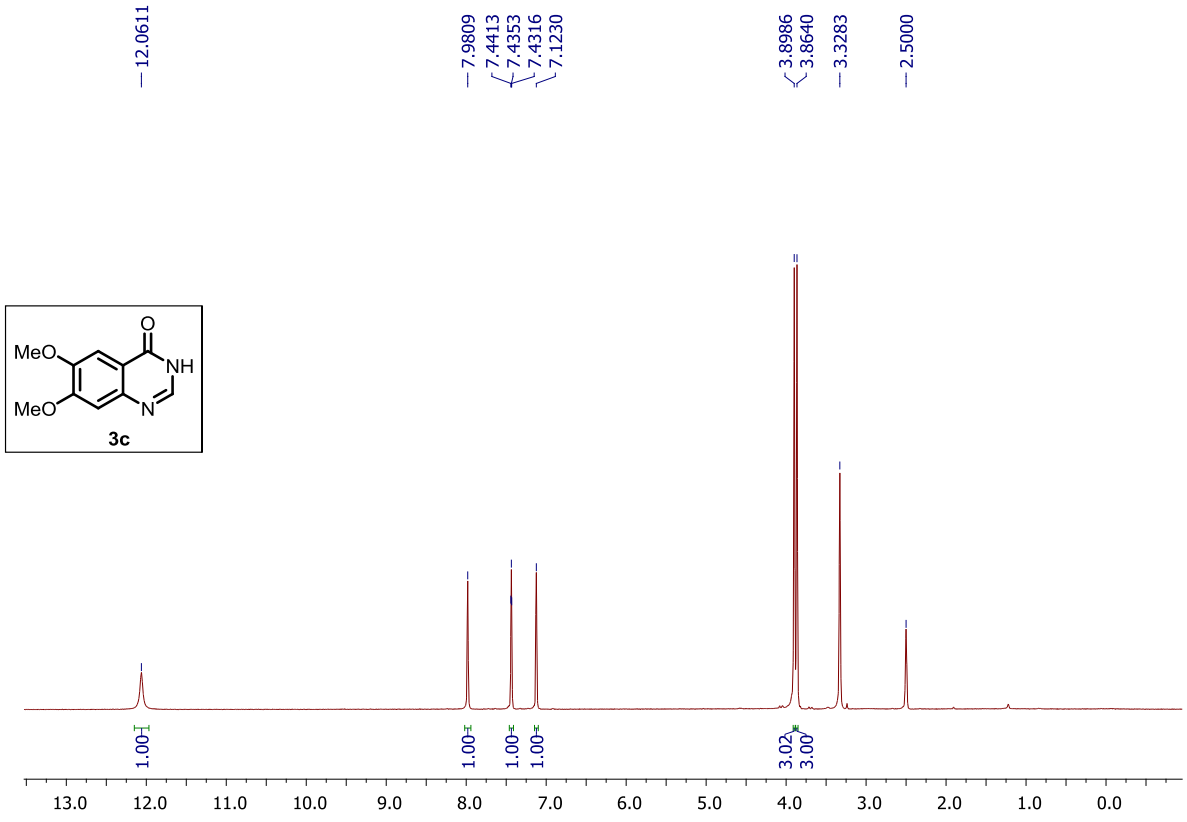
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MeO
NH
N
O
3c
1.00
1.00
1.00
1.00
3.02
3.00
13.0
12.0
11.0
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8.0
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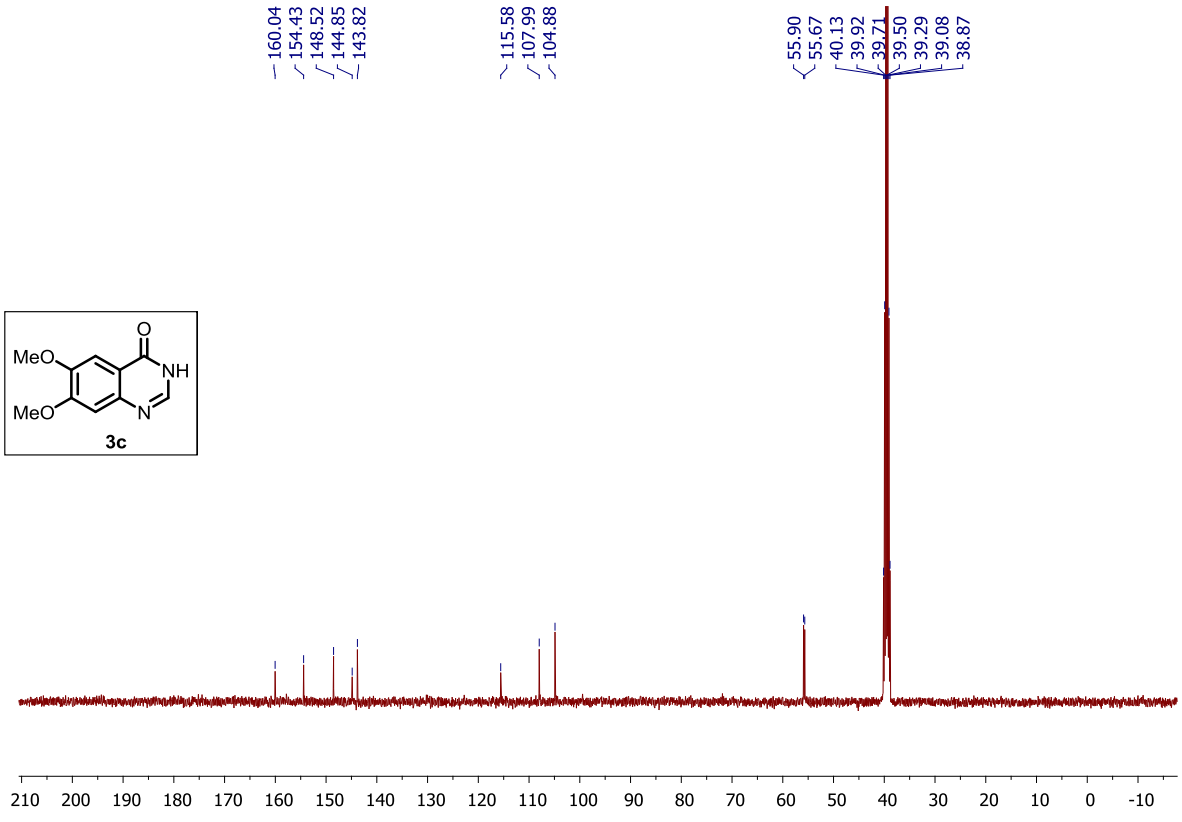
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39.29
39.08
38.87
MeO
MeO
NH
N
O
3c
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200
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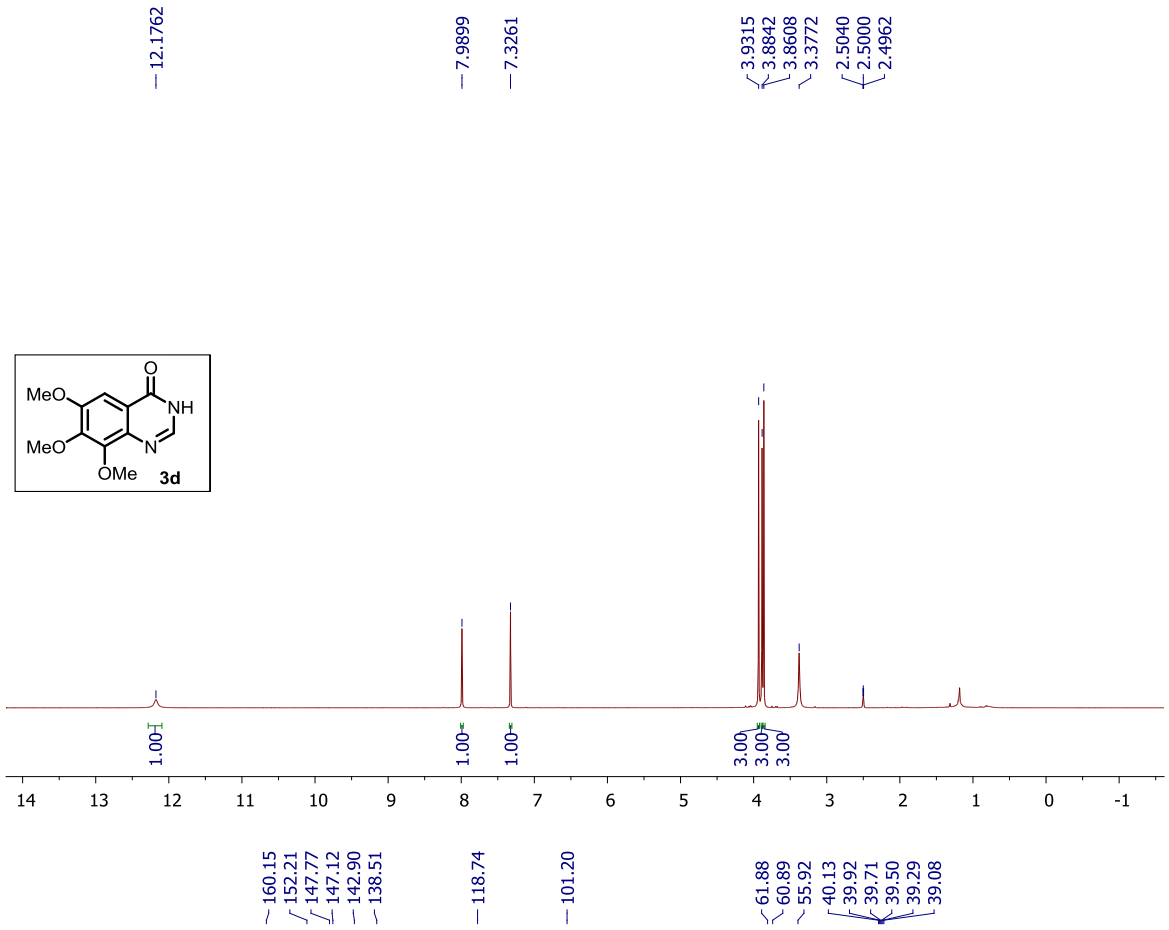
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MeO
MeO
OMe
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1.00
3.00
3.00
3.00
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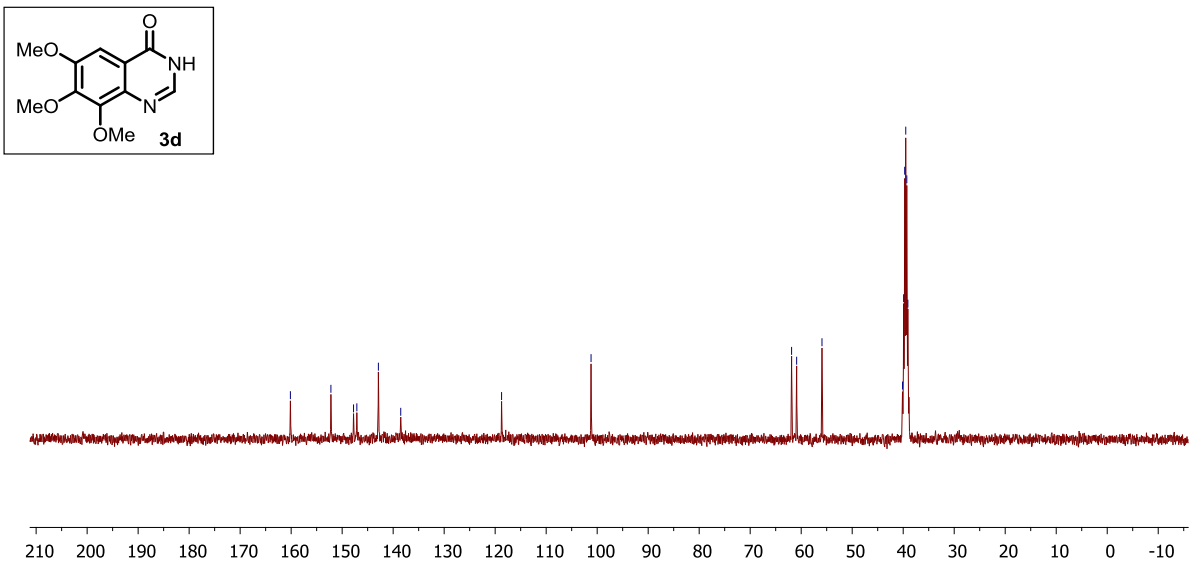
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39.50
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MeO
OMe
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O
N
3d
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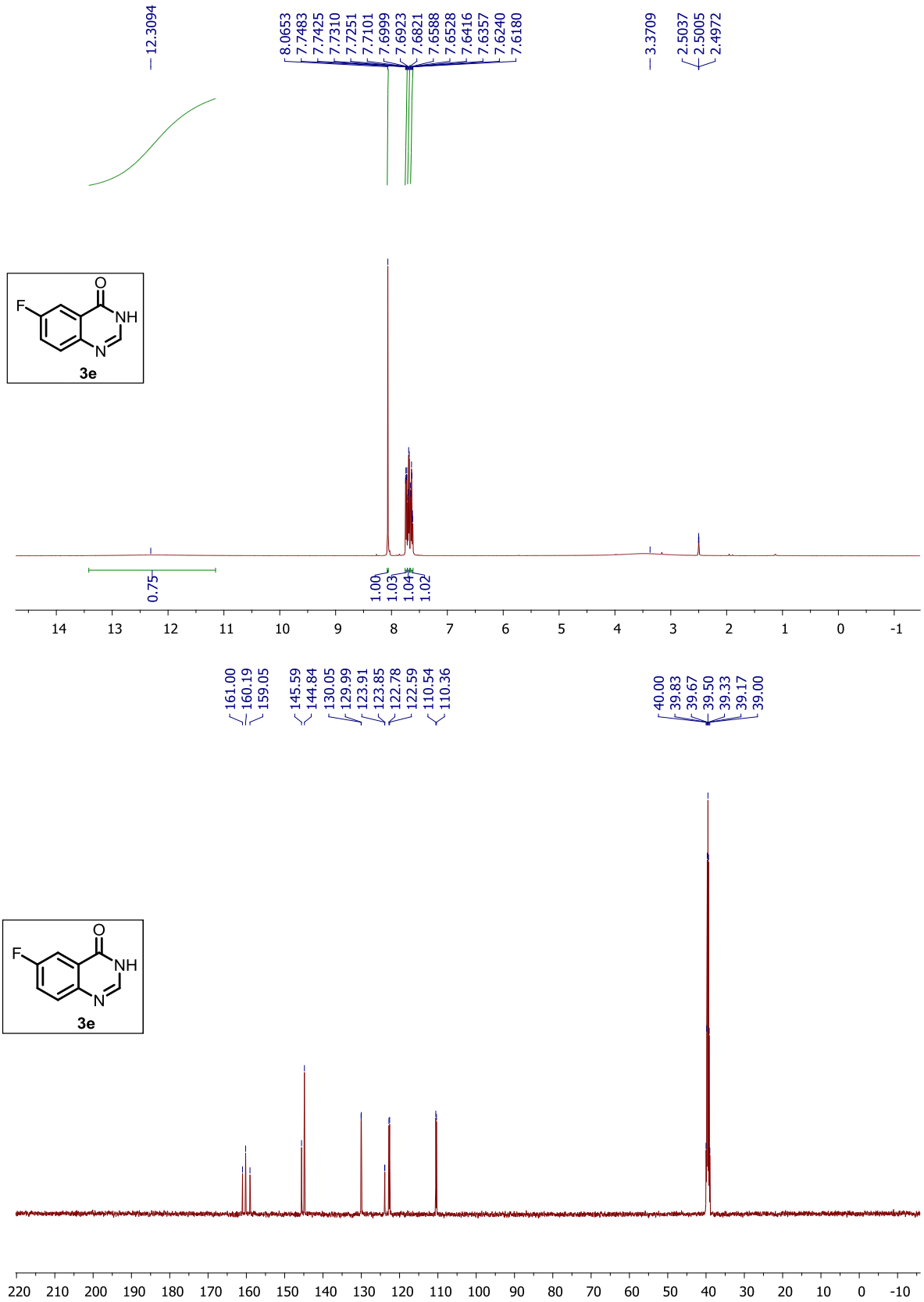
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7.6357
7.6240
7.6180
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2.5037
2.5005
2.4972
F
O
NH
N
3e
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1.03
1.04
1.02
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145.59
144.84
130.05
129.99
123.91
123.85
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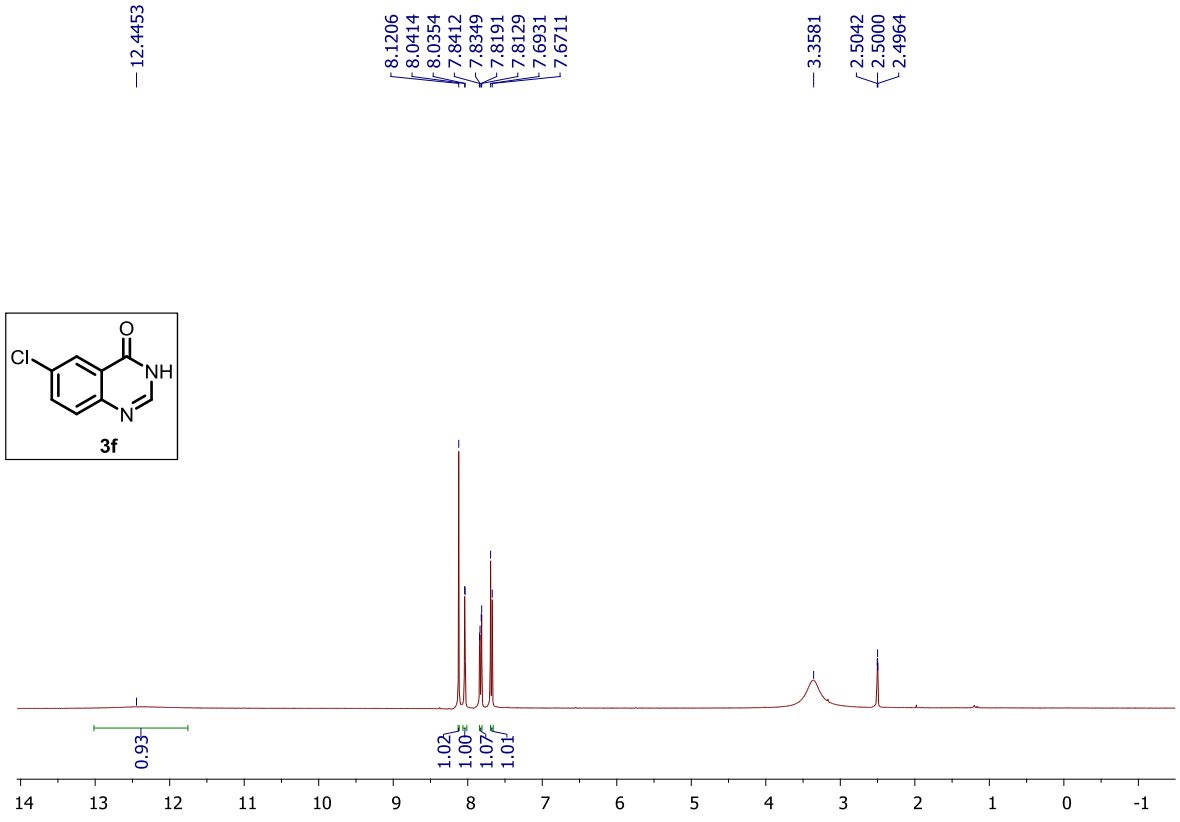
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2.4964
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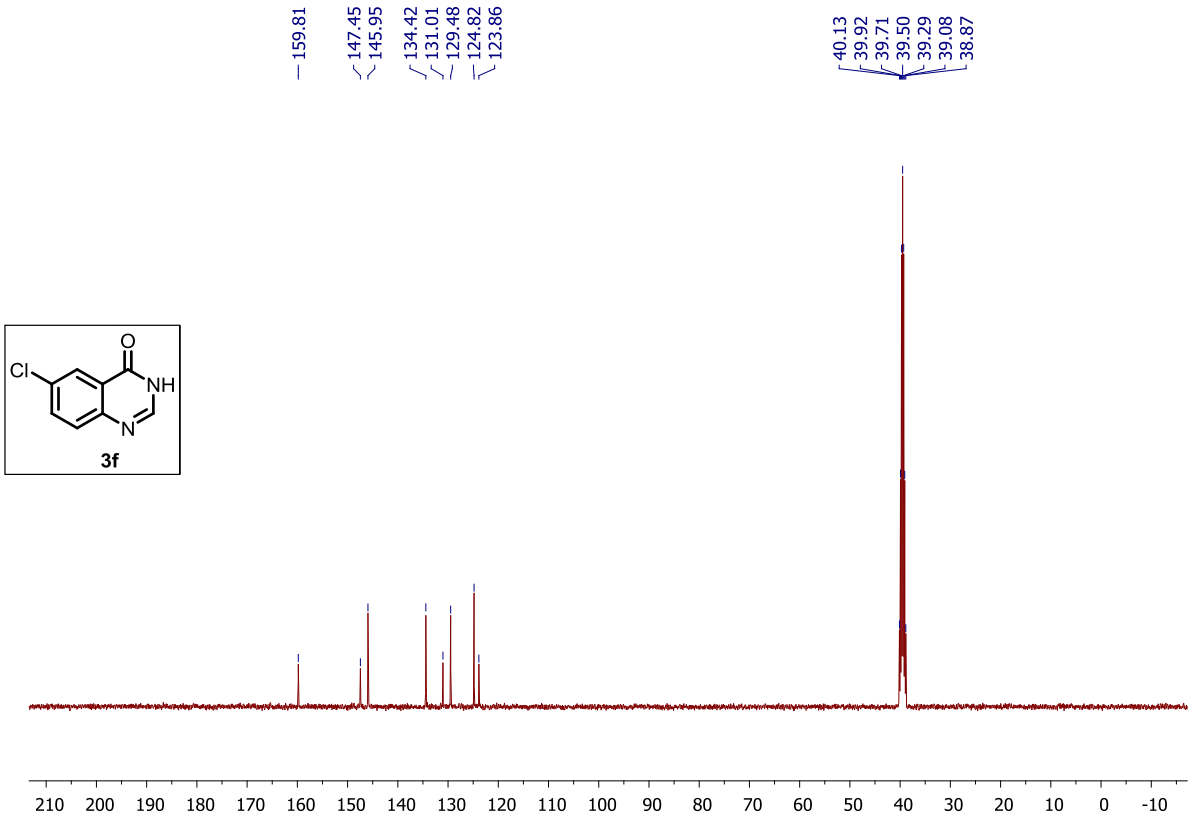
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Cl
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NH
N
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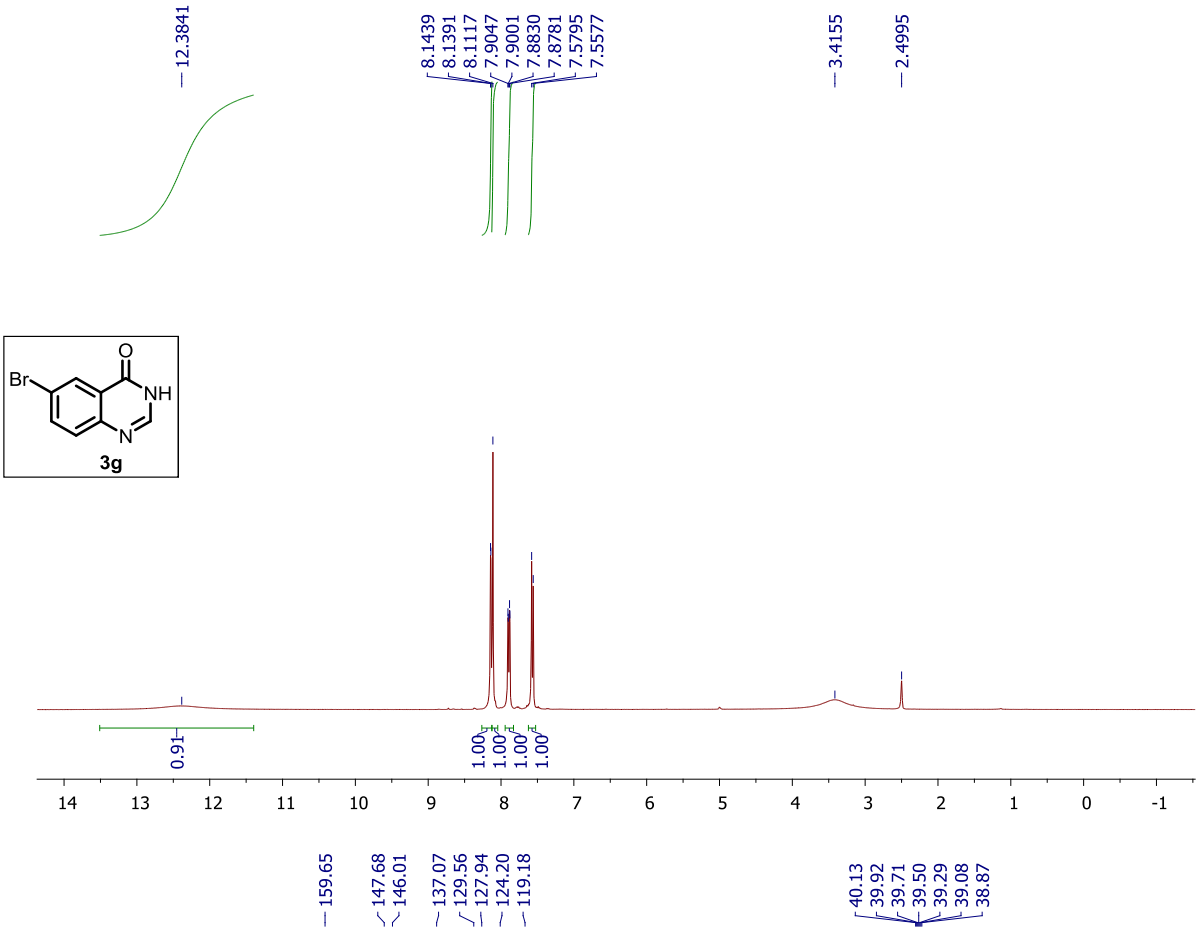
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2.4995
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1.00
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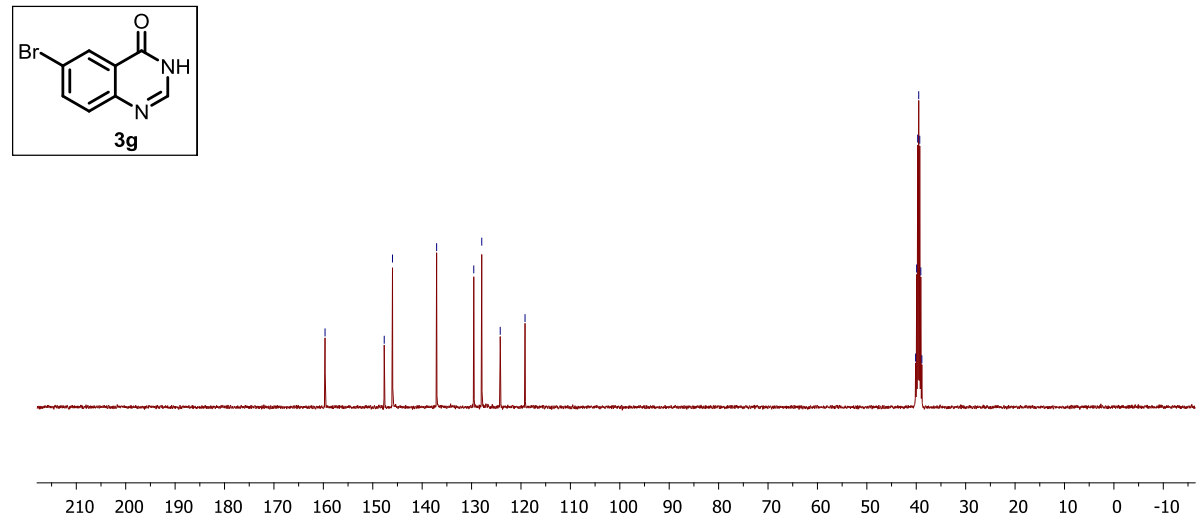
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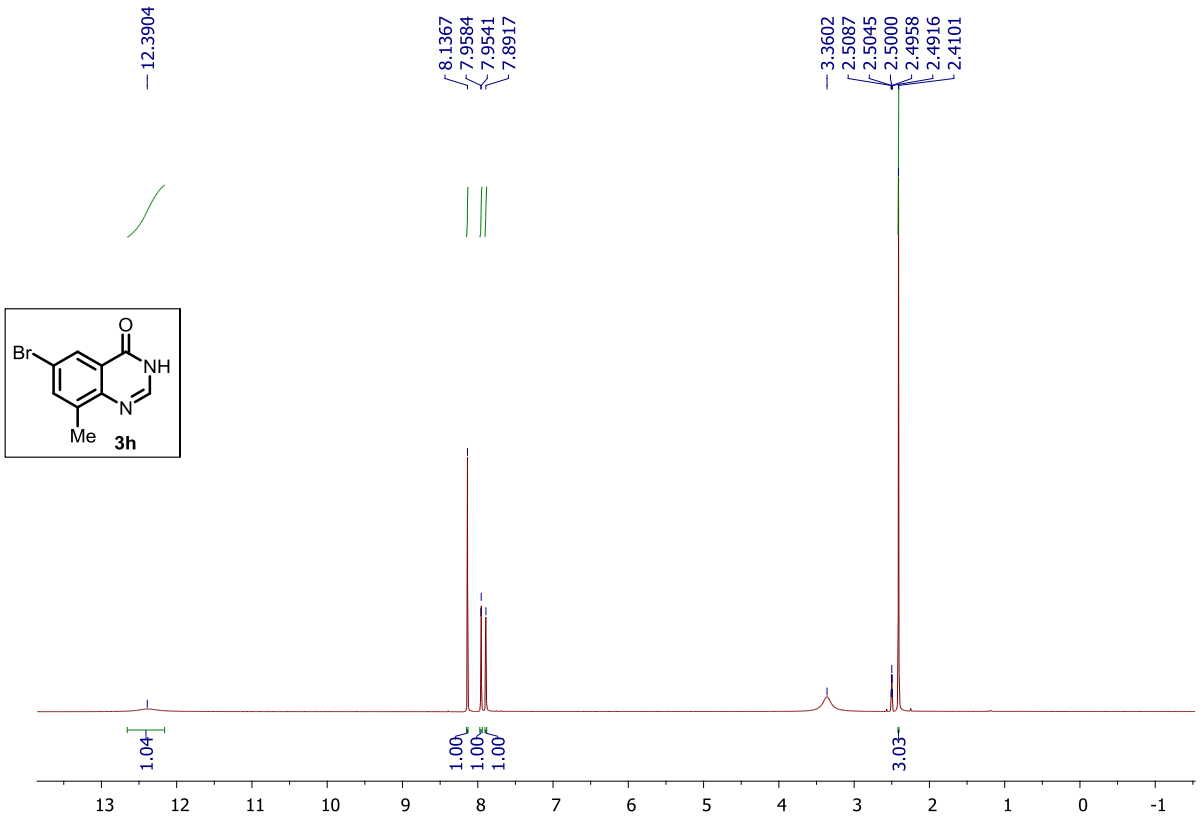
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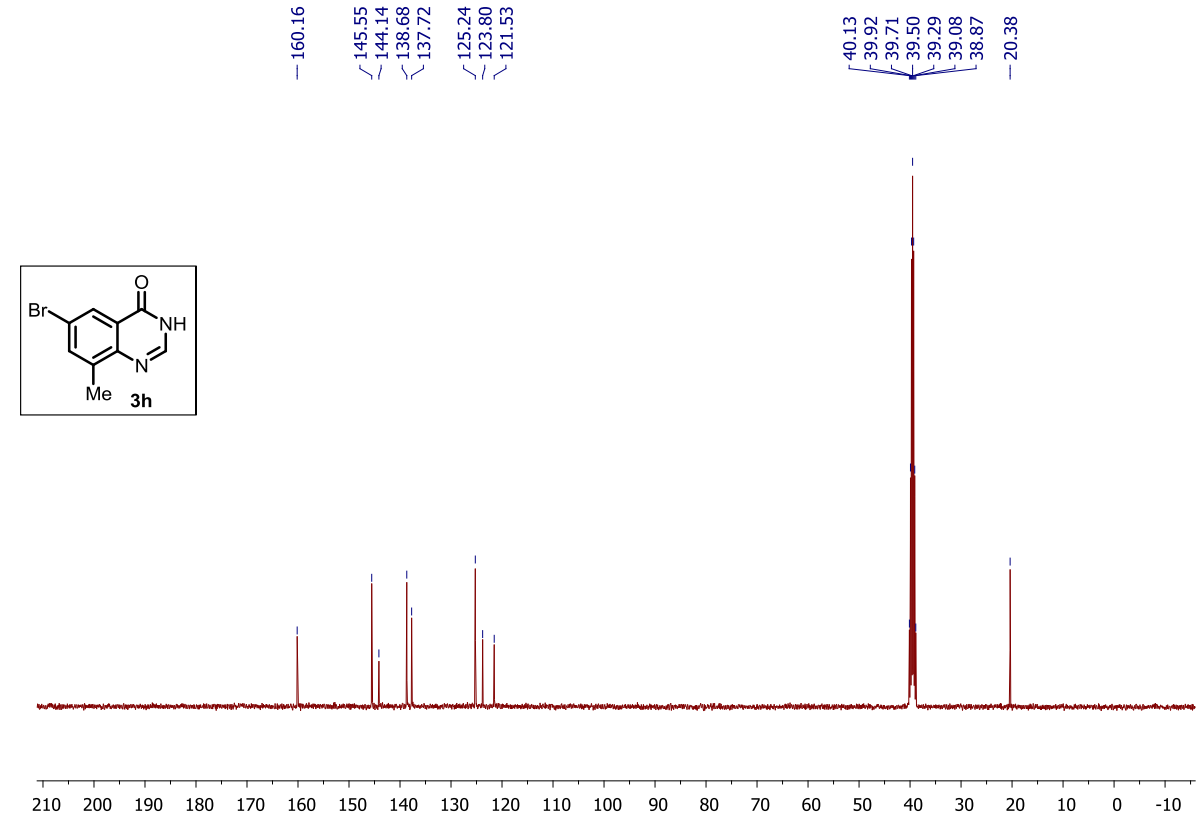
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O
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N
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3h
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200
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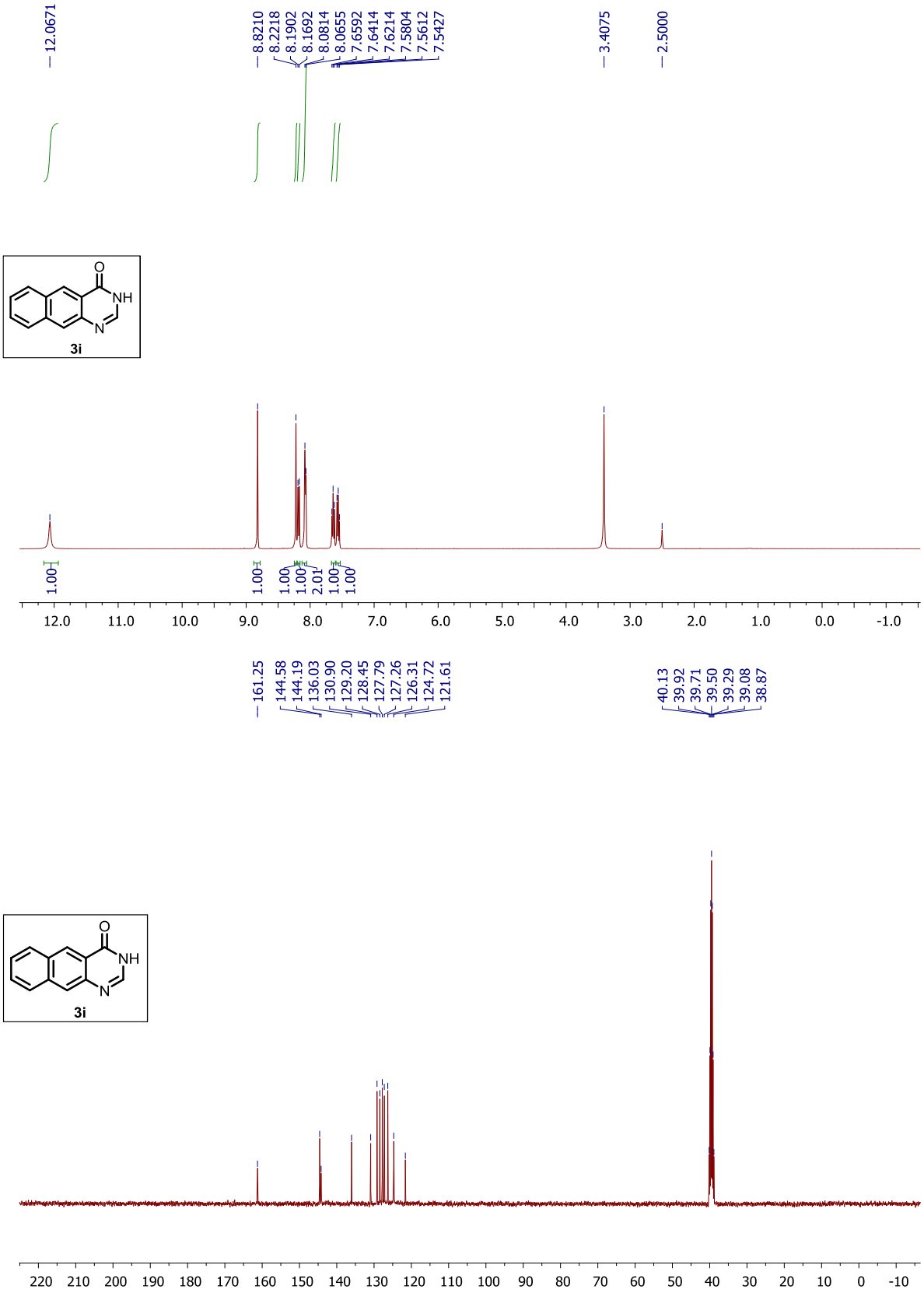
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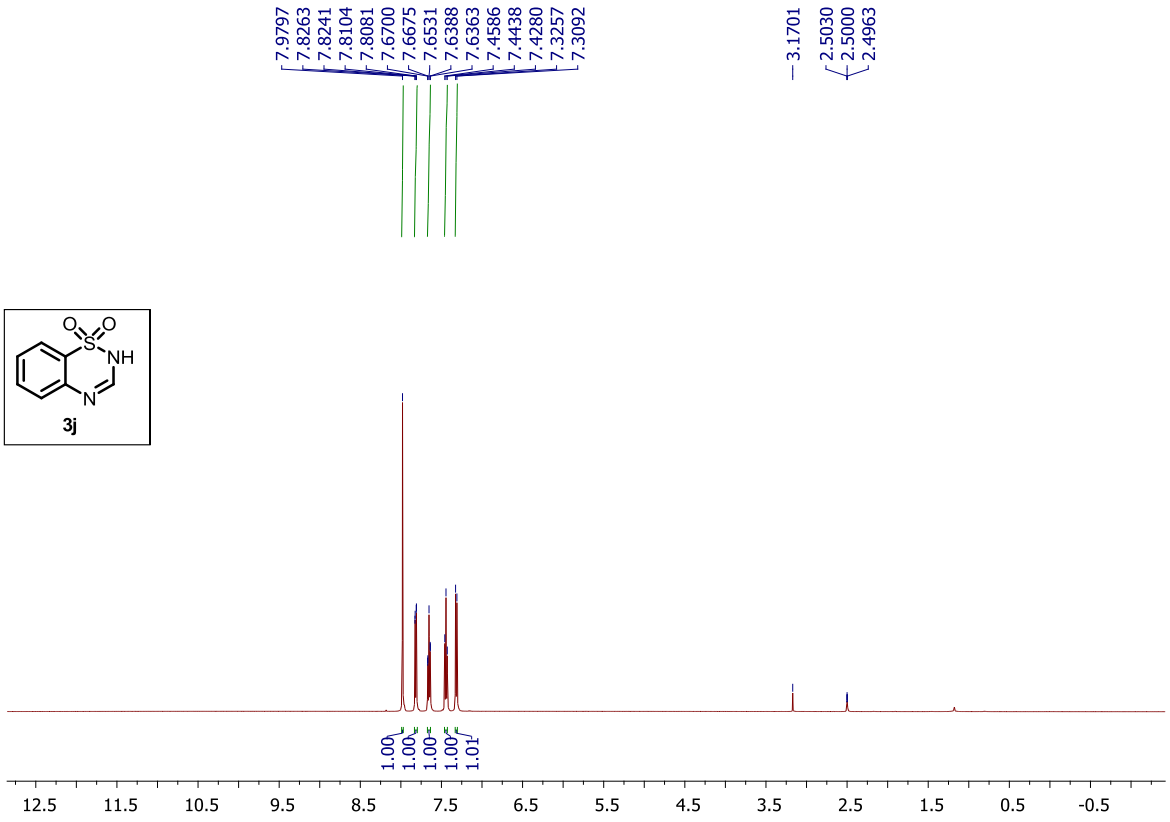
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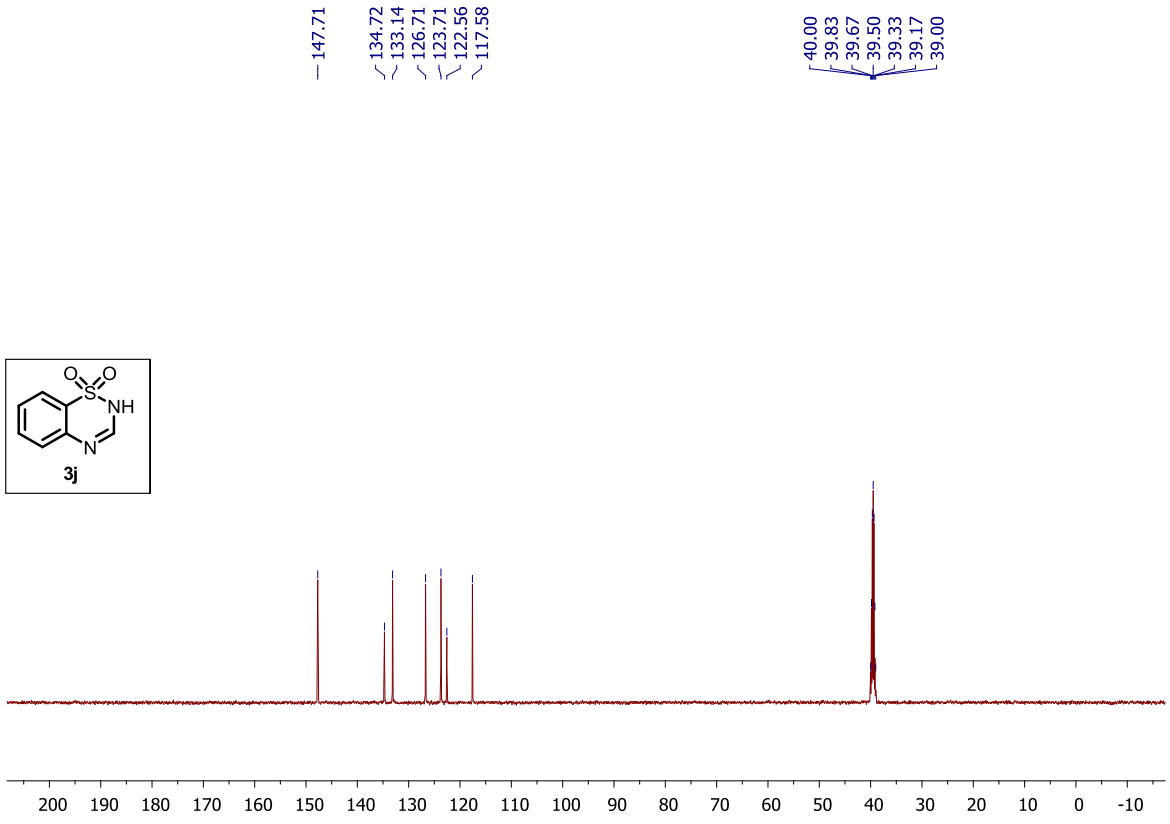
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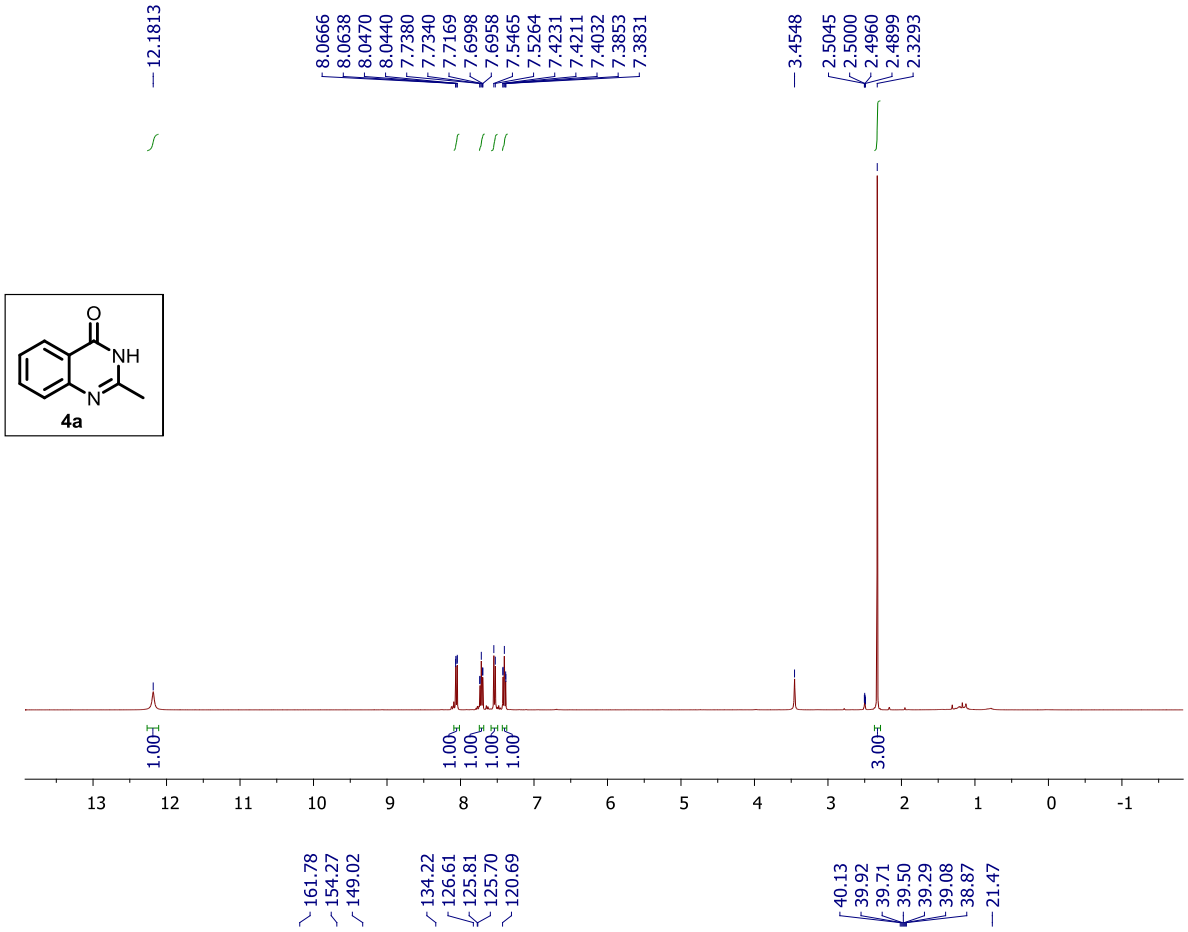
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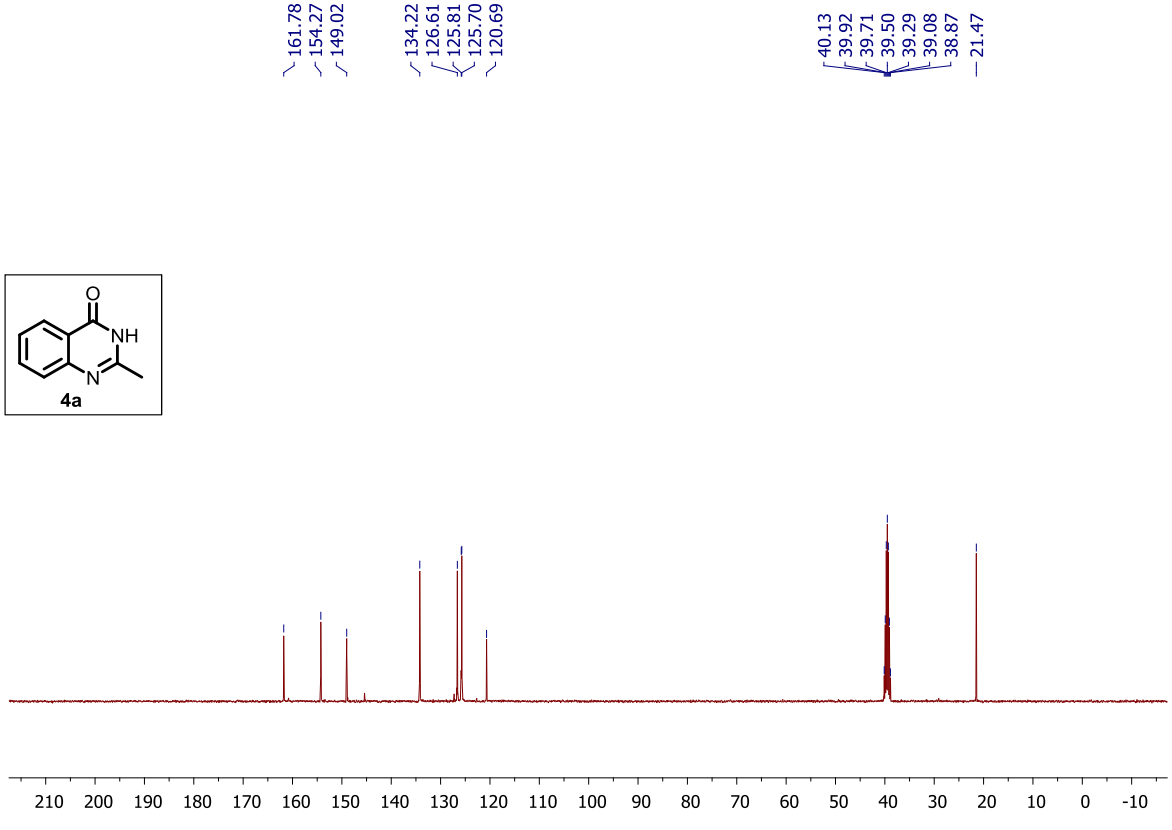
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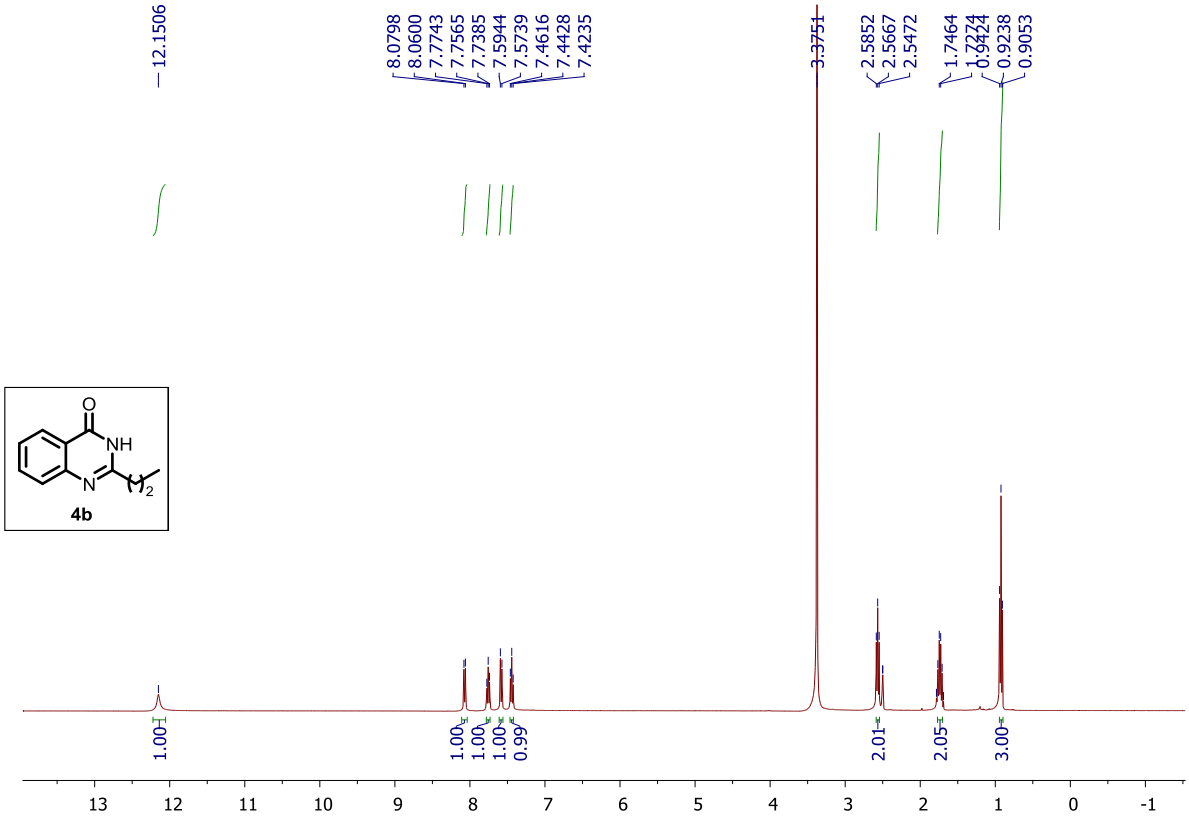
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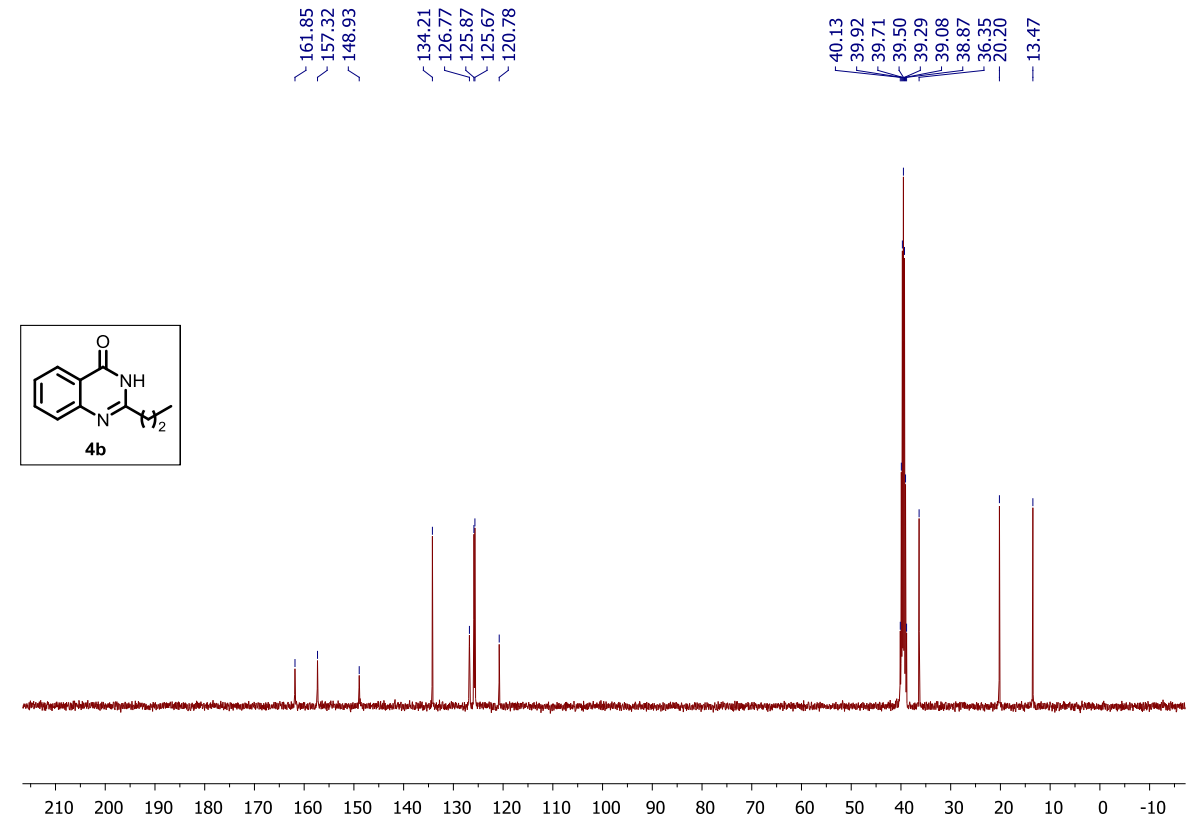
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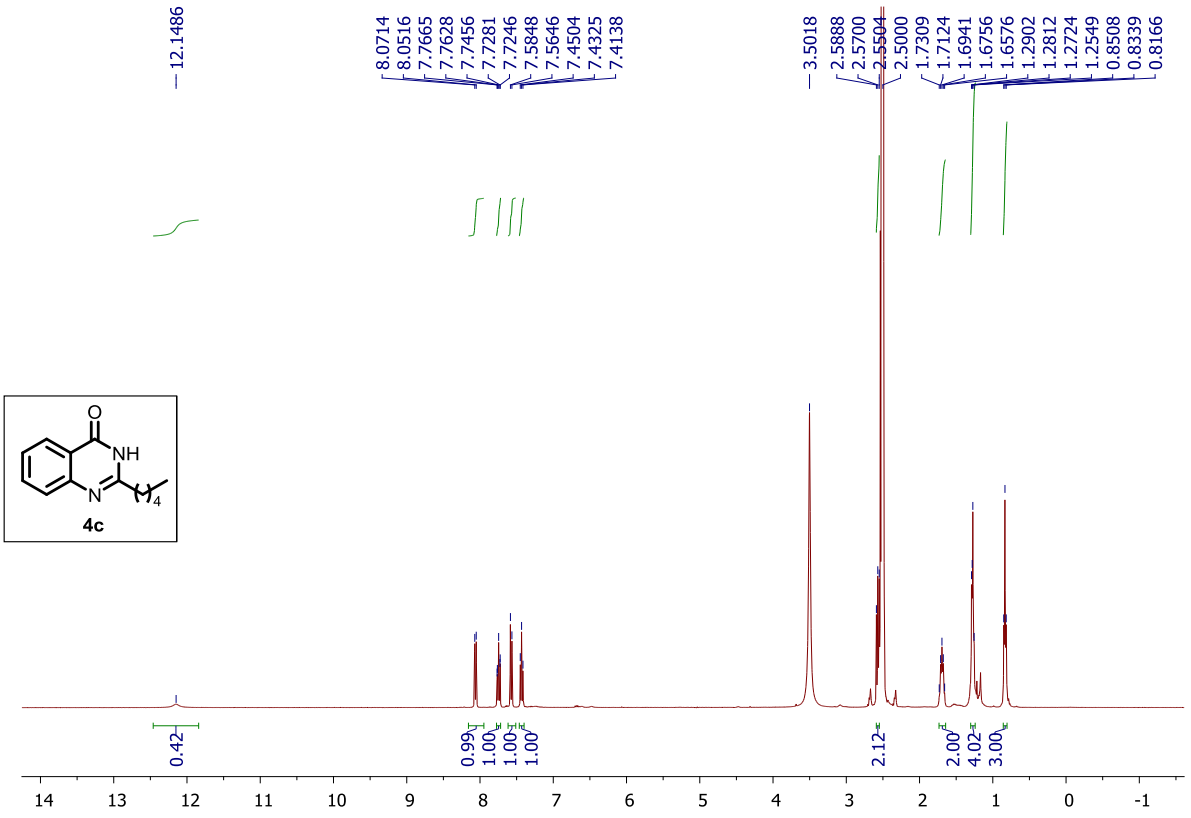
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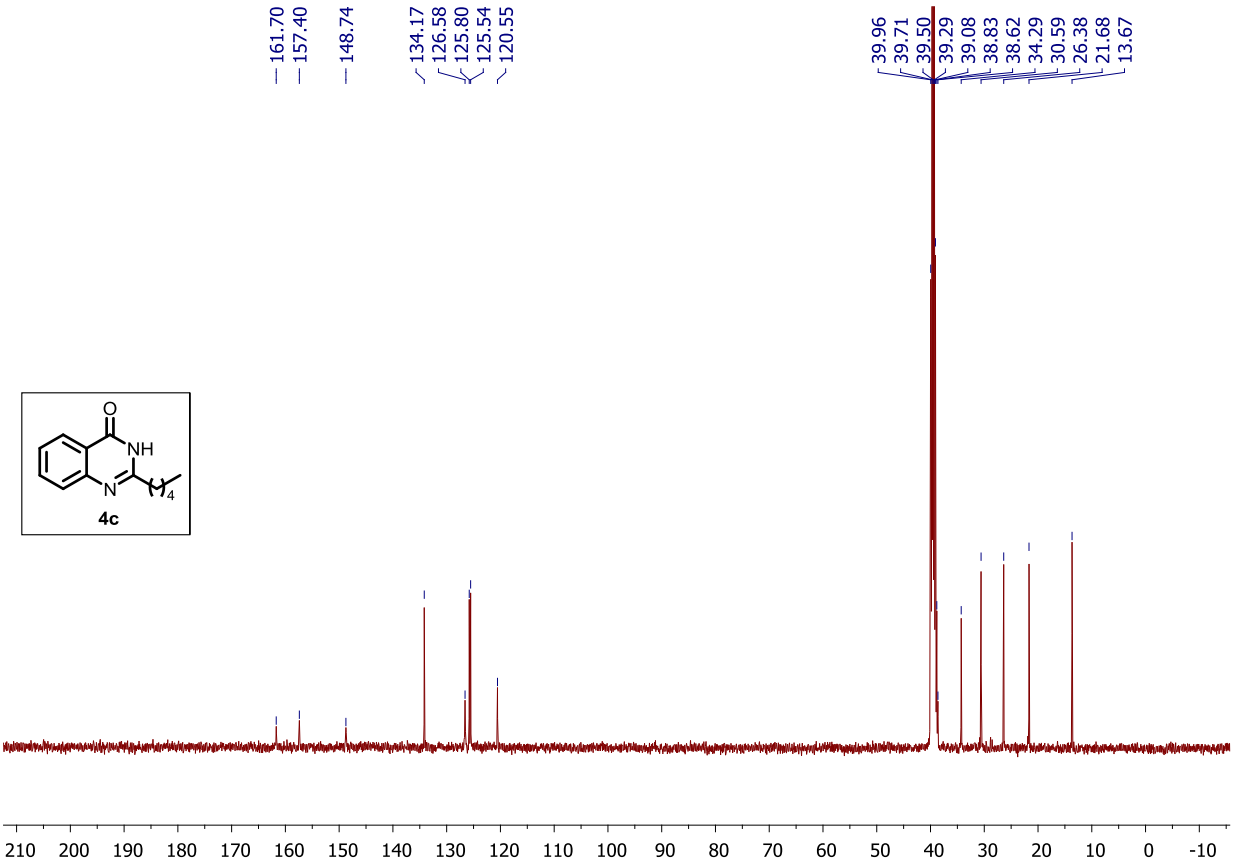
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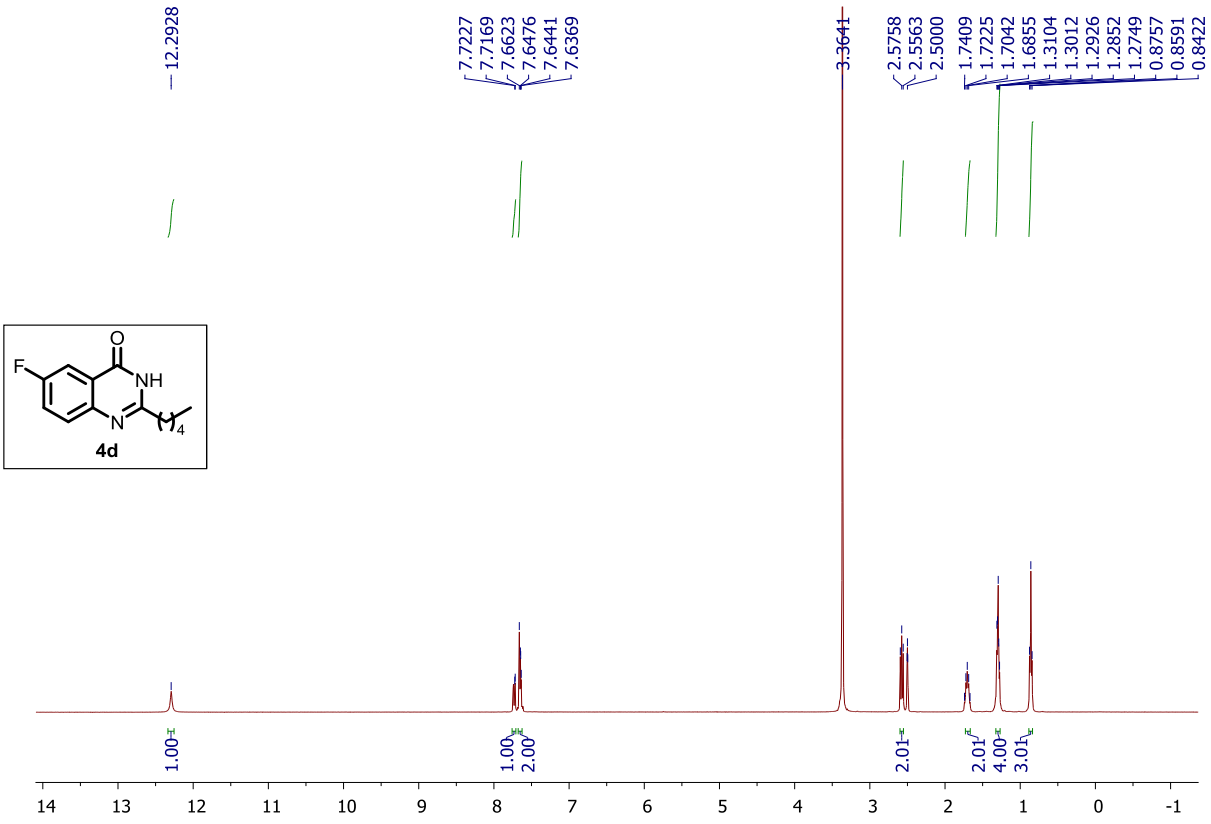
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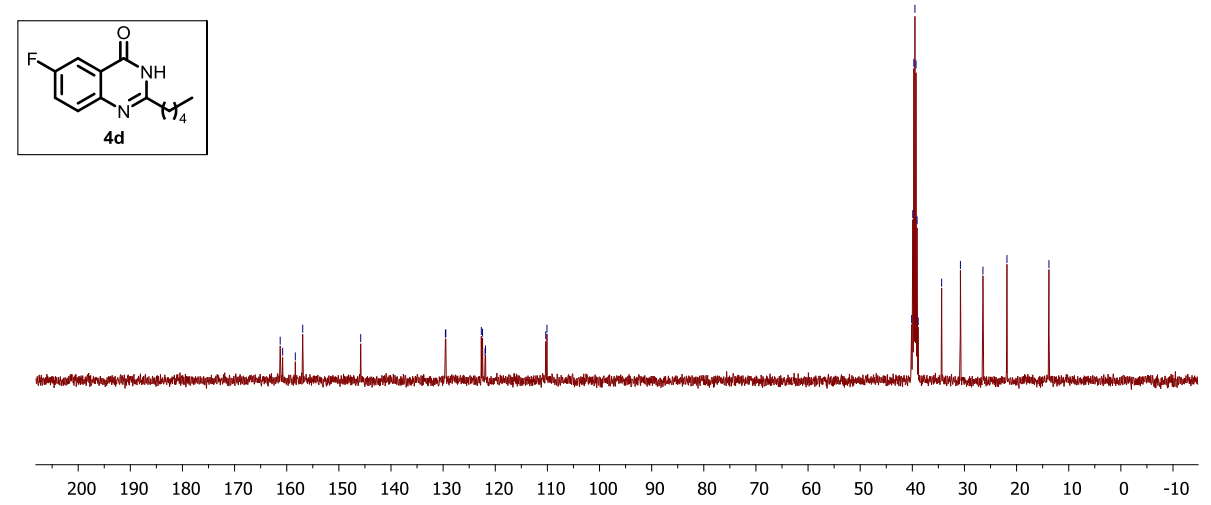
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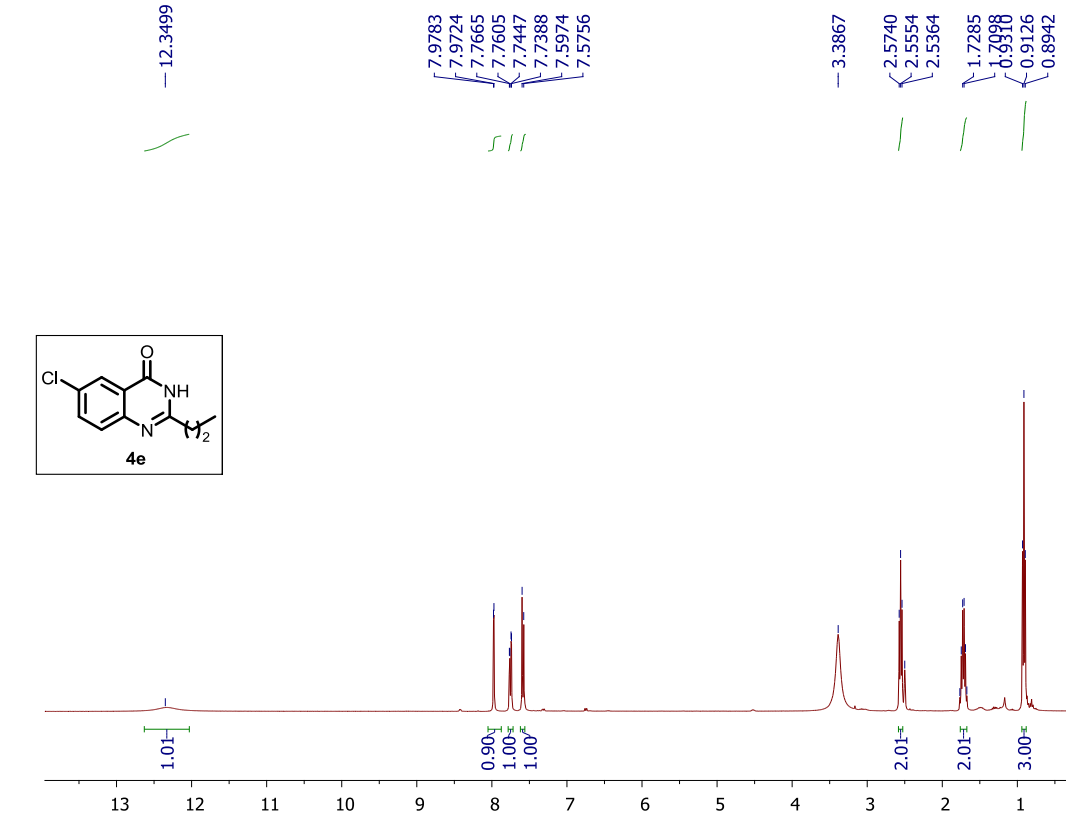
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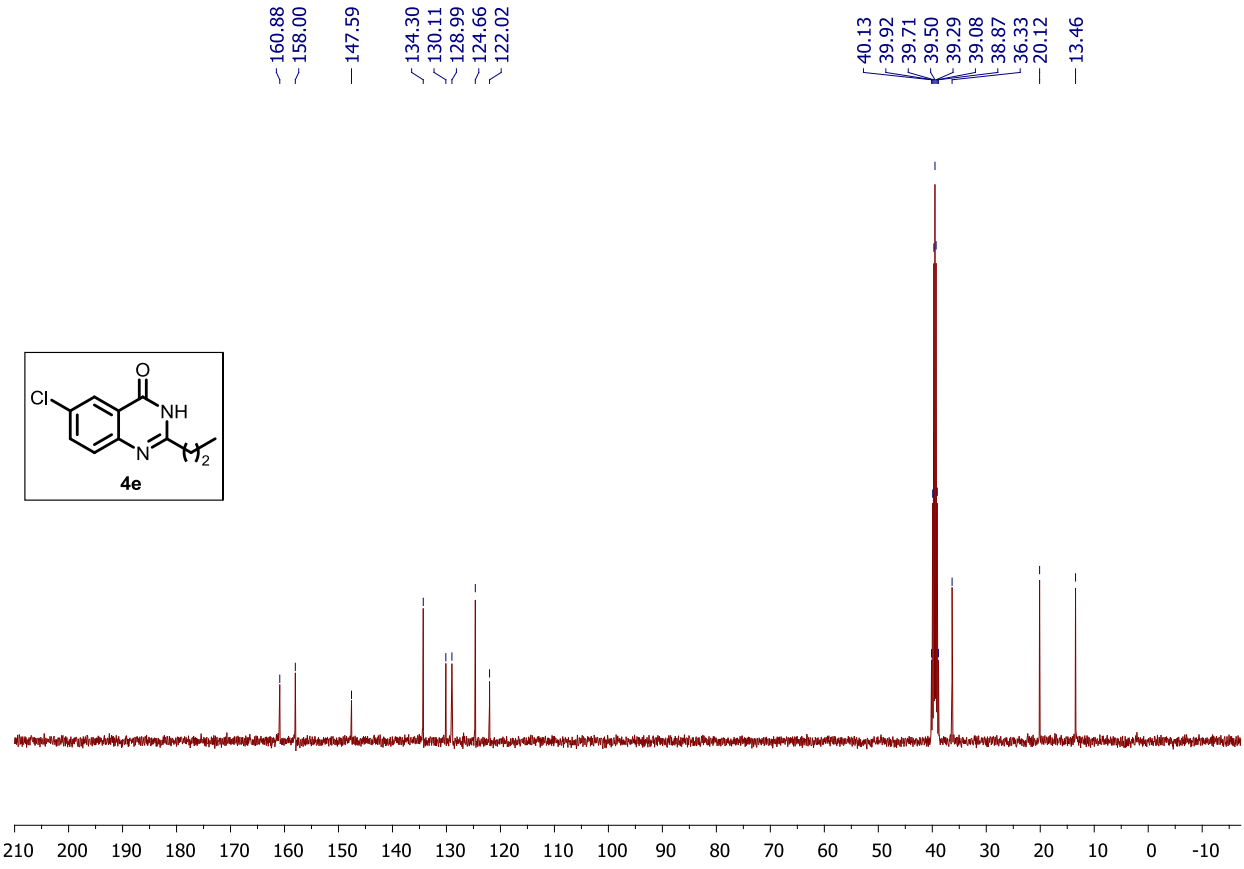
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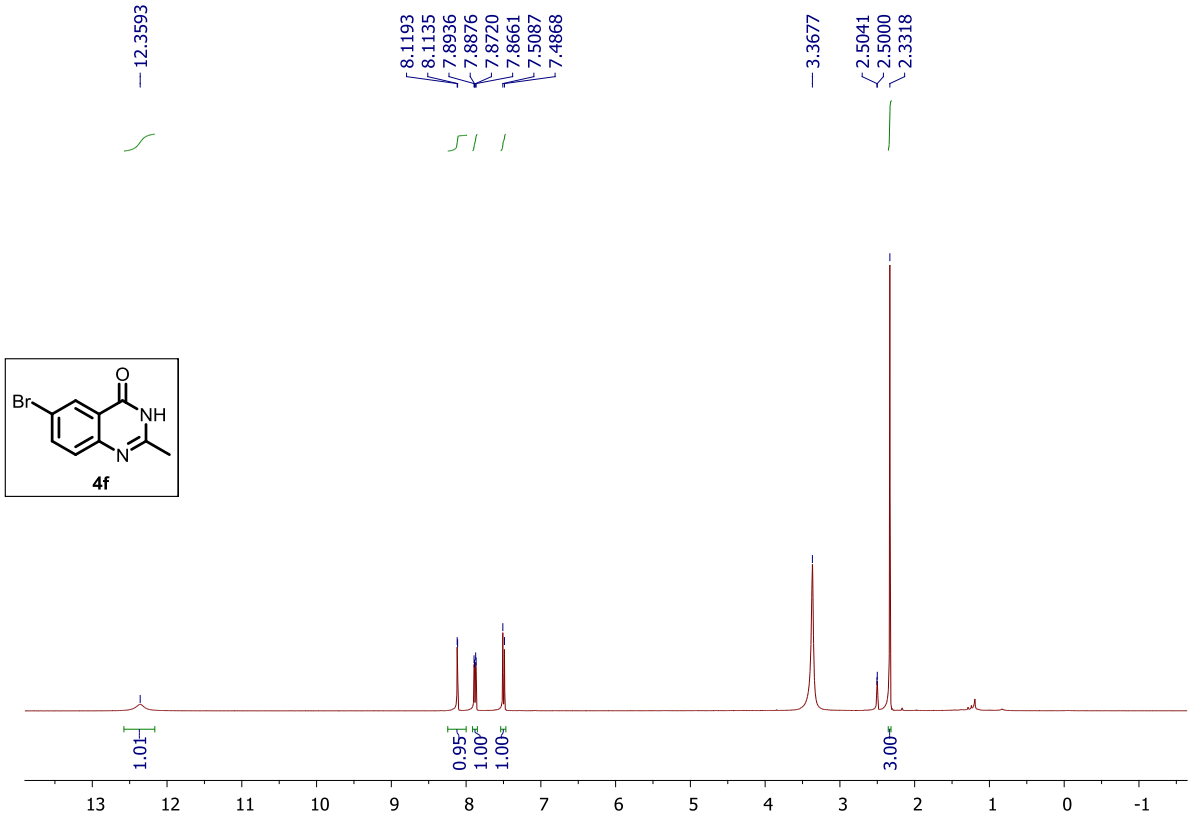
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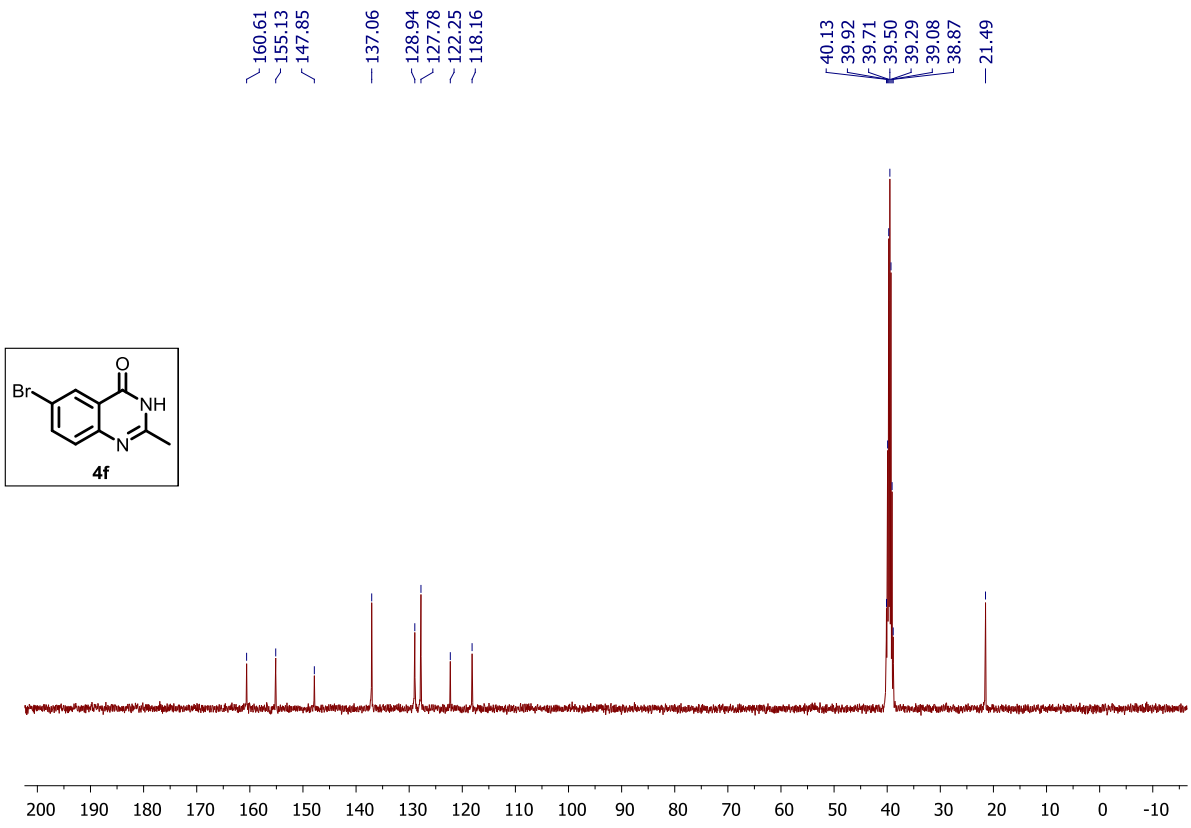
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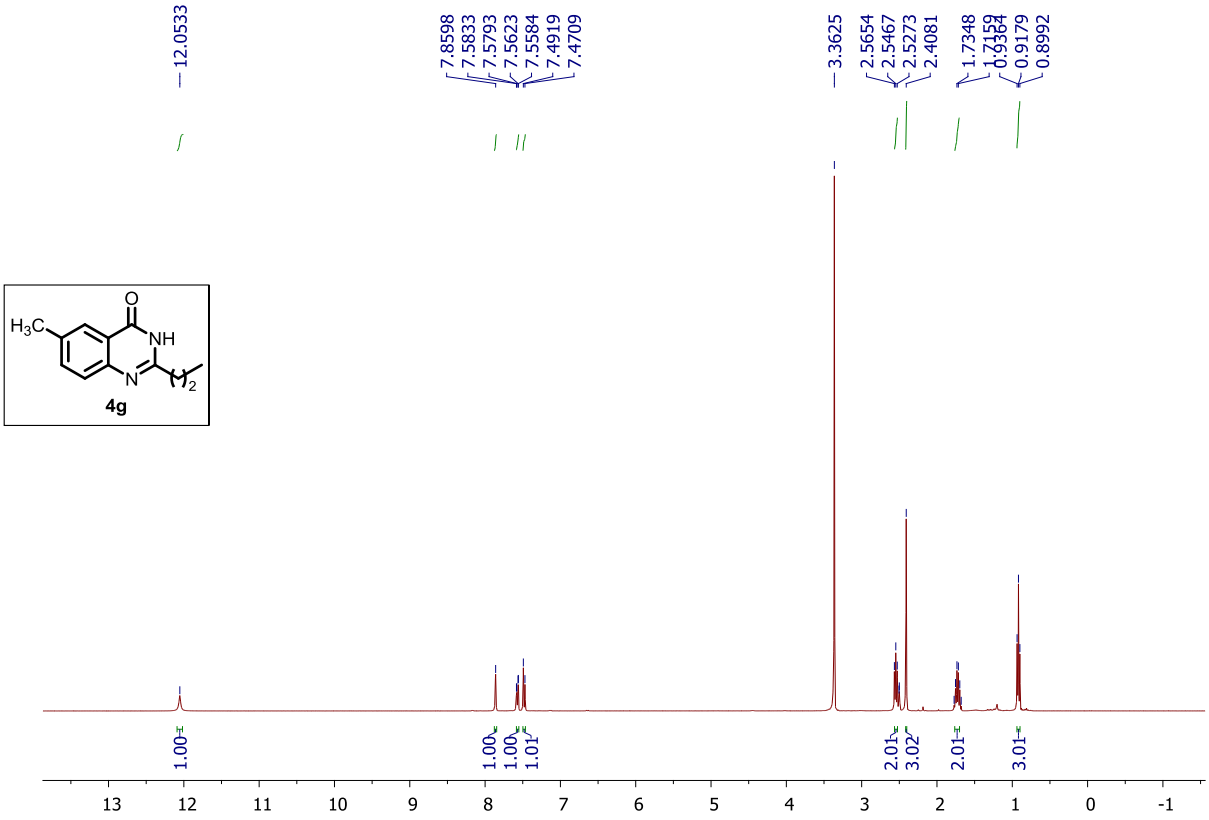
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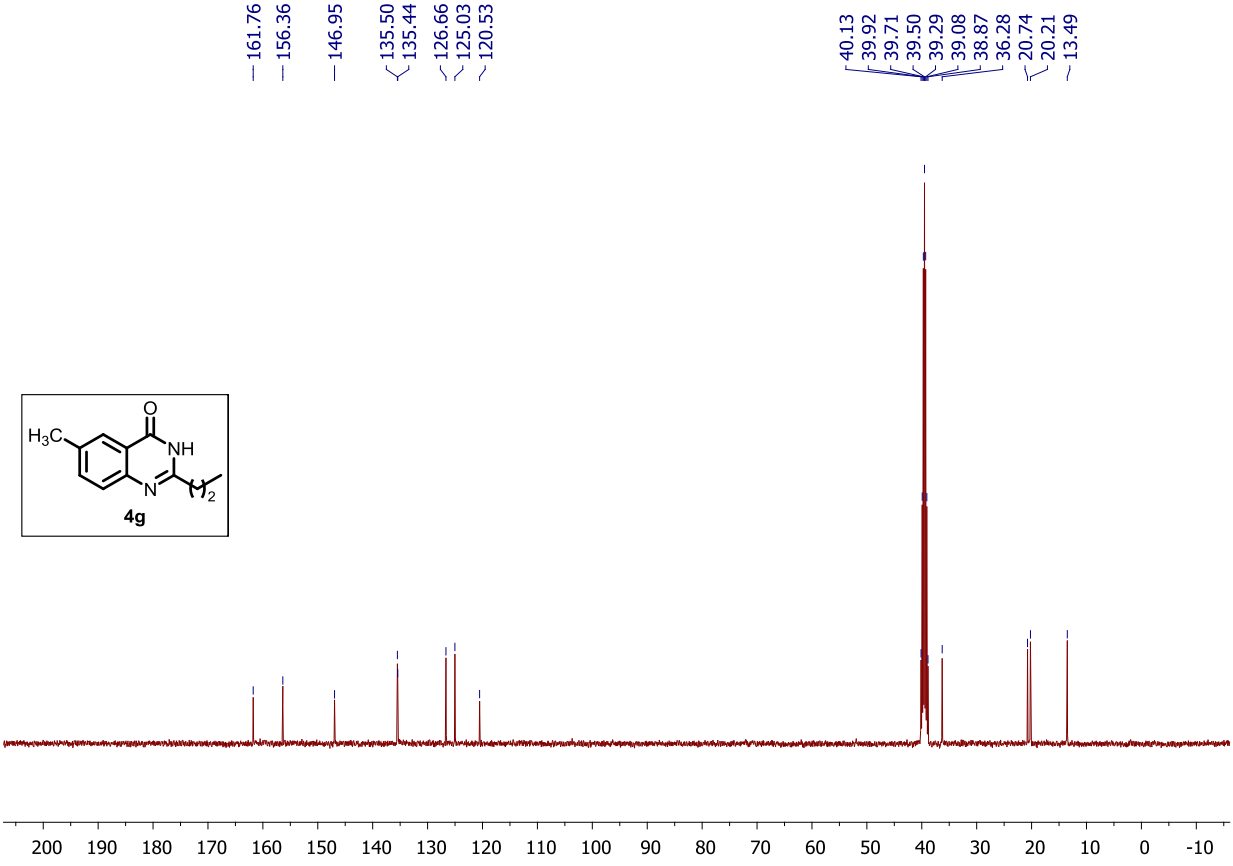
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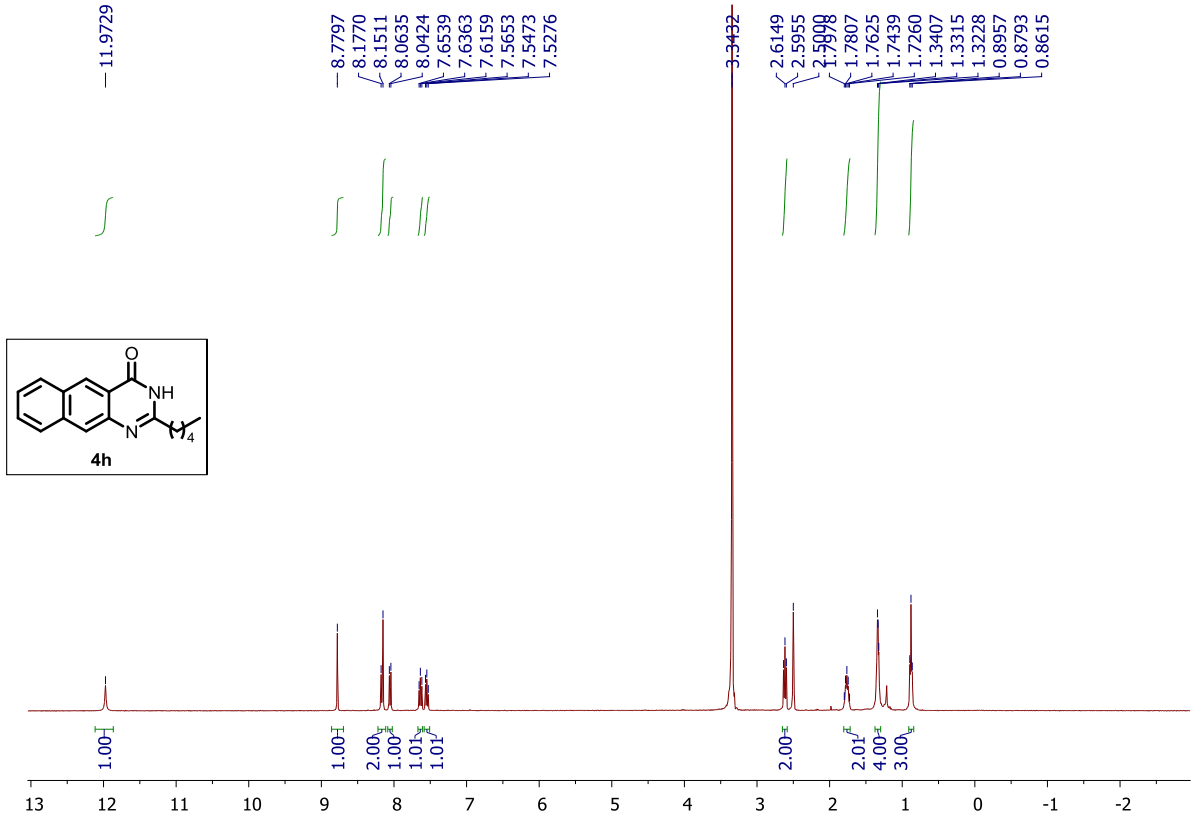
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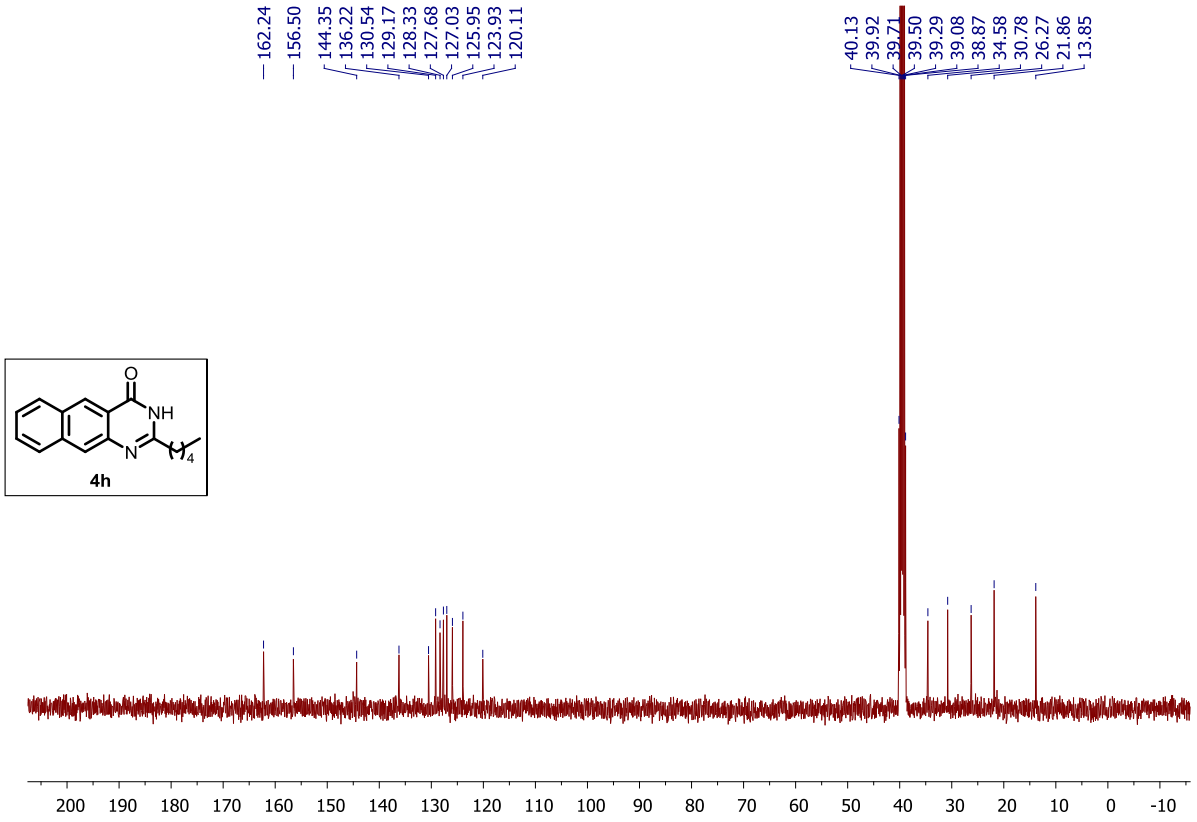
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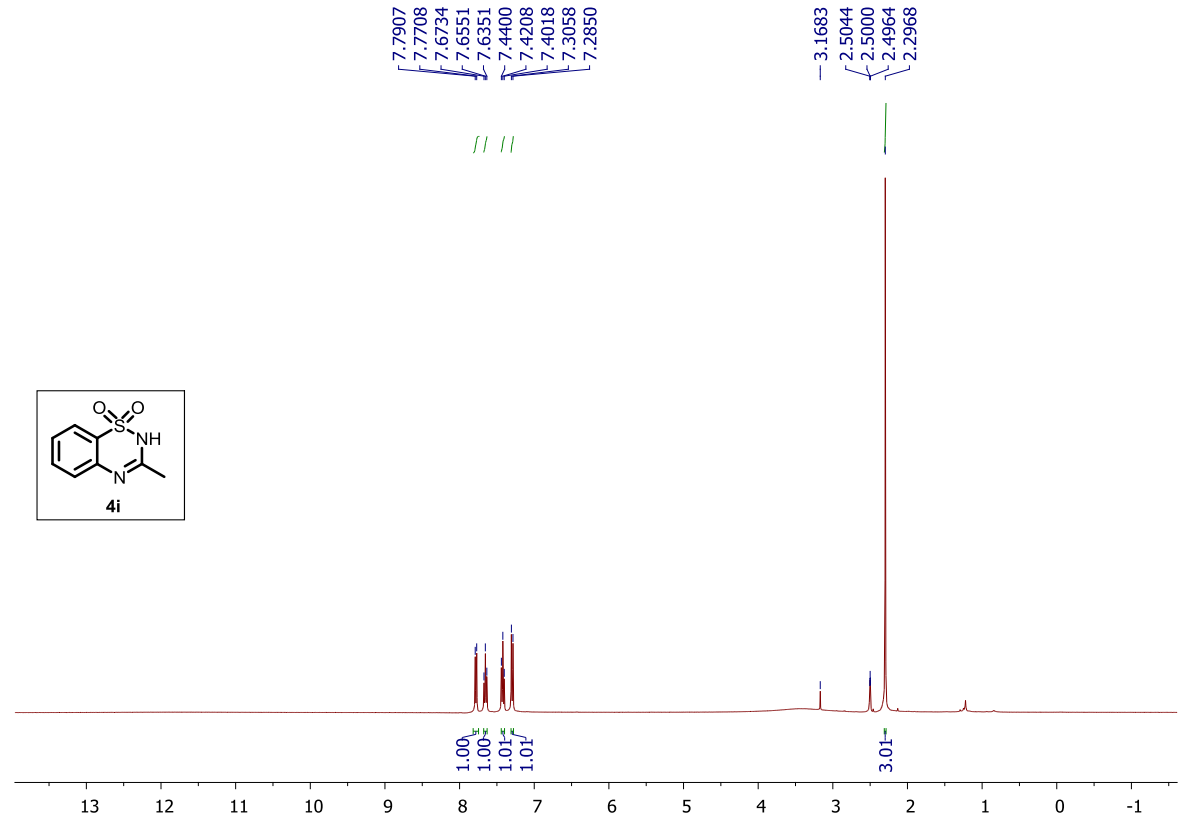
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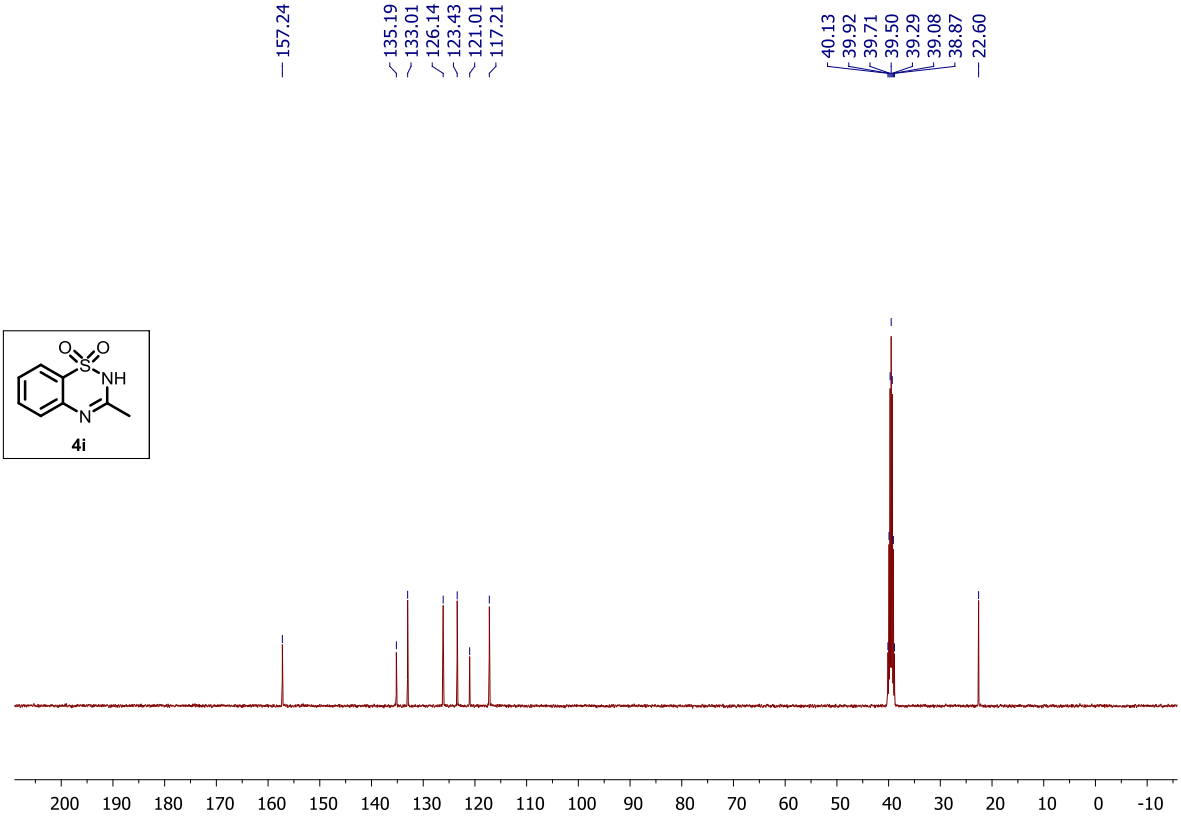
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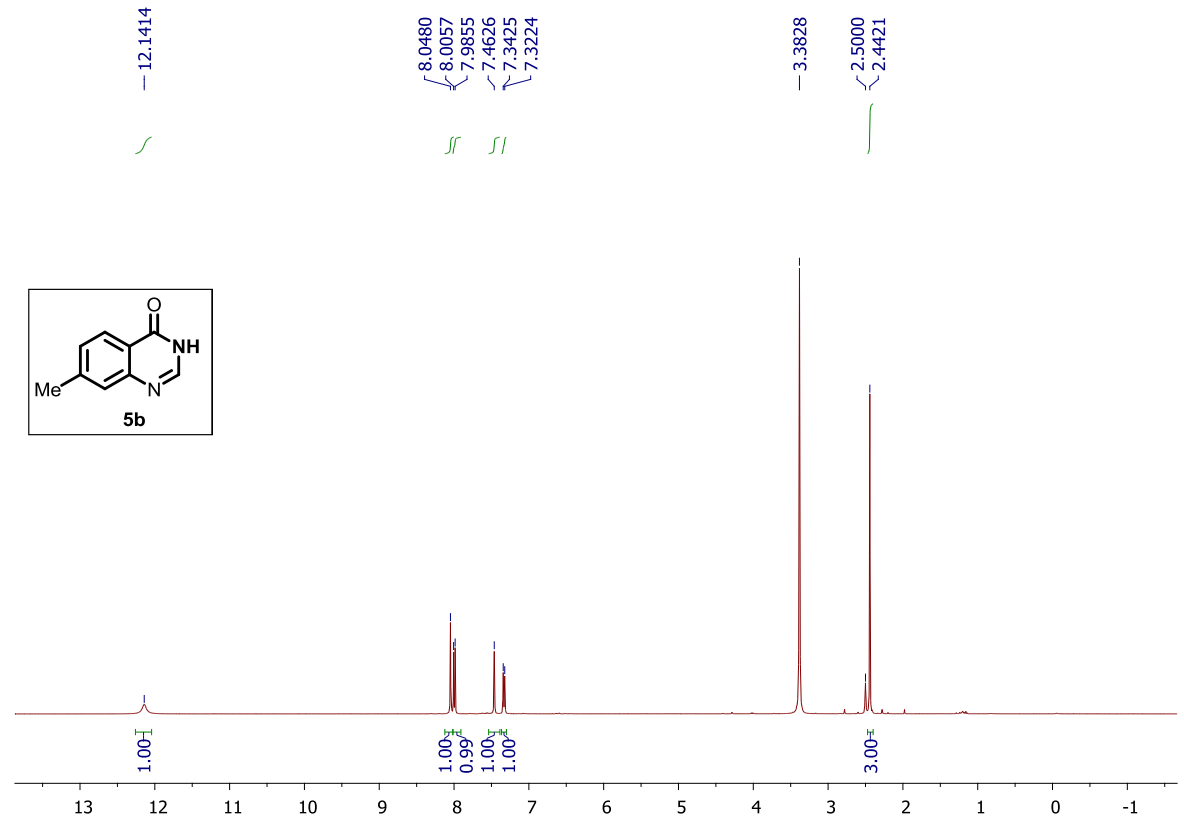
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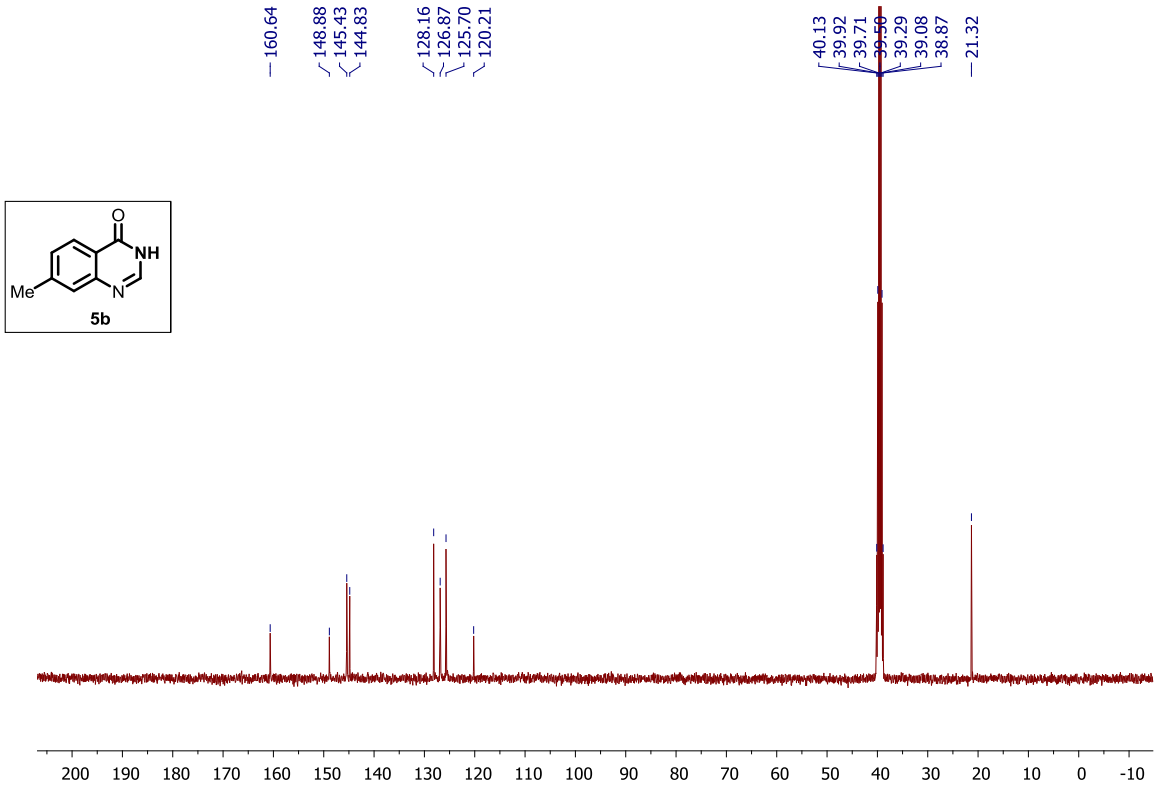
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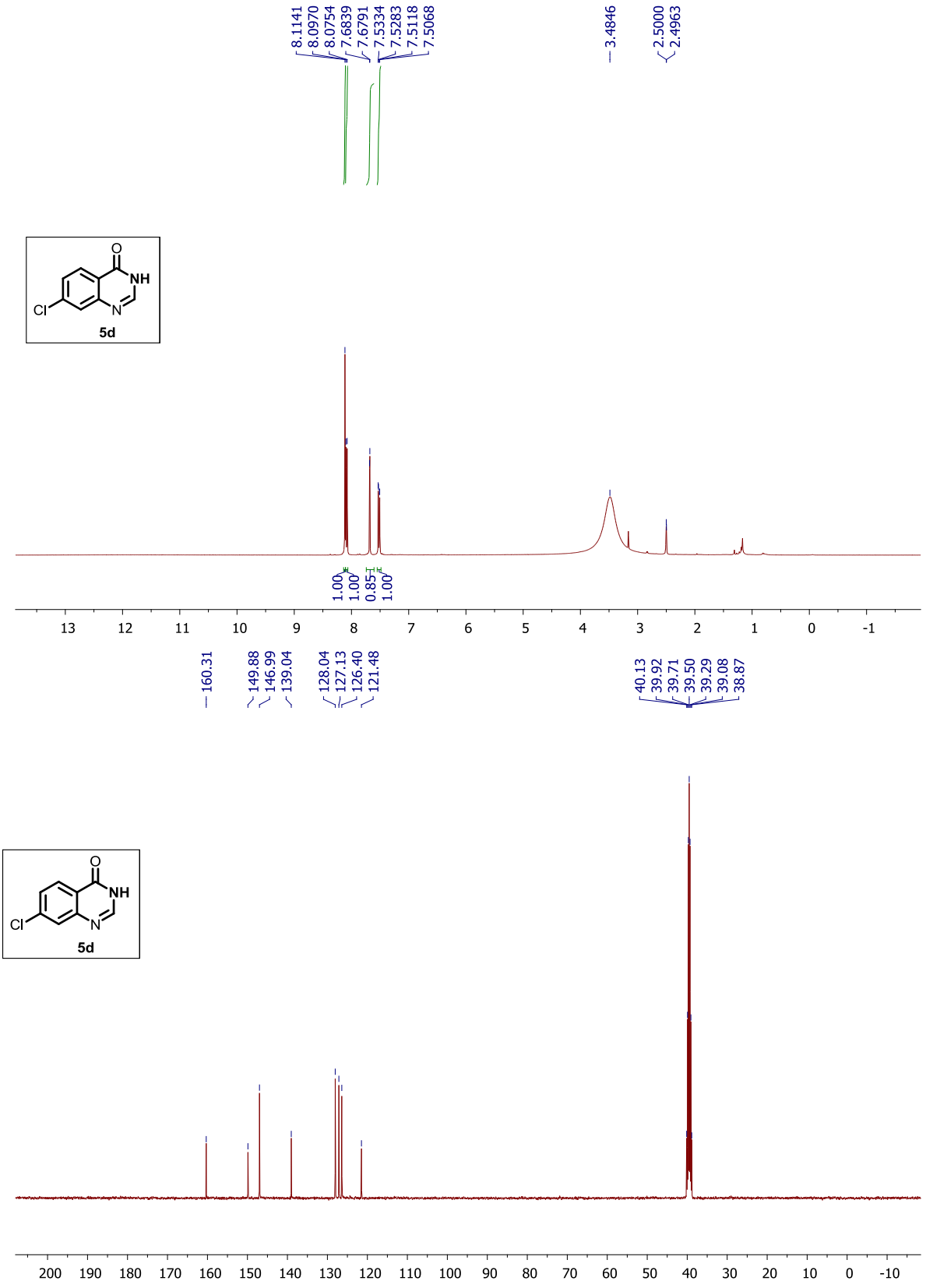
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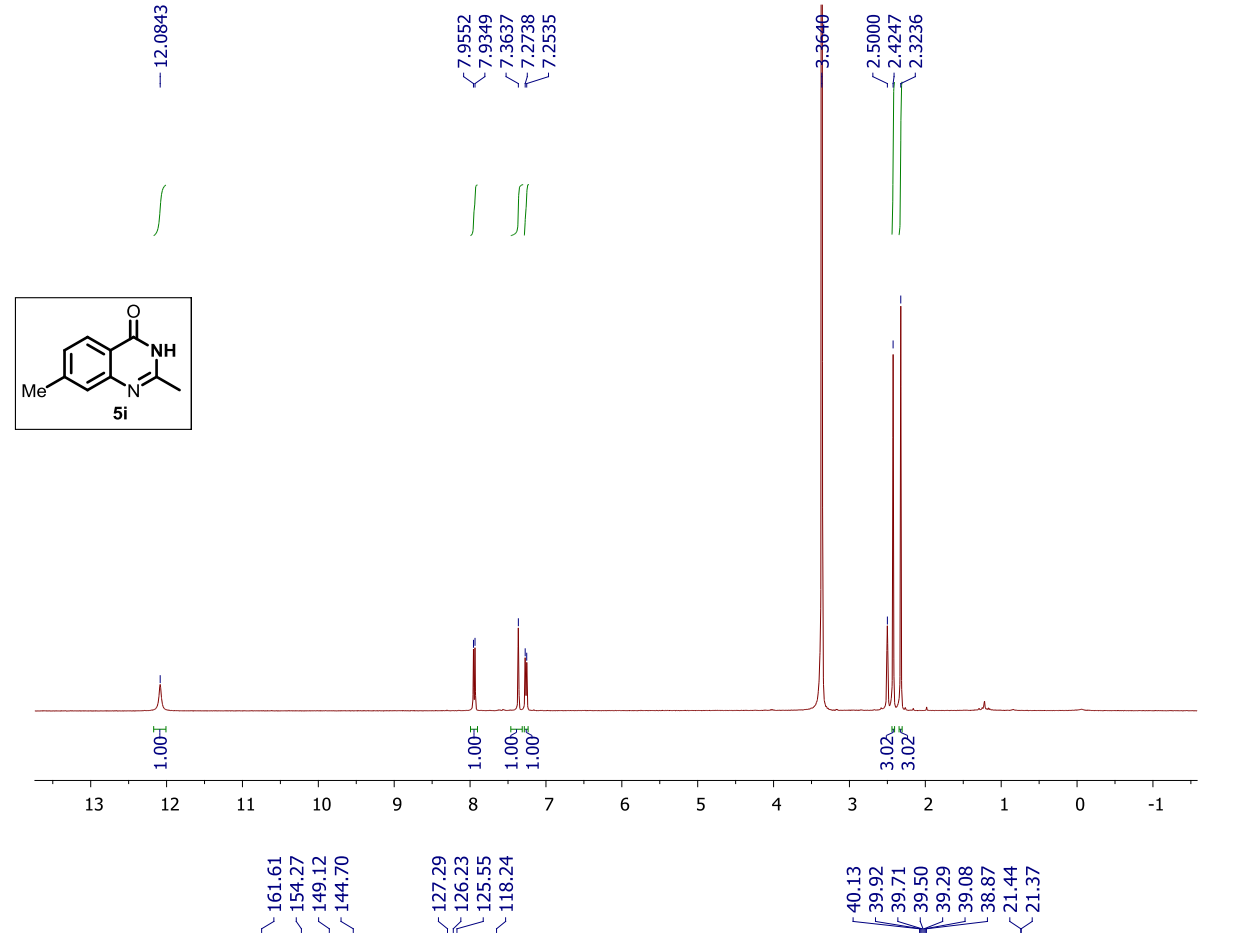
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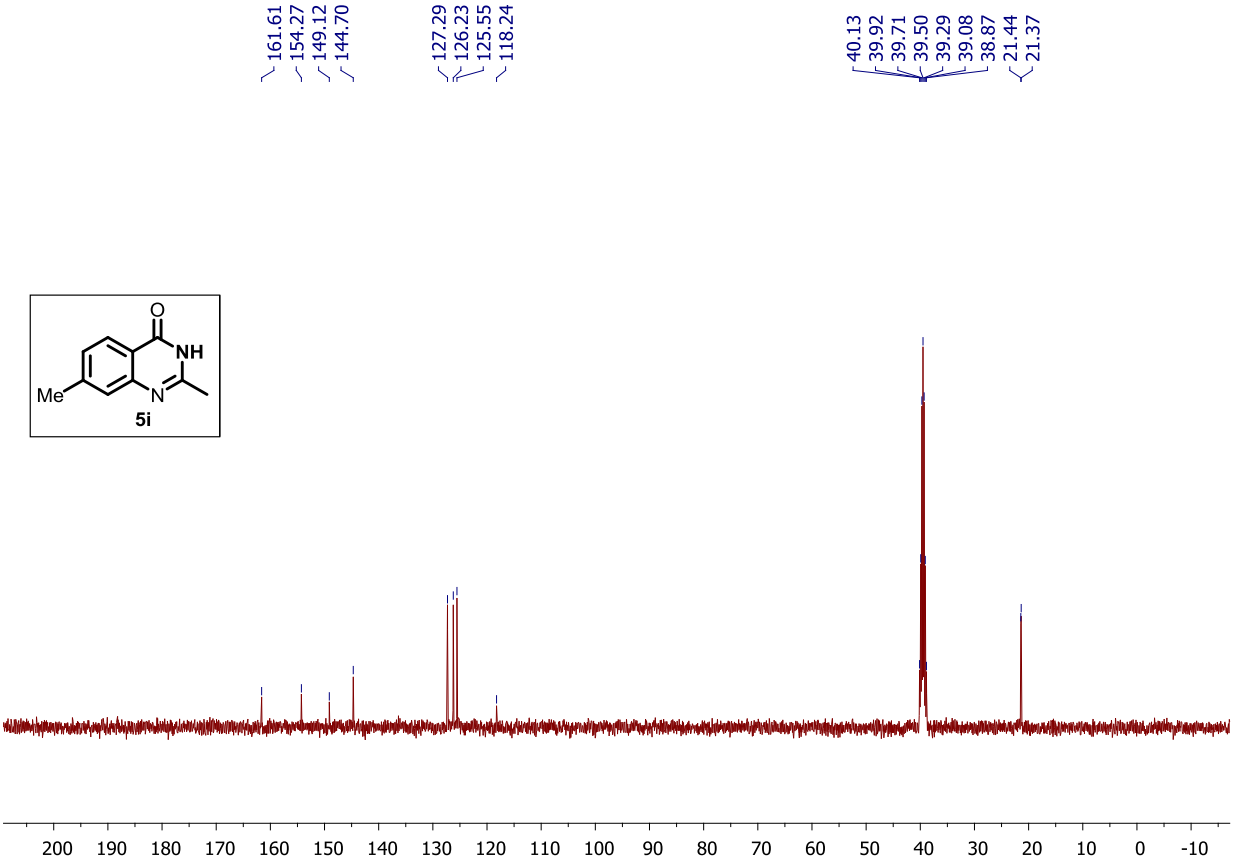
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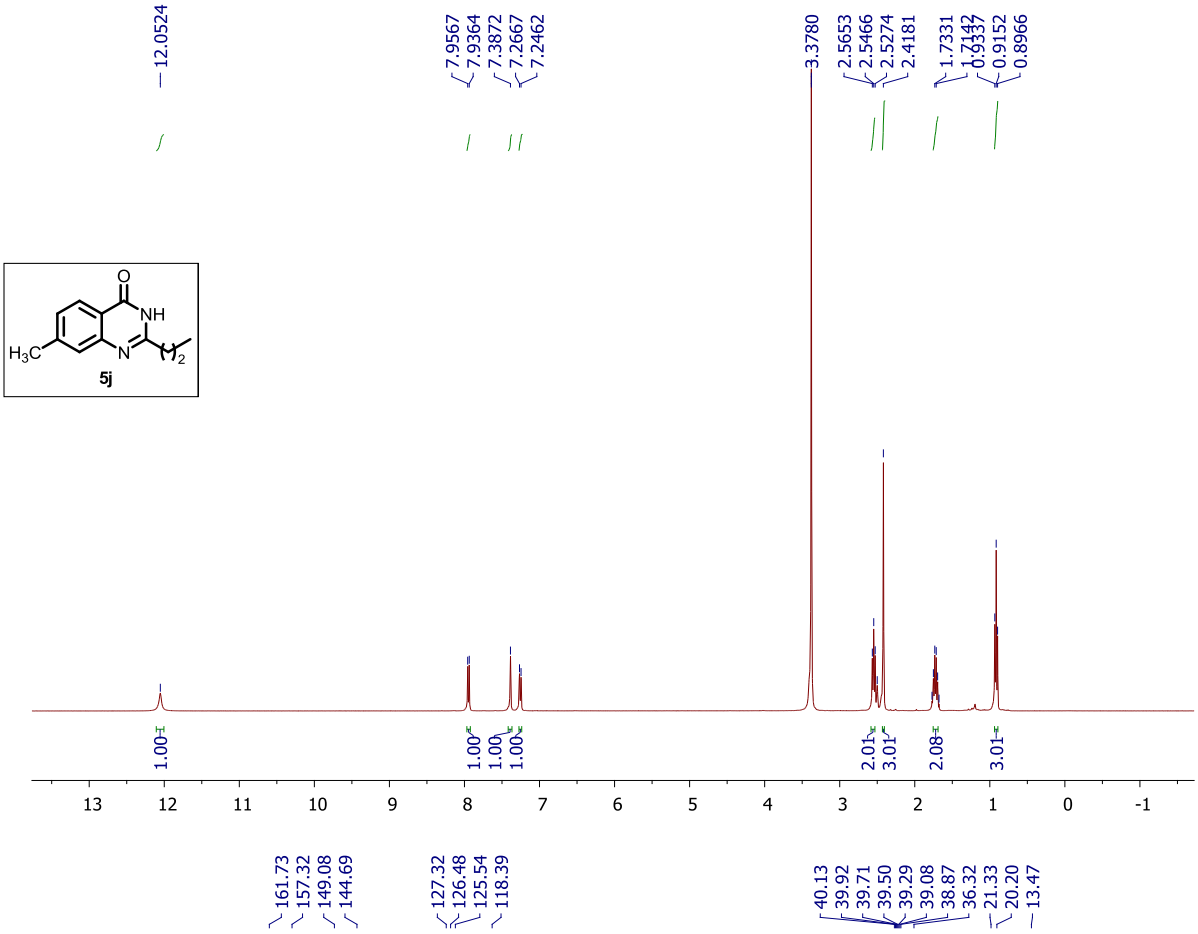
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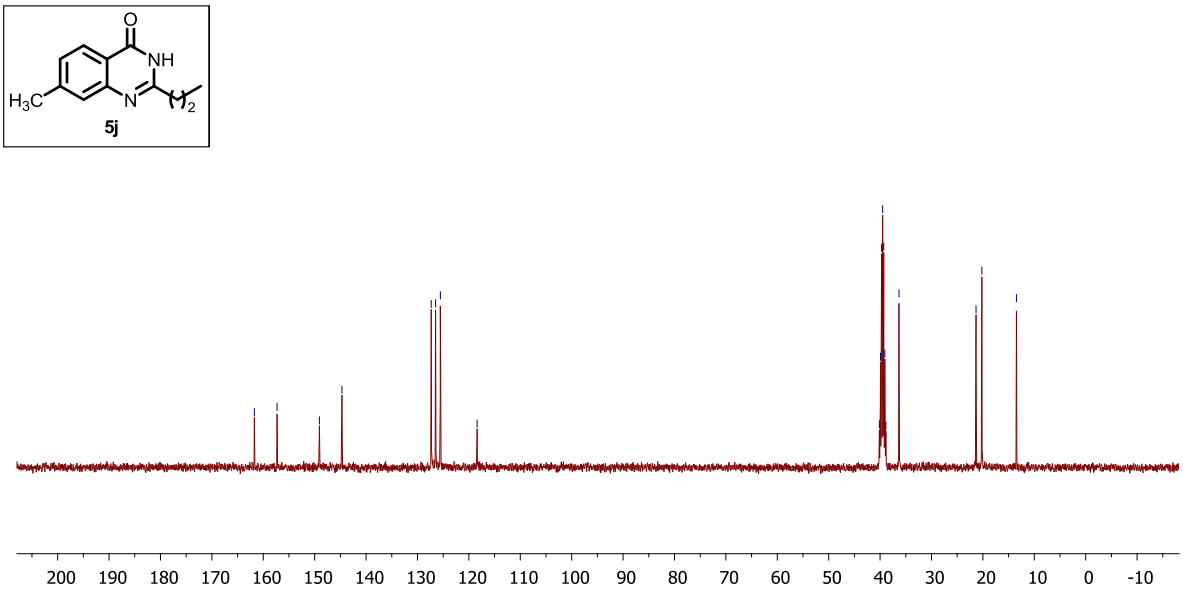
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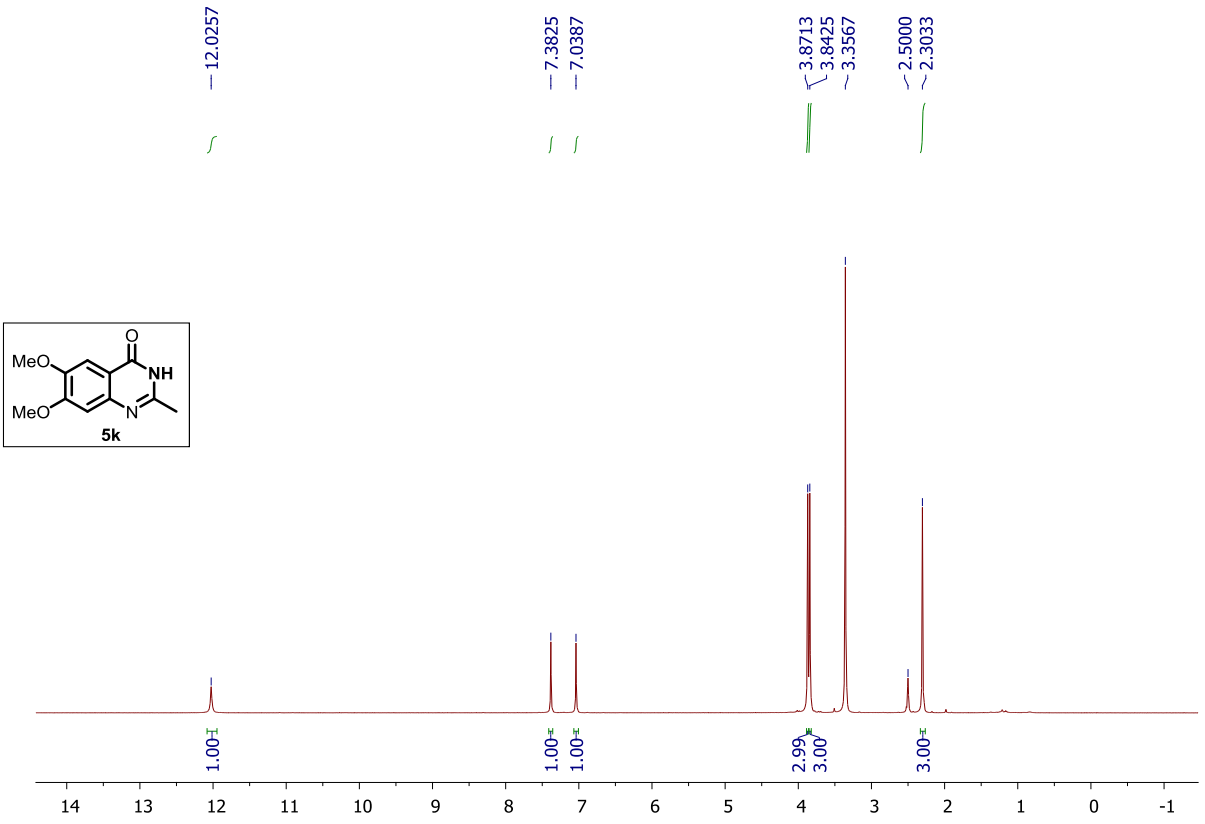
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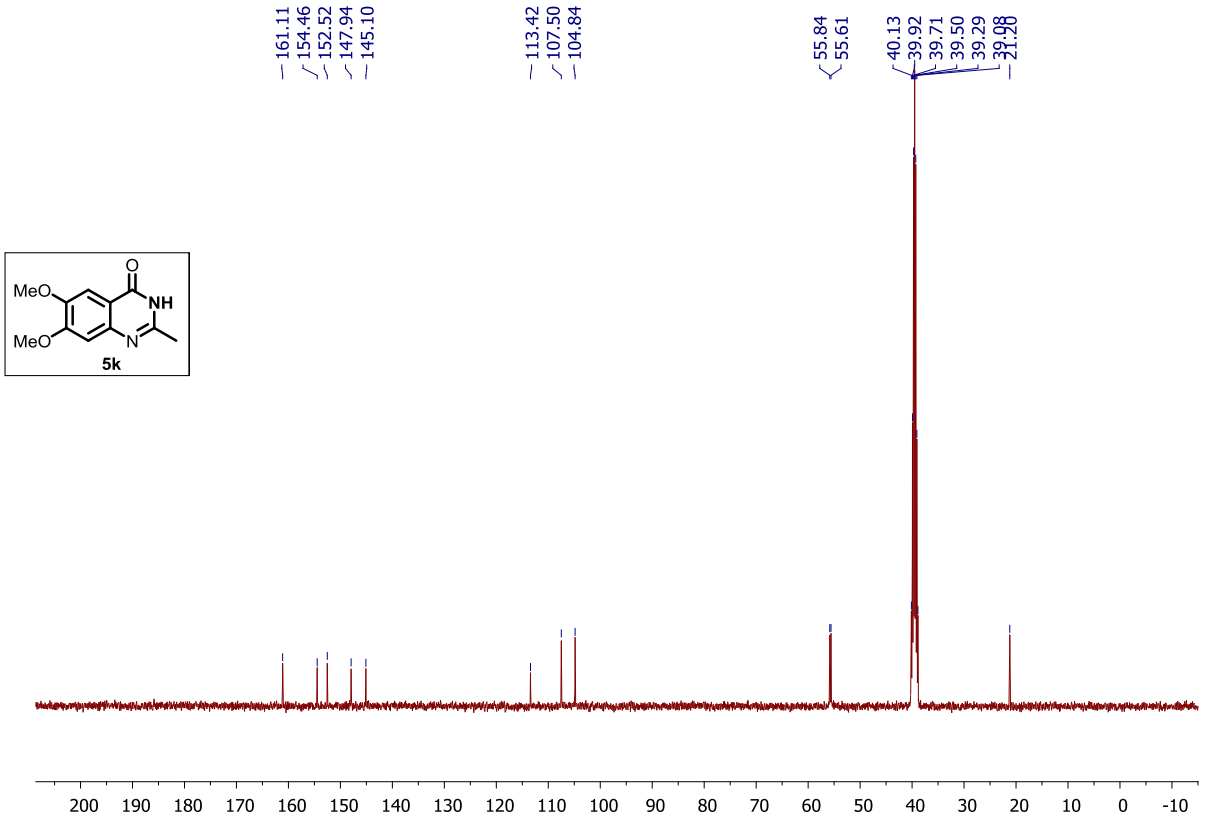
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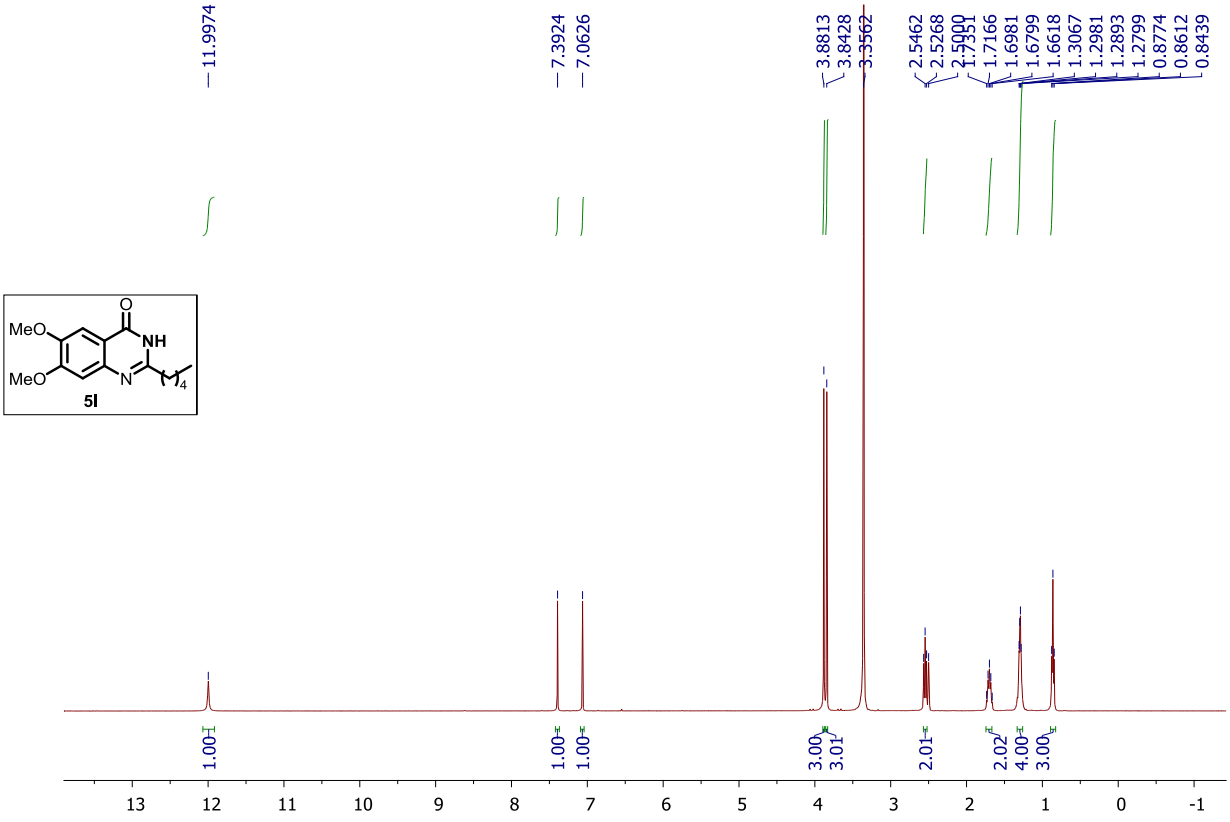
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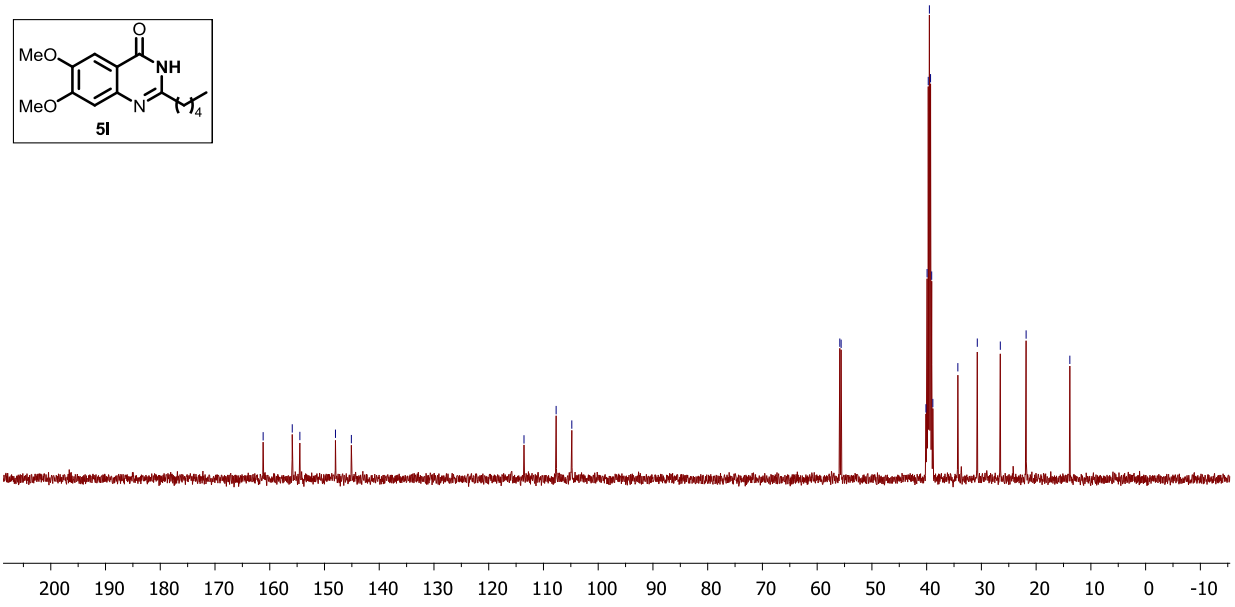
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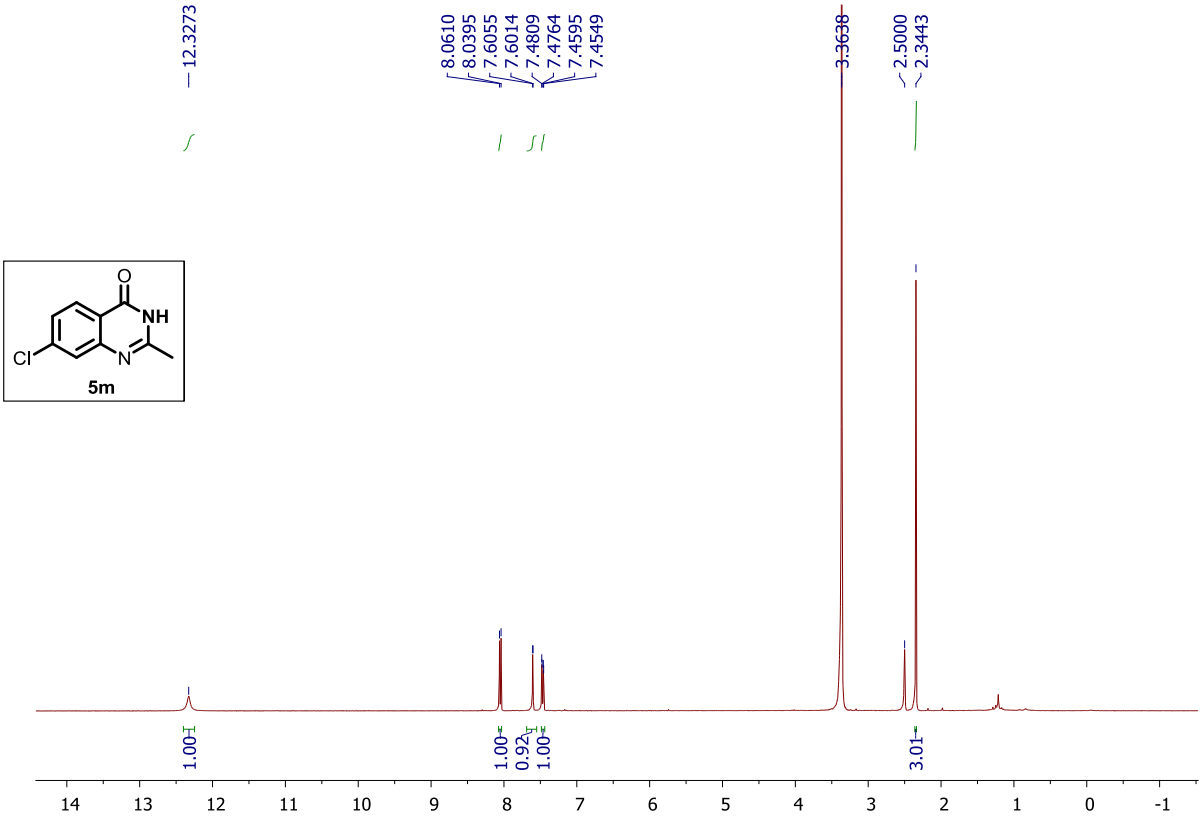
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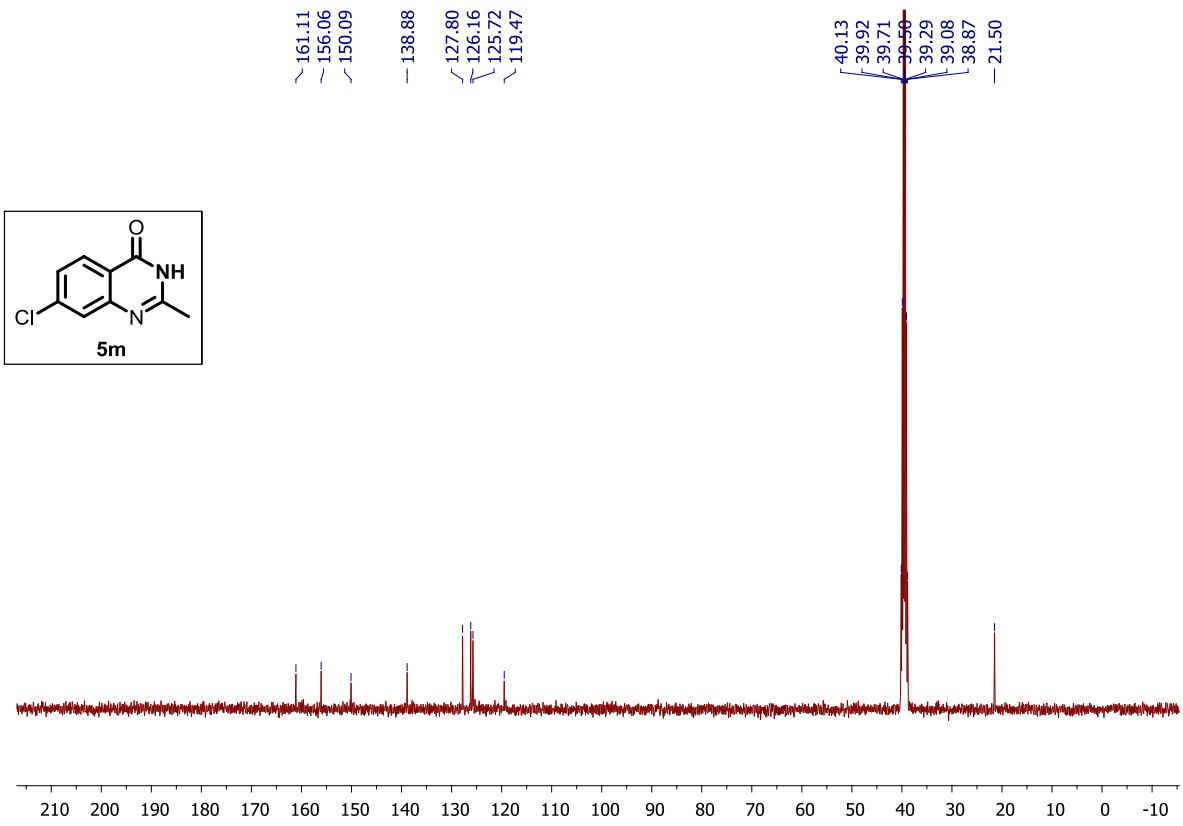
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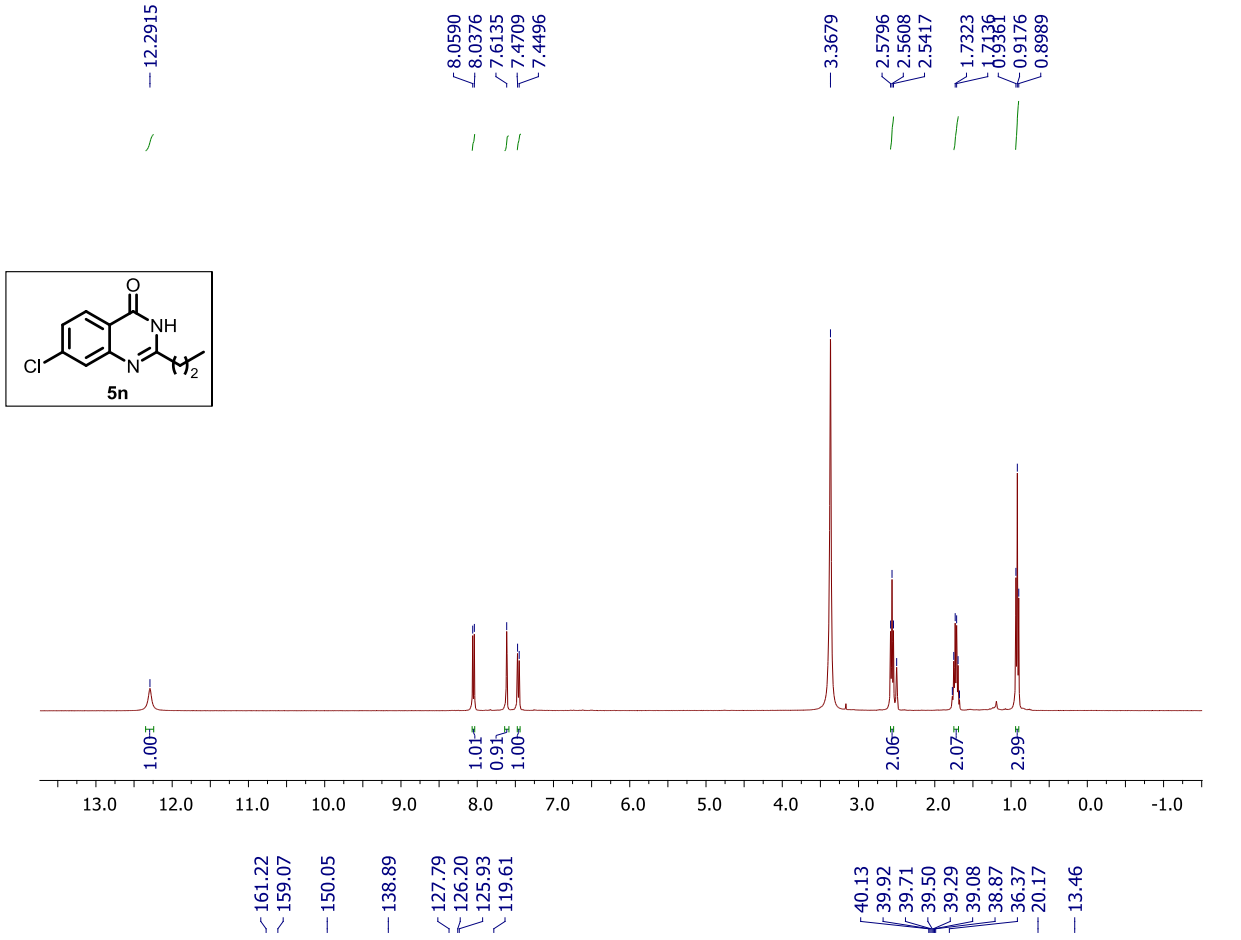
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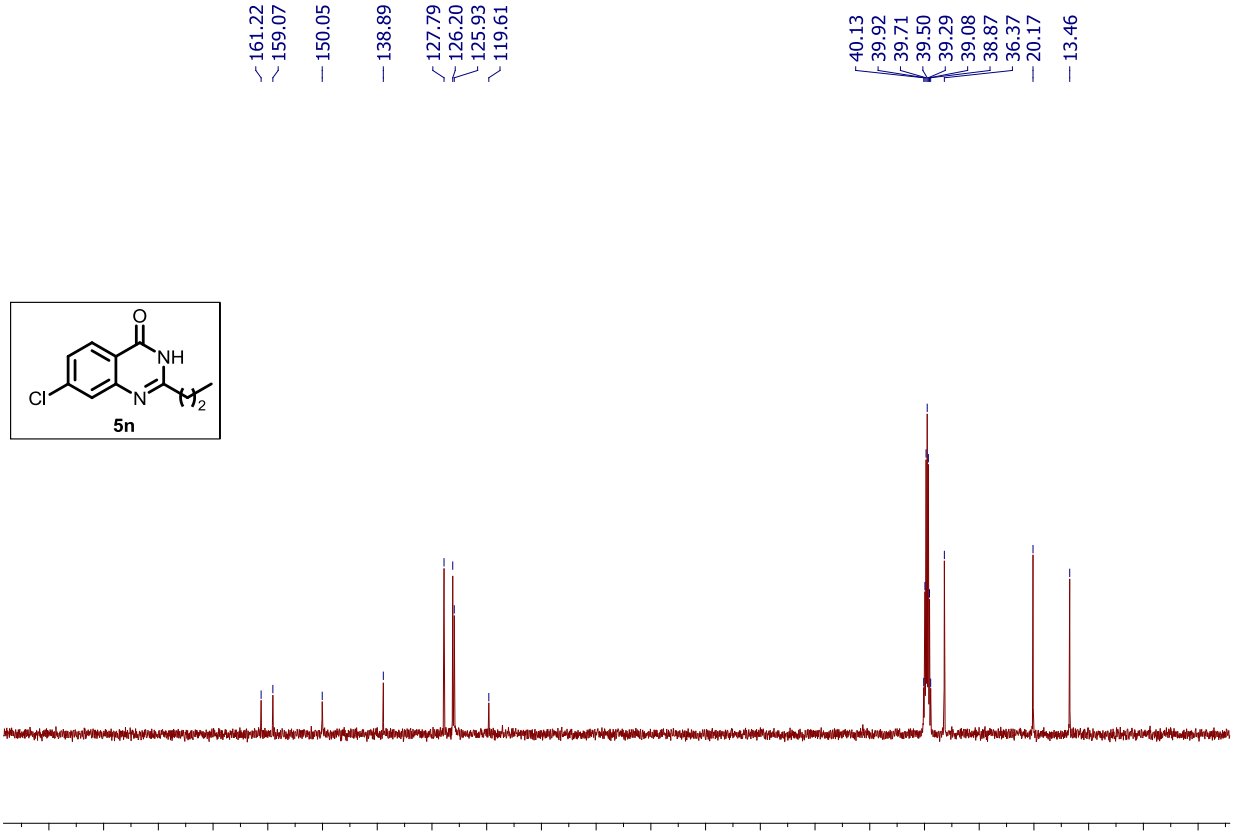
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134.24
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125.87
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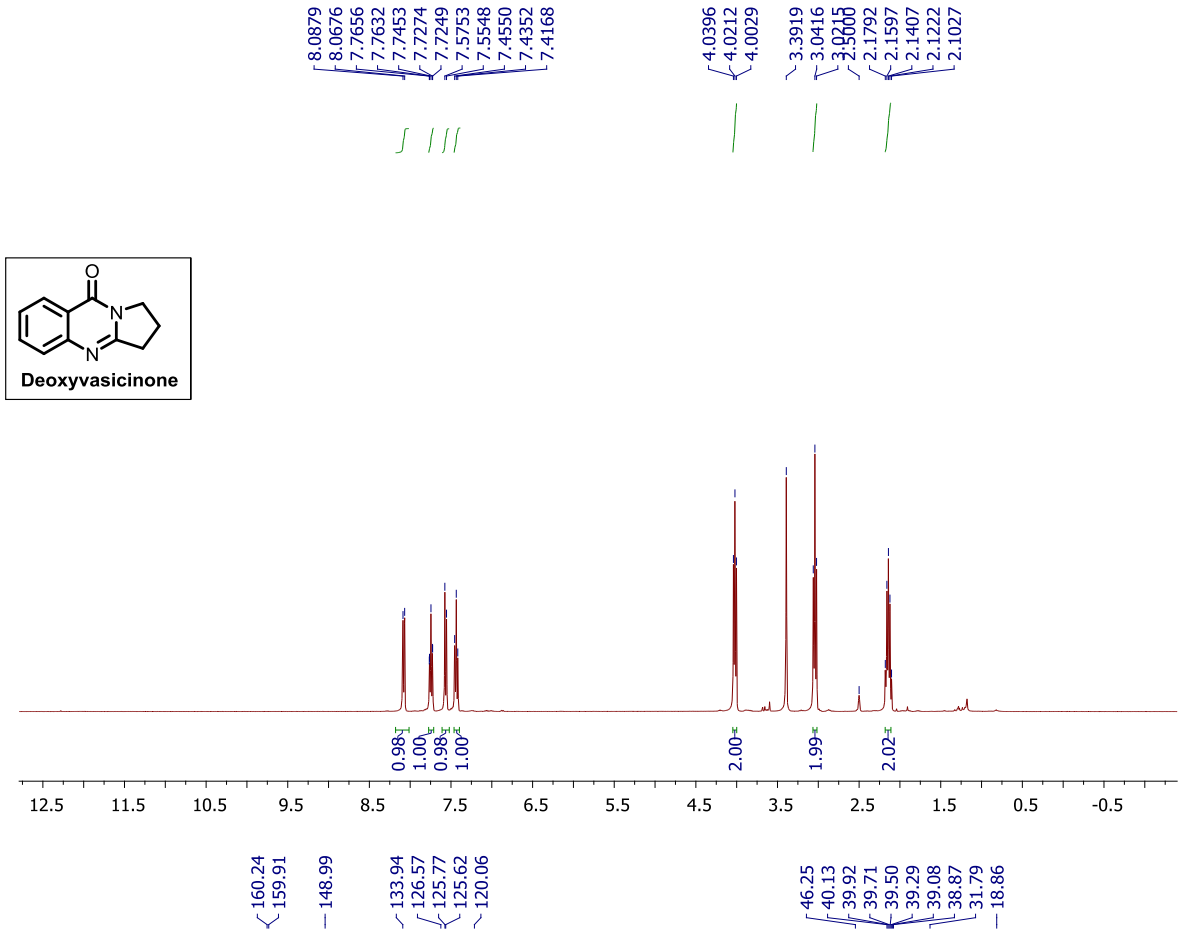
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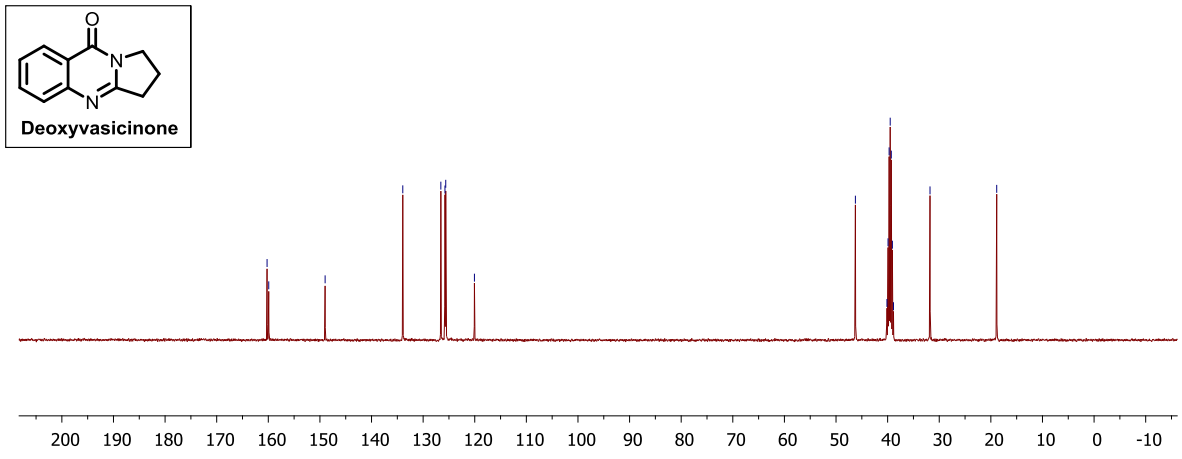
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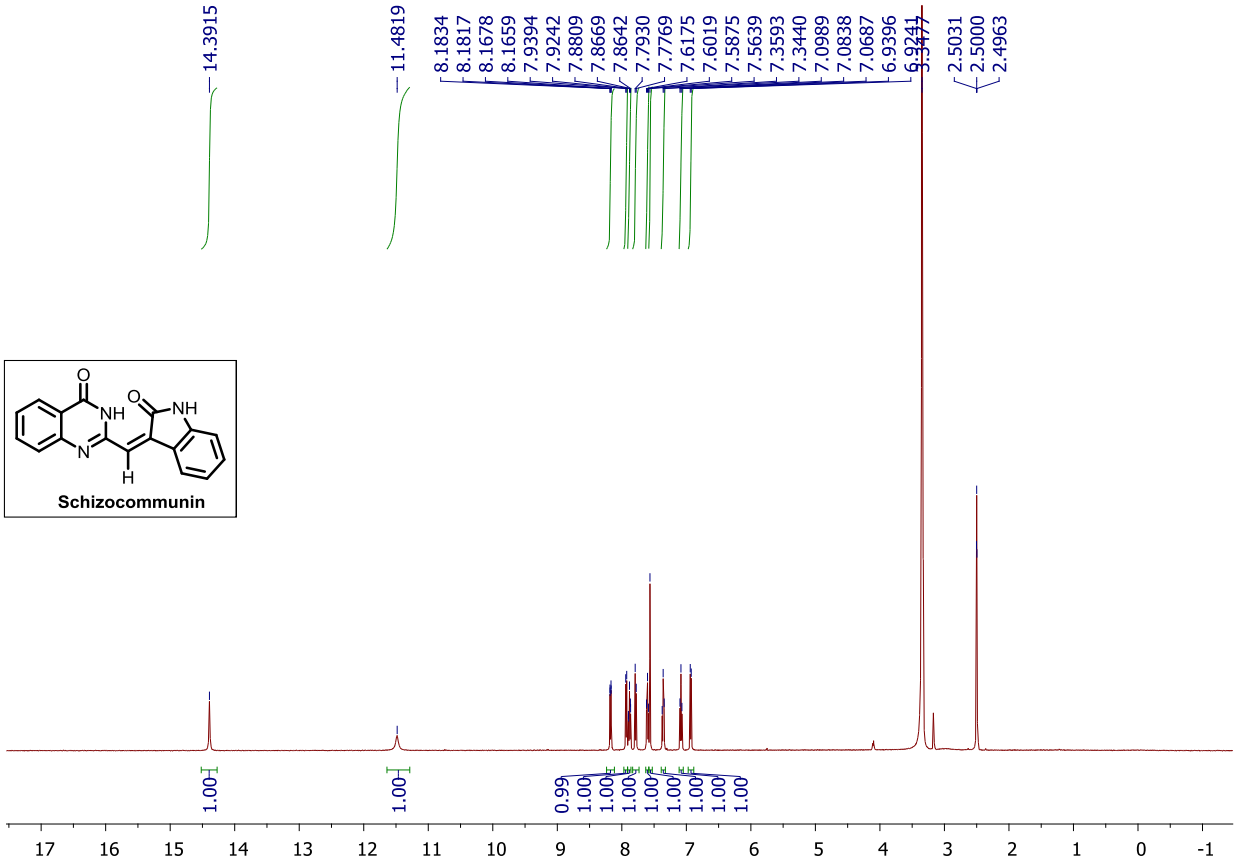
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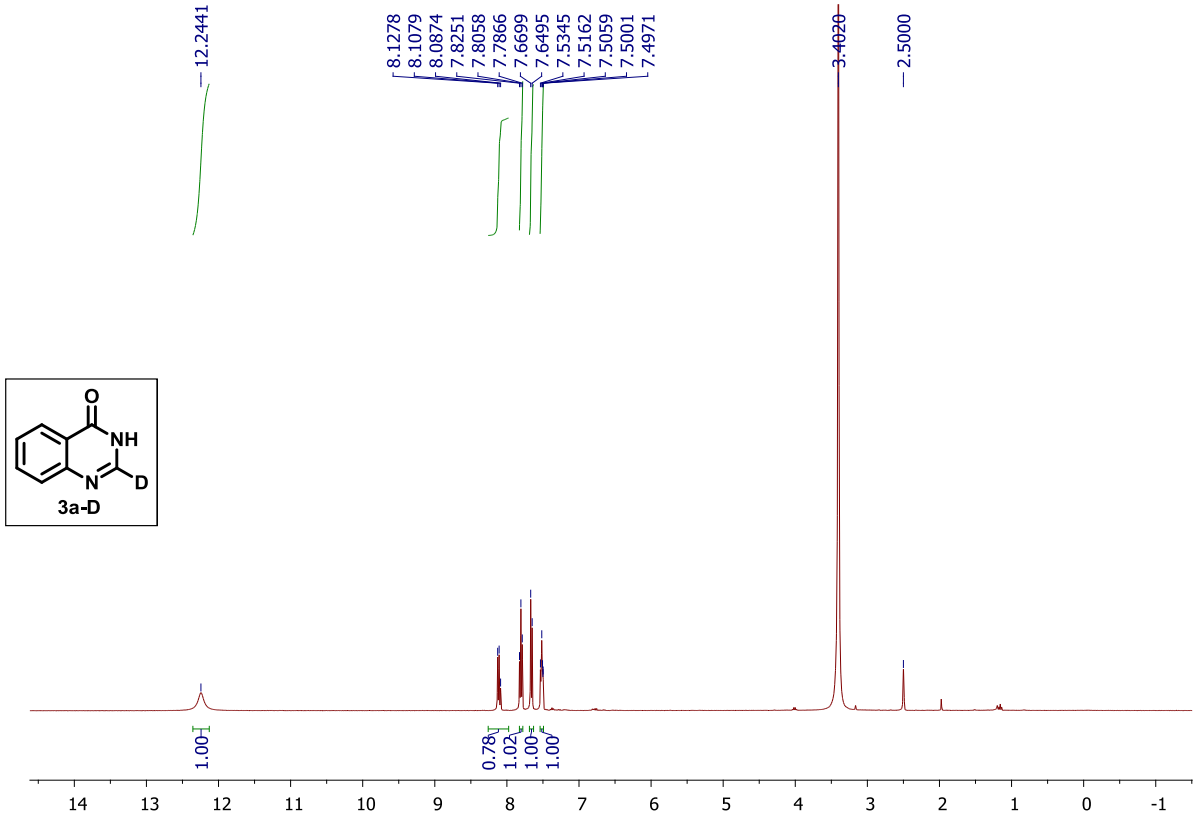
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N
D
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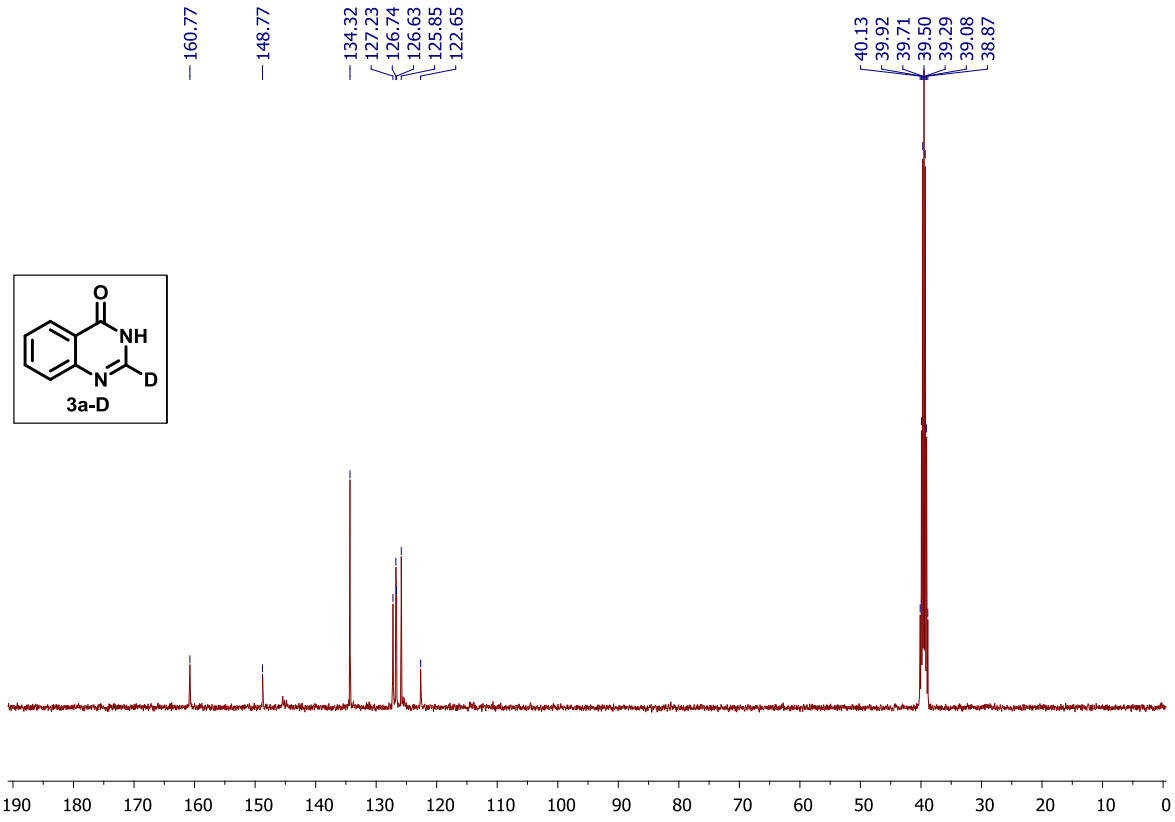
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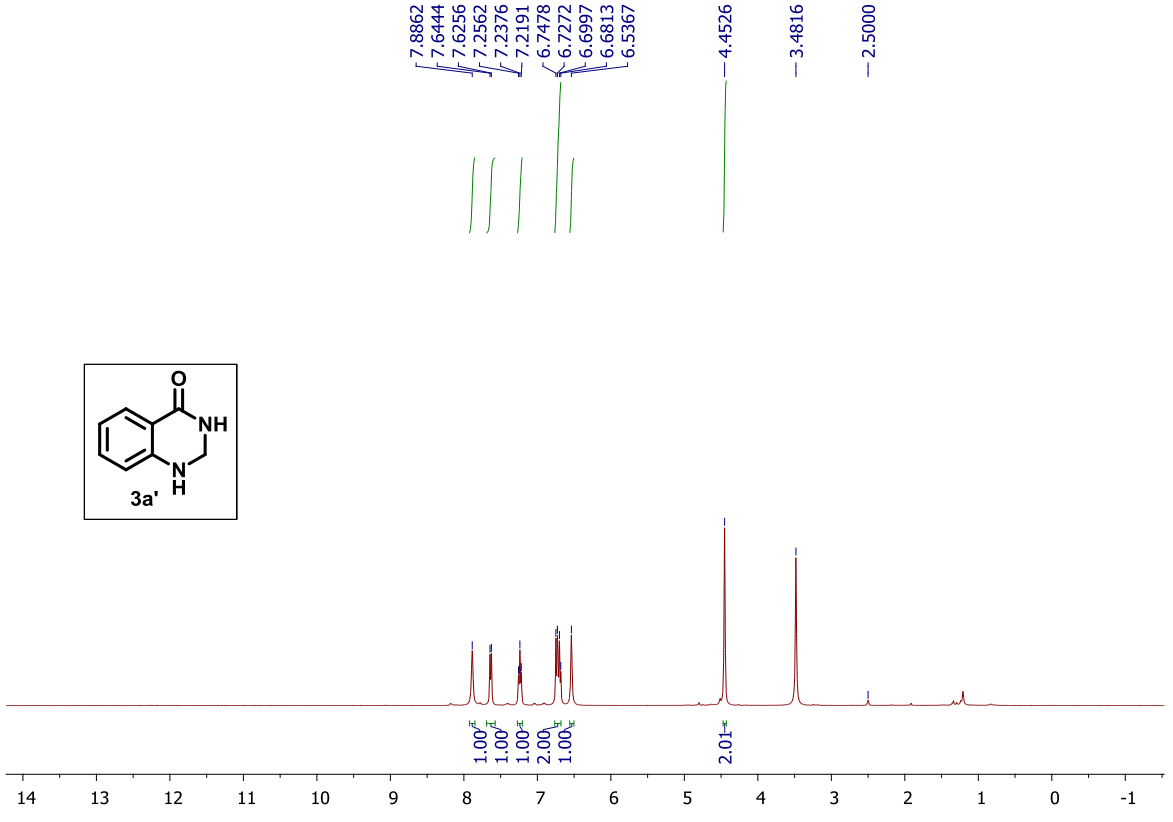
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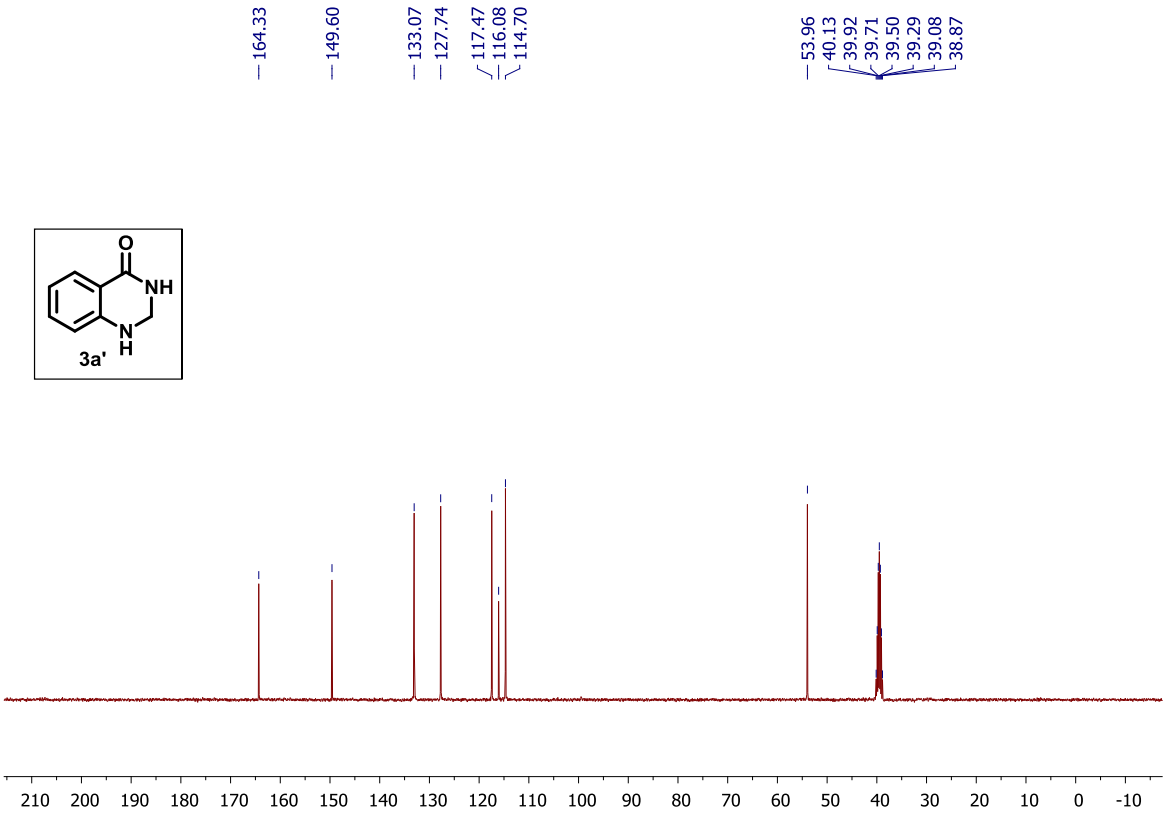
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3a'
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