

Supporting Information

Lossen Rearrangement vs C-N Reductive Elimination enabled by Rh(III)-Catalyzed C–H Activation/Selective Lactone Ring-Opening: Chemodivergent Synthesis of Quinolinones and Dihydroisoquinolinones

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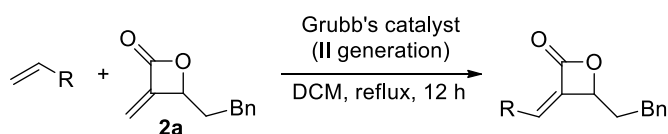
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I. General

NMR spectra were recorded on JEOL 400 NMR (^1H 400 MHz; ^{13}C 100 MHz) in either CDCl_3 , $\text{DMSO}-d_6$ or CD_3OD . Abbreviations for data quoted are s, singlet; brs, broad singlet; d, doublet; t, triplet; dd, doublet of doublets; m, multiplet. The residual solvent signals were used as references and the chemical shifts converted to the TMS scale ($\delta_{\text{H}} = 7.26$ ppm, $\delta_{\text{C}} = 77.16$ ppm; DMSO: $\delta_{\text{H}} = 2.50$ ppm, $\delta_{\text{C}} = 39.52$ ppm; CD_3OD : $\delta_{\text{H}} = 3.31$ ppm, $\delta_{\text{C}} = 49.00$ ppm). Mass spectra and high-resolution mass spectra were measured on an agilent TOF-G6230B mass spectrometer and Thermo-DFS mass spectrometer. Infrared spectra were obtained on a Nicolet 6700 FT-IR instrument. Thin-layer chromatographies were done on pre-coated silica gel 60 F254 plates (Merck). Silica gel 60H (200-300 mesh) and preparative TLC (200x200 mm, 0.2-0.25 mm in thickness) manufactured by Qingdao Haiyang Chemical Group Co. (China) were used for general chromatography. $[\text{Cp}^*\text{IrCl}_2]_2$, $[\text{Cp}^*\text{RhCl}_2]_2$ and $[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ were purchased from Aldrich and used without further purification. Substrates aromatic or vinylic amides^{S1} and methyleneoxetanones^{S2} were synthesized according to published procedures. Other chemicals were purchased from commercial suppliers and were dried and purified when necessary. No attempts were made to optimize yields for substrate synthesis.

II. Experimental Information and Characterization Data

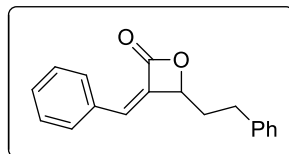
Synthesis of substituted methyleneoxetanones:



The substituted methyleneoxetanones were synthesized according to a known procedure:^{S2c} The olefin cross partner (1.5 equiv) was added to a solution of methyleneoxetanone **2a** (1 equiv) under N_2 in DCM (0.4 M). Catalyst (0.05 equiv) was added and the resultant solution was heated at reflux for 12 h. Afterwards, the solution was cooled and concentrated, and the brown residue was purified by flash

chromatography on silica gel to give the desired product.

(Z)-3-benzylidene-4-phenethyloxetan-2-one (2f)



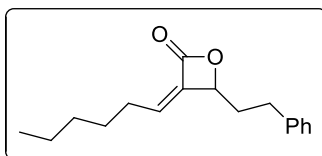
This compound was obtained in 35% yield (92.4 mg) as a light yellow solid. Eluent: PE/EA = 10/1, $R_f = 0.5$.

^1H NMR (400 MHz, CDCl_3): δ 7.90 (dd, $J = 7.3, 2.0$ Hz, 2H), 7.44-7.38 (m, 3H), 7.34-7.29 (m, 2H), 7.26-7.21 (m, 3H), 6.38 (s, 1H), 4.99-4.93 (m, 1H), 2.98-2.88 (m, 1H), 2.86-2.78 (m, 1H), 2.27-2.19 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3): δ 163.1, 140.5, 135.5, 133.7, 133.0, 130.8, 130.4, 129.0, 128.8, 128.6, 126.5, 77.5, 35.7, 31.1.

HRMS (ESI) calculated for $\text{C}_{18}\text{H}_{17}\text{O}_2$ ($[\text{M}+\text{Na}]^+$): 287.1043; found: 287.1039.

(Z)-3-hexylidene-4-phenethyloxetan-2-one (2g)



This compound was obtained in 70% yield (180 mg) as a colorless oil. Eluent: PE/EA = 10/1, $R_f = 0.5$.

^1H NMR (400 MHz, CDCl_3): δ 7.30 (t, $J = 7.4$ Hz, 2H), 7.24-7.17 (m, 3H), 5.74 (t, $J = 8.0$ Hz, 1H), 4.85 (t, $J = 6.2$ Hz, 1H), 2.88-2.70 (m, 2H), 2.46 (q, $J = 7.5$ Hz, 2H), 2.16-2.09 (m, 2H), 1.48-1.39 (m, 2H), 1.35-1.25 (m, 4H), 0.89 (t, $J = 7.8$ Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 164.1, 140.5, 137.2, 136.9, 128.7, 128.5, 126.4, 77.8, 35.6, 31.2, 31.0, 29.0, 28.6, 22.5, 14.1.

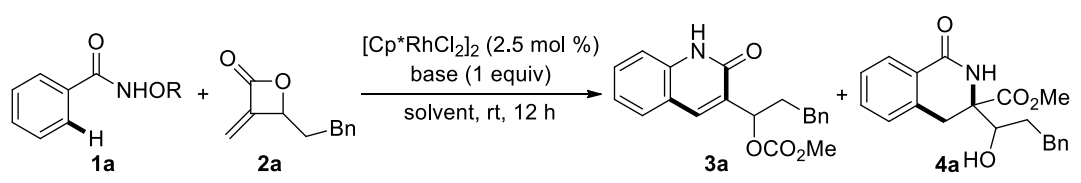
HRMS (ESI) calculated for $\text{C}_{17}\text{H}_{23}\text{O}_2$ ($[\text{M}+\text{Na}]^+$): 281.1512; found: 281.1508.

Optimization studies:

The mixture of *N*-acetoxybenzamide or *N*-pivaloyloxybenzamide (0.1 mmol, 1.0 equiv), methyleneoxetanone **2a** (0.1 mmol, 1.0 equiv), $[\text{Cp}^*\text{RhCl}_2]_2$ (2.5 mol %),

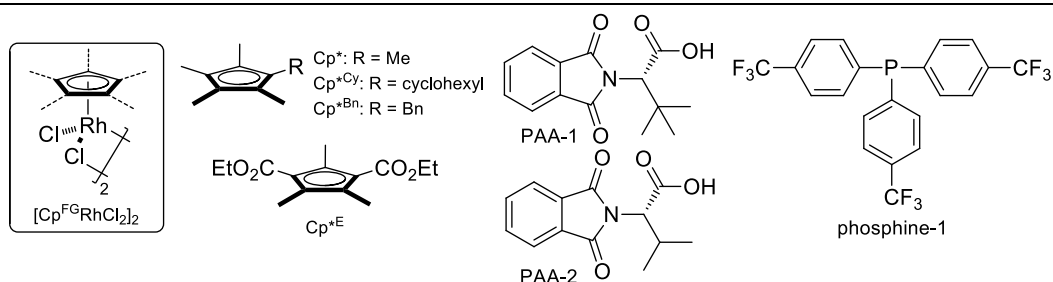
additive (1 equiv) and base (1 equiv) in the solvent (1.0 mL) was stirred in a sealed tube at room temperature for 12 h without exclusion of air or moisture. Afterwards, the mixture was diluted with EA, transferred to a round-bottom flask and concentrated. The crude product was analyzed by ¹H-NMR with 1,3,5-trimethoxybenzene as an internal standard.

Table S1 Reaction Conditions Screening^a



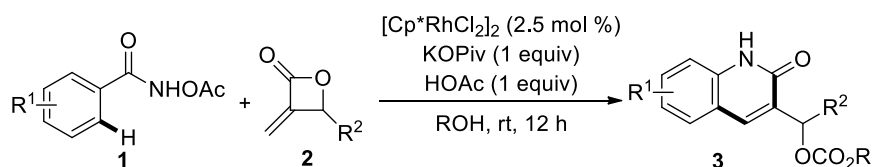
| Entry | R | Base | Additive | Solvent | ¹ H-NMRYield (%) | |
|-----------------|----|---------------------------------|--------------------------------|--------------------|-----------------------------|------|
| | | | | | 3a | 4a |
| 1 | Ac | CsOAc | - | MeOH | 27 | 26 |
| 2 ^b | Ac | CsOAc | - | EtOH | 36 | 43 |
| 3 | Ac | CsOAc | - | TFE | | n.d. |
| 4 | Ac | CsOAc | - | CH ₃ CN | | n.d. |
| 5 | Ac | CsOAc | - | dioxane | | n.d. |
| 6 | Ac | CsOAc | - | THF | | n.d. |
| 7 | Ac | CsOAc | - | DCE | | n.d. |
| 8 | Ac | CsOAc | - | HFIP | | n.d. |
| 9 | Ac | CsOAc | - | ^t BuOH | | n.d. |
| 10 | Ac | NaOAc | - | MeOH | 46 | 10 |
| 11 | Ac | AgOAc | - | MeOH | 40 | n.d. |
| 12 | Ac | CsOAc | - | MeOH | 44 | 15 |
| 13 | Ac | KO ^t Bu | - | MeOH | 28 | 10 |
| 14 | Ac | KOPiv | - | MeOH | 51 | 11 |
| 15 | Ac | Zn(OAc) ₂ | - | MeOH | 36 | n.d. |
| 16 | Ac | Cu(OAc) ₂ | - | MeOH | n.d. | n.d. |
| 17 | Ac | K ₂ HPO ₄ | - | MeOH | n.d. | n.d. |
| 18 | Ac | KH ₂ PO ₄ | - | MeOH | n.d. | n.d. |
| 19 | Ac | KOPiv | HOAc (1 equiv) | MeOH | 70 | 18 |
| 20 | Ac | KOPiv | 4Å MS (20 mg) | MeOH | 46 | 14 |
| 21 | Ac | KOPiv | Amberlite IRA-400 | MeOH | 56 | 16 |
| 22 | Ac | KOPiv | Amberlite IR-120 | MeOH | 48 | 14 |
| 23 | Ac | KOPiv | HCOOH (1 equiv) | MeOH | 37 | 10 |
| 24 | Ac | KOPiv | CF ₃ COOH (1 equiv) | MeOH | n.d. | n.d. |
| 25 | Ac | KOPiv | PivOH (1 equiv) | MeOH | 32 | n.d. |
| 26 ^c | Ac | KOPiv | HOAc (1 equiv) | MeOH | 50 | 11 |

| | | | | | | |
|-----------------|-----|---------------------------------|-------------------------|------|------|------|
| 27 ^d | Ac | KOPiv | HOAc (1 equiv) | MeOH | 36 | 23 |
| 28 ^e | Ac | KOPiv | HOAc (1 equiv) | MeOH | <5 | <5 |
| 29 | Ac | KOPiv | Pyridine (1 equiv) | MeOH | <5 | <5 |
| 30 ^f | Ac | KOPiv | CBZ-leucine (0.2) | MeOH | 35 | 15 |
| 31 ^f | Ac | KOPiv | PAA-1 (0.2) | MeOH | 37 | 16 |
| 32 ^f | Ac | KOPiv | PAA-2 (0.2) | MeOH | 32 | 15 |
| 33 ^f | Ac | KOPiv | Ph ₃ P (0.2) | MeOH | 24 | 7 |
| 34 ^f | Ac | KOPiv | Phosphine-1 (0.2) | MeOH | n.d. | n.d. |
| 35 | Piv | NaOAc | - | MeOH | 39 | 55 |
| 36 | Piv | AgOAc | - | MeOH | 37 | n.d. |
| 37 | Piv | CsOAc | - | MeOH | 38 | 51 |
| 38 | Piv | tBuKO | - | MeOH | 26 | 41 |
| 39 | Piv | KOPiv | - | MeOH | 42 | 54 |
| 40 | Piv | Zn(OAc) ₂ | - | MeOH | 22 | 32 |
| 41 | Piv | Cu(OAc) ₂ | - | MeOH | n.d. | n.d. |
| 42 | Piv | K ₂ HPO ₄ | - | MeOH | 22 | 53 |
| 43 | Piv | KH ₂ PO ₄ | - | MeOH | n.d. | n.d. |
| 44 | Piv | K ₃ PO ₄ | - | MeOH | n.d. | 54 |
| 45 | Piv | NaOAc | 4Å MS (20 mg) | MeOH | 33 | 36 |
| 46 | Piv | NaOAc | Amberlite IRA-400 | MeOH | 37 | 47 |
| 47 | Piv | NaOAc | Amberlite IR-120 | MeOH | 30 | 37 |
| 48 | Piv | NaOAc | HOAc (1 equiv) | MeOH | 35 | 41 |



^aReaction Conditions: **1** (0.1 mmol), **2a** (0.1 mmol), [Cp**RhCl*₂]₂ (2.5 mol %), base (1equiv) and additive in the solvent (0.1 M) at room temperature for 12 h under air, ¹H-NMR yields were reported by using 5.6 mg of 1,3,5-trimethoxybenzene as an internal standard. ^bThe corresponding ethyl ester was detected. ^c[Cp*^{Cy}RhCl₂]₂ was used as the catalyst. ^d[Cp*^{Bn}RhCl₂]₂ was used as the catalyst. ^e[Cp*^ERhCl₂]₂ was used as the catalyst. ^fHOAc (1 equiv) was added as the additive. n.d.: not detected.

General procedure A:

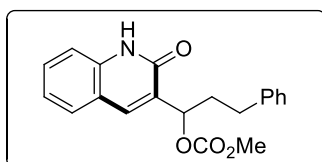


The mixture of *N*-acetoxycyclohexanone **1** (0.2 mmol, 1.0 equiv), methylenecyclohexanones

2 (0.2 mmol, 1.0 equiv), $[\text{Cp}^*\text{RhCl}_2]_2$ (2.5 mol %), HOAc (0.2 mmol, 1.0 equiv) and KO₂Piv (0.2 mmol, 1.0 equiv) in the alcoholic solvent (2.0 mL) in a sealed tube was stirred at room temperature for 12 h without exclusion of air or moisture. Afterwards, the solvent was removed with the reduced pressure and the crude product was purified by preparative TLC to afford the corresponding products **3**.

Characterization of products:

methyl (1-(2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl) carbonate (**3a**)



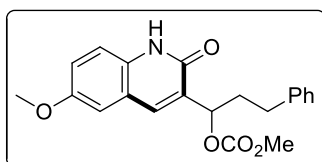
This compound was obtained in 68% yield (45.8 mg) as light yellow oil. Eluent: DCM/PE = 7/1, $R_f = 0.4$.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.40 (s, 1H), 8.21-8.18 (m, 1H), 7.51-7.48 (m, 1H), 7.45-7.39 (m, 1H), 7.34-7.26 (m, 4H), 7.24-7.18 (m, 2H), 7.00 (s, 1H), 5.15-5.09 (m, 1H), 3.67 (s, 3H), 2.89-2.69 (m, 2H), 2.35-2.23 (m, 1H), 2.18-2.05 (m, 1H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.0, 154.9, 140.8, 137.1, 135.1, 131.0, 129.5, 129.4, 128.41, 128.35, 126.3, 126.0, 125.1, 124.8, 77.5, 51.9, 34.9, 30.2.

HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{19}\text{NNaO}_4$ ($[\text{M}+\text{Na}]^+$): 360.1206; found: 360.1199.

1-(6-methoxy-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl methyl carbonate (**3b**)



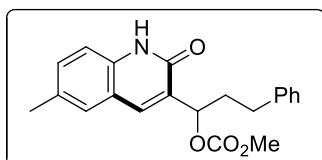
This compound was obtained in 50% yield (36.7 mg) as light yellow oil. Eluent: DCM/PE = 7/1, $R_f = 0.3$.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.17 (brs, 1H), 7.89 (d, *J* = 2.9 Hz, 1H), 7.34-7.25 (m, 5H), 7.23-7.18 (m, 1H), 7.02 (dd, *J* = 8.9, 3.0 Hz, 1H), 6.94 (d, *J* = 1.5 Hz, 1H), 5.13 (ddd, *J* = 7.7, 4.3, 1.3 Hz, 1H), 3.78 (s, 3H), 3.63 (s, 3H), 2.86-2.71 (m, 2H), 2.34-2.23 (m, 1H), 2.18-2.05 (m, 1H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.0, 156.4, 155.3, 140.8, 135.3, 130.3, 129.5, 128.4, 128.3, 128.2, 127.4, 126.0, 117.7, 113.0, 77.5, 55.3, 51.8, 34.8, 30.2.

HRMS (ESI) calculated for C₂₁H₂₁NNaO₅ ([M+Na]⁺): 390.1312; found: 390.1311.

methyl (1-(6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl) carbonate (3c)



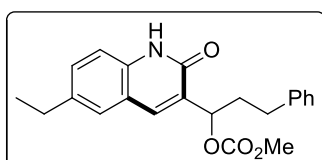
This compound was obtained in 63% yield (44.2 mg) as light yellow oil. Eluent: DCM/PE = 7/1, R_f = 0.4.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.26 (brs, 1H), 8.01 (d, *J* = 1.7 Hz, 1H), 7.35-7.26 (m, 5H), 7.25-7.17 (m, 2H), 6.95 (d, *J* = 1.5 Hz, 1H), 5.11 (ddd, *J* = 7.7, 4.4, 1.4 Hz, 1H), 3.63 (s, 3H), 2.86-2.70 (m, 2H), 2.34-2.23 (m, 4H), 2.16-2.04 (m, 1H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.9, 155.0, 140.8, 134.9, 134.7, 134.0, 131.7, 129.6, 129.5, 128.4, 128.3, 126.0, 125.2, 77.4, 51.8, 34.9, 30.2, 20.5.

HRMS (ESI) calculated for C₂₁H₂₁NNaO₄ ([M+Na]⁺): 374.1363; found: 374.1360.

1-(6-ethyl-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl methyl carbonate (3d)



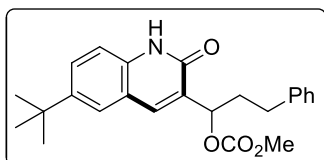
This compound was obtained in 61% yield (44.5 mg) as light yellow oil. Eluent: DCM/PE = 7/1, R_f = 0.5.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.27 (brs, 1H), 8.08 (d, *J* = 1.9 Hz, 1H), 7.37-7.30 (m, 2H), 7.30-7.24 (m, 4H), 7.22-7.17 (m, 1H), 6.96 (d, *J* = 1.4 Hz, 1H), 5.17-5.06 (m, 1H), 3.64 (s, 3H), 2.85-2.71 (m, 2H), 2.60 (q, *J* = 7.6 Hz, 2H), 2.35-2.23 (m, 1H), 2.17-2.04 (m, 1H), 1.20 (t, *J* = 7.6 Hz, 3H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.0, 155.0, 140.8, 140.3, 134.9, 134.8, 130.6, 129.7, 128.4, 128.3, 126.4, 126.0, 125.3, 77.4, 51.8, 34.9, 30.2, 27.6, 15.3.

HRMS (ESI) calculated for C₂₂H₂₃NNaO₄ ([M+Na]⁺): 388.1519; found: 388.1515.

1-(6-(*tert*-butyl)-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl methyl carbonate (3e)



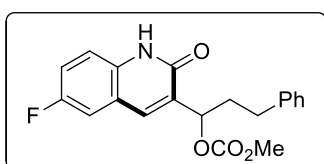
This compound was obtained in 58% yield (45.8 mg) as light yellow oil. Eluent: DCM/PE = 7/1, R_f = 0.55.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.30 (brs, 1H), 8.32 (d, *J* = 2.2 Hz, 1H), 7.44 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.36 (d, *J* = 8.5 Hz, 1H), 7.31-7.25 (m, 4H), 7.21-7.16 (m, 1H), 6.98 (d, *J* = 1.1 Hz, 1H), 5.15-5.08 (m, 1H), 3.65 (s, 3H), 2.85-2.72 (m, 2H), 2.34-2.24 (m, 1H), 2.16-2.06 (m, 1H), 1.29 (s, 9H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.1, 155.0, 147.4, 140.8, 134.7, 134.6, 129.8, 128.4, 128.4, 128.2, 128.14, 128.07, 126.4, 126.0, 125.9, 125.0, 77.4, 51.9, 35.0, 34.4, 31.0, 30.2.

HRMS (ESI) calculated for C₂₄H₂₇NNaO₄ ([M+Na]⁺): 416.1832; found: 416.1825.

1-(6-fluoro-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl methyl carbonate (3f)



This compound was obtained in 49% yield (34.8 mg) as light yellow oil. Eluent: DCM/PE = 7/1, $R_f = 0.5$.

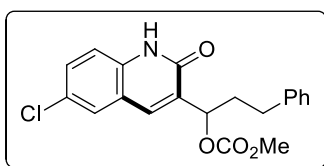
^1H NMR (400 MHz, DMSO- d_6): δ 9.37 (s, 1H), 8.03 (dd, $J = 10.1, 3.0$ Hz, 1H), 7.46 (dd, $J = 8.9, 5.5$ Hz, 1H), 7.34-7.26 (m, 5H), 7.24-7.17 (m, 1H), 6.95 (t, $J = 1.4$ Hz, 1H), 5.15 (ddd, $J = 7.8, 4.4, 1.4$ Hz, 1H), 3.65 (s, 3H), 2.85-2.71 (m, 2H), 2.35-2.26 (m, 1H), 2.20-2.06 (m, 1H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 162.8, 158.7 (d, $J = 240.4$ Hz), 155.0, 140.8, 136.5, 133.6, 128.4, 128.3, 127.5, 126.0, 117.9 (d, $J = 22.6$ Hz), 115.1 (d, $J = 24.1$ Hz), 77.7, 52.0, 34.7, 30.1.

^{19}F NMR (376 MHz, DMSO- d_6): δ -114.4.

HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{18}\text{FNNaO}_4$ ($[\text{M}+\text{Na}]^+$): 378.1112; found: 378.1108.

1-(6-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl methyl carbonate (3g)



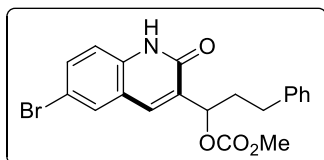
This compound was obtained in 52% yield (38.6 mg) as light yellow oil. Eluent: DCM/PE = 7/1, $R_f = 0.5$.

^1H NMR (400 MHz, DMSO- d_6): δ 9.48 (brs, 1H), 8.22 (d, $J = 2.4$ Hz, 1H), 7.54-7.46 (m, 2H), 7.33-7.26 (m, 4H), 7.22-7.17 (m, 1H), 6.95 (d, $J = 1.5$ Hz, 1H), 5.13 (ddd, $J = 7.8, 4.3, 1.4$ Hz, 1H), 3.66 (s, 3H), 2.85-2.71 (m, 2H), 2.35-2.25 (s, 1H), 2.18-2.06 (m, 1H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 162.8, 154.7, 140.8, 136.5, 136.0, 130.5, 128.7, 128.41, 128.35, 128.2, 128.0, 126.5, 126.0, 77.7, 52.0, 34.7, 30.1.

HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{18}\text{ClNNaO}_4$ ($[\text{M}+\text{Na}]^+$): 394.0817; found: 394.0818.

1-(6-bromo-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl methyl carbonate (3h)



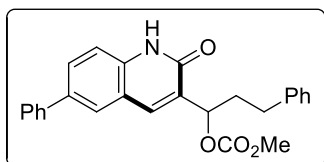
This compound was obtained in 56% yield (46.5 mg) as light yellow oil. Eluent: DCM/PE = 7/1, $R_f = 0.4$.

^1H NMR (400 MHz, DMSO- d_6): δ 9.47 (brs, 1H), 8.36 (d, $J = 2.4$ Hz, 1H), 7.59 (dd, $J = 8.7, 2.4$ Hz, 1H), 7.47 (d, $J = 8.7$ Hz, 1H), 7.35-7.25 (m, 4H), 7.23-7.17 (m, 1H), 6.94 (d, $J = 1.5$ Hz, 1H), 5.13 (ddd, $J = 7.8, 4.4, 1.4$ Hz, 1H), 3.67 (s, 3H), 2.82-2.75 (m, 2H), 2.38-2.23 (m, 1H), 2.19-2.06 (m, 1H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 162.9, 154.7, 140.8, 136.4, 133.4, 131.6, 128.40, 128.35, 128.0, 127.8, 126.7, 126.0, 116.7, 77.7, 52.0, 34.7, 30.2.

HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{18}\text{BrNNaO}_4$ ($[\text{M}+\text{Na}]^+$): 438.0311; found: 438.0308.

methyl (1-(2-oxo-6-phenyl-1,2-dihydroquinolin-3-yl)-3-phenylpropyl) carbonate (3i)



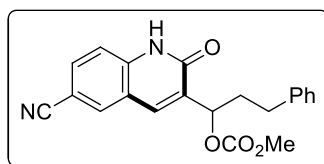
This compound was obtained in 62% yield (51.2 mg) as light yellow oil. Eluent: DCM/PE = 5/1, $R_f = 0.7$.

^1H NMR (400 MHz, DMSO- d_6): δ 9.47 (brs, 1H), 8.52 (d, $J = 2.1$ Hz, 1H), 7.79-7.68 (m, 3H), 7.60 (d, $J = 8.5$ Hz, 1H), 7.49 (t, $J = 8.0$ Hz, 2H), 7.37 (t, $J = 7.3$ Hz, 1H), 7.34-7.27 (m, 4H), 7.23-7.17 (m, 1H), 7.07 (d, $J = 1.3$ Hz, 1H), 5.19-5.12 (m, 1H), 3.69 (s, 3H), 2.88-2.73 (m, 2H), 2.38-2.26 (m, 1H), 2.20-2.10 (m, 1H).

^{13}C NMR (100 MHz, CDCl_3): δ 163.2, 155.0, 140.4, 139.6, 138.6, 137.2, 134.8, 129.8, 129.2, 129.04, 129.01, 128.8, 128.7, 128.6, 128.2, 127.7, 127.1, 126.9, 126.6, 77.7, 52.9, 35.6, 31.0.

HRMS (ESI) calculated for $\text{C}_{26}\text{H}_{23}\text{NNaO}_4$ ($[\text{M}+\text{Na}]^+$): 436.1519; found: 436.1518.

1-(6-cyano-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl methyl carbonate
(3j)



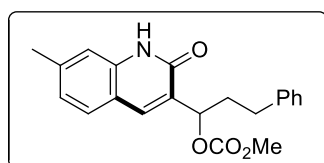
This compound was obtained in 32% yield (23.2 mg) as white solid. Eluent: DCM/PE = 8/1, $R_f = 0.4$.

^1H NMR (400 MHz, DMSO- d_6): δ 9.79 (brs, 1H), 8.43 (d, $J = 1.6$ Hz, 1H), 7.90-7.80 (m, 2H), 7.34-7.26 (m, 4H), 7.23-7.17 (m, 1H), 7.03 (d, $J = 1.5$ Hz, 1H), 5.15 (ddd, $J = 7.7, 4.4, 1.2$ Hz, 1H), 3.70 (s, 3H), 2.87-2.70 (m, 2H), 2.37-2.26 (m, 1H), 2.21-2.08 (m, 1H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 162.8, 154.2, 141.2, 140.8, 137.5, 133.9, 133.7, 128.43, 128.38, 127.4, 126.1, 125.2, 123.8, 118.4, 106.2, 77.9, 52.3, 34.6, 30.2.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{18}\text{N}_2\text{NaO}_4$ ($[\text{M}+\text{Na}]^+$): 385.1159; found: 385.1153.

methyl (1-(7-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl) carbonate
(3k)



This compound was obtained in 51% yield (35.8 mg) as white solid. Eluent: DCM/PE = 8/1, $R_f = 0.7$.

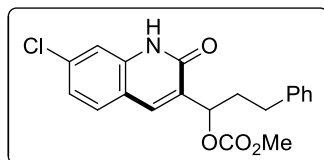
^1H NMR (400 MHz, DMSO- d_6): δ 9.33 (brs, 1H), 8.12 (d, $J = 8.1$ Hz, 1H), 7.34-7.25 (m, 5H), 7.22-7.17 (m, 1H), 7.06 (dd, $J = 8.1, 1.5$ Hz, 1H), 6.95 (d, $J = 1.3$ Hz, 1H), 5.09 (ddd, $J = 7.7, 4.3, 1.3$ Hz, 1H), 3.66 (s, 3H), 2.85-2.71 (m, 2H), 2.31 (s, 3H), 2.30-2.22 (m, 1H), 2.15-2.04 (m, 1H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 163.1, 154.9, 141.2, 140.8, 137.1, 133.9, 129.5, 129.3, 128.41, 128.35, 126.0, 125.8, 125.5, 123.7, 77.4, 51.9, 35.0, 30.2, 21.1.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{22}\text{NO}_4$ ($[\text{M}+\text{H}]^+$): 352.1543; found: 352.1533.

1-(7-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl methyl carbonate

(3l)



This compound was obtained in 45% yield (33.3 mg) as white solid. Eluent: DCM/PE = 8/1, $R_f = 0.7$.

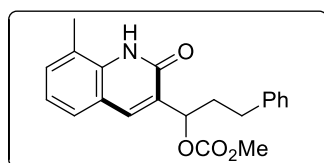
^1H NMR (400 MHz, DMSO- d_6): δ 9.57 (brs, 1H), 8.15 (d, $J = 8.6$ Hz, 1H), 7.63 (d, $J = 2.2$ Hz, 1H), 7.34-7.25 (m, 5H), 7.23-7.17 (m, 1H), 6.97 (d, $J = 1.4$ Hz, 1H), 5.12 (ddd, $J = 7.8, 4.3, 1.4$ Hz, 1H), 3.68 (s, 3H), 2.87-2.70 (m, 2H), 2.36-2.24 (m, 1H), 2.17-2.05 (m, 1H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 162.9, 154.6, 140.8, 138.5, 135.7, 134.9, 130.9, 128.4, 128.3, 128.2, 126.1, 124.5, 124.4, 123.9, 77.7, 52.1, 34.8, 30.2.

HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{18}\text{ClNNaO}_4$ ($[\text{M}+\text{Na}]^+$): 394.0817; found: 394.0815.

methyl (1-(8-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl) carbonate

(3m)



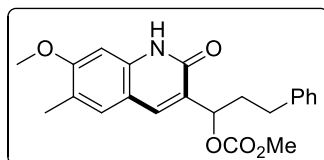
This compound was obtained in 37% yield (26.0 mg) as light yellow oil. Eluent: DCM/PE = 7/1, $R_f = 0.5$.

^1H NMR (400 MHz, DMSO- d_6): δ 9.05 (brs, 1H), 8.09 (d, $J = 7.6$ Hz, 1H), 7.34 (t, $J = 7.5$ Hz, 2H), 7.30-7.25 (m, 4H), 7.23-7.18 (m, 1H), 6.95 (s, 1H), 5.16-5.11 (m, 1H), 3.63 (s, 3H), 2.84-2.69 (m, 2H), 2.33-2.23 (m, 1H), 2.20 (s, 3H), 2.17-2.02 (m, 1H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 162.9, 155.0, 140.8, 136.2, 135.5, 135.4, 132.7, 130.3, 130.1, 128.4, 128.3, 127.1, 126.6, 126.1, 77.5, 52.0, 34.8, 30.1, 17.9.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{21}\text{NNaO}_4$ ($[\text{M}+\text{Na}]^+$): 374.1363; found: 374.1363.

1-(7-methoxy-6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl methyl carbonate (3n)



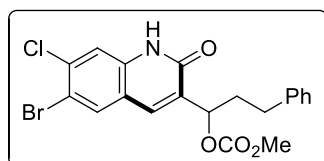
This compound was obtained in 31% yield (23.6 mg) as light yellow oil. Eluent: DCM/PE = 5/1, R_f = 0.4.

^1H NMR (400 MHz, DMSO- d_6): δ 9.36 (brs, 1H), 8.11 (s, 1H), 7.33-7.25 (m, 4H), 7.22-7.17 (m, 1H), 7.07 (s, 1H), 6.89 (d, J = 1.2 Hz, 1H), 5.10-5.02 (m, 1H), 3.80 (s, 3H), 3.65 (s, 3H), 2.85-2.71 (m, 2H), 2.31-2.22 (m, 1H), 2.12 (s, 3H), 2.11-2.00 (m, 1H).

^{13}C NMR (100 MHz, CD $_3$ OD): δ 165.2, 161.4, 157.6, 142.2, 137.9, 133.6, 132.6, 130.1, 129.6, 129.5, 129.3, 127.2, 125.4, 78.7, 56.0, 53.0, 36.8, 31.9, 15.9.

HRMS (ESI) calculated for C $_{22}$ H $_{23}$ NNaO $_5$ ($[\text{M}+\text{Na}]^+$): 404.1468; found: 404.1472.

1-(6-bromo-7-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl methyl carbonate (3o)



This compound was obtained in 37% yield (33.2 mg) as light yellow oil. Eluent: DCM/PE = 8/1, R_f = 0.7.

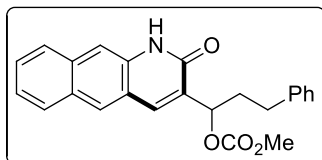
^1H NMR (400 MHz, DMSO- d_6): δ 9.62 (brs, 1H), 8.50 (s, 1H), 7.83 (s, 1H), 7.35-7.25 (m, 4H), 7.22-7.16 (m, 1H), 6.94 (d, J = 1.5 Hz, 1H), 5.13 (ddd, J = 7.8, 4.4, 1.4 Hz, 1H), 3.68 (s, 3H), 2.85-2.71 (m, 2H), 2.36-2.24 (m, 1H), 2.18-2.08 (m, 1H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 162.8, 154.5, 140.7, 137.6, 137.0, 134.6, 133.7, 128.41, 128.36, 126.9, 126.1, 125.8, 125.4, 116.3, 77.8, 52.2, 34.6, 30.2.

HRMS (ESI) calculated for C $_{20}$ H $_{17}$ BrClINNaO $_4$ ($[\text{M}+\text{Na}]^+$): 471.9922; found:

471.9925.

methyl (1-(2-oxo-1,2-dihydrobenzo[g]quinolin-3-yl)-3-phenylpropyl) carbonate (3p)



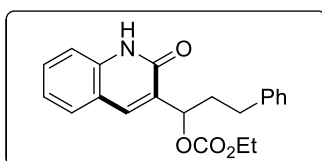
This compound was obtained in 34% yield (26.4 mg) as pink solid. Eluent: DCM/PE = 8/1, $R_f = 0.5$.

^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ 9.63 (brs, 1H), 8.40 (d, $J = 8.7$ Hz, 1H), 8.03-7.91 (m, 3H), 7.67-7.56 (m, 2H), 7.35-7.26 (m, 4H), 7.24-7.18 (m, 1H), 7.14 (s, 1H), 5.20 (ddd, $J = 7.6, 4.4, 1.3$ Hz, 1H), 3.69 (s, 3H), 2.87-2.73 (m, 2H), 2.40-2.27 (m, 1H), 2.24-2.09 (m, 1H).

^{13}C NMR (100 MHz, $\text{DMSO-}d_6$): δ 162.9, 155.6, 140.8, 136.0, 134.5, 133.7, 130.3, 129.8, 128.4, 128.3, 128.1, 127.7, 127.6, 127.0, 126.9, 126.1, 125.6, 124.1, 77.6, 52.2, 34.8, 30.1.

HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{21}\text{NNaO}_4$ ($[\text{M}+\text{Na}]^+$): 410.1363; found: 410.1359.

ethyl (1-(2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl) carbonate (3q)



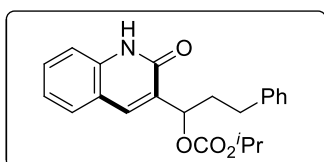
This compound was obtained in 68% yield (47.8 mg) as light yellow oil. Eluent: DCM/PE = 7/1, $R_f = 0.4$.

^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ 9.37 (s, 1H), 8.17 (dd, $J = 7.9, 1.4$ Hz, 1H), 7.49-7.45 (m, 1H), 7.44-7.38 (m, 1H), 7.33-7.26 (m, 4H), 7.25-7.18 (m, 2H), 6.98 (d, $J = 1.4$ Hz, 1H), 5.12 (ddd, $J = 7.8, 4.3, 1.4$ Hz, 1H), 4.14-4.07 (m, 2H), 2.86-2.71 (m, 2H), 2.35-2.23 (m, 1H), 2.16-2.05 (m, 1H), 1.22 (t, $J = 7.1$ Hz, 3H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.0, 154.5, 140.9, 137.2, 135.0, 131.0, 129.6, 129.4, 128.5, 128.4, 126.2, 126.1, 125.0, 124.8, 77.5, 60.6, 35.0, 30.2, 14.5.

HRMS (ESI) calculated for C₂₁H₂₁NNaO₄ ([M+Na]⁺): 374.1363; found: 374.1356.

isopropyl (1-(2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl) carbonate (3r)



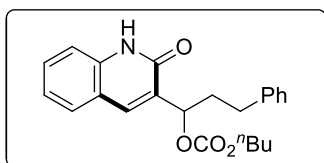
This compound was obtained in 37% yield (27.0 mg) as light yellow oil. Eluent: DCM/PE = 7/1, R_f = 0.6.

¹H NMR (400 MHz, CDCl₃): δ 8.14 (d, *J* = 7.1 Hz, 1H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.39 (td, *J* = 7.8, 1.5 Hz, 1H), 7.35-7.30 (m, 2H), 7.26-7.20 (m, 4H), 6.52 (s, 1H), 6.44 (brs, 1H), 5.05-4.95 (m, 2H), 2.97-2.90 (m, 1H), 2.87-2.78 (m, 1H), 2.29-2.21 (m, 2H), 1.30 (d, *J* = 6.3 Hz, 6H).

¹³C NMR (100 MHz, CDCl₃): δ 163.0, 154.0, 140.5, 136.8, 136.0, 131.5, 130.5, 128.8, 128.7, 128.2, 126.6, 125.8, 124.7, 77.5, 69.6, 35.6, 31.0, 22.2.

HRMS (ESI) calculated for C₂₂H₂₃NNaO₄ ([M+Na]⁺): 388.1519; found: 388.1520.

butyl (1-(2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylpropyl) carbonate (3s)



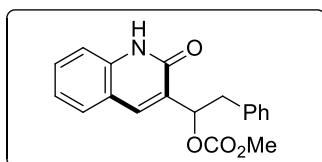
This compound was obtained in 59% yield (46.8 mg) as light yellow oil. Eluent: DCM/PE = 5/1, R_f = 0.6.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.36 (brs, 1H), 8.17 (d, *J* = 7.6 Hz, 1H), 7.47-7.38 (m, 2H), 7.33-7.26 (m, 4H), 7.25-7.18 (m, 2H), 6.97 (d, *J* = 1.1 Hz, 1H), 5.12 (ddd, *J* = 5.7, 4.3, 1.0 Hz, 1H), 4.11-4.00 (m, 2H), 2.87-2.71 (m, 2H), 2.34-2.23 (m, 1H), 2.16-2.06 (m, 1H), 1.62-1.53 (m, 2H), 1.39-1.30 (m, 2H), 0.88 (t, *J* = 7.6 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.1, 154.6, 140.5, 136.8, 135.8, 131.5, 130.5, 128.8, 128.7, 128.3, 126.6, 126.0, 77.4, 65.8, 35.6, 31.04, 31.02, 19.2, 13.9.

HRMS (ESI) calculated for C₂₃H₂₅NNaO₄ ([M+Na]⁺): 402.1676; found: 402.1675.

methyl (1-(2-oxo-1,2-dihydroquinolin-3-yl)-2-phenylethyl) carbonate (3t)



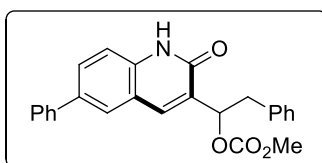
This compound was obtained in 61% yield (39.4 mg) as light yellow oil. Eluent: DCM/PE = 7/1, R_f = 0.5.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.33 (brs, 1H), 8.15-8.11 (m, 1H), 7.47-7.39 (m, 2H), 7.36-7.29 (m, 4H), 7.29-7.21 (m, 2H), 5.34 (ddd, *J* = 7.6, 4.7, 1.5 Hz, 1H), 3.68 (s, 3H), 3.32 (dd, *J* = 14.4, 7.6 Hz, 1H), 3.16 (dd, *J* = 14.4, 7.6 Hz, 1H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.8, 154.9, 137.1, 135.8, 134.9, 131.1, 129.8, 129.6, 129.3, 128.3, 126.7, 126.6, 125.5, 125.1, 77.8, 51.9, 38.9.

HRMS (ESI) calculated for C₁₉H₁₇NNaO₄ ([M+Na]⁺): 346.1050; found: 346.1046.

methyl (1-(2-oxo-6-phenyl-1,2-dihydroquinolin-3-yl)-2-phenylethyl) carbonate (3u)



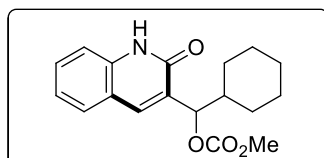
This compound was obtained in 79% yield (63.0 mg) as light yellow oil. Eluent: DCM/PE = 10/1, R_f = 0.55.

¹H NMR (400 MHz, CDCl₃): δ 8.33 (s, 1H), 7.67-7.62 (m, 4H), 7.46-7.41 (m, 2H), 7.40-7.33 (m, 3H), 7.33-7.27 (m, 3H), 6.55 (s, 1H), 6.40 (s, 1H), 5.20 (td, *J* = 6.8, 1.2 Hz, 1H), 3.80 (s, 3H), 3.39 (dd, *J* = 14.0, 6.7 Hz, 1H), 3.10 (dd, *J* = 14.0, 6.9 Hz, 1H).

¹³C NMR (100 MHz, CDCl₃): δ 162.9, 154.8, 139.6, 138.5, 136.9, 134.9, 134.8, 130.0, 129.7, 129.2, 129.1, 129.0, 128.9, 128.8, 128.6, 127.7, 127.6, 127.1, 77.6, 52.9, 40.2.

HRMS (ESI) calculated for C₂₅H₂₁NNaO₄ ([M+Na]⁺): 422.1363; found: 422.1360.

cyclohexyl(2-oxo-1,2-dihydroquinolin-3-yl)methyl methyl carbonate (3v)



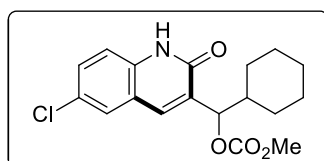
This compound was obtained in 54% yield (34.2 mg) as light yellow oil. Eluent: DCM/PE = 7/1, R_f = 0.5.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.44 (s, 1H), 8.20-8.12 (m, 1H), 7.49-7.38 (m, 2H), 7.27-7.20 (m, 1H), 6.95 (d, *J* = 1.2 Hz, 1H), 4.89 (dd, *J* = 5.9, 1.1 Hz, 1H), 3.66 (s, 3H), 1.83-1.72 (m, 5H), 1.68-1.64 (m, 1H), 1.29-1.08 (m, 5H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.0, 154.9, 137.0, 134.1, 130.9, 129.6, 129.4, 126.5, 125.2, 124.9, 81.1, 51.9, 40.4, 27.0, 26.9, 25.7, 25.1, 25.0.

HRMS (ESI) calculated for C₁₈H₂₁NNaO₄ ([M+Na]⁺): 338.1363; found: 338.1360.

(6-chloro-2-oxo-1,2-dihydroquinolin-3-yl)(cyclohexyl)methyl methyl carbonate (3w)



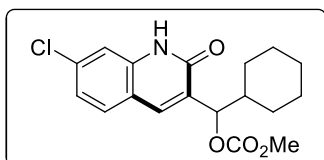
This compound was obtained in 61% yield (42.6 mg) as light yellow oil. Eluent: DCM/PE = 10/1, R_f = 0.55.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.54 (s, 1H), 8.26-8.17 (m, 1H), 7.50-7.46 (m, 2H), 6.92 (d, *J* = 1.4 Hz, 1H), 4.91 (dd, *J* = 6.0, 1.2 Hz, 1H), 3.66 (s, 3H), 1.87-1.70 (m, 5H), 1.67-1.63 (m, 1H), 1.32-1.04 (m, 5H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.9, 154.8, 136.0, 135.5, 130.6, 128.8, 128.7, 128.2, 127.8, 126.7, 81.4, 52.1, 40.3, 27.0, 26.8, 25.7, 25.2, 25.0.

HRMS (ESI) calculated for C₁₈H₂₀ClNNaO₄ ([M+Na]⁺): 372.0973; found: 372.0970.

(7-chloro-2-oxo-1,2-dihydroquinolin-3-yl)(cyclohexyl)methyl methyl carbonate (3x)



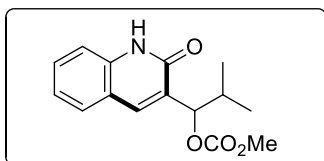
This compound was obtained in 32% yield (22.4 mg) as light yellow oil. Eluent: DCM/PE = 10/1, R_f = 0.7.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.64 (brs, 1H), 8.14 (d, *J* = 8.6 Hz, 1H), 7.60 (d, *J* = 2.2 Hz, 1H), 7.31 (dd, *J* = 8.6, 2.2 Hz, 1H), 6.99-6.90 (m, 1H), 4.89 (dd, *J* = 5.9, 1.1 Hz, 1H), 3.68 (s, 3H), 1.86-1.70 (m, 6H), 1.17-1.09 (m, 5H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.9, 154.7, 138.4, 134.9, 134.8, 131.0, 129.2, 128.4, 124.6, 124.1, 81.4, 52.2, 40.3, 27.0, 26.9, 25.7, 25.2, 25.0.

HRMS (ESI) calculated for C₁₈H₂₀ClNNaO₄ ([M+Na]⁺): 372.0973; found: 372.0971.

methyl (2-methyl-1-(2-oxo-1,2-dihydroquinolin-3-yl)propyl) carbonate (3y)



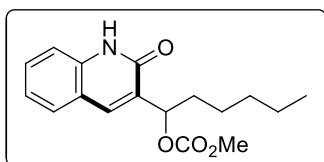
This compound was obtained in 50% yield (27.4 mg) as light yellow oil. Eluent: DCM/PE = 7/1, R_f = 0.5.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.44 (s, 1H), 8.16 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.53-7.39 (m, 2H), 7.27-7.21 (m, 1H), 6.97 (d, *J* = 1.5 Hz, 1H), 4.91 (dd, *J* = 6.2, 1.5 Hz, 1H), 3.66 (s, 3H), 2.15-2.06 (m, 1H), 1.05-1.00 (m, 6H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.0, 154.9, 137.1, 134.1, 131.0, 129.6, 129.4, 126.5, 125.2, 124.9, 81.9, 51.9, 31.0, 17.0, 16.8.

HRMS (ESI) calculated for C₁₅H₁₇NNaO₄ ([M+Na]⁺): 298.1050; found: 298.1048.

methyl (1-(2-oxo-1,2-dihydroquinolin-3-yl)hexyl) carbonate (3z)



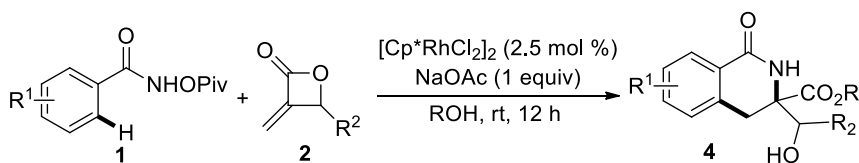
This compound was obtained in 60% yield (36.4 mg) as light yellow oil. Eluent: DCM/PE = 7/1, R_f = 0.5.

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.39 (brs, 1H), 8.18 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.48-7.39 (m, 2H), 7.27-7.19 (m, 1H), 6.98 (d, *J* = 1.4 Hz, 1H), 5.11 (ddd, *J* = 7.6, 4.5, 1.4 Hz, 1H), 3.66 (s, 3H), 2.02-1.90 (m, 1H), 1.84-1.74 (m, 1H), 1.47-1.43 (m, 2H), 1.36-1.29 (m, 4H), 0.91-0.86 (m, 3H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.0, 154.9, 137.1, 135.4, 130.9, 129.4, 129.2, 126.4, 125.2, 124.9, 78.1, 51.9, 33.0, 31.0, 23.7, 21.9, 13.8.

HRMS (ESI) calculated for C₁₇H₂₁NNaO₄ ([M+Na]⁺): 326.1363; found: 326.1356.

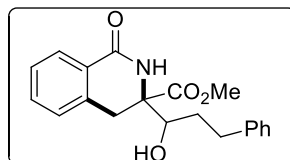
General procedure B:



The mixture of *N*-(pivaloyloxy)benzamide **1** (0.2 mmol, 1.0 equiv), methyleneoxetanones **2** (0.2 mmol, 1.0 equiv), [Cp*RhCl₂]₂ (2.5 mol %) and NaOAc (0.2 mmol, 1.0 equiv) in the alcoholic solvent (2.0 mL) in a sealed tube was stirred at room temperature for 12 h without exclusion of air or moisture. Afterwards, the solvent was removed with the reduced pressure and the crude product was purified by preparative TLC to afford the corresponding products **4**.

Characterization of products:

methyl 3-(1-hydroxy-3-phenylpropyl)-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4a)



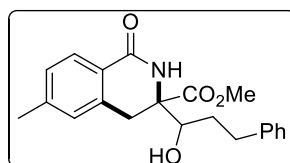
This compound was obtained in 52% yield (35.4 mg) as white solid. Eluent: PE/EA= 1/1, $R_f = 0.3$.

^1H NMR (400 MHz, CD_3OD): δ 7.89 (dd, $J = 7.8, 1.2$ Hz, 1H), 7.46 (td, $J = 7.5, 1.4$ Hz, 1H), 7.32 (t, $J = 7.6$ Hz, 1H), 7.27-7.22 (m, 3H), 7.21-7.18 (m, 2H), 7.17-7.10 (m, 1H), 3.82-3.73 (m, 1H), 3.55 (s, 3H), 3.33 (d, $J = 15.9$ Hz, 1H), 3.16 (d, $J = 15.9$ Hz, 1H), 2.90 (dt, $J = 13.9, 7.1$ Hz, 1H), 2.62 (dt, $J = 13.6, 8.3$ Hz, 1H), 1.89-1.80 (m, 2H).

^{13}C NMR (100 MHz, CD_3OD): δ 173.7, 168.1, 142.9, 138.0, 134.1, 132.9, 129.5, 129.4, 129.1, 128.7, 128.6, 128.4, 128.3, 127.0, 75.6, 67.9, 53.1, 34.4, 34.2, 33.4.

HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{22}\text{NO}_4$ ($[\text{M}+\text{H}]^+$): 340.1543; found: 340.1543.

methyl 3-(1-hydroxy-3-phenylpropyl)-6-methyl-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4b)



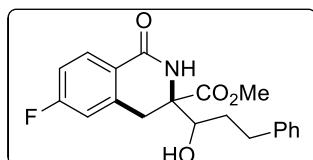
This compound was obtained in 49% yield (34.6 mg) as white solid. Eluent: PE/EA= 1/1, $R_f = 0.3$.

^1H NMR (400 MHz, CD_3OD): δ 7.78 (d, $J = 7.9$ Hz, 1H), 7.26 (t, $J = 7.6$ Hz, 2H), 7.21 (d, $J = 6.8$ Hz, 2H), 7.18-7.14 (m, 2H), 7.09 (s, 1H), 3.77 (dd, $J = 9.5, 3.3$ Hz, 1H), 3.58 (s, 3H), 3.28 (d, $J = 15.9$ Hz, 1H), 3.13 (d, $J = 15.9$ Hz, 1H), 2.97-2.87 (m, 1H), 2.68-2.60 (m, 1H), 2.36 (s, 3H), 1.89-1.82 (m, 2H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 172.7, 164.5, 142.3, 141.9, 136.7, 128.33, 128.29, 128.23, 127.7, 127.0, 125.7, 125.3, 73.8, 66.5, 52.3, 32.6, 32.3, 32.2, 21.1.

HRMS (ESI) calculated for C₂₁H₂₃NNaO₄ ([M+Na]⁺): 376.1519; found: 376.1511.

methyl 6-fluoro-3-(1-hydroxy-3-phenylpropyl)-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4c)



This compound was obtained in 30% yield (21.4 mg) as light yellow solid. Eluent: PE/EA= 1/1, R_f = 0.3.

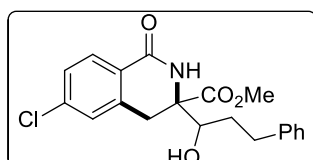
¹H NMR (400 MHz, CD₃OD): δ 7.93 (dd, *J* = 8.5, 5.8 Hz, 1H), 7.27-7.21 (m, 2H), 7.21-7.12 (m, 3H), 7.08-7.00 (m, 2H), 3.81-3.74 (m, 1H), 3.58 (s, 3H), 3.35 (d, *J* = 16.1 Hz, 1H), 3.18 (d, *J* = 16.1 Hz, 1H), 2.90 (dt, *J* = 13.9, 7.1 Hz, 1H), 2.62 (dt, *J* = 13.6, 8.3 Hz, 1H), 1.89-1.77 (m, 2H).

¹³C NMR (100 MHz, CD₃OD): δ 173.6, 167.1, 166.8 (d, *J* = 251.1 Hz), 142.9, 141.5 (d, *J* = 9.2 Hz), 131.5 (d, *J* = 9.9 Hz), 129.6, 129.4, 127.0, 125.3, 115.7 (d, *J* = 22.5 Hz), 115.4 (d, *J* = 22.2 Hz), 75.5, 67.9, 53.2, 34.4, 34.1, 33.4.

¹⁹F NMR (376 MHz, CD₃OD): δ -108.00- -108.06 (m).

HRMS (ESI) calculated for C₂₀H₂₁FNO₄ ([M+H]⁺): 358.1449; found: 358.1441.

methyl 6-chloro-3-(1-hydroxy-3-phenylpropyl)-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4d)



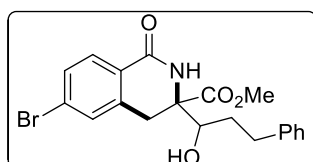
This compound was obtained in 48% yield (35.8 mg) as light yellow solid. Eluent: PE/EA= 1/1, R_f = 0.3.

¹H NMR (400 MHz, CD₃OD): δ 7.85 (d, *J* = 8.2 Hz, 1H), 7.34-7.30 (m, 2H), 7.27-7.22 (m, 2H), 7.20-7.12 (m, 3H), 3.82-3.72 (m, 1H), 3.60 (s, 3H), 3.33 (d, *J* = 16.1 Hz, 1H), 3.17 (d, *J* = 16.1 Hz, 1H), 2.94-2.86 (m, 1H), 2.62 (dt, *J* = 13.6, 8.3 Hz, 1H), 1.86-1.79 (m, 2H).

¹³C NMR (100 MHz, CD₃OD): δ 173.5, 167.0, 142.8, 140.2, 140.0, 130.2, 129.6, 129.5, 129.0, 128.6, 127.5, 127.0, 75.5, 67.8, 53.3, 34.4, 33.9, 33.4.

HRMS (ESI) calculated for C₂₀H₂₁ClNO₄ ([M+H]⁺): 374.1154; found: 374.1152.

methyl 6-bromo-3-(1-hydroxy-3-phenylpropyl)-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4e)



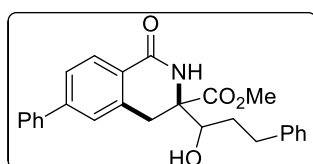
This compound was obtained in 35% yield (29.2 mg) as light yellow solid. Eluent: PE/EA= 1/1, R_f = 0.3.

¹H NMR (400 MHz, CD₃OD): δ 7.79 (d, *J* = 8.1 Hz, 1H), 7.52-7.49 (m, 2H), 7.30-7.24 (m, 2H), 7.23-7.13 (m, 3H), 3.84-3.74 (m, 1H), 3.35 (d, *J* = 16.2 Hz, 1H), 3.20 (d, *J* = 16.1 Hz, 1H), 2.92 (dt, *J* = 13.9, 7.1 Hz, 1H), 2.68-2.57 (m, 1H), 1.88-1.81 (m, 2H).

¹³C NMR (100 MHz, CD₃OD): δ 173.5, 167.1, 142.8, 140.3, 132.0, 131.6, 130.3, 129.6, 129.4, 128.5, 127.9, 127.0, 75.5, 67.8, 53.2, 34.4, 33.8, 33.4.

HRMS (ESI) calculated for C₂₀H₂₁BrNO₄ ([M+H]⁺): 418.0648; found: 418.0647.

methyl 3-(1-hydroxy-3-phenylpropyl)-1-oxo-6-phenyl-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4f)



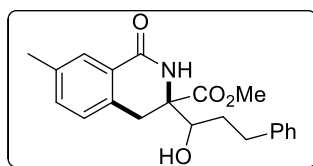
This compound was obtained in 31% yield (25.7 mg) as light yellow solid. Eluent: PE/EA= 1/1, $R_f = 0.4$.

^1H NMR (400 MHz, DMSO- d_6): δ 7.88 (d, $J = 8.5$ Hz, 1H), 7.82 (brs, 1H), 7.72-7.69 (m, 2H), 7.65-7.62 (m, 2H), 7.48 (t, $J = 7.5$ Hz, 2H), 7.43-7.38 (m, 1H), 7.31-7.26 (m, 2H), 7.24-7.21 (m, 2H), 7.20-7.15 (m, 1H), 5.52 (d, $J = 6.6$ Hz, 1H), 3.83-3.75 (m, 1H), 3.50 (s, 3H), 3.38 (d, $J = 15.9$ Hz, 1H), 3.19 (d, $J = 15.9$ Hz, 1H), 2.91-2.78 (m, 1H), 2.63-2.53 (m, 1H), 1.92-1.72 (m, 2H).

^{13}C NMR (100 MHz, DMSO- d_6): 172.7, 167.5, 164.4, 143.7, 142.8, 141.9, 139.2, 137.5, 133.1, 129.0, 128.4, 128.3, 128.2, 128.0, 127.7, 126.9, 126.5, 126.0, 125.8, 125.2, 73.8, 66.6, 52.4, 32.7, 32.5, 32.2.

HRMS (ESI) calculated for $\text{C}_{26}\text{H}_{26}\text{NO}_4$ ($[\text{M}+\text{H}]^+$): 416.1856; found: 416.1850.

methyl 3-(1-hydroxy-3-phenylpropyl)-7-methyl-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4g)



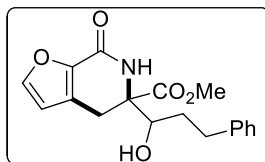
This compound was obtained in 50% yield (35.2 mg) as white solid. Eluent: PE/EA= 1/1, $R_f = 0.3$.

^1H NMR (400 MHz, CD_3OD): δ 7.72 (s, 1H), 7.32-7.27 (m, 1H), 7.25 (d, $J = 7.4$ Hz, 2H), 7.22-7.19 (m, 2H), 7.17-7.12 (m, 2H), 3.79-3.75 (m, 1H), 3.56 (s, 3H), 3.29 (d, $J = 15.8$ Hz, 1H), 3.11 (d, $J = 15.8$ Hz, 1H), 2.91 (dt, $J = 13.9, 7.4$ Hz, 1H), 2.63 (dt, $J = 13.6, 8.2$ Hz, 1H), 2.34 (s, 3H), 1.90-1.81 (m, 2H).

^{13}C NMR (100 MHz, CD_3OD): δ 173.8, 168.3, 142.9, 138.3, 134.9, 134.8, 129.5, 129.4, 129.0, 128.7, 128.5, 127.0, 75.7, 68.0, 53.1, 34.4, 33.9, 33.4, 21.1.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{24}\text{NO}_4$ ($[\text{M}+\text{H}]^+$): 354.1700; found: 354.1698.

methyl 5-(1-hydroxy-3-phenylpropyl)-7-oxo-4,5,6,7-tetrahydrofuro[2,3-*c*]pyridine-5-carboxylate (4h)



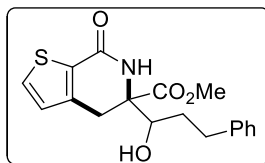
This compound was obtained in 21% yield (13.8 mg) as white solid. Eluent: PE/EA= 1/1, $R_f = 0.3$.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.51 (d, $J = 1.8$ Hz, 1H), 7.32-7.16 (m, 6H), 6.59 (brs, 1H), 6.36 (d, $J = 1.7$ Hz, 1H), 3.81 (dd, $J = 10.7, 2.2$ Hz, 1H), 3.68 (s, 3H), 3.35 (dd, $J = 16.5, 1.1$ Hz, 1H), 3.01-2.86 (m, 2H), 2.69 (dt, $J = 13.9, 8.1$ Hz, 1H), 1.93-1.73 (m, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 172.6, 159.2, 147.1, 142.0, 141.2, 128.73, 128.68, 128.62, 126.3, 110.7, 75.2, 68.4, 53.3, 33.5, 32.4, 27.7.

HRMS (ESI) calculated for $\text{C}_{18}\text{H}_{20}\text{NO}_5$ ($[\text{M}+\text{H}]^+$): 330.1336; found: 330.1330.

methyl 5-(1-hydroxy-3-phenylpropyl)-7-oxo-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-5-carboxylate (4i)



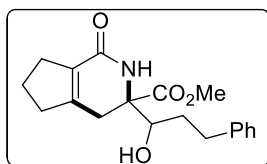
This compound was obtained in 30% yield (20.7 mg) as white solid. Eluent: PE/EA= 1/1, $R_f = 0.5$.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.50 (d, $J = 4.9$ Hz, 1H), 7.28-7.23 (m, 2H), 7.21-7.15 (m, 4H), 6.89 (d, $J = 4.9$ Hz, 1H), 3.85 (dd, $J = 10.1, 2.8$ Hz, 1H), 3.64 (s, 3H), 3.45 (d, $J = 16.2$ Hz, 1H), 3.02-2.94 (m, 2H), 2.68 (dt, $J = 13.8, 8.2$ Hz, 1H), 1.96-1.79 (m, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 172.6, 163.3, 142.9, 141.4, 132.5, 129.8, 128.64, 128.58, 127.1, 126.1, 75.2, 68.4, 53.2, 33.3, 32.5, 30.6.

HRMS (ESI) calculated for $\text{C}_{18}\text{H}_{20}\text{NO}_4\text{S}$ ($[\text{M}+\text{H}]^+$): 346.1108; found: 346.1100.

methyl 3-(1-hydroxy-3-phenylpropyl)-1-oxo-2,3,4,5,6,7-hexahydro-1H-cyclopenta[c]pyridine-3-carboxylate (4j)



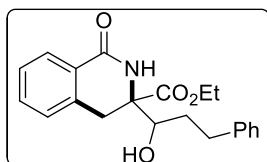
This compound was obtained in 33% yield (21.7 mg) as white solid. Eluent: PE/EA= 1/1, $R_f = 0.3$.

^1H NMR (400 MHz, CDCl_3): δ 7.31-7.24 (m, 2H), 7.21-7.16 (m, 3H), 6.69 (brs, 1H), 3.74-3.69 (m, 4H), 2.95 (dt, $J = 13.9, 7.0$ Hz, 1H), 2.87 (d, $J = 17.9$ Hz, 1H), 2.65 (dt, $J = 13.9, 8.2$ Hz, 1H), 2.58-2.40 (m, 5H), 1.95-1.88 (m, 2H), 1.83-1.69 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3): δ 173.2, 166.5, 153.5, 141.4, 131.3, 128.63, 128.58, 126.2, 75.3, 67.1, 53.1, 36.6, 33.3, 32.4, 31.0, 29.6, 22.0.

HRMS (ESI) calculated for $\text{C}_{19}\text{H}_{24}\text{NO}_4$ ($[\text{M}+\text{H}]^+$): 330.1700; found: 330.1694.

ethyl 3-(1-hydroxy-3-phenylpropyl)-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4k)



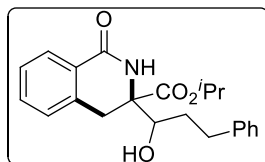
This compound was obtained in 45% yield (31.8 mg) as white solid. Eluent: PE/EA= 1/1, $R_f = 0.3$.

^1H NMR (400 MHz, CD_3OD): δ 7.91 (d, $J = 7.7$ Hz, 1H), 7.48 (td, $J = 7.5, 1.3$ Hz, 1H), 7.34 (t, $J = 7.6$ Hz, 1H), 7.29-7.24 (m, 3H), 7.23-7.13 (m, 3H), 4.06-3.97 (m, 2H), 3.81 (dd, $J = 9.9, 2.9$ Hz, 1H), 3.33 (d, $J = 15.8$ Hz, 1H), 3.20 (d, $J = 15.8$ Hz, 1H), 2.97-2.89 (m, 1H), 2.65 (dt, $J = 13.7, 8.3$ Hz, 1H), 1.97-1.81 (m, 2H), 1.09-0.97 (m, 3H).

^{13}C NMR (100 MHz, CD_3OD): δ 173.2, 168.3, 142.9, 138.0, 134.0, 129.5, 129.4, 129.0, 128.9, 128.4, 128.3, 127.0, 75.4, 67.9, 62.8, 34.5, 34.4, 33.4, 14.3.

HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{24}\text{NO}_4$ ($[\text{M}+\text{H}]^+$): 354.1700; found: 354.1699.

isopropyl 3-(1-hydroxy-3-phenylpropyl)-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4l)



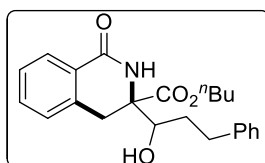
This compound was obtained in 22% yield (16.1 mg) as white solid. Eluent: PE/EA= 1/1, $R_f = 0.4$.

^1H NMR (400 MHz, CD_3OD): δ 7.91 (dd, $J = 7.8, 1.1$ Hz, 1H), 7.48 (td, $J = 7.5, 1.4$ Hz, 1H), 7.35 (t, $J = 7.6$ Hz, 1H), 7.30-7.25 (m, 3H), 7.22 (dd, $J = 8.1, 1.4$ Hz, 2H), 7.19-7.14 (m, 1H), 4.85-4.80 (m, 1H), 3.81 (dd, $J = 10.7, 2.1$ Hz, 1H), 3.29 (d, $J = 15.7$ Hz, 1H), 3.23 (d, $J = 15.7$ Hz, 1H), 2.97-2.89 (m, 1H), 2.66 (dt, $J = 13.7, 8.3$ Hz, 1H), 1.98-1.80 (m, 2H), 1.05 (d, $J = 6.2$ Hz, 3H), 1.00 (d, $J = 6.3$ Hz, 3H).

^{13}C NMR (100 MHz, CD_3OD): δ 172.8, 168.5, 142.9, 138.1, 134.0, 129.6, 129.5, 129.0, 128.4, 128.3, 127.0, 75.2, 70.8, 67.9, 34.9, 34.4, 33.4, 21.74, 21.69.

HRMS (ESI) calculated for $\text{C}_{22}\text{H}_{26}\text{NO}_4$ ($[\text{M}+\text{H}]^+$): 368.1856; found: 368.1854.

butyl 3-(1-hydroxy-3-phenylpropyl)-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4m)



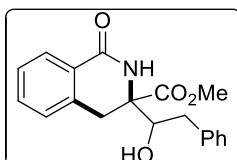
This compound was obtained in 49% yield (37.3 mg) as light yellow solid. Eluent: PE/EA= 1/1, $R_f = 0.6$.

^1H NMR (400 MHz, CD_3OD): δ 7.95-7.89 (m, 1H), 7.48 (td, $J = 7.5, 1.3$ Hz, 1H), 7.34 (t, $J = 7.6$ Hz, 1H), 7.29-7.24 (m, 3H), 7.23-7.13 (m, 3H), 4.00-3.95 (m, 2H), 3.81 (dd, $J = 10.0, 2.8$ Hz, 1H), 3.37-3.31 (m, 1H), 3.21 (d, $J = 15.8$ Hz, 1H), 2.96-2.89 (m, 1H), 2.65 (dt, $J = 13.6, 8.3$ Hz, 1H), 1.99-1.79 (m, 2H), 1.42-1.35 (m, 2H), 1.20-1.10 (m, 2H), 0.78 (t, $J = 7.4$ Hz, 3H).

¹³C NMR (100 MHz, CD₃OD): δ 173.4, 168.3, 142.9, 138.0, 134.0, 129.5, 129.4, 129.1, 128.9, 128.5, 128.3, 127.0, 75.4, 68.0, 66.5, 34.6, 34.5, 33.5, 31.6, 19.9, 13.9.

HRMS (ESI) calculated for C₂₃H₂₈NO₄ ([M+H]⁺): 382.2013; found: 382.2009.

methyl 3-(1-hydroxy-2-phenylethyl)-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4n)



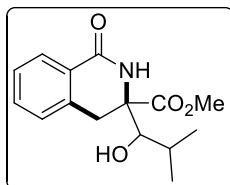
This compound was obtained in 57% yield (37.0 mg) as light yellow solid. Eluent: PE/EA= 1/1, R_f = 0.4.

¹H NMR (400 MHz, DMSO-*d*₆): δ 8.09 (s, 1H), 7.84 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.49 (td, *J* = 7.5, 1.4 Hz, 1H), 7.37-7.26 (m, 6H), 7.22-7.16 (m, 1H), 5.36 (d, *J* = 7.2 Hz, 1H), 3.97 (ddd, *J* = 10.5, 7.2, 1.8 Hz, 1H), 3.52 (s, 3H), 3.40-3.34 (m, 1H), 3.32-3.24 (m, 1H), 2.88 (d, *J* = 12.3 Hz, 1H), 2.71 (dd, *J* = 13.7, 10.7 Hz, 1H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 172.7, 164.6, 139.6, 137.1, 132.4, 129.6, 128.0, 127.93, 127.89, 127.0, 126.9, 126.0, 75.3, 66.6, 52.4, 37.2, 31.8.

HRMS (ESI) calculated for C₁₉H₂₀NO₄ ([M+H]⁺): 326.1387; found: 326.1386.

methyl 3-(1-hydroxy-2-methylpropyl)-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4o)



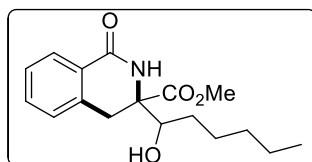
This compound was obtained in 23% yield (13.4 mg) as light yellow solid. Eluent: PE/EA= 1/1, R_f = 0.3.

¹H NMR (400 MHz, CD₃OD): δ 7.91 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.50 (td, *J* = 7.5, 1.4 Hz, 1H), 7.35 (t, *J* = 7.7 Hz, 1H), 7.30 (d, *J* = 7.4 Hz, 1H), 3.68 (d, *J* = 5.4 Hz, 1H), 3.59 (s, 3H), 3.40 (s, 2H), 2.01-1.91 (m, 1H), 1.03-1.00 (m, 6H).

¹³C NMR (100 MHz, CD₃OD): δ 174.2, 168.1, 138.5, 134.1, 129.0, 128.7, 128.4, 128.2, 80.0, 67.6, 53.1, 35.1, 31.3, 21.7, 18.7.

HRMS (ESI) calculated for C₁₅H₂₀NO₄ ([M+H]⁺): 278.1387; found: 278.1388.

methyl 3-(1-hydroxyhexyl)-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4p)



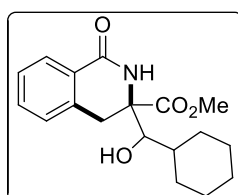
This compound was obtained in 44% yield (26.8 mg) as light yellow solid. Eluent: PE/EA= 1/1, R_f = 0.45.

¹H NMR (400 MHz, CD₃OD): δ 7.92 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.49 (td, *J* = 7.5, 1.4 Hz, 1H), 7.37-7.32 (m, 1H), 7.31-7.27 (m, 1H), 3.80 (dd, *J* = 9.7, 2.8 Hz, 1H), 3.60 (s, 3H), 3.38 (d, *J* = 15.9 Hz, 1H), 3.24 (d, *J* = 15.9 Hz, 1H), 1.67-1.47 (m, 3H), 1.38-1.29 (m, 5H), 0.94-0.88 (m, 3H).

¹³C NMR (100 MHz, CD₃OD): δ 173.8, 168.0, 138.2, 134.1, 129.1, 128.7, 128.5, 128.3, 76.4, 67.9, 53.1, 34.1, 32.7, 32.3, 27.2, 23.7, 14.4.

HRMS (ESI) calculated for C₁₇H₂₄NO₄ ([M+H]⁺): 306.1700; found: 306.1697.

methyl 3-(cyclohexyl(hydroxy)methyl)-1-oxo-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4q)



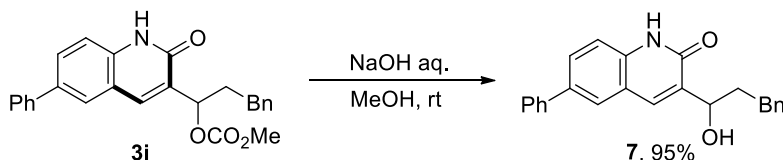
This compound was obtained in 24% yield (16.0 mg) as light yellow solid. Eluent: PE/EA= 1/1, R_f = 0.4.

$^1\text{H NMR}$ (400 MHz, CD_3OD): δ 7.89 (d, J = 7.6 Hz, 1H), 7.48 (td, J = 7.5, 1.1 Hz, 1H), 7.33 (t, J = 7.5 Hz, 1H), 7.28 (d, J = 7.6 Hz, 1H), 3.65 (d, J = 5.3 Hz, 1H), 3.57 (s, 3H), 3.37 (s, 2H), 1.91-1.86 (m, 1H), 1.79-1.72 (m, 2H), 1.70-1.62 (m, 3H), 1.33-1.22 (m, 3H), 1.21-1.13 (m, 2H).

$^{13}\text{C NMR}$ (100 MHz, CD_3OD): δ 174.3, 168.0, 138.5, 134.1, 129.0, 128.7, 128.4, 128.2, 79.5, 67.5, 53.0, 41.4, 34.9, 32.4, 29.7, 27.5, 27.3, 27.2.

HRMS (ESI) calculated for $\text{C}_{18}\text{H}_{24}\text{NO}_4$ ($[\text{M}+\text{H}]^+$): 318.1700; found: 318.1698.

Scale-up synthesis of 3i: The mixture of *N*-acetoxybenzamide **1i** (2.0 mmol, 1.0 equiv), methyleneoxetanone **2a** (2.0 mmol, 1.0 equiv), $[\text{Cp}^*\text{RhCl}_2]_2$ (2.5 mol %), HOAc (2.0 mmol, 1.0 equiv) and KOPiv (2.0 mmol, 1.0 equiv) in MeOH (20 mL) in a sealed tube was stirred at room temperature for 12 h without exclusion of air or moisture. Afterwards, the solvent was removed with the reduced pressure and the crude product was purified by column chromatography to afford the corresponding products **3i** in 61% isolated yield (0.503 g).



The mixture of **3i** (0.5 mmol) and 50% NaOH aqueous solution (3 mL) in MeOH (5 mL) was stirred at room temperature for 24 h without exclusion of air or moisture. Afterwards, it was neutralized by diluted HCl aq. and extracted with EtOAc (10x3 mL), the organic phase was combined and dried over Na_2SO_4 . The resulted mixture was filtered and concentrated to give the corresponding product **7** in 95% isolated yield (0.169 g) as white solid (R_f = 0.3, PE/EA = 1/1).

$^1\text{H NMR}$ (400 MHz, $\text{DMSO}-d_6$): δ 11.83 (s, 1H), 8.05-8.01 (m, 2H), 7.79 (dd, J = 8.5, 2.0 Hz, 1H), 7.74-7.68 (m, 2H), 7.47 (t, J = 7.7 Hz, 2H), 7.42-7.31 (m, 2H), 7.28-7.19 (m, 4H), 7.15 (t, J = 7.1 Hz, 1H), 5.32 (d, J = 4.8 Hz, 1H), 4.77 (dd, J = 7.6, 3.8 Hz, 1H), 2.80-2.65 (m, 2H), 2.17-2.04 (m, 1H), 1.88-1.69 (m, 1H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 161.1, 142.2, 139.5, 137.7, 137.2, 134.2, 133.7, 129.0, 128.3, 128.23, 128.15, 127.1, 126.5, 125.6, 125.4, 119.7, 115.4, 66.7, 37.9, 31.5.

HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{22}\text{NO}_2$ ($[\text{M}+\text{H}]^+$): 356.1645; found: 356.1640.

III. X-Ray Crystallographic Data

Experimental: The sample was dissolved in appropriate amount of acetone to furnish a saturated solution. Afterwards, the mixture was allowed to stand at room temperature to form the crystals. Single crystal was picked and coated in paratone oil carefully, attached to a glass silk which was inserted in a stainless steel stick, then quickly transferred to the Agilent Gemini S Ultra CCD Diffractometer with the Enhance X-ray Source of Cu radiation ($\lambda = 1.54178 \text{ \AA}$) using the ω - ϕ scan technique. All of the structures were solved by direct methods and refined by full-matrix least squares against F^2 using the SHELXL programs. Hydrogen atoms were placed in geometrically calculated positions and included in the refinement process using riding model with isotropic thermal parameters: $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(-\text{CH})$. The crystallographic data have already been deposited at the Cambridge Crystallographic Data Centre (CCDC numbers: 2042748), which can be acquired from www.ccdc.cam.ac.uk/data_request/cif.

The ellipsoid contour percent probability level is 50% for the image of the structure.

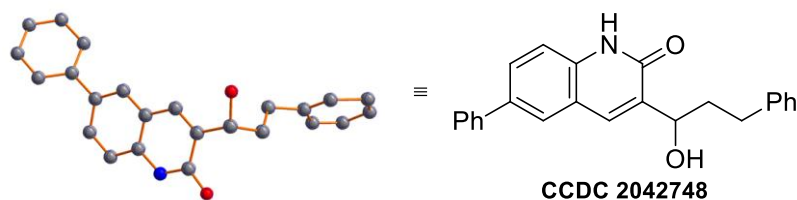


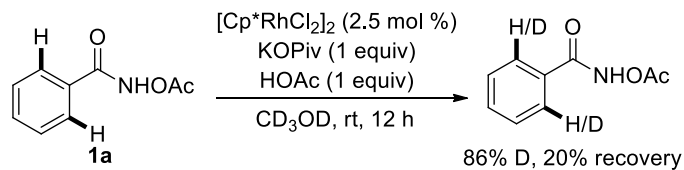
Table S2. Crystal data and structure refinement for **7**

| | |
|---------------------|---|
| Identification code | exp_4407 |
| Empirical formula | $\text{C}_{24}\text{H}_{21}\text{NO}_2$ |

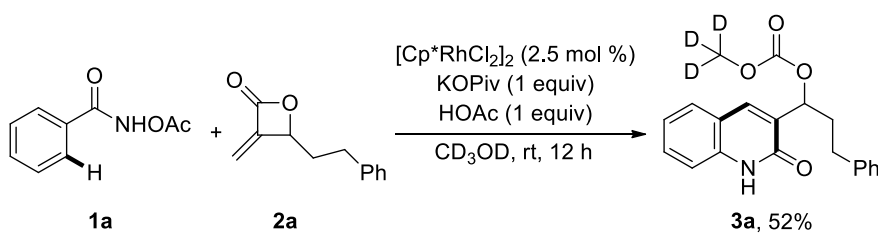
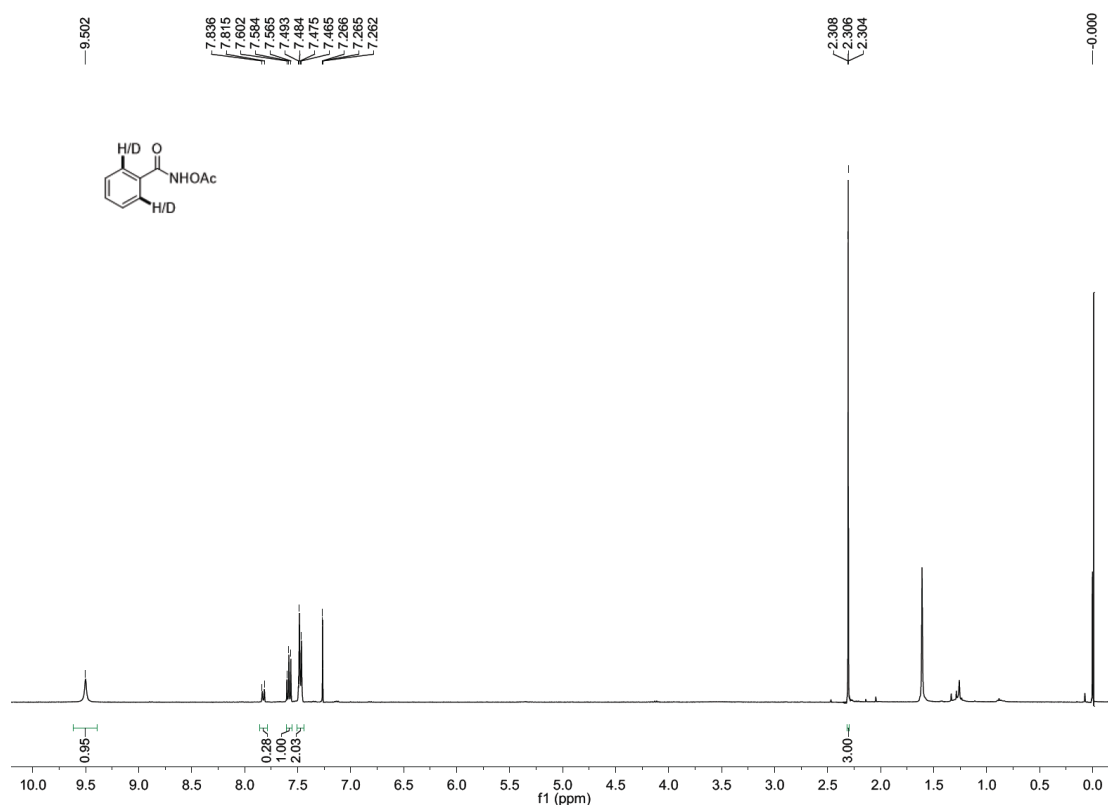
| | |
|---|--|
| Formula weight | 355.42 |
| Temperature/K | 240.00(10) |
| Crystal system | monoclinic |
| Space group | P2 ₁ /n |
| a/Å | 5.6308(2) |
| b/Å | 13.4525(5) |
| c/Å | 25.2525(10) |
| α /° | 90 |
| β /° | 94.702(3) |
| γ /° | 90 |
| Volume/Å ³ | 1906.40(13) |
| Z | 4 |
| ρ_{calc} /cm ³ | 1.238 |
| μ /mm ⁻¹ | 0.619 |
| F(000) | 752.0 |
| Crystal size/mm ³ | 0.12 × 0.11 × 0.10 |
| Radiation | CuK α (λ = 1.54184) |
| 2 Θ range for data collection/° | 7.452 to 133.17 |
| Index ranges | -5 ≤ h ≤ 6, -15 ≤ k ≤ 16, -28 ≤ l ≤ 29 |
| Reflections collected | 6048 |
| Independent reflections | 3342 [R_{int} = 0.0229, R_{sigma} = 0.0327] |
| Data/restraints/parameters | 3342/0/245 |
| Goodness-of-fit on F ² | 1.811 |
| Final R indexes [$I \geq 2\sigma(I)$] | R_1 = 0.1207, wR_2 = 0.3885 |
| Final R indexes [all data] | R_1 = 0.1378, wR_2 = 0.4264 |
| Largest diff. peak/hole / e Å ⁻³ | 1.55/-0.57 |

IV. Experimental Mechanistic Studies

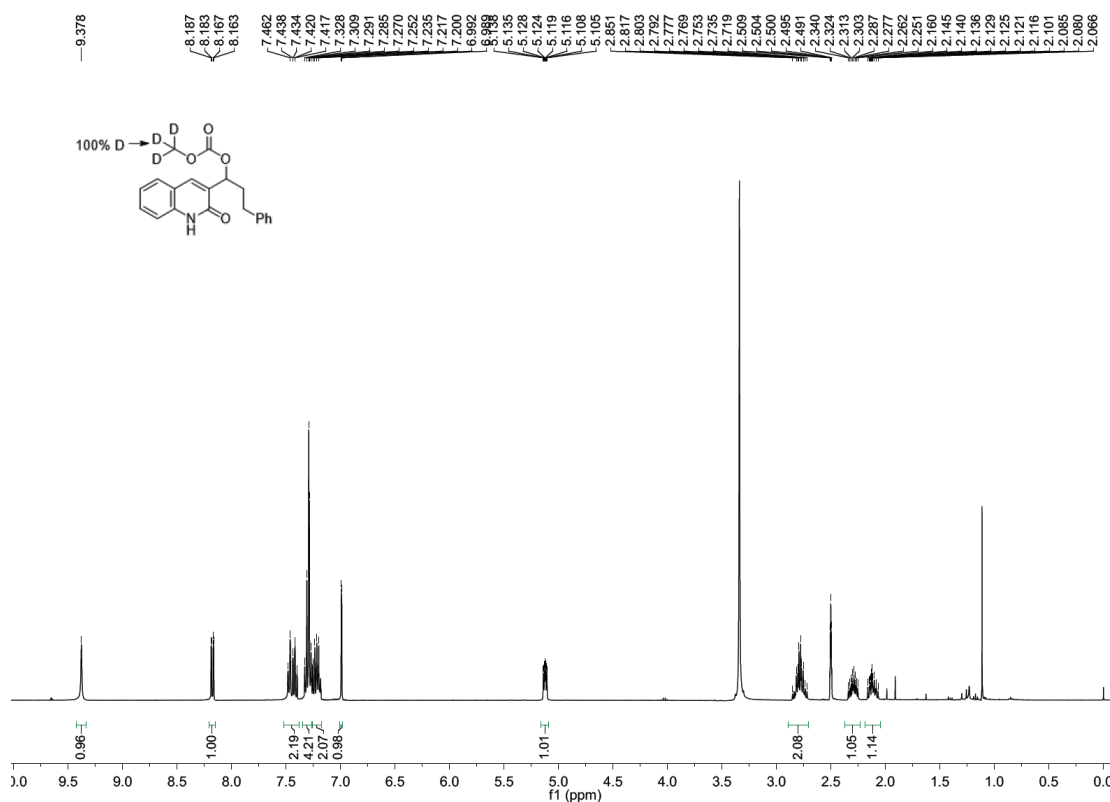
Deuterium labeling experiment:



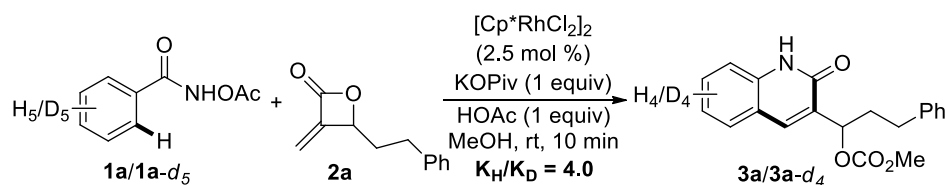
1a (0.1 mmol, 1.0 equiv) was dissolved in CD₃OD (1.0 mL) in the presence of [Cp*RhCl₂]₂ (2.5 mol %), HOAc (0.1 mmol, 1 equiv) and CsOAc (0.1 mmol, 1 equiv). The mixture was stirred at room temperature for 12 h. Afterwards, the mixture was diluted with EtOAc and transferred to a round bottom flask. Silica gel was added to the flask and volatiles were evaporated under reduced pressure. After purification by flash column chromatography, **1a** was recovered and the deuterium incorporation was analyzed by ¹H-NMR. Approximate 86% deuteration was incorporated at the *ortho* position of the DG (the doublet at δ 7.82: 0.28H).



The mixture of *N*-acetoxybenzamide **1a** (0.1 mmol, 1.0 equiv), methyleneoxetanone **2a** (0.1 mmol, 1.0 equiv), [Cp**Rh*Cl₂]₂ (2.5 mol %), HOAc (0.1 mmol, 1.0 equiv) and KO₂Piv (0.1 mmol, 1.0 equiv) in MeOH (1.0 mL) was stirred at room temperature for 12 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduce pressure, and the resulted mixture was purified by preparative TLC to afford the corresponding product **3a**. The deuterium incorporation was analyzed by ¹H-NMR.

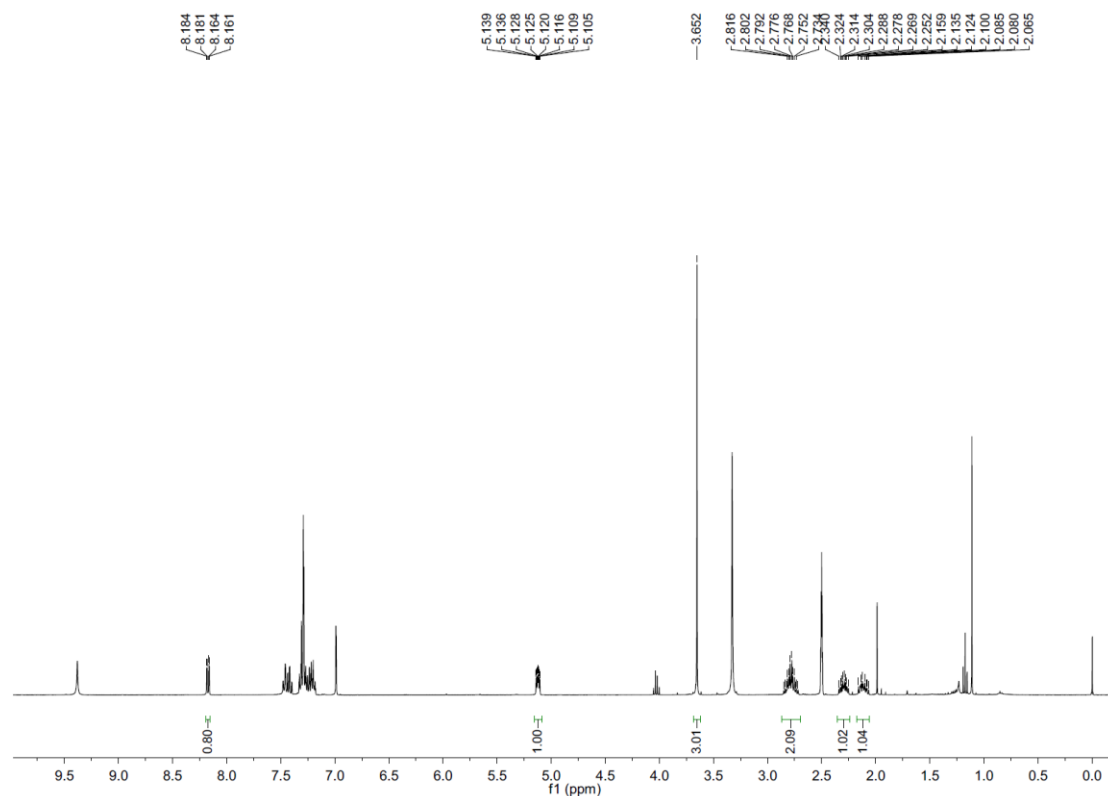


General procedure for estimation of the KIE:



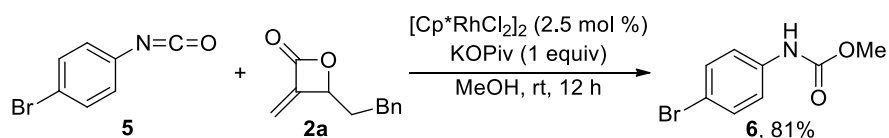
An equimolar mixture of **1a** (0.1 mmol, 1.0 equiv) and **1a-d₅** (0.1 mmol, 1.0 equiv) was allowed to react with **2a** (0.1 mmol, 1.0 equiv) in MeOH (1.0 mL) in the presence of [Cp**Rh*Cl₂]₂ (2.5 mol %), KO₂Piv (0.1 mmol, 1.0 equiv) and HOAc (0.1 mmol, 1.0 equiv). The reaction was stopped after 10 min, and the product was isolated by

preparative TLC and analyzed by $^1\text{H-NMR}$ spectroscopy (DMSO, 400 MHz). The double doublet at δ : 8.17 (0.80H) were used for calculation and an average value of $k_{\text{H}}/k_{\text{D}} = 4.0$ was obtained.



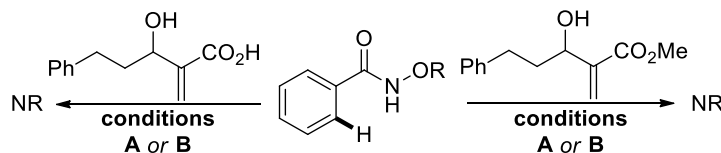
Another two parallel KIE experiments were performed by treating 1 equiv of **1a** or 1 equiv of **1a-d5** with 1.0 equiv of **2a** separately under the standard conditions for 10 min. Afterwards, the solvent was removed under reduce pressure, and the resulted mixture was purified by preparative TLC to afford the corresponding product **3a**. The isolated yields were determined as 36% and 11%, respectively. Thus the KIE was determined to be $k_{\text{H}}/k_{\text{D}} = 3.3$.

Control experiment:



The mixture of aryl isocyanate **5** (0.1 mmol, 1.0 equiv), methyleneoxetanone **2a** (0.1 mmol, 1.0 equiv), $[\text{Cp}^*\text{RhCl}_2]_2$ (2.5 mol %) and KOPIv (0.1 mmol, 1.0 equiv) in MeOH (1.0 mL) was stirred at room temperature for 12 h without exclusion of air or

moisture. Afterwards, the solvent was removed under reduce pressure, and the resulted mixture was purified by preparative TLC to afford the product **6** in 81% isolated yield (18.5 mg). The product **6** was a known compound and all the characterized data was in agreement with that reported.



Condition A: The mixture of *N*-acetoxybenzamide **1a** (0.1 mmol, 1.0 equiv), 2-carboxyl allylic alcohol (0.1 mmol, 1.0 equiv) or its ester form (0.1 mmol, 1.0 equiv), [Cp**Rh*Cl₂]₂ (2.5 mol %), HOAc (0.1 mmol, 1.0 equiv) and KOPiv (0.1 mmol, 1.0 equiv) in MeOH (1.0 mL) was stirred at room temperature for 12 h without exclusion of air or moisture.

Condition B: The mixture of *N*-(*pivaloyloxy*)benzamide (0.1 mmol, 1.0 equiv), 2-carboxyl allylic alcohol (0.1 mmol, 1.0 equiv) or its ester form (0.1 mmol, 1.0 equiv), [Cp**Rh*Cl₂]₂ (2.5 mol %), and NaOAc (0.1 mmol, 1.0 equiv) in MeOH (1.0 mL) was stirred at room temperature for 12 h without exclusion of air or moisture.

Afterwards, the reactions were monitored by TLC analysis and no reaction was detected for any of these cases.

V. Computational Mechanistic Studies

Computational details:

The theoretical calculations were carried out by using Gaussian 09 program.^{S3} Geometry optimizations were performed at the level of the M11L functional^{S4} with a standard 6-31G(d,p) basis set (SDD^{S5} basis set for Rh) using SMD^{S6} solvation model (solvent= methanol). Frequency analyses were done to obtain the thermodynamic energy corrections and to ensure that the optimized structures were at either a minimum or transition state.

$$\text{ODG} = \text{OPiv} \quad \Delta\Delta G = (11.3-11.2) = 0.1 \text{ kcal/mol}$$

both of reduction elimination and Rossen Rearrangement are favorable, leading to competitive products PC1 and PC2

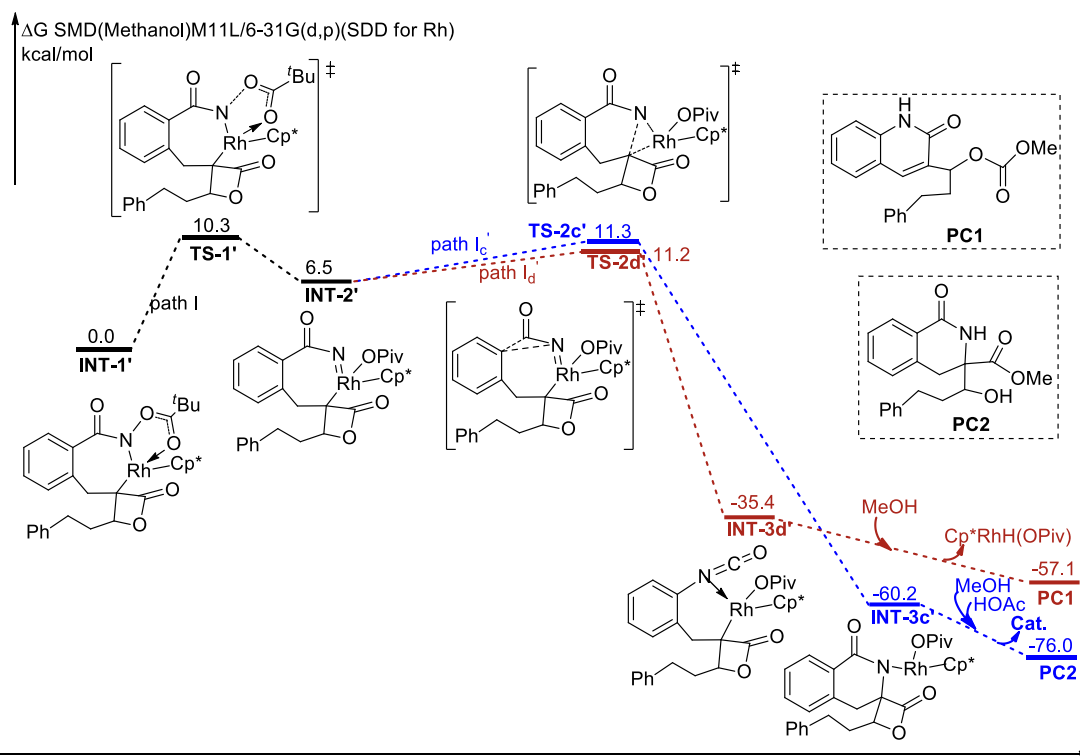


Figure S1. Computed Gibbs free energy changes of the reaction pathway with $-\text{NHOPiv}$ ODG.

Various energy values for all of the relevant species [optimized at the level of M11L/6-31G(d,p) (SDD for Rh) with SMD atomic radii for experimental solvent methanol]

CH₃COOH

| | |
|--|-----------------------------|
| Zero-point correction= | 0.061448 (Hartree/Particle) |
| Thermal correction to Energy= | 0.065198 |
| Thermal correction to Enthalpy= | 0.066142 |
| Thermal correction to Gibbs Free Energy= | 0.035469 |
| Sum of electronic and zero-point Energies= | -228.962477 |
| Sum of electronic and thermal Energies= | -228.958727 |
| Sum of electronic and thermal Enthalpies= | -228.957783 |
| Sum of electronic and thermal Free Energies= | -228.988456 |

MeOH

| | |
|--|-----------------------------|
| Zero-point correction= | 0.050885 (Hartree/Particle) |
| Thermal correction to Energy= | 0.054228 |
| Thermal correction to Enthalpy= | 0.055173 |
| Thermal correction to Gibbs Free Energy= | 0.028141 |

| | |
|--|-------------|
| Sum of electronic and zero-point Energies= | -115.637362 |
| Sum of electronic and thermal Energies= | -115.634019 |
| Sum of electronic and thermal Enthalpies= | -115.633074 |
| Sum of electronic and thermal Free Energies= | -115.660106 |

Cp*RhH(OAc)

| | |
|--|-----------------------------|
| Zero-point correction= | 0.276683 (Hartree/Particle) |
| Thermal correction to Energy= | 0.295753 |
| Thermal correction to Enthalpy= | 0.296697 |
| Thermal correction to Gibbs Free Energy= | 0.230408 |
| Sum of electronic and zero-point Energies= | -729.556720 |
| Sum of electronic and thermal Energies= | -729.537650 |
| Sum of electronic and thermal Enthalpies= | -729.536705 |
| Sum of electronic and thermal Free Energies= | -729.602995 |

Cp*Rh(OAc)₂

| | |
|--|-----------------------------|
| Zero-point correction= | 0.320622 (Hartree/Particle) |
| Thermal correction to Energy= | 0.344585 |
| Thermal correction to Enthalpy= | 0.345530 |
| Thermal correction to Gibbs Free Energy= | 0.267731 |
| Sum of electronic and zero-point Energies= | -957.383982 |
| Sum of electronic and thermal Energies= | -957.360018 |
| Sum of electronic and thermal Enthalpies= | -957.359074 |
| Sum of electronic and thermal Free Energies= | -957.436873 |

Cp*RhH(OPiv)

| | |
|--|-----------------------------|
| Zero-point correction= | 0.359710 (Hartree/Particle) |
| Thermal correction to Energy= | 0.382713 |
| Thermal correction to Enthalpy= | 0.383657 |
| Thermal correction to Gibbs Free Energy= | 0.308803 |
| Sum of electronic and zero-point Energies= | -847.395363 |
| Sum of electronic and thermal Energies= | -847.372360 |
| Sum of electronic and thermal Enthalpies= | -847.371416 |
| Sum of electronic and thermal Free Energies= | -847.446270 |

Cp*RhOAc(OPiv)

| | |
|--|-----------------------------|
| Zero-point correction= | 0.403325 (Hartree/Particle) |
| Thermal correction to Energy= | 0.431271 |
| Thermal correction to Enthalpy= | 0.432215 |
| Thermal correction to Gibbs Free Energy= | 0.345671 |
| Sum of electronic and zero-point Energies= | -1075.223751 |
| Sum of electronic and thermal Energies= | -1075.195805 |
| Sum of electronic and thermal Enthalpies= | -1075.194861 |
| Sum of electronic and thermal Free Energies= | -1075.281405 |

PC1

| | |
|--|-----------------------------|
| Zero-point correction= | 0.351745 (Hartree/Particle) |
| Thermal correction to Energy= | 0.373259 |
| Thermal correction to Enthalpy= | 0.374203 |
| Thermal correction to Gibbs Free Energy= | 0.299348 |
| Sum of electronic and zero-point Energies= | -1128.629073 |
| Sum of electronic and thermal Energies= | -1128.607560 |
| Sum of electronic and thermal Enthalpies= | -1128.606616 |
| Sum of electronic and thermal Free Energies= | -1128.681470 |

PC2

| | |
|--|-----------------------------|
| Zero-point correction= | 0.373755 (Hartree/Particle) |
| Thermal correction to Energy= | 0.396170 |
| Thermal correction to Enthalpy= | 0.397114 |
| Thermal correction to Gibbs Free Energy= | 0.319925 |
| Sum of electronic and zero-point Energies= | -1129.811034 |
| Sum of electronic and thermal Energies= | -1129.788619 |
| Sum of electronic and thermal Enthalpies= | -1129.787675 |
| Sum of electronic and thermal Free Energies= | -1129.864865 |

INT-1

| | |
|--|-----------------------------|
| Zero-point correction= | 0.577464 (Hartree/Particle) |
| Thermal correction to Energy= | 0.615285 |
| Thermal correction to Enthalpy= | 0.616229 |
| Thermal correction to Gibbs Free Energy= | 0.506875 |
| Sum of electronic and zero-point Energies= | -1742.462209 |
| Sum of electronic and thermal Energies= | -1742.424388 |
| Sum of electronic and thermal Enthalpies= | -1742.423444 |
| Sum of electronic and thermal Free Energies= | -1742.532798 |

TS-1

| | |
|--|-----------------------------|
| Zero-point correction= | 0.573725 (Hartree/Particle) |
| Thermal correction to Energy= | 0.611798 |
| Thermal correction to Enthalpy= | 0.612743 |
| Thermal correction to Gibbs Free Energy= | 0.503419 |
| Sum of electronic and zero-point Energies= | -1742.446433 |
| Sum of electronic and thermal Energies= | -1742.408360 |
| Sum of electronic and thermal Enthalpies= | -1742.407415 |
| Sum of electronic and thermal Free Energies= | -1742.516739 |

INT-2

| | |
|-------------------------------|-----------------------------|
| Zero-point correction= | 0.574471 (Hartree/Particle) |
| Thermal correction to Energy= | 0.613288 |

| | |
|--|--------------|
| Thermal correction to Enthalpy= | 0.614232 |
| Thermal correction to Gibbs Free Energy= | 0.503149 |
| Sum of electronic and zero-point Energies= | -1742.450694 |
| Sum of electronic and thermal Energies= | -1742.411877 |
| Sum of electronic and thermal Enthalpies= | -1742.410933 |
| Sum of electronic and thermal Free Energies= | -1742.522016 |

TS-2a

| | |
|--|-----------------------------|
| Zero-point correction= | 0.569044 (Hartree/Particle) |
| Thermal correction to Energy= | 0.607957 |
| Thermal correction to Enthalpy= | 0.608901 |
| Thermal correction to Gibbs Free Energy= | 0.497808 |
| Sum of electronic and zero-point Energies= | -1742.398974 |
| Sum of electronic and thermal Energies= | -1742.360061 |
| Sum of electronic and thermal Enthalpies= | -1742.359117 |
| Sum of electronic and thermal Free Energies= | -1742.470210 |

TS-2b

| | |
|--|-----------------------------|
| Zero-point correction= | 0.571078 (Hartree/Particle) |
| Thermal correction to Energy= | 0.609927 |
| Thermal correction to Enthalpy= | 0.610871 |
| Thermal correction to Gibbs Free Energy= | 0.500234 |
| Sum of electronic and zero-point Energies= | -1742.416211 |
| Sum of electronic and thermal Energies= | -1742.377362 |
| Sum of electronic and thermal Enthalpies= | -1742.376418 |
| Sum of electronic and thermal Free Energies= | -1742.487055 |

TS-2c

| | |
|--|-----------------------------|
| Zero-point correction= | 0.574122 (Hartree/Particle) |
| Thermal correction to Energy= | 0.612401 |
| Thermal correction to Enthalpy= | 0.613345 |
| Thermal correction to Gibbs Free Energy= | 0.502158 |
| Sum of electronic and zero-point Energies= | -1742.441930 |
| Sum of electronic and thermal Energies= | -1742.403651 |
| Sum of electronic and thermal Enthalpies= | -1742.402707 |
| Sum of electronic and thermal Free Energies= | -1742.513894 |

TS-2d

| | |
|--|-----------------------------|
| Zero-point correction= | 0.571617 (Hartree/Particle) |
| Thermal correction to Energy= | 0.610564 |
| Thermal correction to Enthalpy= | 0.611508 |
| Thermal correction to Gibbs Free Energy= | 0.499615 |
| Sum of electronic and zero-point Energies= | -1742.444320 |
| Sum of electronic and thermal Energies= | -1742.405373 |

| | |
|--|--------------|
| Sum of electronic and thermal Enthalpies= | -1742.404429 |
| Sum of electronic and thermal Free Energies= | -1742.516323 |

INT-3a

| | |
|--|-----------------------------|
| Zero-point correction= | 0.575627 (Hartree/Particle) |
| Thermal correction to Energy= | 0.614974 |
| Thermal correction to Enthalpy= | 0.615919 |
| Thermal correction to Gibbs Free Energy= | 0.502201 |
| Sum of electronic and zero-point Energies= | -1742.527491 |
| Sum of electronic and thermal Energies= | -1742.488144 |
| Sum of electronic and thermal Enthalpies= | -1742.487200 |
| Sum of electronic and thermal Free Energies= | -1742.600917 |

INT-3b

| | |
|--|-----------------------------|
| Zero-point correction= | 0.571565 (Hartree/Particle) |
| Thermal correction to Energy= | 0.611421 |
| Thermal correction to Enthalpy= | 0.612365 |
| Thermal correction to Gibbs Free Energy= | 0.498563 |
| Sum of electronic and zero-point Energies= | -1742.427960 |
| Sum of electronic and thermal Energies= | -1742.388104 |
| Sum of electronic and thermal Enthalpies= | -1742.387160 |
| Sum of electronic and thermal Free Energies= | -1742.500962 |

INT-3c

| | |
|--|-----------------------------|
| Zero-point correction= | 0.577684 (Hartree/Particle) |
| Thermal correction to Energy= | 0.615860 |
| Thermal correction to Enthalpy= | 0.616804 |
| Thermal correction to Gibbs Free Energy= | 0.507035 |
| Sum of electronic and zero-point Energies= | -1742.559153 |
| Sum of electronic and thermal Energies= | -1742.520977 |
| Sum of electronic and thermal Enthalpies= | -1742.520033 |
| Sum of electronic and thermal Free Energies= | -1742.629802 |

INT-3d

| | |
|--|-----------------------------|
| Zero-point correction= | 0.574732 (Hartree/Particle) |
| Thermal correction to Energy= | 0.613860 |
| Thermal correction to Enthalpy= | 0.614804 |
| Thermal correction to Gibbs Free Energy= | 0.503116 |
| Sum of electronic and zero-point Energies= | -1742.516340 |
| Sum of electronic and thermal Energies= | -1742.477212 |
| Sum of electronic and thermal Enthalpies= | -1742.476268 |
| Sum of electronic and thermal Free Energies= | -1742.587956 |

INT-4b

| | |
|--|-----------------------------|
| Zero-point correction= | 0.572764 (Hartree/Particle) |
| Thermal correction to Energy= | 0.612298 |
| Thermal correction to Enthalpy= | 0.613242 |
| Thermal correction to Gibbs Free Energy= | 0.499427 |
| Sum of electronic and zero-point Energies= | -1742.460056 |
| Sum of electronic and thermal Energies= | -1742.420522 |
| Sum of electronic and thermal Enthalpies= | -1742.419578 |
| Sum of electronic and thermal Free Energies= | -1742.533393 |

TS-3

| | |
|--|-----------------------------|
| Zero-point correction= | 0.571797 (Hartree/Particle) |
| Thermal correction to Energy= | 0.610159 |
| Thermal correction to Enthalpy= | 0.611103 |
| Thermal correction to Gibbs Free Energy= | 0.502002 |
| Sum of electronic and zero-point Energies= | -1742.370400 |
| Sum of electronic and thermal Energies= | -1742.332039 |
| Sum of electronic and thermal Enthalpies= | -1742.331095 |
| Sum of electronic and thermal Free Energies= | -1742.440196 |

INT-5

| | |
|--|-----------------------------|
| Zero-point correction= | 0.575936 (Hartree/Particle) |
| Thermal correction to Energy= | 0.614007 |
| Thermal correction to Enthalpy= | 0.614951 |
| Thermal correction to Gibbs Free Energy= | 0.505597 |
| Sum of electronic and zero-point Energies= | -1742.432871 |
| Sum of electronic and thermal Energies= | -1742.394800 |
| Sum of electronic and thermal Enthalpies= | -1742.393856 |
| Sum of electronic and thermal Free Energies= | -1742.503210 |

TS-4

| | |
|--|-----------------------------|
| Zero-point correction= | 0.572334 (Hartree/Particle) |
| Thermal correction to Energy= | 0.610182 |
| Thermal correction to Enthalpy= | 0.611126 |
| Thermal correction to Gibbs Free Energy= | 0.502353 |
| Sum of electronic and zero-point Energies= | -1742.425470 |
| Sum of electronic and thermal Energies= | -1742.387622 |
| Sum of electronic and thermal Enthalpies= | -1742.386678 |
| Sum of electronic and thermal Free Energies= | -1742.495452 |

INT-6

| | |
|---------------------------------|-----------------------------|
| Zero-point correction= | 0.573604 (Hartree/Particle) |
| Thermal correction to Energy= | 0.611640 |
| Thermal correction to Enthalpy= | 0.612584 |

| | |
|--|--------------|
| Thermal correction to Gibbs Free Energy= | 0.502746 |
| Sum of electronic and zero-point Energies= | -1742.429083 |
| Sum of electronic and thermal Energies= | -1742.391047 |
| Sum of electronic and thermal Enthalpies= | -1742.390103 |
| Sum of electronic and thermal Free Energies= | -1742.499941 |

TS-5

| | |
|--|-----------------------------|
| Zero-point correction= | 0.571731 (Hartree/Particle) |
| Thermal correction to Energy= | 0.609480 |
| Thermal correction to Enthalpy= | 0.610424 |
| Thermal correction to Gibbs Free Energy= | 0.502143 |
| Sum of electronic and zero-point Energies= | -1742.408007 |
| Sum of electronic and thermal Energies= | -1742.370258 |
| Sum of electronic and thermal Enthalpies= | -1742.369314 |
| Sum of electronic and thermal Free Energies= | -1742.477595 |

INT-7

| | |
|--|-----------------------------|
| Zero-point correction= | 0.576690 (Hartree/Particle) |
| Thermal correction to Energy= | 0.614819 |
| Thermal correction to Enthalpy= | 0.615763 |
| Thermal correction to Gibbs Free Energy= | 0.506144 |
| Sum of electronic and zero-point Energies= | -1742.435820 |
| Sum of electronic and thermal Energies= | -1742.397691 |
| Sum of electronic and thermal Enthalpies= | -1742.396747 |
| Sum of electronic and thermal Free Energies= | -1742.506366 |

INT-1'

| | |
|--|-----------------------------|
| Zero-point correction= | 0.659647 (Hartree/Particle) |
| Thermal correction to Energy= | 0.701484 |
| Thermal correction to Enthalpy= | 0.702428 |
| Thermal correction to Gibbs Free Energy= | 0.586037 |
| Sum of electronic and zero-point Energies= | -1860.302988 |
| Sum of electronic and thermal Energies= | -1860.261151 |
| Sum of electronic and thermal Enthalpies= | -1860.260207 |
| Sum of electronic and thermal Free Energies= | -1860.376598 |

TS-1'

| | |
|--|-----------------------------|
| Zero-point correction= | 0.657184 (Hartree/Particle) |
| Thermal correction to Energy= | 0.698885 |
| Thermal correction to Enthalpy= | 0.699829 |
| Thermal correction to Gibbs Free Energy= | 0.583967 |
| Sum of electronic and zero-point Energies= | -1860.287005 |
| Sum of electronic and thermal Energies= | -1860.245304 |
| Sum of electronic and thermal Enthalpies= | -1860.244360 |

Sum of electronic and thermal Free Energies= -1860.360222

INT-2'

Zero-point correction= 0.657818 (Hartree/Particle)
Thermal correction to Energy= 0.700299
Thermal correction to Enthalpy= 0.701243
Thermal correction to Gibbs Free Energy= 0.583031
Sum of electronic and zero-point Energies= -1860.291489
Sum of electronic and thermal Energies= -1860.249008
Sum of electronic and thermal Enthalpies= -1860.248064
Sum of electronic and thermal Free Energies= -1860.366276

TS-2c'

Zero-point correction= 0.656467 (Hartree/Particle)
Thermal correction to Energy= 0.698732
Thermal correction to Enthalpy= 0.699676
Thermal correction to Gibbs Free Energy= 0.580501
Sum of electronic and zero-point Energies= -1860.282553
Sum of electronic and thermal Energies= -1860.240288
Sum of electronic and thermal Enthalpies= -1860.239344
Sum of electronic and thermal Free Energies= -1860.358519

TS-2d'

Zero-point correction= 0.655428 (Hartree/Particle)
Thermal correction to Energy= 0.697901
Thermal correction to Enthalpy= 0.698846
Thermal correction to Gibbs Free Energy= 0.580824
Sum of electronic and zero-point Energies= -1860.284216
Sum of electronic and thermal Energies= -1860.241743
Sum of electronic and thermal Enthalpies= -1860.240798
Sum of electronic and thermal Free Energies= -1860.358820

INT-3c'

Zero-point correction= 0.660738 (Hartree/Particle)
Thermal correction to Energy= 0.702921
Thermal correction to Enthalpy= 0.703865
Thermal correction to Gibbs Free Energy= 0.585892
Sum of electronic and zero-point Energies= -1860.397757
Sum of electronic and thermal Energies= -1860.355575
Sum of electronic and thermal Enthalpies= -1860.354631
Sum of electronic and thermal Free Energies= -1860.472604

INT-3d'

Zero-point correction= 0.657455 (Hartree/Particle)

| | |
|--|--------------|
| Thermal correction to Energy= | 0.700483 |
| Thermal correction to Enthalpy= | 0.701427 |
| Thermal correction to Gibbs Free Energy= | 0.581863 |
| Sum of electronic and zero-point Energies= | -1860.357468 |
| Sum of electronic and thermal Energies= | -1860.314440 |
| Sum of electronic and thermal Enthalpies= | -1860.313495 |
| Sum of electronic and thermal Free Energies= | -1860.433060 |

Cartesian coordinates for all of the species [optimized at the level of M11L/6-31G(d,p) (SDD for Rh) with SMD atomic radii for experimental solvent methanol]:

CH₃COOH

| | | | |
|---|-------------|-------------|-------------|
| C | -0.09628600 | 0.11466100 | -0.00008500 |
| O | -0.65414700 | 1.17901400 | -0.00000600 |
| O | -0.74483600 | -1.03294700 | 0.00000500 |
| H | -1.68953800 | -0.84167900 | 0.00002100 |
| C | 1.37096000 | -0.09007400 | 0.00004400 |
| H | 1.67073600 | -0.67324100 | 0.88165400 |
| H | 1.67088100 | -0.67329100 | -0.88148200 |
| H | 1.89174400 | 0.87215500 | 0.00006200 |

MeOH

| | | | |
|---|-------------|-------------|-------------|
| C | -0.64547300 | 0.01856900 | -0.00006500 |
| H | -1.02566900 | 0.54846000 | 0.89499200 |
| H | -1.08297800 | -0.99120800 | -0.00004100 |
| H | -1.02572300 | 0.54979600 | -0.89441400 |
| O | 0.73666600 | -0.12203500 | -0.00013600 |
| H | 1.11388600 | 0.75782300 | 0.00094000 |

Cp*RhH(OAc)

| | | | |
|----|-------------|-------------|-------------|
| C | -2.09096600 | 0.24372800 | -0.22726500 |
| C | -1.66612000 | -1.05337000 | 0.11957600 |
| C | -0.60433100 | -0.90020200 | 1.07576100 |
| C | -0.51258900 | 0.50953500 | 1.42769600 |
| C | -1.40322800 | 1.20752600 | 0.62542900 |
| Rh | 0.00467900 | -0.00205000 | -0.72475200 |
| C | -1.63299100 | 2.66217300 | 0.55611800 |
| H | -2.64148100 | 2.92036800 | 0.92158400 |
| H | -0.90898400 | 3.22941700 | 1.15567000 |
| H | -1.57492000 | 3.03400400 | -0.47938600 |
| C | -3.14175200 | 0.60830600 | -1.19497400 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.08164600 | 0.85772800 | -0.67266900 |
| H | -2.86390600 | 1.49581500 | -1.78392400 |
| H | -3.36158600 | -0.20797500 | -1.89619400 |
| C | -2.21227200 | -2.33716100 | -0.36786800 |
| H | -3.02538800 | -2.68590500 | 0.29136700 |
| H | -2.62599400 | -2.25301800 | -1.38221800 |
| H | -1.44748000 | -3.12594600 | -0.38626300 |
| C | 0.06445600 | -1.99356000 | 1.80410000 |
| H | -0.55037000 | -2.30409100 | 2.66779700 |
| H | 0.21207200 | -2.88085900 | 1.17289200 |
| H | 1.04498400 | -1.68953900 | 2.19513700 |
| C | 0.45985800 | 1.04195200 | 2.39973500 |
| H | 0.18473100 | 0.75698700 | 3.42907700 |
| H | 1.46836700 | 0.63297700 | 2.22191700 |
| H | 0.53030500 | 2.13704900 | 2.36525800 |
| O | 2.85043800 | -1.15788300 | 0.15144800 |
| H | 0.35308200 | -1.16449500 | -1.74739300 |
| C | 2.93610900 | -0.06029900 | -0.38432600 |
| O | 1.96357600 | 0.60052600 | -0.86312800 |
| C | 4.26460800 | 0.62753400 | -0.51703700 |
| H | 5.08086000 | 0.00546500 | -0.12916600 |
| H | 4.46754700 | 0.87507800 | -1.56912100 |
| H | 4.25244900 | 1.58108400 | 0.03124500 |

Cp*Rh(OAc)₂

| | | | |
|----|-------------|-------------|-------------|
| Rh | 0.05029200 | 0.21250800 | -0.10050600 |
| C | 1.36611700 | -0.85823100 | 1.22564500 |
| C | 1.16707600 | -1.63983000 | 0.06028300 |
| C | 1.61135700 | -0.87623200 | -1.06592300 |
| C | 2.16494200 | 0.35354300 | -0.56995700 |
| C | 1.99306700 | 0.38309100 | 0.83304100 |
| C | -1.45037900 | 2.21457000 | -0.01608600 |
| O | -0.76832700 | 1.95294900 | -1.03699500 |
| O | -1.27129700 | 1.51804500 | 1.00838800 |
| C | -2.45974600 | 3.29691300 | -0.03987900 |
| H | -3.41120400 | 2.88524300 | -0.40829700 |
| H | -2.63305100 | 3.69849200 | 0.96570900 |
| H | -2.15862600 | 4.09999500 | -0.72373000 |
| O | -1.73729300 | -0.56616800 | -0.78028100 |
| C | -2.42679300 | -1.25760100 | 0.03556100 |
| O | -2.14001700 | -1.46098400 | 1.20850800 |
| C | -3.65931400 | -1.87311500 | -0.55844300 |
| H | -4.04452000 | -1.29738800 | -1.40998900 |
| H | -3.40636800 | -2.87990800 | -0.92649400 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.44351000 | -1.98945100 | 0.20101500 |
| C | 2.73349400 | 1.41393400 | -1.41844900 |
| H | 3.74817300 | 1.13067100 | -1.74420600 |
| H | 2.13677200 | 1.56507000 | -2.33003300 |
| H | 2.80779000 | 2.37509900 | -0.89408900 |
| C | 2.40419200 | 1.44601900 | 1.76832100 |
| H | 3.36246400 | 1.18798000 | 2.24986800 |
| H | 2.53712500 | 2.41289600 | 1.26538200 |
| H | 1.66696000 | 1.58251400 | 2.57296900 |
| C | 1.61428900 | -1.32905100 | -2.46860500 |
| H | 1.55686800 | -0.48654200 | -3.17180900 |
| H | 2.54083900 | -1.88327100 | -2.69678200 |
| H | 0.77155900 | -2.00257900 | -2.67940700 |
| C | 0.56532900 | -2.98302400 | -0.02611400 |
| H | -0.15695200 | -3.04970700 | -0.85415000 |
| H | 1.35039100 | -3.73085900 | -0.22617200 |
| H | 0.05139900 | -3.27352900 | 0.89819300 |
| C | 1.03208700 | -1.21493300 | 2.61513500 |
| H | 0.38364700 | -2.09793700 | 2.67586800 |
| H | 1.95237300 | -1.43162600 | 3.18333800 |
| H | 0.52592900 | -0.38507600 | 3.13145200 |

Cp*RhH(OPiv)

| | | | |
|----|-------------|-------------|-------------|
| C | -2.75461100 | 0.10704300 | -0.30803600 |
| C | -2.25621700 | -1.05303900 | 0.31619800 |
| C | -1.23119100 | -0.62635900 | 1.23007000 |
| C | -1.25683200 | 0.82767200 | 1.29221400 |
| C | -2.16386800 | 1.27183700 | 0.34464100 |
| Rh | -0.62722700 | -0.11532000 | -0.71372400 |
| C | -2.48441200 | 2.65814400 | -0.03945500 |
| H | -3.53207600 | 2.90075100 | 0.20704300 |
| H | -1.84340300 | 3.39303400 | 0.46469500 |
| H | -2.38073900 | 2.80995500 | -1.12603800 |
| C | -3.82875200 | 0.18245100 | -1.31702300 |
| H | -4.80014700 | 0.40314500 | -0.84034100 |
| H | -3.64595800 | 0.98327500 | -2.04939400 |
| H | -3.94131800 | -0.75982800 | -1.87075100 |
| C | -2.70868800 | -2.44427800 | 0.10962300 |
| H | -3.50519000 | -2.69626200 | 0.83061900 |
| H | -3.11706900 | -2.60105500 | -0.89817400 |
| H | -1.89487300 | -3.16777100 | 0.25642400 |
| C | -0.47771400 | -1.48306800 | 2.16382400 |
| H | -1.02093700 | -1.57453100 | 3.12146400 |
| H | -0.33124000 | -2.49761800 | 1.76862300 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.51324600 | -1.06233300 | 2.39196300 |
| C | -0.36616100 | 1.62025300 | 2.16013000 |
| H | -0.62209900 | 1.48060400 | 3.22392300 |
| H | 0.68655100 | 1.30706900 | 2.05026900 |
| H | -0.41869200 | 2.69546300 | 1.94327600 |
| O | 2.09995600 | -1.63984300 | 0.03613600 |
| H | -0.30837100 | -1.43797100 | -1.50921800 |
| C | 2.27790600 | -0.47474100 | -0.29330700 |
| O | 1.38086600 | 0.31894000 | -0.71445100 |
| C | 3.66635500 | 0.16806300 | -0.17697500 |
| C | 4.02097200 | 0.86665000 | -1.47530000 |
| H | 3.30027800 | 1.66088100 | -1.72206800 |
| H | 5.01859300 | 1.33185500 | -1.40223900 |
| H | 4.04805900 | 0.16098500 | -2.32226600 |
| C | 3.60246700 | 1.18701800 | 0.94861200 |
| H | 3.30401800 | 0.71780800 | 1.90232200 |
| H | 4.59003600 | 1.65306100 | 1.10582500 |
| H | 2.88390500 | 1.99269000 | 0.72735800 |
| C | 4.70268500 | -0.88457100 | 0.14507900 |
| H | 4.75705500 | -1.65672300 | -0.63872200 |
| H | 5.70143700 | -0.42484700 | 0.23088200 |
| H | 4.48593100 | -1.39343800 | 1.09684100 |

Cp*RhOAc(OPiv)

| | | | |
|----|-------------|-------------|-------------|
| Rh | 0.66593000 | 0.25710900 | -0.04500000 |
| C | 1.55848700 | -1.38735100 | 1.02699300 |
| C | 1.20712700 | -1.82099900 | -0.28199600 |
| C | 1.91574000 | -1.01590900 | -1.21922500 |
| C | 2.76351400 | -0.11274700 | -0.47791500 |
| C | 2.53861300 | -0.33663500 | 0.89522000 |
| C | -0.26824000 | 2.56376100 | 0.08812900 |
| O | 0.25068700 | 2.13780500 | -0.97220900 |
| O | -0.14024500 | 1.87390900 | 1.12617400 |
| C | -1.05007000 | 3.81996400 | 0.09992600 |
| H | -2.09499000 | 3.58093900 | -0.15585900 |
| H | -1.04587300 | 4.28179900 | 1.09454600 |
| H | -0.67763600 | 4.52651900 | -0.65175700 |
| O | -1.32235200 | 0.04459400 | -0.52631500 |
| C | -2.12837700 | -0.39125700 | 0.35418000 |
| O | -1.82358600 | -0.72441200 | 1.49104000 |
| C | -3.57748900 | -0.46632200 | -0.13904400 |
| C | 3.67078700 | 0.87205800 | -1.09245500 |
| H | 4.58278900 | 0.37257100 | -1.45998500 |
| H | 3.20582700 | 1.36454100 | -1.95934700 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.98116400 | 1.65248000 | -0.38586400 |
| C | 3.16054000 | 0.35789600 | 2.03600800 |
| H | 3.94441300 | -0.27540100 | 2.48452600 |
| H | 3.62692200 | 1.30822300 | 1.74648400 |
| H | 2.42676100 | 0.56529800 | 2.82881300 |
| C | 1.87749800 | -1.12644500 | -2.68813000 |
| H | 1.96063100 | -0.14229500 | -3.17182900 |
| H | 2.72192500 | -1.73711100 | -3.05060300 |
| H | 0.95257900 | -1.60062600 | -3.04263800 |
| C | 0.21466800 | -2.85698500 | -0.62314300 |
| H | -0.33948200 | -2.60087400 | -1.53831800 |
| H | 0.71771800 | -3.82075500 | -0.80543100 |
| H | -0.51450900 | -3.00955200 | 0.18446300 |
| C | 1.12150500 | -1.96398800 | 2.31112100 |
| H | 0.23296600 | -2.59863700 | 2.20242300 |
| H | 1.92688200 | -2.58601600 | 2.73781600 |
| H | 0.89156100 | -1.18330000 | 3.05114300 |
| C | -3.62703600 | -1.38454800 | -1.34704100 |
| H | -3.01073900 | -1.00238900 | -2.17551900 |
| H | -3.26815500 | -2.39849400 | -1.09815100 |
| H | -4.66178700 | -1.48388500 | -1.71604900 |
| C | -4.47587800 | -1.00135700 | 0.95227000 |
| H | -4.46046400 | -0.35850600 | 1.84622100 |
| H | -5.51827900 | -1.05653600 | 0.59709100 |
| H | -4.17581900 | -2.01337700 | 1.26674900 |
| C | -4.01461300 | 0.93304800 | -0.53498700 |
| H | -5.06309900 | 0.92973800 | -0.87788300 |
| H | -3.94906500 | 1.63138800 | 0.31718900 |
| H | -3.39579800 | 1.33609100 | -1.35223000 |

PC1

| | | | |
|---|------------|-------------|-------------|
| N | 3.53488000 | 0.68147100 | -0.28310500 |
| C | 3.92075200 | -0.60826300 | -0.09966500 |
| C | 5.26846800 | -0.95693300 | -0.06203900 |
| H | 6.02951100 | -0.18016400 | -0.17973300 |
| C | 5.61883800 | -2.27419500 | 0.12432900 |
| H | 6.67786500 | -2.54567900 | 0.15341600 |
| C | 4.64637500 | -3.26268200 | 0.27529400 |
| H | 4.94393000 | -4.30362500 | 0.42255100 |
| C | 3.31648300 | -2.92094200 | 0.23848100 |
| H | 2.53814200 | -3.68191000 | 0.35451100 |
| C | 2.92614600 | -1.59109300 | 0.05115200 |
| C | 2.25415800 | 1.12807900 | -0.34767500 |
| O | 2.01507400 | 2.31210500 | -0.54018800 |

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|---|-------------|-------------|-------------|
| C | 1.56860300 | -1.17753300 | 0.00944400 |
| C | 1.22863700 | 0.11731400 | -0.17952300 |
| H | 0.79743100 | -1.94772000 | 0.13046200 |
| C | -0.43319400 | 2.84806200 | 0.66863000 |
| O | -0.24981200 | 3.63420300 | 1.55380900 |
| O | -0.27529400 | 1.56530400 | 0.86497200 |
| C | -0.16415500 | 0.64503000 | -0.24289600 |
| C | -1.26552500 | -0.36404800 | -0.10381200 |
| H | -0.28580300 | 1.20791700 | -1.18334600 |
| C | -2.63913800 | 0.26353200 | -0.22250900 |
| H | -1.13767400 | -1.12945600 | -0.88971800 |
| H | -1.17172700 | -0.88832600 | 0.86563300 |
| H | -2.76585900 | 1.02409200 | 0.56811000 |
| H | -2.70771100 | 0.79829100 | -1.18785400 |
| C | -3.73226700 | -0.74984600 | -0.12480200 |
| C | -4.37514800 | -0.99708300 | 1.08297100 |
| C | -4.09803700 | -1.50445500 | -1.23540500 |
| C | -5.35847400 | -1.96776900 | 1.17914400 |
| H | -4.09971200 | -0.40901300 | 1.96627000 |
| C | -5.07974600 | -2.47557400 | -1.14362500 |
| H | -3.60330300 | -1.31833800 | -2.19621000 |
| C | -5.71396300 | -2.71089600 | 0.06586700 |
| H | -5.85716900 | -2.14363700 | 2.13740500 |
| H | -5.35721500 | -3.05462600 | -2.03002100 |
| H | -6.49301000 | -3.47555100 | 0.13961900 |
| C | -0.97637300 | 4.54138300 | -0.76093800 |
| H | -0.00261500 | 5.03874500 | -0.64563400 |
| H | -1.70561600 | 4.99158200 | -0.07278500 |
| H | -1.32677100 | 4.63919200 | -1.79386600 |
| O | -0.85793200 | 3.15414900 | -0.52995000 |
| H | 4.25222900 | 1.38932800 | -0.40074800 |

PC2

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|---|-------------|-------------|-------------|
| N | -1.85223600 | -1.17056000 | -1.13520400 |
| C | -3.53456600 | 0.34952100 | -0.39318200 |
| C | -4.85591100 | 0.57738900 | -0.02902100 |
| H | -5.58648300 | -0.22655600 | -0.15952000 |
| C | -5.22976200 | 1.79904500 | 0.49241200 |
| H | -6.26746000 | 1.97790600 | 0.78637000 |
| C | -4.28050600 | 2.79984500 | 0.64091400 |
| H | -4.57137000 | 3.76971000 | 1.05532400 |
| C | -2.96422000 | 2.57884700 | 0.27614500 |
| H | -2.21871600 | 3.37105400 | 0.39996100 |
| C | -2.57456600 | 1.35258800 | -0.24139100 |

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|---|-------------|-------------|-------------|
| C | -3.16774700 | -0.95823600 | -0.97618800 |
| O | -3.99845900 | -1.77659500 | -1.32875300 |
| C | -1.16932500 | 1.07680000 | -0.65614900 |
| C | -0.85007800 | -0.38970600 | -0.46964500 |
| H | -0.47268700 | 1.70302900 | -0.08111900 |
| H | -1.02910200 | 1.32868400 | -1.72354900 |
| C | -0.79930800 | -0.69603400 | 1.02540800 |
| O | -0.41373400 | 0.07648300 | 1.85824700 |
| O | 0.58282700 | -2.16876400 | -1.24517900 |
| C | 0.49795900 | -0.78293500 | -1.11763200 |
| C | 1.71655300 | -0.20387900 | -0.44240900 |
| H | 0.43387100 | -0.40320700 | -2.15742500 |
| C | 2.97494100 | -0.43367800 | -1.25492900 |
| H | 1.58085300 | 0.87787600 | -0.26610000 |
| H | 1.83413400 | -0.66410200 | 0.55918200 |
| H | 3.10052100 | -1.51565700 | -1.43395700 |
| H | 2.85035800 | 0.03622300 | -2.24750500 |
| C | 4.19148800 | 0.11524000 | -0.58492600 |
| C | 4.94305400 | -0.66846600 | 0.28436800 |
| C | 4.57138300 | 1.43976500 | -0.77674000 |
| C | 6.04450600 | -0.14617200 | 0.94114500 |
| H | 4.65878700 | -1.71546900 | 0.44345100 |
| C | 5.67207700 | 1.96594800 | -0.12245300 |
| H | 3.99081800 | 2.06935200 | -1.46155900 |
| C | 6.41282000 | 1.17396200 | 0.73982600 |
| H | 6.62697300 | -0.78058700 | 1.61653500 |
| H | 5.95850700 | 3.00874200 | -0.29116900 |
| H | 7.28535200 | 1.58723200 | 1.25452600 |
| C | -1.10884800 | -2.28877300 | 2.64910900 |
| H | -0.07259200 | -2.23319500 | 3.01209300 |
| H | -1.47223600 | -3.32014300 | 2.70077100 |
| H | -1.74555500 | -1.63335800 | 3.25983100 |
| O | -1.18155300 | -1.92469600 | 1.28399000 |
| H | -1.58152000 | -2.11581900 | -1.38335300 |
| H | 0.81088700 | -2.54564900 | -0.39076900 |

INT-1

| | | | |
|---|-------------|------------|-------------|
| N | 2.24688600 | 0.60813600 | -1.22919700 |
| C | 1.30642100 | 2.70780400 | -0.83056900 |
| C | 1.62490000 | 3.95692400 | -0.30890600 |
| H | 2.66920700 | 4.28444500 | -0.34561700 |
| C | 0.65763600 | 4.76182100 | 0.26033200 |
| H | 0.92688300 | 5.73697100 | 0.67587200 |
| C | -0.65422300 | 4.31939900 | 0.29845600 |

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|----|-------------|-------------|-------------|
| H | -1.43451600 | 4.94340000 | 0.74480600 |
| C | -0.98633000 | 3.09913200 | -0.26575500 |
| H | -2.03684000 | 2.78419200 | -0.29404600 |
| C | -0.02821400 | 2.27302200 | -0.84666300 |
| C | 2.43004600 | -1.61868400 | 1.87404700 |
| C | 2.85110400 | -0.28043100 | 1.89017800 |
| C | 1.68347100 | 0.53028100 | 2.12162200 |
| C | 0.56260000 | -0.32807100 | 2.29753100 |
| C | 0.99979000 | -1.66264800 | 2.08931100 |
| Rh | 1.39022700 | -0.55765500 | 0.24088000 |
| C | 2.44220400 | 1.91321800 | -1.37782100 |
| O | 3.41745300 | 2.44682600 | -1.89821300 |
| C | -0.47940700 | 1.05085800 | -1.58781300 |
| C | -0.38135100 | -0.30838200 | -0.93255100 |
| C | 0.22653700 | -2.91329300 | 2.24611000 |
| H | 0.56100600 | -3.46870200 | 3.13890900 |
| H | -0.84967200 | -2.72833800 | 2.36695800 |
| H | 0.35395600 | -3.58814000 | 1.38512600 |
| C | 3.25624500 | -2.81221100 | 1.62002000 |
| H | 3.50071300 | -3.31516800 | 2.57088400 |
| H | 2.72384600 | -3.54898800 | 0.99998000 |
| H | 4.20592600 | -2.56809300 | 1.12346200 |
| C | 4.21373900 | 0.24553400 | 1.66748400 |
| H | 4.68836300 | 0.54856400 | 2.61599200 |
| H | 4.87083700 | -0.49953800 | 1.19707800 |
| H | 4.20250400 | 1.13574800 | 1.01751400 |
| C | 1.69231800 | 1.97777800 | 2.39095500 |
| H | 1.82664800 | 2.14339100 | 3.47483000 |
| H | 2.51801900 | 2.49304900 | 1.88167000 |
| H | 0.74910900 | 2.46417000 | 2.10314300 |
| C | -0.77184500 | 0.15014600 | 2.71741100 |
| H | -0.70928700 | 0.56913400 | 3.73602500 |
| H | -1.14789300 | 0.95837600 | 2.06842800 |
| H | -1.52513000 | -0.64835500 | 2.74507400 |
| O | 3.34368000 | -0.08222900 | -1.83432500 |
| H | 0.10168900 | 0.98448400 | -2.52415000 |
| H | -1.52405800 | 1.23518000 | -1.90685900 |
| C | -0.45314800 | -1.44172300 | -1.87380700 |
| O | 0.02819500 | -1.78327100 | -2.91574000 |
| O | -1.40449500 | -2.12509900 | -1.19823400 |
| C | -1.58475400 | -1.00074500 | -0.27927600 |
| C | -2.95780400 | -0.42137400 | -0.40952600 |
| H | -1.42865600 | -1.38132700 | 0.74124500 |
| C | -4.02761700 | -1.35296700 | 0.12388200 |

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|---|-------------|-------------|-------------|
| H | -2.98141500 | 0.53572300 | 0.14782700 |
| H | -3.16602700 | -0.17205500 | -1.46695300 |
| H | -3.99616300 | -2.30129800 | -0.44198100 |
| H | -3.78797400 | -1.60605800 | 1.17417700 |
| C | -5.39627600 | -0.76116500 | 0.04728600 |
| C | -6.20925800 | -0.97877400 | -1.05982500 |
| C | -5.86876300 | 0.06404000 | 1.06304600 |
| C | -7.46067300 | -0.39240200 | -1.14902600 |
| H | -5.85129700 | -1.62899000 | -1.86679000 |
| C | -7.11900600 | 0.65208100 | 0.97793300 |
| H | -5.24092400 | 0.24128000 | 1.94466800 |
| C | -7.91983900 | 0.42558200 | -0.12984800 |
| H | -8.08823800 | -0.58044200 | -2.02581100 |
| H | -7.47607600 | 1.29264400 | 1.79048900 |
| H | -8.90996800 | 0.88610600 | -0.19674000 |
| C | 3.15961400 | -1.36689000 | -1.79487100 |
| O | 2.23679400 | -1.88885700 | -1.18562700 |
| C | 4.15970700 | -2.13240200 | -2.55471900 |
| H | 4.52681900 | -2.96403800 | -1.94008200 |
| H | 3.66847500 | -2.56918500 | -3.43586200 |
| H | 4.99174800 | -1.50233000 | -2.88512900 |

TS-1

| | | | |
|----|-------------|-------------|-------------|
| N | -2.45122000 | 0.45025000 | 0.67833400 |
| C | -2.01366600 | 2.63665600 | 0.54740500 |
| C | -2.98221500 | 3.61974300 | 0.32538900 |
| H | -3.96633600 | 3.49638500 | 0.78828600 |
| C | -2.70128800 | 4.73041800 | -0.43579100 |
| H | -3.46544300 | 5.49585500 | -0.59524200 |
| C | -1.43458800 | 4.86478600 | -0.98916500 |
| H | -1.18955300 | 5.73828000 | -1.60015300 |
| C | -0.48373500 | 3.89103100 | -0.77618200 |
| H | 0.51331700 | 4.00573200 | -1.21720700 |
| C | -0.74507100 | 2.73970600 | -0.02854200 |
| C | -2.19104600 | -2.25775300 | -1.61979900 |
| C | -2.61391200 | -0.98593600 | -2.03780500 |
| C | -1.44121000 | -0.21734300 | -2.37087200 |
| C | -0.30190800 | -1.07625000 | -2.25222900 |
| C | -0.75029300 | -2.30502100 | -1.73329400 |
| Rh | -1.27424500 | -0.70199600 | -0.23487900 |
| C | -2.49458400 | 1.51146300 | 1.44281800 |
| O | -3.00792500 | 1.72851600 | 2.52365900 |
| C | 0.41528600 | 1.79450900 | 0.09823300 |
| C | 0.29137500 | 0.40503000 | 0.64489700 |

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|---|-------------|-------------|-------------|
| C | 0.06208800 | -3.49470100 | -1.41551800 |
| H | -0.08868100 | -4.27850200 | -2.17697100 |
| H | 1.13703200 | -3.27092100 | -1.38253200 |
| H | -0.22353800 | -3.93658300 | -0.44774800 |
| C | -3.01449800 | -3.37728000 | -1.12621000 |
| H | -3.03419500 | -4.20308000 | -1.85719500 |
| H | -2.60519600 | -3.79607000 | -0.19227000 |
| H | -4.05303300 | -3.07780900 | -0.93455300 |
| C | -3.98793000 | -0.45582300 | -2.08554600 |
| H | -4.32825300 | -0.35859000 | -3.12968400 |
| H | -4.70380000 | -1.10011300 | -1.55840000 |
| H | -4.04531800 | 0.54942200 | -1.63789900 |
| C | -1.46112600 | 1.13084100 | -2.97245700 |
| H | -1.68109200 | 1.05991800 | -4.05198300 |
| H | -2.23755600 | 1.77185500 | -2.52694000 |
| H | -0.49580900 | 1.64656000 | -2.87167200 |
| C | 1.07270800 | -0.74758700 | -2.67379800 |
| H | 1.19616700 | -0.98461400 | -3.74427300 |
| H | 1.30615400 | 0.32013300 | -2.55808200 |
| H | 1.83242500 | -1.32752500 | -2.12988100 |
| O | -2.98483400 | -1.09709400 | 2.21520600 |
| H | 1.18575300 | 2.34341600 | 0.68200700 |
| H | 0.86202100 | 1.71457200 | -0.90981700 |
| C | 0.29538300 | 0.19310000 | 2.12429700 |
| O | -0.31905900 | 0.53168100 | 3.08885000 |
| O | 1.36796900 | -0.61432300 | 2.13344000 |
| C | 1.55271200 | -0.46391700 | 0.69502100 |
| C | 2.89949500 | 0.11209000 | 0.38599800 |
| H | 1.43166100 | -1.46364900 | 0.23255500 |
| C | 4.01482800 | -0.88652000 | 0.62236600 |
| H | 2.91131900 | 0.44042600 | -0.66958600 |
| H | 3.06402200 | 1.01836700 | 0.99805600 |
| H | 4.00703200 | -1.19832100 | 1.68199200 |
| H | 3.80910100 | -1.79546100 | 0.02584100 |
| C | 5.35655600 | -0.34008800 | 0.26163600 |
| C | 6.14162500 | 0.31200000 | 1.20627300 |
| C | 5.82879500 | -0.42944000 | -1.04396200 |
| C | 7.36661300 | 0.85584900 | 0.85814000 |
| H | 5.78360500 | 0.38773400 | 2.23972100 |
| C | 7.05303500 | 0.11233700 | -1.39610500 |
| H | 5.22175900 | -0.94472000 | -1.79847100 |
| C | 7.82666900 | 0.75759000 | -0.44479900 |
| H | 7.97325400 | 1.36006700 | 1.61683000 |
| H | 7.41107600 | 0.02496700 | -2.42668000 |

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|---|-------------|-------------|-------------|
| H | 8.79645000 | 1.18282900 | -0.71979300 |
| C | -2.02724400 | -1.86457000 | 2.24840200 |
| O | -1.07479300 | -1.90889900 | 1.40799500 |
| C | -1.89275600 | -2.82414500 | 3.38784300 |
| H | -1.43804700 | -3.76743400 | 3.06006300 |
| H | -1.21876800 | -2.36873400 | 4.12990100 |
| H | -2.85940700 | -3.01001700 | 3.86993100 |

INT-2

| | | | |
|----|-------------|-------------|-------------|
| N | -2.46992700 | 0.92776300 | -0.19067800 |
| C | -1.56247600 | 3.16149300 | -0.10409600 |
| C | -2.09430600 | 4.44847600 | -0.03749300 |
| H | -3.08519200 | 4.57466900 | 0.40900200 |
| C | -1.39849800 | 5.53496300 | -0.52111500 |
| H | -1.83097500 | 6.53747500 | -0.46480000 |
| C | -0.14274300 | 5.33698900 | -1.07214000 |
| H | 0.43124500 | 6.18504800 | -1.45697100 |
| C | 0.39659200 | 4.06627200 | -1.12470800 |
| H | 1.40062300 | 3.92567000 | -1.54016900 |
| C | -0.29246400 | 2.94994700 | -0.65725300 |
| C | -2.34611500 | -2.66850400 | -0.77715900 |
| C | -2.77469600 | -1.71717900 | -1.73228100 |
| C | -1.61004400 | -1.17501100 | -2.35156700 |
| C | -0.45809600 | -1.86335400 | -1.82783300 |
| C | -0.91017200 | -2.76784900 | -0.85025500 |
| Rh | -1.47428400 | -0.64410100 | -0.17369900 |
| C | -2.43692400 | 2.09283100 | 0.44199800 |
| O | -3.24647400 | 2.31793800 | 1.33970700 |
| C | 0.40716100 | 1.62893700 | -0.79730100 |
| C | 0.21250500 | 0.58161000 | 0.26403500 |
| C | -0.11145200 | -3.71595800 | -0.05382100 |
| H | -0.38423100 | -4.75206100 | -0.31409500 |
| H | 0.96714700 | -3.60375800 | -0.22502600 |
| H | -0.30208800 | -3.60112000 | 1.02581500 |
| C | -3.18703900 | -3.50569200 | 0.09405400 |
| H | -3.33252500 | -4.49784000 | -0.36700200 |
| H | -2.70958600 | -3.68012100 | 1.07026900 |
| H | -4.18004500 | -3.07116500 | 0.26663500 |
| C | -4.15581500 | -1.31101900 | -2.03715500 |
| H | -4.50702300 | -1.80930100 | -2.95603900 |
| H | -4.85290000 | -1.56955000 | -1.22941400 |
| H | -4.22545700 | -0.22742600 | -2.21486600 |
| C | -1.61550000 | -0.22551400 | -3.47862800 |
| H | -1.89849200 | -0.75559100 | -4.40428000 |

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|---|-------------|-------------|-------------|
| H | -2.34779700 | 0.58230200 | -3.33642700 |
| H | -0.62918400 | 0.22431100 | -3.65257700 |
| C | 0.91515900 | -1.71252500 | -2.33731700 |
| H | 1.01626800 | -2.27013800 | -3.28391500 |
| H | 1.16666500 | -0.66597800 | -2.56273500 |
| H | 1.66864900 | -2.11069900 | -1.64408300 |
| O | -3.25765500 | -0.96926300 | 2.32922500 |
| H | 1.48533800 | 1.85914000 | -0.88121400 |
| H | 0.15051900 | 1.19562900 | -1.78278400 |
| C | 0.17280100 | 0.95875000 | 1.71305500 |
| O | -0.45471300 | 1.66339600 | 2.44098700 |
| O | 1.19009100 | 0.16938400 | 2.07423800 |
| C | 1.39008600 | -0.29494300 | 0.70489800 |
| C | 2.78334900 | 0.00775400 | 0.24966400 |
| H | 1.18416300 | -1.38110400 | 0.68336400 |
| C | 3.80784000 | -0.88672700 | 0.91845500 |
| H | 2.83832700 | -0.11631800 | -0.84703000 |
| H | 3.01569900 | 1.06875700 | 0.45739000 |
| H | 3.76042000 | -0.74171400 | 2.01239800 |
| H | 3.53803100 | -1.94260400 | 0.72831600 |
| C | 5.19289600 | -0.62330000 | 0.42664800 |
| C | 6.01310400 | 0.30624600 | 1.05676300 |
| C | 5.67185200 | -1.26663000 | -0.70997300 |
| C | 7.27873200 | 0.58264700 | 0.56744500 |
| H | 5.64989600 | 0.82018600 | 1.95444700 |
| C | 6.93654100 | -0.99376400 | -1.20194700 |
| H | 5.03625000 | -2.00473600 | -1.21435300 |
| C | 7.74488300 | -0.06687700 | -0.56384800 |
| H | 7.91228800 | 1.31350700 | 1.07958900 |
| H | 7.29843700 | -1.51602500 | -2.09308800 |
| H | 8.74657500 | 0.14698600 | -0.94840400 |
| C | -2.10096100 | -1.24910600 | 2.58402600 |
| O | -1.13125900 | -1.24824600 | 1.74433700 |
| C | -1.65540500 | -1.61478300 | 3.96604800 |
| H | -1.02109900 | -2.51195800 | 3.95072000 |
| H | -1.03904200 | -0.79512600 | 4.36710100 |
| H | -2.51333300 | -1.77385600 | 4.63026500 |

TS-2a

| | | | |
|---|-------------|------------|-------------|
| N | -2.72352100 | 0.75391900 | 0.37423000 |
| C | -1.72939200 | 3.00877500 | -0.09864000 |
| C | -2.12685700 | 4.34080900 | -0.14405800 |
| H | -3.07080900 | 4.60937700 | 0.33661100 |
| C | -1.37073700 | 5.30080700 | -0.78992800 |

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|----|-------------|-------------|-------------|
| H | -1.71623500 | 6.33812800 | -0.81807800 |
| C | -0.18716100 | 4.94532900 | -1.41402300 |
| H | 0.41415500 | 5.69417900 | -1.93638200 |
| C | 0.23044400 | 3.62903600 | -1.38084400 |
| H | 1.16760600 | 3.33420300 | -1.86457300 |
| C | -0.52052900 | 2.66848000 | -0.71148600 |
| C | -1.57945200 | -2.85631500 | -0.61098500 |
| C | -2.71595900 | -2.09887400 | -1.11595800 |
| C | -2.25520900 | -1.29436600 | -2.16673100 |
| C | -0.81136800 | -1.48366100 | -2.26115200 |
| C | -0.42481100 | -2.46581000 | -1.31445400 |
| Rh | -1.34282500 | -0.45964400 | -0.33243300 |
| C | -2.67951000 | 2.04689000 | 0.57113500 |
| O | -3.54056600 | 2.56639900 | 1.31505500 |
| C | 0.05905900 | 1.31567900 | -0.65882100 |
| C | 0.30711800 | 0.62717100 | 0.52588800 |
| C | 0.93278000 | -3.01538700 | -1.14042900 |
| H | 1.09971000 | -3.85864100 | -1.83124400 |
| H | 1.71344600 | -2.26952400 | -1.35461900 |
| H | 1.09627600 | -3.39685500 | -0.12249300 |
| C | -1.62956800 | -3.90076000 | 0.41180200 |
| H | -1.63858400 | -4.88465700 | -0.09008900 |
| H | -0.73776200 | -3.88440200 | 1.05394800 |
| H | -2.52323400 | -3.83819700 | 1.04260200 |
| C | -4.13500400 | -2.25466500 | -0.74969800 |
| H | -4.71985300 | -2.56650900 | -1.63014600 |
| H | -4.28334900 | -2.99989900 | 0.04044800 |
| H | -4.56307300 | -1.30270700 | -0.39610900 |
| C | -3.10402000 | -0.50990800 | -3.08064900 |
| H | -3.50986600 | -1.17177900 | -3.86413300 |
| H | -3.95967300 | -0.06616400 | -2.55250300 |
| H | -2.55131300 | 0.29595200 | -3.58125000 |
| C | 0.05058700 | -0.90654600 | -3.30221800 |
| H | 0.03790400 | -1.57170600 | -4.18263300 |
| H | -0.29624500 | 0.08092000 | -3.63686400 |
| H | 1.09771500 | -0.82452500 | -2.97761000 |
| O | -3.25059100 | -1.64992400 | 2.30958900 |
| H | 0.73381700 | 1.06525700 | -1.49377000 |
| H | -1.27413300 | 0.70751400 | -1.37512700 |
| C | 0.18863300 | 1.01679000 | 1.95764400 |
| O | -0.46886900 | 1.71789000 | 2.65225100 |
| O | 1.24478500 | 0.27515900 | 2.32001600 |
| C | 1.45631100 | -0.23824500 | 0.96511200 |
| C | 2.81447100 | 0.07080100 | 0.43008600 |

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|---|-------------|-------------|-------------|
| H | 1.24184600 | -1.32067000 | 0.98131100 |
| C | 3.90637800 | -0.74478000 | 1.09027000 |
| H | 2.79199000 | -0.14120300 | -0.65691600 |
| H | 3.01314600 | 1.15380200 | 0.53184800 |
| H | 3.92284100 | -0.52366500 | 2.17200400 |
| H | 3.65701300 | -1.81779800 | 0.99046400 |
| C | 5.24850200 | -0.47749100 | 0.49290200 |
| C | 6.09083200 | 0.49011400 | 1.02906900 |
| C | 5.66164300 | -1.15862300 | -0.64753100 |
| C | 7.31502700 | 0.76778900 | 0.44423000 |
| H | 5.77876600 | 1.03316600 | 1.92878600 |
| C | 6.88453800 | -0.88410500 | -1.23499500 |
| H | 5.00837100 | -1.92772000 | -1.07771500 |
| C | 7.71583700 | 0.08137400 | -0.69010400 |
| H | 7.96748500 | 1.52887800 | 0.88327900 |
| H | 7.19590900 | -1.43526000 | -2.12780800 |
| H | 8.68435000 | 0.29726900 | -1.15088200 |
| C | -2.07449500 | -1.42527200 | 2.55457900 |
| O | -1.14636200 | -1.24845700 | 1.70400600 |
| C | -1.60718000 | -1.32746900 | 3.98215300 |
| H | -0.59259200 | -1.73017200 | 4.10897600 |
| H | -1.56638500 | -0.26185600 | 4.26149300 |
| H | -2.30008000 | -1.83212100 | 4.66872100 |

TS-2b

| | | | |
|----|-------------|-------------|-------------|
| N | -2.45125100 | 0.51628700 | -0.36792700 |
| C | -2.14717500 | 2.87250100 | -0.23723100 |
| C | -2.98681100 | 3.96204200 | -0.47135900 |
| H | -4.05899600 | 3.83125000 | -0.29641100 |
| C | -2.48801100 | 5.17045000 | -0.90322700 |
| H | -3.16024700 | 6.01401600 | -1.08148600 |
| C | -1.12199500 | 5.29887200 | -1.10194500 |
| H | -0.69986200 | 6.24891200 | -1.44213900 |
| C | -0.28622300 | 4.22783500 | -0.85991900 |
| H | 0.79384800 | 4.34871300 | -1.00064000 |
| C | -0.76525600 | 2.98868900 | -0.43619100 |
| C | -1.46778000 | -2.92228800 | -0.89000400 |
| C | -2.04930600 | -2.06588700 | -1.86276700 |
| C | -1.00683800 | -1.25386100 | -2.39592400 |
| C | 0.23866300 | -1.68159600 | -1.81377600 |
| C | -0.05111600 | -2.68654400 | -0.86241300 |
| Rh | -1.14575100 | -0.79511400 | -0.20933000 |
| C | -2.84963000 | 1.63895800 | 0.20330600 |
| O | -3.88207400 | 1.67502300 | 0.86691300 |

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|---|-------------|-------------|-------------|
| C | 0.28484300 | 1.92932700 | -0.25998700 |
| C | 0.09081400 | 0.75999600 | 0.66529900 |
| C | 0.89211700 | -3.46590700 | -0.03986900 |
| H | 0.85581600 | -4.52968600 | -0.32715800 |
| H | 1.92871600 | -3.12601200 | -0.15703700 |
| H | 0.63449100 | -3.42020900 | 1.03069400 |
| C | -2.14548000 | -3.96000800 | -0.09806500 |
| H | -1.97571900 | -4.94479500 | -0.56628000 |
| H | -1.73643400 | -4.02303900 | 0.92169800 |
| H | -3.22942400 | -3.80473900 | -0.03340900 |
| C | -3.47257800 | -2.00234600 | -2.22912900 |
| H | -3.68640500 | -2.71356200 | -3.04392100 |
| H | -4.12409900 | -2.26260200 | -1.38336400 |
| H | -3.75774100 | -1.00315800 | -2.58500400 |
| C | -1.14218900 | -0.26238100 | -3.47724000 |
| H | -1.02886500 | -0.75653400 | -4.45705100 |
| H | -2.12649700 | 0.22486400 | -3.46810200 |
| H | -0.37062100 | 0.51847500 | -3.41710800 |
| C | 1.56098800 | -1.24891700 | -2.28978000 |
| H | 1.75813200 | -1.73056000 | -3.26294100 |
| H | 1.61195300 | -0.16435400 | -2.46795100 |
| H | 2.37417300 | -1.53764900 | -1.61108700 |
| O | -3.33095700 | -1.53063400 | 1.79860600 |
| H | 1.19504500 | 2.47157900 | 0.06839100 |
| H | 0.55603000 | 1.54530500 | -1.26502000 |
| C | -0.35039500 | 1.07816000 | 2.09367700 |
| O | -1.42436700 | 1.56752300 | 2.38991400 |
| O | 0.61139000 | 0.82340500 | 2.86691200 |
| C | 1.26725300 | -0.00715900 | 0.95409300 |
| C | 2.62333600 | 0.33292100 | 0.54397700 |
| H | 1.11157800 | -0.93881600 | 1.51479100 |
| C | 3.70180300 | -0.65255100 | 0.93664900 |
| H | 2.63087800 | 0.54567000 | -0.54389700 |
| H | 2.82825200 | 1.33410700 | 0.97938600 |
| H | 3.69015600 | -0.77121900 | 2.03384400 |
| H | 3.46795200 | -1.64254500 | 0.50798000 |
| C | 5.05141900 | -0.20986300 | 0.47515900 |
| C | 5.54781300 | -0.62241300 | -0.75627300 |
| C | 5.81465700 | 0.66534200 | 1.24045500 |
| C | 6.77729700 | -0.17725900 | -1.21137600 |
| H | 4.95726000 | -1.31721800 | -1.36653500 |
| C | 7.04414800 | 1.11298900 | 0.78840100 |
| H | 5.43709400 | 0.99625000 | 2.21502900 |
| C | 7.52923200 | 0.69304100 | -0.43947100 |

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|---|-------------|-------------|-------------|
| H | 7.15513900 | -0.51832200 | -2.18013600 |
| H | 7.63471500 | 1.79664600 | 1.40597700 |
| H | 8.50294900 | 1.04288700 | -0.79499100 |
| C | -2.23678100 | -1.56919900 | 2.32804100 |
| O | -1.11417900 | -1.38883800 | 1.73010300 |
| C | -2.06956300 | -1.80746900 | 3.79596400 |
| H | -2.98744400 | -2.21455400 | 4.23678700 |
| H | -1.22186200 | -2.47481100 | 4.00043300 |
| H | -1.84444000 | -0.84282700 | 4.27796700 |

TS-2c

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|----|-------------|-------------|-------------|
| N | -2.07860700 | 0.64708300 | 0.79413200 |
| C | -1.96924200 | 2.93820200 | -0.02942800 |
| C | -2.74613100 | 4.09407900 | -0.09169000 |
| H | -3.82403600 | 3.99904600 | 0.06472900 |
| C | -2.17953800 | 5.32862300 | -0.32518600 |
| H | -2.80559900 | 6.22422700 | -0.36048500 |
| C | -0.80881500 | 5.41734600 | -0.49875500 |
| H | -0.33467300 | 6.38696200 | -0.67671300 |
| C | -0.03206300 | 4.27606300 | -0.44294100 |
| H | 1.05047400 | 4.35599600 | -0.59071200 |
| C | -0.58245900 | 3.01932500 | -0.20862000 |
| C | -2.11285700 | -2.58089900 | -1.16908300 |
| C | -2.63998800 | -1.41067000 | -1.81050700 |
| C | -1.55062500 | -0.66380100 | -2.32698000 |
| C | -0.35197800 | -1.42449300 | -2.07890600 |
| C | -0.69552600 | -2.58818400 | -1.35955400 |
| Rh | -1.36483200 | -0.83483000 | -0.12046500 |
| C | -2.71603300 | 1.69471600 | 0.28092200 |
| O | -3.94724600 | 1.65992100 | 0.23011300 |
| C | 0.36272900 | 1.85999200 | -0.29261400 |
| C | 0.22238000 | 0.68920800 | 0.61503500 |
| C | 0.21751500 | -3.64485200 | -0.88397800 |
| H | 0.20730900 | -4.50772400 | -1.57071100 |
| H | 1.25747000 | -3.29600700 | -0.81278500 |
| H | -0.07917100 | -4.01973100 | 0.10689700 |
| C | -2.89758900 | -3.65949900 | -0.54220200 |
| H | -3.06183900 | -4.47473200 | -1.26789700 |
| H | -2.37599300 | -4.09640000 | 0.32139900 |
| H | -3.88339800 | -3.31247500 | -0.20599500 |
| C | -4.06526200 | -1.05394000 | -1.90403000 |
| H | -4.52626200 | -1.59411800 | -2.74843400 |
| H | -4.62043400 | -1.33639800 | -0.99845200 |
| H | -4.21416800 | 0.01945200 | -2.08013000 |

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|---|-------------|-------------|-------------|
| C | -1.66436000 | 0.57243200 | -3.12745500 |
| H | -2.00103500 | 0.33613400 | -4.15079300 |
| H | -2.40071100 | 1.27126100 | -2.70101300 |
| H | -0.70718800 | 1.10302100 | -3.21829200 |
| C | 0.99202900 | -1.08228300 | -2.56784700 |
| H | 1.09319800 | -1.43442600 | -3.60867700 |
| H | 1.18118800 | -0.00013400 | -2.58615300 |
| H | 1.78660200 | -1.56964100 | -1.98564300 |
| O | -3.01596600 | -1.92133300 | 2.34628500 |
| H | 1.38186000 | 2.27019200 | -0.15501000 |
| H | 0.36838700 | 1.48824800 | -1.33399800 |
| C | 0.27413900 | 0.83305300 | 2.10576800 |
| O | -0.28229100 | 1.42724300 | 2.97142000 |
| O | 1.32972000 | 0.02179300 | 2.25910800 |
| C | 1.42795000 | -0.24632600 | 0.83380800 |
| C | 2.77608200 | 0.15812000 | 0.31695400 |
| H | 1.22562400 | -1.31864500 | 0.66448200 |
| C | 3.84010800 | -0.86455700 | 0.66449200 |
| H | 2.72652300 | 0.28947200 | -0.77838300 |
| H | 3.04537100 | 1.14297100 | 0.74038300 |
| H | 3.85843600 | -1.01628600 | 1.75843000 |
| H | 3.55889100 | -1.83643200 | 0.21605600 |
| C | 5.19286400 | -0.45355300 | 0.18459400 |
| C | 6.06397300 | 0.24255800 | 1.01551100 |
| C | 5.58978800 | -0.71341800 | -1.12318800 |
| C | 7.30043300 | 0.66270800 | 0.55516300 |
| H | 5.76492300 | 0.45289400 | 2.04898700 |
| C | 6.82488300 | -0.29509900 | -1.58728400 |
| H | 4.91465400 | -1.26551600 | -1.78861500 |
| C | 7.68498800 | 0.39521000 | -0.74834900 |
| H | 7.97524400 | 1.20385200 | 1.22565100 |
| H | 7.12263200 | -0.51505700 | -2.61719600 |
| H | 8.66344300 | 0.72313500 | -1.11177900 |
| C | -1.82703700 | -1.80912500 | 2.60349000 |
| O | -0.90518300 | -1.51094100 | 1.77485000 |
| C | -1.31389500 | -2.01138300 | 3.99955600 |
| H | -1.02225300 | -1.03306600 | 4.41434400 |
| H | -2.07776700 | -2.45543400 | 4.65011100 |
| H | -0.41104000 | -2.63764400 | 4.00403000 |

TS-2d

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|---|-------------|------------|------------|
| N | -2.39440900 | 0.56162300 | 0.84817000 |
| C | -1.94432100 | 2.45832800 | 0.80040500 |
| C | -2.99607900 | 3.34332000 | 0.53507600 |

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|----|-------------|-------------|-------------|
| H | -4.00378700 | 3.09162000 | 0.87948500 |
| C | -2.73964300 | 4.53801000 | -0.09227900 |
| H | -3.55040700 | 5.24783400 | -0.27400700 |
| C | -1.43965700 | 4.82380100 | -0.49665300 |
| H | -1.22073600 | 5.76495300 | -1.00851100 |
| C | -0.42801100 | 3.90793400 | -0.29720300 |
| H | 0.58104800 | 4.12763300 | -0.66338900 |
| C | -0.65137500 | 2.67534400 | 0.31611700 |
| C | -2.34768100 | -1.93491400 | -1.75765700 |
| C | -2.75804000 | -0.61787300 | -2.00229200 |
| C | -1.58625200 | 0.15954800 | -2.33203200 |
| C | -0.46876800 | -0.72500700 | -2.38184200 |
| C | -0.91392400 | -1.99863700 | -1.96451400 |
| Rh | -1.30714000 | -0.59051900 | -0.28441400 |
| C | -2.33289000 | 1.34960600 | 1.84047700 |
| O | -2.61712200 | 1.52684800 | 2.99287100 |
| C | 0.51424700 | 1.73584200 | 0.36716500 |
| C | 0.36747100 | 0.27133300 | 0.66775500 |
| C | -0.12022700 | -3.23772000 | -1.85477400 |
| H | -0.36873800 | -3.93019100 | -2.67672000 |
| H | 0.96058300 | -3.04673700 | -1.90155100 |
| H | -0.33004900 | -3.77354700 | -0.91529800 |
| C | -3.17171900 | -3.08816800 | -1.34778200 |
| H | -3.30531400 | -3.79233800 | -2.18659500 |
| H | -2.69304000 | -3.65714200 | -0.53445000 |
| H | -4.17080200 | -2.78641900 | -1.00628500 |
| C | -4.11915100 | -0.05927600 | -1.89813800 |
| H | -4.54954400 | 0.10142600 | -2.90059300 |
| H | -4.79964600 | -0.72067400 | -1.34533300 |
| H | -4.11672300 | 0.91940000 | -1.39232300 |
| C | -1.60153100 | 1.57082000 | -2.76365000 |
| H | -1.88808000 | 1.64438400 | -3.82732900 |
| H | -2.32905600 | 2.17022500 | -2.19433100 |
| H | -0.61535000 | 2.04551100 | -2.66008500 |
| C | 0.89010000 | -0.36744500 | -2.83231400 |
| H | 0.95217700 | -0.45004200 | -3.93077200 |
| H | 1.15738000 | 0.66868900 | -2.57751400 |
| H | 1.66147800 | -1.03333200 | -2.41954400 |
| O | -3.05658100 | -1.49971600 | 2.08238600 |
| H | 1.24108200 | 2.19216100 | 1.07342700 |
| H | 1.01264900 | 1.82805100 | -0.61605000 |
| C | 0.43620100 | -0.18619600 | 2.08607400 |
| O | -0.10545200 | 0.01412100 | 3.13037800 |
| O | 1.46984900 | -1.02358400 | 1.90171800 |

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|---|-------------|-------------|-------------|
| C | 1.60241000 | -0.62291200 | 0.50662300 |
| C | 2.94913300 | -0.01784000 | 0.25855000 |
| H | 1.44314400 | -1.52211600 | -0.11987000 |
| C | 4.06826600 | -1.03547800 | 0.34964400 |
| H | 2.95011200 | 0.44686800 | -0.74488600 |
| H | 3.12361700 | 0.79986600 | 0.98301000 |
| H | 4.04940000 | -1.50970100 | 1.34698400 |
| H | 3.88137500 | -1.84050000 | -0.38572000 |
| C | 5.40819200 | -0.42303500 | 0.10560300 |
| C | 6.18943700 | 0.03054900 | 1.16286900 |
| C | 5.87960800 | -0.24243700 | -1.19092900 |
| C | 7.40921500 | 0.64466000 | 0.93290000 |
| H | 5.83120000 | -0.10604100 | 2.19000600 |
| C | 7.09818300 | 0.37104000 | -1.42518100 |
| H | 5.27621100 | -0.59904400 | -2.03459800 |
| C | 7.86785400 | 0.81688800 | -0.36268700 |
| H | 8.01187100 | 0.99076600 | 1.77846900 |
| H | 7.45541700 | 0.49844200 | -2.45187800 |
| H | 8.83303400 | 1.29837200 | -0.54608000 |
| C | -2.03728100 | -2.17457100 | 2.02059300 |
| O | -1.09931800 | -2.02865400 | 1.17244200 |
| C | -1.78095000 | -3.26038300 | 3.02117800 |
| H | -1.31920300 | -4.13805700 | 2.54928700 |
| H | -1.06579300 | -2.87989800 | 3.76745600 |
| H | -2.70125400 | -3.55135600 | 3.54203600 |

INT-3a

| | | | |
|----|-------------|-------------|-------------|
| N | -1.98161500 | 1.09603300 | -0.43149900 |
| C | -1.09765300 | 3.33128500 | -0.31309300 |
| C | -1.72645400 | 4.56938100 | -0.28483900 |
| H | -2.68007000 | 4.65753400 | 0.24592900 |
| C | -1.18912700 | 5.66330600 | -0.93691400 |
| H | -1.71198500 | 6.62377900 | -0.91612600 |
| C | 0.00106400 | 5.53134400 | -1.63428800 |
| H | 0.42962900 | 6.38665300 | -2.16392900 |
| C | 0.65291700 | 4.31451200 | -1.65304400 |
| H | 1.60947100 | 4.21393300 | -2.17671300 |
| C | 0.13512800 | 3.21005600 | -0.97562100 |
| C | -2.59088500 | -3.04092400 | -0.23834100 |
| C | -3.50431200 | -2.27180300 | -1.03720700 |
| C | -2.75332900 | -1.50806900 | -1.97111700 |
| C | -1.36067800 | -1.77515100 | -1.73763300 |
| C | -1.28142700 | -2.75681300 | -0.69560700 |
| Rh | -2.21213600 | -0.90610400 | 0.02067300 |

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|---|-------------|-------------|-------------|
| C | -1.83467200 | 2.17302100 | 0.31598200 |
| O | -2.31167000 | 2.33320300 | 1.44042500 |
| C | 0.93546100 | 1.98851600 | -0.95625800 |
| C | 1.22685700 | 1.27528800 | 0.12831600 |
| C | -0.05251900 | -3.34445500 | -0.13122500 |
| H | -0.06356000 | -4.43769500 | -0.27004200 |
| H | 0.85501700 | -2.95810800 | -0.61226500 |
| H | 0.02662900 | -3.16501700 | 0.95252500 |
| C | -2.95692000 | -3.99596700 | 0.82448000 |
| H | -3.19209500 | -4.98737000 | 0.40128700 |
| H | -2.13769600 | -4.13359400 | 1.54451400 |
| H | -3.84419400 | -3.66471900 | 1.38333700 |
| C | -4.96790700 | -2.28494000 | -0.87763300 |
| H | -5.39140100 | -3.18645300 | -1.35134900 |
| H | -5.25736600 | -2.31548800 | 0.18326200 |
| H | -5.44689000 | -1.41129900 | -1.33807500 |
| C | -3.29067200 | -0.61213700 | -3.01139200 |
| H | -3.40320400 | -1.15911100 | -3.96226700 |
| H | -4.27663200 | -0.20923800 | -2.74378900 |
| H | -2.62181800 | 0.23811400 | -3.20837500 |
| C | -0.23745400 | -1.23027900 | -2.52506500 |
| H | -0.06856400 | -1.83245900 | -3.43383900 |
| H | -0.43439900 | -0.19965700 | -2.85746400 |
| H | 0.70385400 | -1.22374600 | -1.95595500 |
| O | -3.28434800 | -0.41758900 | 1.82477900 |
| H | 1.37885900 | 1.66737800 | -1.91045200 |
| H | -1.53014800 | 1.20814000 | -1.33567600 |
| C | 1.08880500 | 1.43949800 | 1.58689200 |
| O | 0.60335900 | 2.17991400 | 2.38132800 |
| O | 1.86266400 | 0.36827900 | 1.85930600 |
| C | 2.05110500 | 0.06672000 | 0.43773900 |
| C | 3.49209000 | 0.04593000 | 0.04703400 |
| H | 1.54772600 | -0.89641000 | 0.22458100 |
| C | 4.25672600 | -1.10675100 | 0.66431000 |
| H | 3.53495300 | -0.01811200 | -1.05643200 |
| H | 3.95574500 | 1.01095300 | 0.32285600 |
| H | 4.19541000 | -1.03273200 | 1.76457900 |
| H | 3.76449900 | -2.05621000 | 0.38415300 |
| C | 5.68720700 | -1.12796400 | 0.23582400 |
| C | 6.65536400 | -0.43242800 | 0.95224100 |
| C | 6.07346700 | -1.79965100 | -0.91935700 |
| C | 7.97357500 | -0.41099100 | 0.52909900 |
| H | 6.36605200 | 0.09996200 | 1.86602100 |
| C | 7.39063600 | -1.78118400 | -1.34549800 |

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|---|-------------|-------------|-------------|
| H | 5.32162800 | -2.35529600 | -1.49256700 |
| C | 8.34573800 | -1.08583300 | -0.62198400 |
| H | 8.72232000 | 0.13766100 | 1.10905600 |
| H | 7.67662900 | -2.32140700 | -2.25346000 |
| H | 9.38767900 | -1.07346200 | -0.95518700 |
| C | -2.20078400 | -0.22196900 | 2.42290400 |
| O | -1.13400500 | -0.48271800 | 1.81443300 |
| C | -2.16459100 | 0.26475500 | 3.81986300 |
| H | -1.93972100 | -0.57646200 | 4.49234400 |
| H | -1.36199600 | 1.00471700 | 3.94026200 |
| H | -3.12547000 | 0.70114700 | 4.11587200 |

INT-3b

| | | | |
|----|-------------|-------------|-------------|
| N | -1.95099600 | 0.13738700 | -0.86848500 |
| C | -2.72318600 | 2.41673300 | -0.70943200 |
| C | -3.81022600 | 3.14347400 | -1.18663000 |
| H | -4.72243500 | 2.60179000 | -1.45324800 |
| C | -3.74597800 | 4.51610600 | -1.30405700 |
| H | -4.60691300 | 5.07774400 | -1.67618500 |
| C | -2.58264800 | 5.17099600 | -0.93474500 |
| H | -2.51450300 | 6.25977300 | -1.01449800 |
| C | -1.50108900 | 4.45116000 | -0.46157400 |
| H | -0.58839000 | 4.98066900 | -0.16721100 |
| C | -1.53679200 | 3.06570600 | -0.35049200 |
| C | -0.39567200 | -3.16053600 | -0.55095700 |
| C | -1.01252600 | -2.53744800 | -1.68176200 |
| C | -0.05017100 | -1.66121900 | -2.26697500 |
| C | 1.16704800 | -1.79394400 | -1.53172700 |
| C | 0.93670200 | -2.67321000 | -0.43361100 |
| Rh | -0.57266900 | -0.94558500 | -0.18056200 |
| C | -2.94351100 | 0.95885400 | -0.57616900 |
| O | -4.06466800 | 0.47473400 | -0.42718500 |
| C | -0.27760000 | 2.37888200 | 0.07120700 |
| C | -0.29316000 | 1.20757800 | 0.99643700 |
| C | 1.90989500 | -3.18662300 | 0.54992000 |
| H | 1.92655900 | -4.28811900 | 0.52333700 |
| H | 2.92912800 | -2.83602100 | 0.34624400 |
| H | 1.64792500 | -2.89981500 | 1.58086100 |
| C | -0.97294200 | -4.20520600 | 0.30285900 |
| H | -0.55929200 | -5.17825400 | -0.01425700 |
| H | -0.69013400 | -4.07354400 | 1.35769600 |
| H | -2.06439800 | -4.26533000 | 0.22543600 |
| C | -2.35750800 | -2.82491400 | -2.20040800 |
| H | -2.31146700 | -3.71200900 | -2.85435000 |

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|---|-------------|-------------|-------------|
| H | -3.07004300 | -3.04661000 | -1.39504000 |
| H | -2.75458800 | -1.99421800 | -2.79742300 |
| C | -0.24383400 | -0.87548500 | -3.49503000 |
| H | -0.05667100 | -1.50761600 | -4.37910900 |
| H | -1.27259500 | -0.49856600 | -3.57482500 |
| H | 0.44194700 | -0.01945500 | -3.54855100 |
| C | 2.45624100 | -1.25244200 | -1.96966900 |
| H | 2.83639700 | -1.90864700 | -2.77243400 |
| H | 2.37259500 | -0.24943900 | -2.41072500 |
| H | 3.21307600 | -1.23974200 | -1.17738300 |
| O | -3.18811000 | -2.00211100 | 1.15881800 |
| H | 0.35620000 | 3.13729600 | 0.57592500 |
| H | 0.30139400 | 2.11244300 | -0.83364700 |
| C | -1.30536000 | 1.16881100 | 2.15103800 |
| O | -2.50643800 | 1.21701200 | 1.88814600 |
| O | -0.76002000 | 1.17602600 | 3.25884000 |
| C | 0.86988900 | 0.46560800 | 1.11036300 |
| C | 2.17148200 | 0.91581600 | 0.54491700 |
| H | 0.91520100 | -0.22126000 | 1.96761400 |
| C | 3.36456500 | 0.25904300 | 1.21026300 |
| H | 2.21984900 | 0.81620600 | -0.55297200 |
| H | 2.23694600 | 2.01114500 | 0.70749900 |
| H | 3.30780400 | 0.46388400 | 2.29565600 |
| H | 3.30270700 | -0.83676400 | 1.10788400 |
| C | 4.67520000 | 0.73742400 | 0.67300700 |
| C | 5.05525700 | 2.07095900 | 0.80384600 |
| C | 5.54443600 | -0.13286800 | 0.02465700 |
| C | 6.25995400 | 2.51985200 | 0.29256400 |
| H | 4.39533800 | 2.77203400 | 1.32845000 |
| C | 6.75257200 | 0.31197600 | -0.48714100 |
| H | 5.26914200 | -1.19050300 | -0.07058900 |
| C | 7.11276500 | 1.64206700 | -0.35823800 |
| H | 6.54083300 | 3.57126600 | 0.40848500 |
| H | 7.42157900 | -0.39228000 | -0.99129500 |
| H | 8.06594000 | 1.99720800 | -0.76095900 |
| C | -2.31813900 | -1.78809500 | 1.97924900 |
| O | -1.11895700 | -1.41074200 | 1.71687300 |
| C | -2.55763200 | -1.92379000 | 3.45136600 |
| H | -1.70923200 | -2.40791700 | 3.95313900 |
| H | -2.65443000 | -0.91453600 | 3.88146200 |
| H | -3.48103300 | -2.48211600 | 3.64731600 |

INT-3c

| | | | |
|---|-------------|------------|-------------|
| N | -0.90129000 | 0.82354300 | -0.19427000 |
|---|-------------|------------|-------------|

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|----|-------------|-------------|-------------|
| C | -1.61938200 | 3.07103400 | -0.78024800 |
| C | -2.68211600 | 3.92894600 | -1.03128900 |
| H | -3.68798400 | 3.51193900 | -1.13545500 |
| C | -2.46523400 | 5.28925300 | -1.14333800 |
| H | -3.30399900 | 5.96490400 | -1.33440500 |
| C | -1.18026800 | 5.79500900 | -1.01523100 |
| H | -1.00452800 | 6.87140500 | -1.10353200 |
| C | -0.11681000 | 4.94325200 | -0.76999500 |
| H | 0.89814600 | 5.34213500 | -0.66810600 |
| C | -0.33114600 | 3.57950600 | -0.64568200 |
| C | -2.20003000 | -3.17509900 | -0.35832400 |
| C | -2.57076000 | -2.27673000 | -1.42632300 |
| C | -1.38720400 | -1.75848900 | -2.00720000 |
| C | -0.27275500 | -2.29928100 | -1.28749900 |
| C | -0.78682800 | -3.20152300 | -0.29781500 |
| Rh | -1.47884500 | -1.17500200 | 0.08595800 |
| C | -1.85413300 | 1.60433500 | -0.69471100 |
| O | -2.92863600 | 1.15213700 | -1.10328000 |
| C | 0.76571800 | 2.60655800 | -0.41038700 |
| C | 0.26006100 | 1.41553900 | 0.37826200 |
| C | 0.04214000 | -3.93604900 | 0.67271400 |
| H | 0.47885100 | -4.83228800 | 0.20193900 |
| H | 0.88306600 | -3.32071200 | 1.02924000 |
| H | -0.53474600 | -4.26516700 | 1.54696000 |
| C | -3.15348200 | -3.94692600 | 0.46056500 |
| H | -3.49723600 | -4.84404500 | -0.08164700 |
| H | -2.70714400 | -4.28577700 | 1.40502700 |
| H | -4.04910400 | -3.35626500 | 0.70398900 |
| C | -3.96335900 | -1.98257200 | -1.80379500 |
| H | -4.42601900 | -2.87557600 | -2.25655700 |
| H | -4.57012500 | -1.72351000 | -0.92215200 |
| H | -4.04125200 | -1.15920200 | -2.52417900 |
| C | -1.26707900 | -0.84254800 | -3.15678000 |
| H | -0.88742900 | -1.39425000 | -4.03294400 |
| H | -2.22483300 | -0.38714600 | -3.43596700 |
| H | -0.55119200 | -0.03119400 | -2.95374900 |
| C | 1.14643000 | -2.10207200 | -1.63776300 |
| H | 1.44345300 | -2.80527400 | -2.43505600 |
| H | 1.33465900 | -1.08658100 | -2.01722000 |
| H | 1.81313100 | -2.28139200 | -0.78145600 |
| O | -2.93600700 | -0.39829900 | 1.48057800 |
| H | 1.61077700 | 3.09344900 | 0.10273200 |
| H | 1.15512900 | 2.22873900 | -1.37754500 |
| C | 0.20365500 | 1.71026000 | 1.87955900 |

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|---|-------------|-------------|-------------|
| O | -0.48245800 | 2.31575600 | 2.63907100 |
| O | 1.28127400 | 0.98107700 | 2.17898300 |
| C | 1.38025500 | 0.45185300 | 0.81870900 |
| C | 2.77075300 | 0.54589700 | 0.28589100 |
| H | 1.02269900 | -0.59381000 | 0.83567700 |
| C | 3.70878400 | -0.44286500 | 0.95121800 |
| H | 2.73441500 | 0.35227800 | -0.80219900 |
| H | 3.16513500 | 1.57022400 | 0.40700600 |
| H | 3.79376100 | -0.20206300 | 2.02553100 |
| H | 3.26435700 | -1.45489200 | 0.89211000 |
| C | 5.06185300 | -0.45046800 | 0.31965700 |
| C | 6.11387000 | 0.28098200 | 0.85825300 |
| C | 5.28079000 | -1.15696600 | -0.85916200 |
| C | 7.35295100 | 0.30357000 | 0.23922200 |
| H | 5.95621200 | 0.84172400 | 1.78693900 |
| C | 6.51699000 | -1.13781800 | -1.48061200 |
| H | 4.45822600 | -1.74049000 | -1.29382600 |
| C | 7.55851200 | -0.40613400 | -0.93198200 |
| H | 8.17092900 | 0.88154800 | 0.68046100 |
| H | 6.67210200 | -1.70549400 | -2.40335600 |
| H | 8.53777700 | -0.39214000 | -1.41961200 |
| C | -2.09457800 | -0.44844700 | 2.40408100 |
| O | -0.95527700 | -0.90467700 | 2.13403700 |
| C | -2.43098000 | -0.00550300 | 3.77539500 |
| H | -3.02402600 | -0.79038400 | 4.26805200 |
| H | -1.52778400 | 0.17188300 | 4.37073100 |
| H | -3.04923100 | 0.90070100 | 3.74692700 |

INT-3d

| | | | |
|---|-------------|-------------|-------------|
| N | -2.15316500 | 0.96770400 | 0.98620000 |
| C | -1.90044800 | 2.31065200 | 0.60282600 |
| C | -2.96194100 | 3.20658200 | 0.57259500 |
| H | -3.95668000 | 2.86123300 | 0.87335000 |
| C | -2.75510600 | 4.50728700 | 0.16060000 |
| H | -3.59171500 | 5.21059800 | 0.13805800 |
| C | -1.48436700 | 4.90439400 | -0.22448200 |
| H | -1.30372000 | 5.93006900 | -0.55741000 |
| C | -0.44335100 | 3.99876100 | -0.19051900 |
| H | 0.55975700 | 4.31535400 | -0.49905100 |
| C | -0.61600200 | 2.67752000 | 0.21699200 |
| C | -2.39552500 | -1.80509400 | -1.79682900 |
| C | -2.74064300 | -0.46984000 | -2.00693400 |
| C | -1.53631500 | 0.27668700 | -2.31812300 |
| C | -0.45672700 | -0.64437700 | -2.35802200 |

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|----|-------------|-------------|-------------|
| C | -0.95831200 | -1.90968300 | -1.94097600 |
| Rh | -1.25501600 | -0.52974400 | -0.30653200 |
| C | -2.68914800 | 0.72557300 | 2.05869700 |
| O | -3.19024300 | 0.48577700 | 3.06456700 |
| C | 0.57984800 | 1.77414900 | 0.17851000 |
| C | 0.43489600 | 0.33805800 | 0.59434100 |
| C | -0.20324200 | -3.17263300 | -1.83641200 |
| H | -0.38025700 | -3.80621100 | -2.72256600 |
| H | 0.88055400 | -3.00596300 | -1.76397100 |
| H | -0.51429700 | -3.76005400 | -0.95855000 |
| C | -3.28073900 | -2.94934500 | -1.50342900 |
| H | -3.40959400 | -3.57634900 | -2.40269700 |
| H | -2.86498900 | -3.60436000 | -0.72188800 |
| H | -4.28079300 | -2.63458500 | -1.17675600 |
| C | -4.07640900 | 0.14646500 | -1.90313200 |
| H | -4.46107100 | 0.41394900 | -2.90181700 |
| H | -4.80992900 | -0.51932400 | -1.42930700 |
| H | -4.04440600 | 1.08342900 | -1.32242300 |
| C | -1.51790500 | 1.67401800 | -2.79787600 |
| H | -1.76214700 | 1.71184400 | -3.87429600 |
| H | -2.25920500 | 2.30287700 | -2.28106200 |
| H | -0.53237900 | 2.14675700 | -2.67520300 |
| C | 0.92037900 | -0.36973200 | -2.80961300 |
| H | 1.00159000 | -0.57380900 | -3.89103800 |
| H | 1.21557300 | 0.67894900 | -2.66368600 |
| H | 1.66330400 | -1.01088100 | -2.31298500 |
| O | -3.26088300 | -1.88923200 | 1.56825800 |
| H | 1.37530800 | 2.27346400 | 0.77211800 |
| H | 0.96779700 | 1.79591300 | -0.85750000 |
| C | 0.45238500 | 0.02169900 | 2.04618300 |
| O | -0.12983600 | 0.32114900 | 3.04817700 |
| O | 1.48359500 | -0.83869400 | 1.98172000 |
| C | 1.66142100 | -0.57464000 | 0.55557400 |
| C | 3.02193700 | -0.01117300 | 0.28573300 |
| H | 1.50977800 | -1.52966400 | 0.01365900 |
| C | 4.12421200 | -1.03224700 | 0.48345100 |
| H | 3.04559500 | 0.36783000 | -0.75328400 |
| H | 3.19512600 | 0.86254000 | 0.94171700 |
| H | 4.08417100 | -1.41197300 | 1.52019700 |
| H | 3.93210700 | -1.89861400 | -0.17660500 |
| C | 5.47912600 | -0.47165800 | 0.20121400 |
| C | 6.20504400 | 0.17424200 | 1.19678000 |
| C | 6.02379200 | -0.53807200 | -1.07682100 |
| C | 7.44147600 | 0.73457700 | 0.92448900 |

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|---|-------------|-------------|-------------|
| H | 5.79076200 | 0.23154200 | 2.21031800 |
| C | 7.26042700 | 0.02004800 | -1.35318300 |
| H | 5.46500800 | -1.04799800 | -1.87071200 |
| C | 7.97399800 | 0.65886600 | -0.35231100 |
| H | 7.99982400 | 1.23391300 | 1.72250300 |
| H | 7.67514200 | -0.04931900 | -2.36365200 |
| H | 8.95289300 | 1.09746700 | -0.56776000 |
| C | -2.13062800 | -2.28172800 | 1.83609900 |
| O | -1.06882100 | -1.89042800 | 1.25761000 |
| C | -1.89856800 | -3.26017300 | 2.94654900 |
| H | -1.18315400 | -4.03899900 | 2.64847300 |
| H | -1.44843300 | -2.72660700 | 3.79836200 |
| H | -2.83550900 | -3.72214300 | 3.28154500 |

INT-4b

| | | | |
|----|-------------|-------------|-------------|
| N | -1.72707300 | 0.89033700 | -1.29564200 |
| C | -0.68308900 | 3.09943400 | -0.68239100 |
| C | -1.02643800 | 4.45100800 | -0.62576500 |
| H | -2.06294100 | 4.73700600 | -0.82513300 |
| C | -0.08327200 | 5.40824600 | -0.32386000 |
| H | -0.36488700 | 6.46360500 | -0.28358200 |
| C | 1.22382600 | 5.01776800 | -0.07449100 |
| H | 1.98529800 | 5.76587700 | 0.16497000 |
| C | 1.56928500 | 3.68187900 | -0.13232400 |
| H | 2.60375400 | 3.37692900 | 0.06542700 |
| C | 0.63442900 | 2.70009800 | -0.44099800 |
| C | -2.72866000 | -2.62987100 | 0.13715700 |
| C | -2.59083600 | -2.26953100 | -1.24957200 |
| C | -1.20524700 | -2.06290700 | -1.50545300 |
| C | -0.49887500 | -2.24783500 | -0.28417300 |
| C | -1.45538100 | -2.57507800 | 0.74287500 |
| Rh | -1.90185400 | -0.51335700 | -0.05851600 |
| C | -1.80268500 | 2.19386700 | -0.99070300 |
| O | -2.95878700 | 2.60578900 | -1.10903700 |
| C | 1.10096400 | 1.27758000 | -0.46078900 |
| C | 1.33321600 | 0.74201200 | 0.91506000 |
| C | -1.12476800 | -2.87832000 | 2.14658900 |
| H | -0.76012000 | -3.91466900 | 2.24169800 |
| H | -0.33186100 | -2.22042400 | 2.53183700 |
| H | -1.99765700 | -2.77343000 | 2.80408000 |
| C | -3.99325400 | -2.95271500 | 0.81343100 |
| H | -4.12885600 | -4.04708700 | 0.82526200 |
| H | -4.00043500 | -2.61489400 | 1.85858300 |
| H | -4.86257300 | -2.52264900 | 0.29912700 |

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|---|-------------|-------------|-------------|
| C | -3.63564900 | -2.29777000 | -2.28712900 |
| H | -3.50900900 | -3.20368900 | -2.90391900 |
| H | -4.64785000 | -2.31628400 | -1.86728700 |
| H | -3.56044300 | -1.43429400 | -2.96312800 |
| C | -0.62001800 | -1.75375800 | -2.81885400 |
| H | -0.46831600 | -2.68720600 | -3.38580000 |
| H | -1.28272700 | -1.11376600 | -3.41822600 |
| H | 0.35653900 | -1.25831500 | -2.73092500 |
| C | 0.96250600 | -2.31415500 | -0.13934200 |
| H | 1.29157300 | -3.32324900 | -0.44396100 |
| H | 1.48683600 | -1.59749100 | -0.78733900 |
| H | 1.28852400 | -2.16168300 | 0.89704600 |
| O | -4.89008400 | 0.11969500 | -0.67677100 |
| H | 2.03537400 | 1.23611500 | -1.04241300 |
| H | 0.38927200 | 0.63908800 | -1.00897300 |
| C | 0.15838200 | 0.60625800 | 1.83017900 |
| O | 0.32467300 | 0.43593600 | 3.02930600 |
| O | -1.01329100 | 0.74769300 | 1.32794700 |
| C | 2.53308700 | 0.39564600 | 1.39983600 |
| C | 3.85301000 | 0.39752300 | 0.73859800 |
| H | 2.53901700 | 0.02459500 | 2.43528800 |
| C | 4.50965800 | -0.97688500 | 0.78675400 |
| H | 3.80789900 | 0.75179100 | -0.30540600 |
| H | 4.51233600 | 1.11211900 | 1.27111200 |
| H | 4.54112600 | -1.32310300 | 1.83563700 |
| H | 3.87876000 | -1.69927800 | 0.23699800 |
| C | 5.88712800 | -0.96770200 | 0.21061400 |
| C | 6.98486500 | -0.63994100 | 0.99987200 |
| C | 6.09758000 | -1.23733600 | -1.13733800 |
| C | 8.25804800 | -0.58779000 | 0.45904400 |
| H | 6.83483100 | -0.42839100 | 2.06525100 |
| C | 7.36943600 | -1.18593100 | -1.68233700 |
| H | 5.24173200 | -1.50011200 | -1.77046100 |
| C | 8.45448000 | -0.86061600 | -0.88515100 |
| H | 9.11066200 | -0.33554200 | 1.09725800 |
| H | 7.51599900 | -1.40725700 | -2.74412900 |
| H | 9.46079500 | -0.82390900 | -1.31291100 |
| C | -4.63830400 | 0.28506600 | 0.50145500 |
| O | -3.49026700 | 0.10890100 | 1.05001800 |
| C | -5.69372100 | 0.68687900 | 1.48529700 |
| H | -6.09987200 | -0.22527200 | 1.95008600 |
| H | -5.29000800 | 1.31295700 | 2.29096300 |
| H | -6.51603900 | 1.20579400 | 0.97743800 |

TS-3

| | | | |
|----|-------------|-------------|-------------|
| N | 1.53502400 | 1.29183800 | -0.09233700 |
| C | 2.71289000 | 0.65879500 | 1.73088900 |
| C | 3.89951300 | 0.42506000 | 2.42007300 |
| H | 4.74686900 | 1.10001000 | 2.25607900 |
| C | 4.01882600 | -0.67478700 | 3.23915000 |
| H | 4.96015500 | -0.87615300 | 3.75742800 |
| C | 2.93722200 | -1.55442400 | 3.38566700 |
| H | 3.04510200 | -2.44402700 | 4.01442100 |
| C | 1.73648200 | -1.29674800 | 2.77347300 |
| H | 0.87632900 | -1.95553900 | 2.95057900 |
| C | 1.56939500 | -0.17839600 | 1.92895700 |
| C | 0.71488200 | -1.41006100 | -2.20771900 |
| C | 1.91488100 | -1.96355400 | -1.58894600 |
| C | 1.50232800 | -2.79251400 | -0.53627300 |
| C | 0.06938100 | -2.70943200 | -0.44438500 |
| C | -0.40727600 | -1.95707700 | -1.56008500 |
| Rh | 0.82453100 | -0.67609200 | -0.12478400 |
| C | 2.60459800 | 1.66488000 | 0.70515500 |
| O | 3.27541300 | 2.67237100 | 0.52493900 |
| C | 0.15021500 | 0.46828700 | 1.94640500 |
| C | -0.10063600 | 1.40074600 | 0.82566800 |
| C | -1.81348400 | -1.72592200 | -1.94778300 |
| H | -2.08658300 | -2.33391300 | -2.82900100 |
| H | -2.51747900 | -1.99497300 | -1.14613500 |
| H | -2.00373700 | -0.67514100 | -2.22808200 |
| C | 0.65023000 | -0.55215800 | -3.41174100 |
| H | 0.23125100 | -1.11046000 | -4.26670200 |
| H | -0.00765700 | 0.32186200 | -3.25960200 |
| H | 1.63510200 | -0.17782000 | -3.72039100 |
| C | 3.31386300 | -1.79913300 | -2.03670900 |
| H | 3.72665100 | -2.76216000 | -2.38408900 |
| H | 3.41143600 | -1.08519300 | -2.86397000 |
| H | 3.97125500 | -1.44995300 | -1.22255000 |
| C | 2.39644700 | -3.58845000 | 0.32575100 |
| H | 2.63581200 | -4.55744200 | -0.14664500 |
| H | 3.35606600 | -3.07735700 | 0.50896800 |
| H | 1.94752500 | -3.81396700 | 1.30403500 |
| C | -0.77732200 | -3.43993000 | 0.52324500 |
| H | -1.08004000 | -4.42727800 | 0.13215700 |
| H | -0.25554600 | -3.61857700 | 1.47498300 |
| H | -1.70448000 | -2.89190400 | 0.75367500 |
| O | 1.28650700 | 2.22838900 | -1.10157300 |
| H | 0.08339400 | 0.99932300 | 2.91116500 |

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|---|-------------|-------------|-------------|
| H | -0.62361600 | -0.32268800 | 1.97566600 |
| C | -0.23713600 | 2.87383400 | 0.97226600 |
| O | 0.30544500 | 3.75434200 | 1.56117100 |
| O | -1.31168300 | 2.96507400 | 0.17246100 |
| C | -1.32928100 | 1.51619500 | -0.05141500 |
| C | -2.60003300 | 0.89118000 | 0.42334600 |
| H | -1.15231200 | 1.33809000 | -1.13072000 |
| C | -3.79283000 | 1.28003500 | -0.42730000 |
| H | -2.46189300 | -0.20642900 | 0.40643500 |
| H | -2.77065800 | 1.16825800 | 1.48024900 |
| H | -3.94086100 | 2.37264800 | -0.35865500 |
| H | -3.56955900 | 1.05874600 | -1.48694800 |
| C | -5.03798800 | 0.56598100 | -0.01722400 |
| C | -5.79168500 | 1.01062200 | 1.06454000 |
| C | -5.44553700 | -0.58703000 | -0.67962100 |
| C | -6.92156500 | 0.32276600 | 1.47210300 |
| H | -5.48705000 | 1.92190000 | 1.59277100 |
| C | -6.57642000 | -1.27697800 | -0.27572800 |
| H | -4.86686800 | -0.94161400 | -1.54200100 |
| C | -7.31762200 | -0.82431900 | 0.80316300 |
| H | -7.50523900 | 0.69049300 | 2.32177600 |
| H | -6.88609700 | -2.17752300 | -0.81507800 |
| H | -8.21320000 | -1.36588000 | 1.12180400 |
| C | 2.17049500 | 2.15678000 | -2.10693300 |
| O | 3.09483600 | 1.40151100 | -2.11347900 |
| C | 1.82072200 | 3.14279800 | -3.15076000 |
| H | 0.74091400 | 3.32958100 | -3.19393500 |
| H | 2.31803500 | 4.09537700 | -2.91663500 |
| H | 2.19244100 | 2.79521000 | -4.12096300 |

INT-5

| | | | |
|---|-------------|-------------|-------------|
| N | 0.93168800 | 1.56984600 | 0.20989800 |
| C | 2.22851200 | 0.37182000 | 1.71883200 |
| C | 3.41089500 | -0.13638500 | 2.32023900 |
| H | 4.36214400 | 0.37336000 | 2.13569300 |
| C | 3.33748200 | -1.24667200 | 3.10020800 |
| H | 4.24316300 | -1.66240400 | 3.55117500 |
| C | 2.08548800 | -1.87169900 | 3.34506600 |
| H | 2.05089100 | -2.77041300 | 3.96884700 |
| C | 0.93103400 | -1.34472500 | 2.85416100 |
| H | -0.03516600 | -1.79289400 | 3.11846100 |
| C | 0.92797300 | -0.18888400 | 2.01758000 |
| C | 1.11384600 | -1.18077500 | -2.23277800 |
| C | 2.38763400 | -1.62726700 | -1.81595600 |

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|----|-------------|-------------|-------------|
| C | 2.17367400 | -2.47080900 | -0.69088000 |
| C | 0.75427500 | -2.65530400 | -0.51303600 |
| C | 0.09745900 | -1.85272200 | -1.45861100 |
| Rh | 1.31101100 | -0.53732500 | -0.08132800 |
| C | 2.20564200 | 1.56430200 | 0.92820700 |
| O | 3.05742100 | 2.39154700 | 0.69904700 |
| C | -0.21513500 | 0.77929100 | 2.15932300 |
| C | -0.30691600 | 1.69402300 | 0.96420100 |
| C | -1.34837000 | -1.82264500 | -1.76799500 |
| H | -1.58873800 | -2.48148900 | -2.62380200 |
| H | -1.96342000 | -2.16479600 | -0.92170700 |
| H | -1.69554800 | -0.81375500 | -2.04640000 |
| C | 0.78660800 | -0.30613800 | -3.38019100 |
| H | 0.28059900 | -0.88763100 | -4.17088300 |
| H | 0.08662200 | 0.49931300 | -3.09619800 |
| H | 1.67128400 | 0.16466000 | -3.82739200 |
| C | 3.71134300 | -1.27059000 | -2.37138700 |
| H | 4.20106100 | -2.14224900 | -2.84133300 |
| H | 3.64104000 | -0.48863400 | -3.14019900 |
| H | 4.40577800 | -0.90333100 | -1.59672600 |
| C | 3.23703400 | -3.17802900 | 0.05124900 |
| H | 3.52493100 | -4.11165200 | -0.46427700 |
| H | 4.15089400 | -2.56895000 | 0.13998600 |
| H | 2.92459100 | -3.45888100 | 1.06808800 |
| C | 0.12479800 | -3.59249500 | 0.43959100 |
| H | 0.03325800 | -4.60022300 | -0.00244000 |
| H | 0.71193200 | -3.70496600 | 1.36349700 |
| H | -0.88809800 | -3.27189700 | 0.72886800 |
| O | 0.87504200 | 2.64927100 | -0.69021300 |
| H | -0.07285000 | 1.39630900 | 3.06879500 |
| H | -1.16110300 | 0.23522800 | 2.30014000 |
| C | -0.73860100 | 3.14672000 | 1.18771400 |
| O | -0.36718200 | 4.08542200 | 1.80817300 |
| O | -1.78806900 | 3.07019200 | 0.37347200 |
| C | -1.53380000 | 1.66713100 | 0.03633900 |
| C | -2.70469500 | 0.80778000 | 0.36836800 |
| H | -1.26208600 | 1.60465800 | -1.03408000 |
| C | -3.85394900 | 0.99566300 | -0.60185500 |
| H | -2.36689700 | -0.24513400 | 0.35805600 |
| H | -3.03938600 | 1.01821800 | 1.40093500 |
| H | -4.19492000 | 2.04567100 | -0.55903300 |
| H | -3.48810700 | 0.82585500 | -1.63125200 |
| C | -4.99256000 | 0.07389200 | -0.31253000 |
| C | -5.93488200 | 0.39122500 | 0.66029600 |

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|---|-------------|-------------|-------------|
| C | -5.10716400 | -1.14461200 | -0.97349400 |
| C | -6.96428100 | -0.48321500 | 0.96327600 |
| H | -5.86057000 | 1.35068400 | 1.18574500 |
| C | -6.13630200 | -2.02175600 | -0.67378300 |
| H | -4.37752500 | -1.40345700 | -1.75132300 |
| C | -7.06786300 | -1.69384200 | 0.29724000 |
| H | -7.69969400 | -0.21349500 | 1.72760600 |
| H | -6.21431100 | -2.97275700 | -1.20979800 |
| H | -7.88360300 | -2.38369600 | 0.53283900 |
| C | 1.68698900 | 2.55933800 | -1.76295200 |
| O | 2.50884200 | 1.71085600 | -1.89805100 |
| C | 1.35761100 | 3.65366200 | -2.69880000 |
| H | 2.16635500 | 3.76997300 | -3.42677100 |
| H | 0.42959300 | 3.39635900 | -3.23156100 |
| H | 1.17947800 | 4.59713000 | -2.16836900 |

TS-4

| | | | |
|----|-------------|-------------|-------------|
| N | -2.36882200 | 0.92168300 | 0.15543100 |
| C | -1.22168900 | 2.87922100 | -0.68726200 |
| C | -1.36076400 | 4.24695700 | -0.91628700 |
| H | -2.28459200 | 4.72624100 | -0.58487000 |
| C | -0.38433800 | 4.98692800 | -1.55085800 |
| H | -0.53036100 | 6.05837500 | -1.71312600 |
| C | 0.76777400 | 4.36050500 | -1.99136500 |
| H | 1.54854400 | 4.92512200 | -2.50872800 |
| C | 0.92778000 | 3.00646500 | -1.77393300 |
| H | 1.83972300 | 2.50346800 | -2.11383600 |
| C | -0.03857700 | 2.25367500 | -1.11171300 |
| C | -2.38526700 | -2.46432700 | 0.23079400 |
| C | -2.64584100 | -2.17717200 | -1.15821900 |
| C | -1.43174200 | -2.36992200 | -1.86615100 |
| C | -0.40963100 | -2.68075100 | -0.91996500 |
| C | -1.02949400 | -2.80214200 | 0.37016000 |
| Rh | -1.19776500 | -0.65906200 | -0.47609900 |
| C | -2.42236400 | 2.23330800 | -0.07051900 |
| O | -3.40195500 | 2.92144900 | 0.21101800 |
| C | 0.32789500 | 0.84099800 | -0.86837500 |
| C | 0.46715400 | 0.34762400 | 0.45364700 |
| C | -0.40970300 | -3.26163300 | 1.63016200 |
| H | -0.92479100 | -4.16848300 | 1.98933400 |
| H | 0.64987100 | -3.52161200 | 1.50824900 |
| H | -0.49016000 | -2.51715200 | 2.43888600 |
| C | -3.38753000 | -2.55519900 | 1.31010700 |
| H | -3.59406200 | -3.61622800 | 1.53401100 |

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|---|-------------|-------------|-------------|
| H | -3.03477700 | -2.10222300 | 2.25001900 |
| H | -4.34452500 | -2.09271300 | 1.03812700 |
| C | -3.97527600 | -1.92869000 | -1.75207400 |
| H | -4.63161800 | -1.36524900 | -1.07523800 |
| H | -3.90568200 | -1.36720400 | -2.69428000 |
| H | -4.48165000 | -2.88308400 | -1.97799600 |
| C | -1.24537300 | -2.29593300 | -3.32962300 |
| H | -1.37532500 | -3.29661600 | -3.77562400 |
| H | -1.97311700 | -1.62743900 | -3.80917500 |
| H | -0.23744700 | -1.95196400 | -3.60117800 |
| C | 0.98912600 | -3.00852000 | -1.27059800 |
| H | 1.05070900 | -4.01447600 | -1.71965100 |
| H | 1.40212300 | -2.30560300 | -2.01050500 |
| H | 1.65507800 | -3.00586900 | -0.39635300 |
| O | -3.67066100 | 0.46321200 | 0.45194300 |
| H | 1.07883200 | 0.46282100 | -1.57871100 |
| H | -0.97468200 | 0.24005200 | -1.74746600 |
| C | 0.43308500 | 1.08868500 | 1.72411200 |
| O | -0.11996100 | 2.01147700 | 2.23620900 |
| O | 1.42120400 | 0.35695600 | 2.28445700 |
| C | 1.61841300 | -0.41873900 | 1.06341700 |
| C | 2.97976900 | -0.19120600 | 0.48872900 |
| H | 1.44477400 | -1.48021200 | 1.30206100 |
| C | 4.08618200 | -0.77650200 | 1.34163100 |
| H | 3.00456700 | -0.64126700 | -0.52226400 |
| H | 3.13124600 | 0.89678900 | 0.34832200 |
| H | 4.02087300 | -0.35346300 | 2.35981000 |
| H | 3.92339700 | -1.86564500 | 1.44139700 |
| C | 5.44051900 | -0.51185800 | 0.77102900 |
| C | 6.16676000 | 0.61026500 | 1.15515800 |
| C | 5.98255100 | -1.35250800 | -0.19585200 |
| C | 7.40172700 | 0.88451000 | 0.59225000 |
| H | 5.75254100 | 1.27998600 | 1.91793700 |
| C | 7.21689000 | -1.08173900 | -0.76125700 |
| H | 5.42378300 | -2.24392300 | -0.50544200 |
| C | 7.93104600 | 0.03883800 | -0.36869400 |
| H | 7.96085400 | 1.76949100 | 0.91167700 |
| H | 7.63015400 | -1.75791600 | -1.51615900 |
| H | 8.90821800 | 0.25208900 | -0.81215600 |
| C | -4.07566000 | 0.57709000 | 1.71609300 |
| O | -5.22609800 | 0.30571000 | 1.92769200 |
| C | -3.09084500 | 0.95877500 | 2.75055800 |
| H | -2.18665200 | 0.33669300 | 2.67792000 |
| H | -2.77445200 | 2.00321900 | 2.62558800 |

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|--------------|-------------|-------------|-------------|
| H | -3.55590300 | 0.83752900 | 3.73466800 |
| INT-6 | | | |
| N | 2.40958200 | 0.81878400 | -0.26673900 |
| C | 1.43246300 | 2.85971600 | 0.59089300 |
| C | 1.70202200 | 4.20212300 | 0.84761400 |
| H | 2.62949900 | 4.61976900 | 0.44971400 |
| C | 0.85227800 | 4.99223400 | 1.59512500 |
| H | 1.10059100 | 6.04134000 | 1.77741700 |
| C | -0.29966800 | 4.43977000 | 2.12535500 |
| H | -0.97810500 | 5.04203900 | 2.73630100 |
| C | -0.59439200 | 3.11502100 | 1.87206500 |
| H | -1.51502300 | 2.67658600 | 2.27215800 |
| C | 0.23723700 | 2.31202900 | 1.09227900 |
| C | 2.17694700 | -2.60569400 | -0.09683200 |
| C | 2.40810500 | -2.25084000 | 1.27700900 |
| C | 1.14100900 | -2.28932700 | 1.94975200 |
| C | 0.14408100 | -2.53672300 | 0.97369300 |
| C | 0.80169100 | -2.78253900 | -0.28833800 |
| Rh | 1.17893600 | -0.59894600 | 0.55421800 |
| C | 2.54126900 | 2.13675300 | -0.10771000 |
| O | 3.52924300 | 2.75734300 | -0.49140600 |
| C | -0.27954800 | 0.96498400 | 0.81340500 |
| C | -0.42420800 | 0.46725800 | -0.48532500 |
| C | 0.18727200 | -3.25574500 | -1.54680900 |
| H | 0.66343200 | -4.19868300 | -1.86350200 |
| H | -0.88720800 | -3.45774700 | -1.44235300 |
| H | 0.32073500 | -2.54742000 | -2.38137500 |
| C | 3.20942900 | -2.83826500 | -1.12421000 |
| H | 3.36223900 | -3.92336400 | -1.25754600 |
| H | 2.91775900 | -2.44406300 | -2.11078800 |
| H | 4.18252600 | -2.41092200 | -0.85058500 |
| C | 3.73504100 | -2.12240600 | 1.91428400 |
| H | 4.45708100 | -1.61350700 | 1.26051500 |
| H | 3.68593200 | -1.55996200 | 2.85650000 |
| H | 4.15259700 | -3.11761700 | 2.14445500 |
| C | 0.90440700 | -2.18457200 | 3.40457500 |
| H | 0.82679600 | -3.19301300 | 3.84562800 |
| H | 1.71730700 | -1.66004800 | 3.92408600 |
| H | -0.03491500 | -1.66156100 | 3.63407300 |
| C | -1.28954400 | -2.73305800 | 1.27719800 |
| H | -1.44703300 | -3.72746100 | 1.72894800 |
| H | -1.66345600 | -1.99423400 | 2.00209400 |
| H | -1.92684700 | -2.68556500 | 0.38313800 |

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|---|-------------|-------------|-------------|
| O | 3.67392600 | 0.26772300 | -0.56755500 |
| H | -1.02186200 | 0.61371200 | 1.54519800 |
| H | 1.54876800 | 0.15574100 | 1.85432800 |
| C | -0.31391800 | 1.18053800 | -1.77318200 |
| O | 0.29812500 | 2.06602100 | -2.28004200 |
| O | -1.33291900 | 0.50098500 | -2.33894800 |
| C | -1.58925700 | -0.25846000 | -1.11772100 |
| C | -2.95339700 | 0.01586000 | -0.57179300 |
| H | -1.44688800 | -1.32509900 | -1.34987100 |
| C | -4.05611600 | -0.61069200 | -1.39943200 |
| H | -2.99070500 | -0.37893000 | 0.46091500 |
| H | -3.09482600 | 1.11022900 | -0.48897300 |
| H | -4.01945900 | -0.20454100 | -2.42580800 |
| H | -3.86256100 | -1.69668000 | -1.48410500 |
| C | -5.40768500 | -0.38412700 | -0.80684700 |
| C | -6.18274700 | 0.70578900 | -1.18738800 |
| C | -5.89819600 | -1.23411700 | 0.17940800 |
| C | -7.41639800 | 0.93842800 | -0.60281300 |
| H | -5.80929200 | 1.38326100 | -1.96413400 |
| C | -7.13094900 | -1.00529300 | 0.76590700 |
| H | -5.29946900 | -2.10046100 | 0.48650000 |
| C | -7.89493400 | 0.08296300 | 0.37577200 |
| H | -8.01438800 | 1.79870500 | -0.91921800 |
| H | -7.50384500 | -1.68910000 | 1.53482900 |
| H | -8.87134000 | 0.26297500 | 0.83540800 |
| C | 4.00508700 | 0.18402800 | -1.85613900 |
| O | 5.12127300 | -0.18954000 | -2.09047700 |
| C | 2.98693300 | 0.50982500 | -2.87602500 |
| H | 2.04422500 | -0.02063300 | -2.67551300 |
| H | 2.75862600 | 1.58418700 | -2.86588100 |
| H | 3.37684700 | 0.23010600 | -3.86040400 |

TS-5

| | | | |
|---|-------------|------------|-------------|
| N | 2.40454000 | 0.98914000 | -0.34877200 |
| C | 1.22738800 | 2.93899000 | 0.45069800 |
| C | 1.40812000 | 4.29702000 | 0.70804400 |
| H | 2.23016700 | 4.80742300 | 0.20023400 |
| C | 0.60807100 | 4.98294700 | 1.59712600 |
| H | 0.78135600 | 6.04639300 | 1.78176200 |
| C | -0.39574600 | 4.30450900 | 2.26818900 |
| H | -1.03038700 | 4.82444100 | 2.99167900 |
| C | -0.60569700 | 2.96578600 | 2.00985000 |
| H | -1.42079200 | 2.43648400 | 2.51475800 |
| C | 0.16733900 | 2.25913700 | 1.08566000 |

| | | | |
|----|-------------|-------------|-------------|
| C | 2.34918600 | -2.63245400 | 0.10389500 |
| C | 2.60182300 | -2.03011000 | 1.39294400 |
| C | 1.37606700 | -1.98604100 | 2.10610300 |
| C | 0.35442600 | -2.42335500 | 1.21008800 |
| C | 0.98581000 | -2.90027600 | 0.00036200 |
| Rh | 1.23292300 | -0.57513400 | 0.42315400 |
| C | 2.30303300 | 2.33974000 | -0.38102900 |
| O | 3.10635600 | 3.02529400 | -0.99004600 |
| C | -0.25486500 | 0.88334900 | 0.81026000 |
| C | -0.44362300 | 0.38834700 | -0.50093500 |
| C | 0.33592900 | -3.57039300 | -1.14509100 |
| H | 0.68968200 | -4.61185300 | -1.23311900 |
| H | -0.75700600 | -3.61420500 | -1.04518200 |
| H | 0.56868600 | -3.08257200 | -2.10655600 |
| C | 3.37009700 | -2.96980900 | -0.90749200 |
| H | 3.63078900 | -4.04086000 | -0.84514500 |
| H | 3.01534200 | -2.79546700 | -1.93598500 |
| H | 4.30450200 | -2.40975800 | -0.76527000 |
| C | 3.94465300 | -1.71228700 | 1.92513700 |
| H | 4.59699800 | -1.26365500 | 1.16172200 |
| H | 3.89809000 | -1.01467400 | 2.77285100 |
| H | 4.44978500 | -2.62756100 | 2.27931000 |
| C | 1.17274900 | -1.59044300 | 3.51605600 |
| H | 1.17311800 | -2.47531600 | 4.17641400 |
| H | 1.96230600 | -0.91571300 | 3.87575300 |
| H | 0.20899400 | -1.08126000 | 3.66668300 |
| C | -1.06372600 | -2.61228400 | 1.58419200 |
| H | -1.18684300 | -3.55350800 | 2.14723700 |
| H | -1.43178100 | -1.80341100 | 2.23305500 |
| H | -1.72820000 | -2.67337500 | 0.71061200 |
| O | 3.69876500 | 0.59508800 | -0.71123900 |
| H | -0.95360600 | 0.48715400 | 1.56342000 |
| H | 2.15707100 | 0.56950500 | 1.04033500 |
| C | -0.41038100 | 1.08231500 | -1.79609200 |
| O | 0.14011000 | 1.99147700 | -2.33833500 |
| O | -1.38566000 | 0.32135800 | -2.33994900 |
| C | -1.58729500 | -0.40536500 | -1.08852200 |
| C | -2.95456600 | -0.15602400 | -0.53651200 |
| H | -1.40480000 | -1.47717200 | -1.28005700 |
| C | -4.05268700 | -0.79996900 | -1.35696800 |
| H | -2.98330700 | -0.54171400 | 0.49975800 |
| H | -3.11361500 | 0.93710900 | -0.46392800 |
| H | -4.00079200 | -0.42172300 | -2.39351900 |
| H | -3.86912700 | -1.88925800 | -1.40892800 |

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|---|-------------|-------------|-------------|
| C | -5.40859100 | -0.53886300 | -0.78855100 |
| C | -6.14542100 | 0.57185500 | -1.18577800 |
| C | -5.94056700 | -1.37020800 | 0.19176500 |
| C | -7.38069700 | 0.84357600 | -0.62241700 |
| H | -5.73930600 | 1.23470300 | -1.95889400 |
| C | -7.17548400 | -1.10226100 | 0.75735300 |
| H | -5.37259200 | -2.25198400 | 0.51219500 |
| C | -7.90013500 | 0.00680000 | 0.35173000 |
| H | -7.94799600 | 1.71969400 | -0.95171000 |
| H | -7.58058100 | -1.77146800 | 1.52285000 |
| H | -8.87761500 | 0.21814100 | 0.79545100 |
| C | 3.85466700 | 0.14354700 | -1.96716800 |
| O | 4.96983200 | -0.17342100 | -2.26317800 |
| C | 2.67255900 | 0.07685200 | -2.84587200 |
| H | 1.84770100 | -0.46663900 | -2.35769700 |
| H | 2.30344600 | 1.08965000 | -3.06004800 |
| H | 2.95714600 | -0.41664700 | -3.78074000 |

INT-7

| | | | |
|----|-------------|-------------|-------------|
| N | 2.57154800 | 1.00412200 | -0.12237200 |
| C | 1.19603400 | 2.89421900 | 0.50749600 |
| C | 1.38930500 | 4.24189200 | 0.81301300 |
| H | 2.16744900 | 4.78878600 | 0.27207000 |
| C | 0.66249400 | 4.86105100 | 1.80523400 |
| H | 0.83909900 | 5.91272400 | 2.04270200 |
| C | -0.27338300 | 4.12053700 | 2.51328300 |
| H | -0.84916300 | 4.58845600 | 3.31741000 |
| C | -0.50482000 | 2.79999500 | 2.19129200 |
| H | -1.28352700 | 2.24207200 | 2.72224500 |
| C | 0.18939900 | 2.14918700 | 1.16469400 |
| C | 2.49670800 | -2.52124500 | 0.18184100 |
| C | 2.54846100 | -1.98739100 | 1.53093100 |
| C | 1.25833300 | -2.05537600 | 2.07971500 |
| C | 0.37862300 | -2.52317400 | 1.04389700 |
| C | 1.18171600 | -2.90390700 | -0.09414100 |
| Rh | 1.19049400 | -0.65232300 | 0.34081200 |
| C | 2.19839800 | 2.34908000 | -0.41582900 |
| O | 2.76620500 | 2.95315400 | -1.28060800 |
| C | -0.23822600 | 0.79775300 | 0.81352700 |
| C | -0.44529500 | 0.36332000 | -0.53649200 |
| C | 0.70313600 | -3.58006000 | -1.31677300 |
| H | 0.72009200 | -4.67840100 | -1.19959700 |
| H | -0.33464200 | -3.31522200 | -1.57083500 |
| H | 1.32909100 | -3.34456300 | -2.19132900 |

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|---|-------------|-------------|-------------|
| C | 3.67582400 | -2.73001600 | -0.68574600 |
| H | 4.09209000 | -3.74340900 | -0.54564400 |
| H | 3.43700700 | -2.63553000 | -1.75678900 |
| H | 4.49103700 | -2.02759200 | -0.45742500 |
| C | 3.78789300 | -1.54457400 | 2.20497100 |
| H | 4.42010500 | -0.92839300 | 1.54494800 |
| H | 3.58010100 | -0.95113200 | 3.10688900 |
| H | 4.40885100 | -2.40358500 | 2.51450300 |
| C | 0.83453900 | -1.70478200 | 3.45200000 |
| H | 0.70910900 | -2.60839000 | 4.07450900 |
| H | 1.56432000 | -1.05946600 | 3.96167500 |
| H | -0.13470000 | -1.18071300 | 3.46617700 |
| C | -1.04778600 | -2.85561100 | 1.25416800 |
| H | -1.14801400 | -3.80324400 | 1.81259100 |
| H | -1.57036600 | -2.08664600 | 1.84478400 |
| H | -1.59691400 | -2.98543400 | 0.31016000 |
| O | 3.83256200 | 0.72629900 | -0.68895500 |
| H | -0.96675200 | 0.39593600 | 1.53674500 |
| H | 2.79913700 | 0.97344900 | 0.88011200 |
| C | -0.44631900 | 1.11596700 | -1.78813400 |
| O | 0.10087700 | 2.04651700 | -2.30638800 |
| O | -1.43276300 | 0.38419100 | -2.35814100 |
| C | -1.61571800 | -0.38692700 | -1.13041200 |
| C | -2.97340400 | -0.15434600 | -0.54896000 |
| H | -1.44777900 | -1.45269900 | -1.37110200 |
| C | -4.09023600 | -0.73789000 | -1.38987600 |
| H | -2.99589700 | -0.59678700 | 0.46500900 |
| H | -3.11915400 | 0.93482000 | -0.41303400 |
| H | -4.03895700 | -0.31122500 | -2.40756000 |
| H | -3.92796500 | -1.82645900 | -1.49686300 |
| C | -5.43824000 | -0.48070000 | -0.80129600 |
| C | -6.16302900 | 0.65385500 | -1.15066000 |
| C | -5.97572600 | -1.34203600 | 0.14989900 |
| C | -7.39184800 | 0.91931900 | -0.57032100 |
| H | -5.75280700 | 1.34106600 | -1.89994600 |
| C | -7.20415300 | -1.08038500 | 0.73246900 |
| H | -5.41819600 | -2.24297800 | 0.43301000 |
| C | -7.91694100 | 0.05221700 | 0.37375700 |
| H | -7.94968200 | 1.81441300 | -0.86287400 |
| H | -7.61400200 | -1.77334700 | 1.47392900 |
| H | -8.88955800 | 0.25838100 | 0.83041100 |
| C | 3.88425100 | 0.31023200 | -1.97420200 |
| O | 4.99439300 | 0.13014900 | -2.37781100 |
| C | 2.64503900 | 0.11072900 | -2.74193300 |

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|---|------------|-------------|-------------|
| H | 1.91442500 | -0.49665700 | -2.18264800 |
| H | 2.16651900 | 1.07590600 | -2.95651300 |
| H | 2.90622300 | -0.37655200 | -3.68693100 |

INT-1'

| | | | |
|----|-------------|-------------|-------------|
| N | 2.21086200 | 0.26086000 | -0.87166500 |
| C | 1.52261000 | 2.36990800 | -1.69346800 |
| C | 2.35285400 | 3.45742500 | -1.97842600 |
| H | 3.38547700 | 3.25199600 | -2.28053800 |
| C | 1.90533900 | 4.75718300 | -1.88988700 |
| H | 2.58207700 | 5.59030100 | -2.09899000 |
| C | 0.58073300 | 4.98558000 | -1.54952400 |
| H | 0.19135800 | 6.00610400 | -1.48719500 |
| C | -0.24786200 | 3.91681900 | -1.28533000 |
| H | -1.29463200 | 4.10521400 | -1.01750300 |
| C | 0.19143800 | 2.59048800 | -1.32630800 |
| C | 2.04821600 | -0.25008200 | 2.76583900 |
| C | 2.28794000 | 1.04969400 | 2.31169900 |
| C | 1.01361000 | 1.70716000 | 2.12788500 |
| C | -0.00840800 | 0.81001200 | 2.56903200 |
| C | 0.61160100 | -0.41319800 | 2.89507400 |
| Rh | 1.03454400 | 0.00647000 | 0.77604900 |
| C | 2.17817100 | 1.04595900 | -1.94003200 |
| O | 2.71806200 | 0.82576000 | -3.01680000 |
| C | -0.87401300 | 1.56830800 | -1.03245900 |
| C | -0.55615700 | 0.15803400 | -0.61439900 |
| C | -0.03785000 | -1.65247900 | 3.36435000 |
| H | 0.16713800 | -1.81895300 | 4.43549700 |
| H | -1.12888900 | -1.62622600 | 3.23772400 |
| H | 0.34257900 | -2.53837100 | 2.83030800 |
| C | 3.03182500 | -1.31562700 | 3.04261300 |
| H | 3.20521800 | -1.42721000 | 4.12675000 |
| H | 2.68186800 | -2.29606200 | 2.68089200 |
| H | 4.00630900 | -1.11260800 | 2.57644700 |
| C | 3.58505500 | 1.67627100 | 1.99416100 |
| H | 3.86281100 | 2.41064400 | 2.76855900 |
| H | 4.39958700 | 0.94276100 | 1.92521300 |
| H | 3.54309000 | 2.22520600 | 1.03897400 |
| C | 0.84646800 | 3.15128600 | 1.87276400 |
| H | 0.98813500 | 3.71694500 | 2.81112300 |
| H | 1.58028100 | 3.53895800 | 1.14983800 |
| H | -0.15768200 | 3.39437000 | 1.49865700 |
| C | -1.44061000 | 1.13771200 | 2.71170700 |

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|---|-------------|-------------|-------------|
| H | -1.62464100 | 1.58957000 | 3.70155100 |
| H | -1.78075900 | 1.86849000 | 1.96395300 |
| H | -2.08636500 | 0.25018900 | 2.64296100 |
| O | 2.84081900 | -0.97828200 | -1.27642500 |
| H | -1.54839200 | 1.55267400 | -1.91674200 |
| H | -1.50187900 | 2.00805200 | -0.23547500 |
| C | -0.40357900 | -0.88061500 | -1.66194500 |
| O | 0.23180500 | -1.08732600 | -2.65480300 |
| O | -1.33017600 | -1.71921600 | -1.15709000 |
| C | -1.70499000 | -0.74160900 | -0.13979800 |
| C | -3.12810800 | -0.31201200 | -0.31566900 |
| H | -1.55405700 | -1.21080200 | 0.85282600 |
| C | -4.11402000 | -1.41314300 | 0.01847000 |
| H | -3.31320800 | 0.56180400 | 0.33723000 |
| H | -3.28461900 | 0.03616000 | -1.35406000 |
| H | -3.93535200 | -2.27711700 | -0.64633200 |
| H | -3.92017800 | -1.76413500 | 1.04965100 |
| C | -5.53192400 | -0.96114400 | -0.10237500 |
| C | -6.23392600 | -1.11338900 | -1.29318600 |
| C | -6.16410100 | -0.32572600 | 0.96181700 |
| C | -7.53242700 | -0.64817200 | -1.41673000 |
| H | -5.74960500 | -1.61341800 | -2.14021600 |
| C | -7.46196600 | 0.14043300 | 0.84264000 |
| H | -5.62378400 | -0.20235500 | 1.90833600 |
| C | -8.15114900 | -0.01947300 | -0.34869900 |
| H | -8.07083300 | -0.78187500 | -2.36026700 |
| H | -7.94467300 | 0.63155800 | 1.69340000 |
| H | -9.17851200 | 0.34462400 | -0.44357800 |
| C | 2.26929000 | -2.01356700 | -0.76495900 |
| O | 1.32850500 | -1.94499600 | 0.01797600 |
| C | 2.86021500 | -3.33734100 | -1.17702500 |
| C | 3.95907900 | -3.15810700 | -2.20084700 |
| H | 4.34583300 | -4.14520900 | -2.49713100 |
| H | 3.59393000 | -2.65433800 | -3.10862300 |
| H | 4.80295300 | -2.57476700 | -1.80258400 |
| C | 3.40337700 | -3.98756500 | 0.08546500 |
| H | 3.84533800 | -4.96412800 | -0.16592200 |
| H | 4.19000700 | -3.37309400 | 0.55343600 |
| H | 2.60722000 | -4.15695400 | 0.82724700 |
| C | 1.72759700 | -4.17467400 | -1.74733200 |
| H | 0.91154100 | -4.30274200 | -1.02024600 |
| H | 1.30777000 | -3.72241400 | -2.65947100 |
| H | 2.10894300 | -5.17363100 | -2.00983000 |

TS-1'

| | | | |
|----|-------------|-------------|-------------|
| N | 2.24494200 | 0.68243100 | -0.65353200 |
| C | 1.58148400 | 2.60997800 | -1.57274900 |
| C | 2.42562200 | 3.69537700 | -1.82280300 |
| H | 3.45031500 | 3.49436200 | -2.15100400 |
| C | 1.97798100 | 4.98877300 | -1.68349600 |
| H | 2.64817000 | 5.82823900 | -1.88724800 |
| C | 0.66505800 | 5.20742200 | -1.28828300 |
| H | 0.28690400 | 6.22685700 | -1.16963200 |
| C | -0.16434000 | 4.13677000 | -1.03578700 |
| H | -1.19959000 | 4.31926500 | -0.72459600 |
| C | 0.26674400 | 2.81189200 | -1.14276500 |
| C | 2.09066300 | -0.58586000 | 2.65015100 |
| C | 2.31976000 | 0.78360100 | 2.44044800 |
| C | 1.03967700 | 1.44129200 | 2.36330500 |
| C | 0.02567300 | 0.46843600 | 2.63366700 |
| C | 0.65986300 | -0.78415600 | 2.74954900 |
| Rh | 1.11338200 | 0.00294600 | 0.70207500 |
| C | 2.24042700 | 1.26639400 | -1.82407100 |
| O | 2.80285300 | 1.01613300 | -2.87287700 |
| C | -0.78462300 | 1.78258200 | -0.83477300 |
| C | -0.47325400 | 0.32791300 | -0.64809100 |
| C | 0.02617200 | -2.09353100 | 2.99543500 |
| H | 0.22825100 | -2.43189300 | 4.02560200 |
| H | -1.06403200 | -2.06151200 | 2.86613400 |
| H | 0.42542500 | -2.87233000 | 2.32443200 |
| C | 3.08308500 | -1.67381400 | 2.73937500 |
| H | 3.18404100 | -2.03246900 | 3.77764700 |
| H | 2.77927700 | -2.54536300 | 2.13547800 |
| H | 4.07814800 | -1.35950300 | 2.39814900 |
| C | 3.61050900 | 1.47112100 | 2.25827700 |
| H | 3.84846800 | 2.08510000 | 3.14251800 |
| H | 4.44142600 | 0.77049400 | 2.10400700 |
| H | 3.58240900 | 2.15506000 | 1.39465500 |
| C | 0.84843100 | 2.90251900 | 2.26877200 |
| H | 0.97915700 | 3.36850900 | 3.26109200 |
| H | 1.58073800 | 3.37266300 | 1.59418300 |
| H | -0.15766300 | 3.17006000 | 1.91640400 |
| C | -1.40964800 | 0.75256000 | 2.82232100 |
| H | -1.59970400 | 1.01188600 | 3.87771000 |
| H | -1.75112900 | 1.60697700 | 2.22084300 |
| H | -2.04794200 | -0.11155900 | 2.58724800 |
| O | 3.03554400 | -1.24887900 | -1.23784700 |
| H | -1.55249800 | 1.89019900 | -1.63164700 |

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|---|-------------|-------------|-------------|
| H | -1.30534100 | 2.13092000 | 0.07670200 |
| C | -0.33705500 | -0.54736800 | -1.84980800 |
| O | 0.29233700 | -0.60628600 | -2.86152800 |
| O | -1.29456400 | -1.41616600 | -1.48474300 |
| C | -1.62096300 | -0.62788600 | -0.30166200 |
| C | -3.04365800 | -0.16472100 | -0.34611300 |
| H | -1.43497900 | -1.26138600 | 0.58807500 |
| C | -4.02169000 | -1.29843300 | -0.11289600 |
| H | -3.18542500 | 0.61563500 | 0.42441700 |
| H | -3.24483900 | 0.31740800 | -1.32094600 |
| H | -3.87240900 | -2.07375500 | -0.88544300 |
| H | -3.78862000 | -1.77405800 | 0.85859900 |
| C | -5.44234500 | -0.83912000 | -0.12350700 |
| C | -6.19287800 | -0.86333500 | -1.29395700 |
| C | -6.03055800 | -0.32980200 | 1.02990700 |
| C | -7.49654700 | -0.39655500 | -1.31168200 |
| H | -5.74346400 | -1.26467600 | -2.20985100 |
| C | -7.33348800 | 0.13759900 | 1.01661300 |
| H | -5.45130000 | -0.30835600 | 1.96115100 |
| C | -8.07137200 | 0.10569400 | -0.15578600 |
| H | -8.07372400 | -0.42963100 | -2.24097700 |
| H | -7.78124000 | 0.52828600 | 1.93571800 |
| H | -9.10290100 | 0.46998200 | -0.16695400 |
| C | 2.21953700 | -2.08680600 | -0.85760900 |
| O | 1.19805800 | -1.86003100 | -0.14889700 |
| C | 2.40127600 | -3.54391700 | -1.30411500 |
| C | 3.88056400 | -3.85777400 | -1.38220500 |
| H | 4.02701900 | -4.90453900 | -1.69344500 |
| H | 4.39736100 | -3.21346900 | -2.10831300 |
| H | 4.37323400 | -3.72895400 | -0.40423000 |
| C | 1.71376200 | -4.48558400 | -0.33936900 |
| H | 1.86889100 | -5.52732000 | -0.66473100 |
| H | 2.12023900 | -4.39434300 | 0.68199900 |
| H | 0.62893700 | -4.30793200 | -0.29082000 |
| C | 1.76695600 | -3.65518200 | -2.68004200 |
| H | 0.68515100 | -3.44579300 | -2.64654300 |
| H | 2.22869800 | -2.95868700 | -3.39756800 |
| H | 1.89897800 | -4.67857900 | -3.06787400 |

INT-2'

| | | | |
|---|------------|------------|-------------|
| N | 2.20200300 | 1.42533600 | 0.11640500 |
| C | 1.12622300 | 3.35911600 | -0.83207600 |
| C | 1.55605900 | 4.58285000 | -1.34359900 |
| H | 2.56676800 | 4.64127000 | -1.75864100 |

| | | | |
|----|-------------|-------------|-------------|
| C | 0.73850500 | 5.69154800 | -1.32673500 |
| H | 1.09270500 | 6.64512200 | -1.72738400 |
| C | -0.53816800 | 5.57608500 | -0.80028000 |
| H | -1.20796200 | 6.44088000 | -0.78160600 |
| C | -0.97529500 | 4.36208600 | -0.30764200 |
| H | -1.99474000 | 4.27818100 | 0.08494000 |
| C | -0.16271300 | 3.23063800 | -0.29771600 |
| C | 2.29476300 | -1.65679000 | 2.09397200 |
| C | 2.63939700 | -0.38169700 | 2.59992200 |
| C | 1.42577400 | 0.29327700 | 2.92471200 |
| C | 0.32952200 | -0.61438500 | 2.69991200 |
| C | 0.86392600 | -1.80592700 | 2.17644400 |
| Rh | 1.34333400 | -0.11339600 | 0.71200700 |
| C | 2.12526300 | 2.26250300 | -0.90714800 |
| O | 2.97869000 | 2.22763600 | -1.79218500 |
| C | -0.76154000 | 1.99019500 | 0.29985400 |
| C | -0.38642200 | 0.64278700 | -0.25449000 |
| C | 0.14443500 | -3.04798400 | 1.84260100 |
| H | 0.48132600 | -3.86647300 | 2.50012300 |
| H | -0.94193700 | -2.94929700 | 1.96620800 |
| H | 0.34362700 | -3.37304700 | 0.80828900 |
| C | 3.20782600 | -2.71320400 | 1.62747600 |
| H | 3.41398200 | -3.42286100 | 2.44691800 |
| H | 2.75894100 | -3.30124900 | 0.81102000 |
| H | 4.17023400 | -2.31512600 | 1.28096900 |
| C | 3.98637900 | 0.19358900 | 2.74456200 |
| H | 4.28191700 | 0.21163500 | 3.80666700 |
| H | 4.74436900 | -0.38078700 | 2.19601100 |
| H | 4.02040000 | 1.23432200 | 2.38778900 |
| C | 1.33948600 | 1.61907500 | 3.56160100 |
| H | 1.54987300 | 1.52467000 | 4.64082600 |
| H | 2.07860700 | 2.32173900 | 3.15060500 |
| H | 0.34125100 | 2.06651800 | 3.46416100 |
| C | -1.07131500 | -0.37033300 | 3.08263600 |
| H | -1.19308900 | -0.56583200 | 4.16167200 |
| H | -1.38162900 | 0.67085200 | 2.91597800 |
| H | -1.77026100 | -1.03185500 | 2.55270100 |
| O | 3.30120900 | -1.14547100 | -1.43578400 |
| H | -1.85813000 | 2.11386700 | 0.23104500 |
| H | -0.55973400 | 1.99935000 | 1.38788000 |
| C | -0.25481800 | 0.43873900 | -1.73148900 |
| O | 0.36780200 | 0.88059200 | -2.64653300 |
| O | -1.16299800 | -0.54159500 | -1.80273800 |
| C | -1.44529000 | -0.45909300 | -0.37201000 |

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|---|-------------|-------------|-------------|
| C | -2.89195300 | -0.15499900 | -0.14056100 |
| H | -1.15551600 | -1.42378800 | 0.08426800 |
| C | -3.78059700 | -1.34468100 | -0.44376200 |
| H | -3.02813600 | 0.15640500 | 0.91148800 |
| H | -3.19023700 | 0.70774300 | -0.76473800 |
| H | -3.62764700 | -1.65647500 | -1.49227700 |
| H | -3.46409900 | -2.19616500 | 0.18765700 |
| C | -5.22435100 | -1.04551200 | -0.20771100 |
| C | -6.03831700 | -0.59123700 | -1.23952400 |
| C | -5.77275900 | -1.16457500 | 1.06535000 |
| C | -7.36466700 | -0.26752100 | -1.00794800 |
| H | -5.62007300 | -0.49405500 | -2.24821100 |
| C | -7.09807700 | -0.84207700 | 1.30107300 |
| H | -5.14352300 | -1.52587600 | 1.88799700 |
| C | -7.89915200 | -0.39209900 | 0.26390700 |
| H | -7.99100300 | 0.08380100 | -1.83390700 |
| H | -7.51334700 | -0.94858600 | 2.30806400 |
| H | -8.94798100 | -0.14080300 | 0.44759800 |
| C | 2.23884100 | -1.73742700 | -1.50068800 |
| O | 1.21574800 | -1.50808200 | -0.77030100 |
| C | 2.02444000 | -2.83768100 | -2.55028800 |
| C | 3.32366800 | -3.60068900 | -2.71081200 |
| H | 3.63327300 | -4.07764100 | -1.76530700 |
| H | 3.20503700 | -4.39851400 | -3.46212900 |
| H | 4.14296500 | -2.94496100 | -3.03983600 |
| C | 0.91052100 | -3.78472500 | -2.16202300 |
| H | 1.12745600 | -4.30403400 | -1.21296200 |
| H | -0.05420200 | -3.26524300 | -2.05193300 |
| H | 0.78676300 | -4.55852300 | -2.93799900 |
| C | 1.67274600 | -2.13739500 | -3.85243200 |
| H | 0.70753500 | -1.60970600 | -3.78354200 |
| H | 2.44323000 | -1.40352700 | -4.13839400 |
| H | 1.59126700 | -2.87584900 | -4.66737500 |

TS-2c'

| | | | |
|---|-------------|------------|-------------|
| N | 1.89566500 | 0.77869000 | -0.86266800 |
| C | 1.55175200 | 3.19136000 | -1.03163600 |
| C | 2.22802300 | 4.36774700 | -1.35519200 |
| H | 3.31763800 | 4.32856200 | -1.43443800 |
| C | 1.55235700 | 5.54580900 | -1.58608500 |
| H | 2.10165400 | 6.45504800 | -1.84466500 |
| C | 0.16995100 | 5.55515200 | -1.49984100 |
| H | -0.39058900 | 6.47535500 | -1.68856400 |
| C | -0.50725400 | 4.39554200 | -1.17930000 |

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|----|-------------|-------------|-------------|
| H | -1.60033300 | 4.41446600 | -1.10696200 |
| C | 0.15506800 | 3.19461700 | -0.93569900 |
| C | 2.13276200 | -1.19084800 | 2.37462400 |
| C | 2.52711900 | 0.18733100 | 2.39842100 |
| C | 1.35248900 | 0.97859600 | 2.49841600 |
| C | 0.23636300 | 0.07593900 | 2.62761700 |
| C | 0.71415200 | -1.24808800 | 2.53271500 |
| Rh | 1.28333800 | -0.19849100 | 0.62796300 |
| C | 2.41643000 | 2.00145600 | -0.84998100 |
| O | 3.64534900 | 2.10123200 | -0.82816500 |
| C | -0.71618000 | 2.06431600 | -0.47855400 |
| C | -0.38596400 | 0.63696300 | -0.73905600 |
| C | -0.07014800 | -2.49619700 | 2.59118000 |
| H | 0.08904600 | -3.01199500 | 3.55282200 |
| H | -1.14904600 | -2.31762200 | 2.48834700 |
| H | 0.23396600 | -3.20017800 | 1.79885500 |
| C | 3.02598200 | -2.36264200 | 2.35169100 |
| H | 3.16111200 | -2.74412600 | 3.37864200 |
| H | 2.60536500 | -3.18745100 | 1.75633500 |
| H | 4.01990600 | -2.12378800 | 1.95231800 |
| C | 3.91309800 | 0.67578700 | 2.31378400 |
| H | 4.39754000 | 0.58933800 | 3.30115900 |
| H | 4.51182300 | 0.08240600 | 1.60772200 |
| H | 3.96515400 | 1.72953800 | 2.01085500 |
| C | 1.31142600 | 2.44792500 | 2.64051000 |
| H | 1.48591900 | 2.73634800 | 3.69081000 |
| H | 2.08833700 | 2.94061300 | 2.03704400 |
| H | 0.33965700 | 2.86987600 | 2.34925200 |
| C | -1.15457100 | 0.46499400 | 2.90712600 |
| H | -1.29129800 | 0.52941100 | 4.00029200 |
| H | -1.41785300 | 1.45126700 | 2.50262800 |
| H | -1.88022300 | -0.27405200 | 2.53888200 |
| O | 3.24223400 | -2.07069600 | -0.85774300 |
| H | -1.72182300 | 2.25404800 | -0.90183200 |
| H | -0.86928500 | 2.17643800 | 0.61061800 |
| C | -0.35950700 | 0.07217200 | -2.12628800 |
| O | 0.18589200 | 0.25952000 | -3.16485400 |
| O | -1.31481700 | -0.83984600 | -1.89252300 |
| C | -1.48459100 | -0.42290200 | -0.51200500 |
| C | -2.89920800 | 0.01294900 | -0.27113300 |
| H | -1.19699300 | -1.26275900 | 0.14699400 |
| C | -3.83126300 | -1.17647500 | -0.14426600 |
| H | -2.94721000 | 0.62838900 | 0.64470600 |
| H | -3.22710900 | 0.66041500 | -1.10482700 |

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|---|-------------|-------------|-------------|
| H | -3.74208800 | -1.80647700 | -1.04718700 |
| H | -3.50024800 | -1.79897700 | 0.70851200 |
| C | -5.25276600 | -0.76217100 | 0.04625900 |
| C | -6.11048900 | -0.63638900 | -1.04104100 |
| C | -5.73526100 | -0.44489700 | 1.31186800 |
| C | -7.41690800 | -0.21084400 | -0.86904100 |
| H | -5.74372800 | -0.88492600 | -2.04381500 |
| C | -7.04045000 | -0.01897000 | 1.48796500 |
| H | -5.07061300 | -0.54334800 | 2.17897000 |
| C | -7.88625800 | 0.09926300 | 0.39672500 |
| H | -8.07930700 | -0.12449500 | -1.73593000 |
| H | -7.40461200 | 0.21933300 | 2.49213400 |
| H | -8.91940300 | 0.43161500 | 0.53487700 |
| C | 2.08795700 | -2.38458500 | -1.10391800 |
| O | 1.04648500 | -1.76930700 | -0.70527200 |
| C | 1.77182400 | -3.62413500 | -1.95357000 |
| C | 3.05251200 | -4.35493800 | -2.28824600 |
| H | 3.58400900 | -4.68274600 | -1.38073600 |
| H | 2.83274300 | -5.25169500 | -2.89103500 |
| H | 3.74364600 | -3.72316500 | -2.86720100 |
| C | 0.84860200 | -4.53383600 | -1.16399900 |
| H | 1.30532100 | -4.84393000 | -0.20731400 |
| H | -0.11225100 | -4.04444700 | -0.93810500 |
| H | 0.63003200 | -5.45201600 | -1.73494500 |
| C | 1.08298500 | -3.17644500 | -3.22981800 |
| H | 0.10851200 | -2.70711100 | -3.02583500 |
| H | 1.69717700 | -2.45285800 | -3.79155300 |
| H | 0.90423900 | -4.04160900 | -3.89045200 |

TS-2d'

| | | | |
|---|-------------|-------------|-------------|
| N | 2.21074400 | 0.86456800 | -0.81506700 |
| C | 1.56400500 | 2.54110500 | -1.56387200 |
| C | 2.48222400 | 3.59627800 | -1.62536000 |
| H | 3.54081800 | 3.37179800 | -1.78793900 |
| C | 2.03604300 | 4.89303200 | -1.55070000 |
| H | 2.74292700 | 5.72241000 | -1.63251300 |
| C | 0.67865800 | 5.13087800 | -1.36112200 |
| H | 0.30901400 | 6.15715400 | -1.28559900 |
| C | -0.20351000 | 4.07945400 | -1.22383500 |
| H | -1.26245000 | 4.28358200 | -1.03012800 |
| C | 0.21173800 | 2.74923200 | -1.27657100 |
| C | 2.12762500 | -0.48242300 | 2.54651200 |
| C | 2.42775500 | 0.86455300 | 2.30055300 |
| C | 1.18223900 | 1.59178800 | 2.23500300 |

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|----|-------------|-------------|-------------|
| C | 0.12439500 | 0.68736700 | 2.54625600 |
| C | 0.68634300 | -0.60305900 | 2.67064900 |
| Rh | 1.14923100 | 0.09371800 | 0.62367900 |
| C | 2.17830800 | 1.17877600 | -2.04299600 |
| O | 2.57296100 | 0.92749100 | -3.14835700 |
| C | -0.83564200 | 1.71138300 | -1.01408900 |
| C | -0.50025400 | 0.28378300 | -0.68728900 |
| C | -0.01160600 | -1.86077400 | 3.00256600 |
| H | 0.27579500 | -2.20663000 | 4.00961800 |
| H | -1.10400600 | -1.74617600 | 2.99246100 |
| H | 0.24975000 | -2.67247900 | 2.30280200 |
| C | 3.06401500 | -1.61796800 | 2.65277500 |
| H | 3.27512000 | -1.85555200 | 3.70929700 |
| H | 2.63936900 | -2.53065400 | 2.20362200 |
| H | 4.02474100 | -1.41410600 | 2.16000900 |
| C | 3.75411700 | 1.47118400 | 2.08233800 |
| H | 4.06499100 | 2.05055700 | 2.96756000 |
| H | 4.52954200 | 0.71785000 | 1.88905300 |
| H | 3.74380300 | 2.17164100 | 1.23195100 |
| C | 1.06461800 | 3.05358400 | 2.06872500 |
| H | 1.26376700 | 3.56821900 | 3.02481000 |
| H | 1.79050200 | 3.44539700 | 1.33867400 |
| H | 0.05851400 | 3.35359100 | 1.74216100 |
| C | -1.29268400 | 1.05271600 | 2.73235800 |
| H | -1.45833700 | 1.38455900 | 3.77137600 |
| H | -1.60054900 | 1.88411400 | 2.08177100 |
| H | -1.97269700 | 0.20761600 | 2.55457600 |
| O | 3.17553200 | -1.50745200 | -1.10716800 |
| H | -1.51635300 | 1.73864800 | -1.89265700 |
| H | -1.45734800 | 2.11240800 | -0.19189700 |
| C | -0.37163000 | -0.69206400 | -1.80731400 |
| O | 0.25094000 | -0.83311200 | -2.81559900 |
| O | -1.32583100 | -1.52704900 | -1.36351300 |
| C | -1.63895600 | -0.64228100 | -0.24656100 |
| C | -3.06183400 | -0.18188800 | -0.30774200 |
| H | -1.44103100 | -1.20042200 | 0.68893200 |
| C | -4.04371000 | -1.29557000 | -0.00536800 |
| H | -3.19630100 | 0.63853000 | 0.42177600 |
| H | -3.26977200 | 0.24919700 | -1.30513300 |
| H | -3.91122400 | -2.10857900 | -0.74124800 |
| H | -3.80141000 | -1.72476400 | 0.98511700 |
| C | -5.45991200 | -0.82240000 | -0.01893500 |
| C | -6.21458300 | -0.85874300 | -1.18655200 |
| C | -6.03788400 | -0.28397500 | 1.12626600 |

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|---|-------------|-------------|-------------|
| C | -7.51191100 | -0.37502300 | -1.20922300 |
| H | -5.77336900 | -1.28270300 | -2.09628600 |
| C | -7.33473200 | 0.20019100 | 1.10810600 |
| H | -5.45532300 | -0.25190000 | 2.05504900 |
| C | -8.07657500 | 0.15633600 | -0.06126600 |
| H | -8.09235300 | -0.41765600 | -2.13610900 |
| H | -7.77431300 | 0.61386900 | 2.02112300 |
| H | -9.10317100 | 0.53423800 | -0.07638700 |
| C | 2.24865100 | -2.21838400 | -0.74112300 |
| O | 1.21560000 | -1.82757900 | -0.11751800 |
| C | 2.28028100 | -3.71881600 | -1.06380200 |
| C | 3.66183000 | -4.24441600 | -0.72672100 |
| H | 3.72853000 | -5.32150000 | -0.95216000 |
| H | 4.44383900 | -3.72764600 | -1.30264200 |
| H | 3.89298900 | -4.11535600 | 0.34504900 |
| C | 1.23113500 | -4.48239400 | -0.28700500 |
| H | 0.21236900 | -4.13306800 | -0.51803800 |
| H | 1.28160500 | -5.55572100 | -0.53635600 |
| H | 1.37974400 | -4.38982200 | 0.80246000 |
| C | 2.02123600 | -3.85767200 | -2.55352500 |
| H | 2.75665100 | -3.28974100 | -3.14494600 |
| H | 2.08731300 | -4.91626600 | -2.85553400 |
| H | 1.01533100 | -3.49503800 | -2.82333200 |

INT-3c'

| | | | |
|----|-------------|-------------|-------------|
| N | -0.62959600 | 0.93263600 | -0.51548000 |
| C | -1.21239300 | 3.23926600 | -1.00263100 |
| C | -2.21549100 | 4.15411400 | -1.29405400 |
| H | -3.21757100 | 3.78436900 | -1.53033200 |
| C | -1.94514600 | 5.50942100 | -1.28032700 |
| H | -2.73819000 | 6.22934100 | -1.50205700 |
| C | -0.66475900 | 5.95331100 | -0.98608800 |
| H | -0.44681000 | 7.02551900 | -0.97361900 |
| C | 0.34046700 | 5.04465100 | -0.70151900 |
| H | 1.35172100 | 5.39510000 | -0.46853700 |
| C | 0.07153800 | 3.68512000 | -0.70253600 |
| C | -1.92260300 | -3.00263100 | -1.18157400 |
| C | -2.16914600 | -2.01559400 | -2.20755100 |
| C | -0.92588200 | -1.46621300 | -2.60951100 |
| C | 0.10066600 | -2.07941900 | -1.81991800 |
| C | -0.52363000 | -3.05789000 | -0.97430700 |
| Rh | -1.24806200 | -1.06429000 | -0.50187400 |
| C | -1.49979800 | 1.78063500 | -1.05208900 |
| O | -2.53527300 | 1.39511200 | -1.60560900 |

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|---|-------------|-------------|-------------|
| C | 1.10701900 | 2.65606600 | -0.42719600 |
| C | 0.48030700 | 1.43991000 | 0.22093400 |
| C | 0.18981600 | -3.88470100 | 0.01300400 |
| H | 0.67377700 | -4.74005900 | -0.48674900 |
| H | 0.98774000 | -3.31508700 | 0.51473100 |
| H | -0.48123100 | -4.28520700 | 0.78386700 |
| C | -2.96483100 | -3.79179700 | -0.49714000 |
| H | -3.24145500 | -4.68438500 | -1.08305500 |
| H | -2.63245900 | -4.13851700 | 0.49182000 |
| H | -3.88329000 | -3.20306000 | -0.35219800 |
| C | -3.50801400 | -1.66318700 | -2.70831500 |
| H | -3.92555000 | -2.50481700 | -3.28590200 |
| H | -4.20723100 | -1.46859600 | -1.88021100 |
| H | -3.49538900 | -0.77955100 | -3.35811200 |
| C | -0.68198900 | -0.45623000 | -3.65591900 |
| H | -0.22855300 | -0.93561600 | -4.53952600 |
| H | -1.60247400 | 0.04439500 | -3.97989200 |
| H | 0.02257000 | 0.31722500 | -3.31369800 |
| C | 1.54974300 | -1.86670700 | -1.99407100 |
| H | 1.93274800 | -2.49826300 | -2.81430500 |
| H | 1.77814000 | -0.82278900 | -2.25693500 |
| H | 2.11923500 | -2.12668600 | -1.08967200 |
| O | -2.89404300 | -0.44489200 | 0.77002500 |
| H | 1.90964900 | 3.07442100 | 0.20158200 |
| H | 1.58261900 | 2.32663400 | -1.37327100 |
| C | 0.24813300 | 1.63561400 | 1.72155200 |
| O | -0.48995300 | 2.23984500 | 2.43210800 |
| O | 1.22670300 | 0.81184300 | 2.09922300 |
| C | 1.49879900 | 0.39600400 | 0.72227700 |
| C | 2.95359600 | 0.48162700 | 0.40087700 |
| H | 1.11816400 | -0.63407900 | 0.59462500 |
| C | 3.75582900 | -0.59883200 | 1.10051900 |
| H | 3.07171000 | 0.38544900 | -0.69420300 |
| H | 3.35248900 | 1.47502700 | 0.67221000 |
| H | 3.68309800 | -0.45931100 | 2.19344700 |
| H | 3.29898700 | -1.58306200 | 0.88057700 |
| C | 5.18866500 | -0.60473700 | 0.68080300 |
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| C | 5.56452000 | -1.19643400 | -0.52145800 |
| C | 7.48815100 | 0.03934600 | 1.02988200 |
| H | 5.88642000 | 0.48394900 | 2.39836300 |
| C | 6.88226700 | -1.17506600 | -0.94302300 |
| H | 4.80075200 | -1.69119000 | -1.13615800 |
| C | 7.84964700 | -0.55583200 | -0.16705100 |

| | | | |
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| H | 8.24622000 | 0.52754700 | 1.65020100 |
| H | 7.15992100 | -1.65253100 | -1.88790200 |
| H | 8.89276200 | -0.54145900 | -0.49642100 |
| C | -2.20471700 | -0.67092600 | 1.78869500 |
| O | -1.01439000 | -1.03506400 | 1.62900200 |
| C | -2.82002900 | -0.58170400 | 3.16603100 |
| C | -3.65665400 | 0.67831600 | 3.26697900 |
| H | -4.45238400 | 0.70201600 | 2.50741200 |
| H | -4.13718500 | 0.73140400 | 4.25720900 |
| H | -3.04248700 | 1.58490100 | 3.14446200 |
| C | -3.71469500 | -1.80614900 | 3.30171000 |
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| H | -4.50844800 | -1.81361000 | 2.53765100 |
| H | -3.13797200 | -2.74148700 | 3.20461300 |
| C | -1.74811900 | -0.60165300 | 4.23286500 |
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| H | -2.21220900 | -0.53881100 | 5.23030100 |

INT-3d'

| | | | |
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| C | 2.02316600 | 4.61999600 | -2.00772700 |
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VI. References

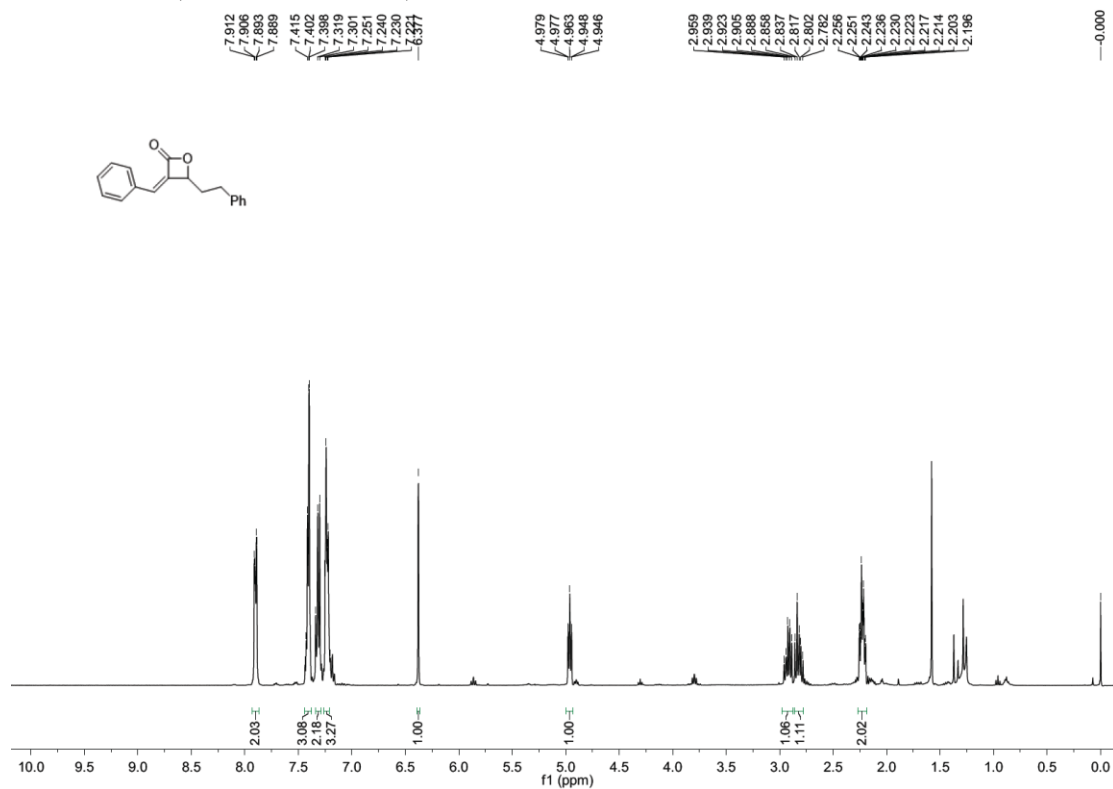
- [S1] Guimond, N.; Gorelsky, S. I.; Fagnou, K. *J. Am. Chem. Soc.* **2011**, *133*, 6449.
- [S2] (a) Malapit, C. A.; Caldwell, D. R.; Sassu, N.; Milbin, S.; Howell, A. R. *Org. Lett.* **2017**, *19*, 1966. (b) Xia, J.; Kong, L.; Zhou, X.; Zheng, G.; Li, X. *Org. Lett.* **2017**, *19*, 5972. (c) Raju, R.; Howell, A. R. *Org. Lett.* **2006**, *8*, 2139.
- [S3] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, Jr., J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, revision D. 01*, Gaussian, Inc., Wallingford CT, **2013**.
- [S4] Peverati, R.; Truhlar, D. G. *J. Phys. Chem. Lett.* **2012**, *3*, 117.

[S5] Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. *J. Chem. Phys.* **1987**, *86*, 866.

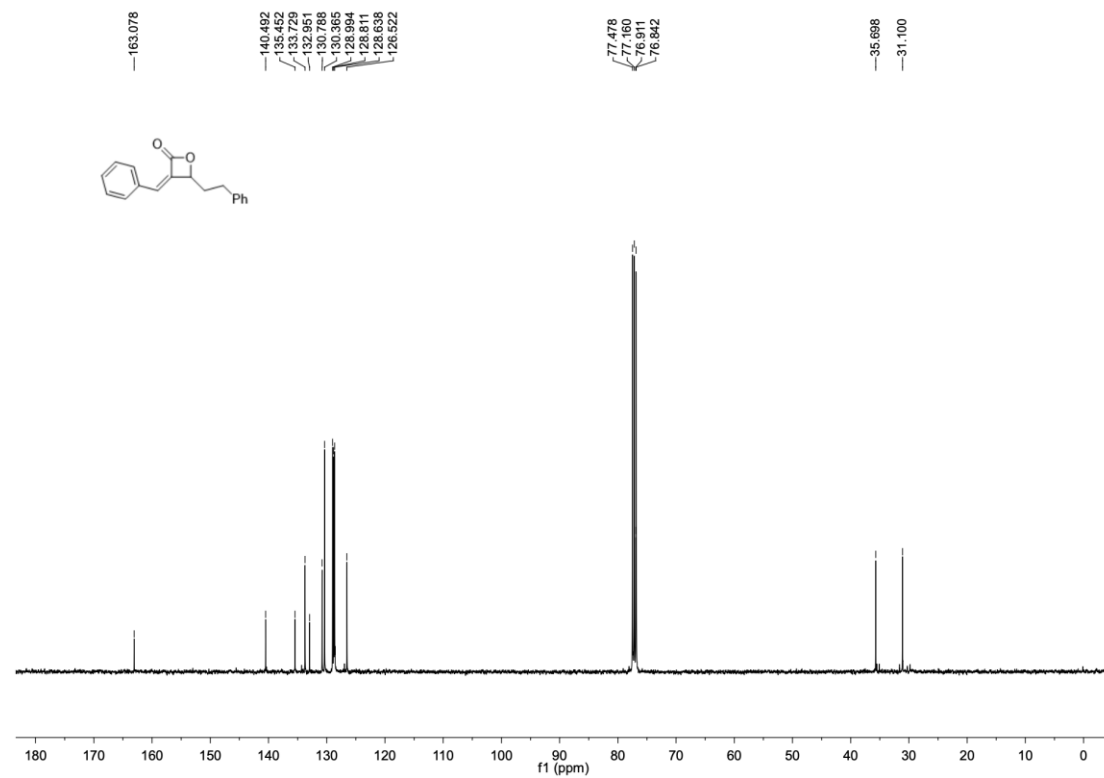
[S6] Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378.

VII. Copies of ^1H , ^{13}C and ^{19}F NMR spectra

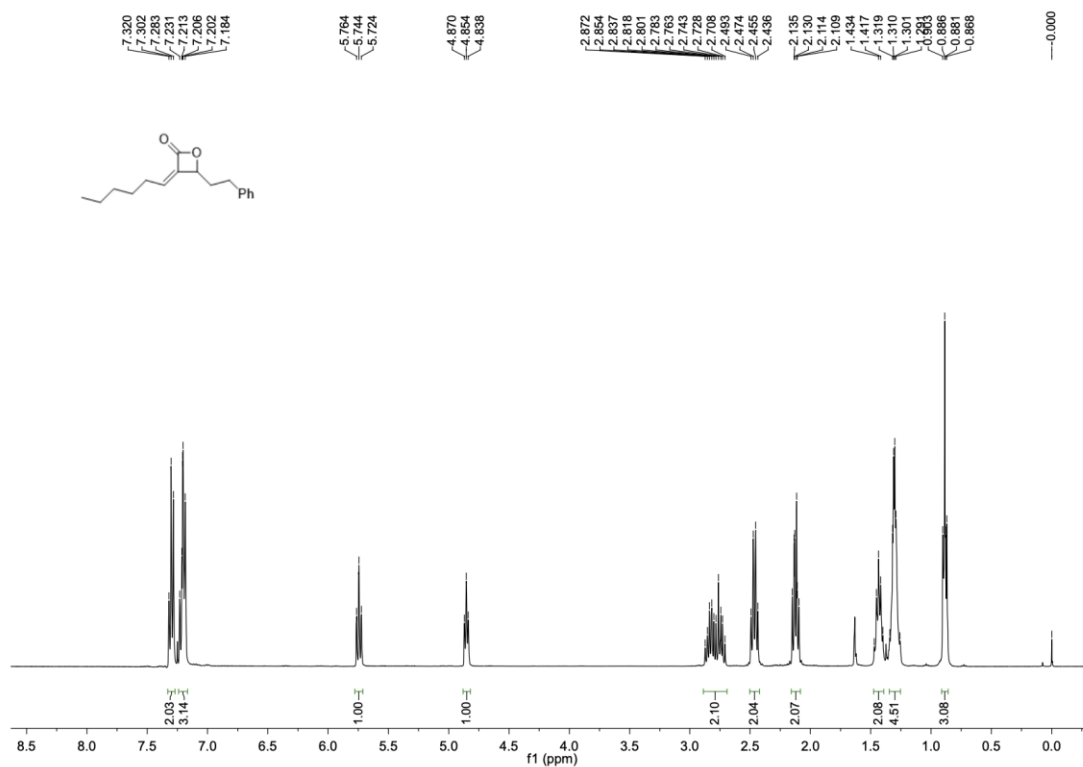
2f- ^1H NMR (400 MHz, CDCl_3)



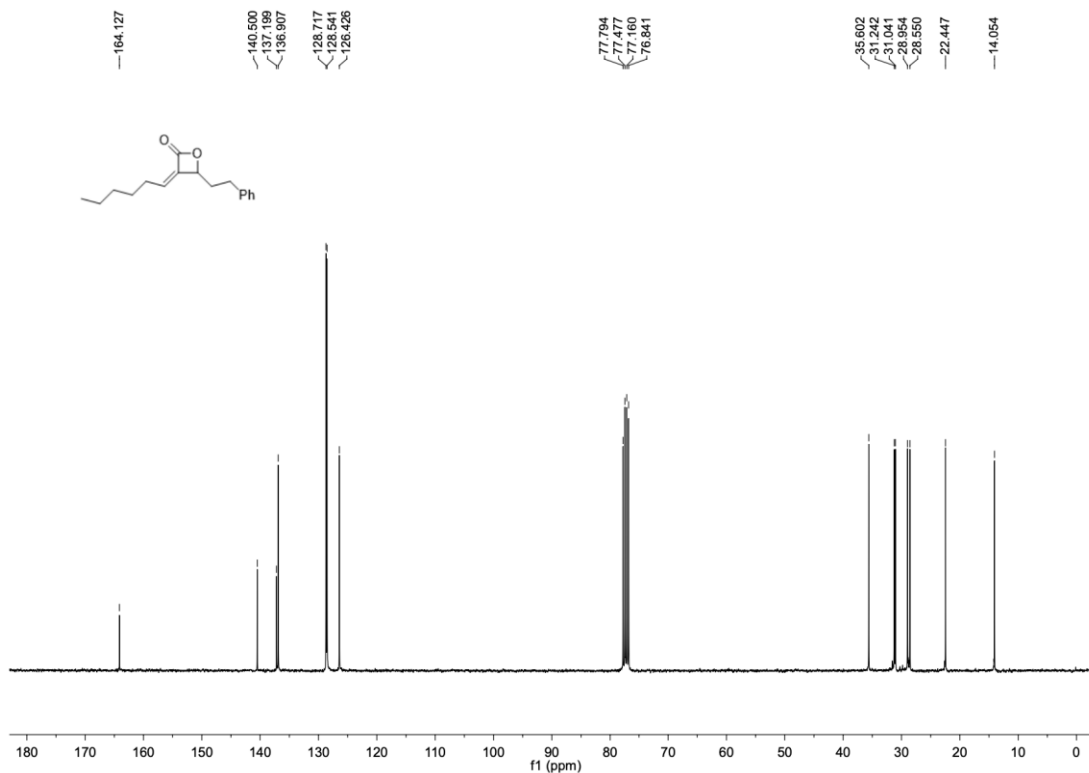
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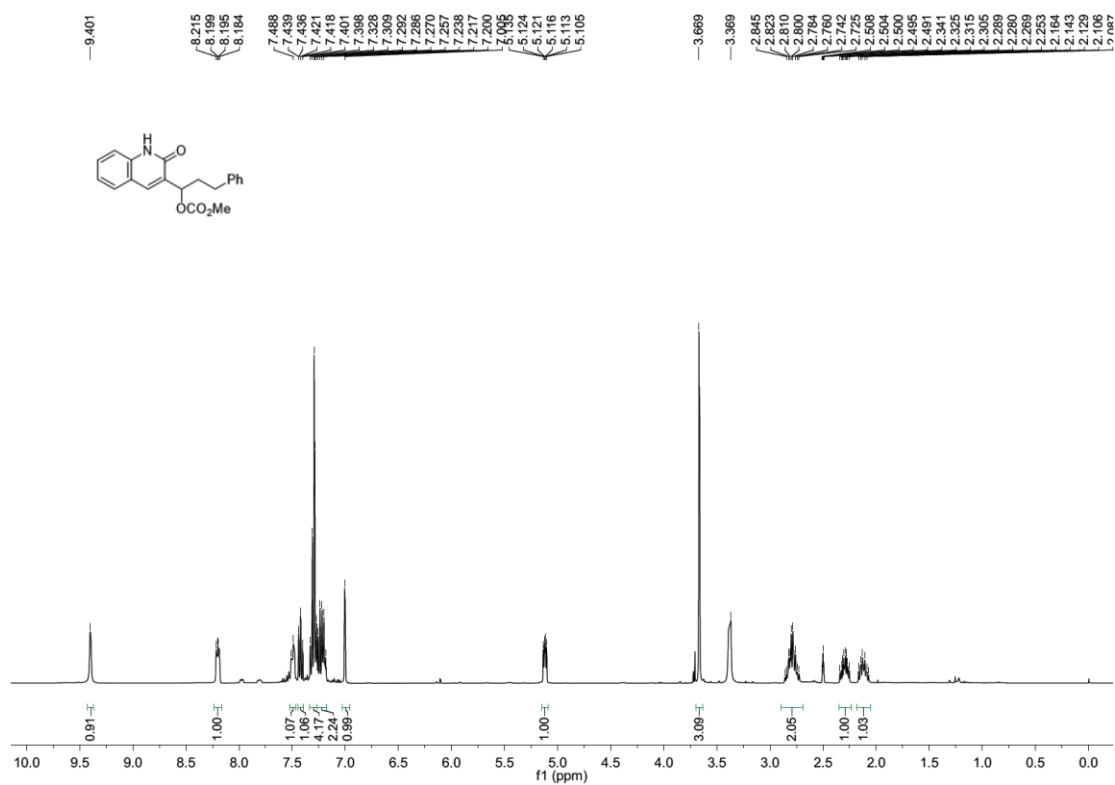
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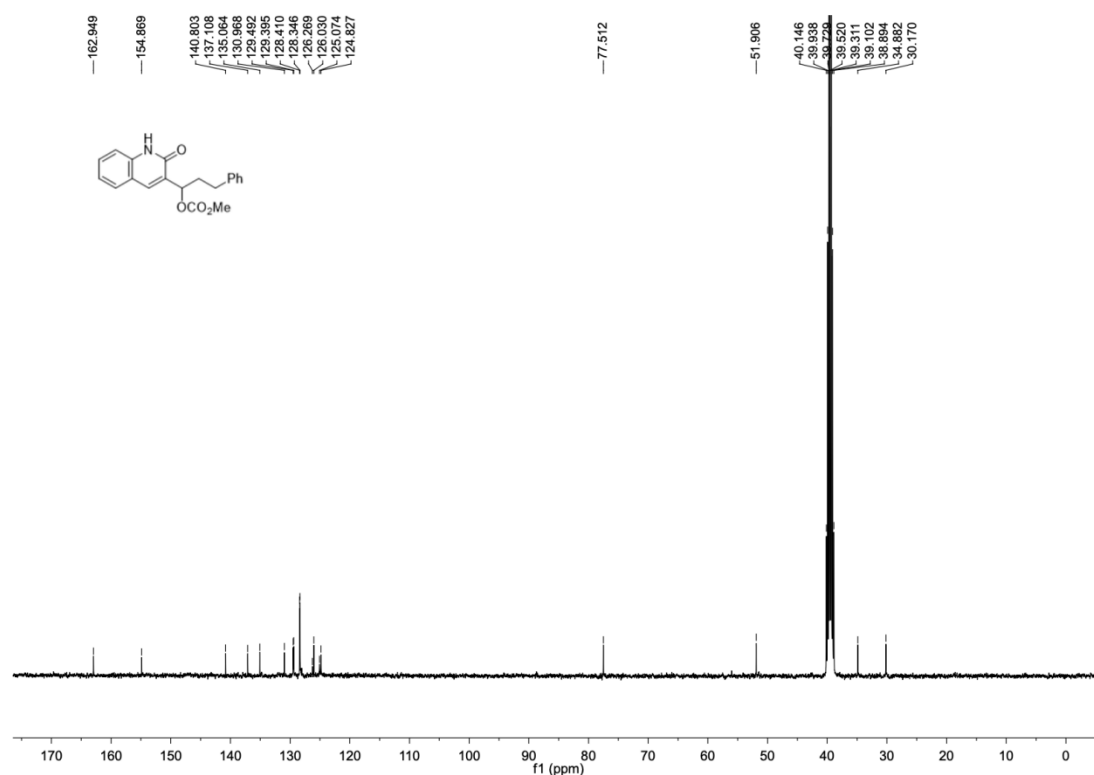
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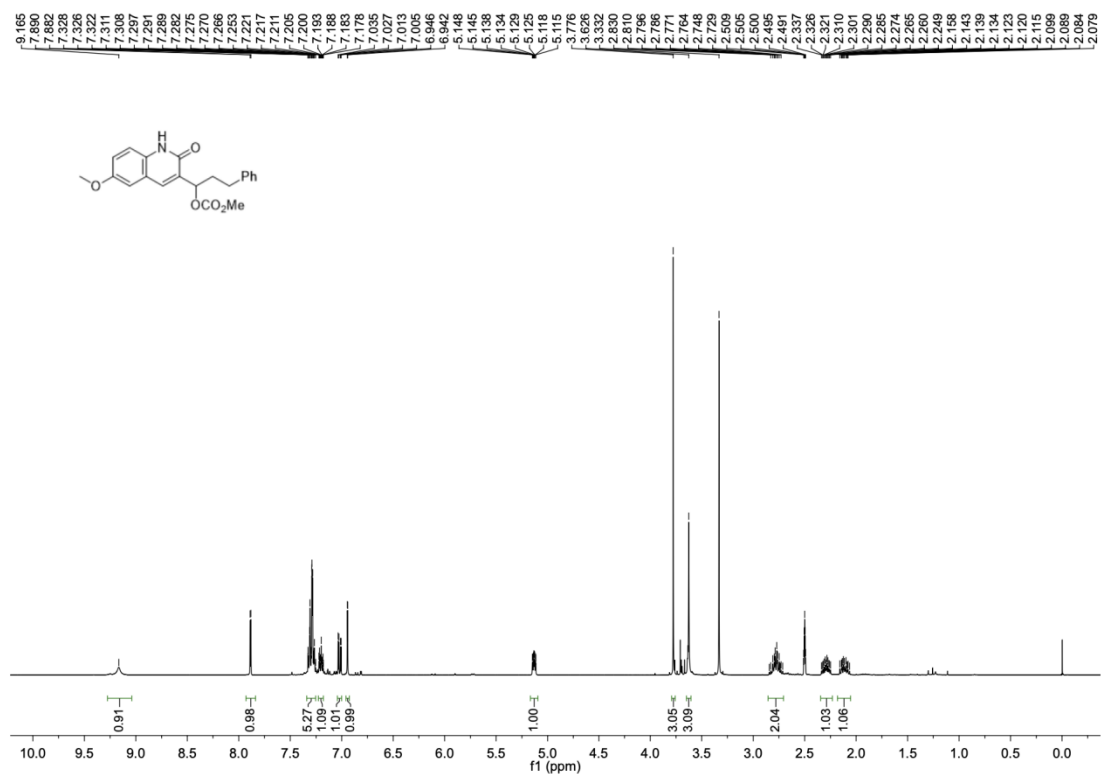
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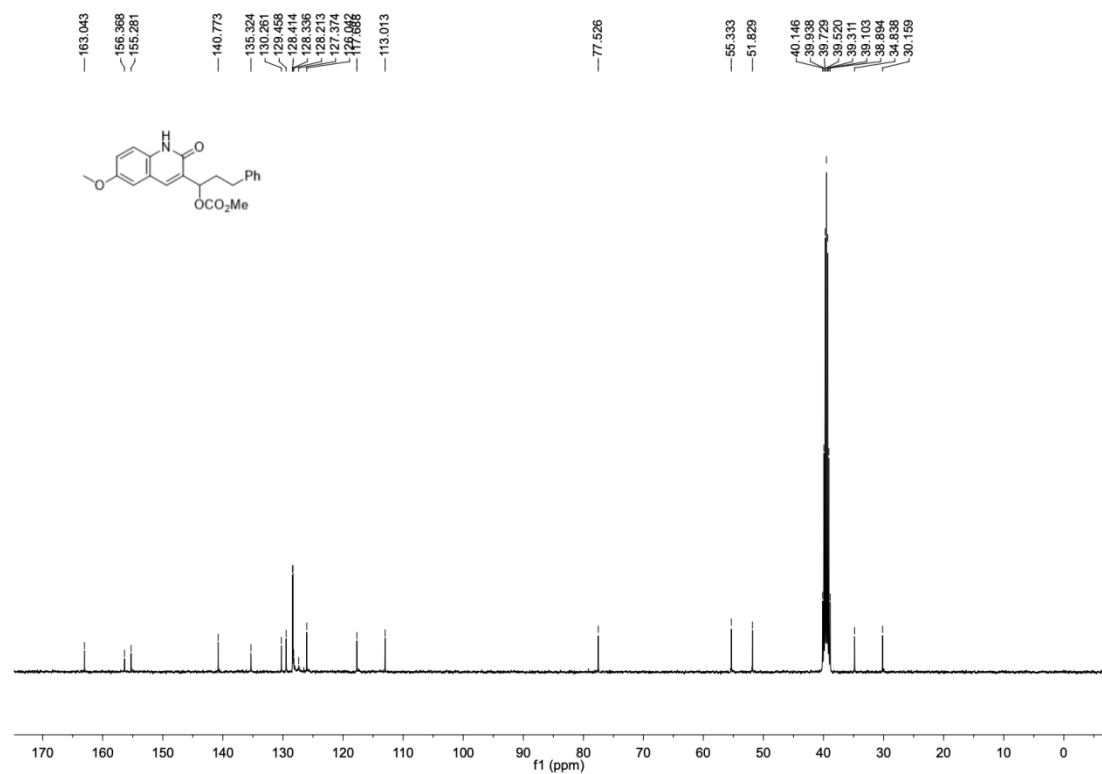
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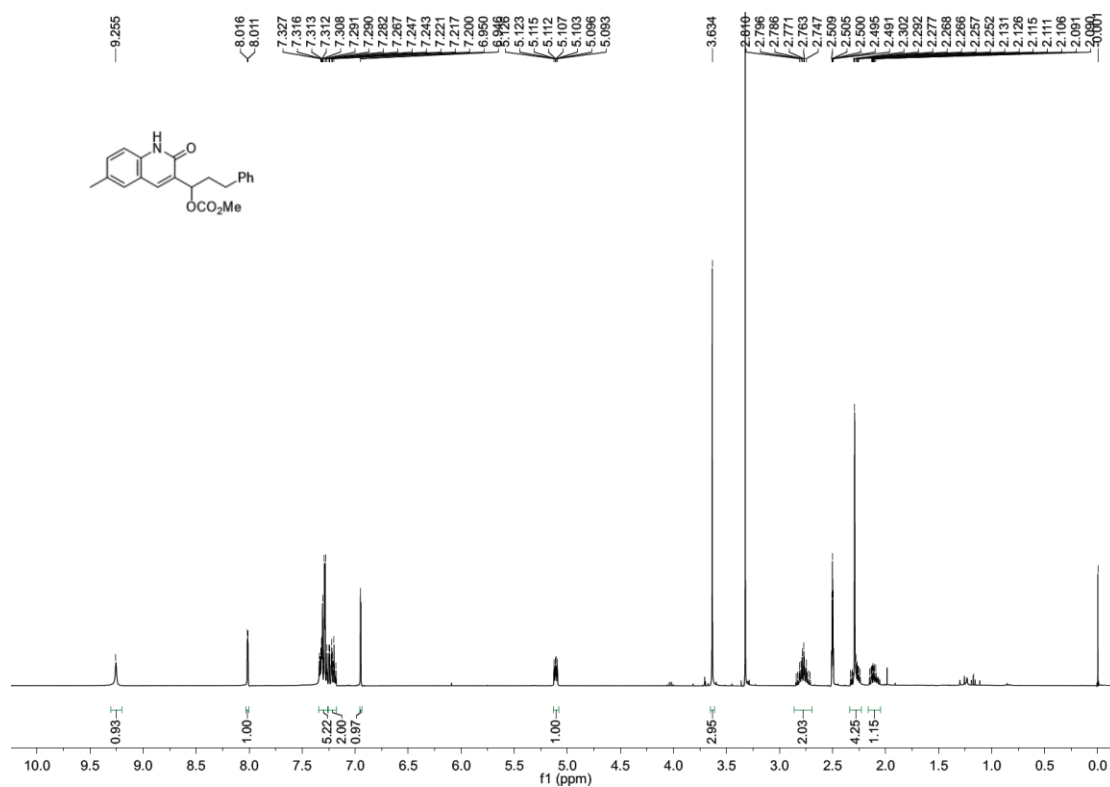
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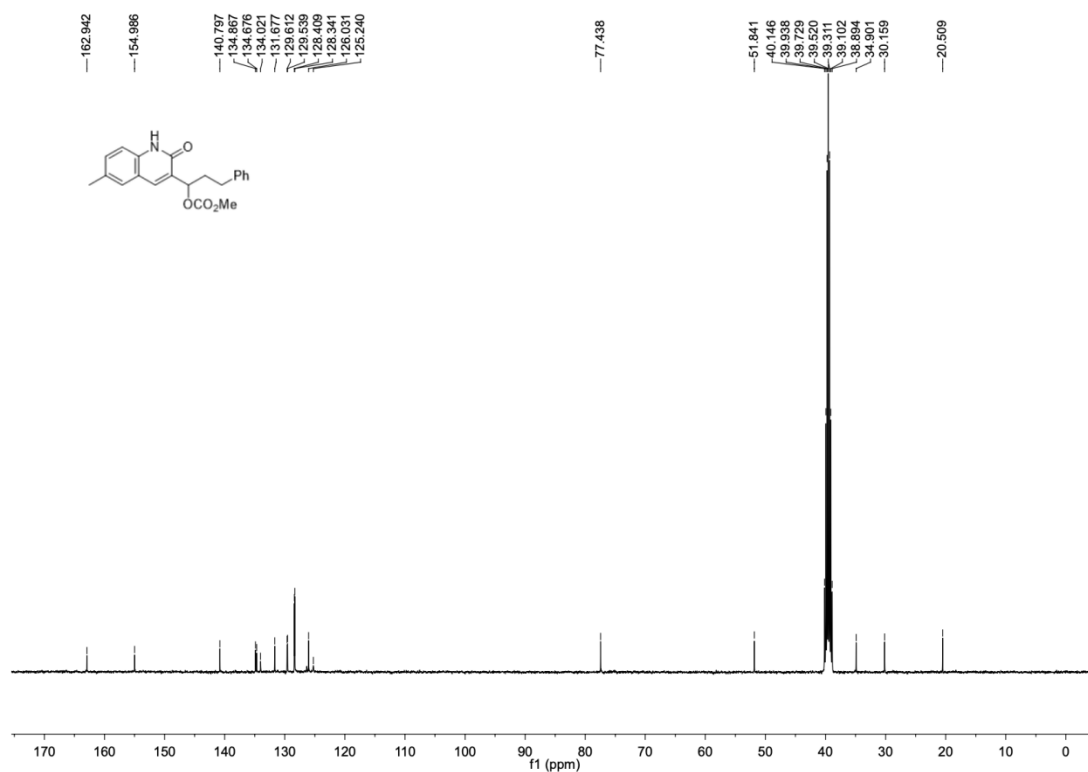
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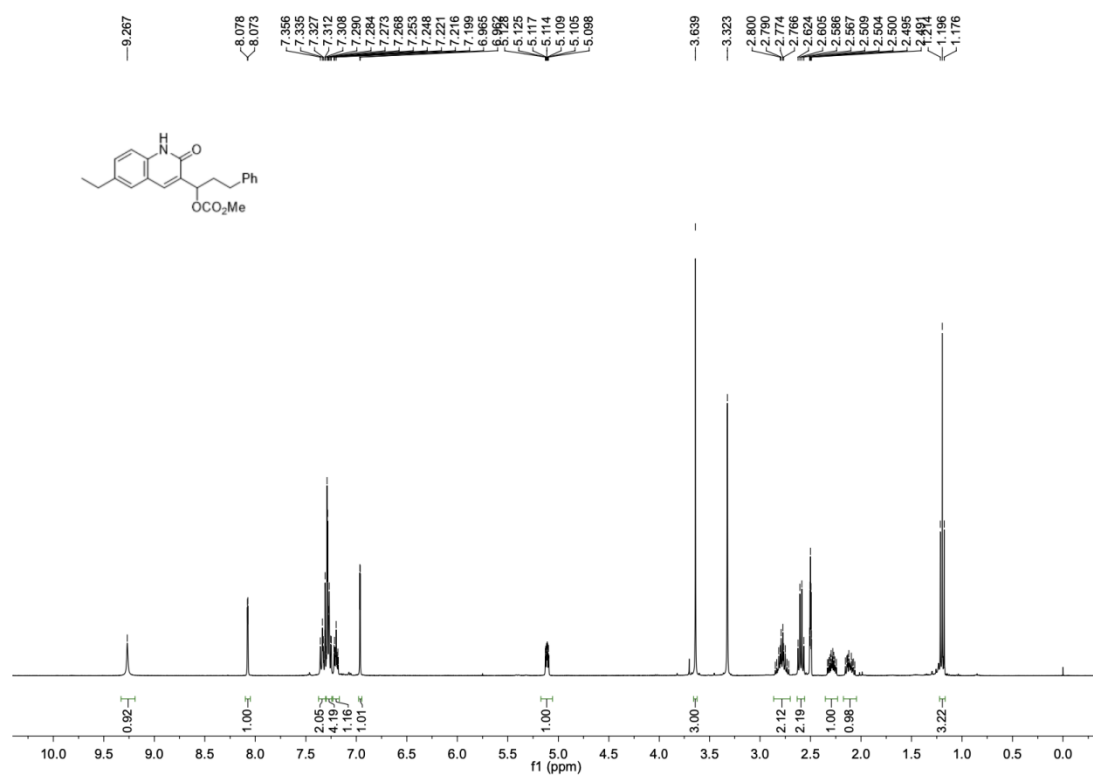
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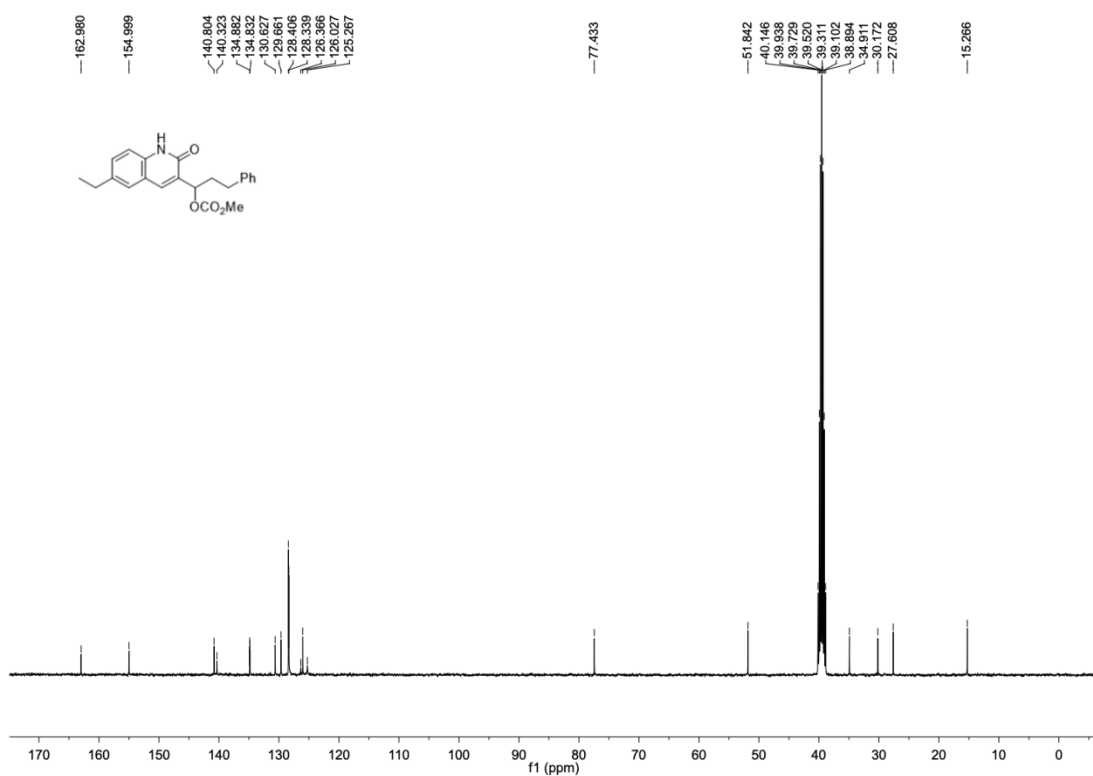
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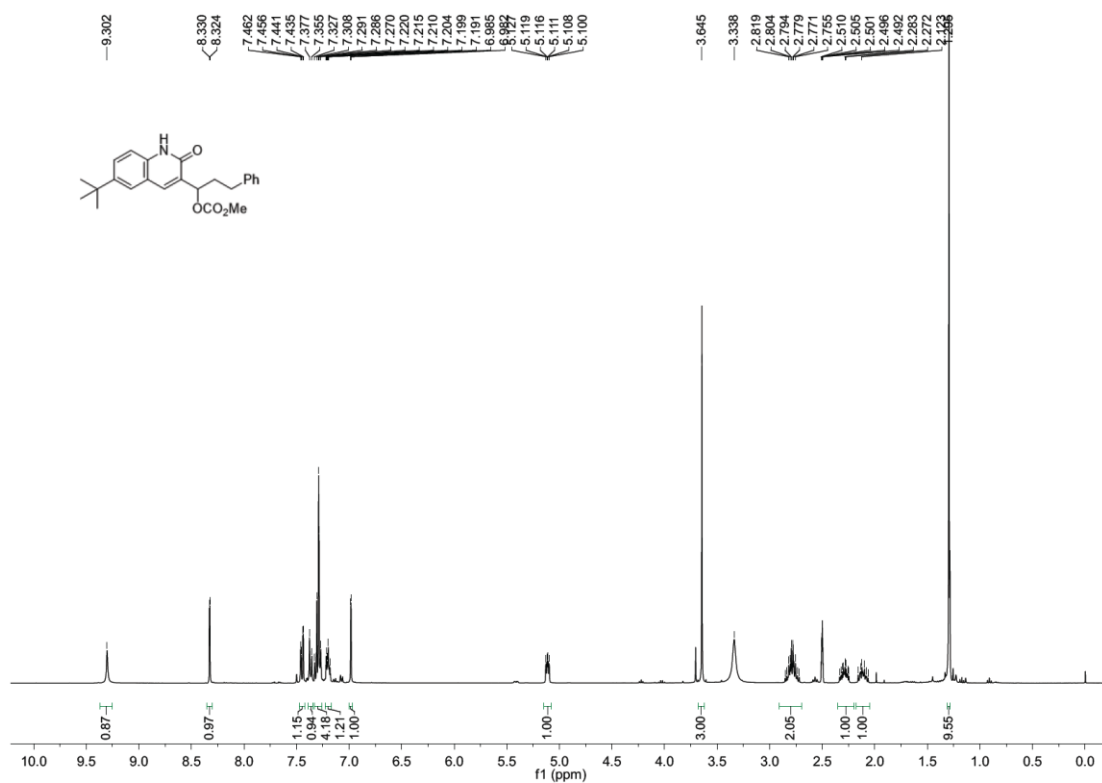
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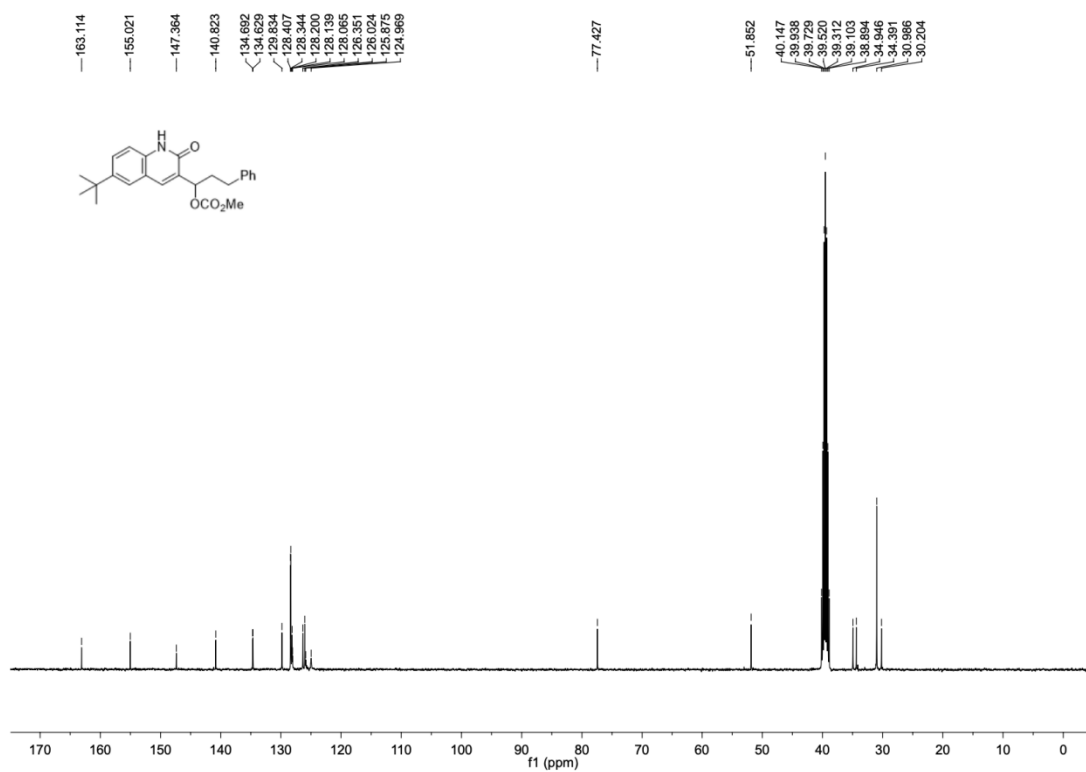
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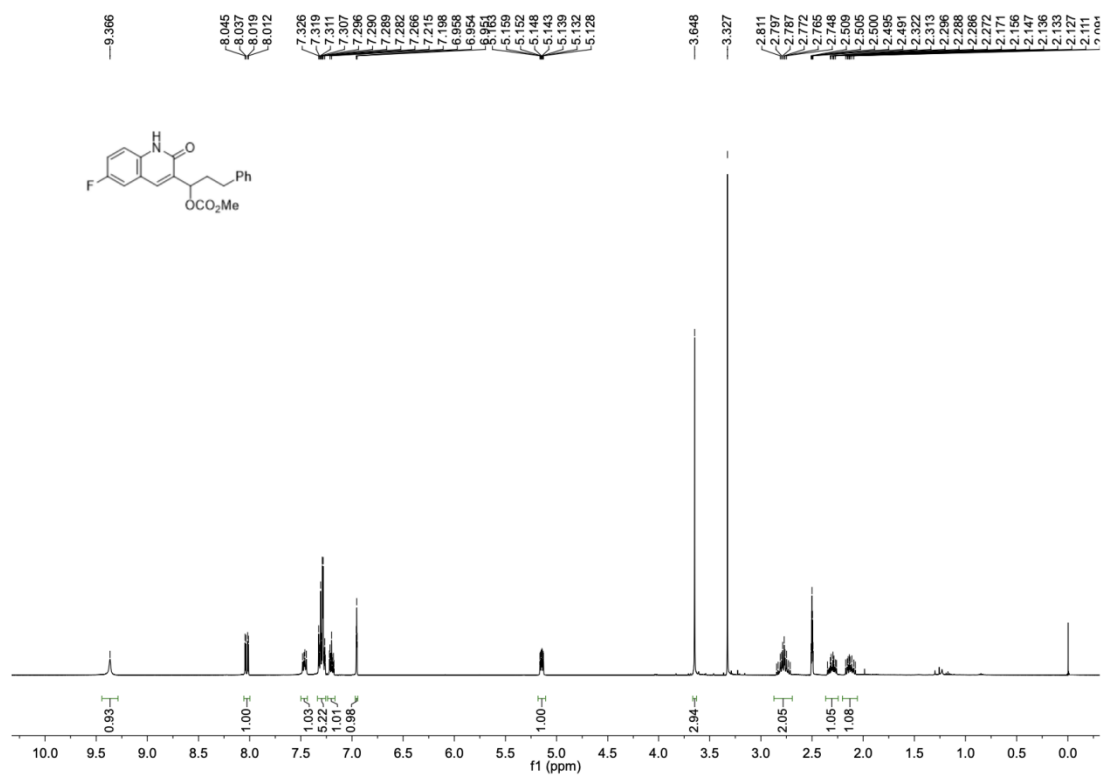
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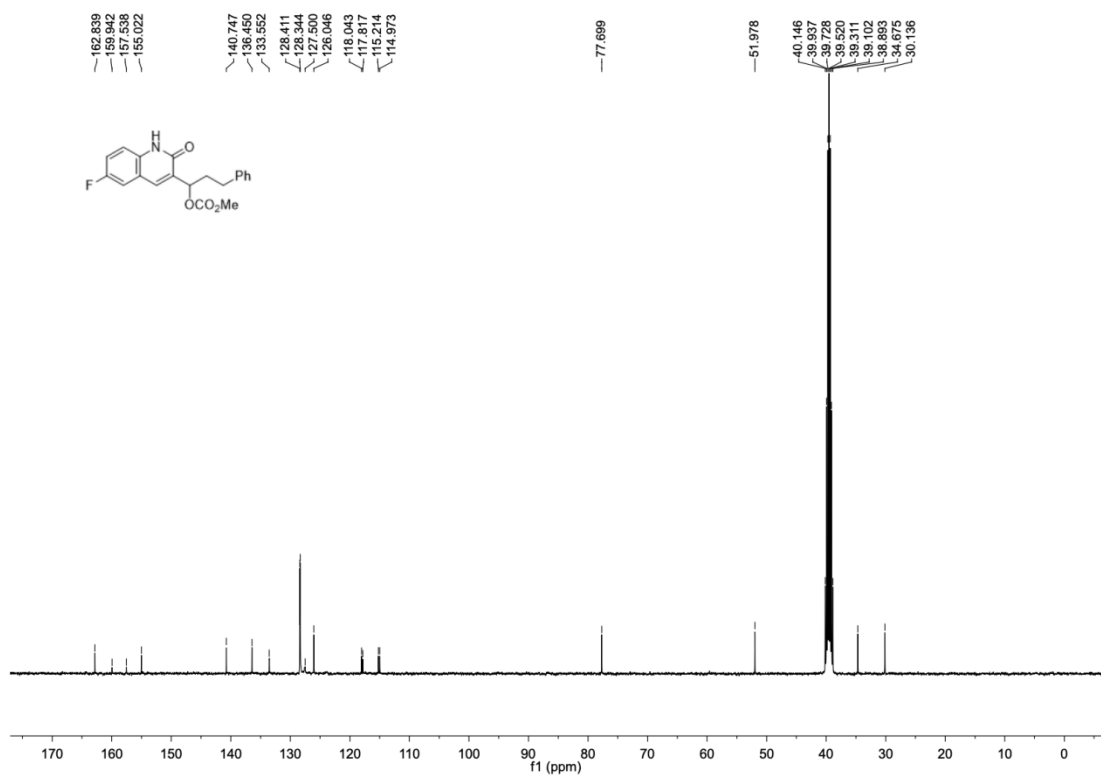
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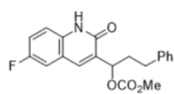
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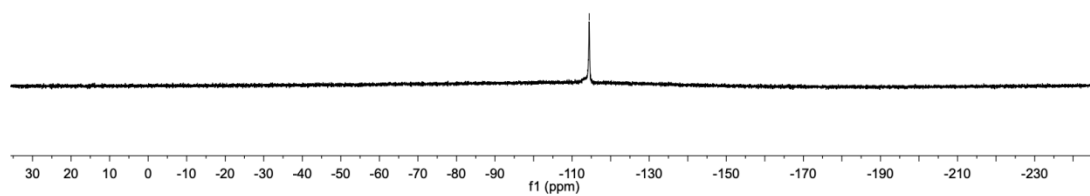
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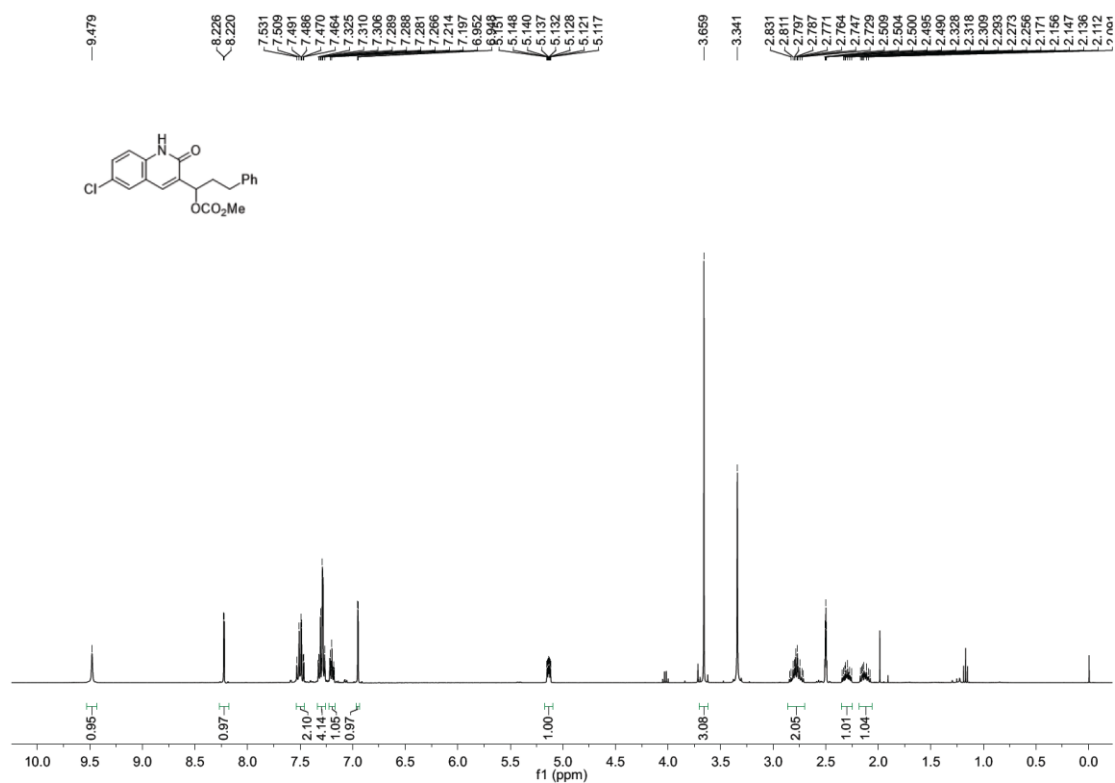
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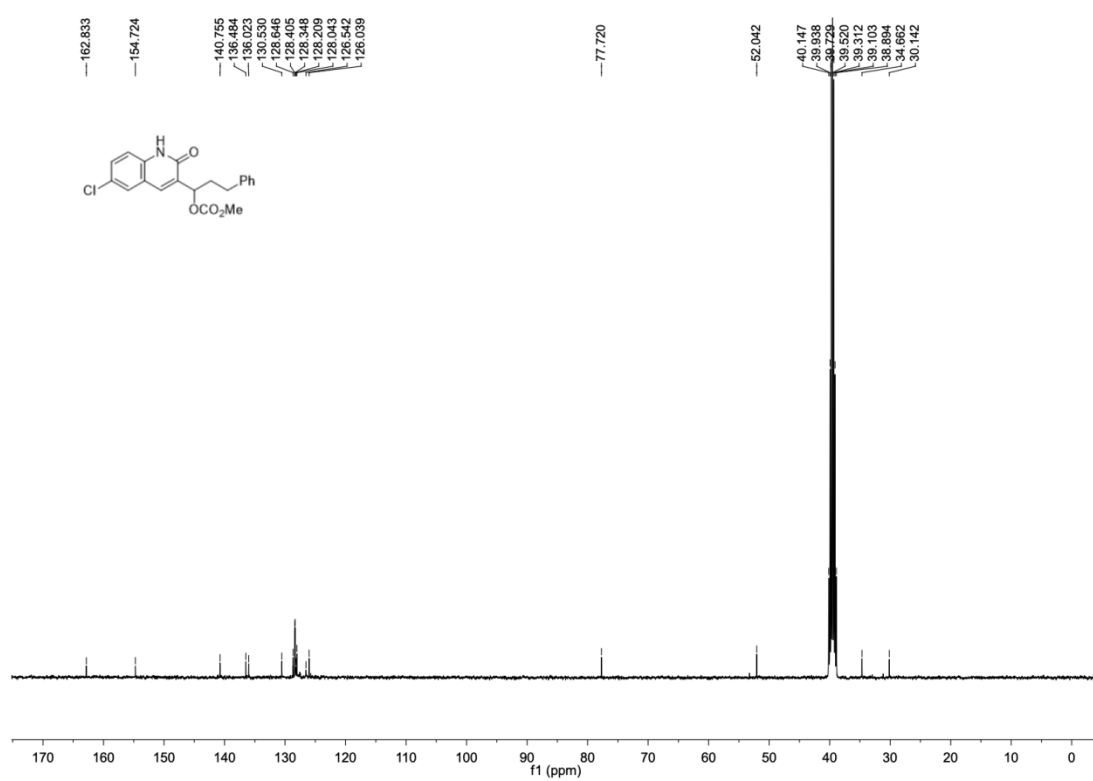
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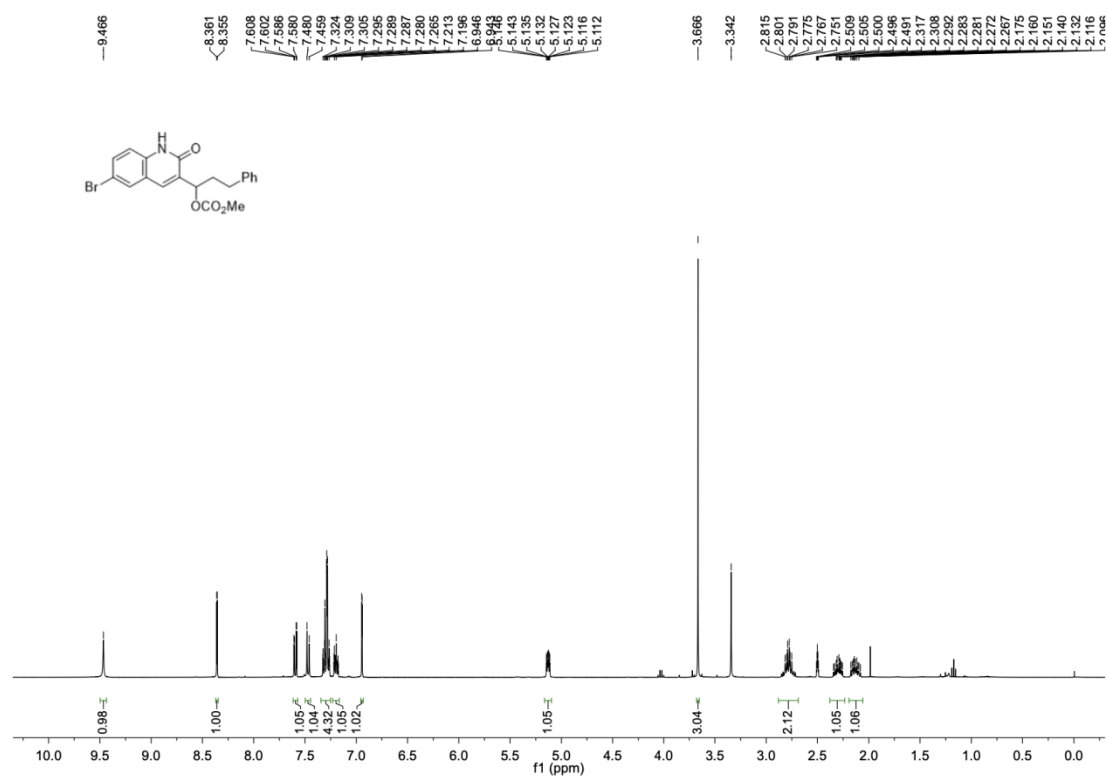
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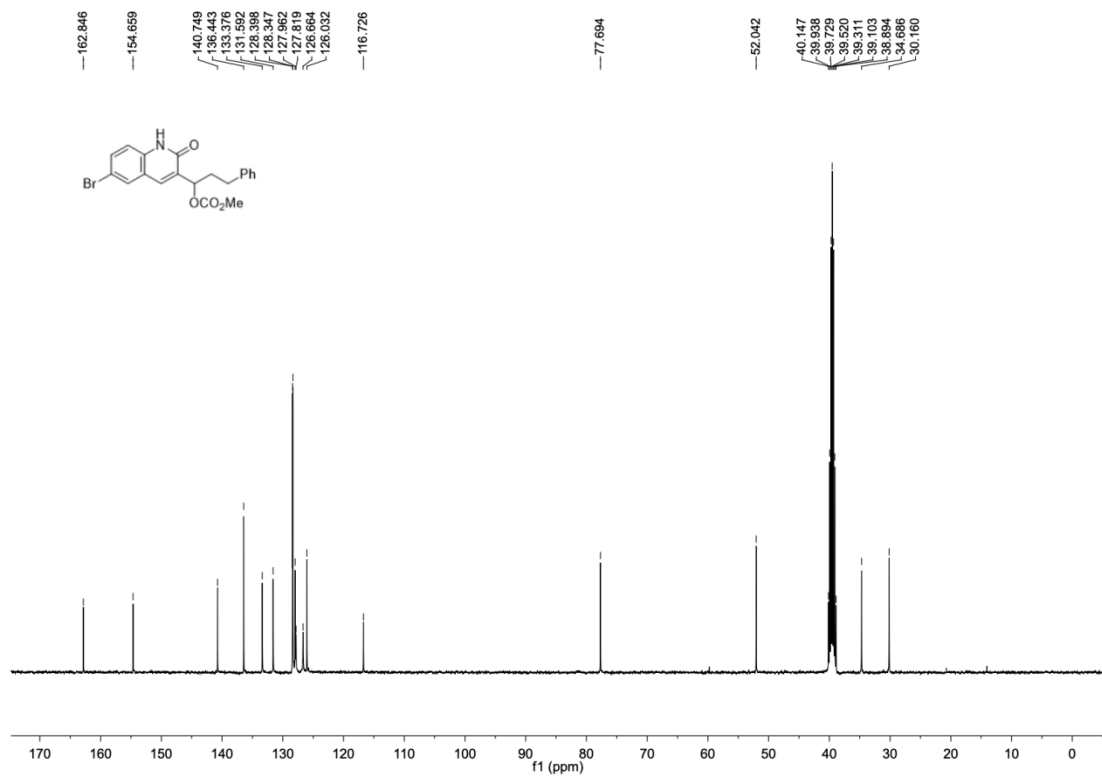
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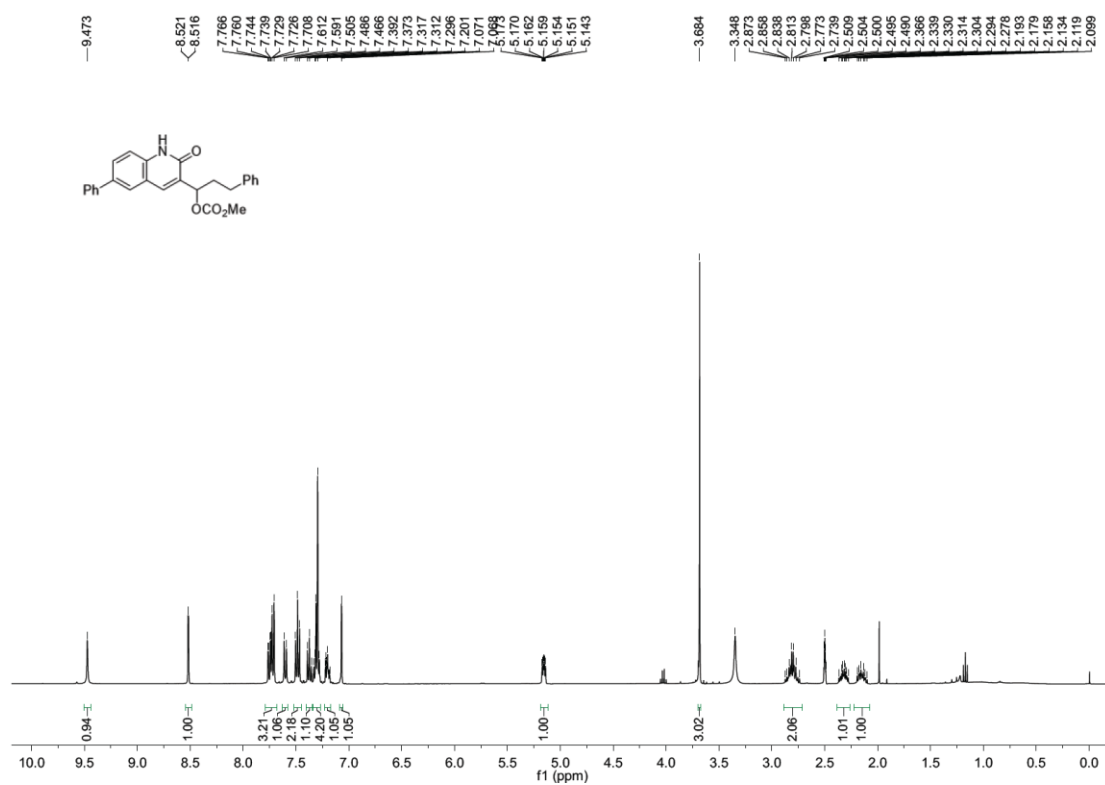
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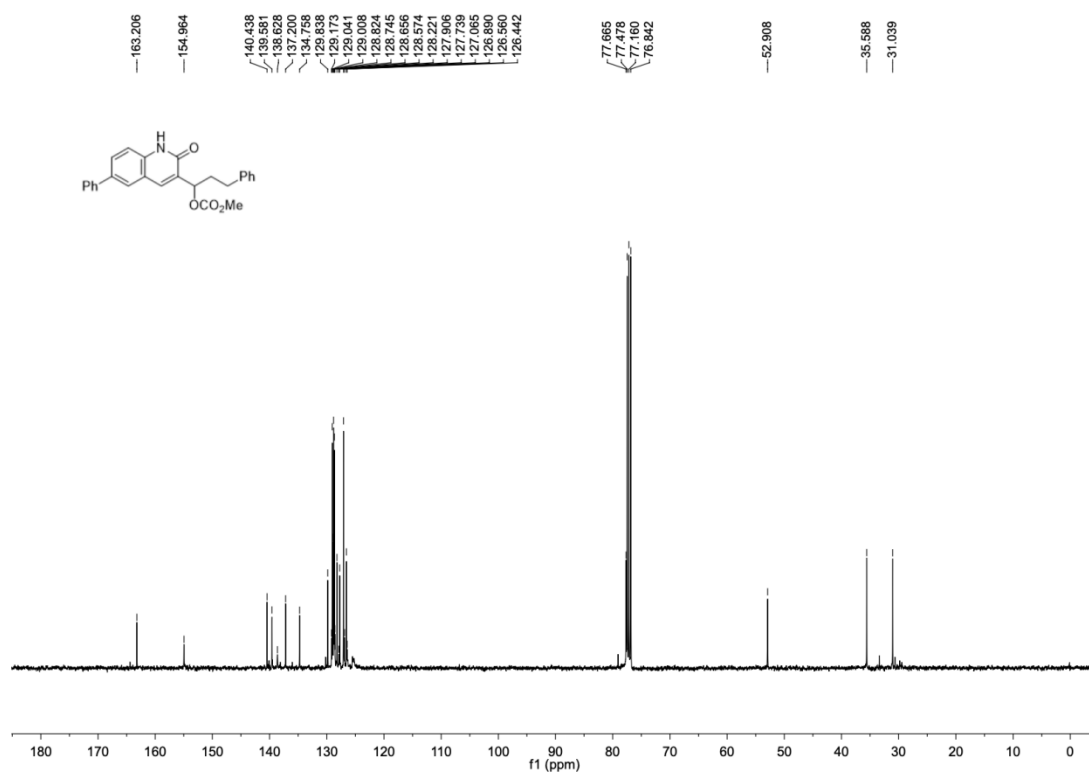
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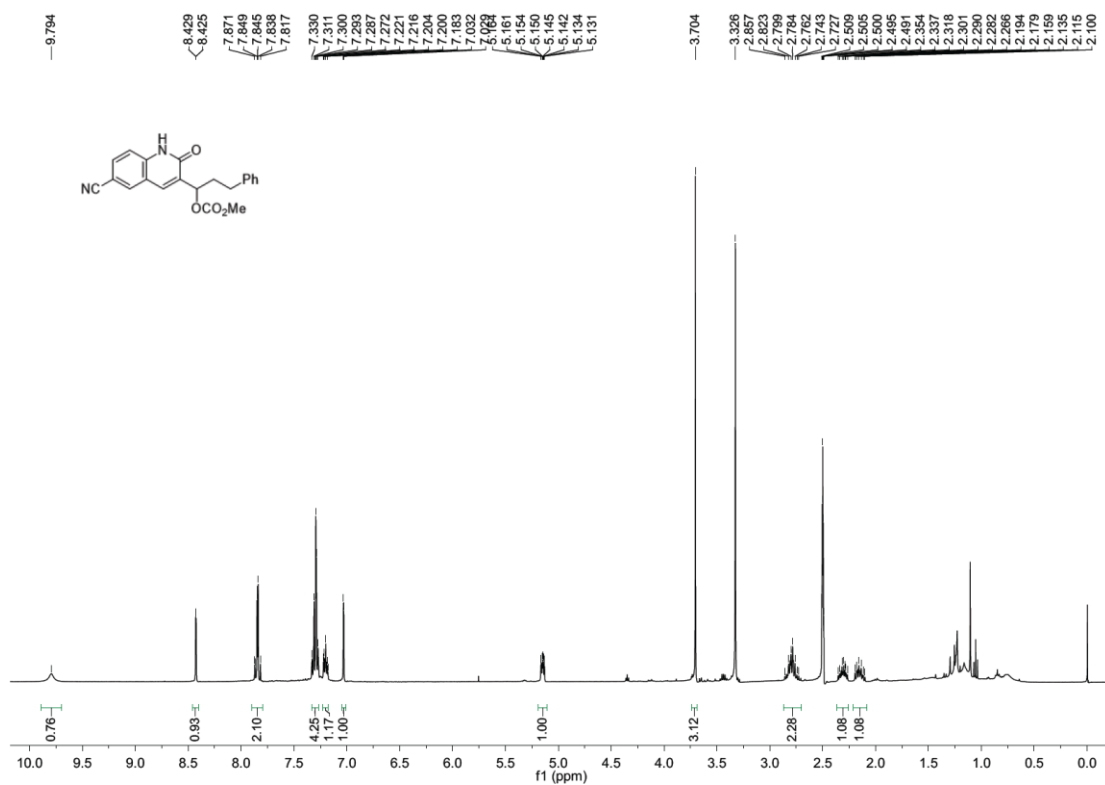
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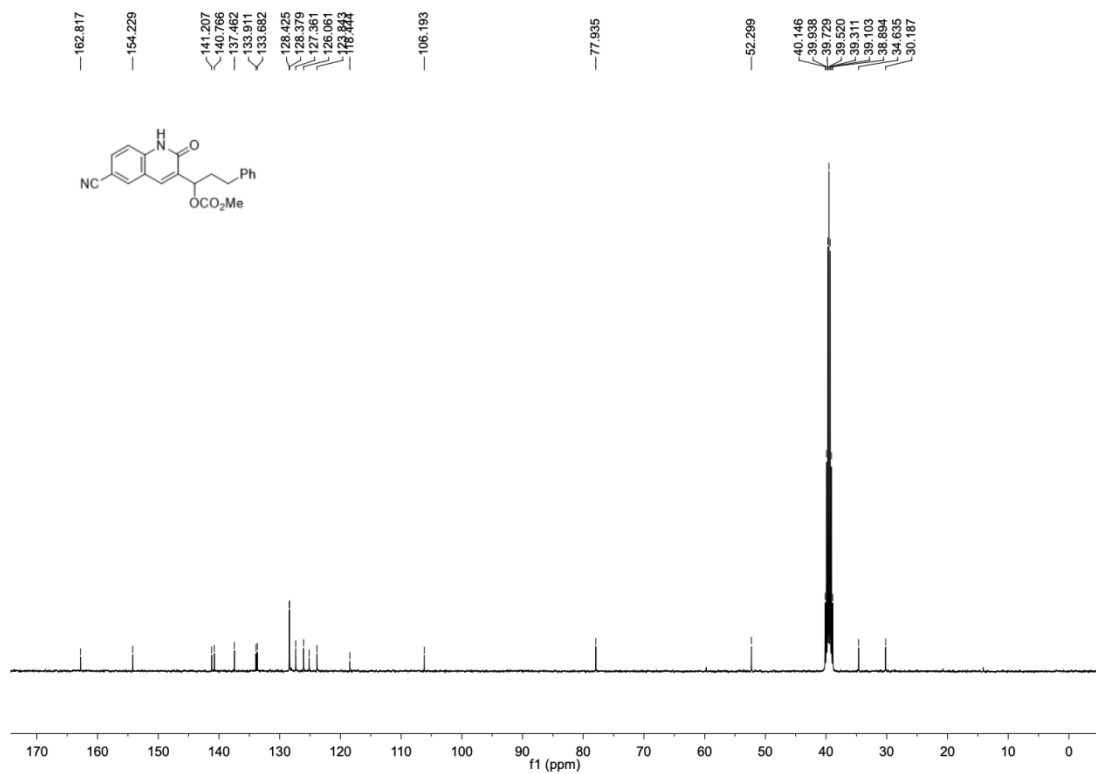
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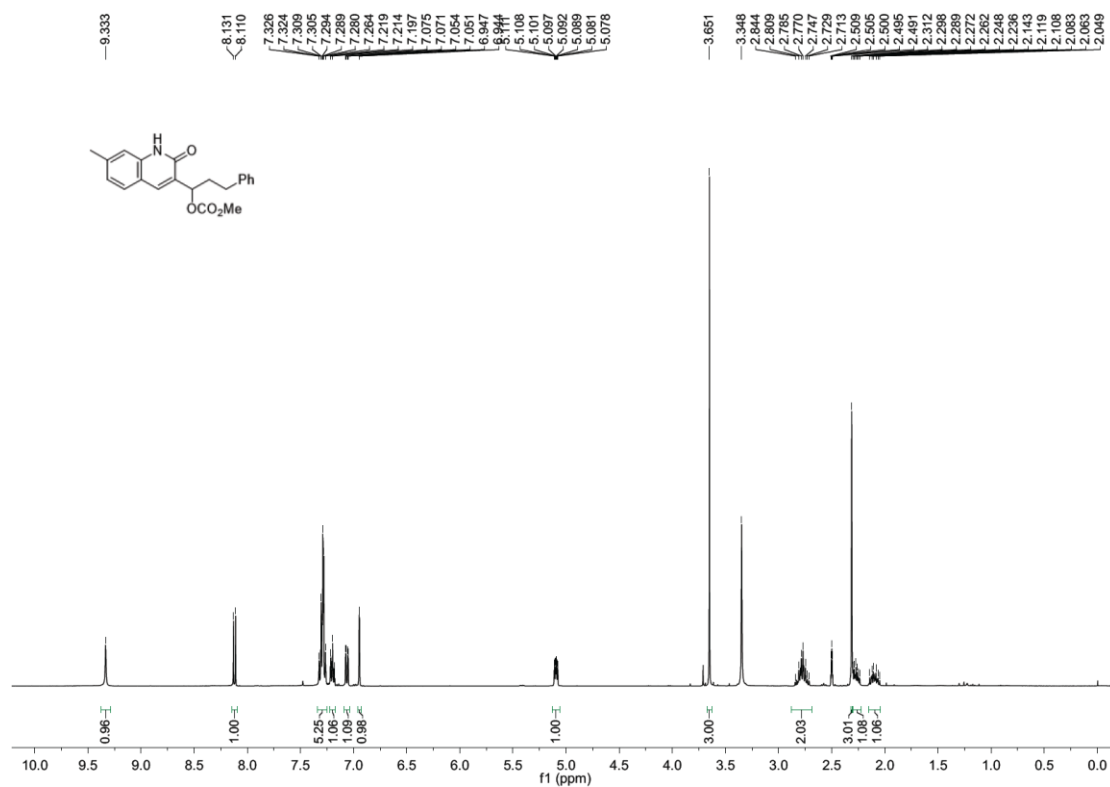
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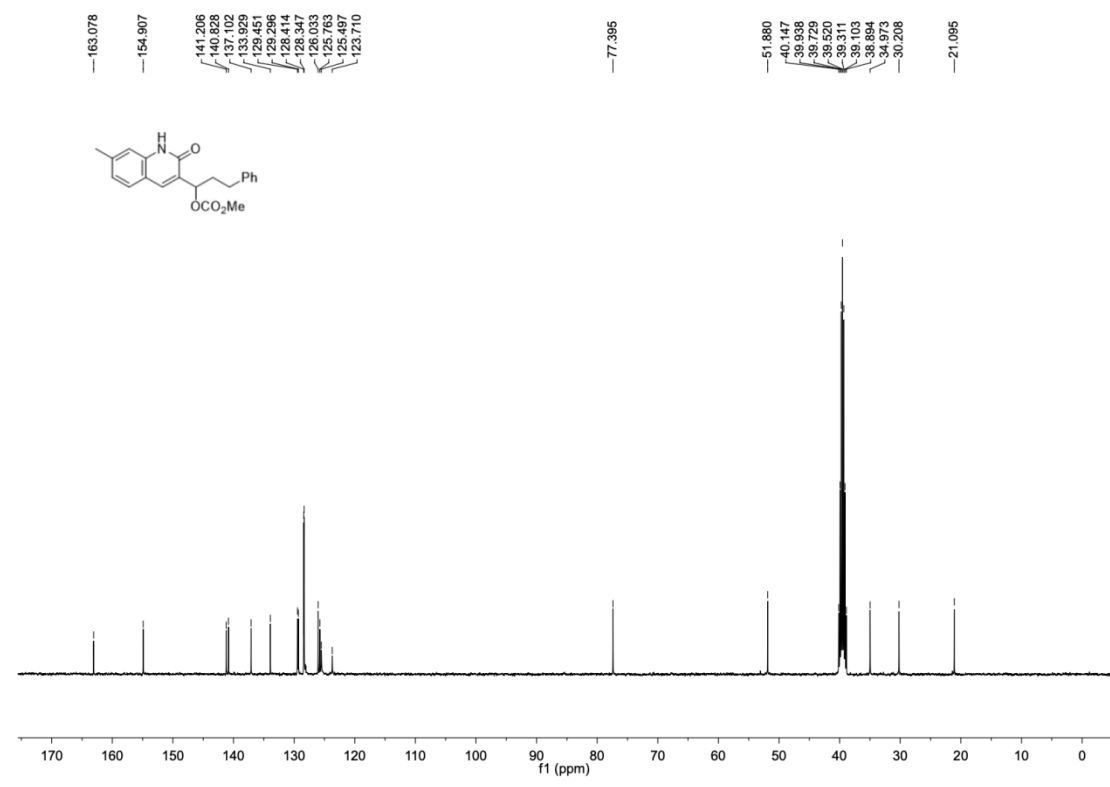
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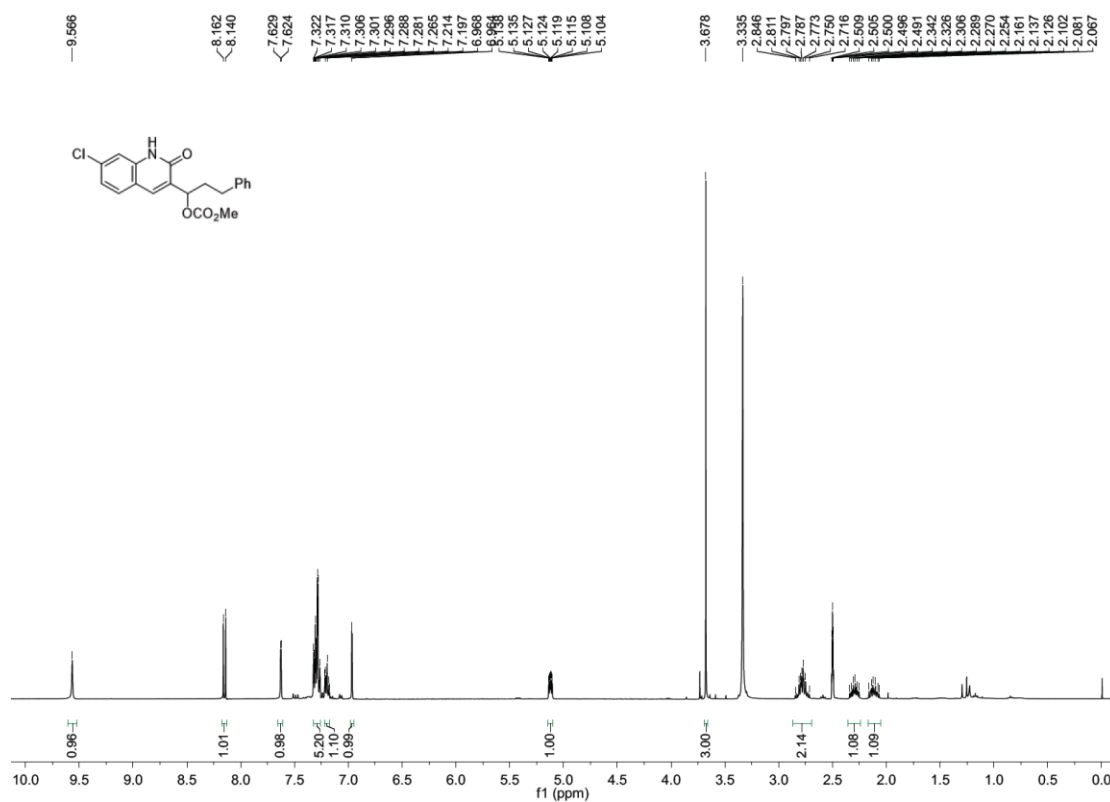
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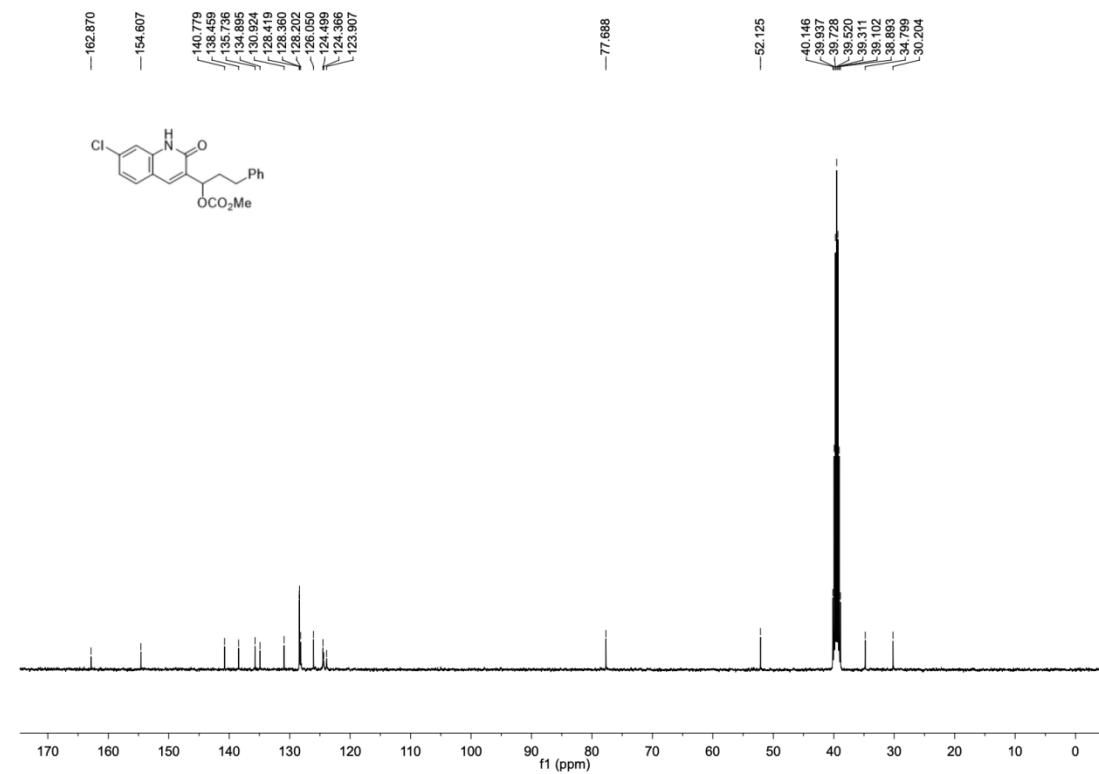
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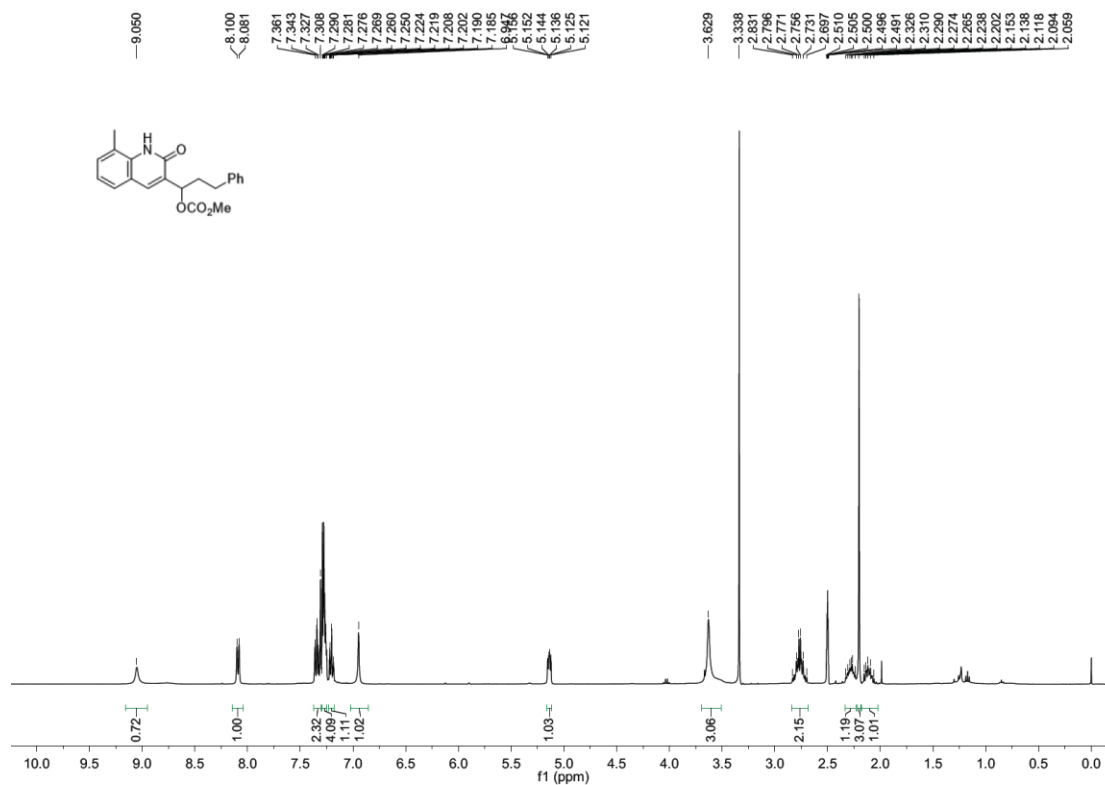
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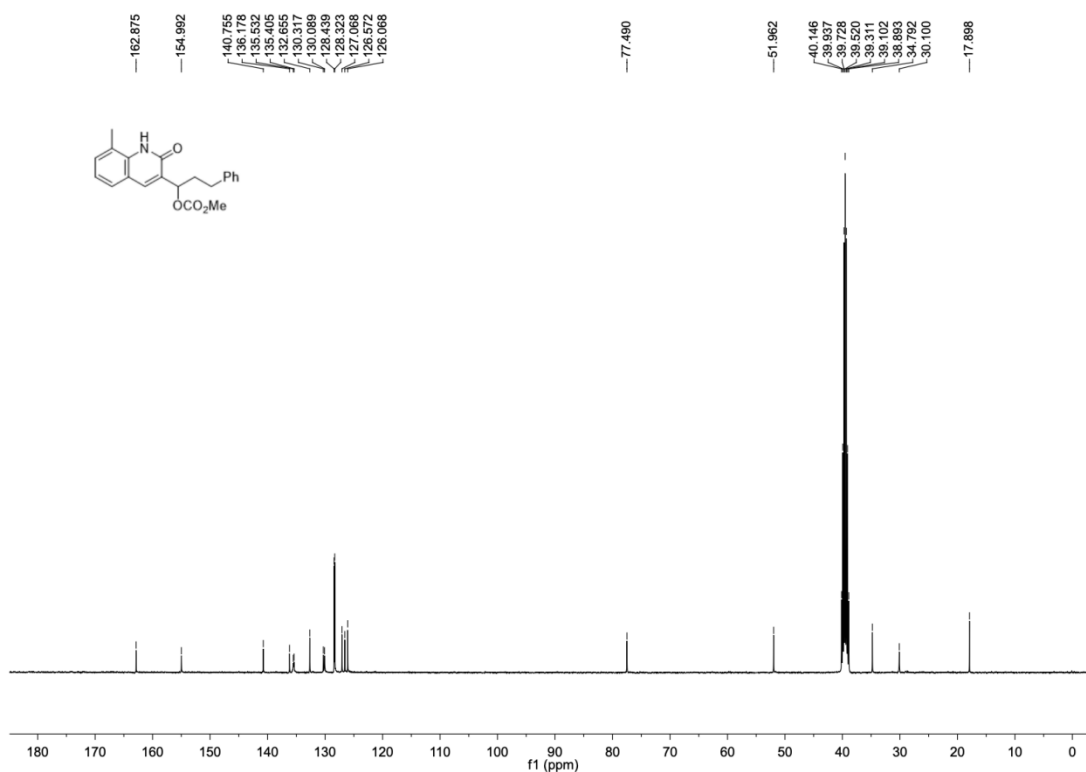
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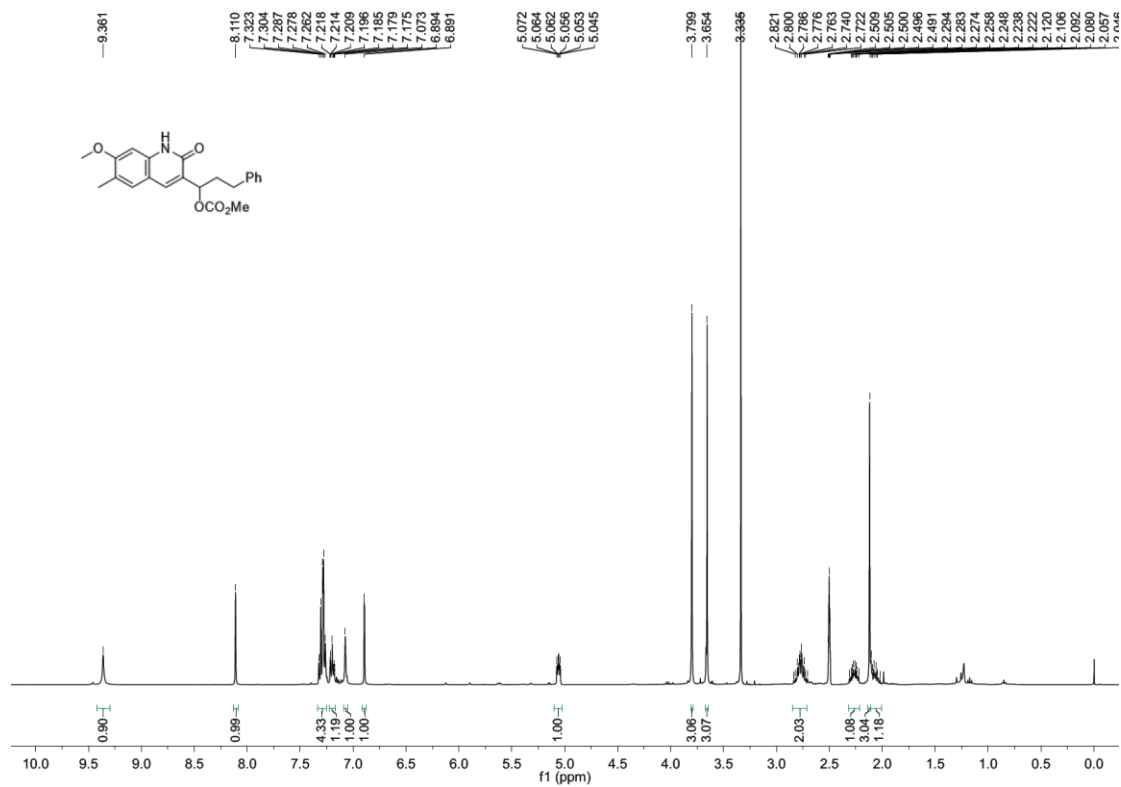
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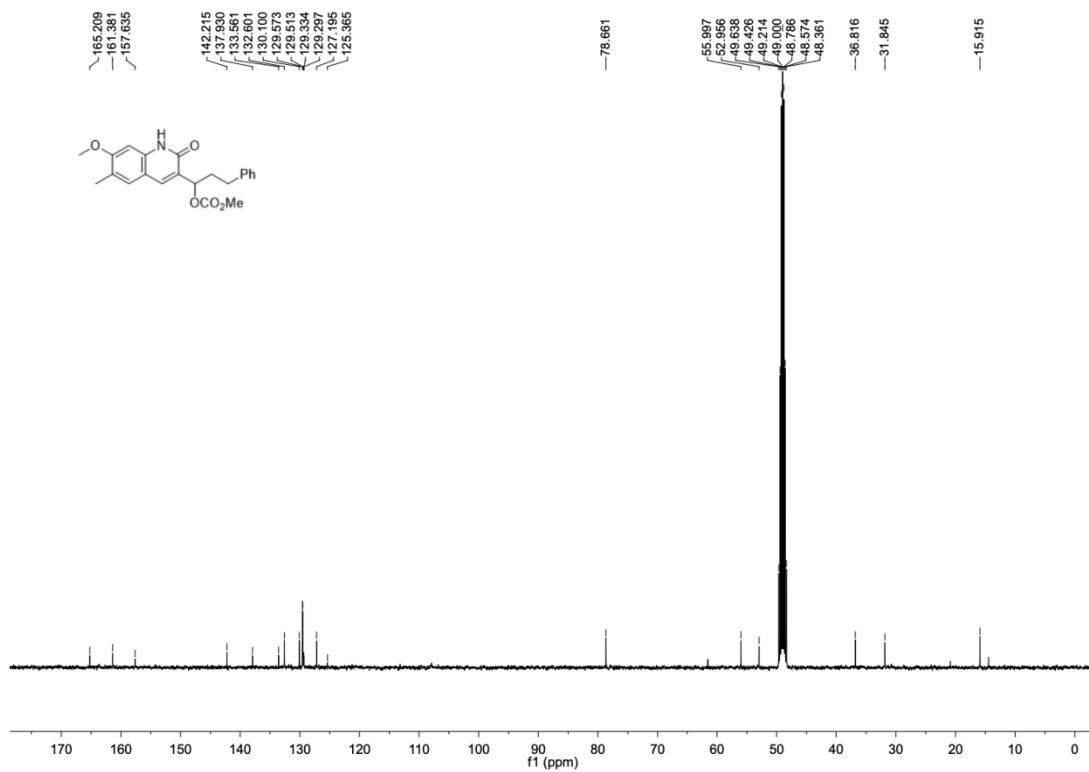
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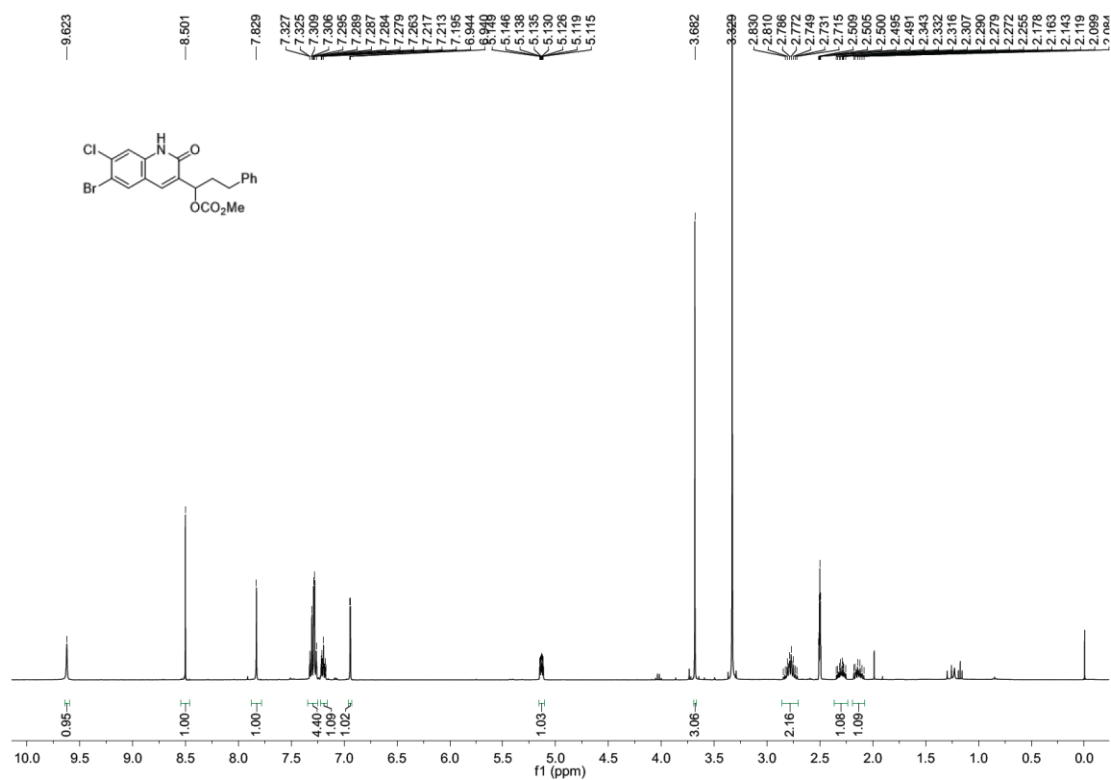
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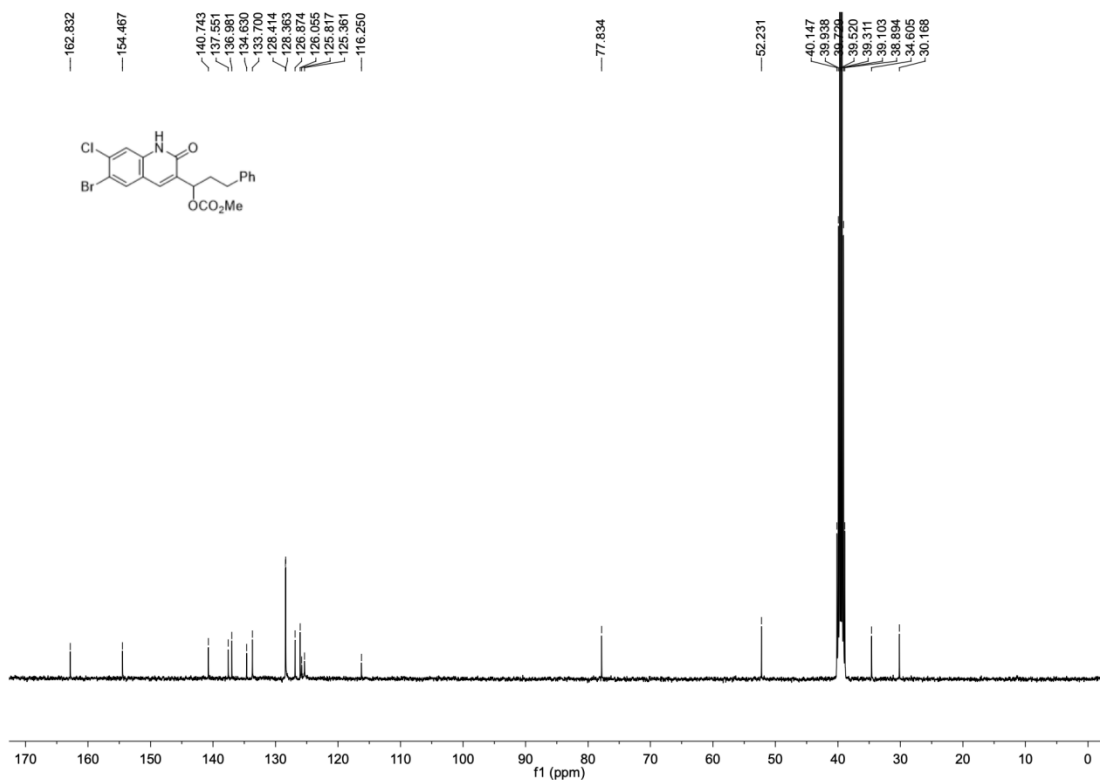
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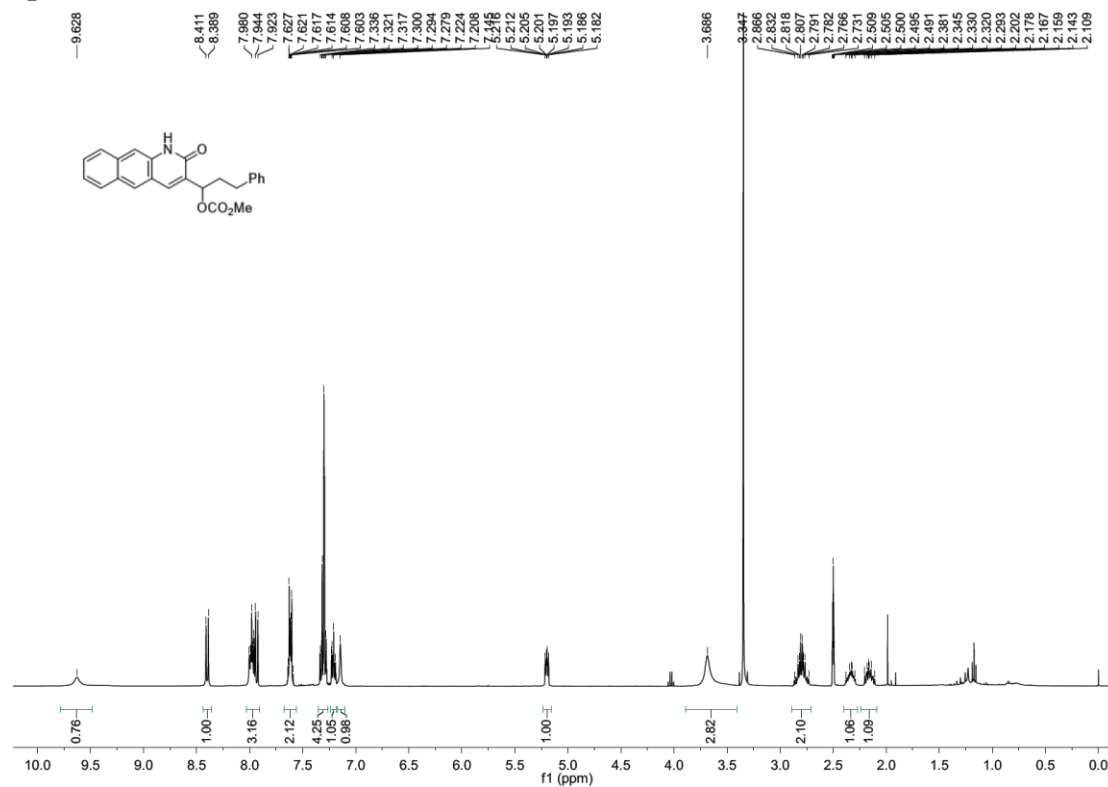
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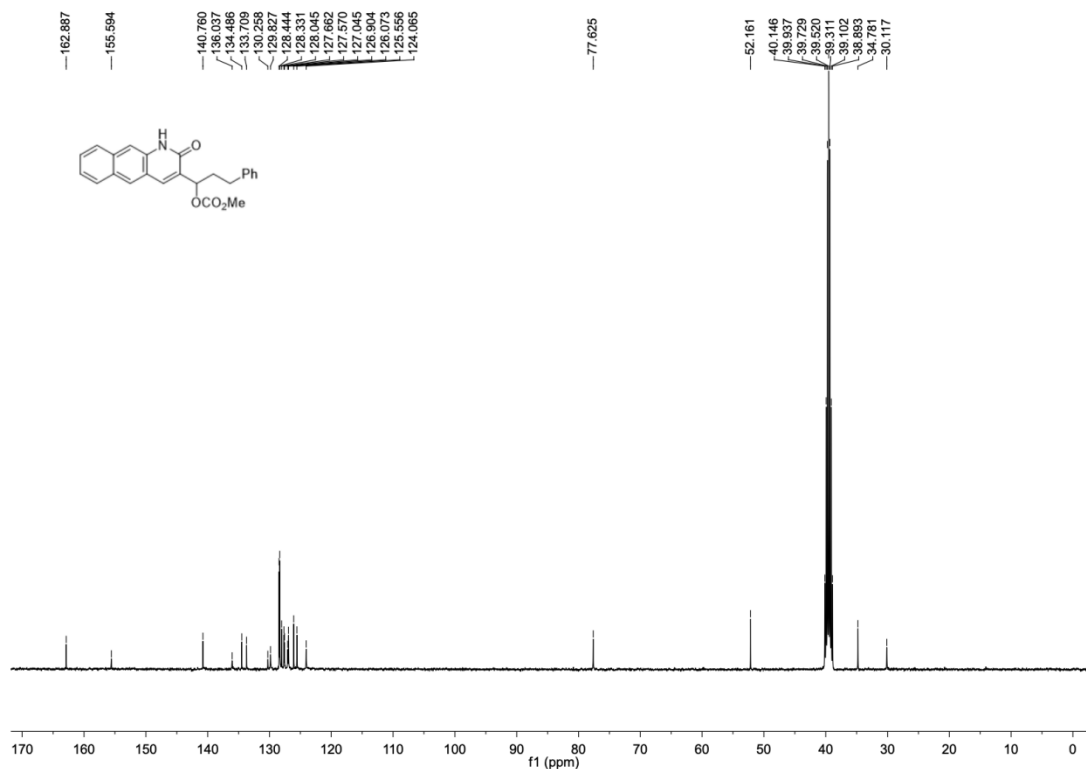
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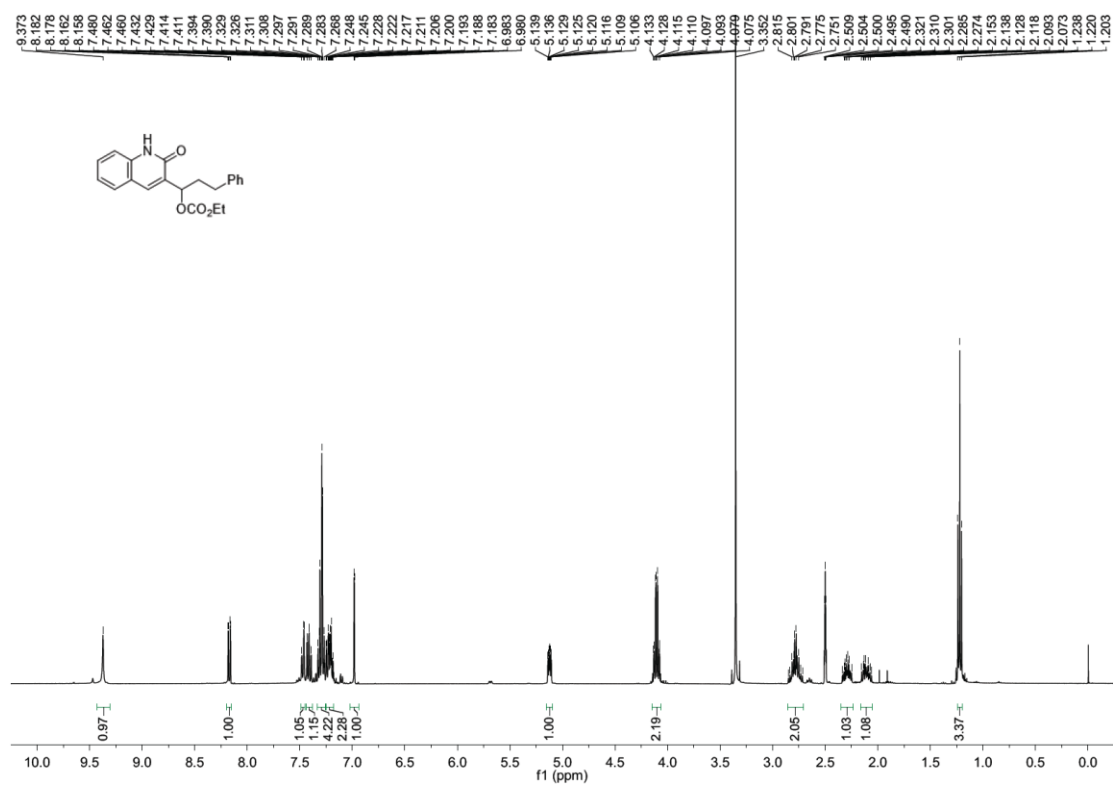
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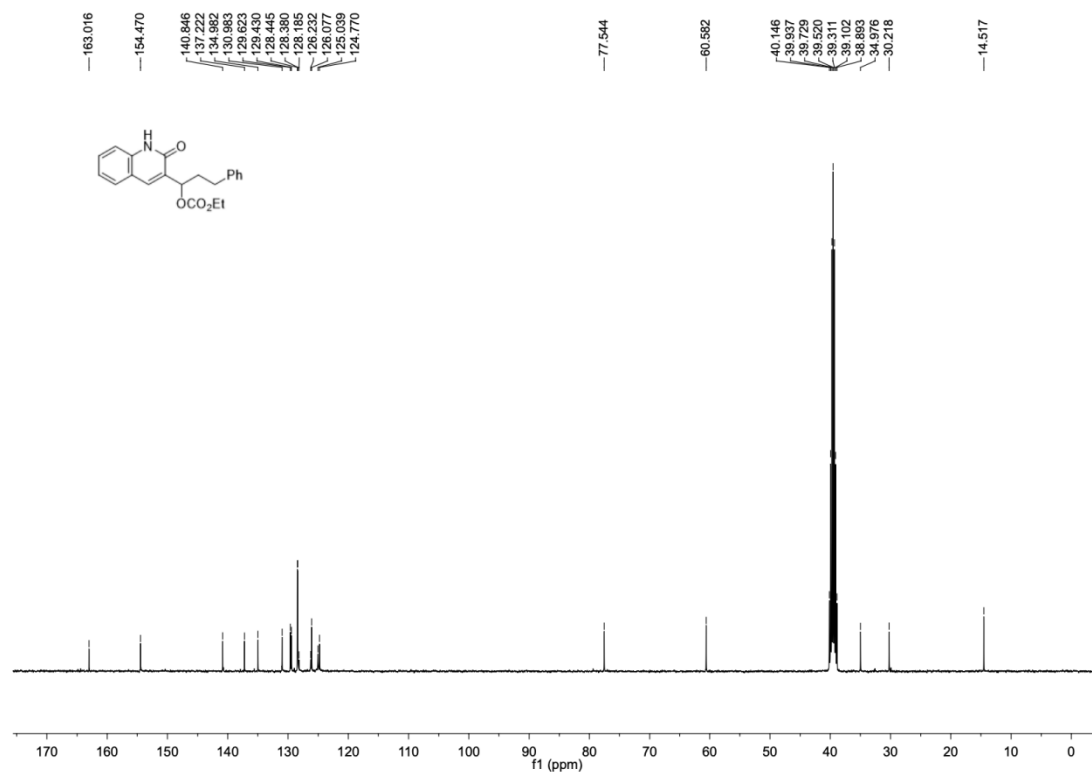
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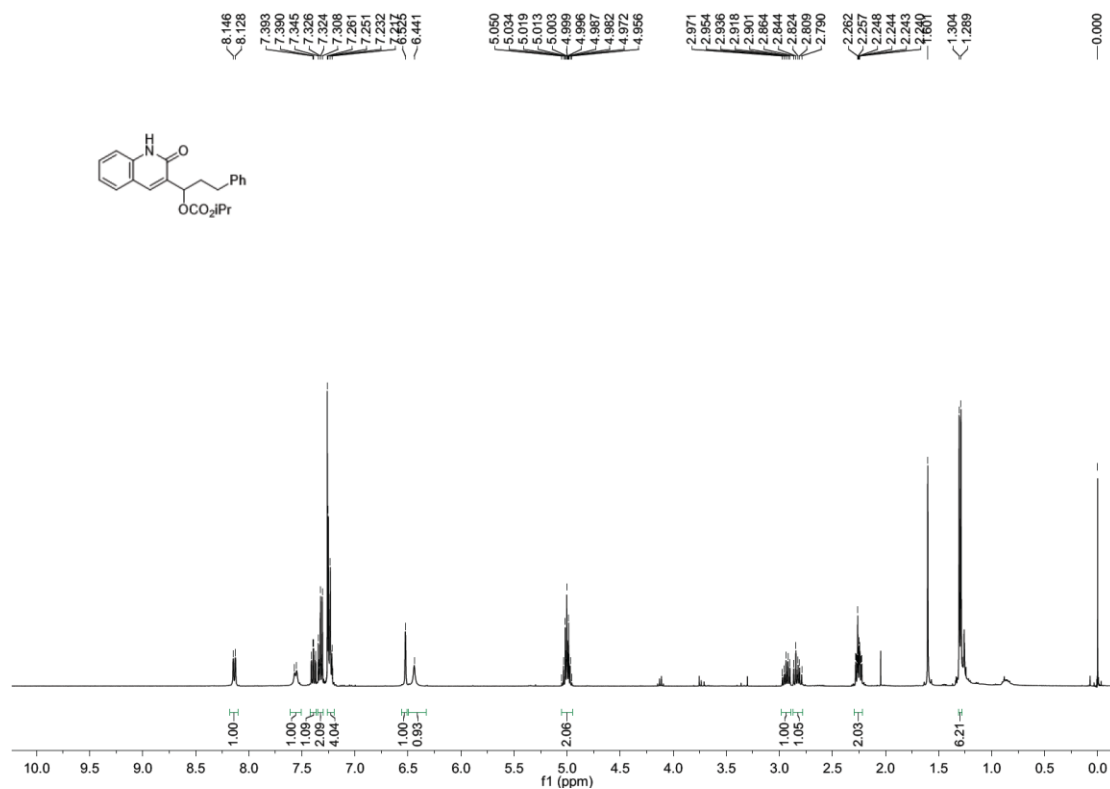
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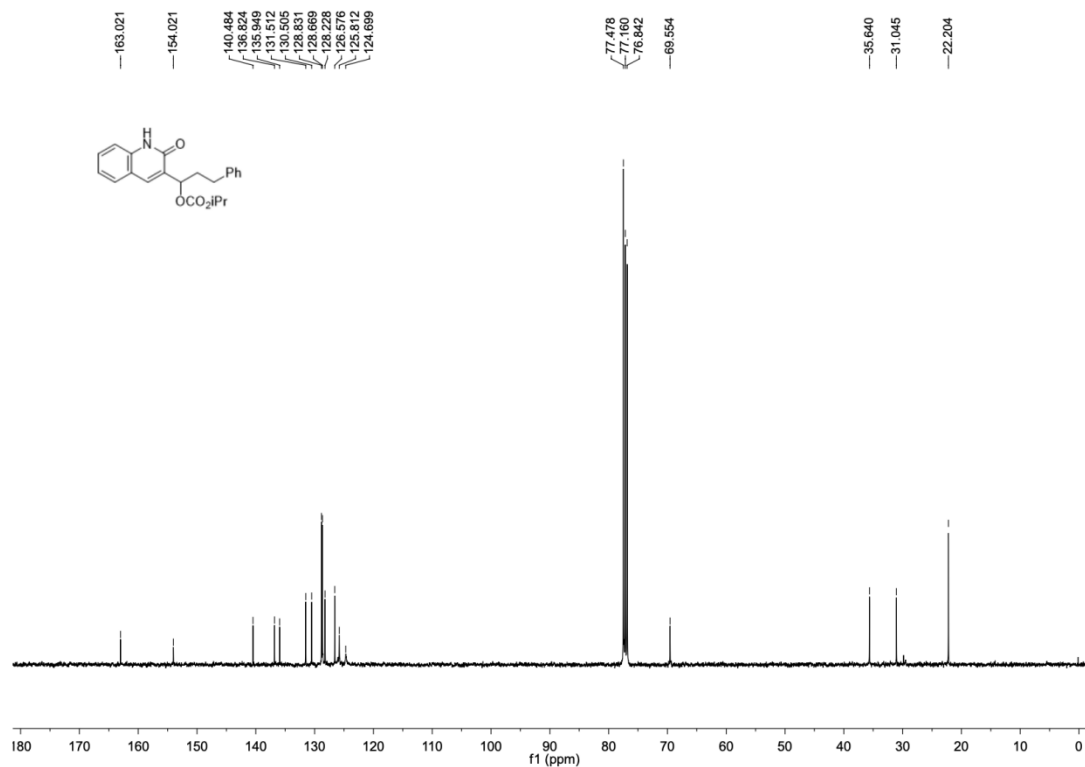
3q-¹³C NMR (100 MHz, DMSO-*d*₆)



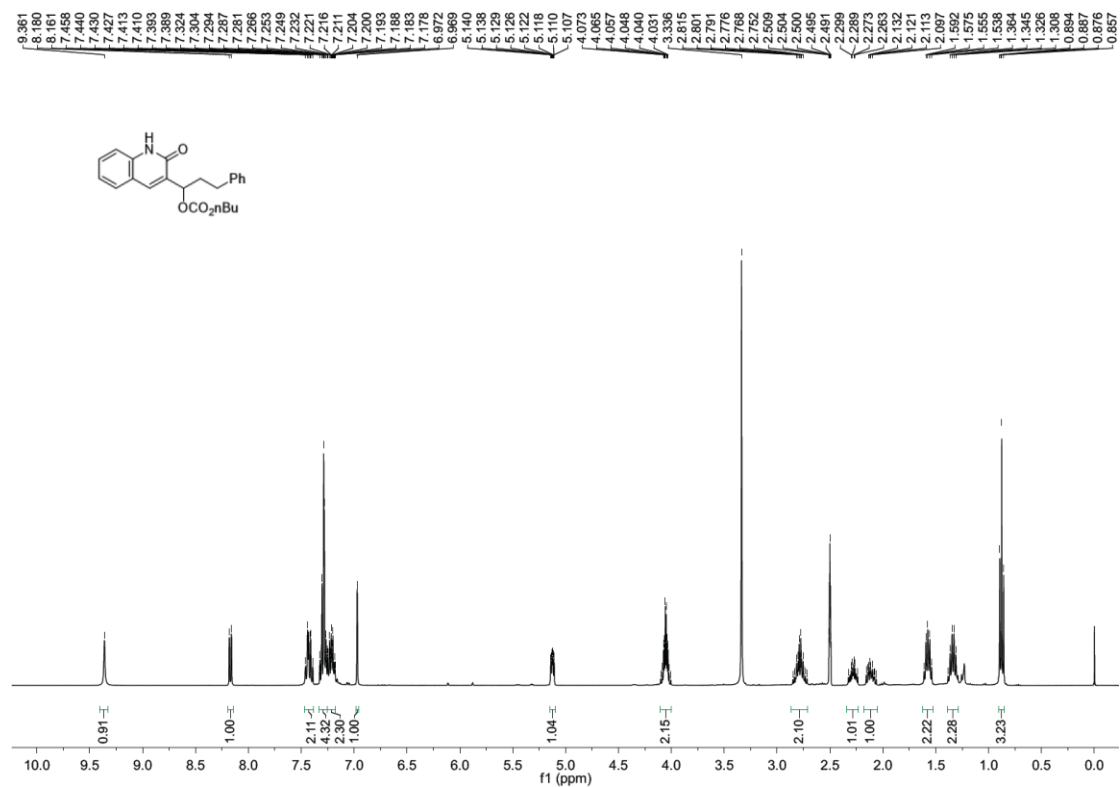
3r-¹H NMR (400 MHz, CDCl₃)



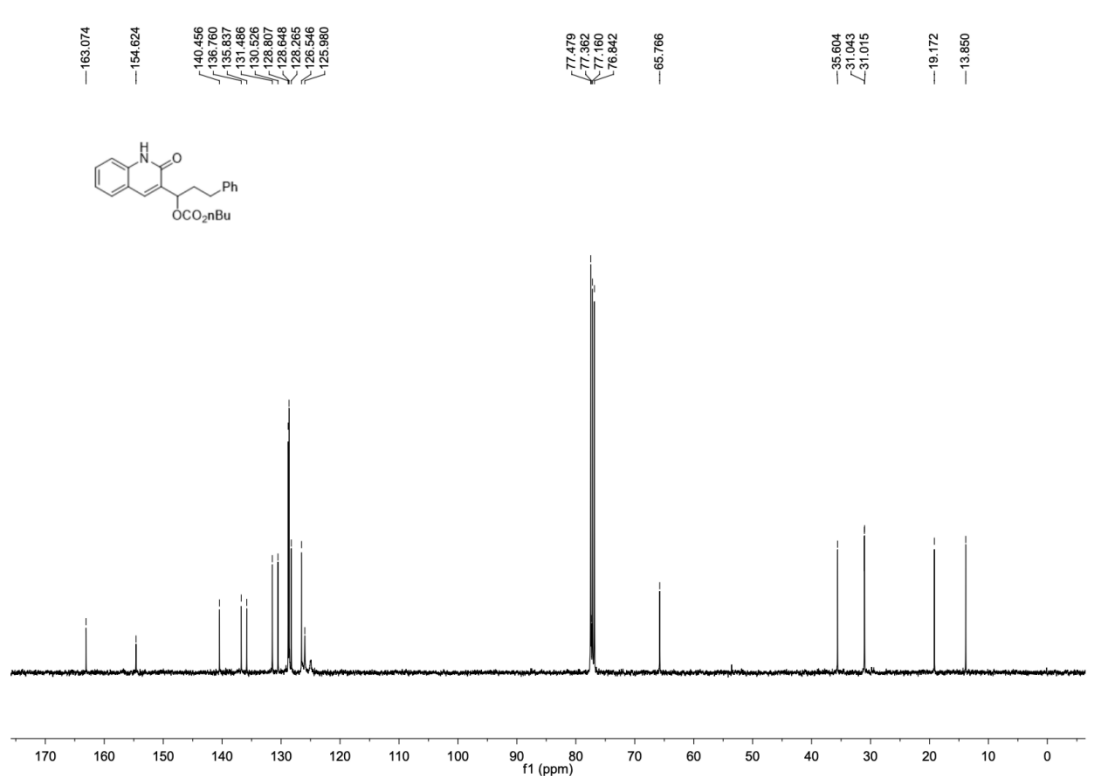
3r-¹³C NMR (100 MHz, CDCl₃)



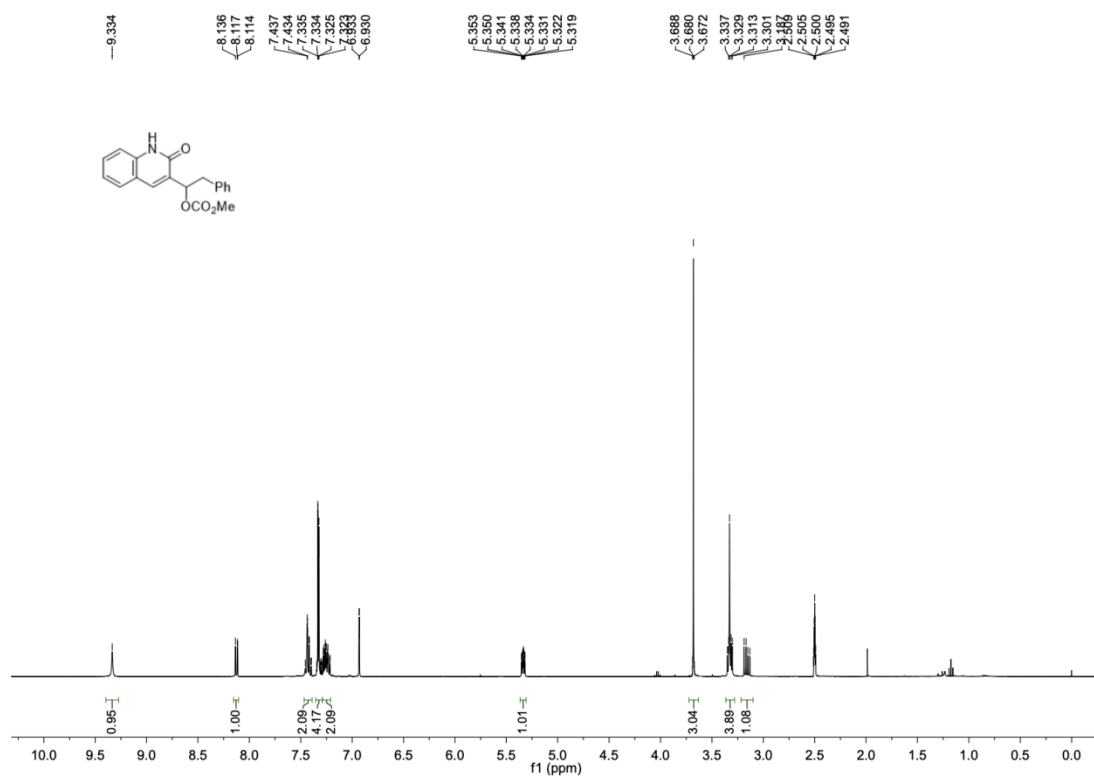
3s-¹H NMR (400 MHz, DMSO-*d*₆)



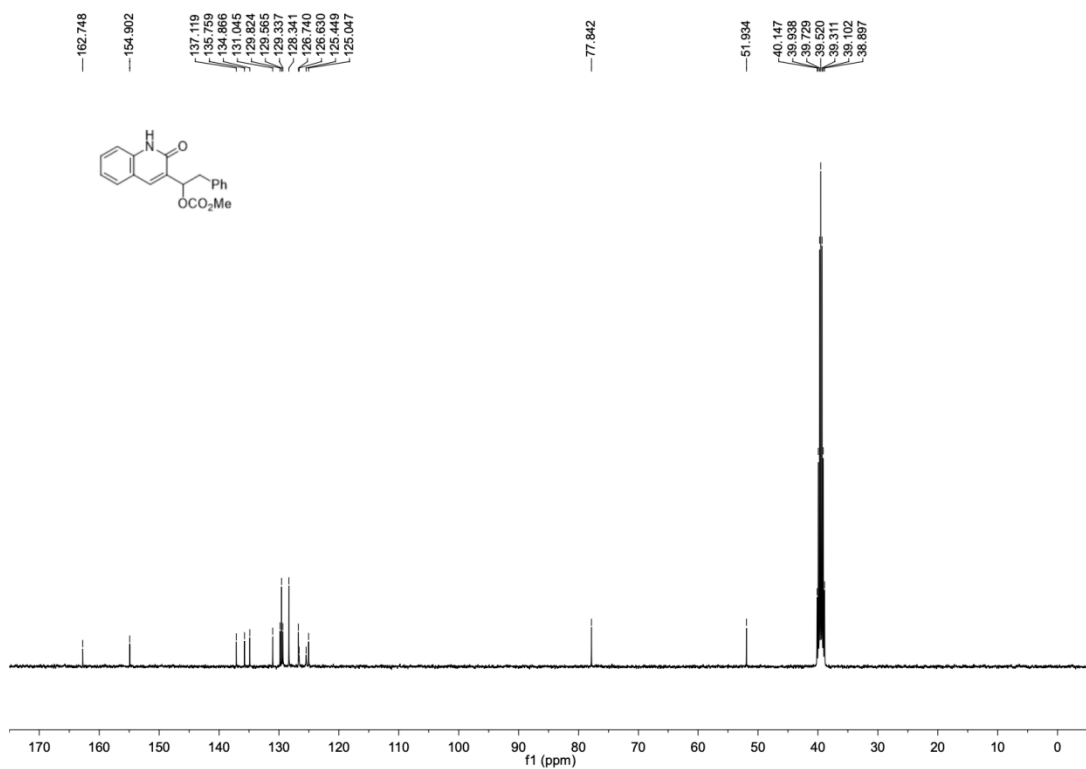
3s-¹³C NMR (100 MHz, CDCl₃)



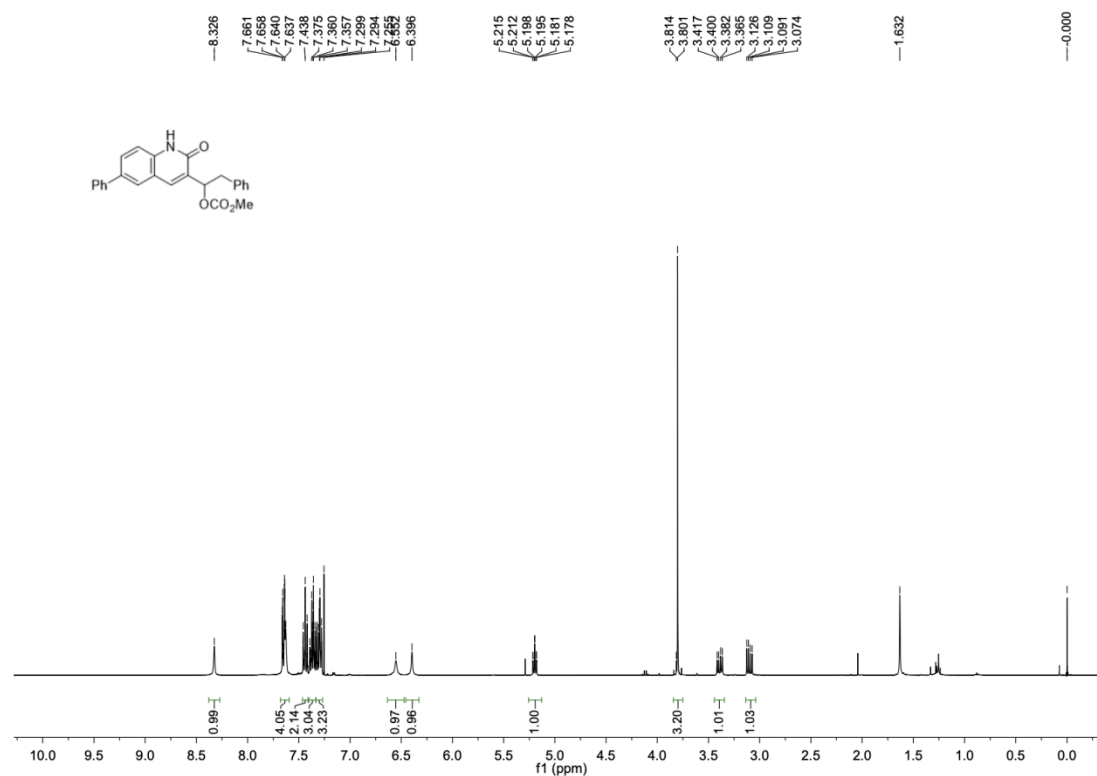
3t-¹H NMR (400 MHz, DMSO-*d*₆)



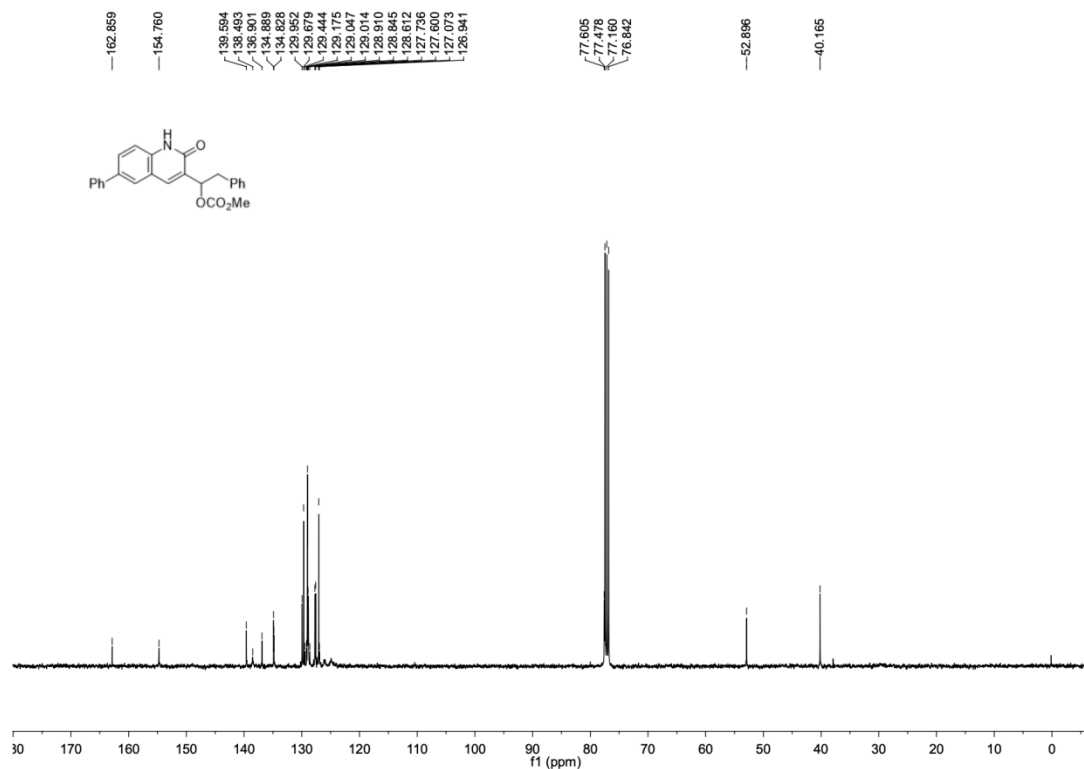
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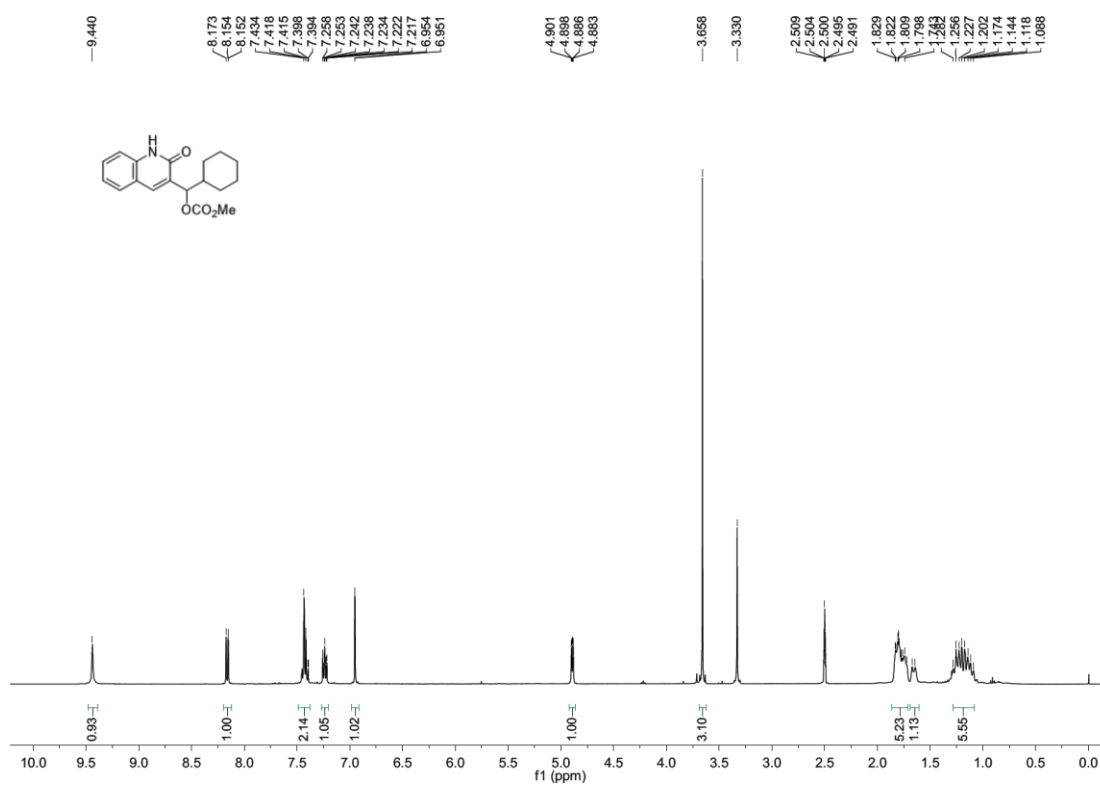
3u-¹H NMR (400 MHz, CDCl₃)



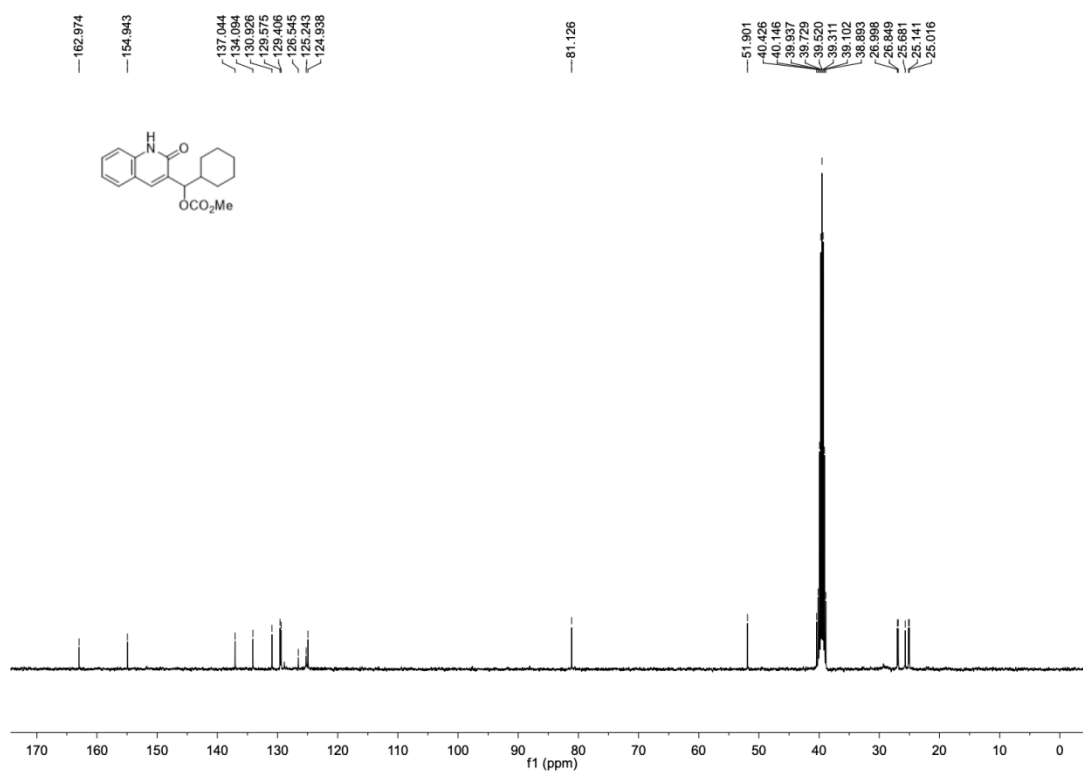
3u-¹³C NMR (100 MHz, CDCl₃)



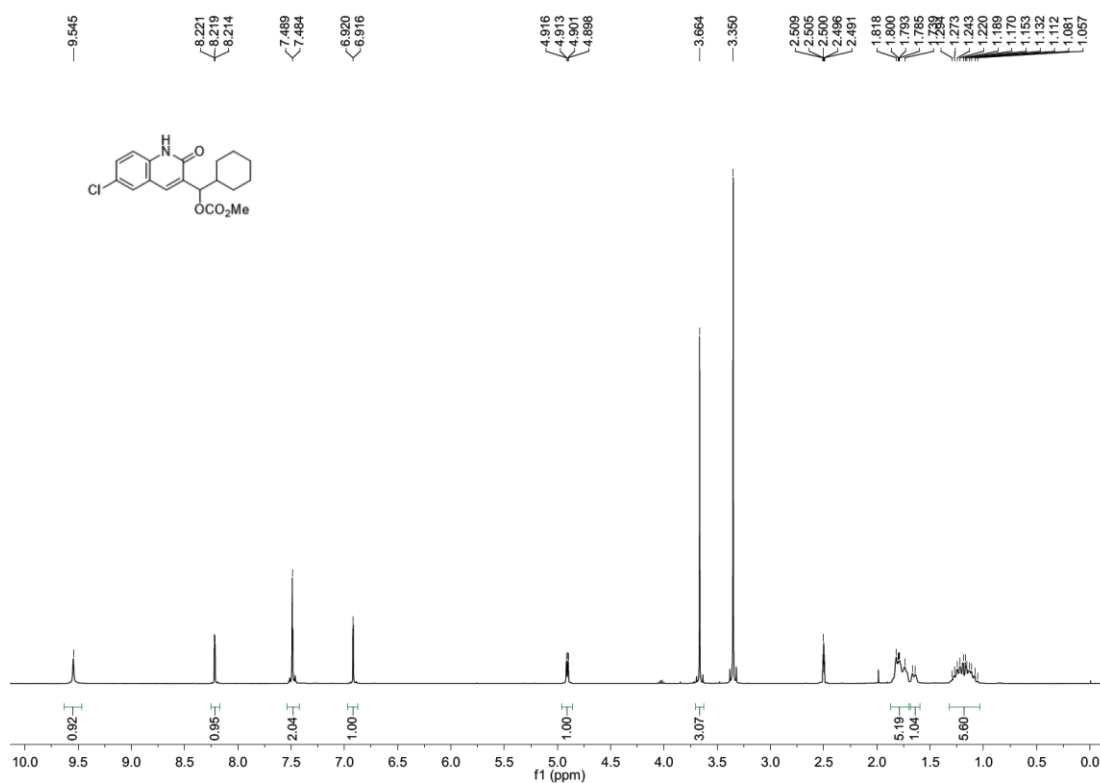
3v-¹H NMR (400 MHz, DMSO-d₆)



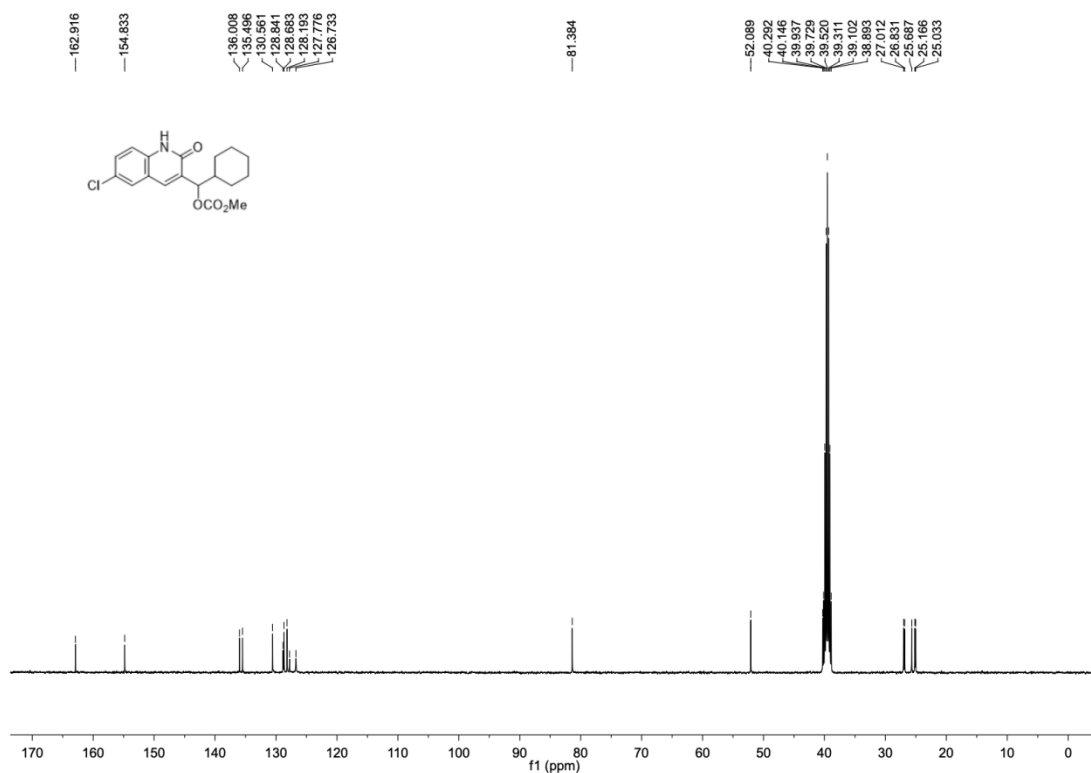
3v-¹³C NMR (100 MHz, DMSO-d₆)



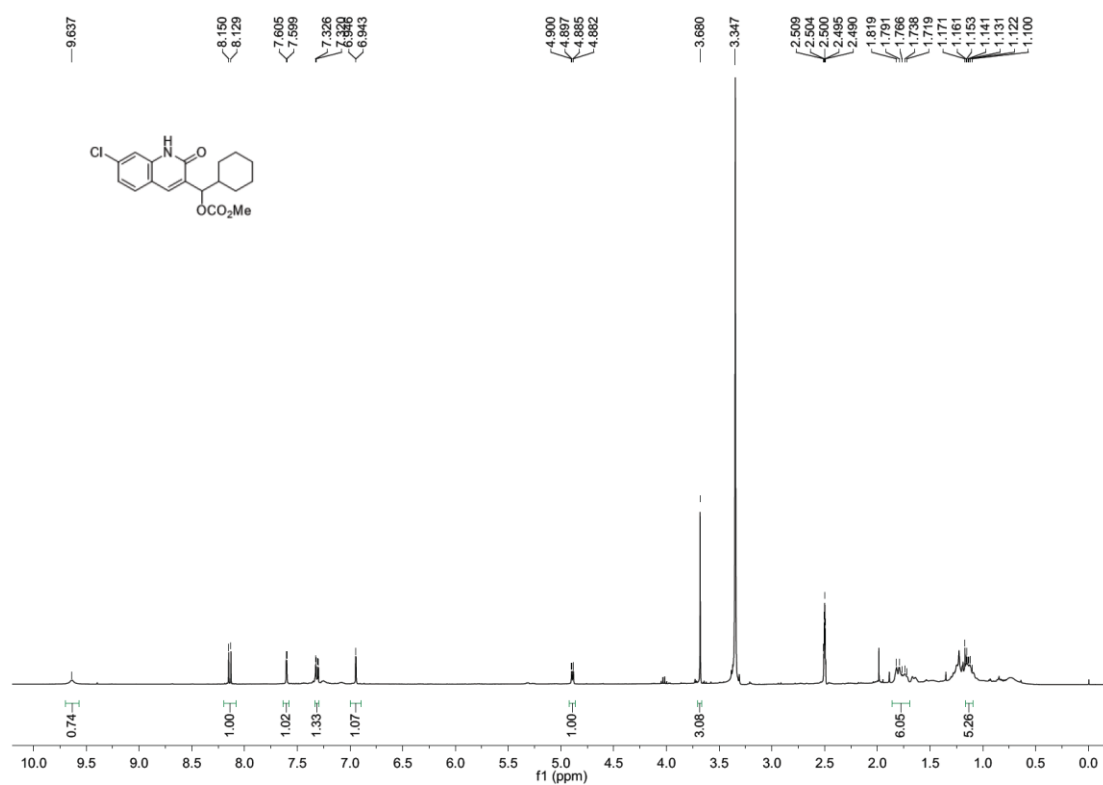
3w-¹H NMR (400 MHz, DMSO-*d*₆)



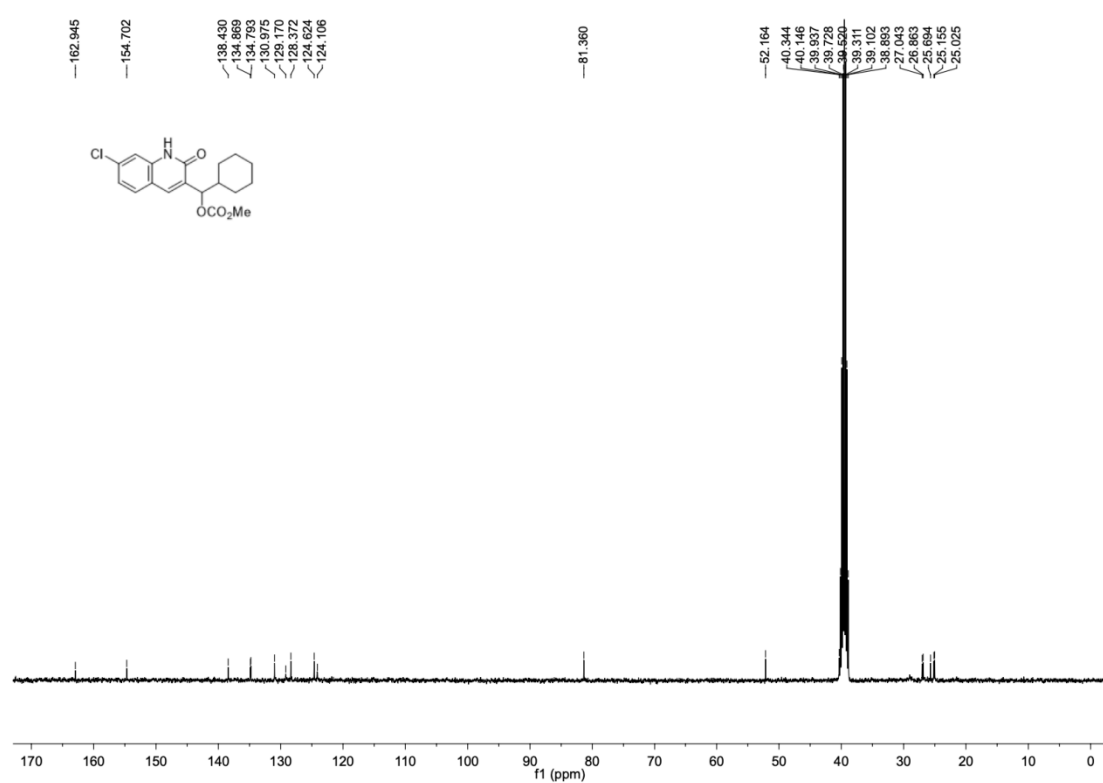
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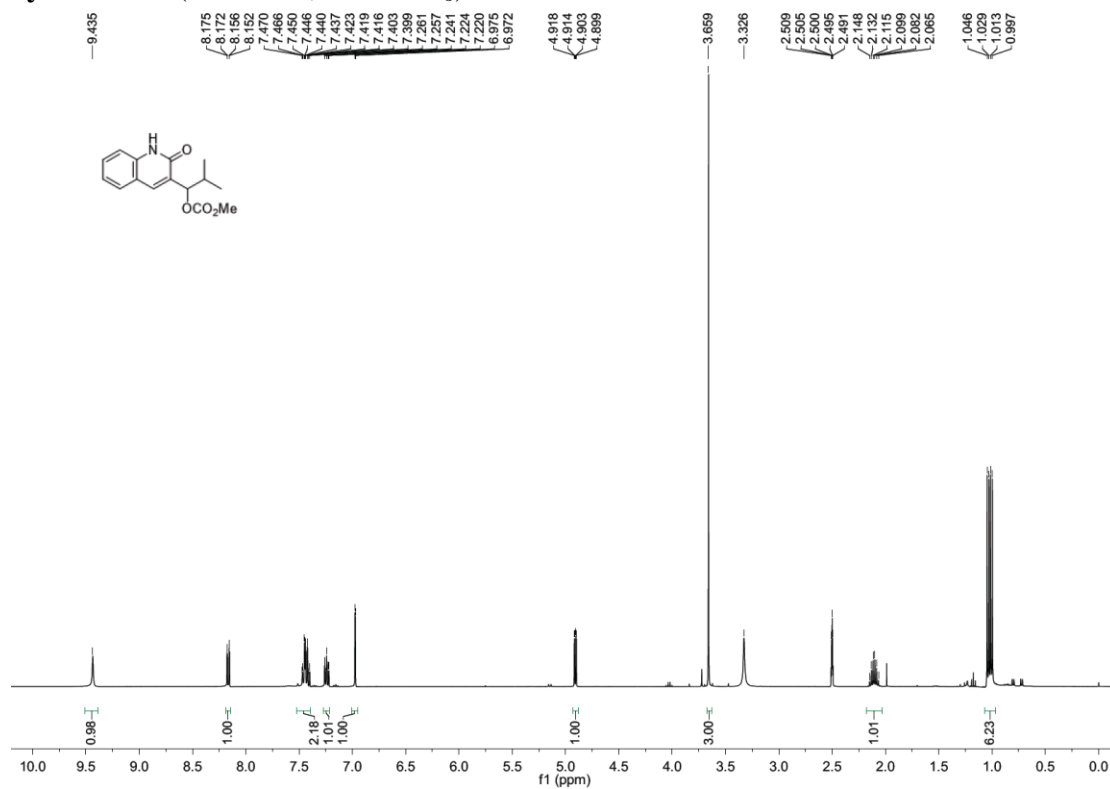
3x-¹H NMR (400 MHz, DMSO-*d*₆)



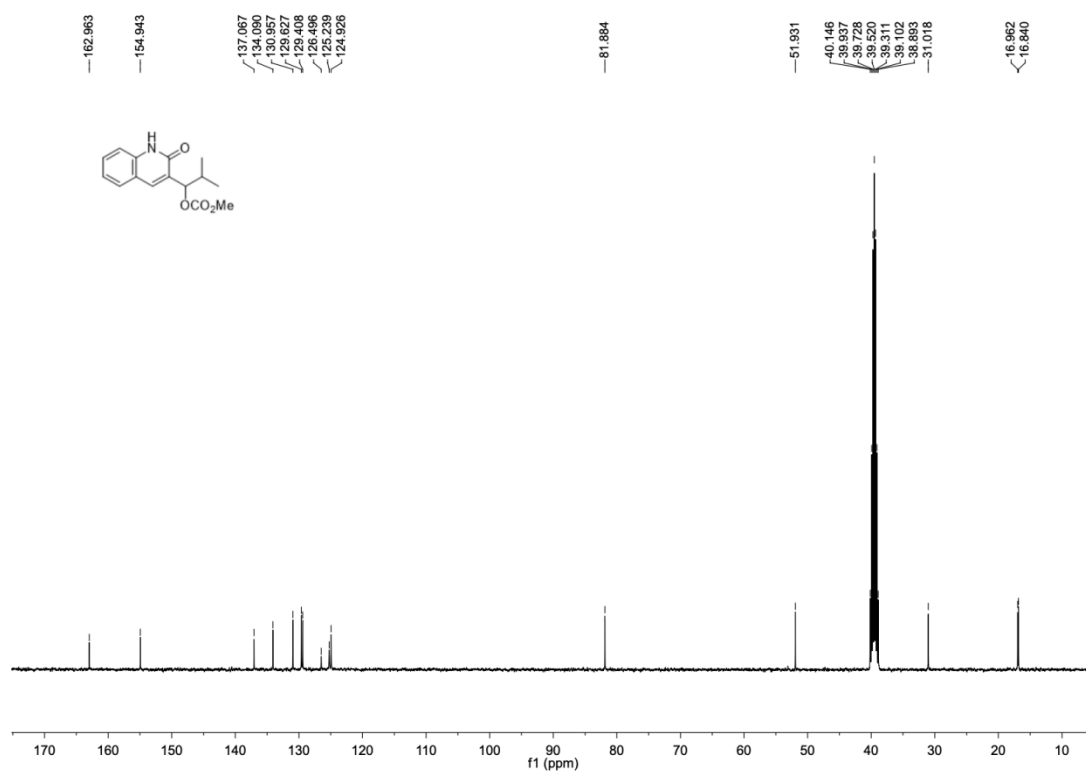
3x-¹³C NMR (100 MHz, DMSO-*d*₆)



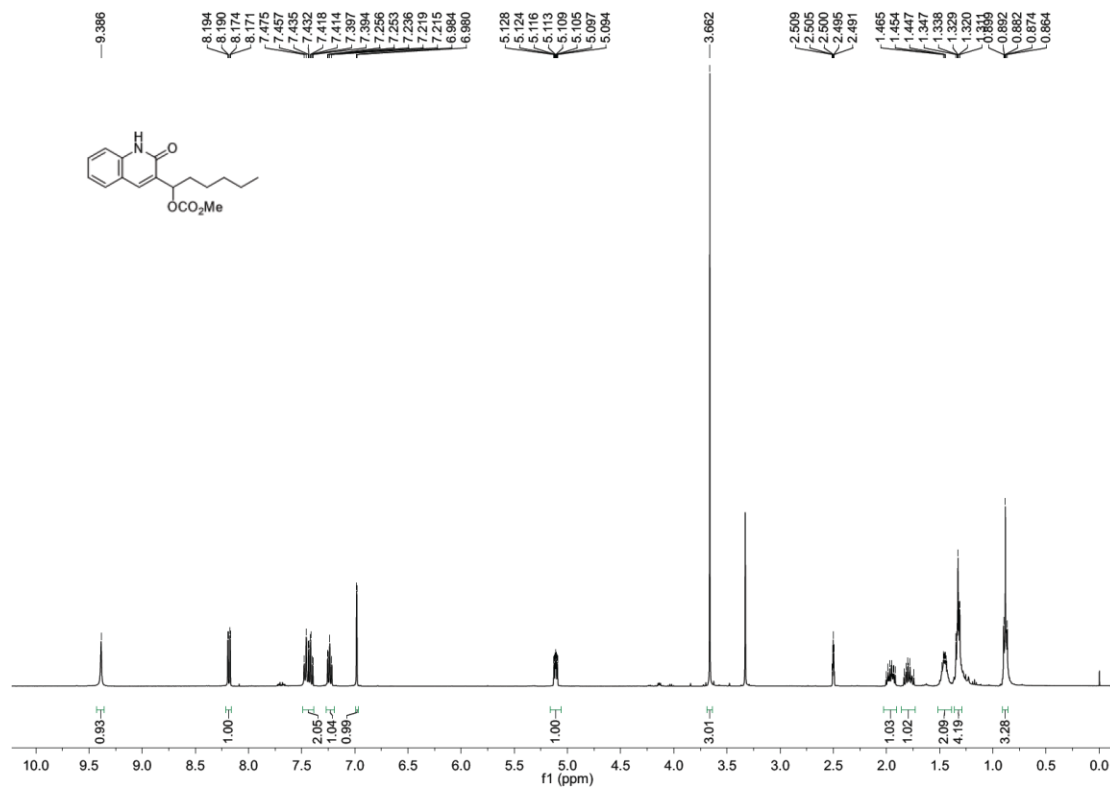
3y-¹H NMR (400 MHz, DMSO-*d*₆)



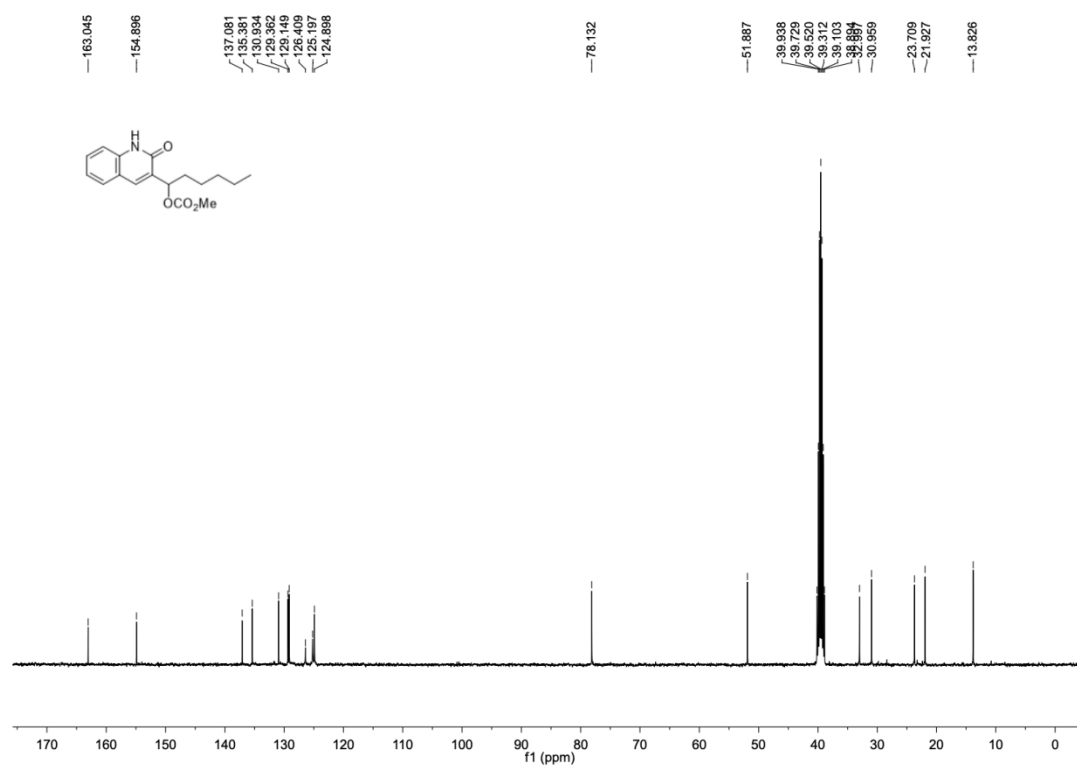
3y-¹³C NMR (100 MHz, DMSO-*d*₆)



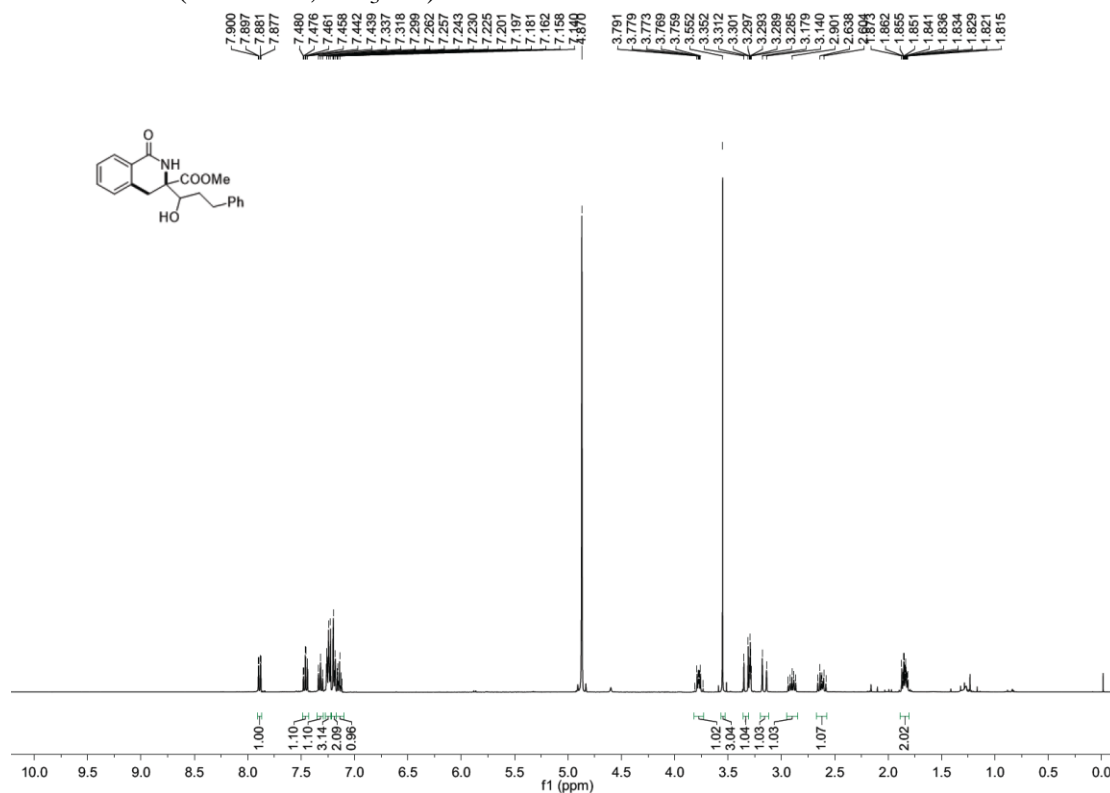
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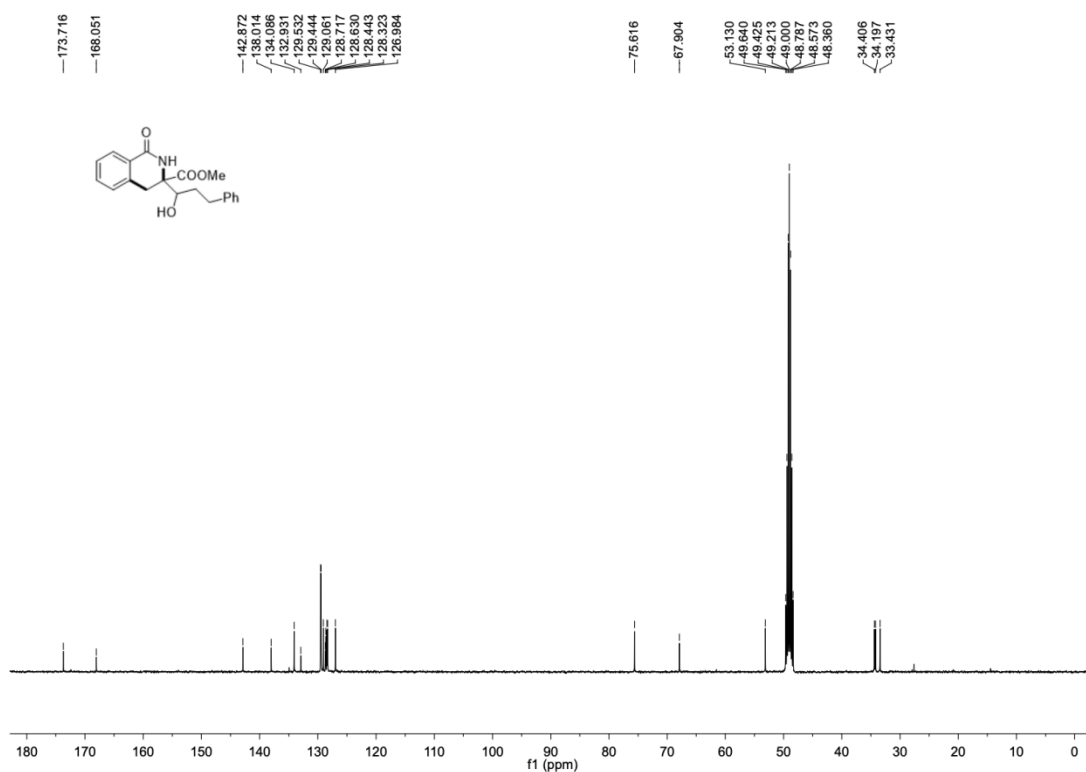
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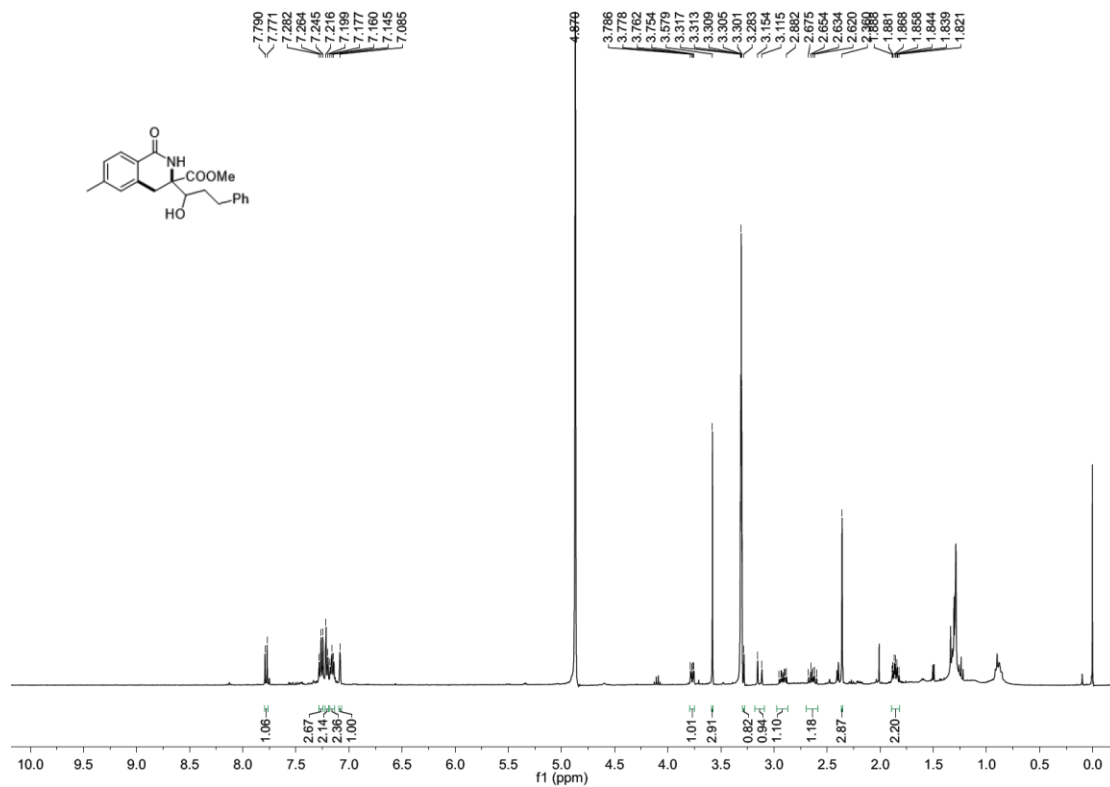
4a-¹H NMR (400 MHz, CD₃OD)



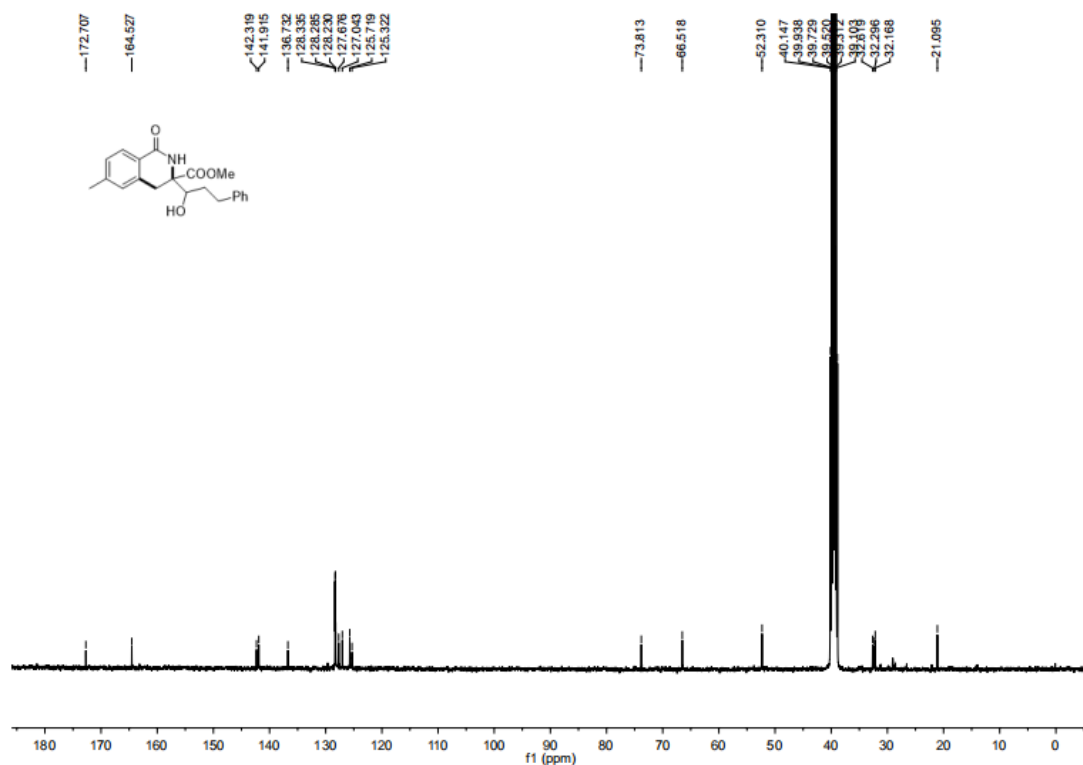
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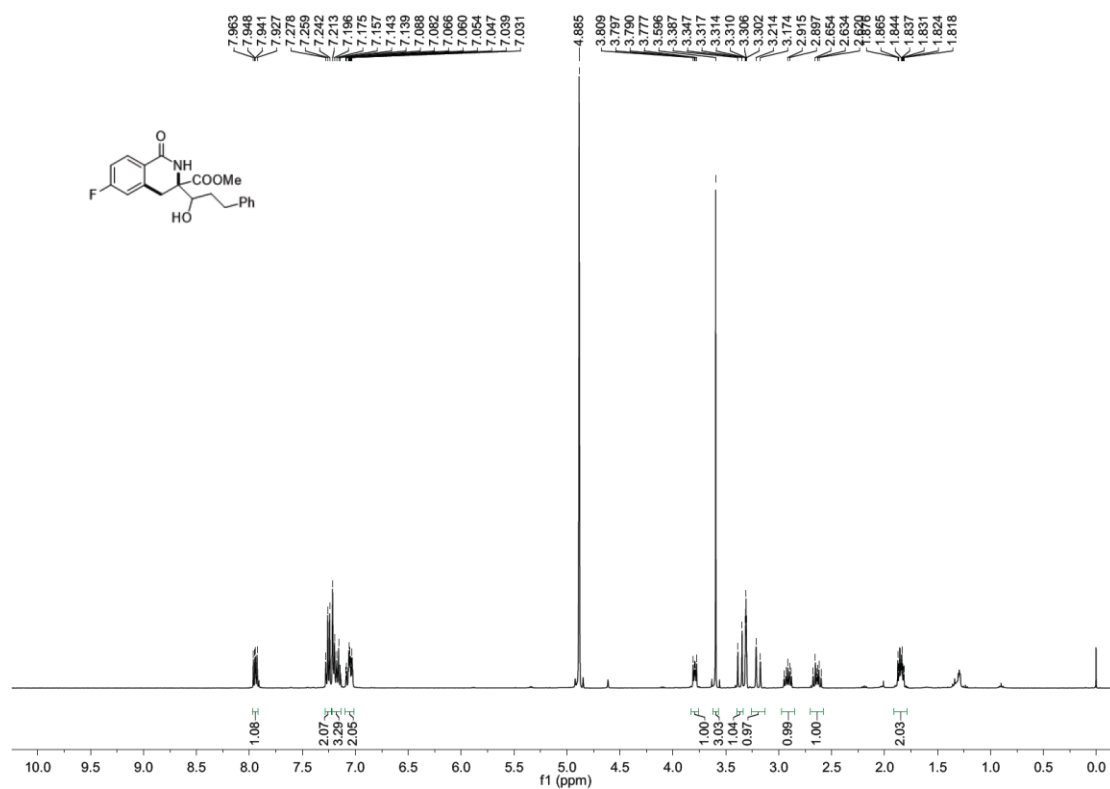
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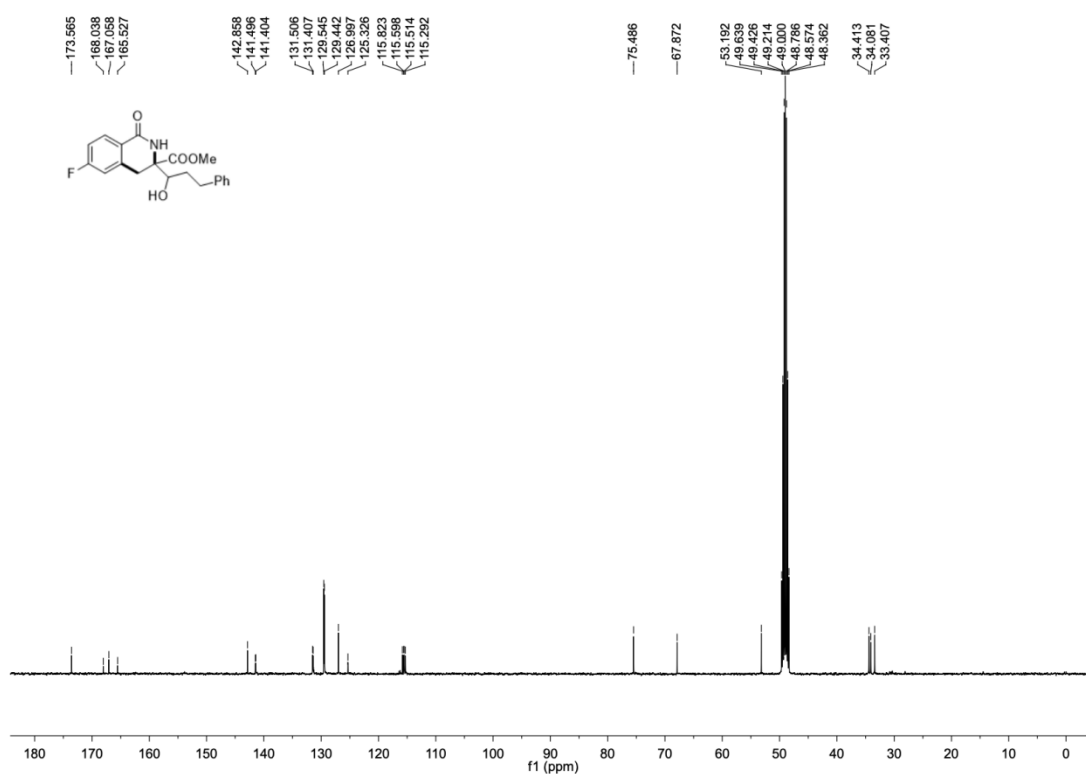
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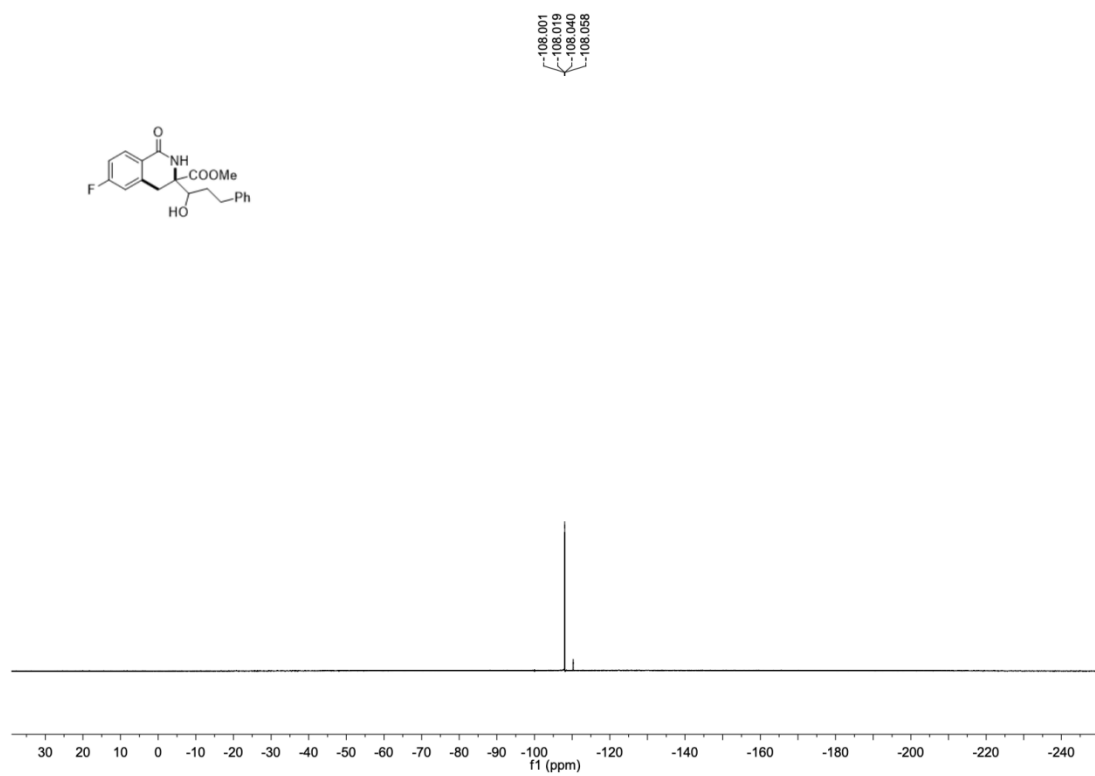
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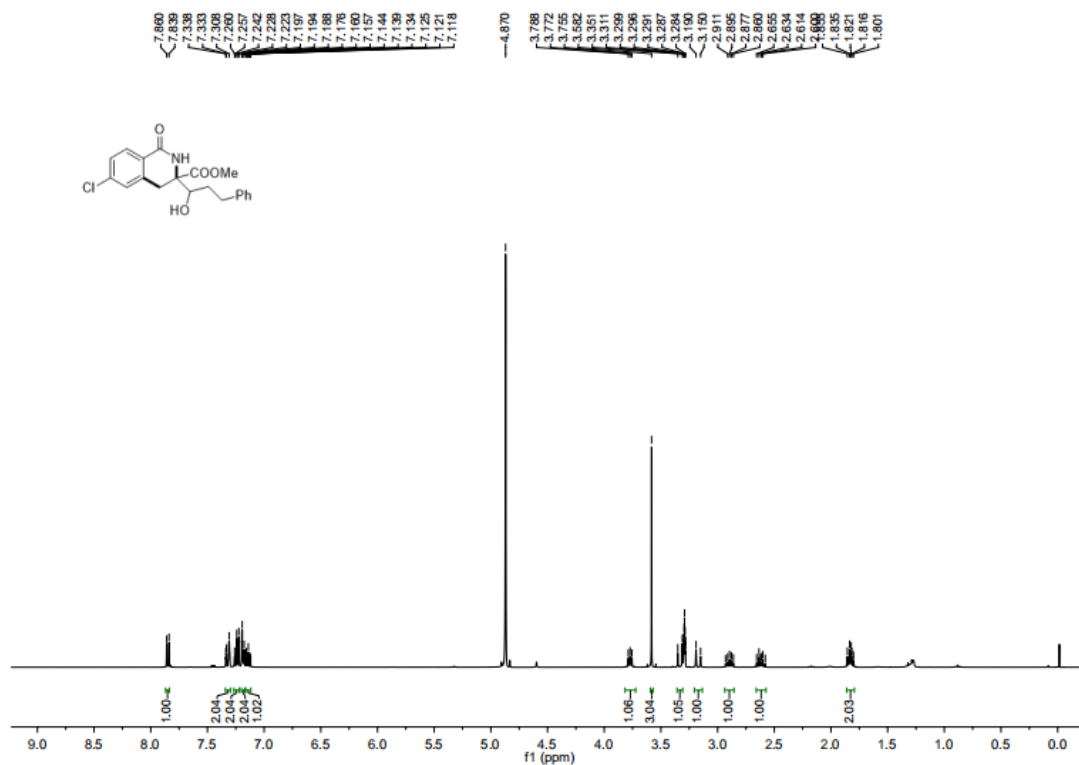
4c-¹³C NMR (100 MHz, CD₃OD)



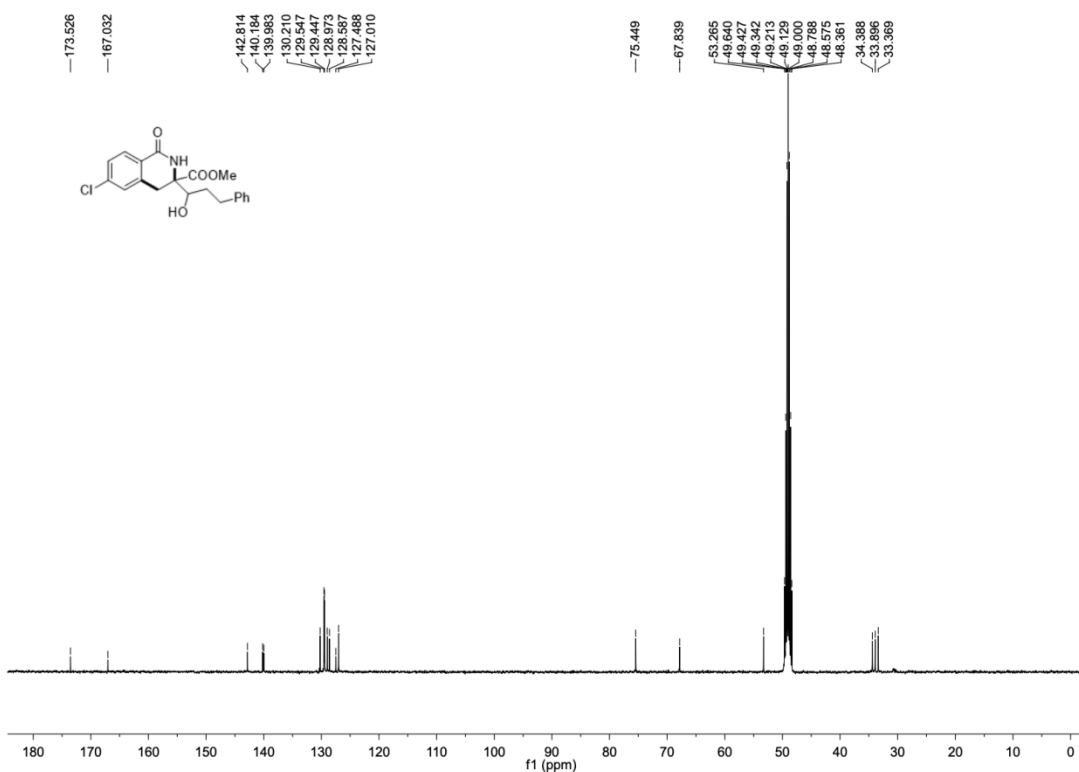
¹⁹F-NMR spectrum of 4c (100 MHz, CD₃OD)



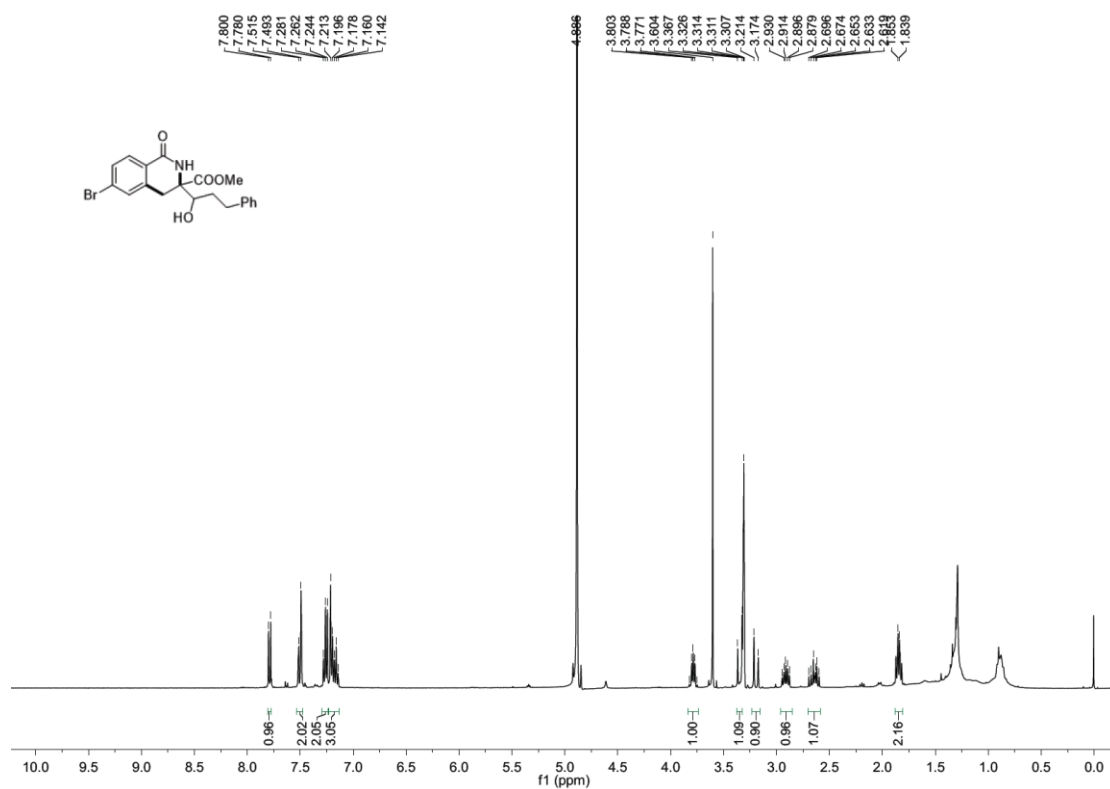
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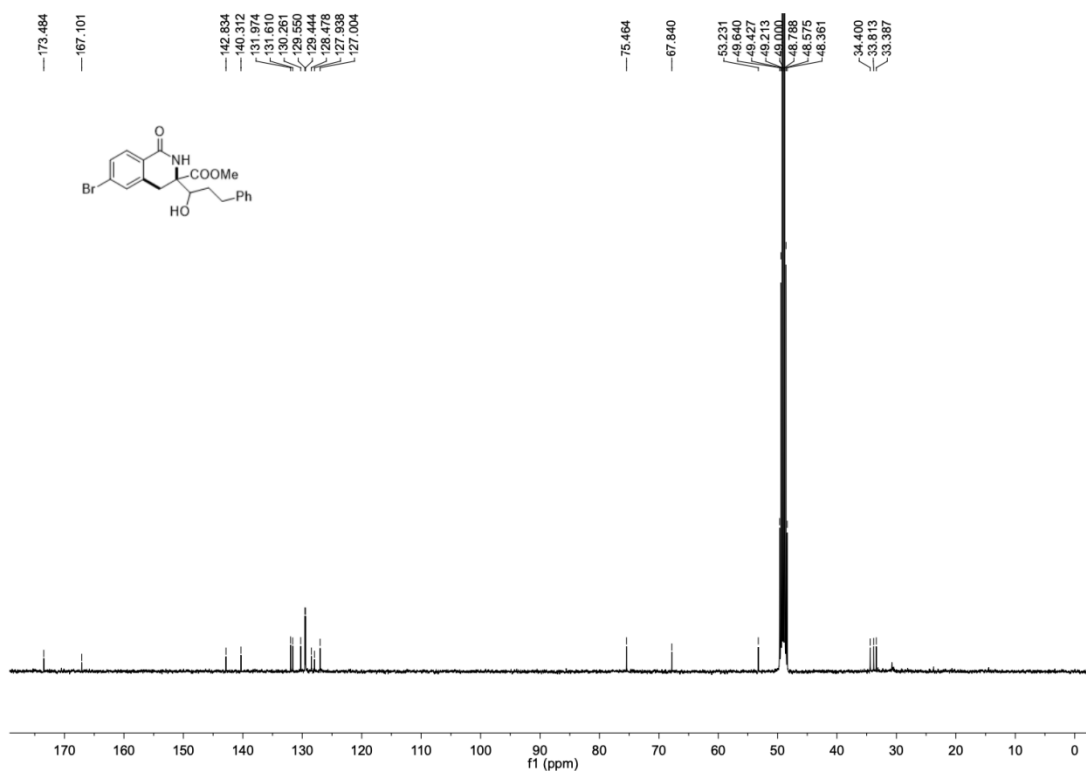
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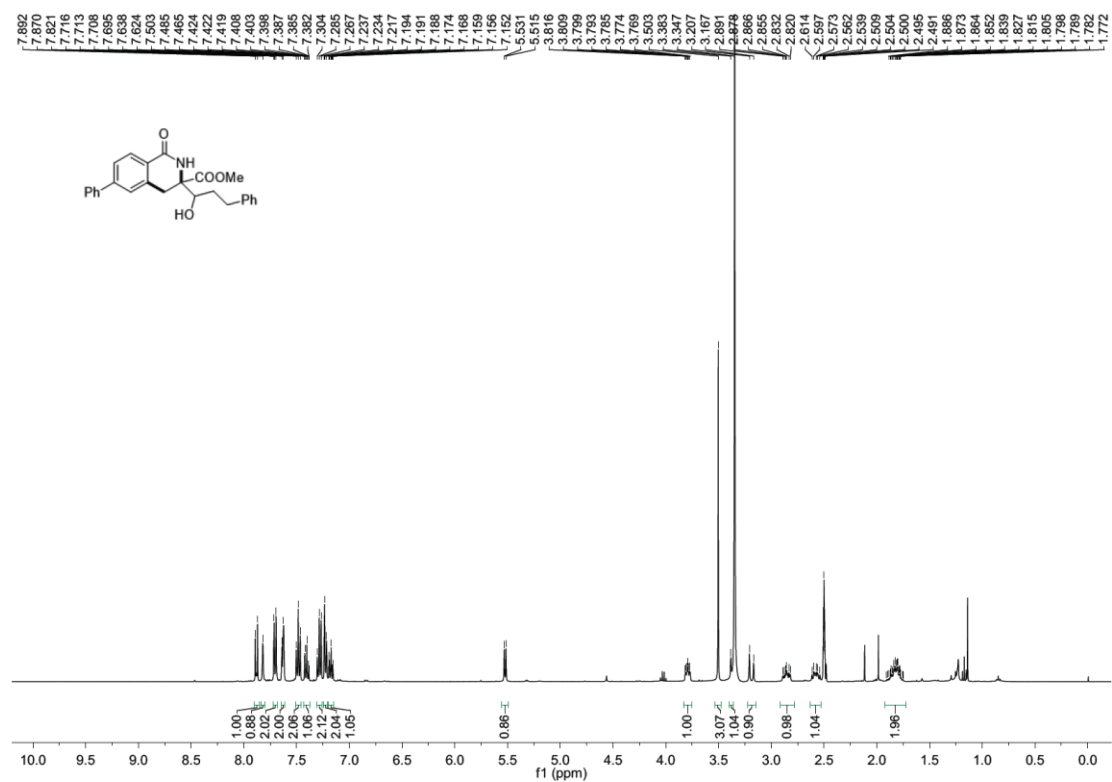
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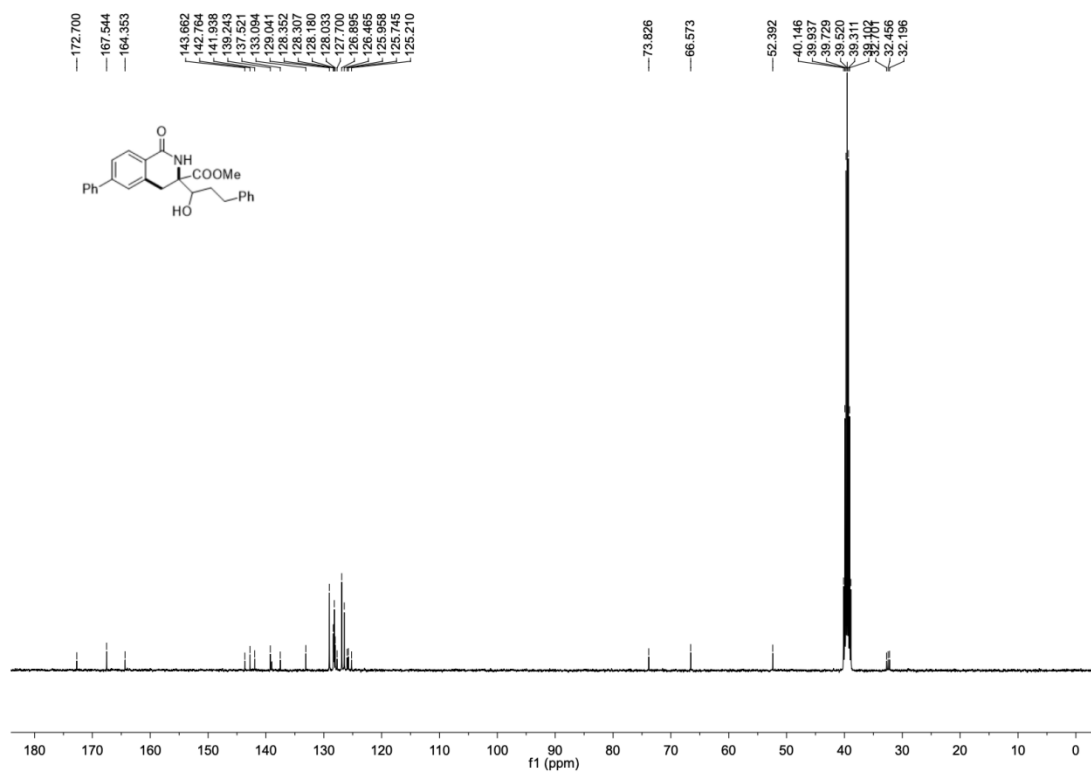
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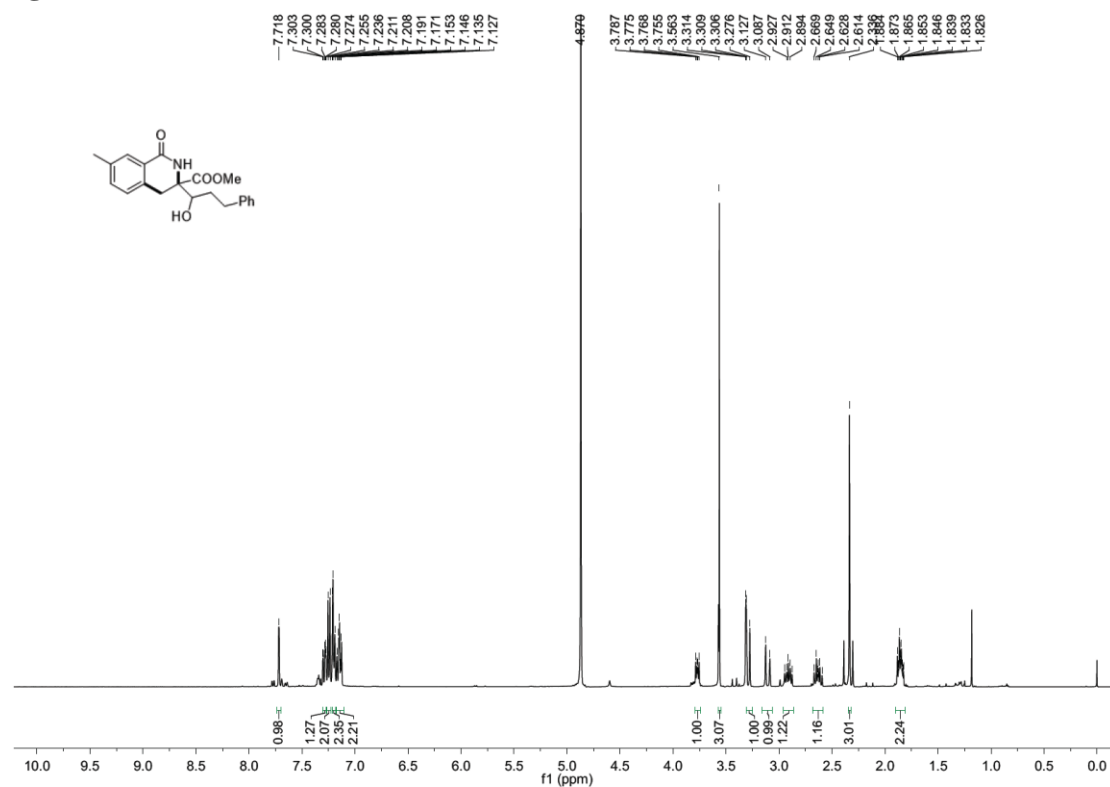
4f-¹H NMR (400 MHz, DMSO-*d*₆)



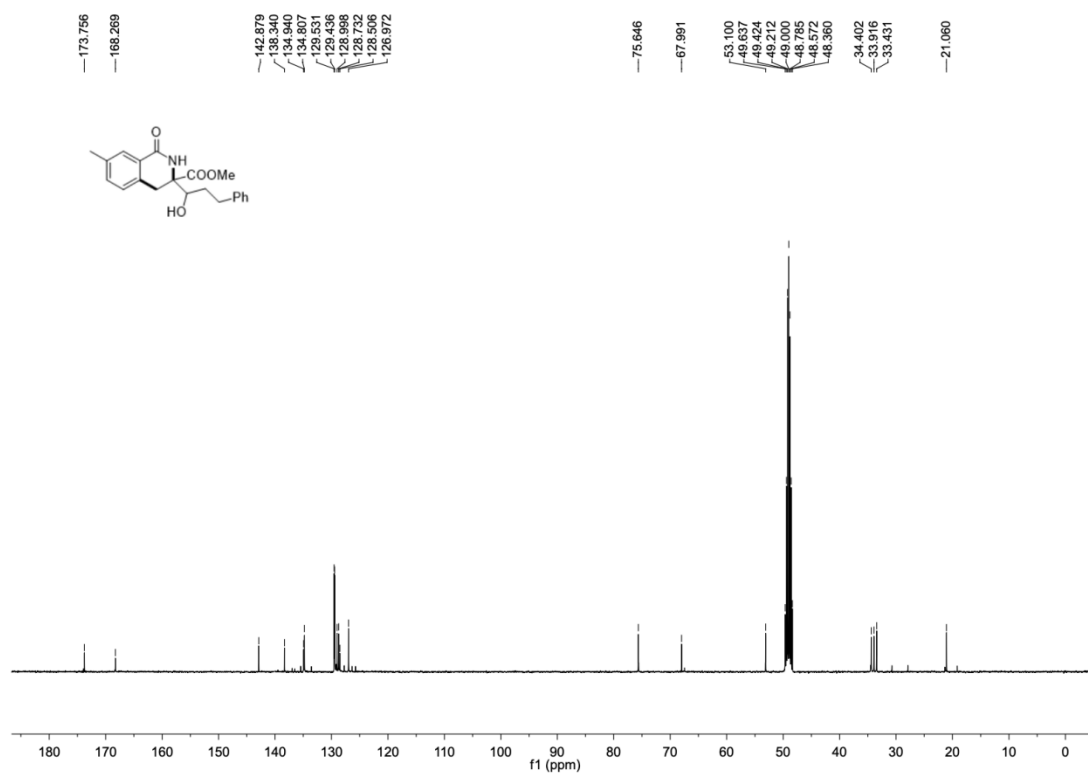
4f-¹³C NMR (100 MHz, DMSO-*d*₆)



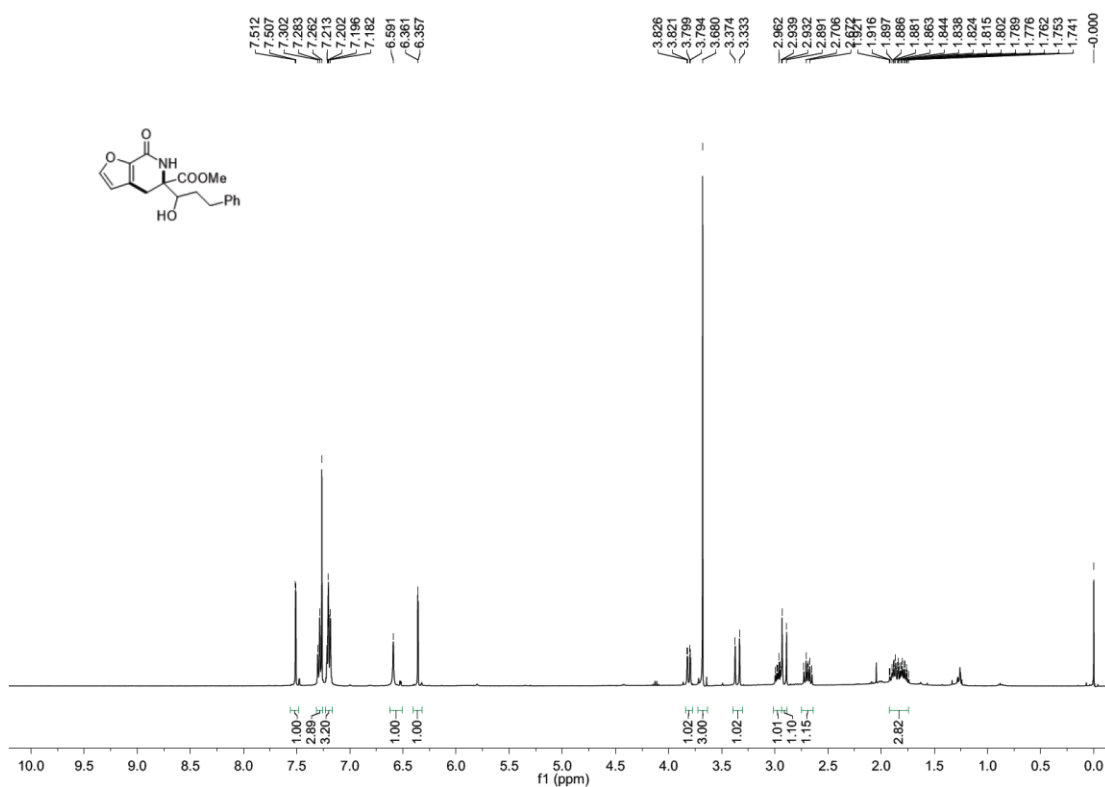
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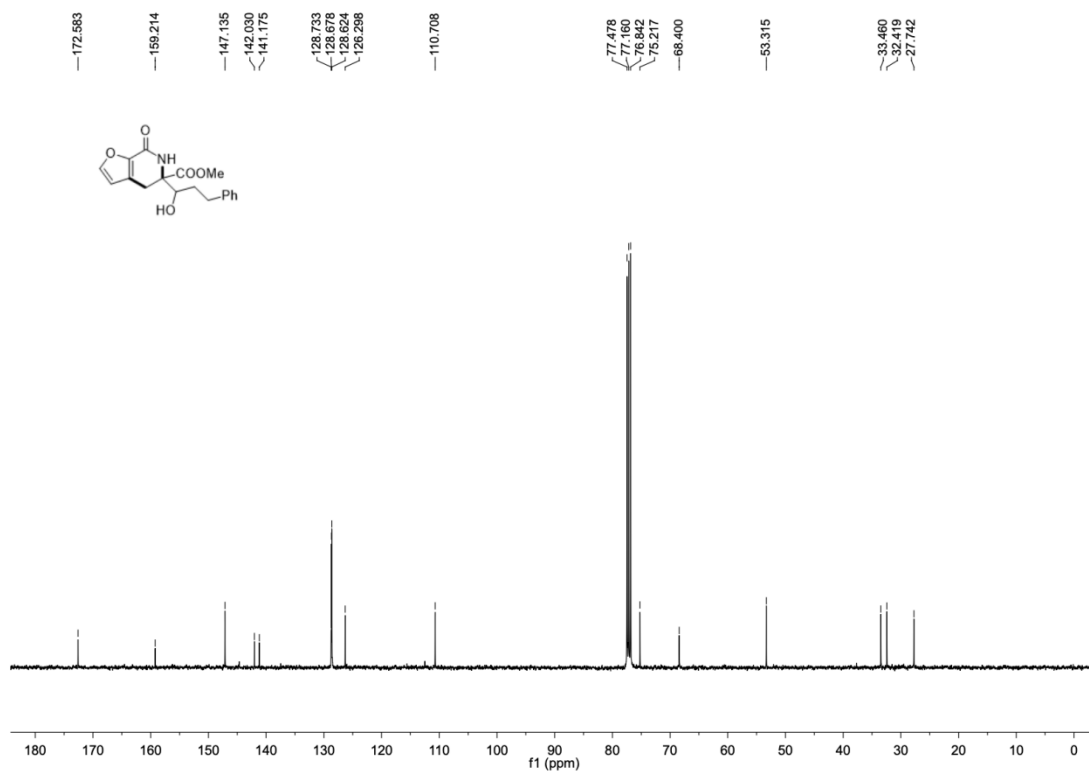
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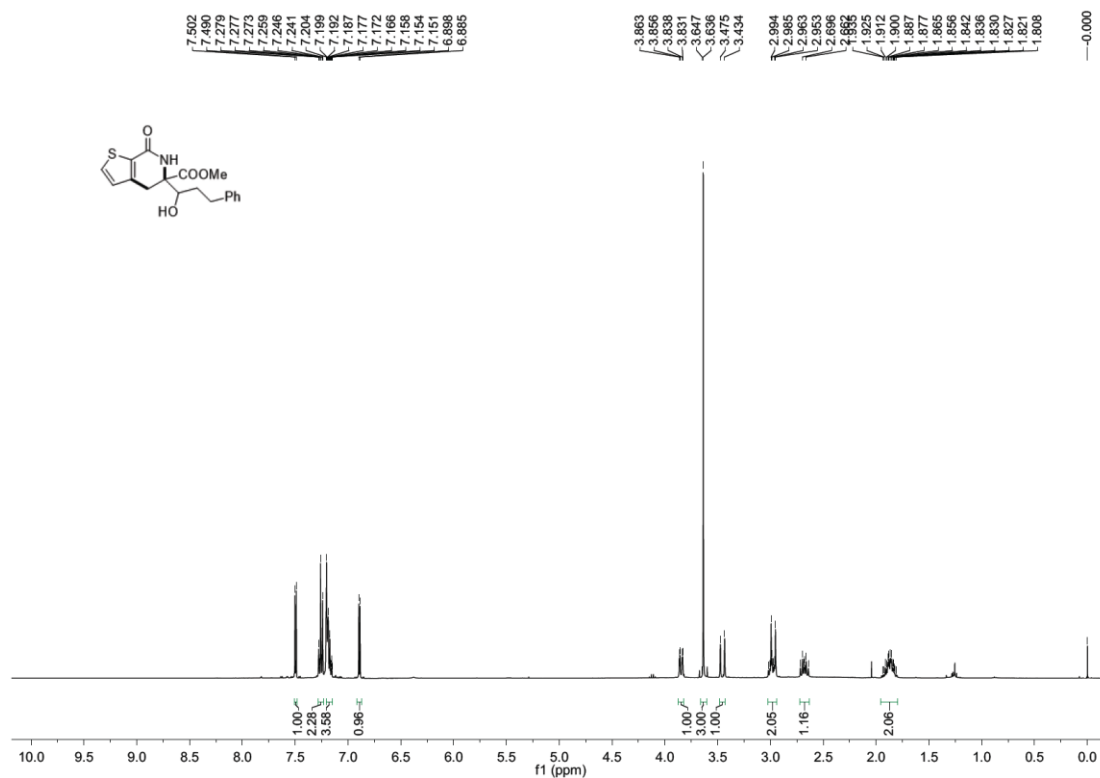
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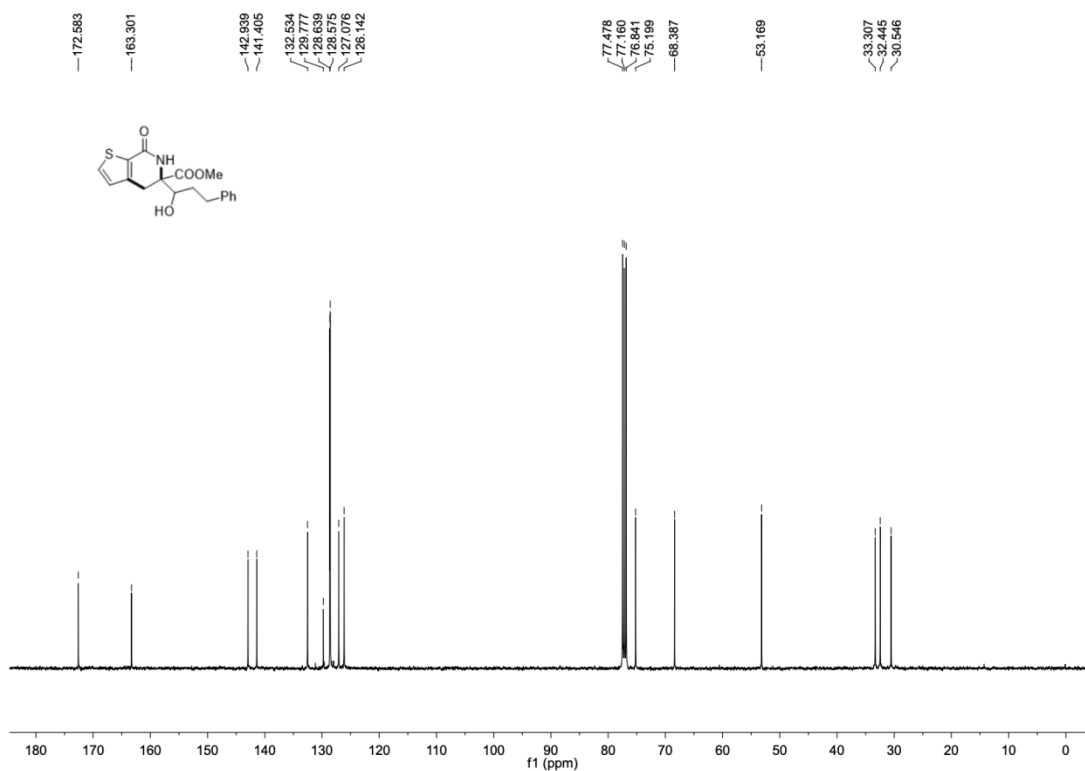
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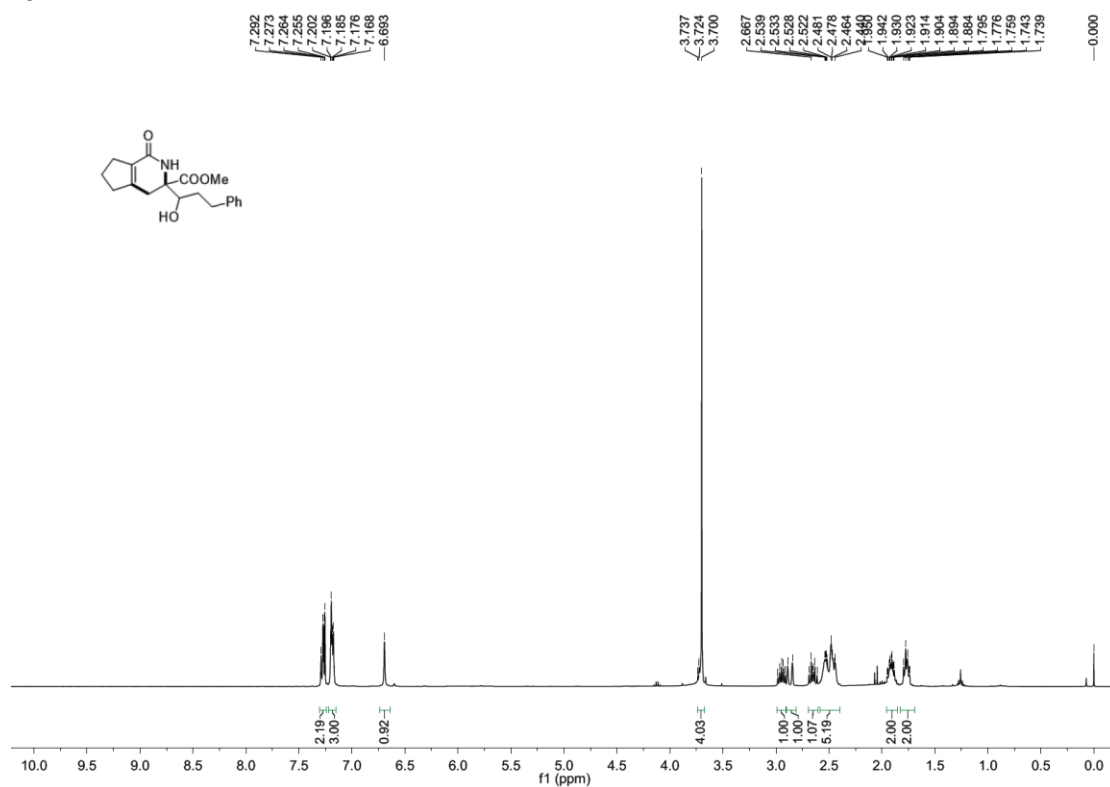
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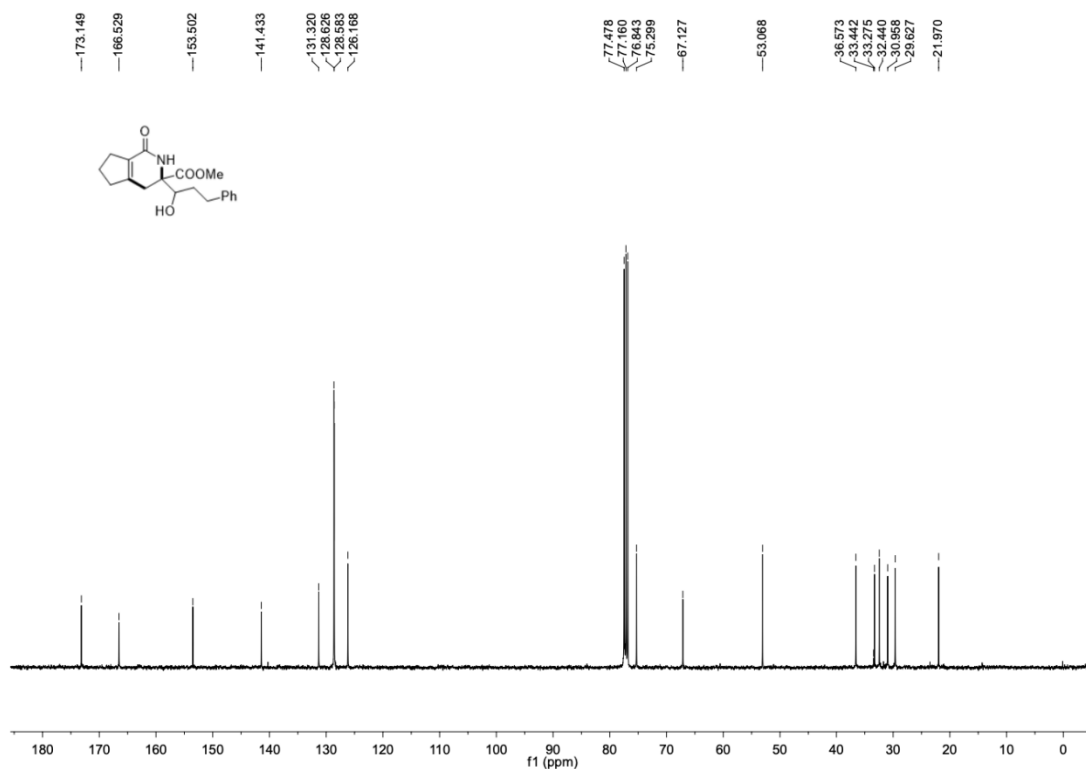
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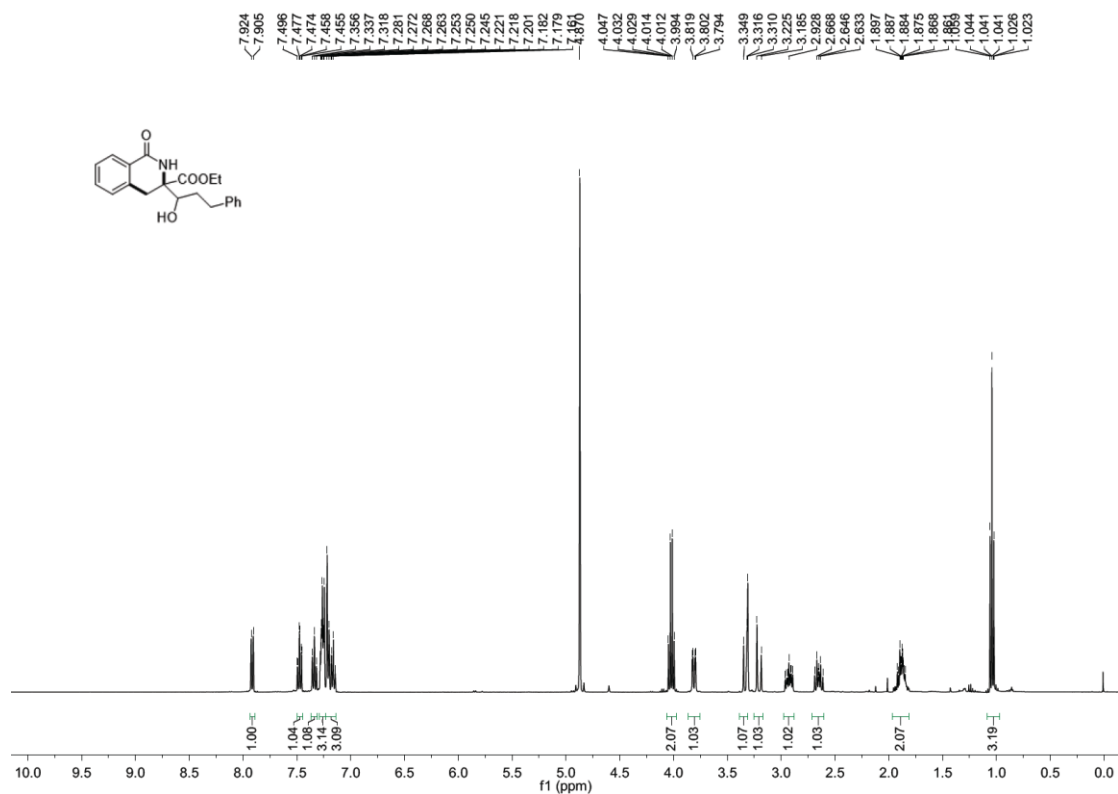
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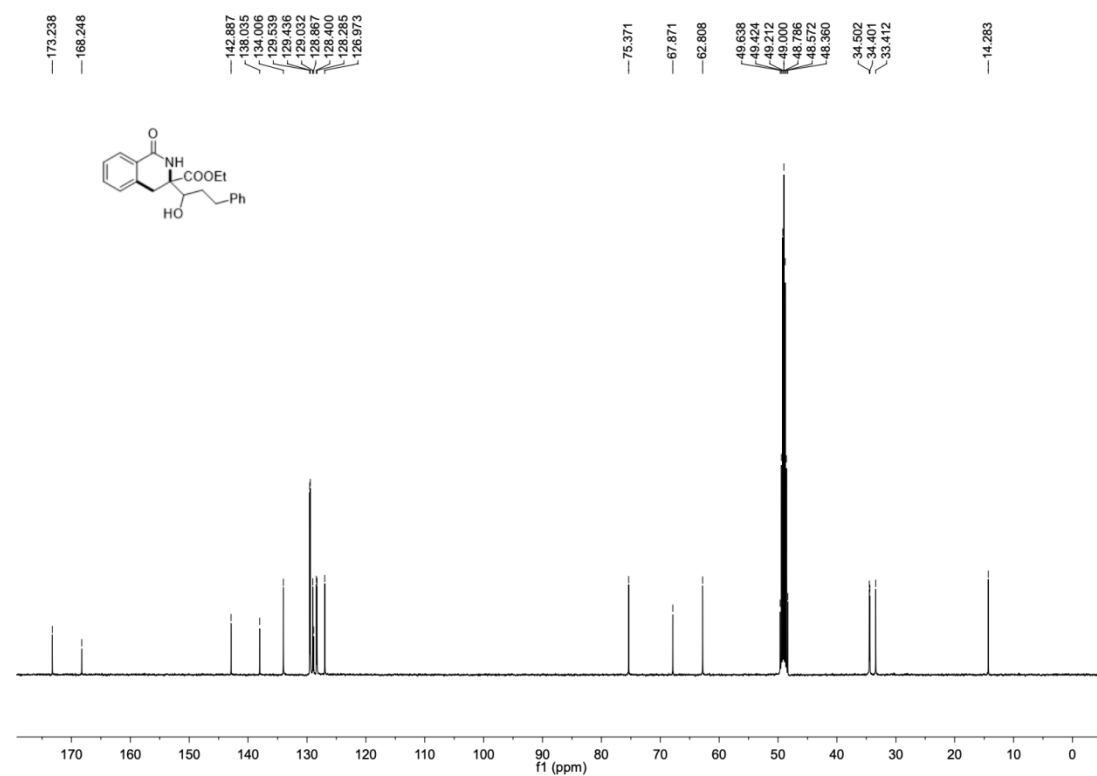
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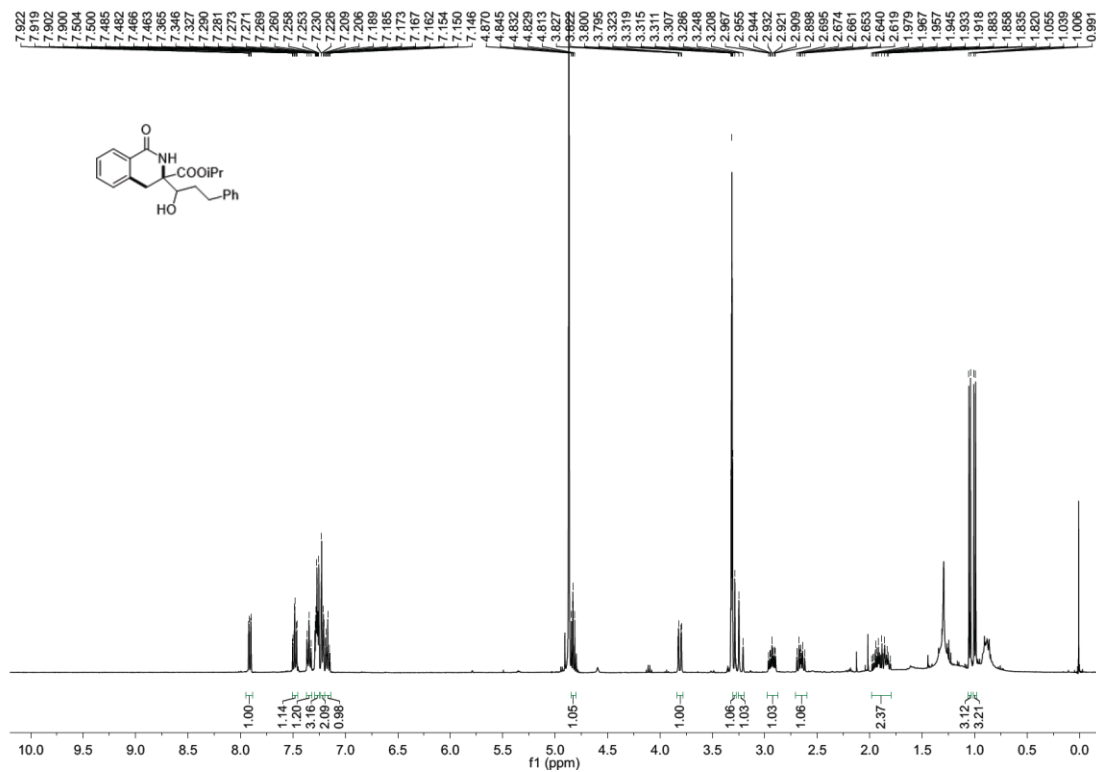
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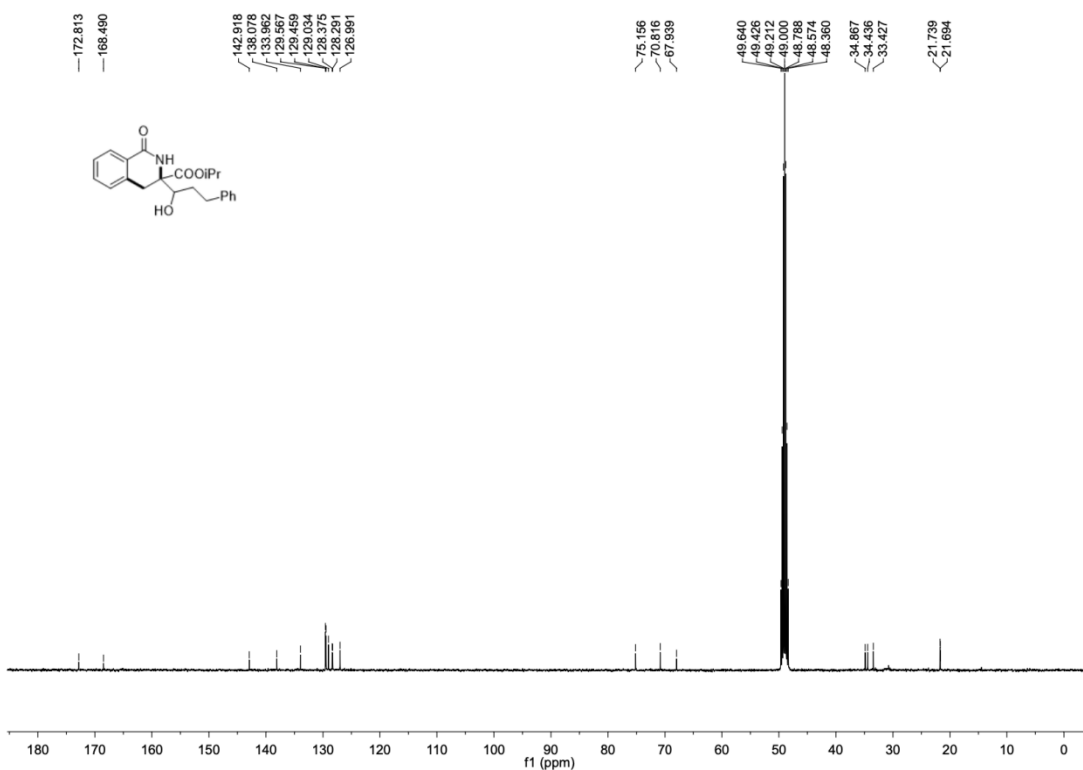
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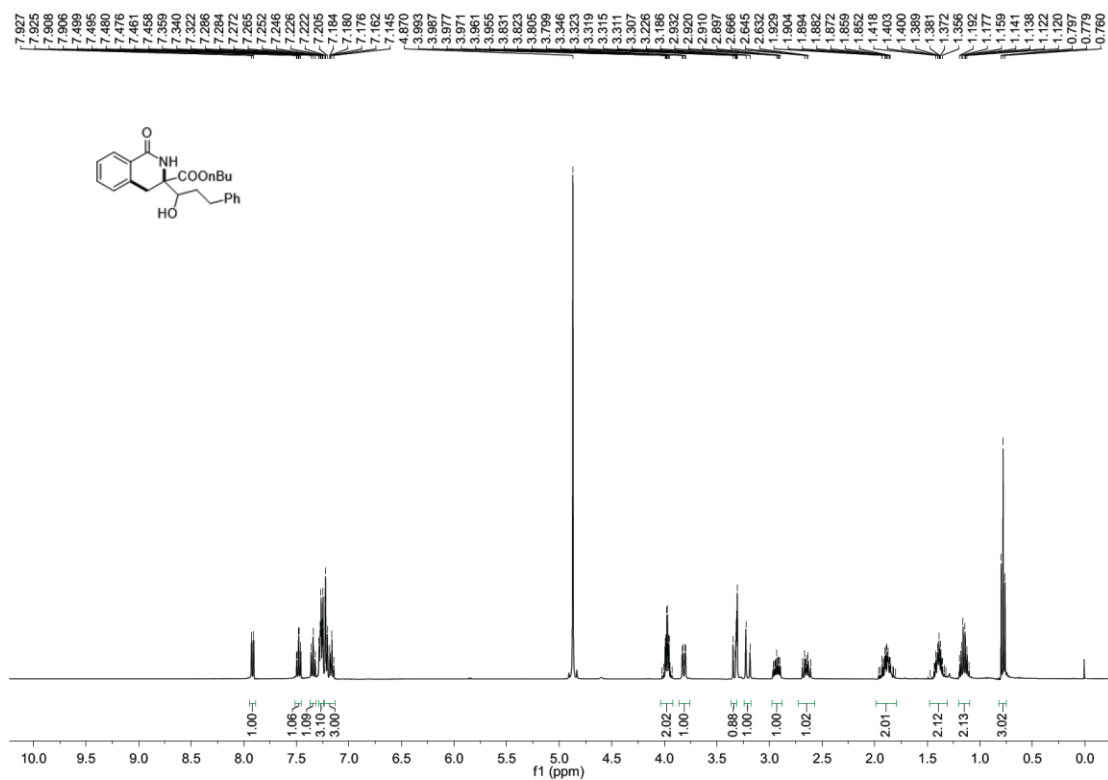
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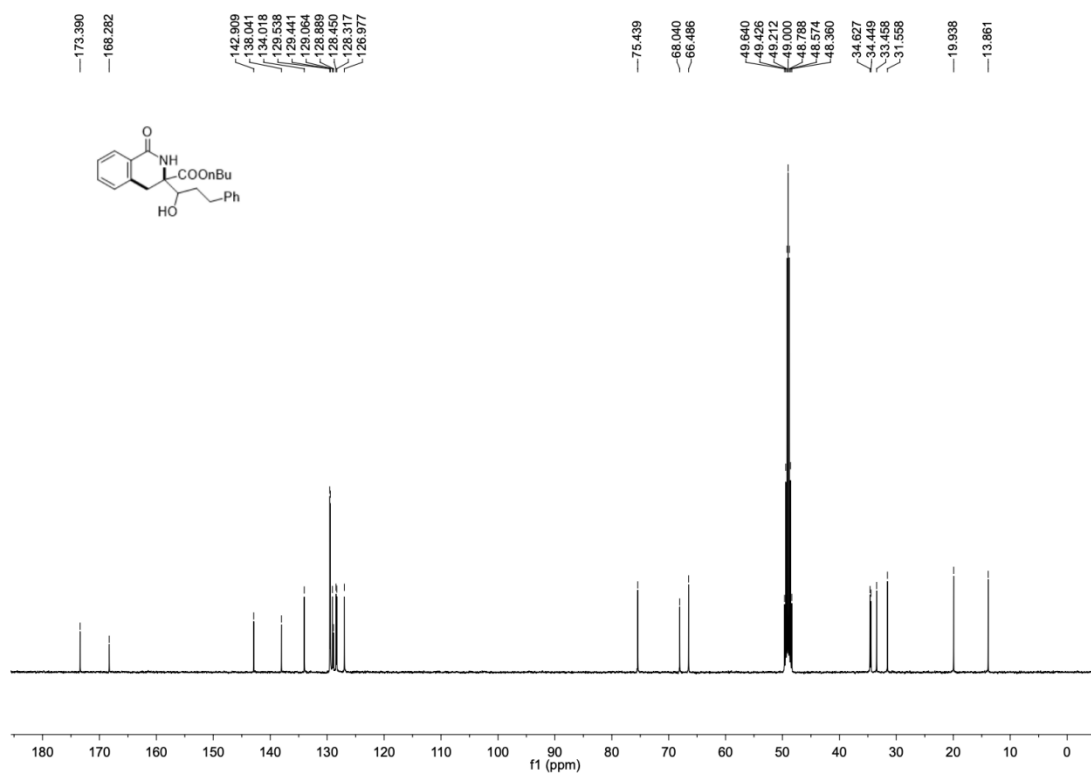
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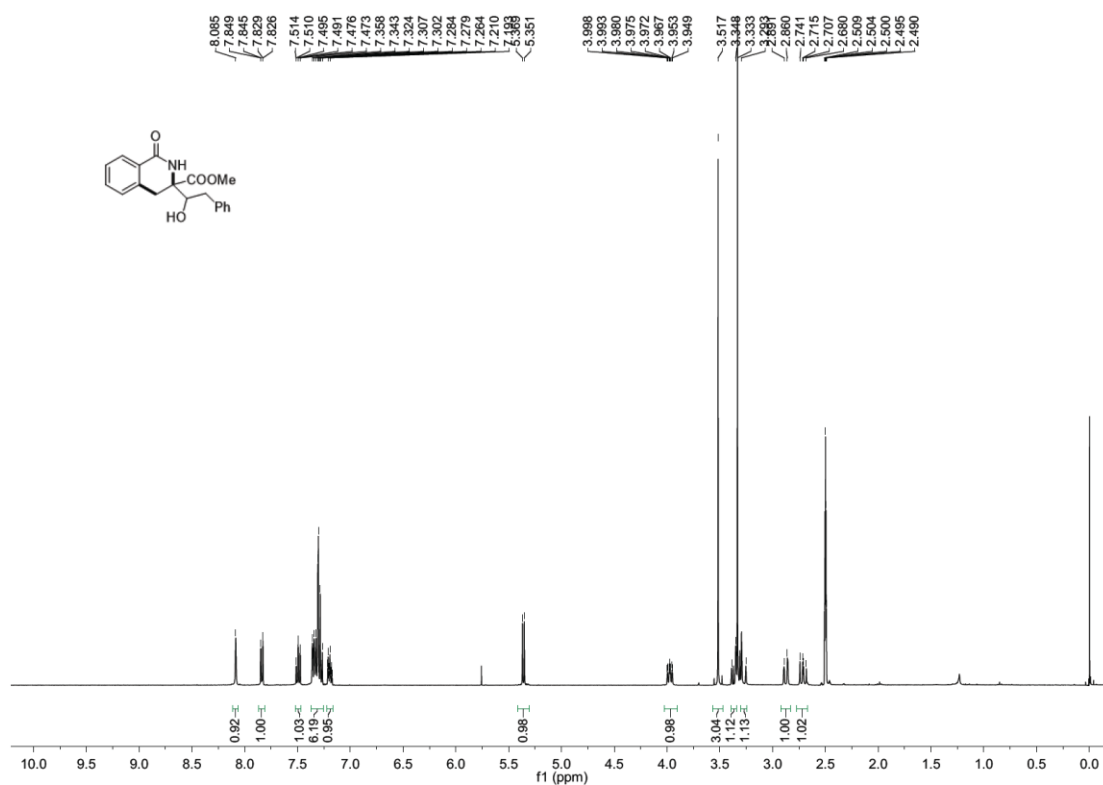
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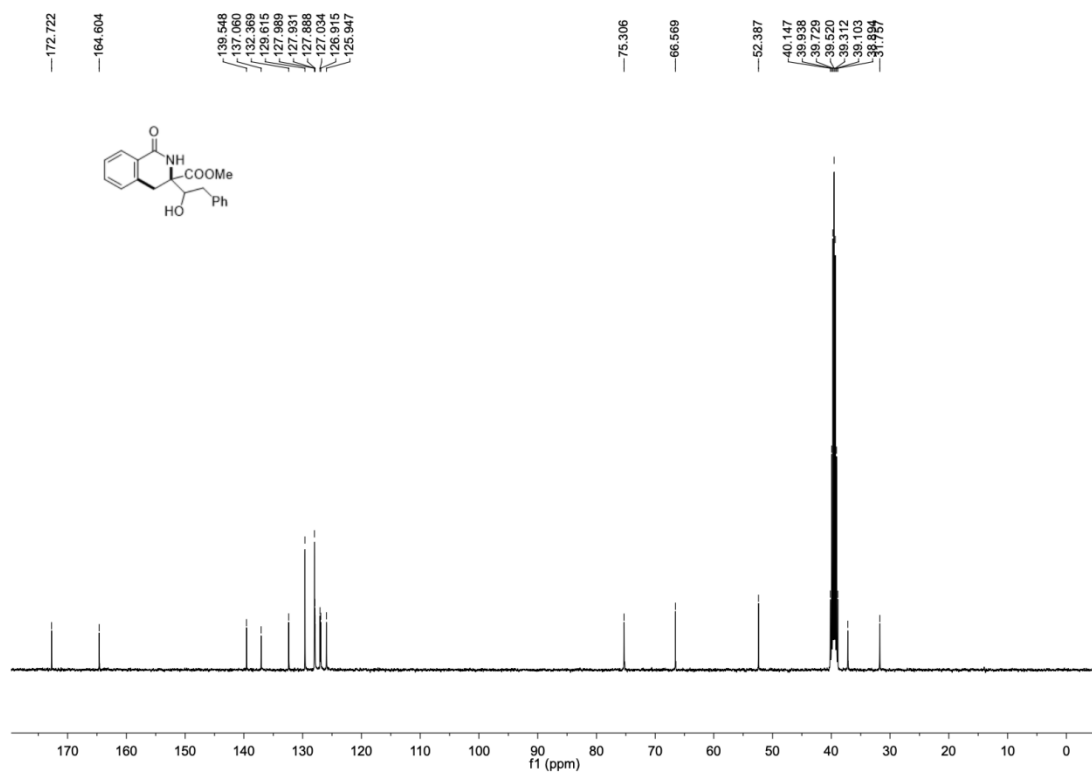
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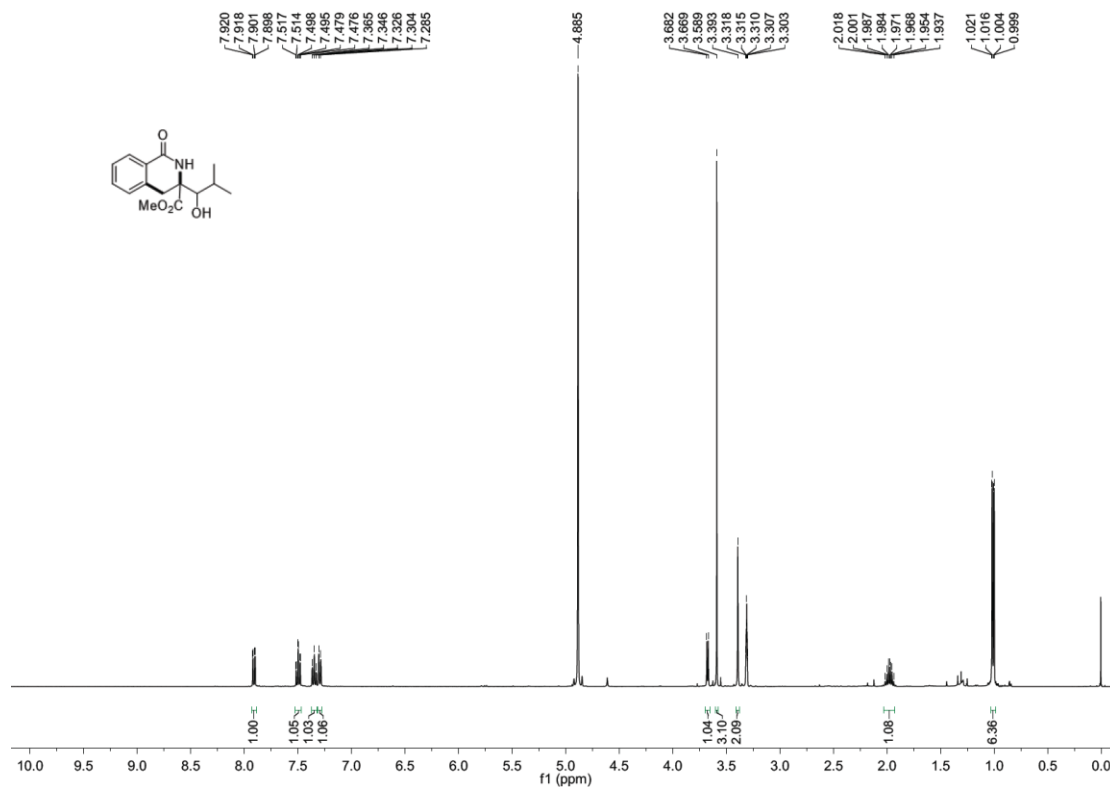
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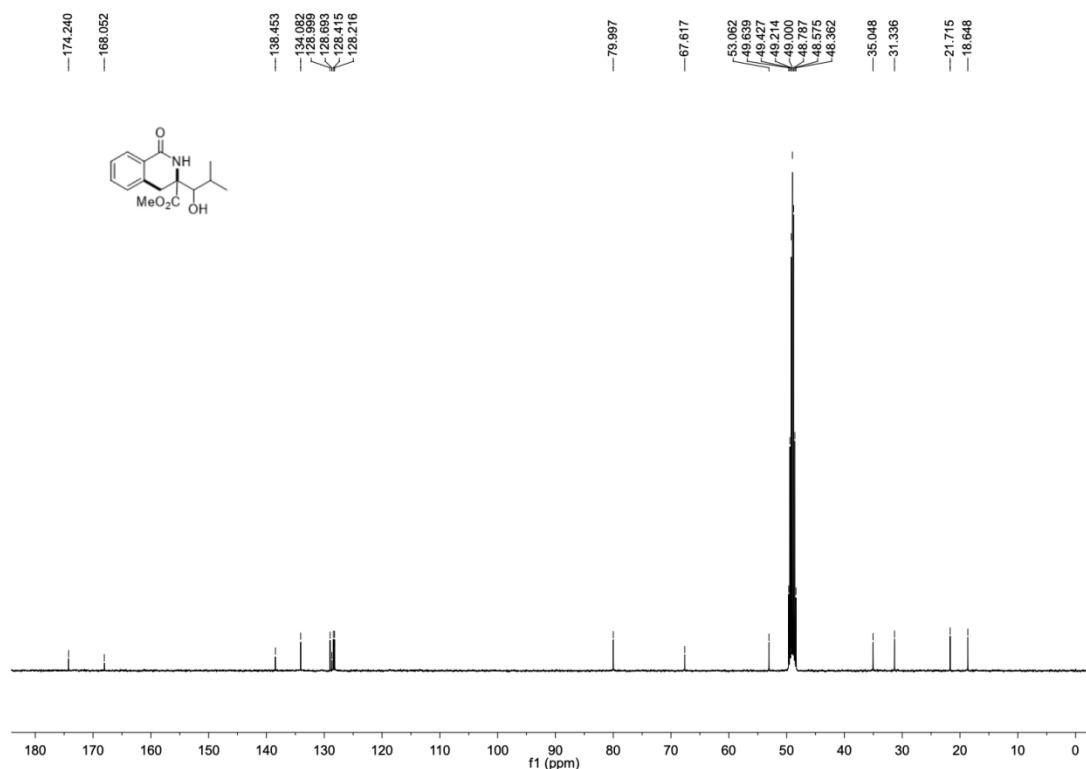
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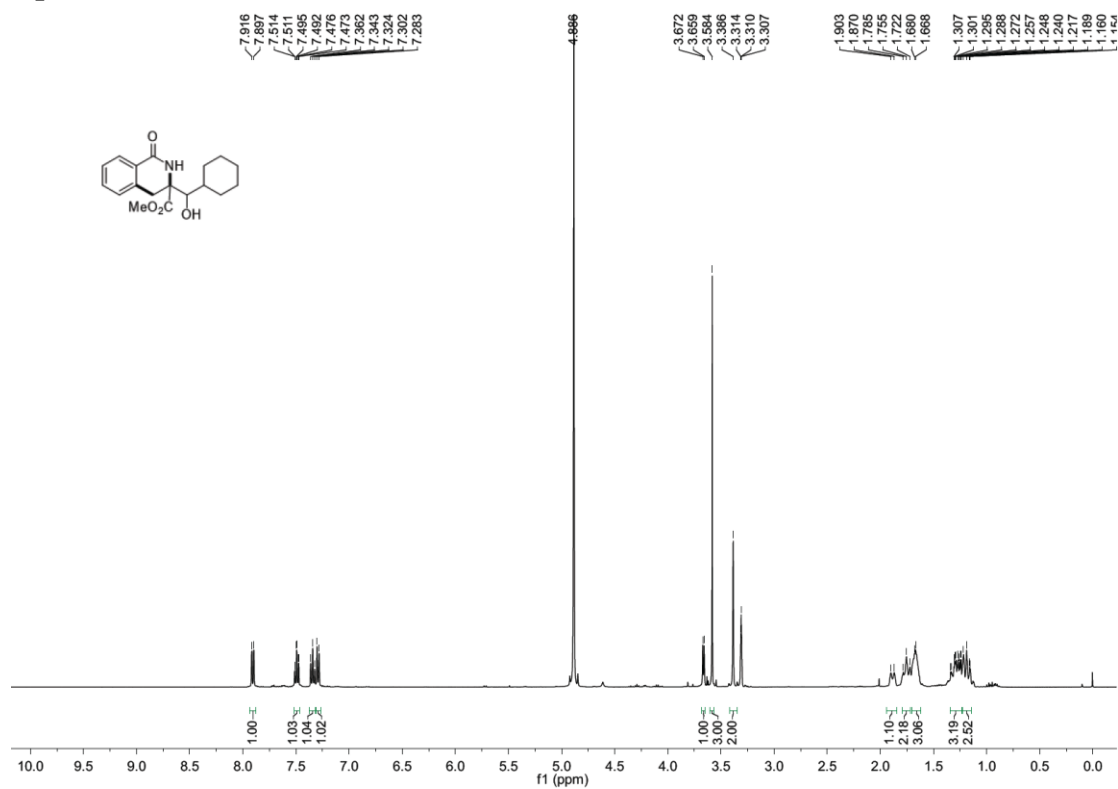
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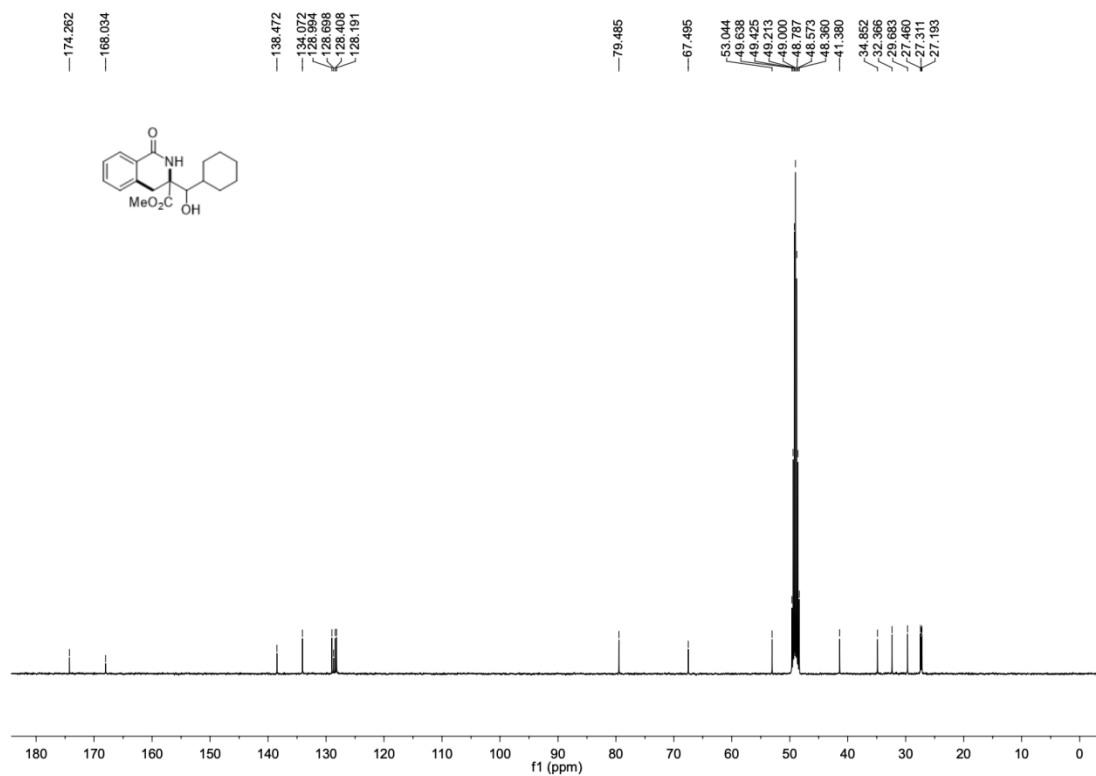
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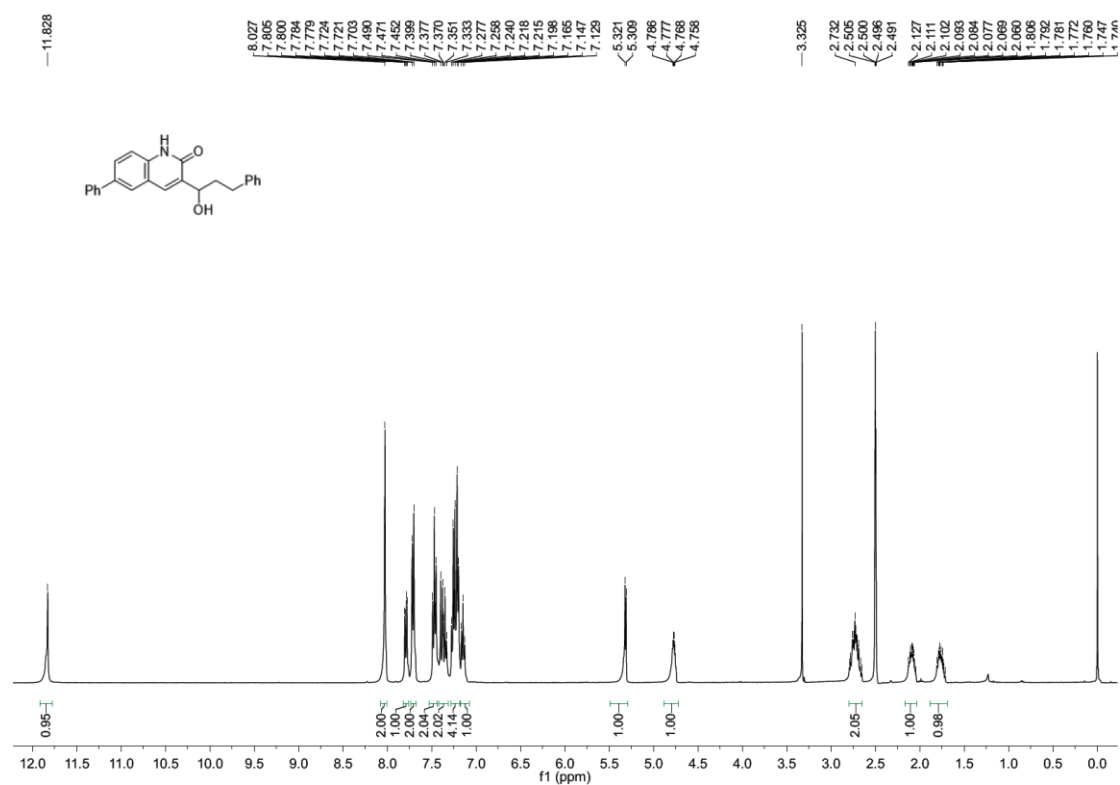
4q-¹H NMR (400 MHz, CD₃OD)



4q-¹³C NMR (100 MHz, CD₃OD)



7-¹H NMR (400 MHz, DMSO-d₆)



7-¹³C NMR (100 MHz, DMSO-d₆)

