

## Supporting Information

### Catalytic Asymmetric Indolization by a Desymmetrizing [3+2] Annulation Strategy

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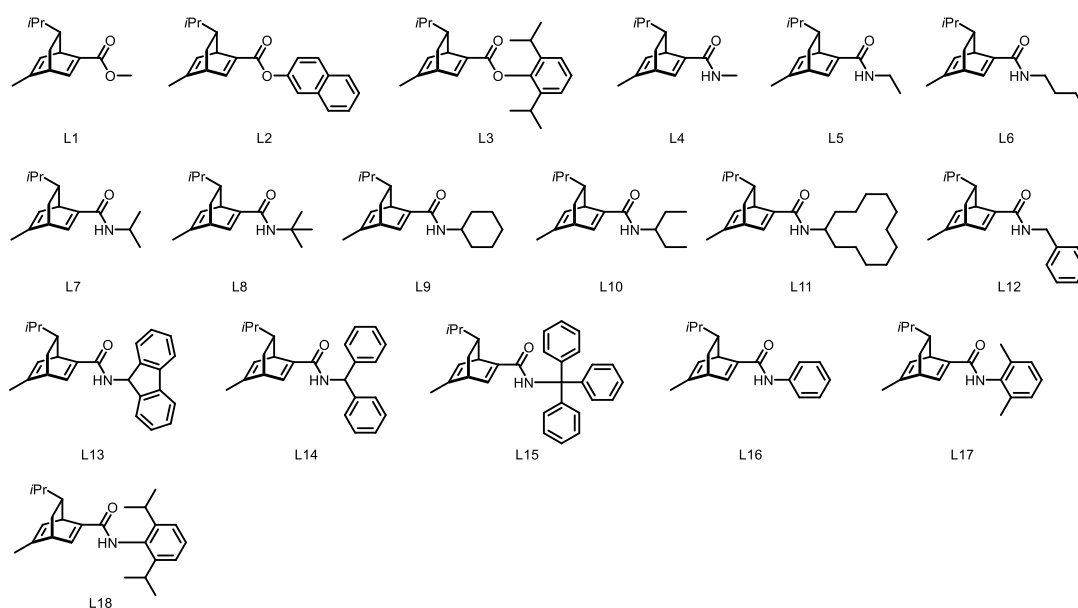
## 1. General information

Unless otherwise noted, all commercialized reagents were used as received without further purification. All air-sensitive manipulations were performed under a dry nitrogen atmosphere using vacuum-line and standard Schlenk techniques. Reaction mixtures were stirred using Teflon-coated magnetic stir bars. Silicone oil bath is used as the heat source for all the reactions that requiring heating. Temperature was maintained using heidolph MR Hei-Tec heating blocks. The abbreviation “rt” refers to reactions carried out approximately between 23–27 °C. Thin layer chromatography (TLC) was performed on pre-coated silica gel HSGF<sub>254</sub> plates and compounds were visualized by observation under UV light at 254 nm and/or by treating the plates with KMnO<sub>4</sub> followed by heating. Flash column chromatography was carried out on silica gel (300–400 mesh).

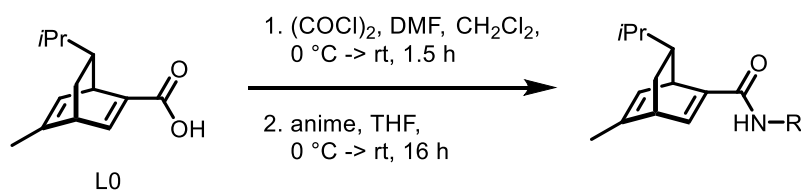
NMR spectra were collected at room temperature on a Bruker AVANCE AV-400 spectrometer (400 MHz for <sup>1</sup>H, 101 MHz for <sup>13</sup>C) or a Bruker AVANCE AV-300 spectrometer (300 MHz for <sup>1</sup>H, 75 MHz for <sup>13</sup>C). Chemical shifts were reported in  $\delta$  (ppm) referenced to the residual solvent peak of CHCl<sub>3</sub>-*d* ( $\delta$  7.26) for <sup>1</sup>H NMR and CHCl<sub>3</sub>-*d* ( $\delta$  77.0) for <sup>13</sup>C NMR, the residual solvent peak of DMSO-*d*<sub>6</sub> ( $\delta$  2.50) for <sup>1</sup>H NMR and DMSO-*d*<sub>6</sub> ( $\delta$  39.52) for <sup>13</sup>C NMR. Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublets), dt (doublet of triplets), dq (doublet of quartets), td (triplet of doublets), tt (triplet of triplets), ddd (doublet of doublet of doublets), ddt (doublet of doublet of triplets), dtd (doublet of triplet of doublets), m (multiplet), br (broad), etc. Coupling constants were reported in Hertz (Hz). Enantiomeric excesses (ee) were determined by HPLC analysis on Shimadzu HPLC system with Daicel chiral columns. Authentic racemic samples of products for chiral HPLC assay determinations were obtained using [Rh(cod)Cl]<sub>2</sub> (3 mol %) as an achiral precatalyst. Optical rotations were measured on an Anton Paar MCP 100 automatic polarimeter. High resolution mass spectra (HRMS) were performed on Waters XEVO G2-S TOF or Agilent 6520B Q-FOF (ESI). Single crystal X-ray diffraction were obtained on Bruker D8 VENTURE diffractometer.

## 2. Materials

All solvents were purchased from commercial suppliers and degassed with N<sub>2</sub> before use. The catalysts [RhCl(L1)]<sub>2</sub>, [RhCl(L2)]<sub>2</sub> were prepared according to the reported procedures.<sup>1a</sup> The catalyst [RhCl(L3)]<sub>2</sub> was prepared according to the reported procedures.<sup>1b</sup> The catalyst [RhCl(L4)]<sub>2</sub> was prepared according to the reported procedures.<sup>1c</sup> The catalysts [RhCl(L7)]<sub>2</sub>, [RhCl(L8)]<sub>2</sub> were prepared according to the reported procedures.<sup>1d</sup> The catalysts [RhCl(L9)]<sub>2</sub>, [RhCl(L12)]<sub>2</sub> were prepared according to the reported procedures.<sup>1e</sup> The catalyst [RhCl(L16)]<sub>2</sub> was prepared according to the reported procedures.<sup>1f</sup> The catalyst [RhCl(L18)]<sub>2</sub> was prepared according to the reported procedures.<sup>1g</sup> The arylboronic acids **2a** was purchased from commercial suppliers and used as received. The 2-aminoarylboronic acid pinacol esters were purchased from commercial suppliers or prepared according to literature methods.<sup>2</sup> The 1,3-diketones were prepared according to literature methods.<sup>3a-3f</sup>

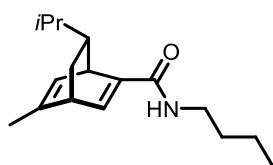


### 2.1 Preparation of ligands and catalysts

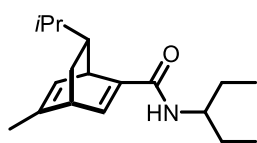


To a solution of carboxylic acid L0 (100 mg, 0.48 mmol, 1.0 equiv.) and DMF (7 μL, 0.01 mmol, 0.2 equiv.) in CH<sub>2</sub>Cl<sub>2</sub> (1.5 mL) at 0 °C was added oxalyl chloride (82

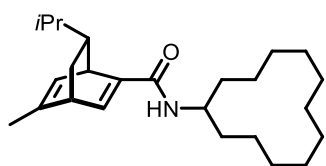
$\mu\text{L}$ , 0.97 mmol, 2.0 equiv.) dropwise over 1 min. The mixture was warmed to room temperature and stirred for 1.5 h to give a solution of the corresponding acyl chloride. The solvent was removed under vacuum, and the residue was dissolved in THF (1.0 mL). To a solution of the corresponding amine (1.21 mmol, 2.5 equiv.) in THF (1.5 mL) was added the solution of acyl chloride dropwise at 0 °C. The mixture was then stirred at room temperature for 16 h. Saturated aqueous  $\text{K}_2\text{CO}_3$  solution was added, and the mixture was extracted with EtOAc for three times. The combined organic extracts were washed with saturated aqueous  $\text{NH}_4\text{Cl}$  solution, dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated under vacuum. Purification of the residue by silica gel column chromatography eluting with petroleum ether/EtOAc (PE/EA) gave the corresponding diene ligands.



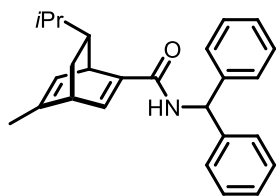
L6: Purified by silica gel column chromatography (PE:EA v/v=5:1) to obtain a white solid (86.7 mg, 68% yield).  $^1\text{H}$  NMR ( $\text{CHCl}_3\text{-}d$ , 300 MHz):  $\delta$  6.77 (dd,  $J$  = 6.2, 1.9 Hz, 1H), 5.90 (t,  $J$  = 5.8 Hz, 1H), 5.74 (dt,  $J$  = 6.0, 1.8 Hz, 1H), 3.98 (dt,  $J$  = 6.1, 2.0 Hz, 1H), 3.31 – 3.18 (m, 3H), 1.76 (d,  $J$  = 1.7 Hz, 3H), 1.56 – 1.48 (m, 1H), 1.48 – 1.40 (m, 2H), 1.35 – 1.25 (m, 2H), 1.18 – 1.11 (m, 1H), 1.08 – 0.99 (m, 1H), 0.94 (d,  $J$  = 5.9 Hz, 3H), 0.92 – 0.89 (m, 1H), 0.87 (t,  $J$  = 7.3 Hz, 4H), 0.76 (d,  $J$  = 6.1 Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CHCl}_3\text{-}d$ , 75 MHz):  $\delta$  166.03, 144.99, 143.84, 137.57, 124.10, 47.76, 43.53, 39.97, 39.26, 33.84, 31.81, 21.84, 21.38, 20.17, 19.00, 13.81. HRMS (ESI+): calcd. for  $\text{C}_{17}\text{H}_{28}\text{NO}^+$   $[\text{M}+\text{H}]^+$  262.2165, found 262.2175. Optical rotation:  $[\alpha]^{25}_{\text{D}} +20.7$  ( $c$  1.08,  $\text{CHCl}_3$ ).



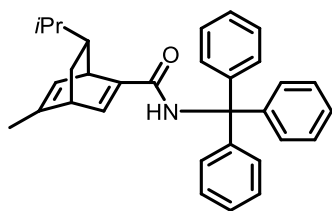
L11: Purified by silica gel column chromatography (PE:EA v/v=10:1) to obtain a white solid (87.5 mg, 66% yield).  $^1\text{H}$  NMR ( $\text{CHCl}_3\text{-}d$ , 300 MHz):  $\delta$  6.76 (dd,  $J$  = 6.2, 1.9 Hz, 1H), 5.80 (dt,  $J$  = 6.0, 1.8 Hz, 1H), 5.35 (d,  $J$  = 9.0 Hz, 1H), 4.01 (dt,  $J$  = 6.1, 2.0 Hz, 1H), 3.88 – 3.75 (m, 1H), 3.37 – 3.28 (m, 1H), 1.81 (d,  $J$  = 1.7 Hz, 3H), 1.61 – 1.51 (m, 3H), 1.43 – 1.33 (m, 2H), 1.23 – 1.17 (m, 1H), 1.12 – 1.04 (m, 1H), 0.99 (d,  $J$  = 5.9 Hz, 3H), 0.92 – 0.85 (m, 7H), 0.81 (d,  $J$  = 6.1 Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CHCl}_3\text{-}d$ , 75 MHz):  $\delta$  166.03, 145.36, 143.92, 137.13, 124.19, 51.88, 47.89, 43.58, 40.17, 33.90, 31.91, 27.58, 27.50, 21.91, 21.43, 19.08, 10.38, 10.34. HRMS (ESI+): calcd. for  $\text{C}_{18}\text{H}_{30}\text{NO}^+$   $[\text{M}+\text{H}]^+$  276.2322, found 276.2331. Optical rotation:  $[\alpha]^{25}_{\text{D}} +24.3$  ( $c$  0.66,  $\text{CHCl}_3$ ).



L12: Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (136.1 mg, 76% yield). **<sup>1</sup>H NMR (CHCl<sub>3</sub>-d, 300 MHz):** δ 6.70 (dd, *J* = 6.2, 1.9 Hz, 1H), 5.75 (dt, *J* = 6.0, 1.9 Hz, 1H), 5.52 (d, *J* = 8.6 Hz, 1H), 4.11 – 4.02 (m, 1H), 3.99 (dt, *J* = 6.1, 2.1 Hz, 1H), 3.30 – 3.22 (m, 1H), 1.77 (d, *J* = 1.7 Hz, 3H), 1.57 – 1.17 (m, 26H), 1.08 – 1.00 (m, 1H), 0.95 (d, *J* = 5.8 Hz, 3H), 0.91 – 0.84 (m, 1H), 0.77 (d, *J* = 6.1 Hz, 3H); **<sup>13</sup>C NMR (CHCl<sub>3</sub>-d, 75 MHz):** δ 165.51, 145.29, 143.77, 137.01, 124.23, 47.73, 45.68, 43.52, 40.04, 33.89, 31.90, 30.45, 30.36, 23.85, 23.80, 23.56, 23.52, 23.42, 23.39, 21.86, 21.59, 21.53, 21.39, 19.02. **HRMS (ESI+):** calcd. for C<sub>25</sub>H<sub>42</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 372.3261, found 372.3266. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +11.8 (*c* 1.28, CHCl<sub>3</sub>).

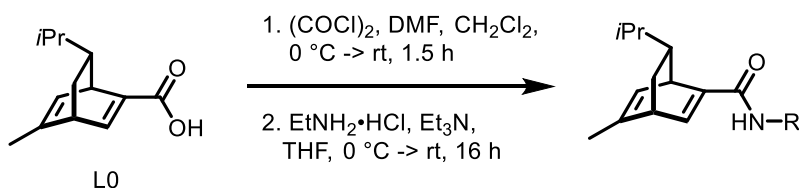


L14: Purified by silica gel column chromatography (PE:EA v/v=10:1) to obtain a white solid (167.3 mg, 93% yield). **<sup>1</sup>H NMR (CHCl<sub>3</sub>-d, 300 MHz):** δ 7.38 – 7.19 (m, 10H), 6.87 (dd, *J* = 6.2, 1.9 Hz, 1H), 6.37 (d, *J* = 7.9 Hz, 1H), 6.30 (d, *J* = 7.8 Hz, 1H), 5.87 – 5.76 (m, 1H), 4.12 (dt, *J* = 6.1, 2.0 Hz, 1H), 3.38 – 3.29 (m, 1H), 1.83 (d, *J* = 1.7 Hz, 3H), 1.59 (ddd, *J* = 11.6, 8.7, 3.0 Hz, 1H), 1.28 – 1.18 (m, 1H), 1.16 – 1.04 (m, 1H), 1.00 (d, *J* = 5.9 Hz, 4H), 0.99 – 0.90 (m, 3H), 0.84 (d, *J* = 6.2 Hz, 3H); **<sup>13</sup>C NMR (CHCl<sub>3</sub>-d, 75 MHz):** δ 165.16, 144.71, 143.69, 141.83, 141.79, 138.19, 128.66, 128.62, 127.49, 127.40, 127.38, 124.24, 56.93, 47.74, 43.61, 40.00, 33.86, 31.83, 21.88, 21.38, 19.05. **HRMS (ESI+):** calcd. for C<sub>26</sub>H<sub>30</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 372.2322, found 372.2323. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +12.7 (*c* 1.42, CHCl<sub>3</sub>).

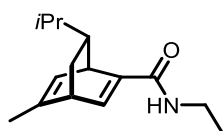


L15: This reaction condition needs to be modified from the standard reaction procedure. The mixture of acyl chloride and amine needed to be heated at reflux for 16 h. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (114.2 mg, 53% yield). **<sup>1</sup>H NMR (CHCl<sub>3</sub>-d, 300 MHz):** δ 7.38 – 7.28 (m, 15H), 7.00 – 6.91 (m, 2H), 5.91 – 5.80 (m, 1H), 4.09 (dt, *J* = 6.1, 2.0 Hz, 1H), 3.47 – 3.34 (m, 1H), 1.89 (d, *J* = 1.7 Hz, 3H), 1.68 (ddd, *J* = 11.6, 8.7, 3.0 Hz, 1H), 1.33 – 1.25 (m, 1H), 1.21 – 1.11 (m, 1H), 1.02 (d, *J* = 6.3 Hz, 3H), 1.01 – 0.94 (m, 1H), 0.89 (d, *J* = 6.3 Hz, 3H); **<sup>13</sup>C NMR (CHCl<sub>3</sub>-d, 75 MHz):** δ 164.92, 145.90, 145.02, 143.69, 137.76, 128.67, 127.96, 126.95, 124.28, 70.24, 47.78, 43.60, 40.09, 33.89, 31.91, 21.88, 21.40, 19.06.

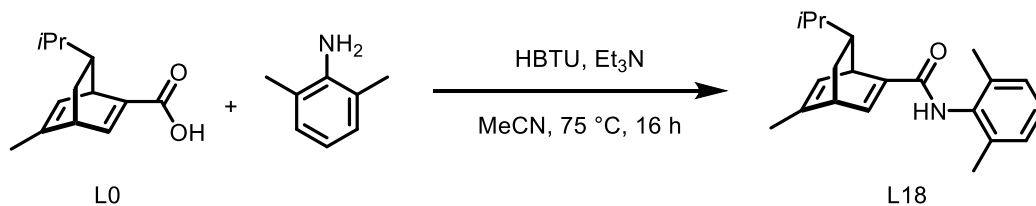
**HRMS (ESI+):** calcd. for C<sub>32</sub>H<sub>34</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 448.2635, found 448.2639. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +8.8 (*c* 2.00, CHCl<sub>3</sub>).



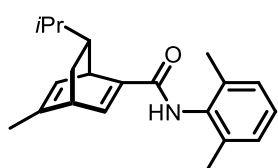
To a solution of carboxylic acid L0 (100 mg, 0.48 mmol, 1.0 equiv.) and DMF (7 μL, 0.01 mmol, 0.2 equiv.) in CH<sub>2</sub>Cl<sub>2</sub> (1.5 mL) at 0 °C was added oxalyl chloride (82 μL, 0.97 mmol, 2.0 equiv.) dropwise over 1 min. The mixture was warmed to room temperature and stirred for 1.5 h to give a solution of the corresponding acyl chloride. The solvent was removed under vacuum, and the residue was dissolved in THF (1.0 mL). To a solution of the corresponding ethylamine hydrochloride (98.8 mg, 1.21 mmol, 2.5 equiv.) in the mixture of THF (1.5 mL) and Et<sub>3</sub>N (0.2 mL, 1.45 mmol, 3.0 equiv.) was added the solution of acyl chloride dropwise at 0 °C. The mixture was then stirred at room temperature for 16 h. Saturated aqueous K<sub>2</sub>CO<sub>3</sub> solution was added, and the mixture was extracted with EtOAc for three times. The combined organic extracts were washed with saturated aqueous NH<sub>4</sub>Cl solution, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under vacuum. Purification of the residue by silica gel column chromatography eluting with petroleum ether/EtOAc (PE/EA) gave the corresponding diene ligands.



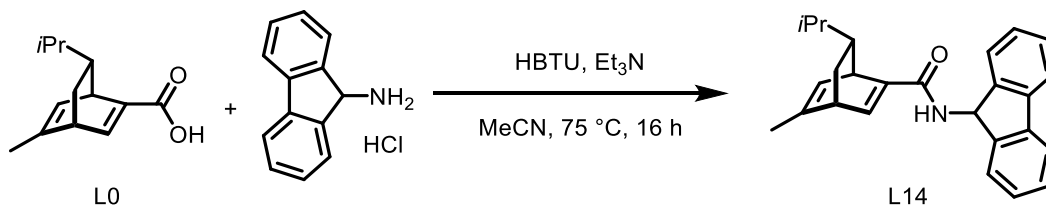
L5: Purified by silica gel column chromatography (PE:EA v/v=3:1) to obtain a white solid (73.2 mg, 65% yield). <sup>1</sup>H NMR (CHCl<sub>3</sub>-*d*, 300 MHz): δ 6.78 (dd, *J* = 6.2, 2.0 Hz, 1H), 5.88 – 5.63 (m, 2H), 4.06 – 3.94 (m, 1H), 3.37 – 3.24 (m, 3H), 1.79 (d, *J* = 1.7 Hz, 3H), 1.54 (ddd, *J* = 11.5, 8.6, 3.0 Hz, 1H), 1.22 – 1.17 (m, 1H), 1.13 (t, *J* = 7.2 Hz, 3H), 1.08 – 1.02 (m, 1H), 0.97 (d, *J* = 5.9 Hz, 3H), 0.93 – 0.88 (m, 1H), 0.79 (d, *J* = 6.1 Hz, 3H); <sup>13</sup>C NMR (CHCl<sub>3</sub>-*d*, 75 MHz): δ 166.05, 145.07, 143.98, 137.75, 124.18, 47.83, 43.62, 40.08, 34.44, 33.94, 31.87, 21.93, 21.47, 19.09, 15.03. **HRMS (ESI+):** calcd. for C<sub>15</sub>H<sub>24</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 234.1852, found 234.1862. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +28.8 (*c* 0.27, CHCl<sub>3</sub>).



To a solution of carboxylic acid L0 (100 mg, 0.48 mmol, 1.0 equiv.) and HBTU (202.2 mg, 0.53 mmol, 1.1 equiv.) in MeCN (10 mL) at room temperature was added Et<sub>3</sub>N (74 μL, 0.53 mmol, 1.1 equiv.) and 2,6-dimethylaniline (58.7 mg, 1.1 mmol, 1.1 equiv.). The mixture was heated at 75 °C for 16 h, then cooled to room temperature, quenched with brine. The mixture was extracted with EtOAc for three times. The combined organic extracts were washed with 1 M aqueous HCl solution, saturated aqueous NaHCO<sub>3</sub> solution, and brine. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under vacuum. Purification of the residue by silica gel column chromatography eluting with petroleum ether/EtOAc (PE/EA) gave the corresponding diene ligands.

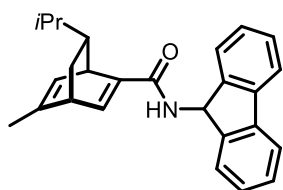


L17: Purified by silica gel column chromatography (PE:EA v/v=10:1) to obtain a white solid (55.6 mg, 37% yield). **<sup>1</sup>H NMR (CHCl<sub>3</sub>-d, 300 MHz):** δ 7.13 – 6.97 (m, 5H), 5.84 (dt, *J* = 6.2, 1.9 Hz, 1H), 4.10 (dt, *J* = 6.1, 2.1 Hz, 1H), 3.44 – 3.35 (m, 1H), 2.21 (s, 6H), 1.86 (d, *J* = 1.6 Hz, 3H), 1.64 (ddd, *J* = 11.6, 8.7, 3.0 Hz, 1H), 1.26 – 1.21 (m, 1H), 1.17 – 1.09 (m, 1H), 1.00 (d, *J* = 6.4 Hz, 3H), 0.98 – 0.96 (m, 1H), 0.84 (d, *J* = 6.3 Hz, 3H); **<sup>13</sup>C NMR (CHCl<sub>3</sub>-d, 75 MHz):** δ 164.24, 144.87, 143.89, 139.02, 135.65, 134.09, 128.19, 127.13, 124.17, 48.09, 43.79, 40.26, 33.93, 31.86, 21.96, 21.49, 19.15, 18.64. **HRMS (ESI+):** calcd. for C<sub>21</sub>H<sub>28</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 310.2165, found 310.2166. **Optical rotation:** [α]<sub>D</sub><sup>25</sup> +7.8 (*c* 0.45, CHCl<sub>3</sub>).



To a solution of carboxylic acid L0 (100 mg, 0.48 mmol, 1.0 equiv.) and HBTU (202.2 mg, 0.53 mmol, 1.1 equiv.) in MeCN (10 mL) at room temperature was added Et<sub>3</sub>N (148 μL, 1.1 mmol, 2.2 equiv.) and 9H-fluoren-9-amine hydrochloride (116.1 mg, 0.53 mmol, 1.1 equiv.). The mixture was heated at reflux for 16 h, then cooled to room

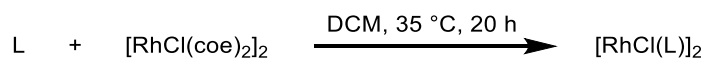
temperature, quenched with brine. The mixture was extracted with EtOAc for three times. The combined organic extracts were washed with 1 M aqueous HCl solution, saturated aqueous NaHCO<sub>3</sub> solution, and brine. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under vacuum. Purification of the residue by silica gel column chromatography eluting with petroleum ether/EtOAc (PE/EA) gave the corresponding diene ligands.



L13: Purified by silica gel column chromatography (PE:EA v/v=10:1) to obtain a white solid (105.0 mg, 59% yield).

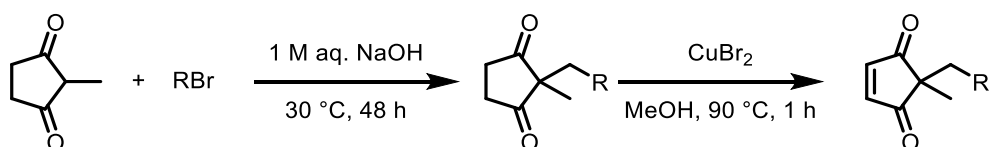
**<sup>1</sup>H NMR (CHCl<sub>3</sub>-d, 300 MHz):** δ 7.68 (d, *J* = 7.5 Hz, 2H), 7.58 (t, *J* = 7.0 Hz, 2H), 7.42 – 7.35 (m, 2H), 7.34 – 7.26 (m, 2H), 6.78 (dd, *J* = 6.2, 1.9 Hz, 1H), 6.28 (d, *J* = 8.8 Hz,

1H), 5.95 (d, *J* = 8.9 Hz, 1H), 5.87 – 5.80 (m, 1H), 4.20 – 4.10 (m, 1H), 3.36 – 3.27 (m, 1H), 1.81 (d, *J* = 1.6 Hz, 3H), 1.59 (ddd, *J* = 11.6, 8.7, 3.0 Hz, 1H), 1.30 – 1.24 (m, 1H), 1.18 – 1.08 (m, 1H), 1.04 (d, *J* = 6.0 Hz, 3H), 0.97 (ddd, *J* = 11.5, 4.8, 2.4 Hz, 1H), 0.85 (d, *J* = 6.1 Hz, 3H); **<sup>13</sup>C NMR (CHCl<sub>3</sub>-d, 75 MHz):** δ 166.59, 144.72, 144.69, 144.62, 143.86, 140.67, 140.60, 138.75, 128.67, 127.82, 127.78, 125.34, 125.32, 124.22, 120.02, 120.00, 54.74, 47.87, 43.68, 40.16, 33.95, 31.82, 21.94, 21.51, 19.06. **HRMS (ESI+):** calcd. for C<sub>26</sub>H<sub>28</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 370.2165, found 370.2171. **Optical rotation:** [α]<sub>D</sub><sup>25</sup> +10.9 (*c* 0.75, CHCl<sub>3</sub>).



[RhCl(coe)<sub>2</sub>]<sub>2</sub> (0.11 mmol) and ligand L (0.20 mmol) were placed in a Schlenk tube under nitrogen. Dichloromethane (2.0 mL) was added and the resulting solution was stirred at 35 °C for 20 h. Upon completion, the crude mixture was concentrated under vacuum and purified by flash silica gel column chromatography eluting with petroleum ether/EtOAc (PE/EA) as eluent to give the corresponding [RhCl(L)]<sub>2</sub> as an orange solid.

## 2.2 Preparation of 1,3-diketones

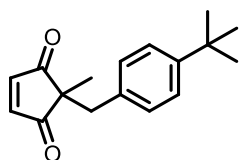


2-Methyl cyclopentane-1,3-dione (8.92 mmol, 1.0 equiv.) was taken with 10.5 mL of 1 M aq. NaOH solution and the suspension was stirred at room temperature for 10

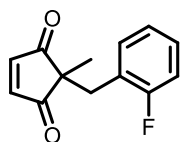


min. To this mixture was added RBr (17.84 mmol, 2.0 equiv.) at once and the resulting biphasic solution was stirred vigorously at room temperature. After being stirred for 48 h, the reaction mixture was diluted with 20 mL of EtOAc, organic phase was separated from aqueous phase, aqueous phase was back-extracted with EtOAc (2 × 20 mL). The combined organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated under reduced pressure. The crude reaction mixture was purified by silica-gel column chromatography eluting with petroleum ether/EtOAc (PE/EA) to obtain 2,2-disubstituted cyclopentane-1,3-dione.

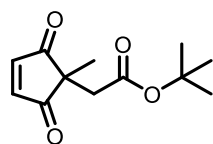
To a solution of 2,2-disubstituted cyclopentane-1,3-dione (1.0 mmol, 1.0 equiv.) in 7 mL MeOH was added copper(II) bromide (2.2 mmol, 2.2 equiv.) and the resulting brown solution was stirred at 90 °C under argon atmosphere for 1 h. After 1 h the reaction mixture was cooled to room temperature, quenched with 2 mL of 1 M aq. HCl solution, 20 mL of Et<sub>2</sub>O was added and the organic phase was separated from aqueous phase. Aqueous phase was back-extracted with Et<sub>2</sub>O (2 × 20 mL). The combined organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated under reduced pressure. The crude reaction mixture was purified by silica-gel column chromatography eluting with petroleum ether/EtOAc (PE/EA) to obtain 2,2-disubstituted cyclopentene-1,3-dione.



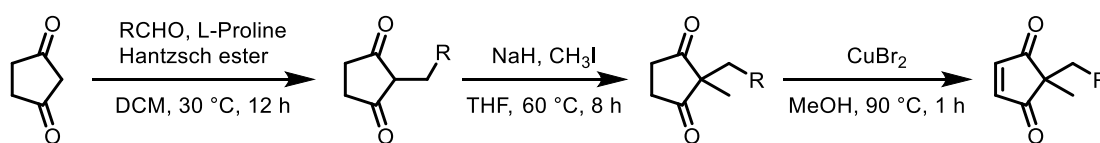
**1c:** Purified by silica gel column chromatography (PE:EA v/v=25:1) to obtain a yellow solid (32% yield in 2 steps). <sup>1</sup>H NMR (CHCl<sub>3</sub>-d, 300 MHz): δ 7.17 – 7.12 (m, 2H), 6.98 (s, 2H), 6.86 – 6.81 (m, 2H), 2.94 (s, 2H), 1.22 (s, 9H), 1.22 (s, 3H); <sup>13</sup>C NMR (CHCl<sub>3</sub>-d, 75 MHz): δ 207.47, 149.82, 148.79, 132.48, 129.42, 125.26, 52.53, 40.41, 34.41, 31.32, 19.37. HRMS (ESI<sup>+</sup>): calcd. for C<sub>17</sub>H<sub>20</sub>NaO<sub>2</sub><sup>+</sup> [M+Na]<sup>+</sup> 279.1355, found 279.1382.



**1j:** Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a yellow solid (45% yield in 2 steps). <sup>1</sup>H NMR (CHCl<sub>3</sub>-d, 300 MHz): δ 7.18 – 7.09 (m, 1H), 7.06 (s, 2H), 7.01 – 6.85 (m, 3H), 2.99 (d, *J* = 1.4 Hz, 2H), 1.22 (s, 3H); <sup>13</sup>C NMR (CHCl<sub>3</sub>-d, 75 MHz): δ 206.51, 162.37, 159.10 (d, *J* = 245.3 Hz), 148.44, 132.24 (d, *J* = 4.1 Hz), 129.14 (d, *J* = 8.1 Hz), 124.00 (d, *J* = 3.6 Hz), 122.54 (d, *J* = 15.9 Hz), 115.64 (d, *J* = 22.3 Hz), 51.33, 33.68 (d, *J* = 2.1 Hz), 18.72; <sup>19</sup>F NMR (CHCl<sub>3</sub>-d, 282 MHz) δ –114.98. HRMS (ESI<sup>+</sup>): calcd. for C<sub>13</sub>H<sub>12</sub>FO<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup> 219.0816, found 219.0818.



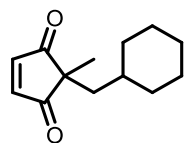
**1s:** This reaction condition needs to be modified from the standard reaction procedure. In the second step of procedure, 2,2-disubstituted cyclopentane-1,3-dione (1.0 mmol, 1.0 equiv.) in 7 mL *t*BuOH was added copper(II) bromide (12.0 mmol, 12.0 equiv.) and the resulting brown solution was stirred at 90 °C under argon atmosphere for 8 h. Purified by silica gel column chromatography (PE:EA v/v=10:1) to obtain a yellow solid (5% yield in 2 steps). **<sup>1</sup>H NMR (CHCl<sub>3</sub>-*d*, 300 MHz):** δ 7.23 (s, 2H), 2.75 (s, 2H), 1.27 (s, 9H), 1.07 (s, 3H); **<sup>13</sup>C NMR (CHCl<sub>3</sub>-*d*, 75 MHz):** δ 206.00, 169.48, 147.55, 81.87, 47.98, 39.05, 27.94, 20.68. **HRMS (ESI+):** calcd. for C<sub>12</sub>H<sub>17</sub>O<sub>4</sub><sup>+</sup> [M+H]<sup>+</sup> 225.1121, found 225.1112.



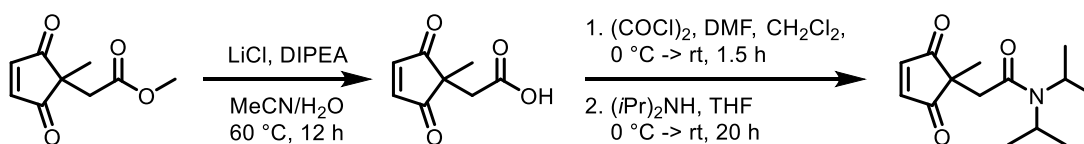
The reaction conditions of the first step are modified from reported procedures.<sup>3f</sup> To a solution of cyclopentane-1,3-dione (981 mg, 10 mmol, 1.0 equiv.), Hantzsch ester (2.78 g, 11 mmol, 1.1 equiv.), and L-proline (57.6 mg, 0.5 mmol, 0.05 equiv.) in 30 mL DCM was added aldehyde (3.37 g, 30 mmol, 3.0 equiv.) and the resulting mixture was stirred at 30 °C for 12 h. After 12 h, the mixture was concentrated to a paste under reduced pressure. The paste was filtered, washed with *n*-hexane, and the filter cake was collected, which was used for the next step without further purification. To a mixture of crude 2-substituted cyclopentane-1,3-dione in 15 mL THF was added a suspension of NaH (60%, 600 mg, 15 mmol, 1.5 equiv.) in 15 mL THF dropwise at 0 °C. The mixture was warm to room temperature and stirred for 10 min. CH<sub>3</sub>I (1.56 mL, 2.28 g, 25 mmol, 2.5 equiv.) was added to the mixture and the resulting mixture was stirred at 60 °C for 8 h. After 8 h the reaction mixture was cooled to room temperature, quenched with 5 mL water, and extracted with EtOAc (3 × 20 mL). The combined organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The crude reaction mixture was purified by silica-gel column chromatography eluting with petroleum ether/EtOAc (PE/EA) to obtain 2,2-disubstituted cyclopentene-1,3-dione.

To a solution of 2,2-disubstituted cyclopentane-1,3-dione (1.0 mmol, 1.0 equiv.) in 7 mL MeOH was added copper(II) bromide (2.2 mmol, 2.2 equiv.) and the resulting brown solution was stirred at 90 °C under argon atmosphere for 1 h. After 1 h the reaction mixture was cooled to room temperature, quenched with 2 mL of 1 M aq. HCl solution, 20 mL of Et<sub>2</sub>O was added and the organic phase was separated from aqueous

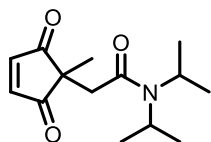
phase. Aqueous phase was back-extracted with Et<sub>2</sub>O (2 × 20 mL). The combined organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated under reduced pressure. The crude reaction mixture was purified by silica-gel column chromatography eluting with petroleum ether/EtOAc (PE/EA) to obtain 2,2-disubstituted cyclopentene-1,3-dione.



**1p:** Purified by silica gel column chromatography (PE:EA v/v=25:1) to obtain a yellow solid (36% yield in 3 steps). <sup>1</sup>H NMR (CHCl<sub>3</sub>-d, 300 MHz): δ 7.23 (s, 2H), 1.60 (d, *J* = 6.3 Hz, 2H), 1.58 – 1.46 (m, 3H), 1.41 – 1.32 (m, 2H), 1.08 (s, 3H), 1.07 – 0.93 (m, 4H), 0.84 – 0.71 (m, 2H); <sup>13</sup>C NMR (CHCl<sub>3</sub>-d, 75 MHz): δ 208.07, 148.22, 50.21, 42.29, 34.58, 34.38, 26.04, 25.96, 21.48. HRMS (ESI<sup>+</sup>): calcd. for C<sub>13</sub>H<sub>19</sub>O<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup> 207.1380, found 207.1389.



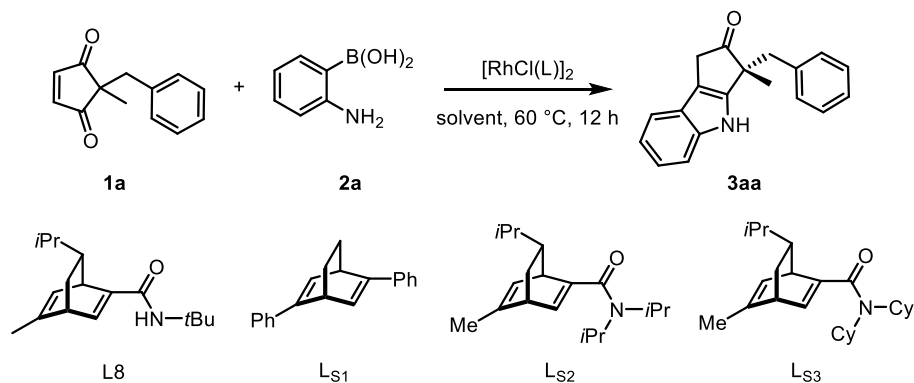
This reaction conditions of the first step are modified from reported procedures.<sup>3g</sup> To a solution of ester (315.0 mg, 1.73 mmol, 1.0 equiv.), LiCl (219.9 mg, 5.19 mmol, 3.0 equiv.) in MeCN/H<sub>2</sub>O (v/v=1:1, 40 mL) was added DIPEA (0.6 mL, 3.46 mmol, 2.0 equiv.). The mixture was stirred for 12 h at 60 °C. The solvent MeCN was removed under vacuum, and 10 mL 1 M aq. HCl solution was added to the residue. The mixture was extracted with EtOAc (3 × 30 mL). The combined organic dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under vacuum, which was used for the next step without further purification. To a solution of carboxylic acid (290.8 mg, 1.73 mmol, 1.0 equiv.) and DMF (27 μL, 0.35 mmol, 0.2 equiv.) in CH<sub>2</sub>Cl<sub>2</sub> (4.8 mL) at 0 °C was added oxalyl chloride (293 μL, 3.46 mmol, 2.0 equiv.) dropwise over 1 min. The mixture was warm to room temperature and stirred for 1.5 h to give a solution of the corresponding acid chloride. The solvent was removed under vacuum, and the residue was dissolved in THF (4.5 mL). To a solution of the diisopropylamine (590 μL, 4.32 mmol, 2.5 equiv.) in THF (4.5 mL) was added the solution of acid chloride dropwise at 0 °C. The mixture was then stirred at room temperature for 20 h. Saturated aqueous K<sub>2</sub>CO<sub>3</sub> solution was added, and the mixture was extracted with EtOAc (3 × 20 mL). The combined organic extracts were washed with saturated aqueous NH<sub>4</sub>Cl solution, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under vacuum. Purification of the residue by silica gel column chromatography eluting with petroleum ether/EtOAc (PE/EA) gave the corresponding amide.



**1t:** Purified by silica gel column chromatography (PE:EA v/v=5:1) to obtain a yellow solid (66% yield in 2 steps). **<sup>1</sup>H NMR (CHCl<sub>3</sub>-*d*, 300 MHz):** δ 7.19 (s, 2H), 3.90 – 3.76 (m, 1H), 3.42 – 3.19 (m, 1H), 2.86 (s, 2H), 1.14 (dd, *J* = 6.8, 1.6 Hz, 12H), 1.06 (s, 3H); **<sup>13</sup>C NMR (CHCl<sub>3</sub>-*d*, 75 MHz):** δ 206.37, 167.76, 147.04, 48.78, 48.40, 45.68, 40.47, 20.77, 20.54, 20.37. **HRMS (ESI+):** calcd. for C<sub>14</sub>H<sub>22</sub>NO<sub>3</sub><sup>+</sup> [M+H]<sup>+</sup> 252.1594, found 252.1602.

### 3. Experimental Section

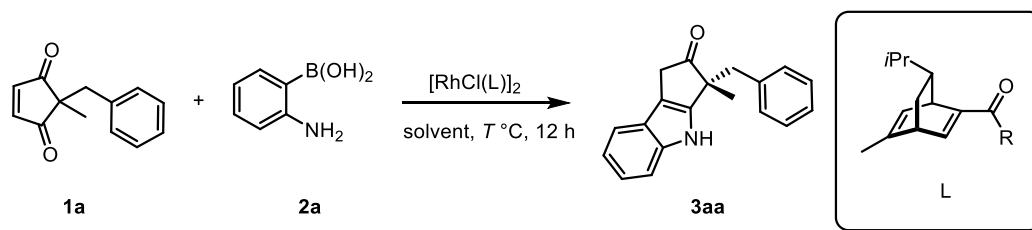
#### 3.1 Evaluation of Reaction Conditions



entry	L	solvent	result
1	$[\text{RhCl}(\text{L8})]_2$	toluene/H <sub>2</sub> O (10:1)	38%, 92.5:7.5 er
2	$[\text{RhCl}(\text{L8})]_2$	1,4-dioxane/H <sub>2</sub> O (10:1)	98%, 81.5:8.5 er
3	$[\text{RhCl}(\text{L8})]_2$	THF/H <sub>2</sub> O (10:1)	98%, 82:8 er
4	$[\text{RhCl}(\text{L8})]_2$	EtOH	98%, 93:7 er
5	$[\text{RhCl}(\text{L}_{\text{S1}})]_2$	EtOH	92%, 85.5:14.5 er
6	$[\text{RhCl}(\text{L}_{\text{S2}})]_2$	EtOH	98%, 87.5:12.5 er
7	$[\text{RhCl}(\text{L}_{\text{S3}})]_2$	EtOH	96%, 90.5:9.5 er
8	$[\text{RhCl}((\text{R})\text{-Binap})]_2$	EtOH	91%, 50:50 er

Condition: **1a** (0.10 mmol), **2a** (0.20 mmol), and Rh catalyst (3 mol% Rh), in the corresponding solvent at  $60\text{ }^\circ\text{C}$  for 12 h. Note: Cy = cyclohexyl.

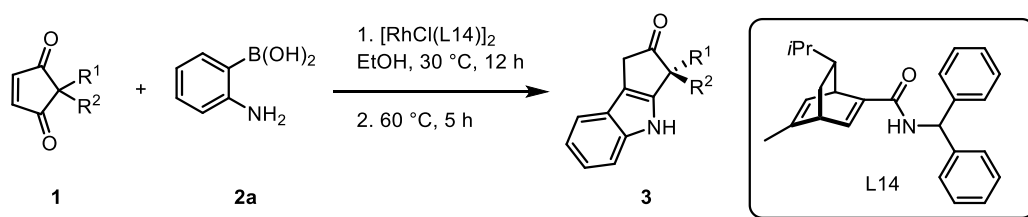
#### 3.2 A General Procedure for Table 1 and Scheme 2



**Procedure:** **1a** (0.10 mmol), **2a** (0.20 mmol),  $[\text{RhCl}(\text{L})]_2$  (3 mol% Rh) were placed in a Schlenk tube under nitrogen. Solvent (1.0 mL) was added and the reaction mixture

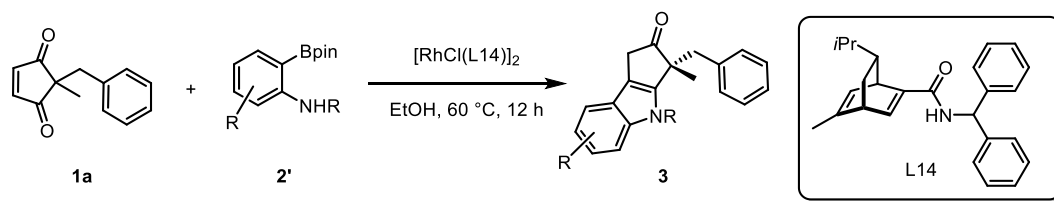
was stirred at  $T$  °C for 12 h. Upon completion, aqueous HCl (0.5 mL, 1 M) was added to remove the deboronated product aniline. The reaction mixture was diluted with ethyl acetate (5 mL) and water (2 mL). The layers were separated and the aqueous layer was extracted again with ethyl acetate for two more times (5 mL  $\times$  2). The combined organic phases were concentrated in vacuo, and the residue was purified by silica gel chromatography eluting with petroleum ether/EtOAc (v/v=15:1) to give product **3aa**.

### 3.3 A General Procedure for Scheme 3



**Procedure:** **1** (0.20 mmol), **2a** (0.30 mmol),  $[\text{RhCl}(\text{L14})]_2$  (3 mol% Rh) were placed in a Schlenk tube under nitrogen. EtOH (2.0 mL) was added and the reaction mixture was stirred at 30 °C for 12 h. The reaction solution was heated and stirred at 60 °C for 5 h. Upon completion, aqueous HCl (0.5 mL, 1 M) was added to remove the deboronated product aniline. The reaction mixture was diluted with ethyl acetate (5 mL) and water (2 mL). The layers were separated and the aqueous layer was extracted again with ethyl acetate for two more times (5 mL  $\times$  2). The combined organic phases were concentrated in vacuo, and the residue was purified by silica gel chromatography eluting with petroleum ether/EtOAc to give product **3**.

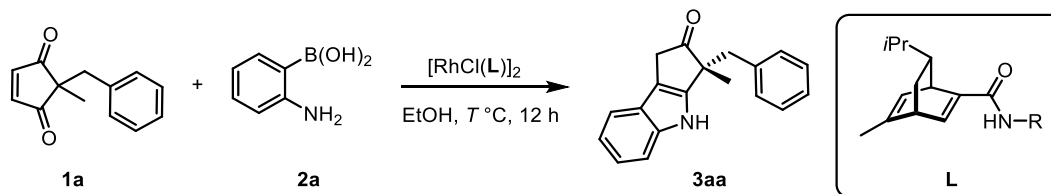
### 3.4 A General Procedure for Scheme 4



**Procedure:** **1** (0.20 mmol), **2'** (0.30 mmol),  $[\text{RhCl}(\text{L14})]_2$  (3 mol% Rh) were placed in a Schlenk tube under nitrogen. EtOH (2.0 mL) was added and the reaction mixture was stirred at 60 °C for 12 h. Upon completion, aqueous HCl (0.5 mL, 1 M) was added to remove the deboronated product aniline. The reaction mixture was diluted with ethyl acetate (5 mL) and water (2 mL). The layers were separated and the aqueous layer was extracted again with ethyl acetate for two more times (5 mL  $\times$  2). The

combined organic phases were concentrated in vacuo, and the residue was purified by silica gel chromatography eluting with petroleum ether/EtOAc to give product **3**.

### 3.5 Eyring Analysis for Reaction



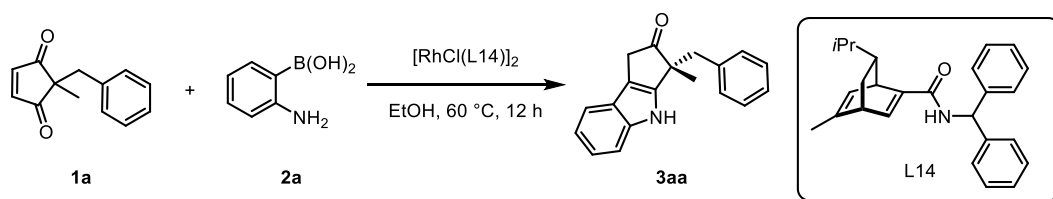
**Procedure:** **1a** (0.10 mmol), **2a** (0.20 mmol),  $[\text{RhCl}(\text{L})_2]_2$  (3 mol% Rh) were placed in a Schlenk tube under nitrogen. EtOH (1.0 mL) was added and the reaction mixture was stirred at  $T$  °C for 12 h. Upon completion, aqueous HCl (0.5 mL, 1 M) was added to remove the deboronated product aniline. The reaction mixture was diluted with ethyl acetate (5 mL) and water (2 mL). The layers were separated and the aqueous layer was extracted again with ethyl acetate for two more times (5 mL  $\times$  2). The combined organic phases were concentrated in vacuo, and the residue was purified by silica gel chromatography eluting with petroleum ether/EtOAc (v/v=15:1) to give product **3aa**. The er was determined by chiral HPLC analysis using Daicel Chiralcel IB column.

Table S1 lists the origin peak area data from HPLC analysis, and the er values are determined as  $A:(100 - A)$ . The activation parameters were calculated using  $R \ln(\text{er}) = -\Delta\Delta H^\ddagger/T + \Delta\Delta S^\ddagger$ , where  $R = 1.98720478 \text{ cal}/(\text{mol} \cdot \text{K})$ . Linear regression models were developed and evaluated using Python package Statsmodels 0.13.2. The visualizations of linear regression models were performed by Python package Matplotlib 3.5.2.<sup>8c</sup>

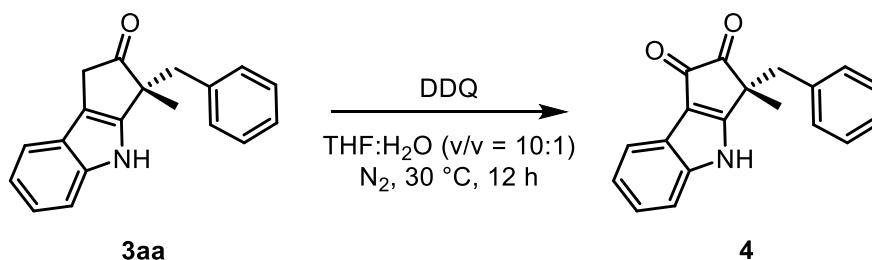
**Table S1: Eyring plot data**

R	$A$ (100 °C)	$A$ (80 °C)	$A$ (60 °C)	$A$ (40 °C)	$A$ (30 °C)	model $R^2$
Me	86.497	87.596	89.367	89.977	90.263	96%
<i>t</i> Bu	91.075	91.830	93.221	94.029	94.398	99%
CHPh <sub>2</sub>	92.277	93.020	94.828	95.554	96.130	98%

### 3.6 Procedures for Scheme 5

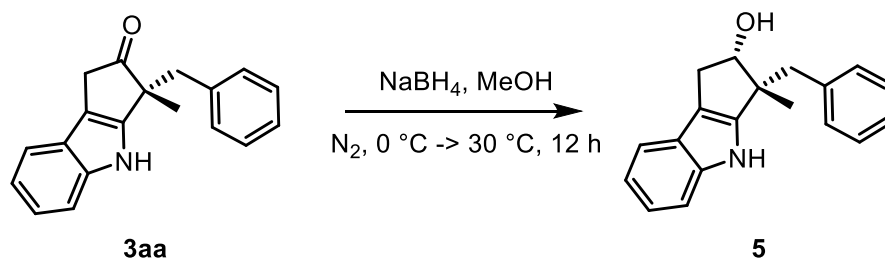


**Procedure:** **1a** (2.00 mmol), **2a** (3.00 mmol),  $[\text{RhCl}(\text{L14})]_2$  (3 mol% Rh) were placed in a Schlenk tube under nitrogen. EtOH (20.0 mL) was added and the reaction mixture was stirred at 30 °C for 12 h. The reaction solution was heated and stirred at 60 °C for 5 h. Upon completion, the reaction mixture was concentrated in vacuo, and then aqueous HCl (5 mL, 1 M) was added to the residue to remove the deboronated product aniline. The mixture was diluted with ethyl acetate (50 mL) and water (20 mL). The layers were separated and the aqueous layer was extracted again with ethyl acetate for two more times (50 mL  $\times$  2). The combined organic phases were concentrated in vacuo, and the residue was purified by silica gel chromatography eluting with petroleum ether/EtOAc (v/v=15:1) to give product **3aa**.

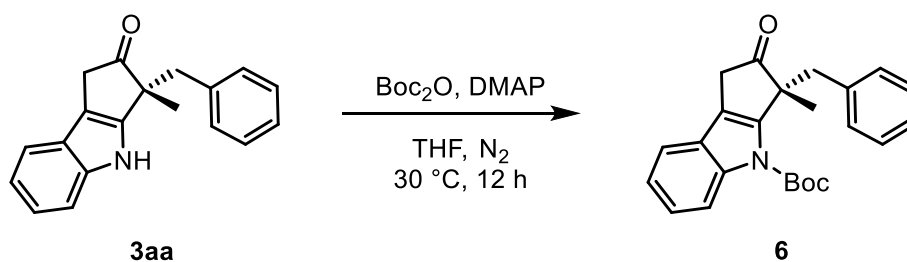


**Procedure:** **3aa** (27.5 mg, 0.10 mmol) and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ, 68.3 mg, 0.30 mmol) were placed in a Schlenk tube under nitrogen. THF:H<sub>2</sub>O (1.5 mL: 0.15 mL) was added and the reaction mixture was stirred at 30 °C for 12 h. Upon completion, saturated aqueous NaHCO<sub>3</sub> (3 mL) was added. The reaction mixture was diluted with ethyl acetate (5 mL). The layers were separated and the aqueous layer was extracted again with ethyl acetate for two more times (5 mL  $\times$  2). The combined organic phases were concentrated in vacuo, and the residue was purified by silica gel chromatography eluting with petroleum ether/EtOAc (v/v=2:1) to give the product **4**.

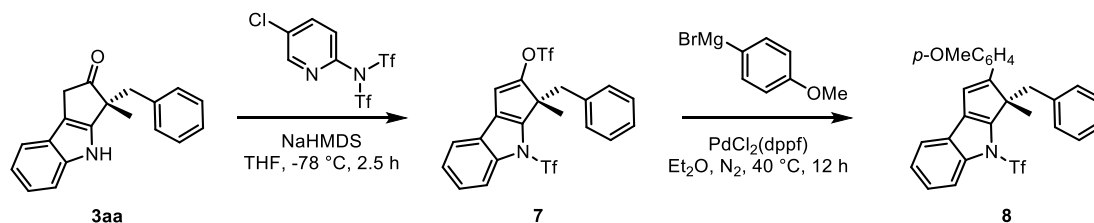




**Procedure:** **3aa** (27.5 mg, 0.10 mmol) and NaBH<sub>4</sub> (11.3 mg, 0.30 mmol) were placed in a Schlenk tube under nitrogen. MeOH (1.0 mL) was added at 0 °C, and the reaction mixture was stirred at 30 °C for 12 h. Upon completion, H<sub>2</sub>O (1 mL) was added. The reaction mixture was diluted with ethyl acetate (5 mL). The layers were separated and the aqueous layer was extracted again with ethyl acetate for two more times (5 mL × 2). The combined organic phases were concentrated in vacuo, and the residue was purified by silica gel chromatography eluting with petroleum ether/EtOAc (v/v=6:1) to give the product **5**.



**Procedure:** **3aa** (27.5 mg, 0.10 mmol) and DMAP (18.3 mg, 0.15 mmol) were placed in a Schlenk tube under nitrogen. Boc<sub>2</sub>O (46 μL, 0.20 mmol) and THF (1 mL) was added and the reaction mixture was stirred at 30 °C for 12 h. Upon completion, the reaction mixture was concentrated in vacuo, and the residue was purified by silica gel chromatography eluting with petroleum ether/EtOAc (v/v=50:1) to give the product **6**.



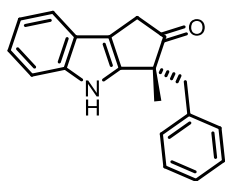
**Procedure:** **3aa** (27.5 mg, 0.10 mmol) and *N*-(5-chloro-2-pyridyl)triflimide (117.7 mg, 0.30 mmol) were placed in a Schlenk tube. Then THF (2.0 mL) was added at -78 °C and NaHMDS (2.0 M in THF, 0.30 mmol, 0.15 mL) was added dropwise and the reaction mixture was stirred at -78 °C for 2.5 h. Upon completion, saturated aqueous

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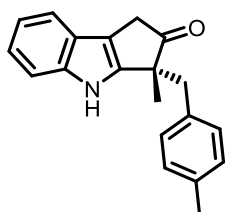
NH<sub>4</sub>Cl (3 mL) was added. The reaction mixture was diluted with ethyl acetate (5 mL). The layers were separated and the aqueous layer was extracted again with ethyl acetate for two more times (5 mL × 2). The combined organic phases were concentrated in vacuo, and the residue was purified by silica gel chromatography eluting with petroleum ether/CH<sub>2</sub>Cl<sub>2</sub> (v/v=10:1) to give the product **7**.

**7** (54.1 mg, 0.10 mmol) and PdCl<sub>2</sub>(dppf) (5 mol%, 3.7 mg) were placed in a Schlenk tube under nitrogen. Et<sub>2</sub>O (1 mL) and *p*-OMeC<sub>6</sub>H<sub>4</sub>MgBr (1.0 M in THF, 0.30 mmol, 0.3 mL) was added, and the reaction mixture was stirred at 40 °C for 12 h. Upon completion, H<sub>2</sub>O (1 mL) was added. The reaction mixture was diluted with ethyl acetate (5 mL). The layers were separated and the aqueous layer was extracted again with ethyl acetate for two more times (5 mL × 2). The combined organic phases were concentrated in vacuo, and the residue was purified by silica gel chromatography eluting with petroleum ether/CH<sub>2</sub>Cl<sub>2</sub> (v/v=8:1) to give the product **8**.

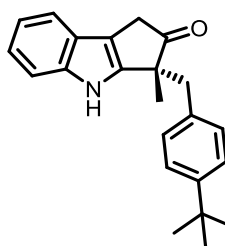
## 4. Product Characterization



**3aa:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (54.0 mg, 98% yield, 96:4 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):** δ 11.36 (s, 1H), 7.42 (d, *J* = 8.1 Hz, 1H), 7.27 (d, *J* = 7.7 Hz, 1H), 7.09 – 7.04 (m, 1H), 7.04 – 6.99 (m, 3H), 6.97 – 6.92 (m, 1H), 6.80 – 6.74 (m, 2H), 3.26 (d, *J* = 21.3 Hz, 1H), 3.07 (s, 2H), 2.67 (d, *J* = 21.3 Hz, 1H), 1.40 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz):** δ 219.10, 144.12, 138.48, 137.13, 129.20, 127.75, 126.25, 123.79, 120.80, 118.97, 118.58, 112.00, 109.40, 52.85, 43.72, 37.95, 23.38. **HRMS (ESI+):** calcd. for C<sub>19</sub>H<sub>18</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 276.1383, found 276.1389. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +31.3 (*c* 0.21, CH<sub>2</sub>Cl<sub>2</sub>) for 96:4 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 16.90 min (*R*), *t*<sub>minor</sub> = 12.04 min (*S*)).

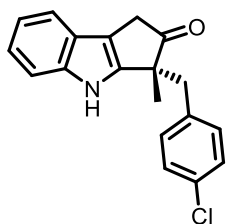


**3ba:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (57.3 mg, 99% yield, 96:4 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz):** δ 11.37 (s, 1H), 7.43 (d, *J* = 8.1 Hz, 1H), 7.28 (d, *J* = 7.7 Hz, 1H), 7.12 – 7.00 (m, 1H), 7.00 – 6.92 (m, 1H), 6.83 (d, *J* = 7.8 Hz, 2H), 6.68 (d, *J* = 8.1 Hz, 2H), 3.28 (d, *J* = 21.3 Hz, 1H), 3.04 (s, 2H), 2.72 (d, *J* = 21.3 Hz, 1H), 2.10 (s, 3H), 1.40 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz):** δ 219.21, 144.29, 138.51, 135.12, 134.10, 129.13, 128.41, 123.85, 120.77, 118.97, 118.61, 112.03, 109.36, 52.91, 43.33, 38.00, 23.45, 20.54. **HRMS (ESI+):** calcd. for C<sub>20</sub>H<sub>20</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 290.1539, found 290.1548. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +8.5 (*c* 0.57, CH<sub>2</sub>Cl<sub>2</sub>) for 96:4 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 16.40 min (*R*), *t*<sub>minor</sub> = 10.39 min (*S*)).



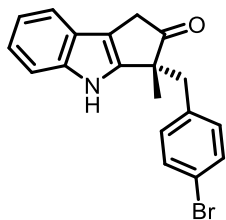
**3ca:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (65.6 mg, 99% yield, 95.5:4.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz):** δ 11.39 (s, 1H), 7.44 (d, *J* = 8.1 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.12 – 7.02 (m, 3H), 7.00 – 6.92 (m, 1H), 6.79 – 6.68 (m, 2H), 3.28 (d, *J* = 21.2 Hz, 1H), 3.05 (s, 2H), 2.74 (d, *J* = 21.2 Hz, 1H), 1.39 (s, 3H), 1.14 (s, 9H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75**

**MHz):**  $\delta$  218.95, 148.34, 144.42, 138.54, 134.08, 129.05, 124.52, 123.91, 120.79, 119.00, 118.60, 112.06, 109.34, 52.62, 43.02, 37.90, 33.99, 31.07, 23.58. **HRMS (ESI+):** calcd. for  $C_{20}H_{20}NO_2^+$   $[M+H]^+$  306.1489, found 306.1521. **Optical rotation:**  $[\alpha]^{25}_D$   $-21.3$  ( $c$  0.66,  $CH_2Cl_2$ ) for 95.5:4.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm,  $t_{major}$  = 12.20 min (*R*),  $t_{minor}$  = 8.82 min (*S*)).



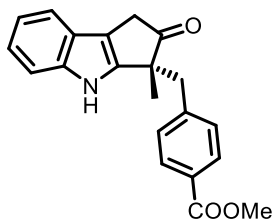
**3da:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (61.3 mg, 99% yield, 95.5:4.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):**  $\delta$  11.34 (s, 1H), 7.43 (d,  $J$  = 8.1 Hz, 1H), 7.30 (d,  $J$  = 7.8 Hz, 1H), 7.13 – 7.03 (m, 3H), 7.00 – 6.93 (m, 1H), 6.83 – 6.77 (m, 2H), 3.31 (d,  $J$  = 21.4 Hz,

1H), 3.07 (s, 2H), 2.78 (d,  $J$  = 21.4 Hz, 1H), 1.40 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz):**  $\delta$  218.94, 143.80, 138.48, 136.15, 131.02, 131.01, 127.76, 123.75, 120.89, 119.03, 118.64, 112.03, 109.44, 52.74, 42.77, 37.91, 23.25. **HRMS (ESI+):** calcd. for  $C_{19}H_{17}^{35}ClNO^+$   $[M+H]^+$  310.0993, found 310.0988. **Optical rotation:**  $[\alpha]^{25}_D$   $+35.4$  ( $c$  0.61,  $CH_2Cl_2$ ) for 95.5:4.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 92/8, 1.0 mL/min, 25 °C, 254 nm,  $t_{major}$  = 14.42 min (*R*),  $t_{minor}$  = 9.14 min (*S*)).

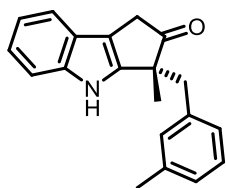


**3ea:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (70.1 mg, 99% yield, 95:5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz):** 11.36 (s, 1H), 7.43 (d,  $J$  = 8.1 Hz, 1H), 7.30 (d,  $J$  = 7.7 Hz, 1H), 7.27 – 7.19 (m, 2H), 7.12 – 7.03 (m, 1H), 7.01 – 6.91 (m, 1H), 6.80 – 6.69 (m, 2H), 3.32 (d,  $J$  = 21.4

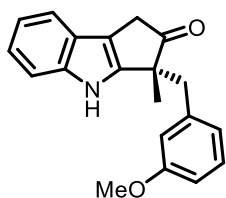
Hz, 1H), 3.05 (s, 2H), 2.78 (d,  $J$  = 21.4 Hz, 1H), 1.39 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz):**  $\delta$  218.98, 143.81, 138.48, 136.59, 131.42, 130.71, 123.76, 120.91, 119.61, 119.05, 118.67, 112.07, 109.44, 52.70, 42.82, 37.94, 23.32. **HRMS (ESI+):** calcd. for  $C_{19}H_{17}^{79}BrNO^+$   $[M+H]^+$  354.0488, found 354.0477. **Optical rotation:**  $[\alpha]^{25}_D$   $+31.7$  ( $c$  0.64,  $CH_2Cl_2$ ) for 95:5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm,  $t_{major}$  = 24.93 min (*R*),  $t_{minor}$  = 14.15 min (*S*)).



**3fa:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (65.3 mg, 98% yield, 95.5:4.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz):** δ 11.37 (s, 1H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.44 (d, *J* = 8.1 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 7.11 – 7.02 (m, 1H), 7.01 – 6.87 (m, 3H), 3.72 (s, 3H), 3.30 (d, *J* = 21.4 Hz, 1H), 3.15 (s, 2H), 2.74 (d, *J* = 21.4 Hz, 1H), 1.42 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz):** δ 218.92, 166.02, 143.73, 142.97, 138.50, 129.61, 128.69, 127.69, 123.73, 120.95, 119.05, 118.66, 112.07, 109.46, 52.83, 51.92, 43.52, 37.93, 23.36. **HRMS (ESI+):** calcd. for C<sub>21</sub>H<sub>20</sub>NO<sub>3</sub><sup>+</sup> [M+H]<sup>+</sup> 334.1438, found 334.1442. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +30.9 (*c* 0.59, CH<sub>2</sub>Cl<sub>2</sub>) for 95.5:4.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 90/10, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 16.26 min (*R*), *t*<sub>minor</sub> = 10.56 min (*S*)).

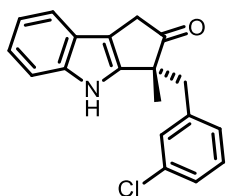


**3ga:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (55.6 mg, 96% yield, 95.5:4.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz):** δ 11.37 (s, 1H), 7.44 (d, *J* = 8.1 Hz, 1H), 7.28 (d, *J* = 7.9 Hz, 1H), 7.12 – 7.03 (m, 1H), 7.00 – 6.79 (m, 3H), 6.62 – 6.53 (m, 2H), 3.27 (d, *J* = 21.2 Hz, 1H), 3.03 (s, 2H), 2.68 (d, *J* = 21.2 Hz, 1H), 2.02 (s, 3H), 1.41 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz):** δ 219.11, 144.21, 138.52, 137.02, 136.59, 130.03, 127.60, 126.89, 126.28, 123.84, 120.81, 118.97, 118.58, 111.97, 109.52, 52.86, 43.81, 38.00, 23.27, 20.85. **HRMS (ESI+):** calcd. for C<sub>20</sub>H<sub>20</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 290.1539, found 290.1546. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +8.9 (*c* 0.55, CH<sub>2</sub>Cl<sub>2</sub>) for 95.5:4.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 16.88 min (*R*), *t*<sub>minor</sub> = 10.89 min (*S*)).

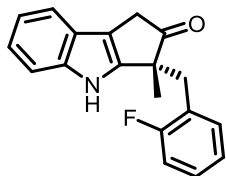


**3ha:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (59.9 mg, 98% yield, 95.5:4.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):** δ 11.39 (s, 1H), 7.44 (d, *J* = 8.1 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.11 – 7.04 (m, 1H), 7.00 – 6.92 (m, 2H), 6.61 – 6.54 (m, 1H), 6.45 – 6.37 (m, 1H), 6.29 – 6.21 (m, 1H), 3.35 (s, 3H), 3.28 (d, *J* = 21.2 Hz, 1H), 3.07 (d, *J* = 13.1 Hz, 1H), 3.03 (d, *J* = 13.0 Hz, 1H), 2.69 (d, *J* = 21.2 Hz, 1H), 1.41 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz):** δ 219.07, 158.52, 144.14,

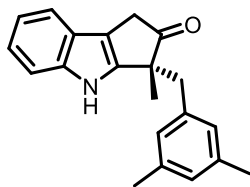
138.64, 138.54, 128.70, 123.84, 121.57, 120.87, 119.03, 118.62, 114.29, 112.24, 111.94, 109.64, 54.36, 52.83, 43.77, 37.98, 23.36. **HRMS (ESI+)**: calcd. for  $C_{20}H_{20}NO_2^+$   $[M+H]^+$  306.1489, found 306.1495. **Optical rotation**:  $[\alpha]^{25}_D +37.8$  ( $c$  0.49,  $CH_2Cl_2$ ) for 95.5:4.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 92/8, 1.0 mL/min, 25 °C, 254 nm,  $t_{major}$  = 14.06 min (*R*),  $t_{minor}$  = 9.97 min (*S*)).



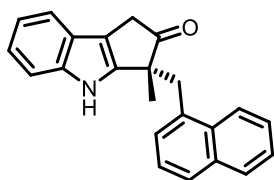
**3ia**: The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (60.7 mg, 98% yield, 94.5:5.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz)**:  $\delta$  11.37 (s, 1H), 7.45 (d,  $J$  = 8.0 Hz, 1H), 7.30 (d,  $J$  = 7.8 Hz, 1H), 7.14 – 7.01 (m, 3H), 7.01 – 6.93 (m, 1H), 6.88 – 6.80 (m, 1H), 6.78 – 6.66 (m, 1H), 3.33 (d,  $J$  = 21.4 Hz, 1H), 3.08 (s, 2H), 2.78 (d,  $J$  = 21.4 Hz, 1H), 1.40 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz)**:  $\delta$  218.89, 143.72, 139.67, 138.50, 132.33, 129.59, 129.14, 127.87, 126.32, 123.75, 120.97, 119.07, 118.67, 112.03, 109.51, 52.74, 42.96, 37.93, 23.33. **HRMS (ESI+)**: calcd. for  $C_{19}H_{17}^{35}ClNO^+$   $[M+H]^+$  310.0993, found 310.0989. **Optical rotation**:  $[\alpha]^{25}_D +50.5$  ( $c$  0.49  $CH_2Cl_2$ ) for 94.5:5.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 92/8, 1.0 mL/min, 25 °C, 254 nm,  $t_{major}$  = 14.94 min (*R*),  $t_{minor}$  = 9.60 min (*S*)).



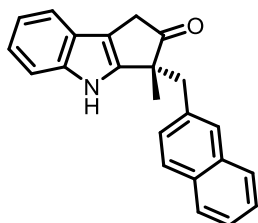
**3ja**: The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (52.8 mg, 93% yield, 90:10 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz)**:  $\delta$  11.32 (s, 1H), 7.42 (d,  $J$  = 8.1 Hz, 1H), 7.31 (d,  $J$  = 7.8 Hz, 1H), 7.17 – 7.02 (m, 2H), 7.01 – 6.79 (m, 4H), 3.31 (d,  $J$  = 21.3 Hz, 1H), 3.14 (d,  $J$  = 13.5 Hz, 1H), 3.08 (d,  $J$  = 13.7 Hz, 1H), 2.90 (d,  $J$  = 21.3 Hz, 1H), 1.41 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz)**:  $\delta$  218.20, 160.44 (d,  $J$  = 244.7 Hz), 144.09, 138.52, 131.79 (d,  $J$  = 4.4 Hz), 128.63 (d,  $J$  = 8.2 Hz), 123.79 (d,  $J$  = 3.4 Hz), 123.77 (d,  $J$  = 15.9 Hz), 123.69, 120.90, 118.98, 118.66, 114.94 (d,  $J$  = 22.5 Hz), 112.04, 109.25, 51.96, 37.73, 36.32, 22.68; **<sup>19</sup>F NMR (DMSO-*d*<sub>6</sub>, 282 MHz)**  $\delta$  -116.29. **HRMS (ESI+)**: calcd. for  $C_{19}H_{17}FNO^+$   $[M+H]^+$  294.1289, found 294.1295. **Optical rotation**:  $[\alpha]^{25}_D +40.5$  ( $c$  0.55,  $CH_2Cl_2$ ) for 90:10 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 92/8, 1.0 mL/min, 25 °C, 254 nm,  $t_{major}$  = 14.94 min (*R*),  $t_{minor}$  = 8.30 min (*S*)).



**3ka:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (60.1 mg, 99% yield, 95:5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz):** δ 11.33 (s, 1H), 7.44 (d, *J* = 8.1 Hz, 1H), 7.28 (d, *J* = 7.6 Hz, 1H), 7.12 – 7.02 (m, 1H), 7.01 – 6.90 (m, 1H), 6.63 (s, 1H), 6.35 (s, 2H), 3.26 (d, *J* = 21.2 Hz, 1H), 2.96 (s, 2H), 2.69 (d, *J* = 21.2 Hz, 1H), 1.96 (s, 6H), 1.39 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz):** δ 219.12, 144.26, 138.50, 136.87, 136.35, 127.68, 127.11, 123.83, 120.80, 118.93, 118.53, 111.89, 109.57, 52.81, 43.83, 38.00, 23.11, 20.74. **HRMS (ESI+):** calcd. for C<sub>21</sub>H<sub>22</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 304.1696, found 304.1701. **Optical rotation:** [α]<sub>D</sub><sup>25</sup> +1.0 (*c* 0.61, CH<sub>2</sub>Cl<sub>2</sub>) for 95:5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 13.85 min (*R*), *t*<sub>minor</sub> = 9.05 min (*S*)).

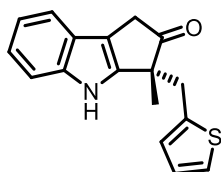


**3la:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (63.8 mg, 98% yield, 94.5:5.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz):** δ 11.35 (s, 1H), 8.17 – 8.05 (m, 1H), 7.80 – 7.72 (m, 1H), 7.65 (d, *J* = 8.2 Hz, 1H), 7.44 – 7.34 (m, 3H), 7.25 – 7.16 (m, 2H), 7.10 – 6.98 (m, 2H), 6.92 (t, *J* = 7.3 Hz, 1H), 3.65 (d, *J* = 13.8 Hz, 1H), 3.53 (d, *J* = 13.8 Hz, 1H), 3.22 (d, *J* = 21.2 Hz, 1H), 2.66 (d, *J* = 21.2 Hz, 1H), 1.52 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz):** δ 218.91, 144.29, 138.39, 133.49, 133.14, 131.78, 128.21, 127.84, 127.05, 125.35, 125.30, 124.97, 124.26, 123.66, 120.82, 118.91, 118.55, 111.91, 109.29, 52.73, 37.96, 23.14. **HRMS (ESI+):** calcd. for C<sub>23</sub>H<sub>20</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 326.1539, found 326.1543. **Optical rotation:** [α]<sub>D</sub><sup>25</sup> +55.4 (*c* 0.70, CH<sub>2</sub>Cl<sub>2</sub>) for 94.5:5.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 90/10, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 12.85 min (*R*), *t*<sub>minor</sub> = 9.48 min (*S*)).

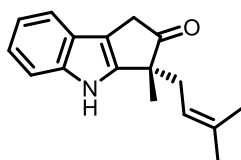


**3ma:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (63.1 mg, 97% yield, 95.5:4.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz):** δ 11.43 (s, 1H), 7.75 – 7.68 (m, 1H), 7.66 – 7.59 (m, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.46 (d, *J* = 8.1 Hz, 1H), 7.41 – 7.33 (m, 3H), 7.23 (d, *J* = 7.8 Hz, 1H), 7.11 – 7.03 (m, 1H), 6.97 – 6.87 (m, 2H), 3.29 (d, *J* = 21.4 Hz, 3H), 3.26 (s, 2H), 2.69 (d, *J* = 21.4 Hz, 1H), 1.46 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz):** δ

219.11, 144.14, 138.52, 134.96, 132.63, 131.57, 127.77, 127.69, 127.35, 127.06, 125.90, 125.46, 123.76, 120.86, 118.99, 118.60, 112.01, 109.41, 52.95, 43.84, 37.96, 23.37. **HRMS (ESI+)**: calcd. for C<sub>23</sub>H<sub>20</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 326.1539, found 326.1542. **Optical rotation**: [ $\alpha$ ]<sub>D</sub><sup>25</sup> +32.2 (*c* 0.43, CH<sub>2</sub>Cl<sub>2</sub>) for 95.5:4.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 92/8, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 16.19 min (*R*), *t*<sub>minor</sub> = 11.10 min (*S*)).

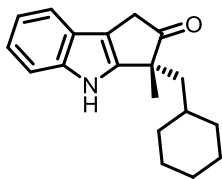


**3na**: The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (50.1 mg, 89% yield, 93.5:6.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz)**:  $\delta$  11.36 (s, 1H), 7.44 (d, *J* = 8.1 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.14 – 7.04 (m, 2H), 7.03 – 6.94 (m, 1H), 6.75 – 6.68 (m, 1H), 6.52 – 6.46 (m, 1H), 3.38 (d, *J* = 21.3 Hz, 1H), 3.35 (d, *J* = 14.4 Hz, 1H), 3.30 (d, *J* = 14.4 Hz, 1H), 2.90 (d, *J* = 21.3 Hz, 1H), 1.40 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz)**:  $\delta$  218.91, 143.83, 138.78, 138.53, 126.36, 126.30, 124.74, 123.90, 120.91, 119.01, 118.67, 112.05, 110.04, 52.65, 37.96, 37.34, 23.34. **HRMS (ESI+)**: calcd. for C<sub>17</sub>H<sub>16</sub>NOS<sup>+</sup> [M+H]<sup>+</sup> 282.0947, found 282.0945. **Optical rotation**: [ $\alpha$ ]<sub>D</sub><sup>25</sup> +31.9 (*c* 0.48, CH<sub>2</sub>Cl<sub>2</sub>) for 93.5:6.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 85/15, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 10.32 min (*R*), *t*<sub>minor</sub> = 6.73 min (*S*)).

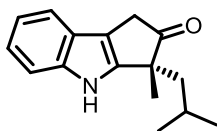


**3oa**: The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (48.1 mg, 95% yield, 87:13 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz)**:  $\delta$  11.22 (s, 1H), 7.44 – 7.35 (m, 2H), 7.11 – 7.05 (m, 1H), 7.04 – 6.97 (m, 1H), 4.82 (t, *J* = 4.2 Hz, 1H), 3.43 (d, *J* = 21.2 Hz, 1H), 3.31 (d, *J* = 21.2 Hz, 1H), 2.49 – 2.35 (m, 2H), 1.52 (s, 3H), 1.48 (s, 3H), 1.28 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz)**:  $\delta$  219.31, 145.09, 138.51, 133.84, 123.94, 120.76, 119.03, 118.97, 118.63, 111.97, 108.87, 51.01, 37.84, 36.24, 25.64, 22.25, 17.59. **HRMS (ESI+)**: calcd. for C<sub>17</sub>H<sub>20</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 254.1539, found 254.1538. **Optical rotation**: [ $\alpha$ ]<sub>D</sub><sup>25</sup> +2.7 (*c* 0.52, CH<sub>2</sub>Cl<sub>2</sub>) for 87:13 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 14.06 min (*R*), *t*<sub>minor</sub> = 8.20 min (*S*)).

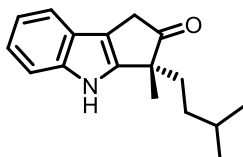




**3pa:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=20:1) to obtain a white solid (53.5 mg, 95% yield, 93:7 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz):** δ 11.27 (s, 1H), 7.48 – 7.35 (m, 2H), 7.13 – 7.04 (m, 1H), 7.04 – 6.96 (m, 1H), 3.51 (d, *J* = 21.3 Hz, 1H), 3.43 (d, *J* = 21.3 Hz, 1H), 1.75 (d, *J* = 6.1 Hz, 2H), 1.53 – 1.38 (m, 3H), 1.35 – 1.26 (m, 2H), 1.23 (s, 3H), 1.05 – 0.67 (m, 6H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz):** δ 219.88, 145.40, 138.51, 124.04, 120.71, 119.01, 118.65, 112.01, 108.62, 50.38, 45.01, 37.84, 34.62, 33.69, 33.58, 25.68, 25.58, 25.56, 25.15. **HRMS (ESI+):** calcd. for C<sub>19</sub>H<sub>24</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 282.1852, found 282.1856. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +14.5 (*c* 0.55, CH<sub>2</sub>Cl<sub>2</sub>) for 93:7 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 13.28 min (*R*), *t*<sub>minor</sub> = 8.08 min (*S*)).

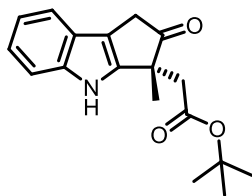


**3qa:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=20:1) to obtain a white solid (44.4 mg, 92% yield, 91.5:8.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):** δ 11.27 (s, 1H), 7.46 – 7.34 (m, 2H), 7.10 – 7.04 (m, 1H), 7.04 – 6.97 (m, 1H), 3.51 (d, *J* = 21.5 Hz, 1H), 3.44 (d, *J* = 21.4 Hz, 1H), 1.82 – 1.70 (m, 2H), 1.32 – 1.25 (m, 1H), 1.24 (s, 3H), 0.61 (dd, *J* = 6.6, 3.1 Hz, 6H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz):** δ 220.03, 145.20, 138.49, 124.01, 120.74, 119.01, 118.59, 111.94, 108.78, 50.61, 46.41, 37.87, 25.53, 25.10, 23.50, 23.49. **HRMS (ESI+):** calcd. for C<sub>16</sub>H<sub>20</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 242.1539, found 242.1539. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +6.3 (*c* 0.46, CH<sub>2</sub>Cl<sub>2</sub>) for 91.5:8.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 13.22 min (*R*), *t*<sub>minor</sub> = 8.21 min (*S*)).

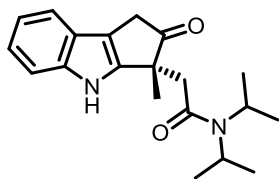


**3ra:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=20:1) to obtain a white solid (48.0 mg, 94% yield, 84.5:15.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz):** δ 11.25 (s, 1H), 7.46 – 7.35 (m, 2H), 7.12 – 7.04 (m, 1H), 7.04 – 6.97 (m, 1H), 3.48 (d, *J* = 21.4 Hz, 1H), 3.37 (d, *J* = 21.4 Hz, 1H), 1.74 (t, *J* = 8.5 Hz, 2H), 1.42 – 1.31 (m, 1H), 1.28 (s, 3H), 0.93 – 0.78 (m, 2H), 0.75 (dd, *J* = 6.6, 1.3 Hz, 6H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz):** δ 220.01, 145.21, 138.51, 124.02, 120.75, 119.05, 118.60, 112.00, 108.94, 50.88, 38.01, 35.67, 33.84, 27.81, 23.07, 22.39, 22.28. **HRMS (ESI+):** calcd. for C<sub>17</sub>H<sub>22</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 256.1696, found 256.1702. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +0.2

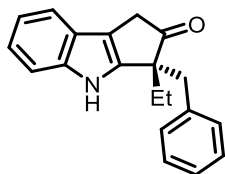
(*c* 0.47, CH<sub>2</sub>Cl<sub>2</sub>) for 84.5:15.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 13.92 min (*R*), *t*<sub>minor</sub> = 7.58 min (*S*)).



**3sa:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (47.9 mg, 80% yield, 85:15 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):** δ 11.20 (s, 1H), 7.46 – 7.38 (m, 2H), 7.11 – 7.05 (m, 1H), 7.04 – 6.97 (m, 1H), 3.50 (d, *J* = 21.0 Hz, 1H), 3.42 (d, *J* = 21.0 Hz, 1H), 2.86 (d, *J* = 15.3 Hz, 1H), 2.75 (d, *J* = 15.3 Hz, 1H), 1.27 (s, 3H), 1.05 (s, 9H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz):** δ 217.56, 169.07, 143.70, 138.35, 123.97, 120.85, 119.04, 118.57, 111.94, 109.47, 80.02, 48.27, 43.32, 37.59, 27.23, 23.64. **HRMS (ESI+):** calcd. for C<sub>18</sub>H<sub>22</sub>NO<sub>3</sub><sup>+</sup> [M+H]<sup>+</sup> 300.1594, found 300.1599. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> –32.1 (*c* 0.41, CH<sub>2</sub>Cl<sub>2</sub>) for 85:15 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 7.39 min (*R*), *t*<sub>minor</sub> = 5.76 min (*S*)).

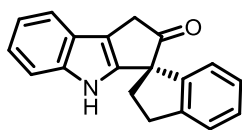


**3ta:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=10:1) to obtain a white solid (37.2 mg, 57% yield, 97:3 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz):** δ 10.98 (s, 1H), 7.43 – 7.33 (m, 2H), 7.07 – 6.94 (m, 2H), 4.07 – 3.92 (m, 1H), 3.53 (d, *J* = 20.4 Hz, 1H), 3.31 (d, *J* = 20.4 Hz, 1H), 3.33 – 3.25 (m, 1H), 3.13 (d, *J* = 16.0 Hz, 1H), 2.79 (d, *J* = 15.9 Hz, 1H), 1.25 (s, 3H), 1.11 (t, *J* = 7.1 Hz, 6H), 1.03 (d, *J* = 6.6 Hz, 3H), 0.86 (d, *J* = 6.7 Hz, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz):** δ 217.89, 167.95, 145.09, 138.14, 124.28, 120.38, 118.88, 118.51, 111.96, 109.43, 48.36, 48.14, 44.55, 42.95, 37.75, 23.78, 20.71, 20.53, 20.48, 20.28. **HRMS (ESI+):** calcd. for C<sub>20</sub>H<sub>27</sub>N<sub>2</sub>O<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup> 327.2067, found 327.2073. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> –18.4 (*c* 0.29, CH<sub>2</sub>Cl<sub>2</sub>) for 97:3 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 98.5/1.5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 8.76 min (*R*), *t*<sub>minor</sub> = 8.07 min (*S*)).

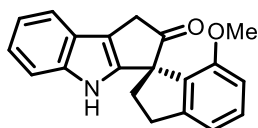


**3ua:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (53.8 mg, 93% yield, 84.5:15.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):** δ 11.39 (s, 1H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.28 (d, *J* = 7.8 Hz, 1H), 7.11 – 7.03 (m, 1H), 7.03 –

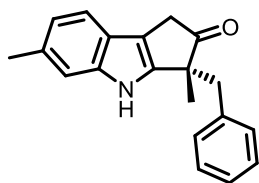
6.90 (m, 4H), 6.84 – 6.72 (m, 2H), 3.17 (d,  $J = 21.4$  Hz, 1H), 3.10 (d,  $J = 13.1$  Hz, 1H), 3.04 (d,  $J = 13.1$  Hz, 1H), 2.65 (d,  $J = 21.4$  Hz, 1H), 1.92 (q,  $J = 7.4$  Hz, 2H), 0.59 (t,  $J = 7.4$  Hz, 3H);  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 101 MHz):  $\delta$  219.64, 142.21, 138.76, 137.04, 129.27, 127.71, 126.17, 123.79, 120.78, 118.92, 118.54, 111.99, 111.06, 58.44, 42.90, 30.37, 9.42. HRMS (ESI+): calcd. for  $\text{C}_{20}\text{H}_{20}\text{NO}^+$   $[\text{M}+\text{H}]^+$  290.1539, found 290.1554. **Optical rotation:**  $[\alpha]^{25}_{\text{D}} +36.9$  ( $c$  0.27,  $\text{CH}_2\text{Cl}_2$ ) for 84.5:15.5 er ( $R$ ). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 92/8, 0.5 mL/min, 25 °C, 254 nm,  $t_{\text{major}} = 17.67$  min ( $R$ ),  $t_{\text{minor}} = 16.01$  min ( $S$ )).



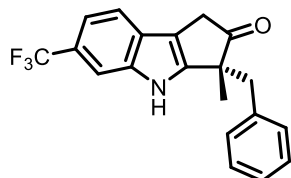
**3va:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (45.9 mg, 84% yield, 78.5:21.5 er).  $^1\text{H}$  NMR (DMSO- $d_6$ , 400 MHz):  $\delta$  11.25 (s, 1H), 7.51 (d,  $J = 7.2$  Hz, 1H), 7.37 (dd,  $J = 11.4, 7.7$  Hz, 2H), 7.28 – 7.21 (m, 1H), 7.15 – 7.02 (m, 3H), 6.71 (d,  $J = 7.2$  Hz, 1H), 3.71 (d,  $J = 21.2$  Hz, 1H), 3.57 (d,  $J = 21.2$  Hz, 1H), 3.29 – 3.13 (m, 2H), 2.56 – 2.47 (m, 1H), 2.46 – 2.36 (m, 1H);  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 101 MHz):  $\delta$  216.84, 144.24, 144.18, 143.58, 138.77, 127.73, 126.69, 124.94, 123.81, 123.37, 121.28, 119.24, 118.85, 112.10, 110.70, 62.74, 37.41, 35.39, 30.89. HRMS (ESI+): calcd. for  $\text{C}_{19}\text{H}_{16}\text{NO}^+$   $[\text{M}+\text{H}]^+$  274.1226, found 274.1230. **Optical rotation:**  $[\alpha]^{25}_{\text{D}} +33.9$  ( $c$  0.45,  $\text{CH}_2\text{Cl}_2$ ) for 78.5:21.5 er ( $R$ ). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm,  $t_{\text{major}} = 16.63$  min ( $R$ ),  $t_{\text{minor}} = 13.45$  min ( $S$ )).



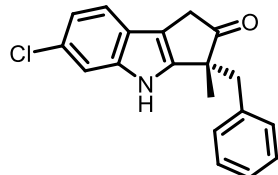
**3wa:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=6:1) to obtain a white solid (59.5 mg, 98% yield, 99:1 er).  $^1\text{H}$  NMR (DMSO- $d_6$ , 400 MHz):  $\delta$  11.11 (s, 1H), 7.49 (d,  $J = 7.8$  Hz, 1H), 7.33 (d,  $J = 7.9$  Hz, 1H), 7.23 (t,  $J = 7.8$  Hz, 1H), 7.12 – 7.06 (m, 1H), 7.06 – 7.01 (m, 1H), 6.97 (d,  $J = 7.5$  Hz, 1H), 6.70 (d,  $J = 8.2$  Hz, 1H), 3.71 (d,  $J = 20.7$  Hz, 1H), 3.52 (d,  $J = 20.7$  Hz, 4H), 3.47 – 3.40 (m, 1H), 3.11 – 2.99 (m, 1H), 2.55 – 2.44 (m, 1H), 2.27 – 2.17 (m, 1H);  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 101 MHz):  $\delta$  217.83, 155.20, 146.35, 143.79, 138.53, 132.08, 129.60, 123.87, 120.88, 119.06, 118.75, 117.00, 111.98, 109.49, 109.05, 60.88, 55.38, 37.99, 36.95, 31.24. HRMS (ESI+): calcd. for  $\text{C}_{20}\text{H}_{18}\text{NO}_2^+$   $[\text{M}+\text{H}]^+$  304.1332, found 304.1342. **Optical rotation:**  $[\alpha]^{25}_{\text{D}} -44.2$  ( $c$  0.59,  $\text{CH}_2\text{Cl}_2$ ) for 99:1 er ( $R$ ). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 92/8, 1.0 mL/min, 25 °C, 254 nm,  $t_{\text{major}} = 14.27$  min ( $R$ ),  $t_{\text{minor}} = 9.71$  min ( $S$ )).



**3ab:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (56.7 mg, 98% yield, 94:6 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):** δ 11.18 (s, 1H), 7.21 (s, 1H), 7.14 (d, *J* = 8.0 Hz, 1H), 7.05 – 6.98 (m, 3H), 6.80 – 6.72 (m, 3H), 3.22 (d, *J* = 21.2 Hz, 1H), 3.05 (s, 2H), 2.61 (d, *J* = 21.2 Hz, 1H), 2.39 (s, 3H), 1.39 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz):** δ 219.16, 143.34, 138.91, 137.15, 129.79, 129.17, 127.70, 126.18, 121.71, 120.58, 118.22, 111.95, 109.17, 52.80, 43.74, 37.98, 23.38, 21.39. **HRMS (ESI+):** calcd. for C<sub>20</sub>H<sub>20</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 290.1539, found 290.1548. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +41.9 (*c* 0.30, CH<sub>2</sub>Cl<sub>2</sub>) for 94:6 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 11.47 min (*R*), *t*<sub>minor</sub> = 10.55 min (*S*)).

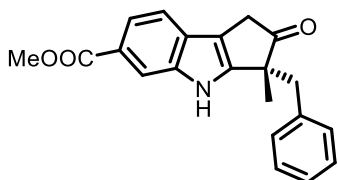


**3ac:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (61.1 mg, 89% yield, 94:6 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):** δ 11.89 (s, 1H), 7.77 (s, 1H), 7.46 (d, *J* = 8.3 Hz, 1H), 7.25 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.05 – 6.99 (m, 3H), 6.81 – 6.74 (m, 2H), 3.33 (d, *J* = 21.3 Hz, 1H), 3.12 (d, *J* = 13.3 Hz, 1H), 3.08 (d, *J* = 13.3 Hz, 1H), 2.71 (d, *J* = 21.3 Hz, 1H), 1.42 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz):** δ 218.92, 148.18, 137.68, 137.31, 129.58, 128.30, 126.82, 126.61, 125.96 (q, *J* = 272.5 Hz), 121.55 (q, *J* = 31.2 Hz), 119.67, 115.86 (q, *J* = 3.8 Hz), 110.48, 109.68 (q, *J* = 4.7 Hz), 53.57, 44.07, 38.22, 23.51; **<sup>19</sup>F NMR (DMSO-*d*<sub>6</sub>, 282 MHz)** δ -58.59. **HRMS (ESI+):** calcd. for C<sub>20</sub>H<sub>17</sub>F<sub>3</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 344.1257, found 344.1255. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +67.4 (*c* 0.14, CH<sub>2</sub>Cl<sub>2</sub>) for 94:6 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 10.53 min (*R*), *t*<sub>minor</sub> = 11.90 min (*S*)).

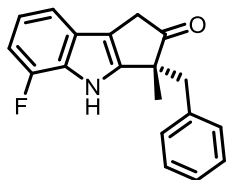


**3ad:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (47.7 mg, 77% yield, 94:6 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):** δ 11.56 (s, 1H), 7.48 (d, *J* = 1.9 Hz, 1H), 7.27 (d, *J* = 8.4 Hz, 1H), 7.04 – 7.00 (m, 3H), 6.96 (dd, *J* = 8.4, 1.9 Hz, 1H), 6.78 – 6.74 (m, 2H), 3.26 (d, *J* = 21.3 Hz, 1H), 3.08 (d, *J* = 13.0 Hz, 1H), 3.04 (d, *J* = 13.2 Hz, 1H), 2.64 (d, *J* = 21.3 Hz, 1H), 1.40 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz):** δ 218.69, 145.30, 138.80,

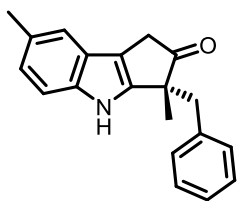
136.98, 129.16, 127.79, 126.31, 125.49, 122.57, 119.78, 119.28, 111.72, 109.73, 53.04, 43.67, 37.87, 23.14. **HRMS (ESI+)**: calcd. for  $C_{19}H_{16}^{35}ClKNO^+$   $[M+K]^+$  348.0552, found 348.0578. **Optical rotation**:  $[\alpha]_D^{25} +46.1$  ( $c$  0.14,  $CH_2Cl_2$ ) for 94:6 er ( $R$ ). The er was determined by HPLC analysis using Daicel Chiralcel IF column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm,  $t_{major}$  = 6.42 min ( $R$ ),  $t_{minor}$  = 6.96 min ( $S$ )).



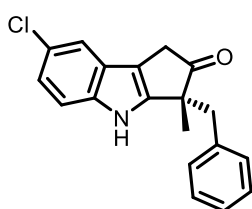
**3ae**: The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=5:1) to obtain a white solid (64.0 mg, 96% yield, 94.5:5.5 er).  **$^1H$  NMR (DMSO- $d_6$ , 400 MHz)**:  $\delta$  11.81 (s, 1H), 8.08 (s, 1H), 7.60 (dd,  $J$  = 8.4, 1.5 Hz, 1H), 7.35 (d,  $J$  = 8.3 Hz, 1H), 7.05 – 6.99 (m, 3H), 6.81 – 6.75 (m, 2H), 3.85 (s, 3H), 3.32 (d,  $J$  = 21.3 Hz, 1H), 3.09 (s, 2H), 2.71 (d,  $J$  = 21.3 Hz, 1H), 1.43 (s, 3H);  **$^{13}C$  NMR (DMSO- $d_6$ , 101 MHz)**:  $\delta$  218.42, 167.21, 148.31, 137.71, 136.81, 129.13, 127.81, 127.13, 126.36, 121.74, 119.92, 118.30, 113.72, 110.19, 53.08, 51.75, 43.70, 37.73, 22.99. **HRMS (ESI+)**: calcd. for  $C_{21}H_{20}NO_3^+$   $[M+H]^+$  334.1438, found 334.1449. **Optical rotation**:  $[\alpha]_D^{25} +92.3$  ( $c$  0.31,  $CH_2Cl_2$ ) for 94.5:5.5 er ( $R$ ). The er was determined by HPLC analysis using Daicel Chiralcel IA column (hexane/isopropanol = 96/4, 1.0 mL/min, 25 °C, 254 nm,  $t_{major}$  = 20.49 min ( $R$ ),  $t_{minor}$  = 15.11 min ( $S$ )).



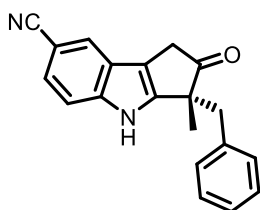
**3af**: The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (43.4 mg, 74% yield, 94.5:5.5 er).  **$^1H$  NMR (DMSO- $d_6$ , 300 MHz)**:  $\delta$  11.86 (s, 1H), 7.12 – 6.98 (m, 4H), 6.96 – 6.86 (m, 2H), 6.81 – 6.72 (m, 2H), 3.28 (d,  $J$  = 21.3 Hz, 1H), 3.12 (d,  $J$  = 13.1 Hz, 1H), 3.06 (d,  $J$  = 13.1 Hz, 1H), 2.63 (d,  $J$  = 21.3 Hz, 1H), 1.42 (s, 3H);  **$^{13}C$  NMR (DMSO- $d_6$ , 75 MHz)**:  $\delta$  219.19, 149.89 (d,  $J$  = 240.6 Hz), 145.76, 137.50, 129.55, 128.25, 127.98 (d,  $J$  = 6.0 Hz), 126.75, 126.26 (d,  $J$  = 12.7 Hz), 119.75 (d,  $J$  = 6.7 Hz), 115.35 (d,  $J$  = 2.9 Hz), 110.97 (d,  $J$  = 2.7 Hz), 106.36 (d,  $J$  = 16.0 Hz), 53.54, 44.01, 38.43, 23.77;  **$^{19}F$  NMR (DMSO- $d_6$ , 282 MHz)**  $\delta$  -133.13. **HRMS (ESI+)**: calcd. for  $C_{19}H_{17}FNO^+$   $[M+H]^+$  294.1289, found 294.1293. **Optical rotation**:  $[\alpha]_D^{25} +9.5$  ( $c$  0.11,  $CH_2Cl_2$ ) for 94.5:5.5 er ( $R$ ). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm,  $t_{major}$  = 12.13 min ( $R$ ),  $t_{minor}$  = 9.37 min ( $S$ )).



**3ag:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (38.2 mg, 66% yield, 94:6 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):** δ 11.22 (s, 1H), 7.30 (d, *J* = 8.2 Hz, 1H), 7.06 – 6.98 (m, 4H), 6.88 (dd, *J* = 8.3, 1.7 Hz, 1H), 6.79 – 6.71 (m, 2H), 3.22 (d, *J* = 21.2 Hz, 1H), 3.05 (s, 2H), 2.61 (d, *J* = 21.2 Hz, 1H), 2.31 (s, 3H), 1.39 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz):** δ 219.24, 144.15, 137.15, 136.81, 129.18, 127.74, 127.41, 126.23, 124.00, 122.28, 118.37, 111.65, 108.91, 52.83, 43.79, 37.94, 23.40, 21.16. **HRMS (ESI+):** calcd. for C<sub>20</sub>H<sub>20</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 290.1539, found 290.1552. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +16.7 (*c* 0.17, CH<sub>2</sub>Cl<sub>2</sub>) for 94:6 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 95/5, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 20.13 min (*R*), *t*<sub>minor</sub> = 10.45 min (*S*)).

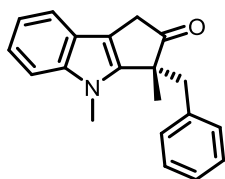


**3ah:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=15:1) to obtain a white solid (53.9 mg, 87% yield, 94:6 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):** δ 11.59 (s, 1H), 7.43 (d, *J* = 8.6 Hz, 1H), 7.31 (d, *J* = 2.1 Hz, 1H), 7.09 – 6.98 (m, 4H), 6.79 – 6.72 (m, 2H), 3.25 (d, *J* = 21.3 Hz, 1H), 3.06 (s, 2H), 2.63 (d, *J* = 21.3 Hz, 1H), 1.40 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz):** δ 218.62, 146.03, 136.92, 136.89, 129.12, 127.78, 126.32, 124.82, 123.60, 120.63, 117.88, 113.37, 109.39, 52.97, 43.70, 37.86, 23.12. **HRMS (ESI+):** calcd. for C<sub>19</sub>H<sub>17</sub><sup>35</sup>ClNO<sup>+</sup> [M+H]<sup>+</sup> 310.0993, found 310.1001. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> +7.8 (*c* 0.28, CH<sub>2</sub>Cl<sub>2</sub>) for 94:6 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IB column (hexane/isopropanol = 92/8, 1.0 mL/min, 25 °C, 254 nm, *t*<sub>major</sub> = 17.37 min (*R*), *t*<sub>minor</sub> = 9.43 min (*S*)).

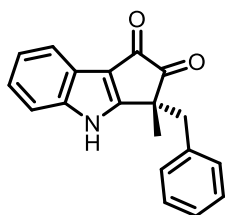


**3ai:** The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=5:1) to obtain a white solid (49.2 mg, 81% yield, 92:8 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):** δ 12.02 (s, 1H), 7.80 (s, 1H), 7.60 (d, *J* = 8.5 Hz, 1H), 7.41 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.06 – 6.99 (m, 3H), 6.80 – 6.73 (m, 2H), 3.31 (d, *J* = 21.4 Hz, 1H), 3.08 (s, 2H), 2.69 (d, *J* = 21.4 Hz, 1H), 1.41 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz):** δ 218.63, 147.39, 140.64, 137.26, 129.55, 128.29, 126.85, 124.51, 124.15, 124.00, 121.07, 113.66, 111.09, 101.59, 53.53, 44.08, 38.32, 23.41. **HRMS (ESI+):** calcd. for C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>NaO<sup>+</sup> [M+Na]<sup>+</sup> 323.1155, found 323.1172. **Optical rotation:** [α]<sup>25</sup><sub>D</sub> –7.6 (*c* 0.24, CH<sub>2</sub>Cl<sub>2</sub>) for 92:8 er (*R*). The er was determined by HPLC analysis using

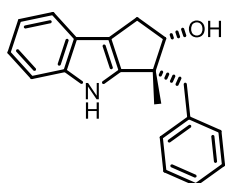
Daicel Chiralcel IB column (hexane/isopropanol = 80/20, 1.0 mL/min, 25 °C, 254 nm,  $t_{\text{major}} = 8.15$  min (*R*),  $t_{\text{minor}} = 6.31$  min (*S*)).



**3aa'**: The reaction was carried out on a 0.20 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=30:1) to obtain a white solid (24.9 mg, 43% yield, 95:5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz)**:  $\delta$  7.47 (d,  $J = 8.3$  Hz, 1H), 7.29 (d,  $J = 7.8$  Hz, 1H), 7.13 (ddd,  $J = 8.3, 7.1, 1.2$  Hz, 1H), 7.09 – 7.00 (m, 3H), 7.03 – 6.93 (m, 1H), 6.81 – 6.72 (m, 2H), 3.80 (s, 3H), 3.29 (d,  $J = 21.4$  Hz, 1H), 3.20 (d,  $J = 13.5$  Hz, 1H), 3.09 (d,  $J = 13.5$  Hz, 1H), 2.75 (d,  $J = 21.4$  Hz, 1H), 1.49 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz)**:  $\delta$  218.66, 144.09, 139.29, 136.98, 129.16, 127.87, 126.38, 123.41, 120.92, 119.18, 118.76, 109.98, 109.66, 53.35, 43.56, 37.67, 30.64, 22.39. **HRMS (ESI+)**: calcd. for C<sub>20</sub>H<sub>20</sub>NO<sup>+</sup> [M+H]<sup>+</sup> 290.1539, found 290.1542. **Optical rotation**:  $[\alpha]^{25}_{\text{D}} +69.2$  ( $c$  0.18, CH<sub>2</sub>Cl<sub>2</sub>) for 95:5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IC column (hexane/isopropanol = 98.5/1.5, 1.0 mL/min, 25 °C, 254 nm,  $t_{\text{major}} = 9.15$  min (*R*),  $t_{\text{minor}} = 8.60$  min (*S*)).

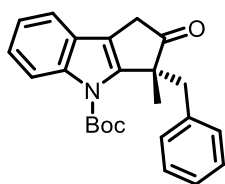


**4**: The reaction was carried out on a 0.10 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=2:1) to obtain a pale yellow solid (26.3 mg, 91% yield, 93.5:6.5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 300 MHz)**:  $\delta$  7.65 (t,  $J = 8.7$  Hz, 2H), 7.40 – 7.32 (m, 1H), 7.24 (td,  $J = 7.5, 1.1$  Hz, 1H), 7.09 – 6.96 (m, 3H), 6.81 – 6.72 (m, 2H), 3.24 (d,  $J = 13.4$  Hz, 1H), 3.18 (d,  $J = 13.4$  Hz, 1H), 1.54 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 75 MHz)**:  $\delta$  206.58, 175.47, 168.30, 139.86, 136.06, 129.11, 128.19, 126.81, 125.38, 123.62, 123.30, 120.91, 120.76, 113.61, 47.75, 42.59, 22.49. **HRMS (ESI+)**: calcd. for C<sub>19</sub>H<sub>16</sub>NO<sub>2</sub><sup>+</sup> [M+H]<sup>+</sup> 290.1176, found 290.1180. **Optical rotation**:  $[\alpha]^{25}_{\text{D}} +56.4$  ( $c$  0.16, CHCl<sub>3</sub>) for 93.5:6.5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IE column (hexane/isopropanol = 80/20, 1.0 mL/min, 25 °C, 254 nm,  $t_{\text{major}} = 20.41$  min (*R*),  $t_{\text{minor}} = 22.50$  min (*S*)).

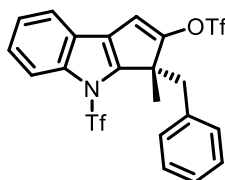


**5**: The reaction was carried out on a 0.10 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=6:1) to obtain a white solid (27.5 mg, 99% yield, >20:1 dr, 95:5 er for both diastereoisomers). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz)**:  $\delta$  10.54 (s, 1H), 7.30 – 7.23 (m, 2H), 7.14 – 7.10 (m, 3H), 6.98 – 6.86 (m, 4H), 5.46 (d,  $J = 5.5$  Hz, 1H), 4.37 – 4.26 (m, 1H), 2.92 (dd,  $J =$

13.5, 7.1 Hz, 1H), 2.90 (d,  $J = 13.1$  Hz, 1H), 2.81 (d,  $J = 13.0$  Hz, 1H), 2.43 (dd,  $J = 13.5, 7.7$  Hz, 1H), 1.28 (s, 3H);  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 101 MHz):  $\delta$  147.78, 139.61, 130.84, 127.83, 126.03, 124.77, 119.83, 118.81, 118.40, 112.22, 111.09, 84.92, 47.65, 41.03, 32.57, 23.53. HRMS (ESI+): calcd. for  $\text{C}_{19}\text{H}_{20}\text{NO}^+$   $[\text{M}+\text{H}]^+$  278.1539, found 278.1545. Optical rotation:  $[\alpha]^{25}_{\text{D}} -102.2$  ( $c$  0.18,  $\text{CH}_2\text{Cl}_2$ ) for 95:5 er ( $R,S$ ). The er was determined by HPLC analysis using Daicel Chiralcel IF column (hexane/isopropanol = 93/7, 1.0 mL/min, 25 °C, 254 nm,  $t_{\text{major}1} = 8.60$  min ( $R,S$ ),  $t_{\text{minor}1} = 11.11$  min ( $S,R$ ),  $t_{\text{major}2} = 11.89$  min ( $R,R$ ),  $t_{\text{minor}2} = 10.42$  min ( $S,S$ )).

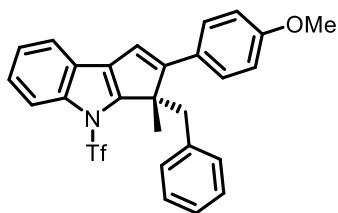


**6:** The reaction was carried out on a 0.10 mmol scale. Purified by silica gel column chromatography (PE:EA v/v=50:1) to obtain a white solid (31.9 mg, 85% yield, 96:4 er).  $^1\text{H}$  NMR ( $\text{CHCl}_3$ - $d$ , 400 MHz):  $\delta$  8.14 (d,  $J = 8.4$  Hz, 1H), 7.32 – 7.25 (m, 2H), 7.22 – 7.17 (m, 1H), 7.03 – 6.98 (m, 3H), 6.87 – 6.80 (m, 2H), 3.70 (d,  $J = 13.1$  Hz, 1H), 3.20 (d,  $J = 21.8$  Hz, 1H), 3.14 (d,  $J = 13.1$  Hz, 1H), 2.66 (d,  $J = 21.8$  Hz, 1H), 1.81 (s, 9H), 1.62 (s, 3H);  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 75 MHz):  $\delta$  218.32, 149.42, 142.85, 137.68, 137.31, 128.62, 128.04, 126.34, 125.58, 124.34, 123.01, 119.47, 118.76, 115.91, 84.93, 56.71, 42.46, 36.90, 27.84, 22.74. HRMS (ESI+): calcd. for  $\text{C}_{24}\text{H}_{26}\text{NO}_3^+$   $[\text{M}+\text{H}]^+$  376.1907, found 376.1908. Optical rotation:  $[\alpha]^{25}_{\text{D}} +130.2$  ( $c$  0.17,  $\text{CH}_2\text{Cl}_2$ ) for 96:4 er ( $R$ ). The er was determined by HPLC analysis using Daicel Chiralcel IC column (hexane/isopropanol = 99/1, 1.0 mL/min, 25 °C, 254 nm,  $t_{\text{major}} = 6.82$  min ( $R$ ),  $t_{\text{minor}} = 6.18$  min ( $S$ )).



**7:** The reaction was carried out on a 0.10 mmol scale. Purified by silica gel column chromatography (PE:DCM v/v=10:1) to obtain a colorless oil (38.3 mg, 71% yield).  $^1\text{H}$  NMR (DMSO- $d_6$ , 400 MHz):  $\delta$  7.90 (d,  $J = 8.3$  Hz, 1H), 7.75 (d,  $J = 7.6$  Hz, 1H), 7.44 (dt,  $J = 22.4, 7.5$  Hz, 2H), 7.07 – 6.97 (m, 3H), 6.94 (s, 1H), 6.83 (d,  $J = 6.4$  Hz, 2H), 3.48 (d,  $J = 13.7$  Hz, 1H), 3.18 (d,  $J = 13.7$  Hz, 1H), 1.61 (s, 3H);  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 101 MHz):  $\delta$  154.53, 140.73, 138.47, 134.72, 128.14, 127.84, 127.49, 126.93, 126.30, 125.96, 124.19, 120.89, 119.31 (q,  $J = 327.6$  Hz), 118.01 (q,  $J = 322.0$  Hz), 114.26, 109.37, 54.46, 40.43, 17.98;  $^{19}\text{F}$  NMR (DMSO- $d_6$ , 282 MHz)  $\delta$  -72.92, -73.20. HRMS (ESI+): calcd. for  $\text{C}_{21}\text{H}_{16}\text{F}_6\text{NO}_5\text{S}_2^+$   $[\text{M}+\text{H}]^+$  540.0369, found 540.0370.





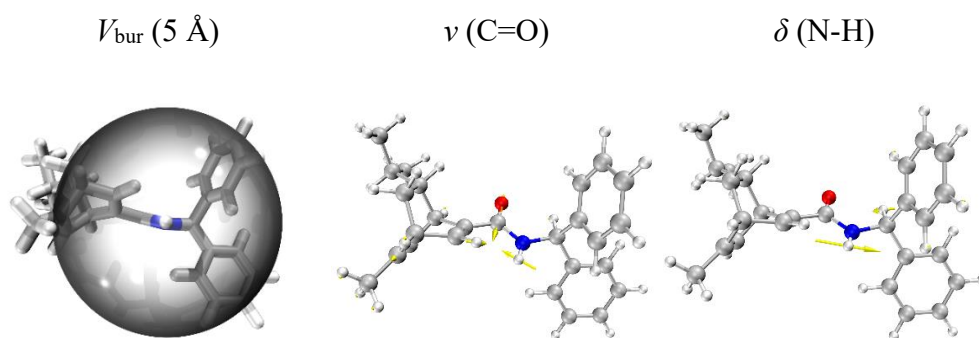
**8:** The reaction was carried out on a 0.10 mmol scale. Purified by silica gel column chromatography (PE:DCM v/v=8:1) to obtain a white solid (42.8 mg, 86% yield, 95:5 er). **<sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz):**  $\delta$  7.91 (d,  $J$  = 8.1 Hz, 1H), 7.77 (d,  $J$  = 8.4 Hz, 2H), 7.64 (d,  $J$  = 7.3 Hz, 1H), 7.40 (p,  $J$  = 7.1 Hz, 2H), 7.10 (s, 1H), 7.05 (d,  $J$  = 8.3 Hz, 2H), 6.91 – 6.81 (m, 3H), 6.70 – 6.61 (m, 2H), 3.82 (s, 3H), 3.63 (q,  $J$  = 13.8 Hz, 2H), 1.70 (s, 3H); **<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz):**  $\delta$  158.75, 152.04, 148.31, 139.79, 136.20, 132.43, 128.09, 128.05, 127.49, 127.36, 126.28, 125.76, 125.62, 124.06, 120.54, 119.50 (q,  $J$  = 328.5 Hz), 117.71, 114.61, 114.23, 56.35, 55.14, 41.89, 20.40; **<sup>19</sup>F NMR (DMSO-*d*<sub>6</sub>, 282 MHz)**  $\delta$  -72.64. **HRMS (ESI+):** calcd. for C<sub>27</sub>H<sub>23</sub>F<sub>3</sub>NO<sub>3</sub>S<sup>+</sup> [M+H]<sup>+</sup> 498.1345, found 498.1343. **Optical rotation:**  $[\alpha]_D^{25}$  -14.6 ( $c$  0.28, CH<sub>2</sub>Cl<sub>2</sub>) for 95:5 er (*R*). The er was determined by HPLC analysis using Daicel Chiralcel IF column (hexane/isopropanol = 97/3, 1.0 mL/min, 25 °C, 254 nm,  $t_{\text{major}}$  = 5.25 min (*R*),  $t_{\text{minor}}$  = 4.74 min (*S*)).

## 5. QSSR Model

The conformational search was implemented for structures of ligands, using ABCluster and xTB.<sup>4,7</sup> The minimized structures of ligands were geometrically optimized in the gas phase by the DFT method with the B3LYP functional in combination with the RI approximation and the def2-TZVP(-f) basis set for all atoms, applying the Grimme's D4 empirical correction as implemented in the ORCA 5.0.2 program package.<sup>4,5</sup> IR frequencies were obtained from the geometry optimized structures at the same level of theory as that used for geometry optimizations. Percent buried volumes of the substituents were calculated for the geometrically optimized structures using the python script DBSTEP developed by the Paton Group.<sup>6c</sup> Measured  $\Delta\Delta G^\ddagger$  values were calculated using the formula  $\Delta\Delta G^\ddagger = -RT\ln(er)$ , where  $R$  is the ideal gas constant,  $T$  is temperature, and  $er$  is the enantiomeric ratio measured by HPLC. Molecular structures were visualized by using VMD 1.9.3.<sup>8a</sup>

Some representative molecular descriptors are listed in the table S2.  $V_{\text{bur}}$  (4 Å) [*resp.*  $V_{\text{bur}}$  (5 Å),  $V_{\text{bur}}$  (6 Å)] is the percent buried volume with a radius of 4 Å [*resp.* 5 Å, 6 Å] centered on the hydrogen atom of the amide in ligand.  $\nu$  (C=O) is the stretching vibration frequency of the C=O.  $\nu$  (N-H) is the stretching vibration frequency of the N-H.  $\delta$  (N-H) is the bending vibration frequency of the N-H. The illustration diagram of  $V_{\text{bur}}$  (5 Å),  $\nu$  (C=O) and  $\delta$  (N-H) is given in figure S1.

**Figure S1: The illustration diagram of  $V_{\text{bur}}$  (5 Å),  $\nu$  (C=O) and  $\delta$  (N-H)**



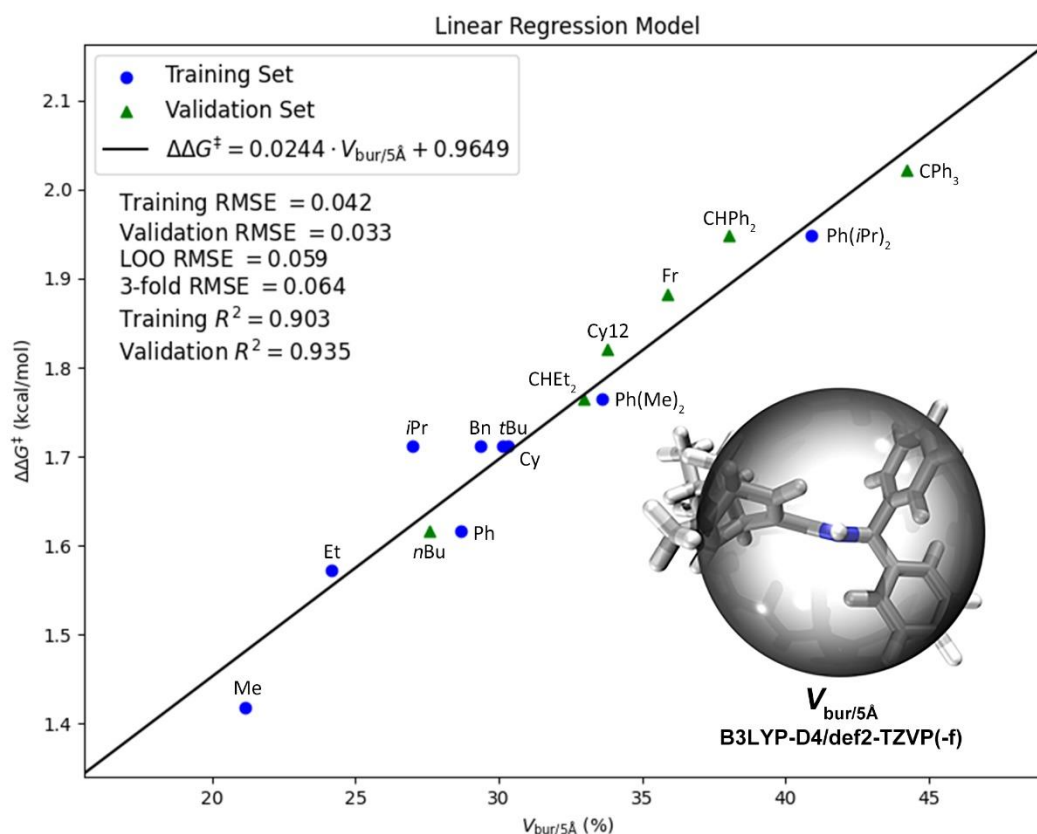
**Table S2: Representative molecular descriptors of ligands**

R	$\Delta\Delta G^\ddagger$	$V_{\text{bur}}$ (4 Å)	$V_{\text{bur}}$ (5 Å)	$V_{\text{bur}}$ (6 Å)	$\nu$ (C=O)	$\nu$ (N-H)	$\delta$ (N-H)
Me	1.4180	29.75	21.16	16.29	1722.44	3637.00	1545.43
Et	1.5725	33.42	24.15	18.02	1721.60	3641.32	1539.33
<i>i</i> Pr	1.7117	38.47	27.00	19.66	1721.13	3625.46	1531.69
<i>n</i> Bu	1.6162	36.71	27.58	21.15	1721.80	3647.86	1537.37
<i>t</i> Bu	1.7117	41.71	30.14	21.52	1720.99	3624.61	1535.91

CHEt <sub>2</sub>	1.7643	45.77	32.96	23.16	1721.03	3626.96	1531.42
Cy	1.7117	39.47	30.31	23.53	1720.99	3614.63	1529.41
Cy12	1.8208	42.28	33.76	27.54	1720.70	3615.27	1539.88
CH <sub>2</sub> Ph	1.7117	37.43	29.36	23.03	1721.26	3626.91	1540.05
CHPh <sub>2</sub>	1.9485	46.89	38.00	29.88	1721.38	3611.54	1523.21
CPh <sub>3</sub>	2.0217	52.99	44.21	35.26	1723.17	3628.17	1515.66
Ph	1.6162	36.58	28.68	22.15	1723.85	3615.01	1558.05
Ph(Me) <sub>2</sub>	1.7643	43.30	33.61	25.38	1724.48	3605.74	1532.72
Ph( <i>i</i> Pr) <sub>2</sub>	1.9485	50.44	40.90	31.64	1724.42	3608.52	1521.92
Fr	1.8819	43.82	35.88	28.70	1721.08	3623.99	1522.71

Note: Cy = cyclohexyl, Cy12 = cyclododecyl, Ph(Me)<sub>2</sub> = 2,6-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, Ph(*i*Pr)<sub>2</sub> = 2,6-*i*Pr<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, Fr = 9-fluorenyl.

**Figure S2: Visualizations of the linear regression models (with labels)**



Linear regression models were developed and evaluated using Python package Scikit-learn. Root mean square error (RMSE) and R-square ( $R^2$ ) were employed for model performance evaluation. Leave-one-out (LOO) cross-validation and 3-fold cross-validation were implemented to avoid overfitting. The 3-fold RMSE was obtained from the mean of 10 independent 3-fold cross-validations. Let  $m$  be the amount of

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data ( $m = 9$  for training set, and  $m = 6$  for validation set) and  $N = 10$  be the number of independent cross-validations, then  $\text{RMSE} = \sqrt{\frac{1}{m} \sum_{i=1}^m (y_i - \hat{y}_i)^2}$ , 3-fold RMSE =  $\sqrt{\frac{1}{3N \sum_i 1} \sum_{k=1}^N \sum_i (y_{ki} - \hat{y}_{ki})^2}$ , LOO RMSE =  $\sqrt{\frac{1}{m} \sum_i (y_i - \hat{y}_i)^2}$ ,  $R^2 = 1 - \frac{\sum_{i=1}^m (y_i - \hat{y}_i)^2}{\sum_{i=1}^m (y_i - \bar{y})^2}$ .

The visualizations of linear regression models were performed by Python package Matplotlib 3.5.2.<sup>8c</sup> A labeled visualizations of the linear regression model was given in figure S2.

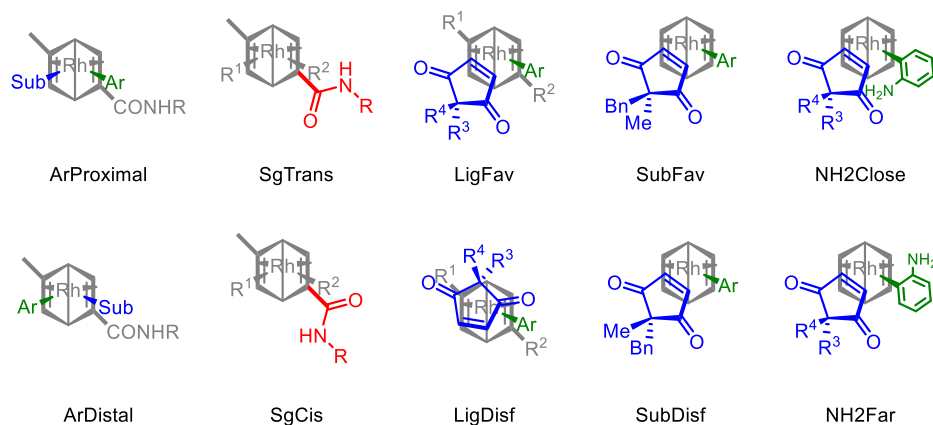
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## 6. DFT Calculation

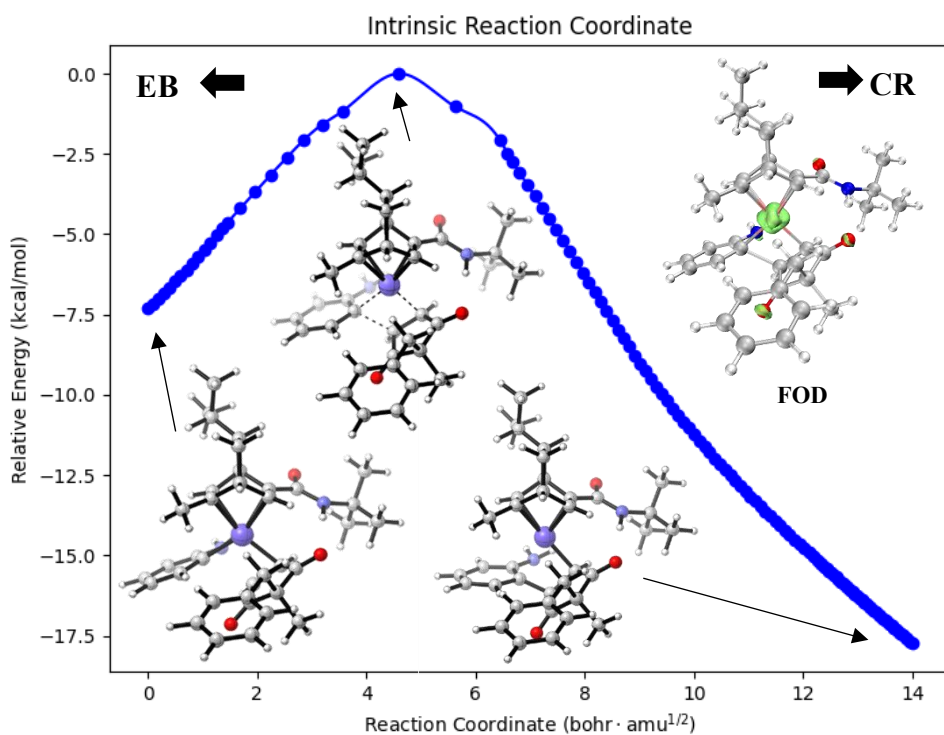
Geometries of transition states and intermediates were optimized by the DFT method with the PBE0 functional in combination with the RI approximation, the def2-TZVP basis set for rhodium atom and the def2-SVP basis set for other atoms, and the implicit solvent model C-PCM using ethanol as the solvent, applying the Grimme's D4 empirical correction as implemented in the ORCA 5.0.2 program package.<sup>4,5</sup> Frequency analyses were performed at the same level of theory as that used for geometry optimizations to characterize the stationary points as either minima (no imaginary frequencies) or saddle points (one imaginary frequency) on the potential energy surface. Intrinsic reaction coordinate (IRC) calculations were performed to confirm that the transition state connects with its respective reactant and product. All geometrically optimized structures have been checked for the wavefunction stability. Grimme's quasi-harmonic approximation implemented in the ORCA 5.0.2 program package was applied to the vibrational entropies to obtain thermal corrections for Gibbs free energies.<sup>6a</sup> The ZPE scale factor 0.98008286 was derived from linear regression to the experimental values available in the ZPVE15/10 Database.<sup>6b</sup> Single point energies were calculated with the PWPB95 functional in combination with the RI approximation and the def2-TZVPP basis set for all atoms, applying the Grimme's D4 empirical correction as implemented in the ORCA 5.0.2 program package.<sup>5</sup> The solvation energies were evaluated with the SMD(ethanol)/M06-2X/Lan12TZ(Rh)/6-31G\*(other atoms).<sup>5</sup> Free energies calculated using the gas phase standard state concentration (1 atm) were converted to reproduce the standard state concentration in solution (1 M) at 30 °C by adding 1.936116029 kcal/mol. Grimme's FOD plot suggests that the multi-reference effects of these systems are not significant.<sup>6c</sup> The non-covalent interaction (NCI) analysis within the  $\text{sign}(\lambda_2)\rho$  colored reduced density gradient (RDG) plot and the topology analysis of the electron density within the framework of Bader's quantum theory of atoms in molecules (QTAIM) were performed with Multiwfn 3.8(dev).<sup>6d</sup> Molecular structures were visualized by using CYLView20, VMD 1.9.3, and Paraview 5.10.1.<sup>8a,8b</sup> The visualizations of IRC path was performed by Python package Matplotlib 3.5.2.<sup>8c</sup> The visualizations of energy barriers was performed by EnePro v1.6 script.<sup>8d</sup>

Different transition states of olefin insertion with ligand L8 (R = *t*Bu) were carefully examined, which was thought to be critical for the enantioselectivity of rhodium catalyzed conjugate addition.<sup>9</sup> Conformational search was also implemented for typical transition states. The relative Gibbs energy of transition states (TS) of olefin

insertion, enone binding (EB) intermediates, carborhodation (CR) intermediates are listed in table S3 and table S4. The illustration diagram of IRC and FOD plot (isovalue = 0.005) are shown in figure S3. Representative structures are shown in figure S4.



**Figure S3: The illustration diagram of IRC and FOD plot (for TS15)**



The relation between absolute configuration of transition state and that of product is illustrated (in Hayashi's style) in scheme S1. The absolute configuration of the product follows the Curtin-Hammett principle and the EB intermediates are in equilibrium. The relative energy difference between favored transition state and disfavored transition state determines the enantiomeric excess value, viz.  $er_{\text{calc}} = \exp(-\Delta\Delta G_{\text{TS}}/RT) = \exp(-\Delta(G_{\text{fav}} - G_{\text{disf}})/RT)$ . If the EB intermediates  $R_i$  obey

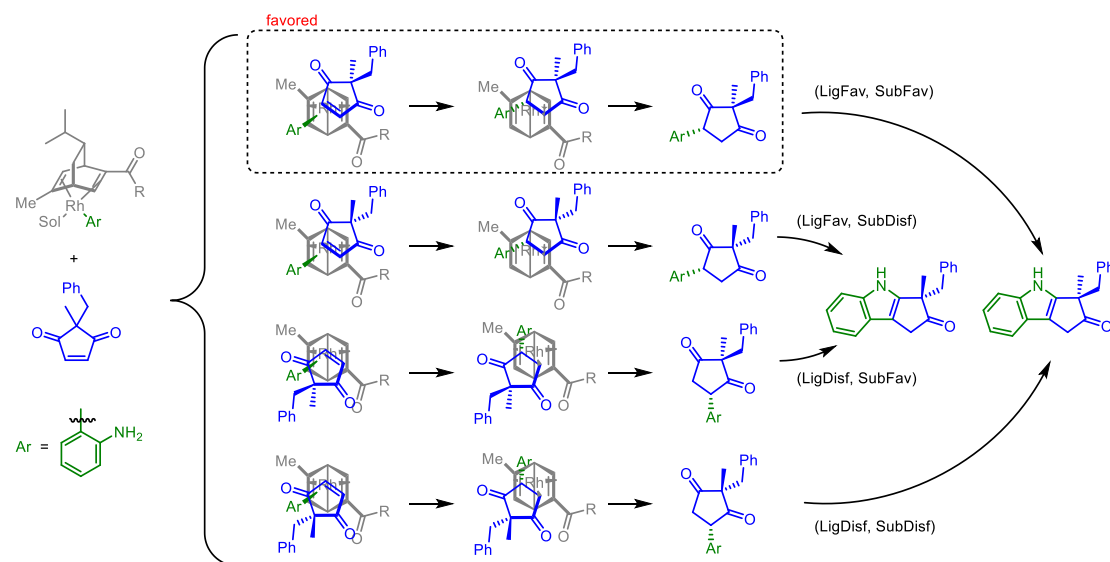
the Boltzmann distribution, then relative energies of an ensemble of transition states need to be taken into consideration,<sup>10</sup> viz.

$$er_{\text{calcB}} = \frac{k_{\text{fav}}}{k_{\text{disf}}} = \frac{\sum_i^{\text{fav}} k_i[\text{R}_i]}{\sum_j^{\text{disf}} k_j[\text{R}_j]} = \frac{\sum_i^{\text{fav}} k_i p_{\text{EB},i}[\text{R}]}{\sum_j^{\text{disf}} k_j p_{\text{EB},j}[\text{R}]} = \frac{\sum_i^{\text{fav}} \frac{k k_{\text{B}} T}{h} e^{-\beta \Delta G_i^\ddagger} \frac{1}{Z} e^{-\beta(G_{\text{EB},i} - G_{\text{ref}})}}{\sum_j^{\text{disf}} \frac{k k_{\text{B}} T}{h} e^{-\beta \Delta G_j^\ddagger} \frac{1}{Z} e^{-\beta(G_{\text{EB},j} - G_{\text{ref}})}} =$$

$\frac{\sum_i^{\text{fav}} e^{-\beta(G_{\text{TS},i} - G_{\text{ref}})}}{\sum_j^{\text{disf}} e^{-\beta(G_{\text{TS},j} - G_{\text{ref}})}}$ , where  $\beta = 1/RT$ . For our system,  $ee_{\text{calc}} = 0.870$  (considering

TS15 and TS16) and  $ee_{\text{calcB}} = 0.879$  (considering from TS1 to TS16), which means multiple transition states of the similar free energies leading to the same enantiomer require no special consideration.

### Scheme S1: The relation between configuration of TS and that of product



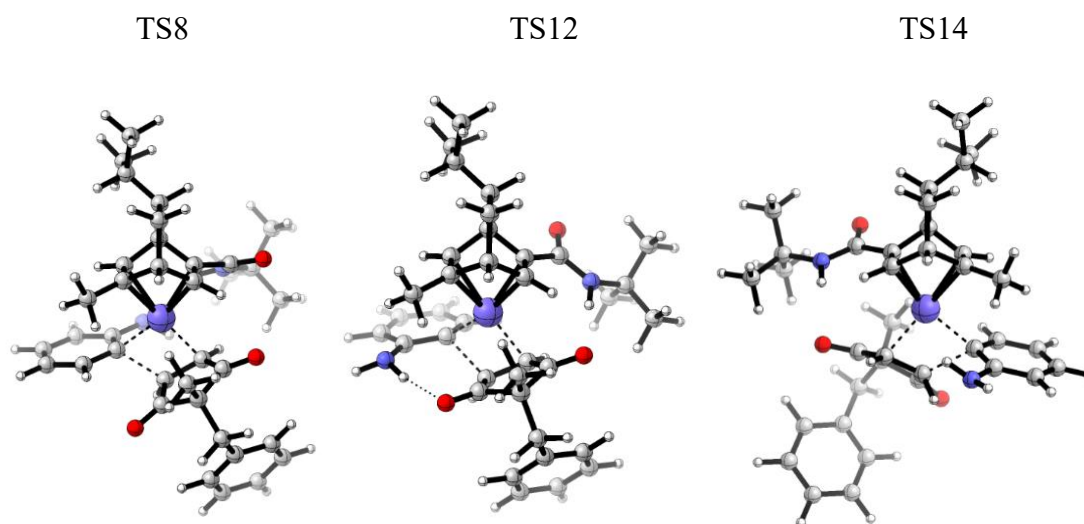
**Table S3: Relative Gibbs energy of TS, EB and CR (unit: kcal/mol)**

#	Name	$\Delta G_{EB,gas}$	$\Delta G_{EB}$	$\Delta G_{TS,gas}$	$\Delta G_{TS}$	$\Delta G_{CR,gas}$	$\Delta G_{CR}$
1	ArDistal-SgCis-NH2Close-LigDisf-SubDisf	0.591611374	-2.47162134	11.89607965	13.05141833	-2.569008773	-3.557867549
2	ArDistal-SgCis-NH2Close-LigDisf-SubFav	-2.511636353	-4.562006069	8.645851547	10.60575983	-5.465332452	-4.822170725
3	ArDistal-SgCis-NH2Close-LigFav-SubDisf	-1.751911579	-0.145801506	7.535453727	10.4023154	-12.59513646	-12.77850397
4	ArDistal-SgCis-NH2Close-LigFav-SubFav	-4.881194638	-2.969036316	4.251000161	6.848349814	-15.18885187	-13.58694696
5	ArDistal-SgCis-NH2Far-LigDisf-SubDisf	-2.763031483	-4.528935568	11.67889029	9.295310592	-6.958252224	-11.80026232
6	ArDistal-SgCis-NH2Far-LigDisf-SubFav	-4.23864491	-6.263200355	9.319275151	7.847111031	-10.72378489	-13.58502231
7	ArDistal-SgCis-NH2Far-LigFav-SubDisf	-6.191350254	-7.210826354	9.026051364	7.665419692	-12.53020959	-16.74504101
8	ArDistal-SgCis-NH2Far-LigFav-SubFav	-9.286146389	-9.673665435	5.856644343	6.622903774	-17.37469013	-17.21873423
9	ArDistal-SgTrans-NH2Close-LigDisf-SubDisf	-2.2337375	4.927215403	5.20188968	13.19343695	-8.171553078	-1.078929049
10	ArDistal-SgTrans-NH2Close-LigDisf-SubFav	-4.76965164	2.15856578	1.393530245	9.552660931	-11.56584981	-3.533877463
11	ArDistal-SgTrans-NH2Close-LigFav-SubDisf	-9.147731162	-1.39506576	-0.324701146	8.643447471	-22.05984599	-14.91440323
12	ArDistal-SgTrans-NH2Close-LigFav-SubFav	-12.62648398	-4.237865998	-3.509129755	5.49608906	-24.58500607	-16.01662127
13	ArDistal-SgTrans-NH2Far-LigDisf-SubDisf	-2.878531919	-3.934165711	6.593798081	9.906884262	-13.13957334	-11.7709077
14	ArDistal-SgTrans-NH2Far-LigDisf-SubFav	-3.146644675	-5.155118213	5.735003197	9.905426368	-15.34689739	-14.99327043
15	ArDistal-SgTrans-NH2Far-LigFav-SubDisf	-12.57724606	-8.248236681	0.161438532	6.141470694	-22.40871019	-17.93466718
16	ArDistal-SgTrans-NH2Far-LigFav-SubFav	-15.48270608	-9.947455038	-2.688221522	4.535110052	-26.05549248	-19.68008554

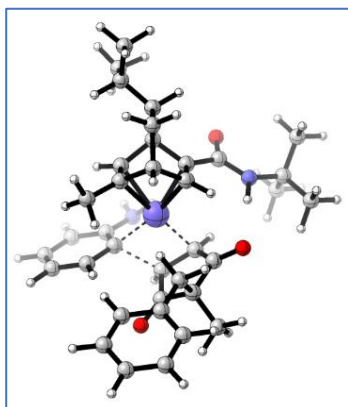


**Table S4: Relative Gibbs energy of TS (unit: kcal/mol)**

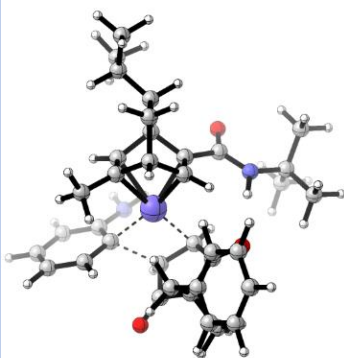
#	Name	$\Delta G_{\text{TS,gas}}$	$\Delta G_{\text{TS}}$
15	ArDistal-SgTrans-NH2Far-LigFav-SubDisf	0.161438532	6.141470694
15'	ArDistal-SgTrans-NH2Far-LigFav-SubDisf	0.769676107	6.505990982
15''	ArDistal-SgTrans-NH2Far-LigFav-SubDisf''	-0.305981119	7.517906019
16	ArDistal-SgTrans-NH2Far-LigFav-SubFav	-2.688221522	4.535110052
16'	ArDistal-SgTrans-NH2Far-LigFav-SubFav'	0.671101238	6.684068448
16''	ArDistal-SgTrans-NH2Far-LigFav-SubFav''	1.003292709	6.989813225
17	ArProximal-SgTrans-NH2Close-LigFav-SubDisf	5.222604322	10.79320121
18	ArProximal-SgTrans-NH2Close-LigFav-SubFav	2.353217641	8.005701598
19	ArProximal-SgTrans-NH2Far-LigDisf-SubDisf	7.526295601	10.65124364
20	ArProximal-SgTrans-NH2Far-LigDisf-SubFav	5.296277505	9.497193382
21	ArProximal-SgTrans-NH2Far-LigFav-SubDisf	5.16603455	7.211572459
22	ArProximal-SgTrans-NH2Far-LigFav-SubFav	3.659484037	7.177479816

**Figure S4: Representative structures of transition states**

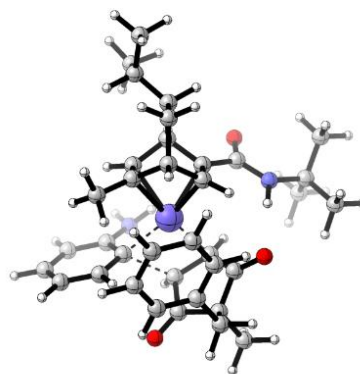
TS15



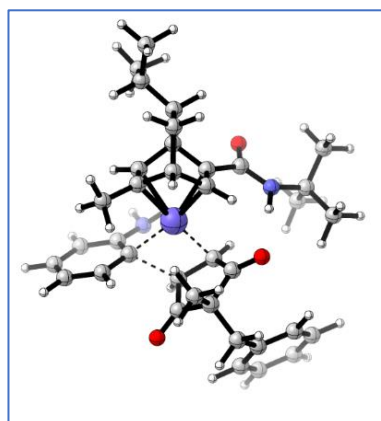
TS15'



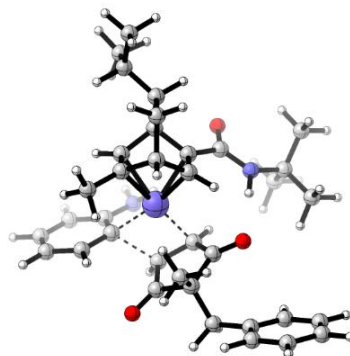
TS15''



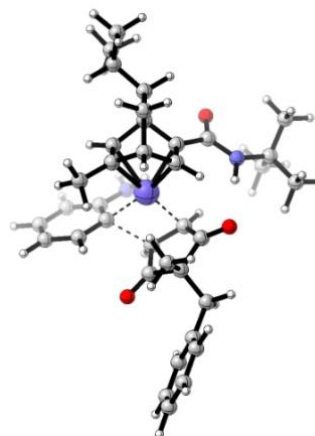
TS16



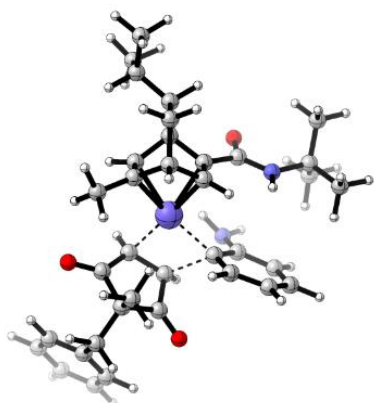
TS16'



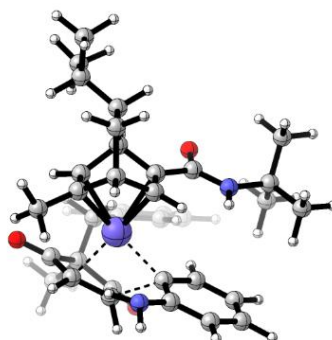
TS16''



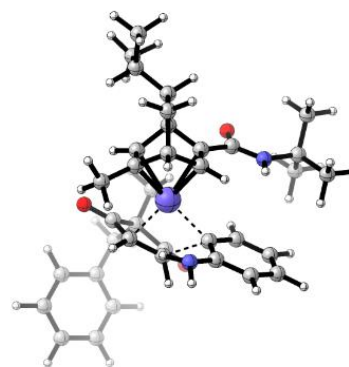
TS20



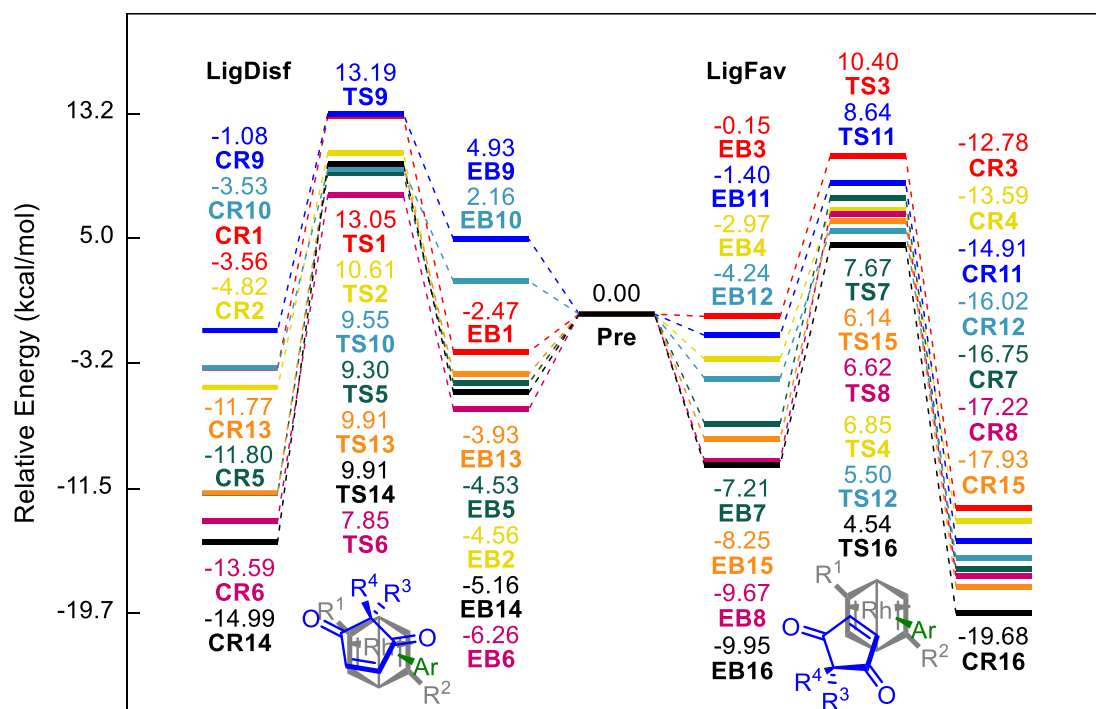
TS21



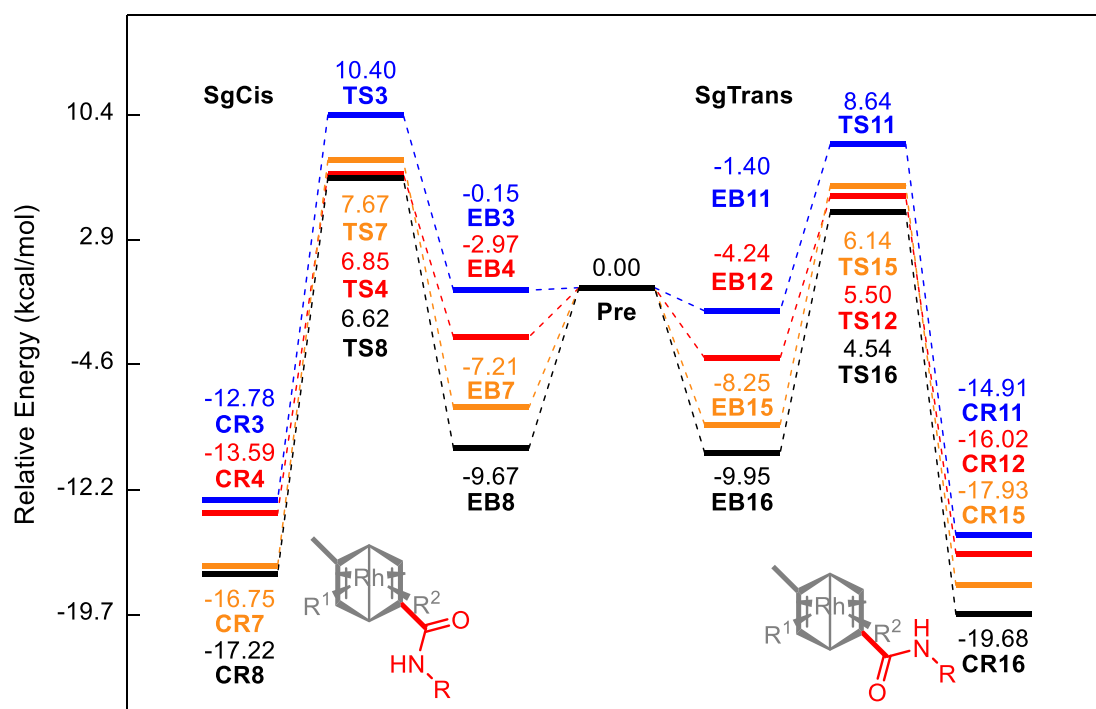
TS22



Scheme S2: Comparison of relative Gibbs energy between LigFav and LigDisf



Scheme S3: Comparison of relative Gibbs energy between SgTrans and SgCis



Scheme S2 and scheme S3 provides an intuitive relative energy comparison. The same color on both sides of the **Pre** indicates similar transition states and intermediates

except for one term, viz. LigFav vs. LigDisf [*resp.* SgTrans vs. SgCis]. The scheme S2 indicates the classic Hayashi's stereochemical model is still valid in our system. The relative energies of LigFav transition states are on average 2–4 kcal/mol lower than that of LigDisf. The scheme S3 reveals that the relative energies of SgTrans transition states are on average 1–2 kcal/mol lower than that of SgCis, which suggests hydrogen bonds between the N-H of the amide-diene ligand and the carbonyl group of the substrate in those SgTrans transition states stabilize the relative energy. The relative energies between NH2Close transition states and NH2Far transition states are closely related to the solvation effect, and those potential hydrogen bonds between N-H of aniline and the carbonyl group of the substrate are not important.

Since the enantioselectivity control has been verified to be determined by the transition states ArDistal-SgTrans-NH2Far-LigFav-SubFav and ArDistal-SgTrans-NH2Far-LigFav-SubDisf, we investigated these two transition states for different ligands. For brevity, TS(ArDistal-SgTrans-NH2Far-LigFav-SubFav) is abbreviated as TSFav, and TS(ArDistal-SgTrans-NH2Far-LigFav-SubDisf) is abbreviated as TSDisf. The Gibbs energies and relative Gibbs energies of TSFav and TSDisf for different ligands were given in table S5 and table S6 respectively.

**Table S5: Gibbs energy of TS for different ligands (unit: a.u.)**

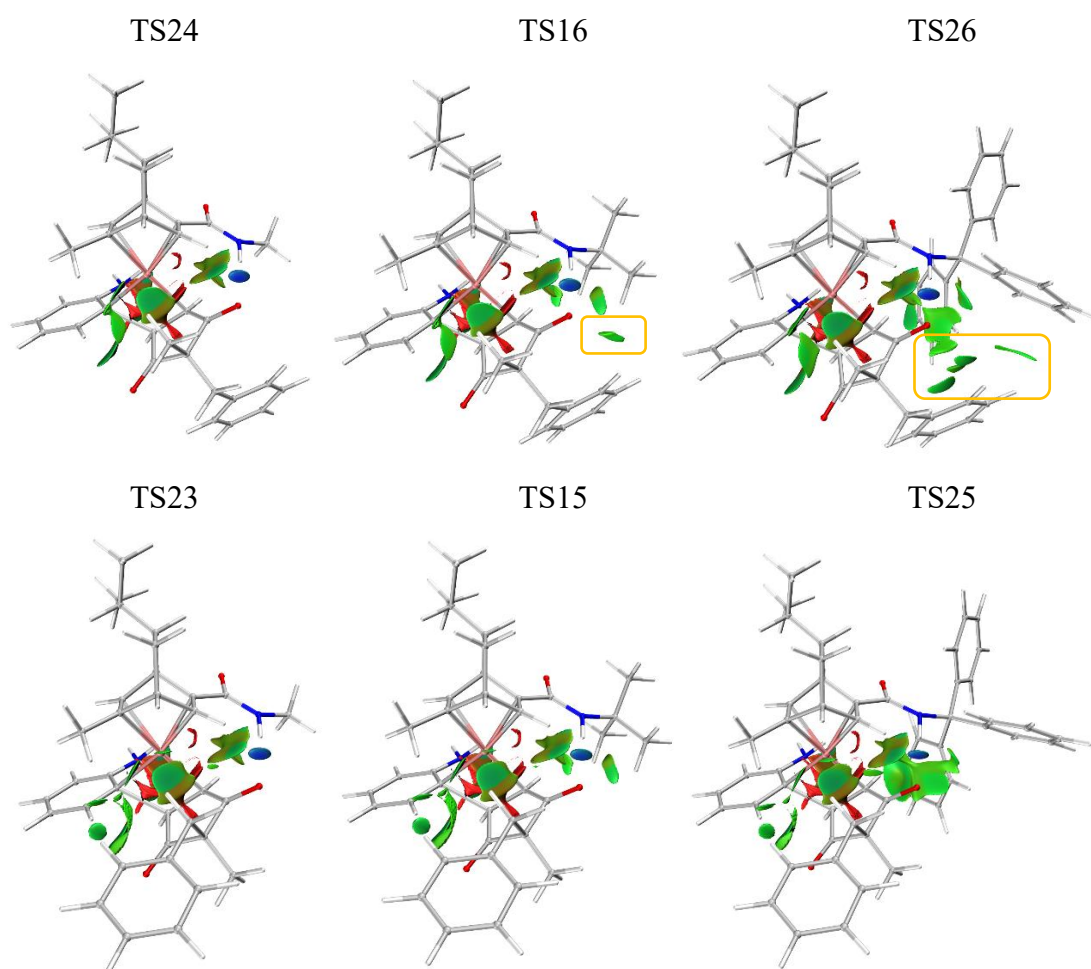
#	Name	$G_{\text{TS,gas}}$	$G_{\text{TS}}$
23	TSDisf for Ligand (R=Me)	-1725.591099	-1725.631241
24	TSFav for Ligand (R=Me)	-1725.594526	-1725.633013
15	TSDisf for Ligand (R= <i>t</i> Bu)	-1843.406825	-1843.446989
16	TSFav for Ligand (R= <i>t</i> Bu)	-1843.411403	-1843.449586
25	TSDisf for Ligand (R=CPh <sub>3</sub> )	-2418.259965	-2418.315173
26	TSFav for Ligand (R=CPh <sub>3</sub> )	-2418.264596	-2418.318262

**Table S6:  $\Delta\Delta G_{\text{TS,gas}}$  and  $\Delta\Delta G_{\text{TS}}$  for different ligands (unit: kcal/mol)**

Name	$\Delta\Delta G_{\text{TS,gas}}$	$\Delta\Delta G_{\text{TS}}$	ee <sub>calc</sub>	ee <sub>exp</sub>
Ligand (R=Me)	2.150488997	1.111910679	69%	79%
Ligand (R= <i>t</i> Bu)	2.872375896	1.629076485	84%	86%
Ligand (R=CPh <sub>3</sub> )	2.906132236	1.938695477	90%	91%

The RDG plots of TS for different ligands are given in figure S5, visualizing the non-covalent interactions in the transition states.<sup>6f</sup> Only non-covalent interactions between ligand-Rh-PhNH<sub>2</sub> complex and substrate are displayed (isovalue = 0.5). Except for the non-covalent interactions framed by the orange boxes (in TS16 and TS26), other major non-covalent interactions exist in both TSFav and TSDif. In other words, these framed non-covalent interactions are thought to have important effects on enantioselectivity. The topology analysis of the electron density was also used to give the properties of the bond critical points (BCPs), which were summarized in table S7.<sup>6g</sup> The illustration of bond critical points in TS16 and TS26 was given in figure S6.

**Figure S5: RDG plots of TS for different ligands**

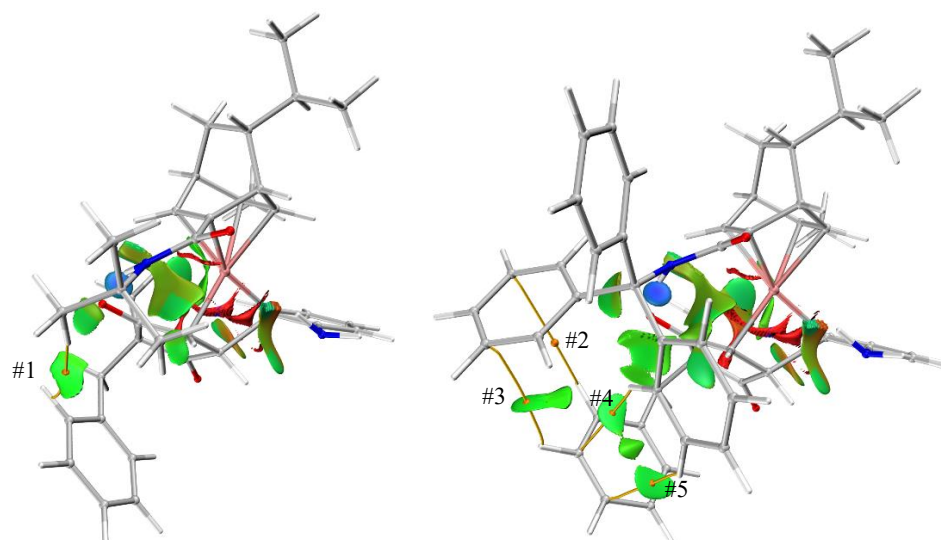


**Table S7: Selected properties of the bond critical points**

BCP	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$H(\mathbf{r})$
#1	0.002696735386	0.01018573320	0.0007224062133
#2	0.0009630038965	0.003544045180	0.0002575394580

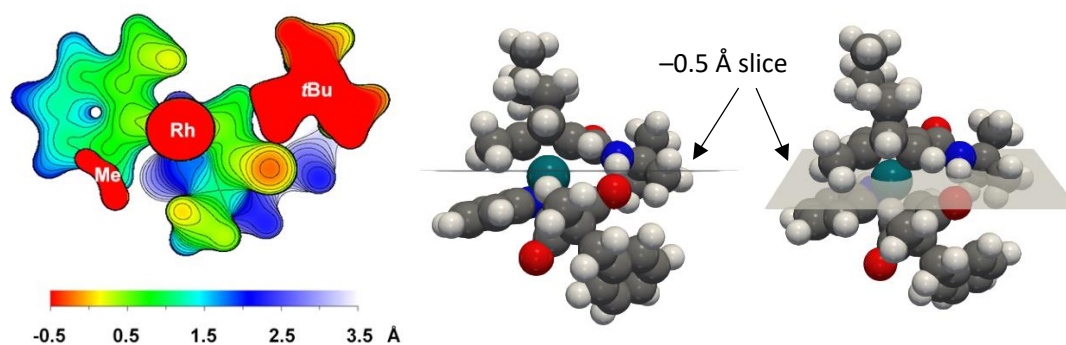
#3	0.002273823597	0.007006044773	0.0004249505022
#4	0.005966468459	0.01720689958	0.0007228245874
#5	0.005892419053	0.01687801384	0.0007236948608

**Figure S6: The illustration of bond critical points in TS16 and TS26**



The surface distance projection maps were displayed from  $-0.5 \text{ \AA}$  to  $3.5 \text{ \AA}$  centered on the rhodium atom.<sup>6h</sup> An illustration of the surface distance projection maps was given in figure S7.

**Figure S7: The illustration of surface distance projection maps (TS16)**



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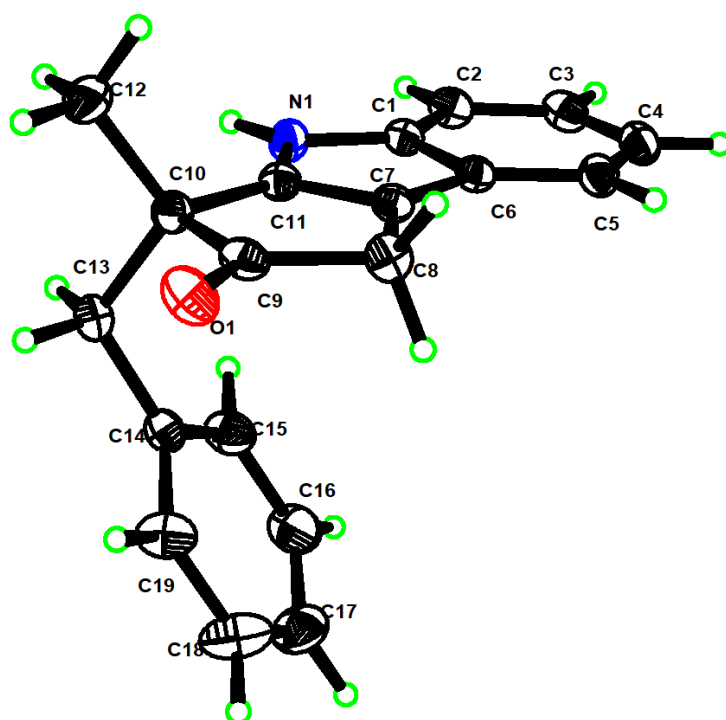
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## 8. Single Crystal X-ray Diffraction

Single crystal of **3aa** for X-ray diffraction was grown by liquid-liquid diffusion in a *n*-hexane/toluene binary solvent system in a 10 mL screw cap vial at room temperature. The X-ray data of **3aa** is deposited in the Cambridge Crystallographic Data Centre with a number of CCDC 2260854.

**Figure S8: ORTEP representation of the X-ray structure of enantiopure 3aa (thermal ellipsoids are drawn at 50% probability)**



**Table S8: Crystal data and structure refinement for 3aa**

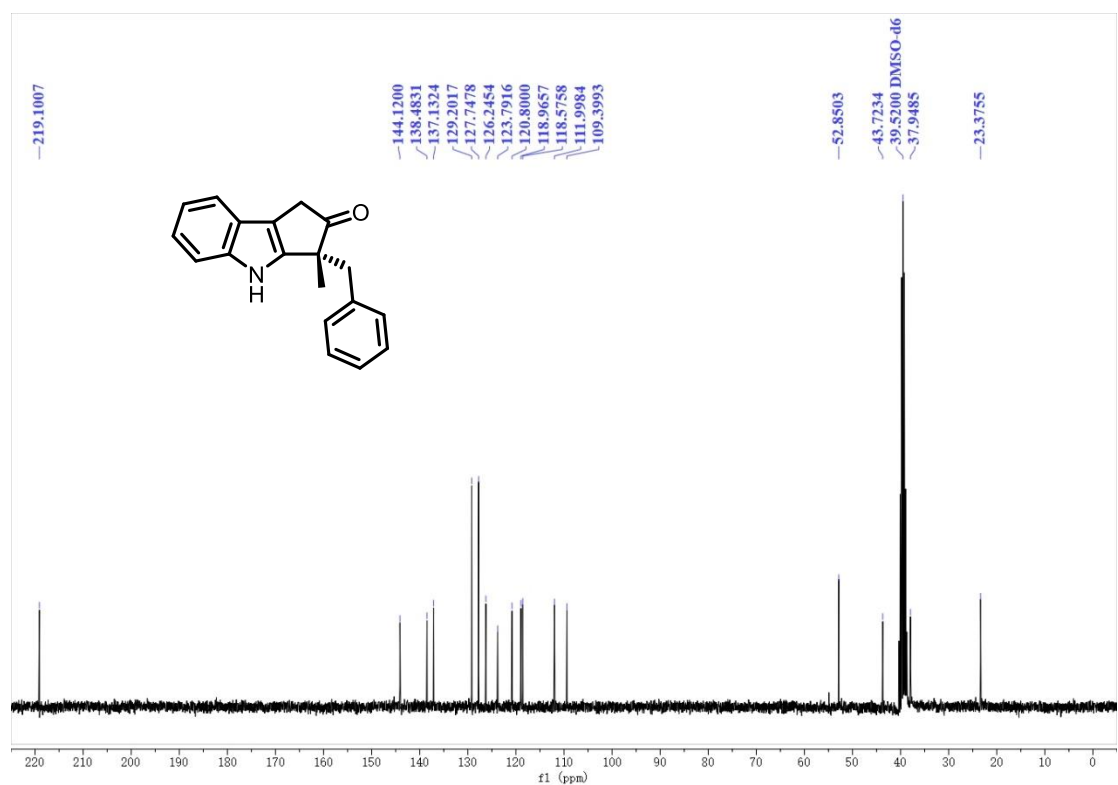
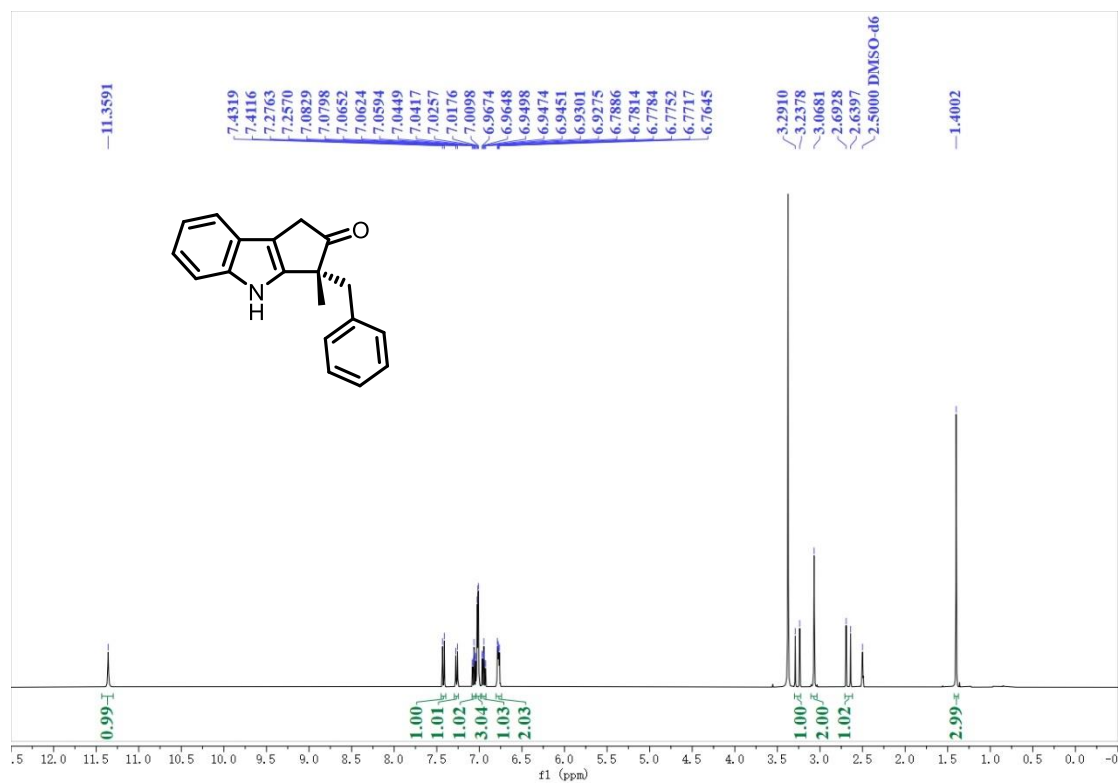
Identification code	WCH262_0m
Empirical formula	C <sub>19</sub> H <sub>16</sub> NO
Formula weight	274.33
Temperature/K	170.0
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
a/Å	9.1061(2)
b/Å	12.0634(2)
c/Å	14.0083(3)

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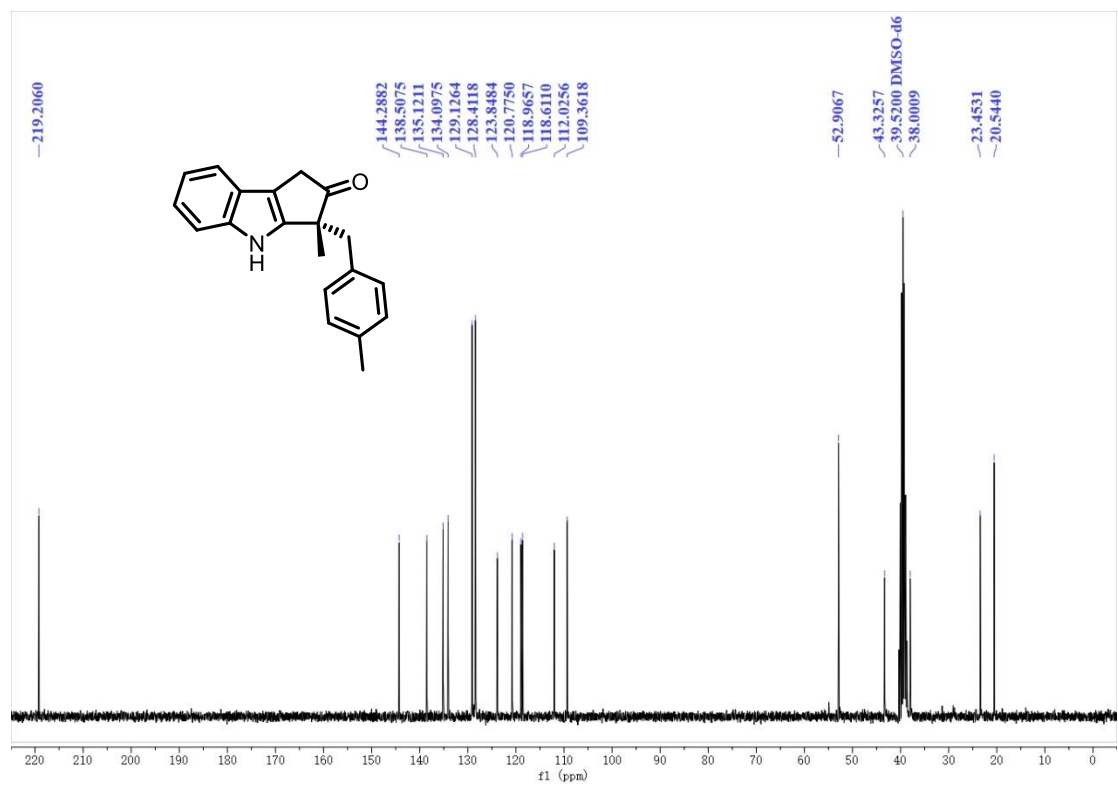
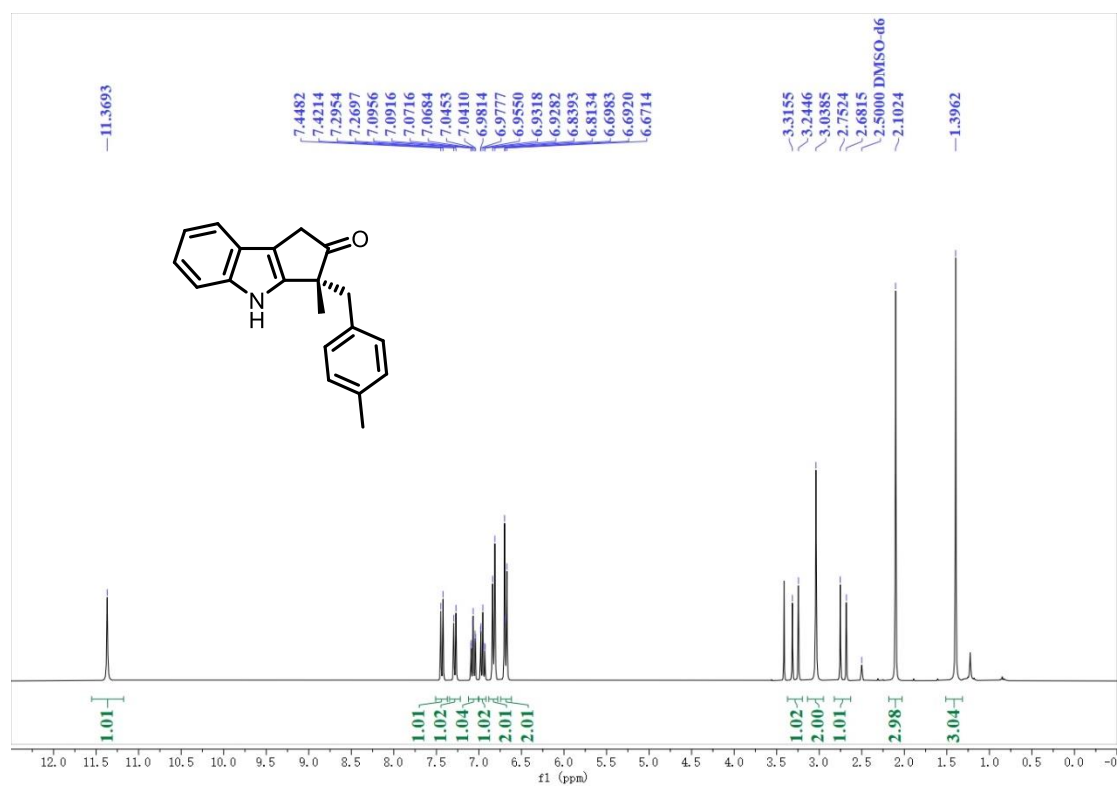
$\alpha/^\circ$	90
$\beta/^\circ$	90
$\gamma/^\circ$	90
Volume/ $\text{\AA}^3$	1538.82(5)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.184
$\mu/\text{mm}^{-1}$	0.571
F(000)	580.0
Crystal size/ $\text{mm}^3$	$0.15 \times 0.08 \times 0.05$
Radiation	CuK $\alpha$ ( $\lambda = 1.54178$ )
$2\Theta$ range for data collection/ $^\circ$	9.676 to 149.092
Index ranges	$-9 \leq h \leq 11, -13 \leq k \leq 14, -17 \leq l \leq 17$
Reflections collected	14446
Independent reflections	3105 [ $R_{\text{int}} = 0.0344, R_{\text{sigma}} = 0.0244$ ]
Data/restraints/parameters	3105/0/191
Goodness-of-fit on $F^2$	1.043
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1 = 0.0403, wR_2 = 0.1089$
Final R indexes [all data]	$R_1 = 0.0425, wR_2 = 0.1116$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	0.36/-0.37
Flack parameter	0.03(11)

## 9. NMR Spectra

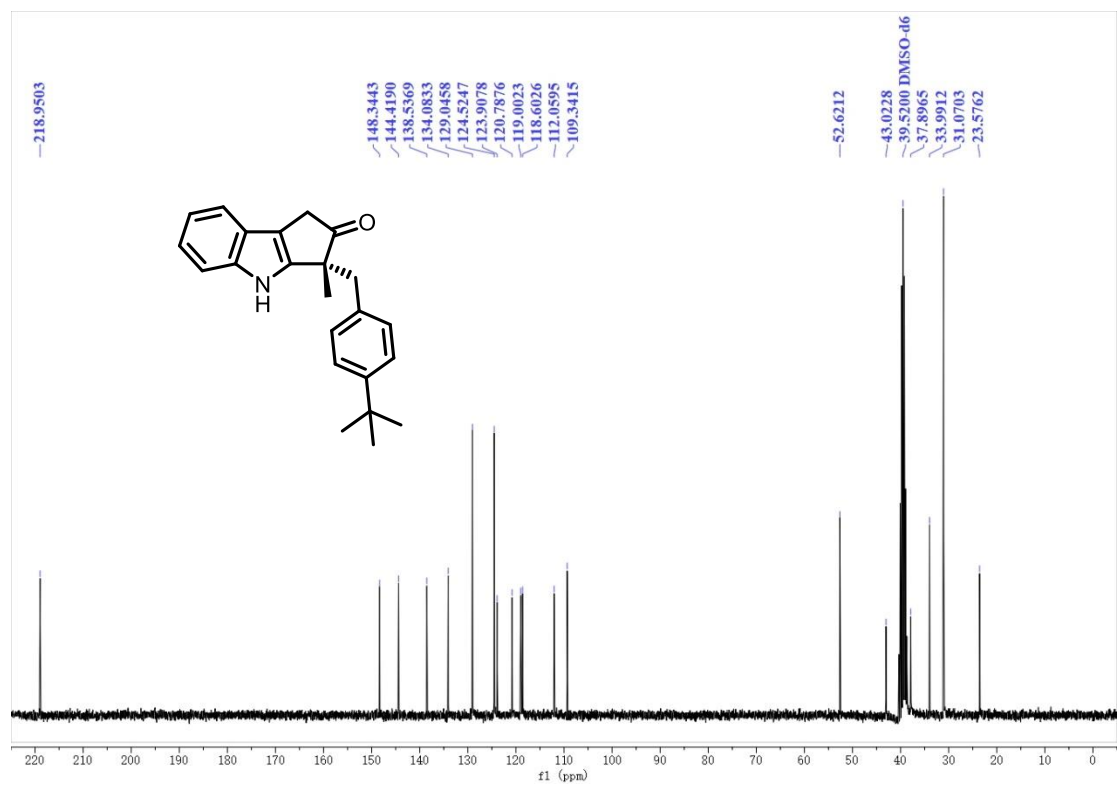
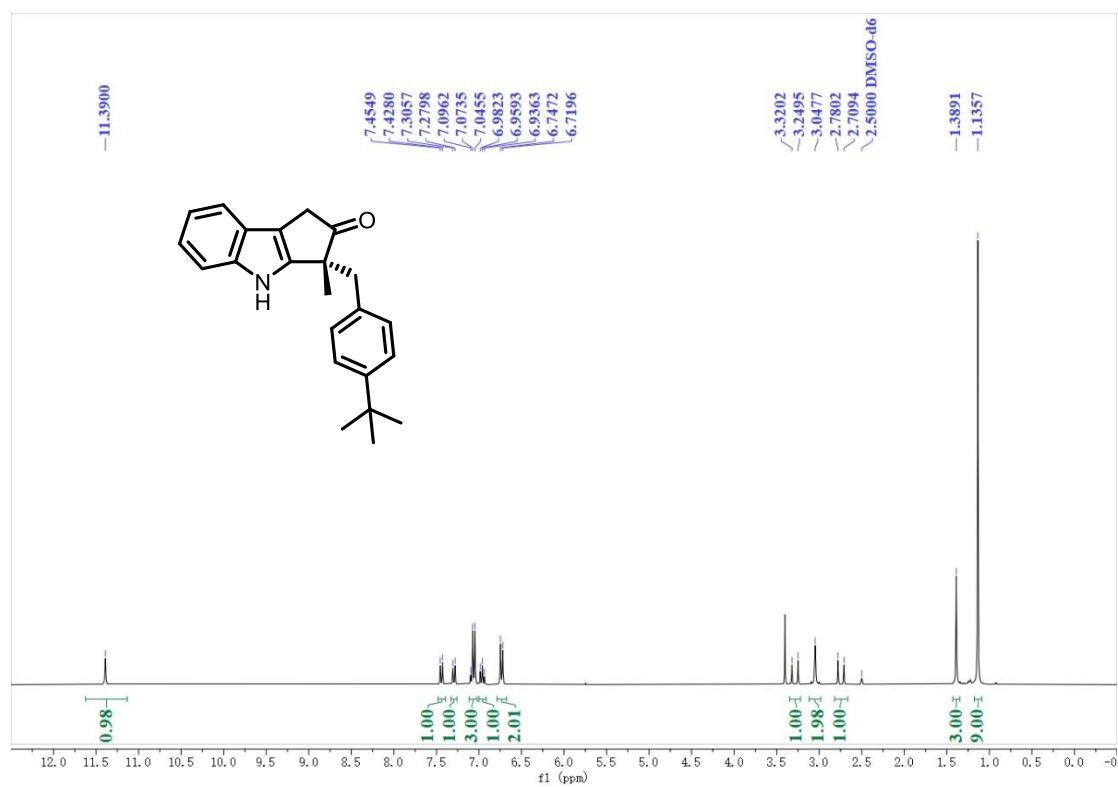
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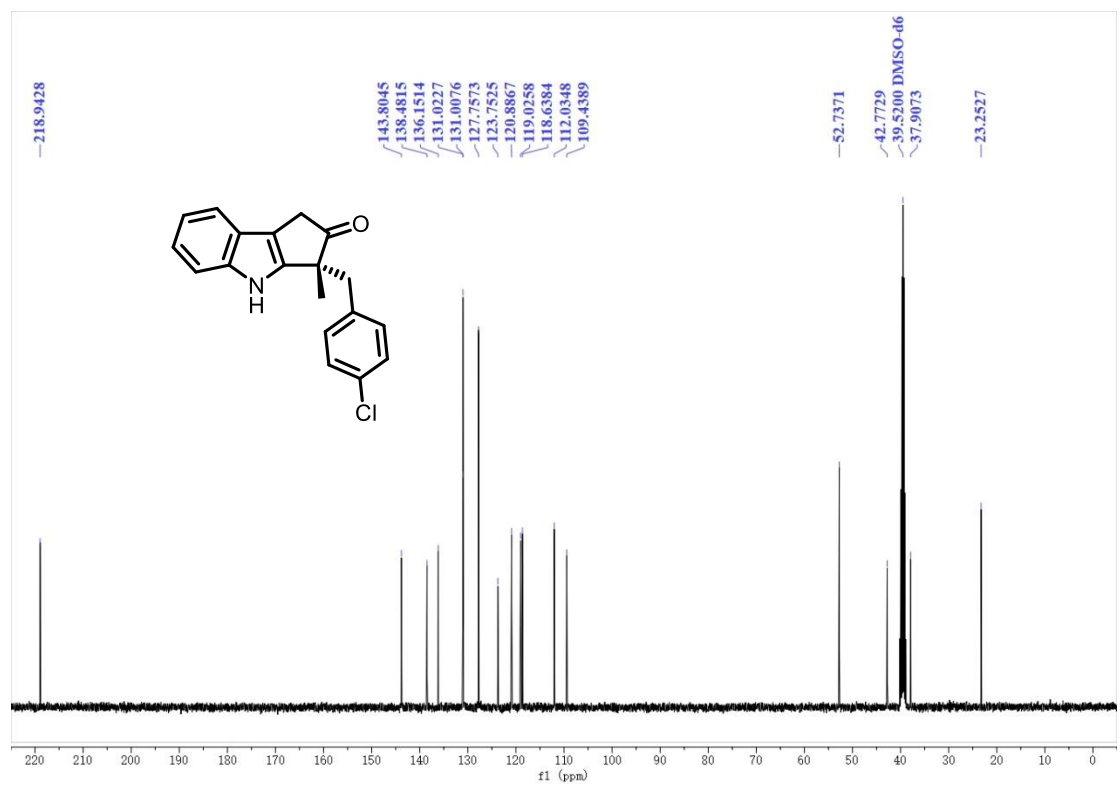
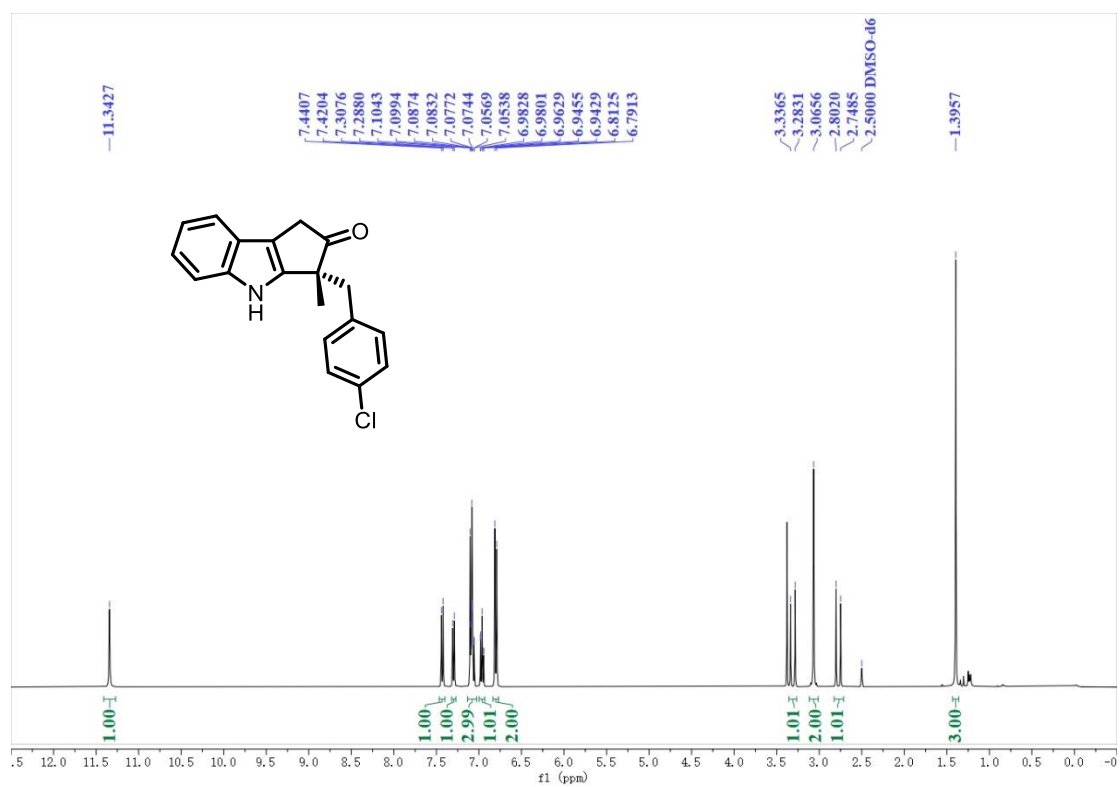
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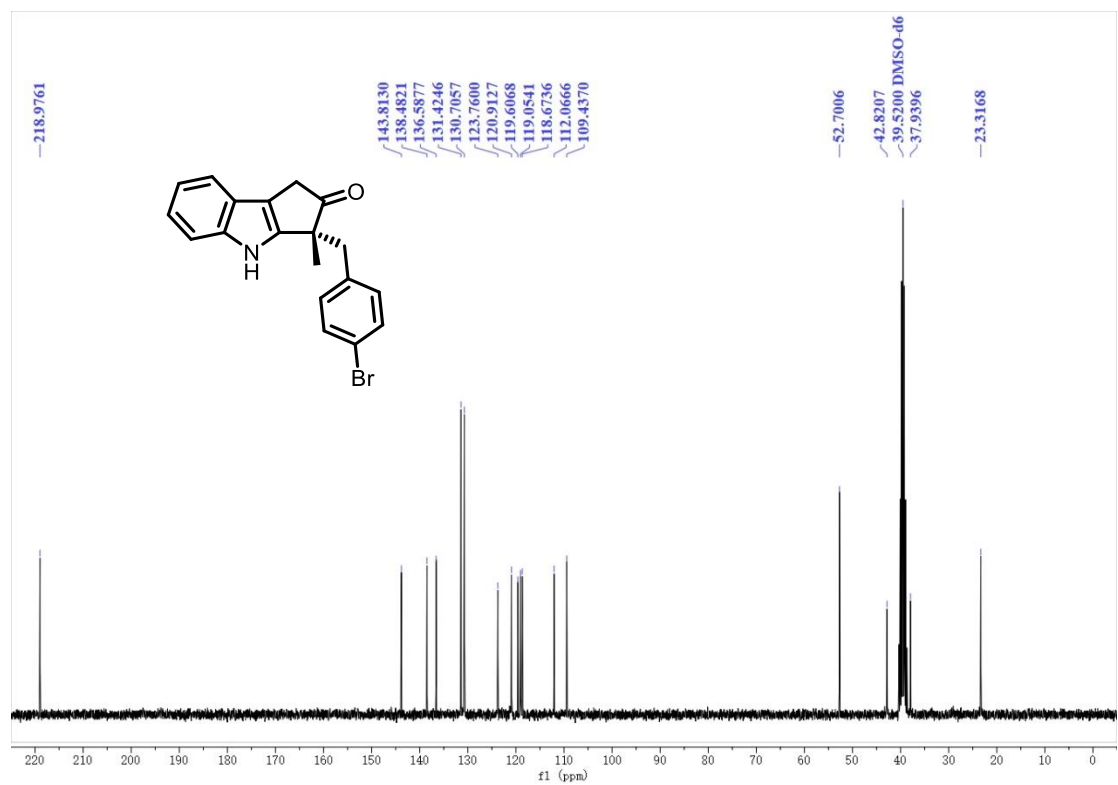
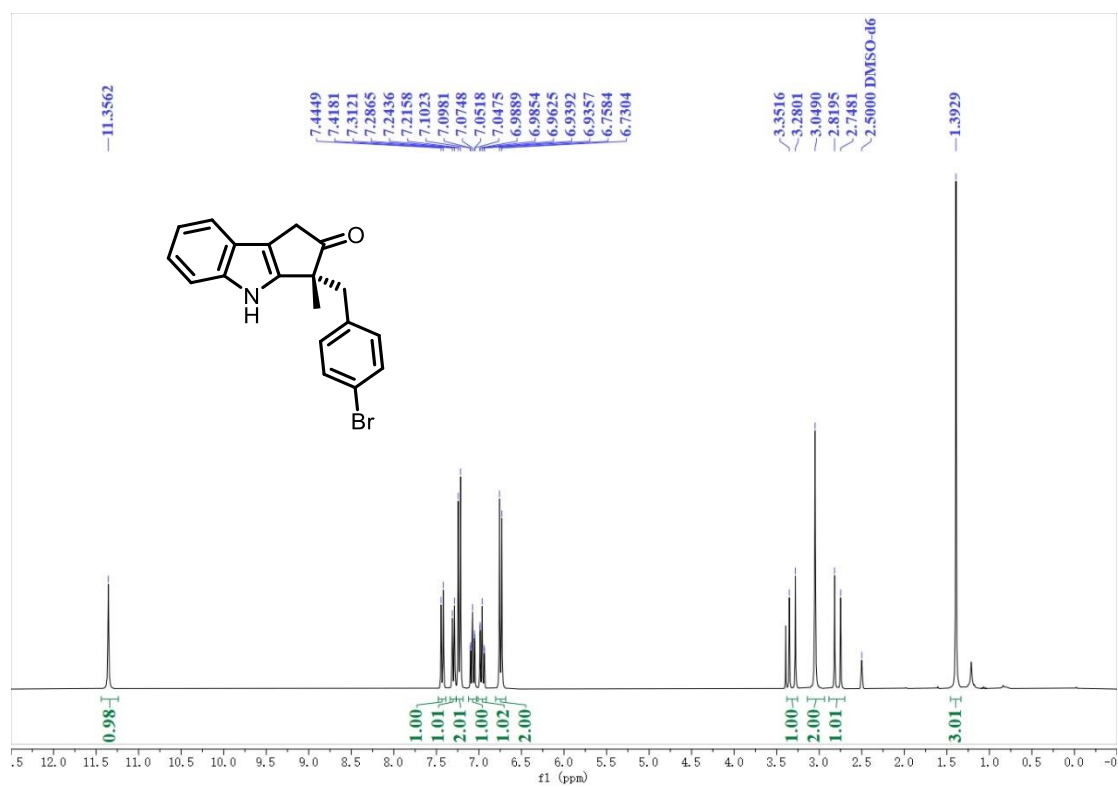
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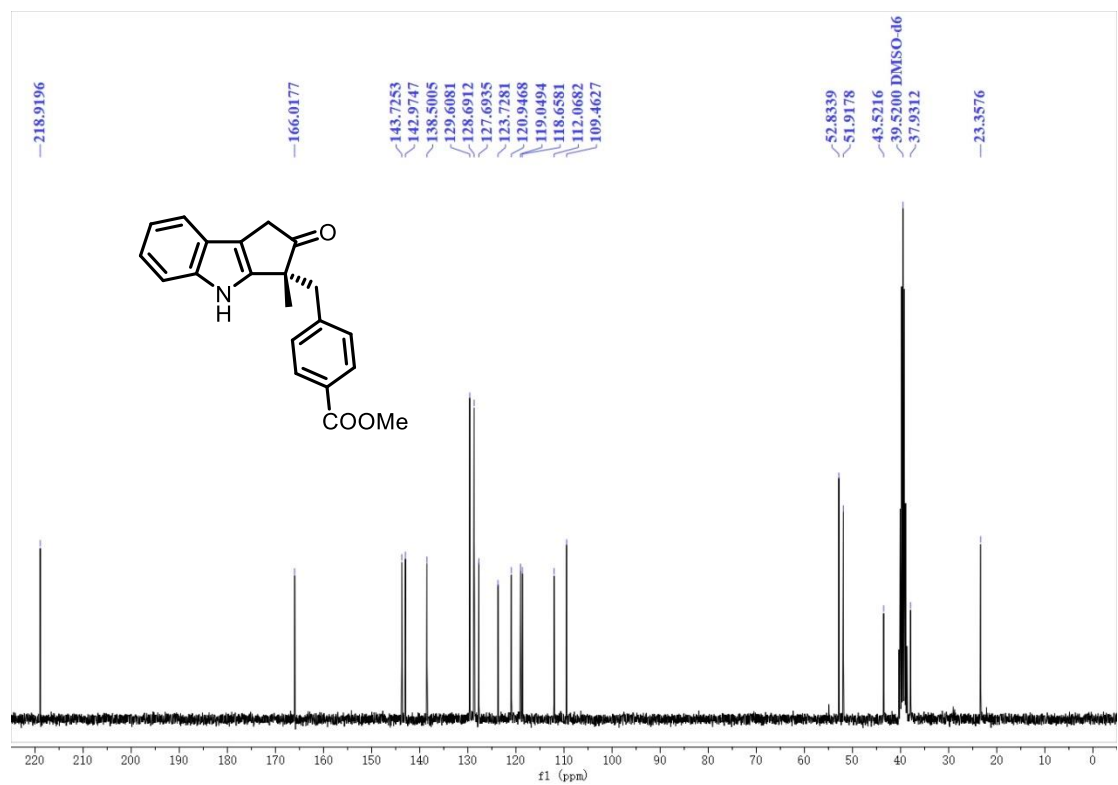
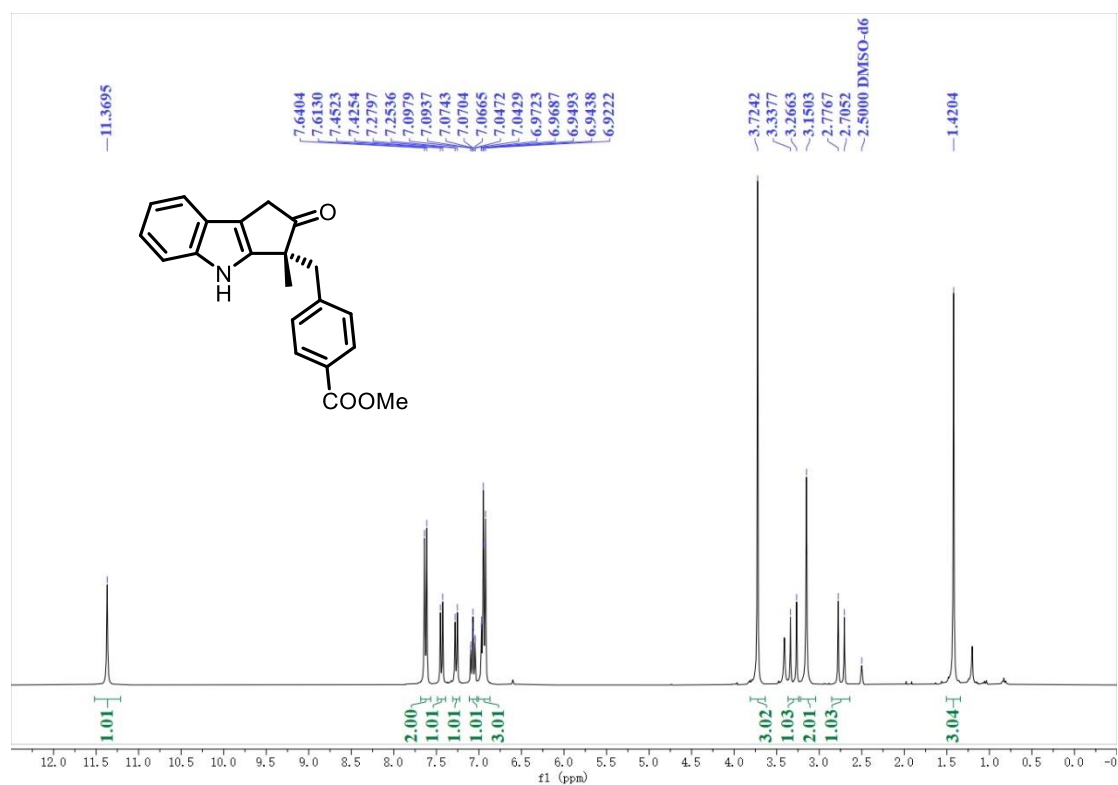
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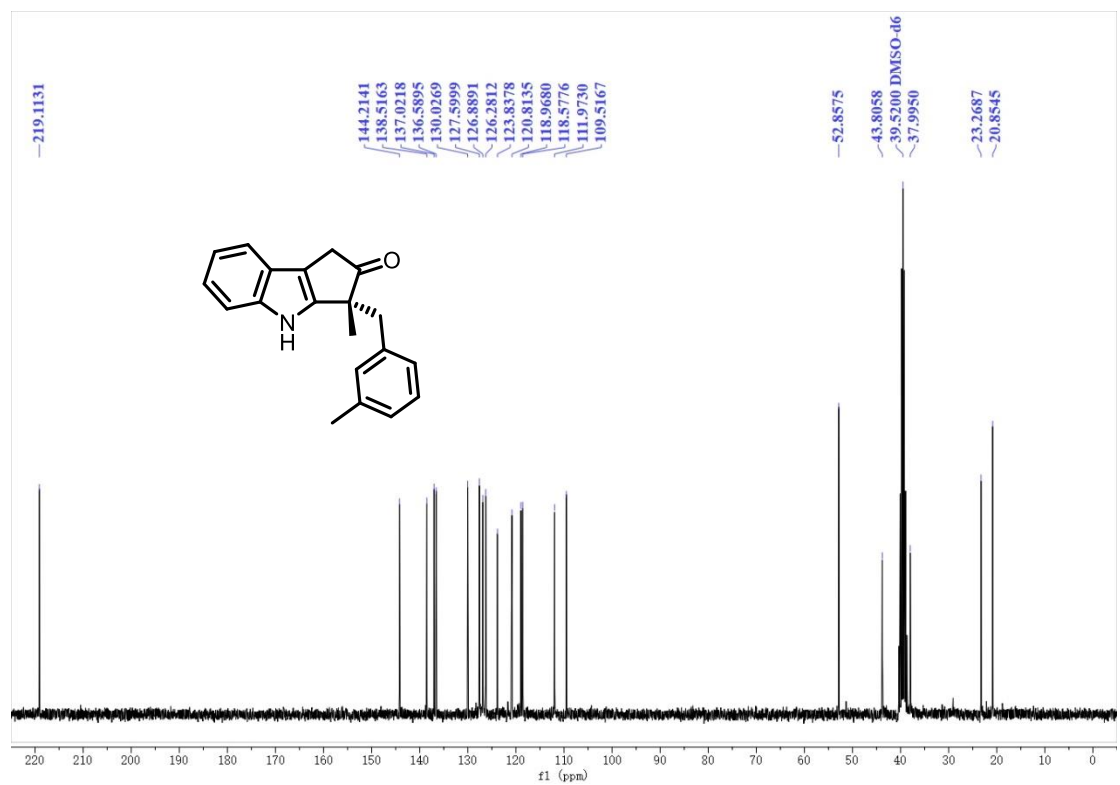
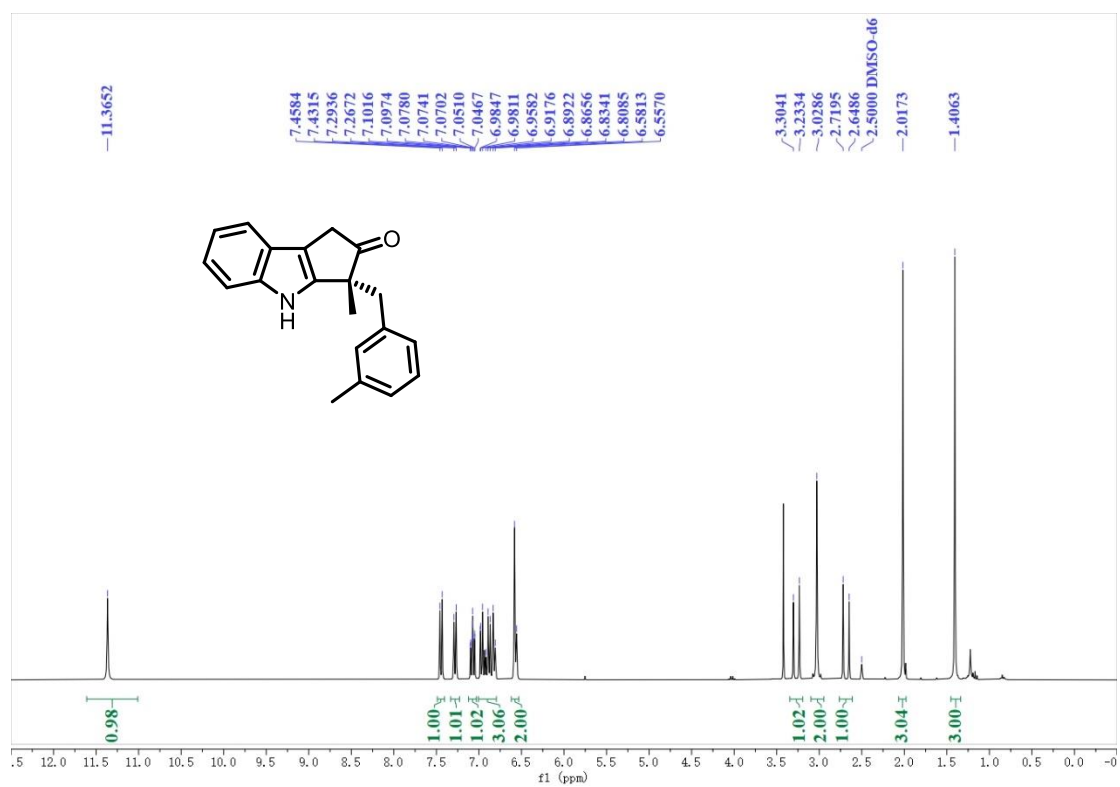


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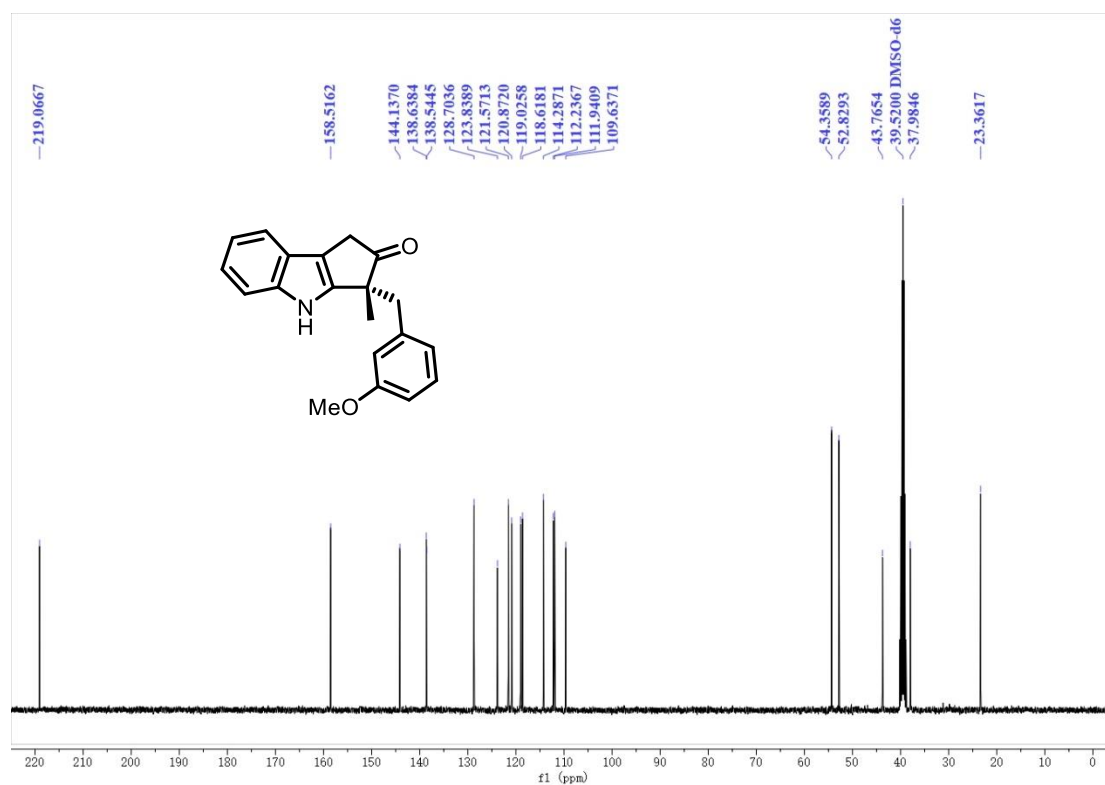
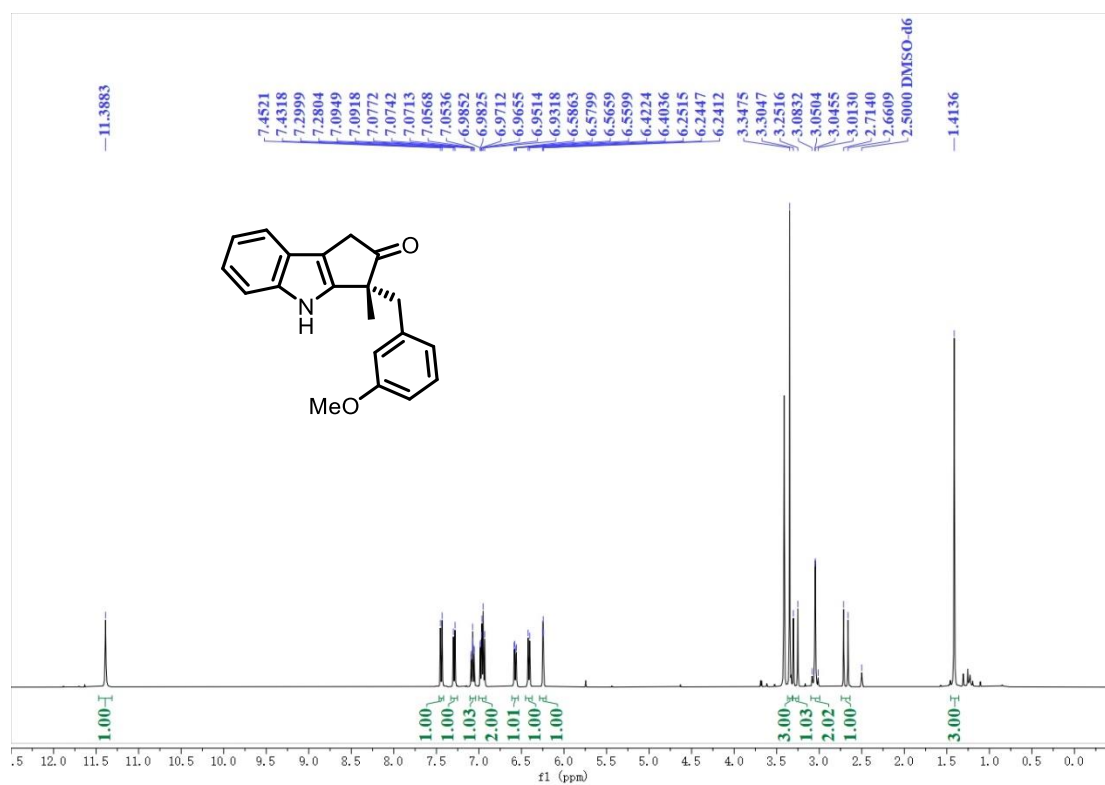




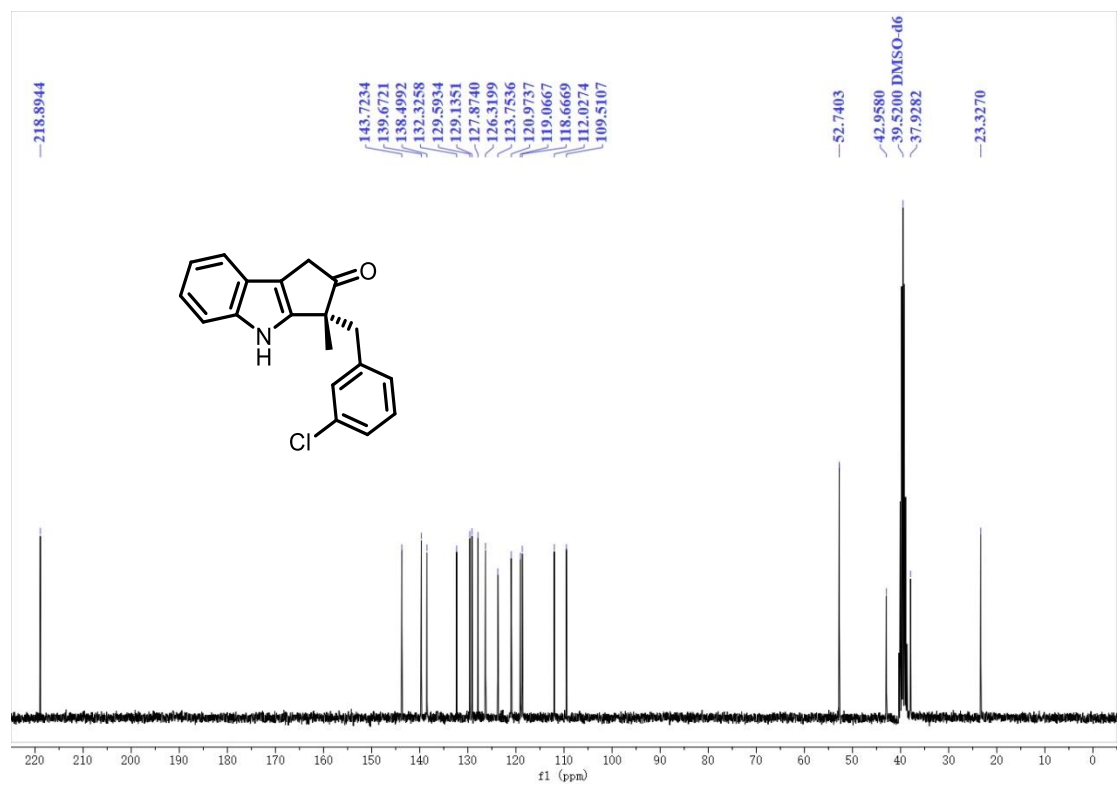
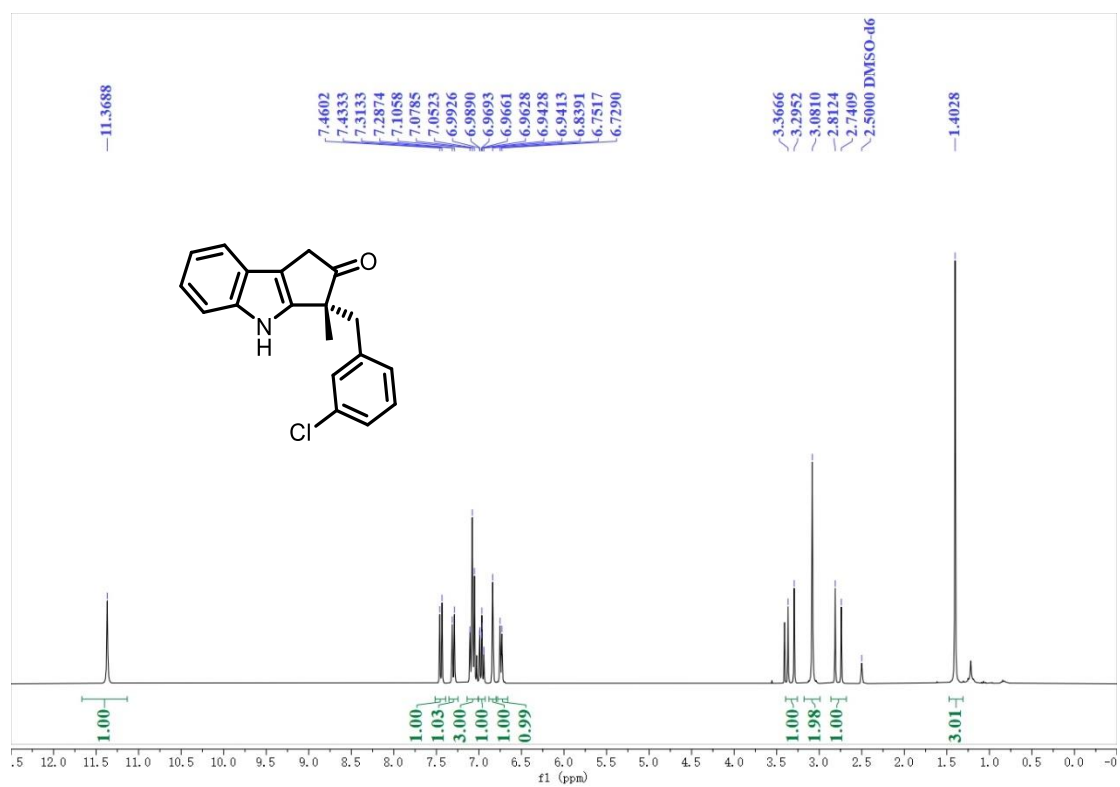
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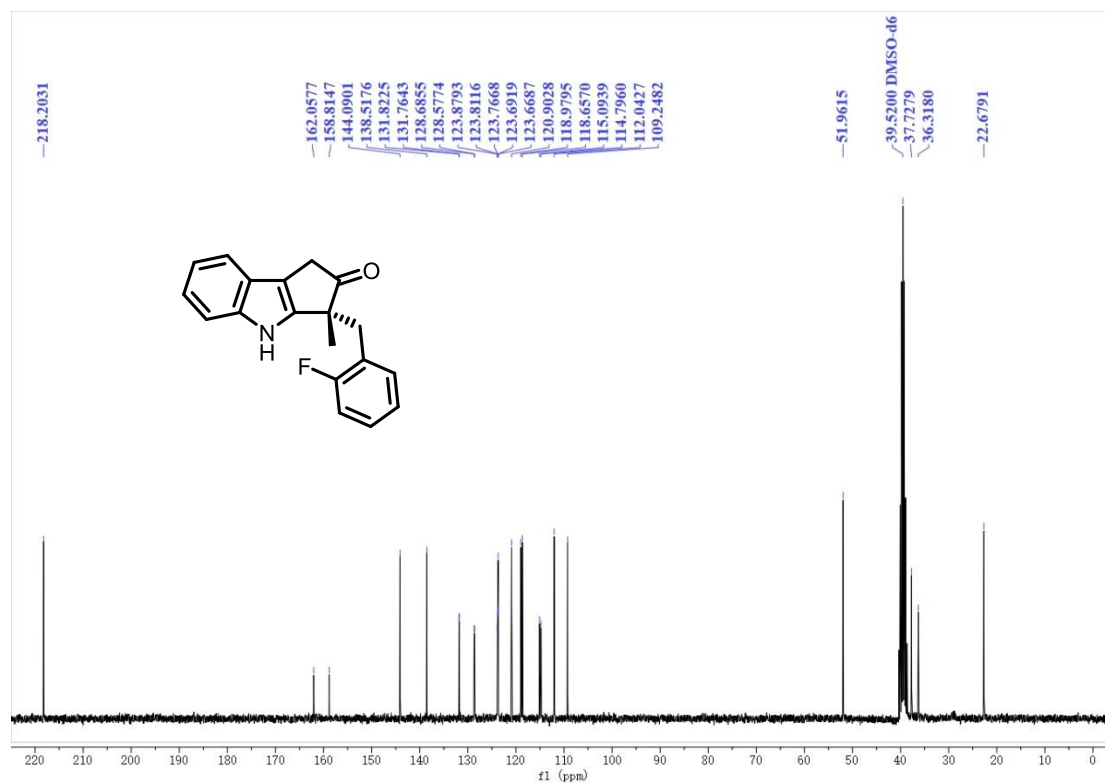
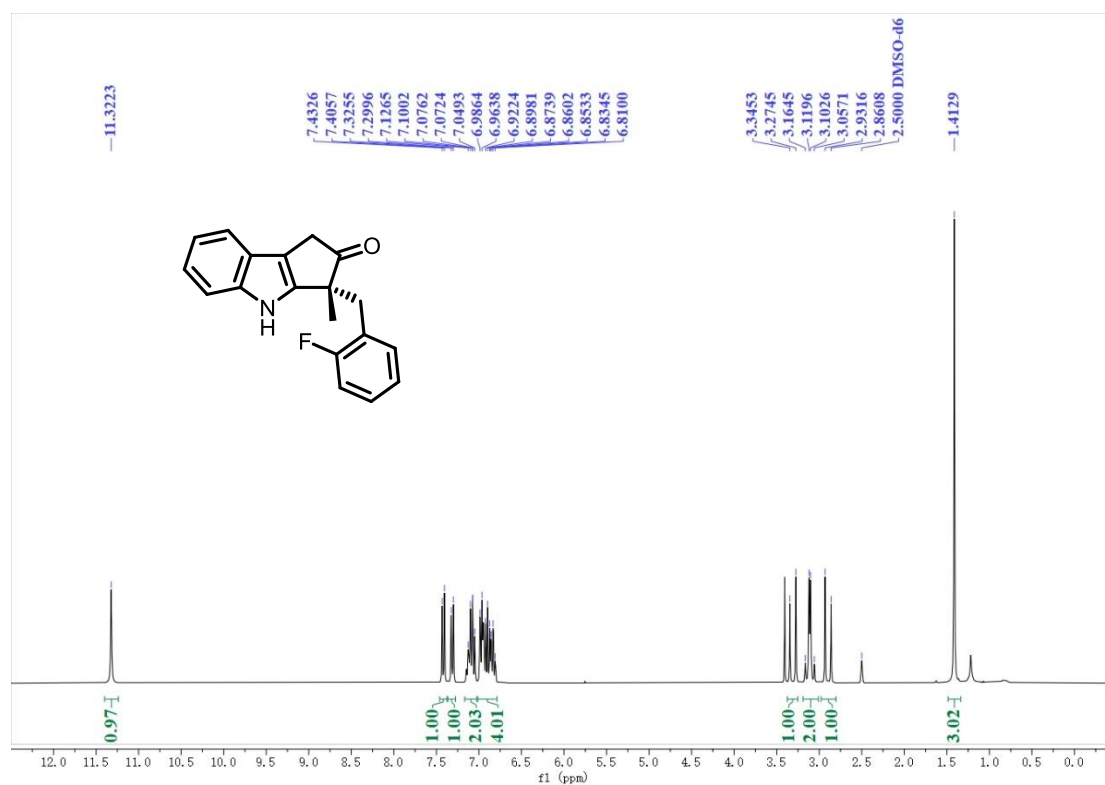
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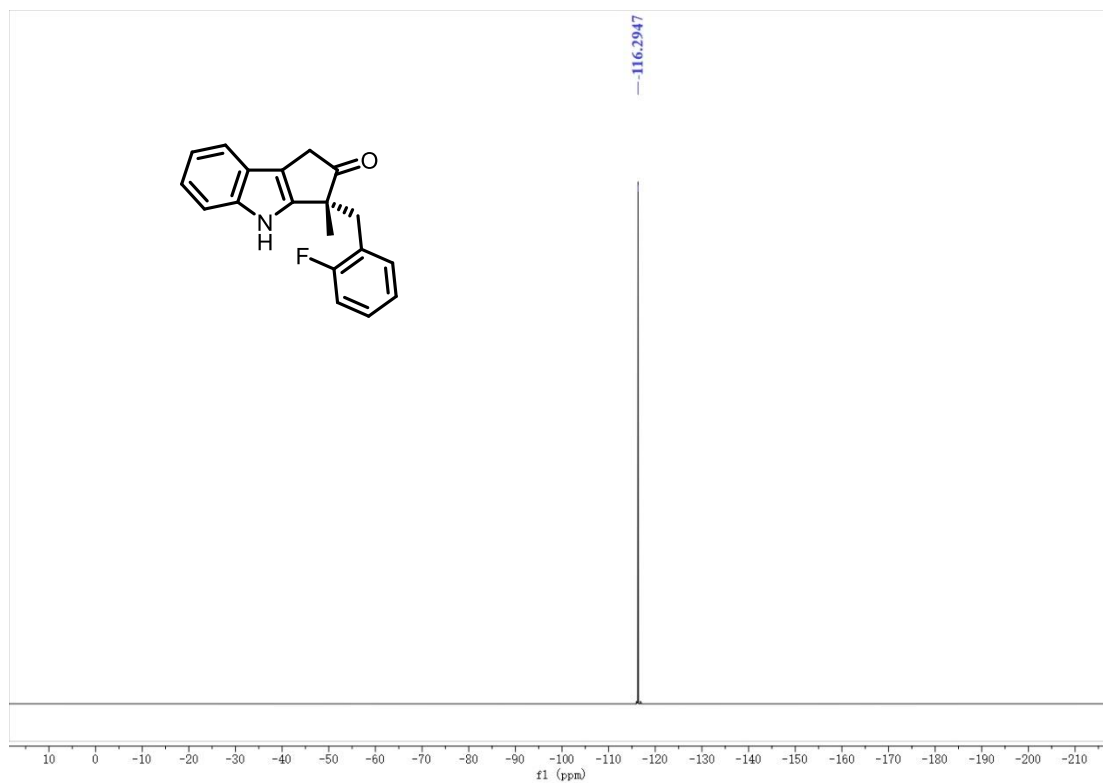
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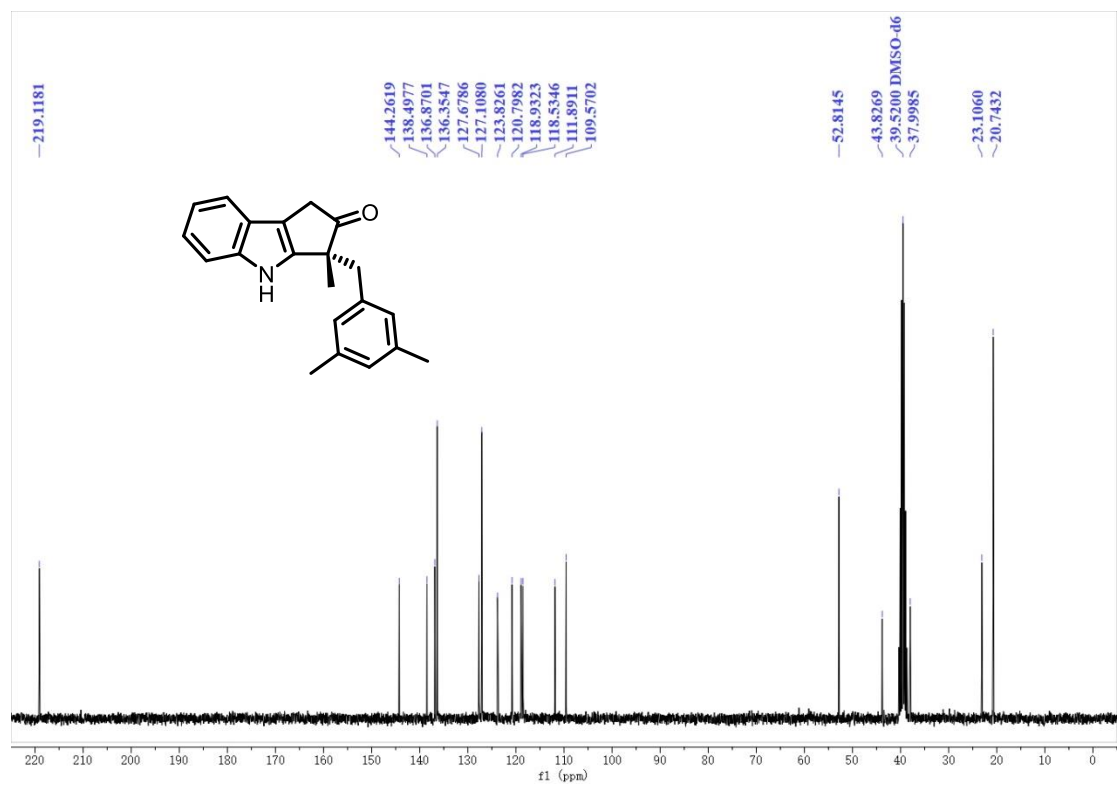
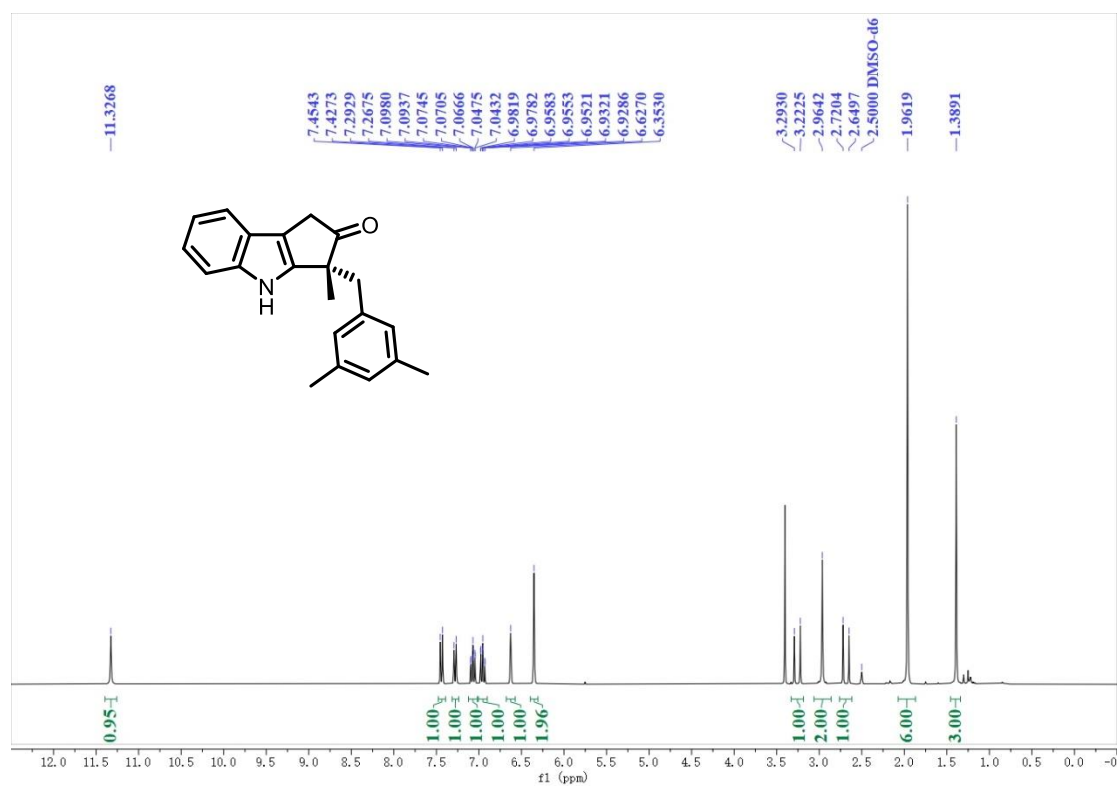
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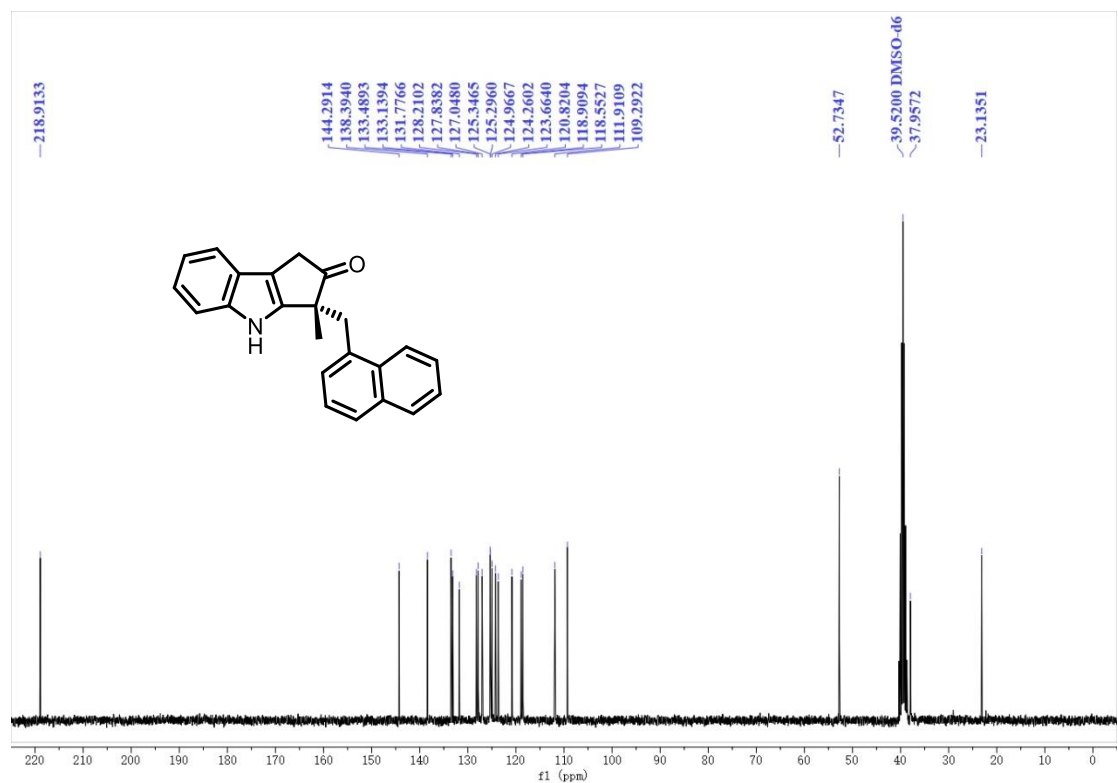
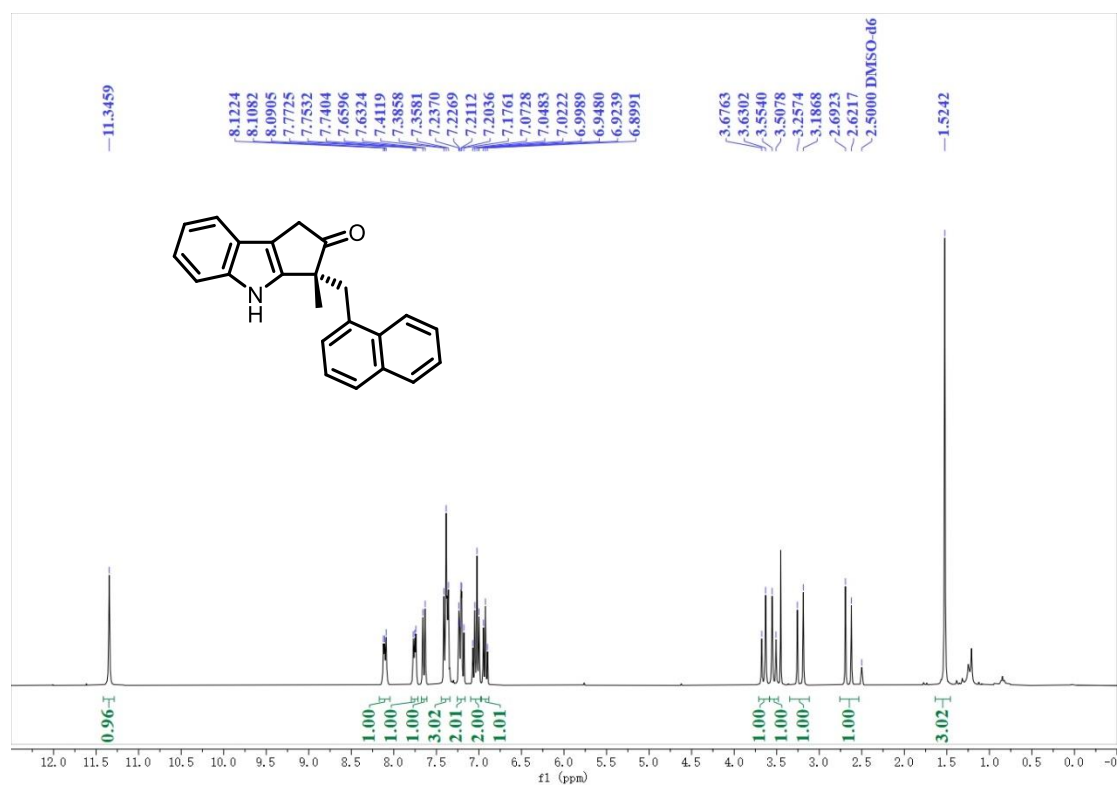
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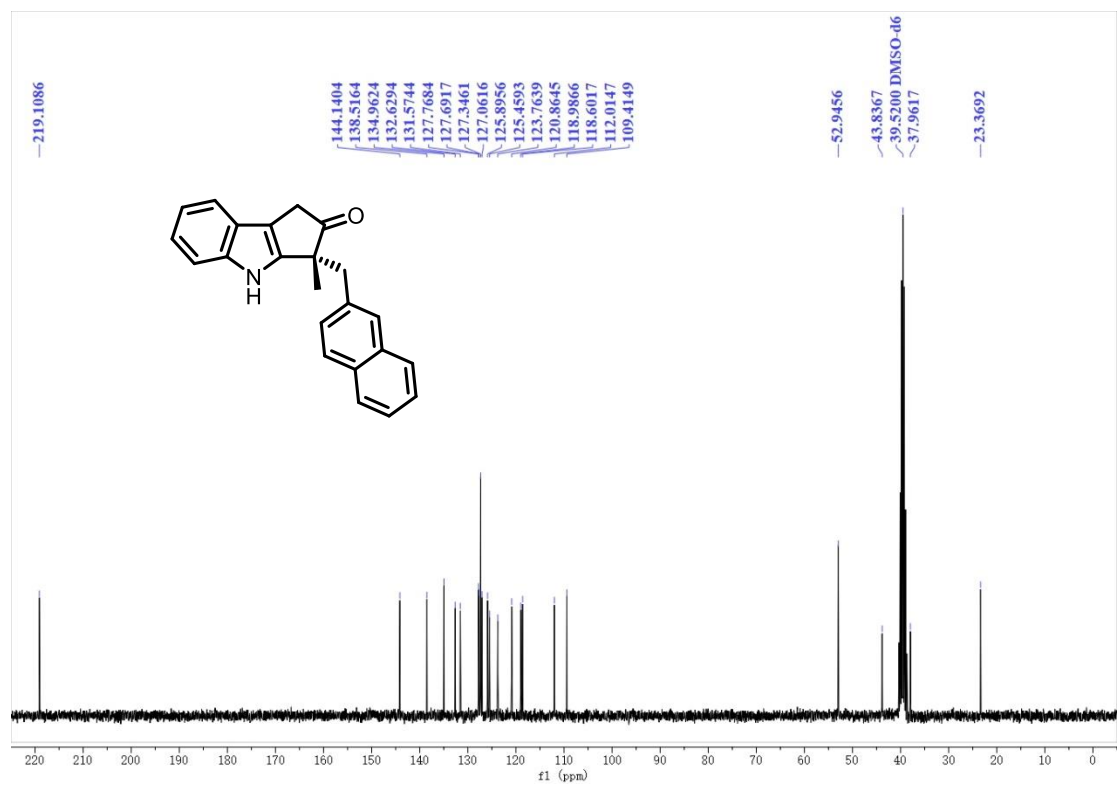
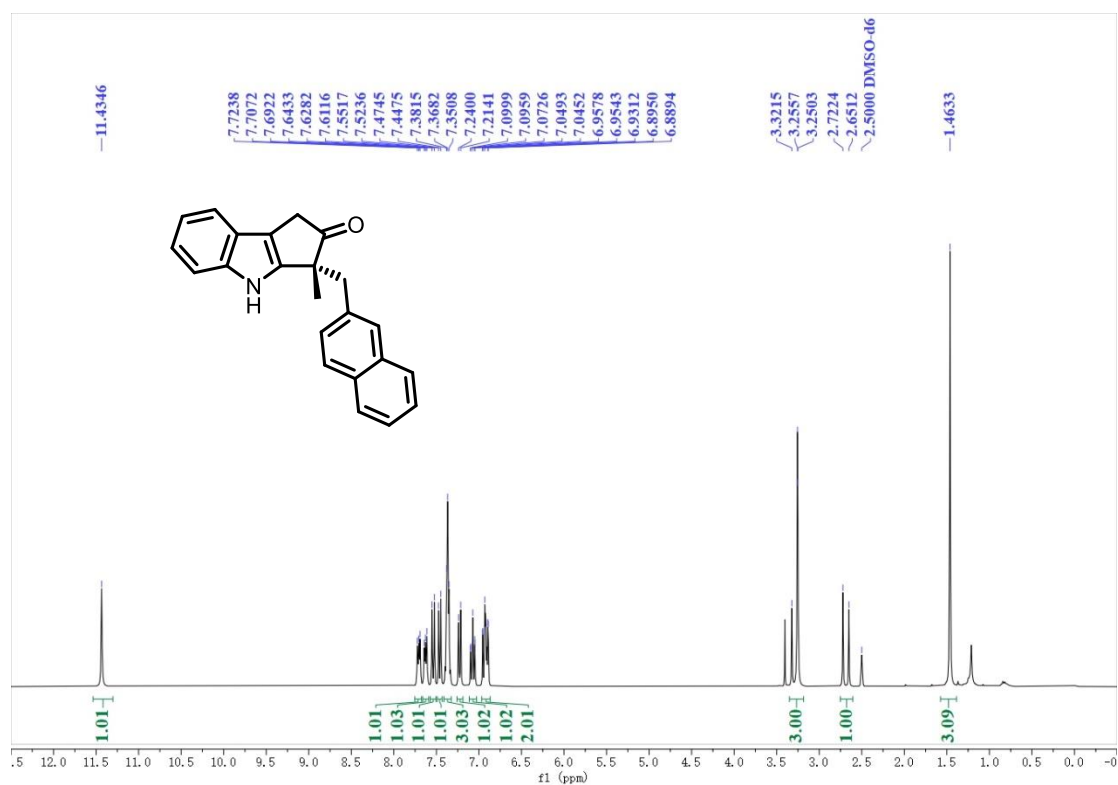
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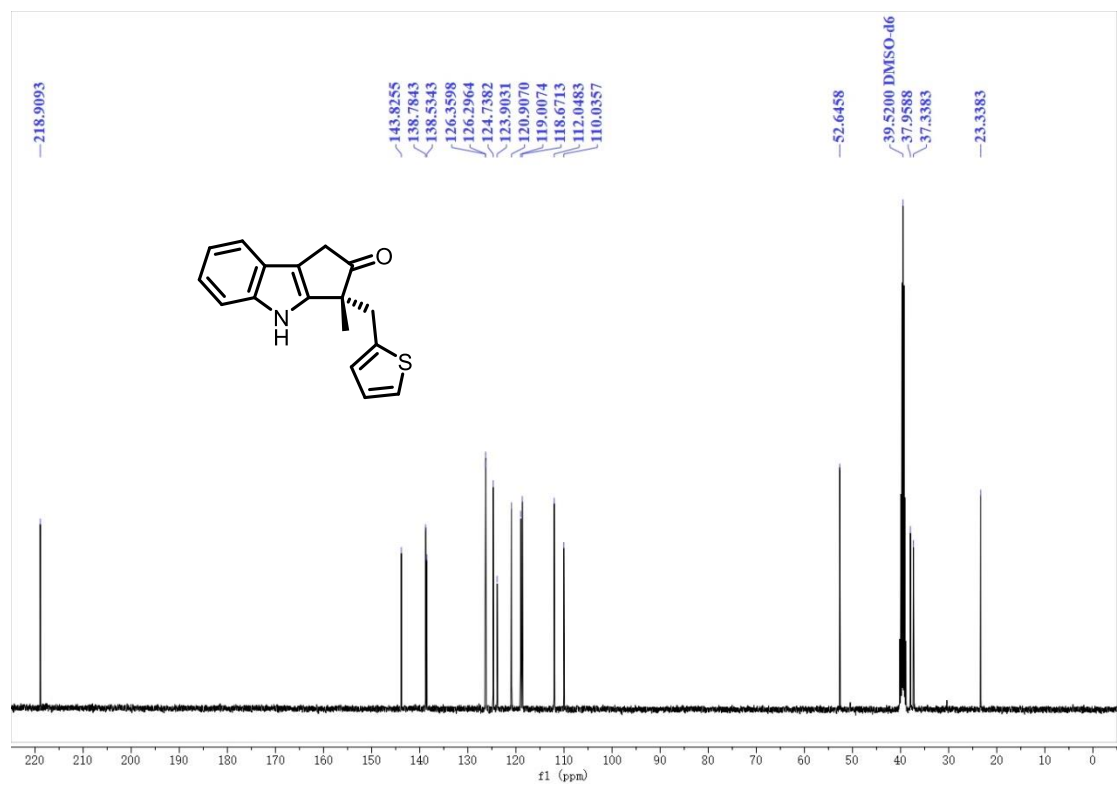
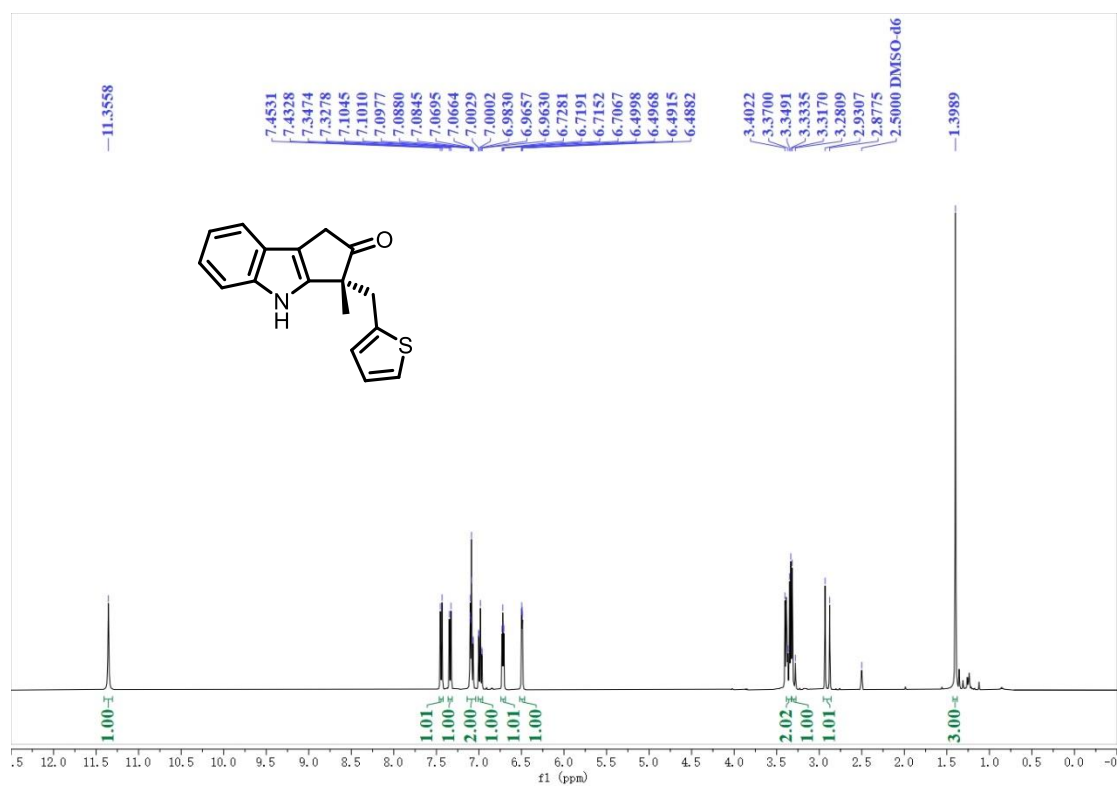


**3ma**  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-}d_6$ )

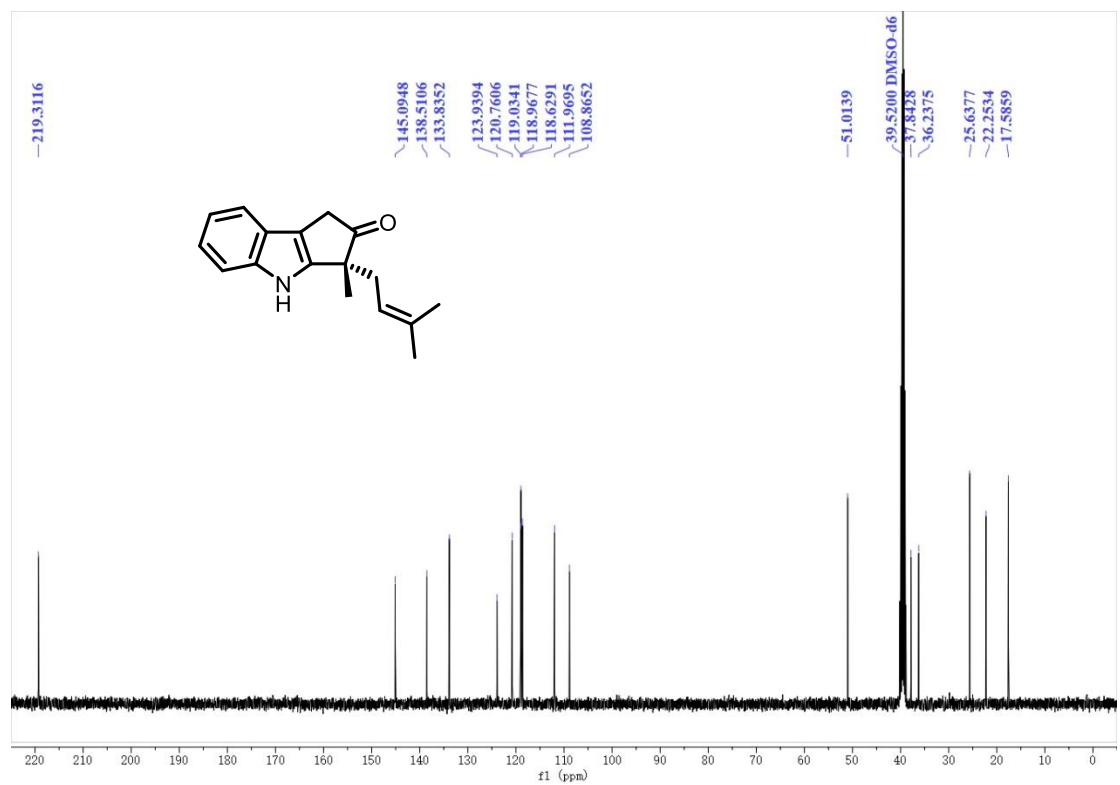
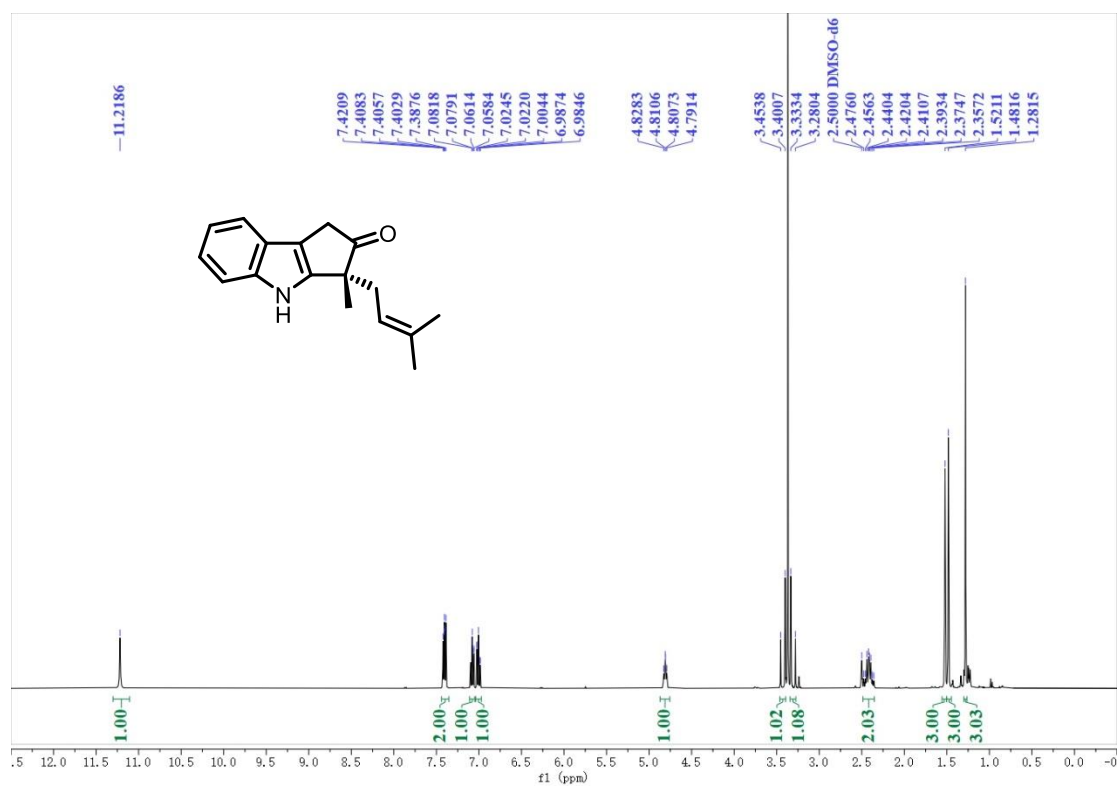




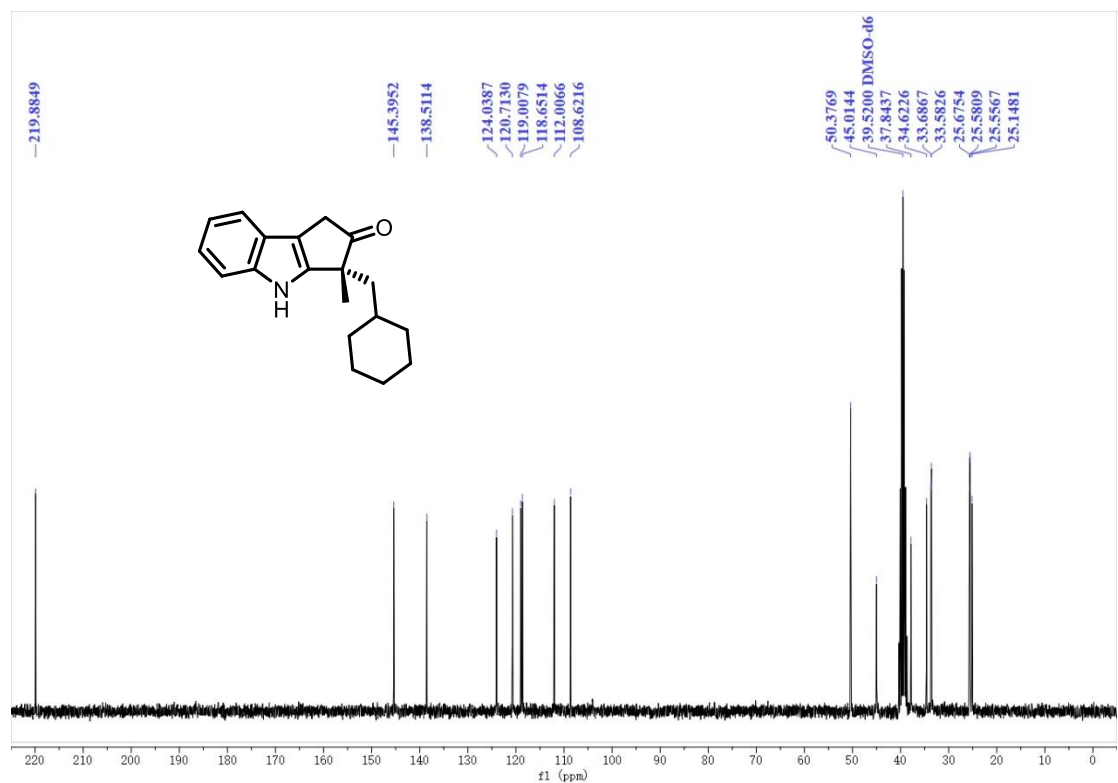
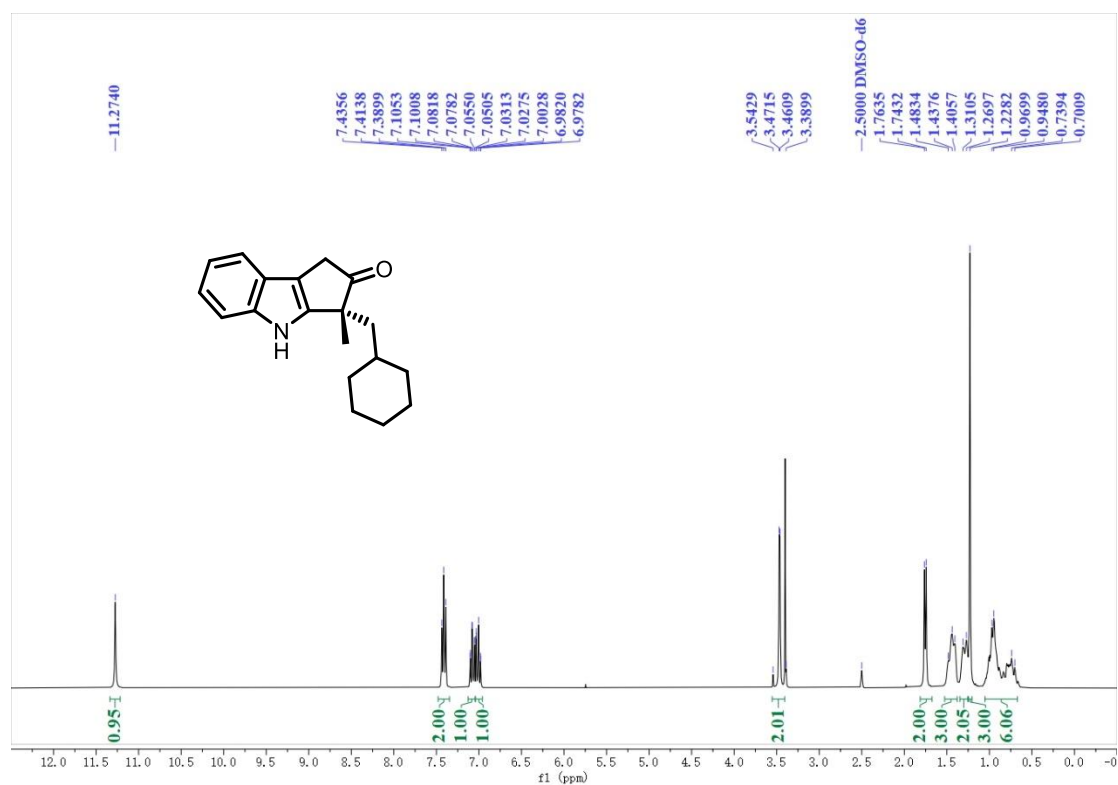
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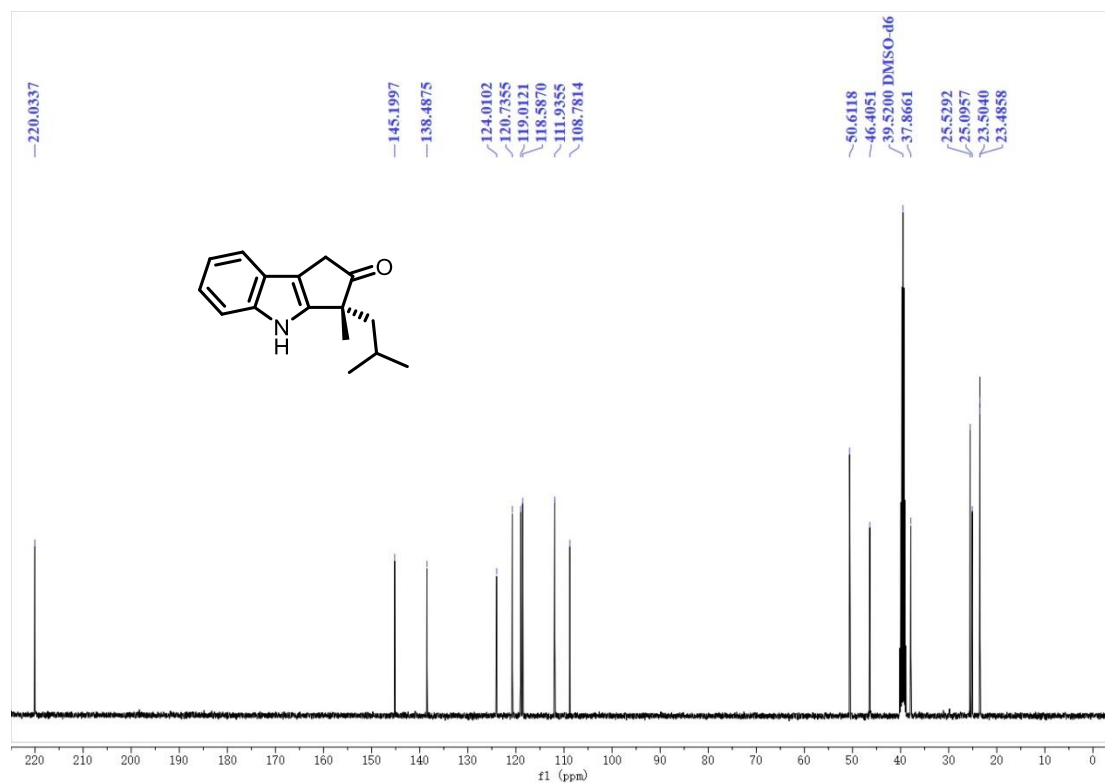
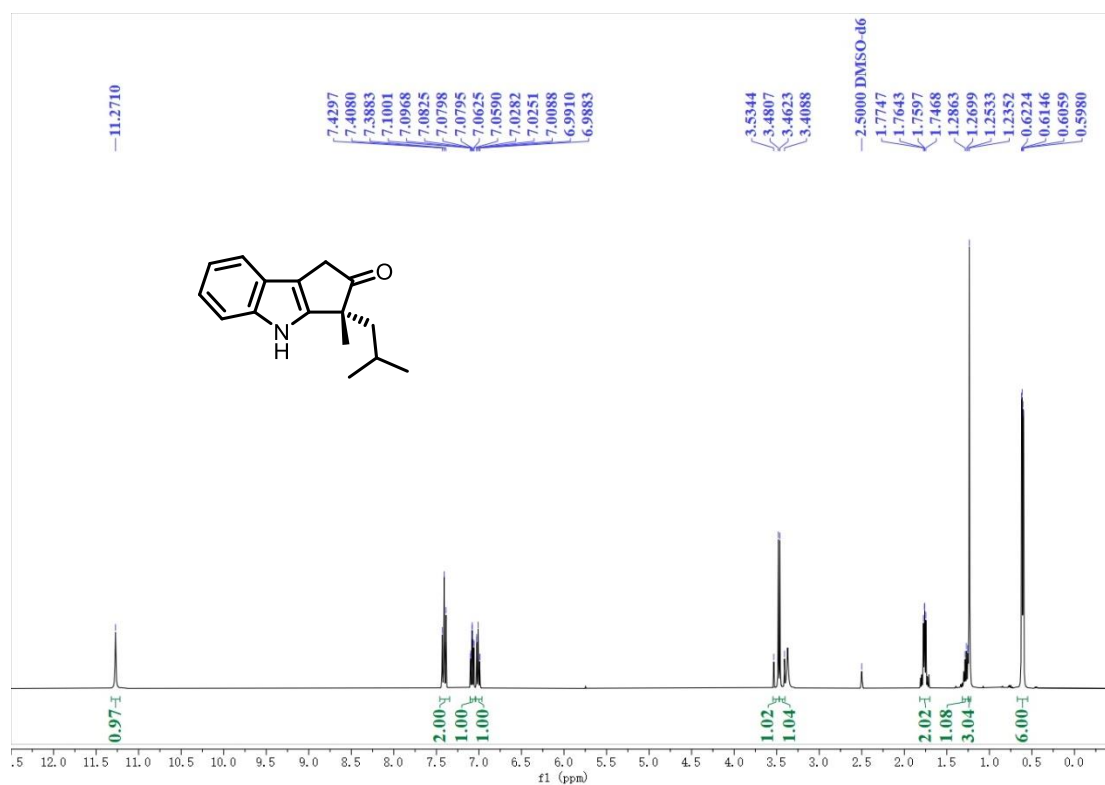
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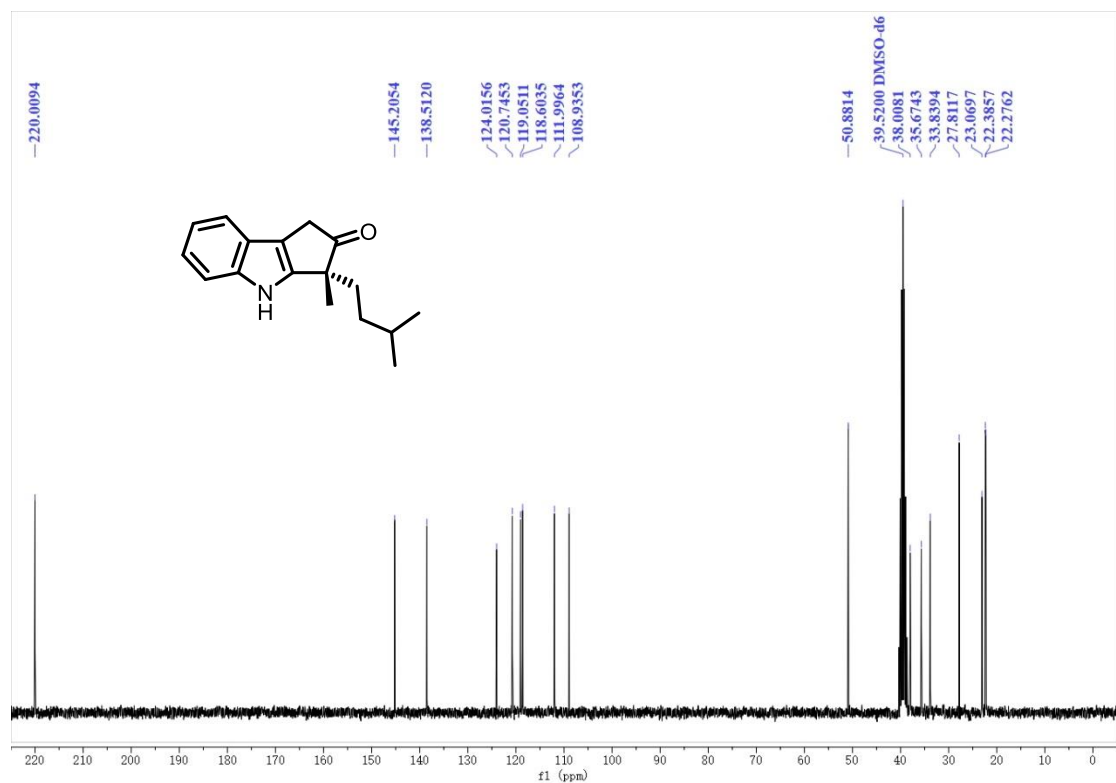
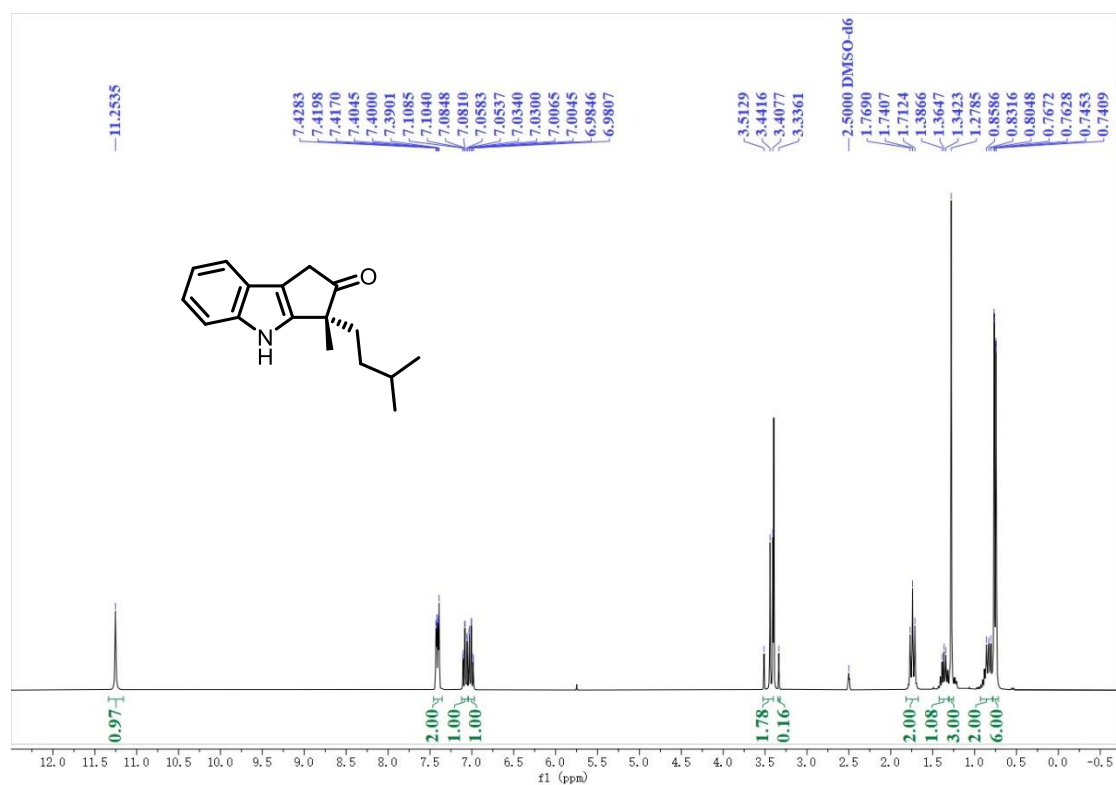
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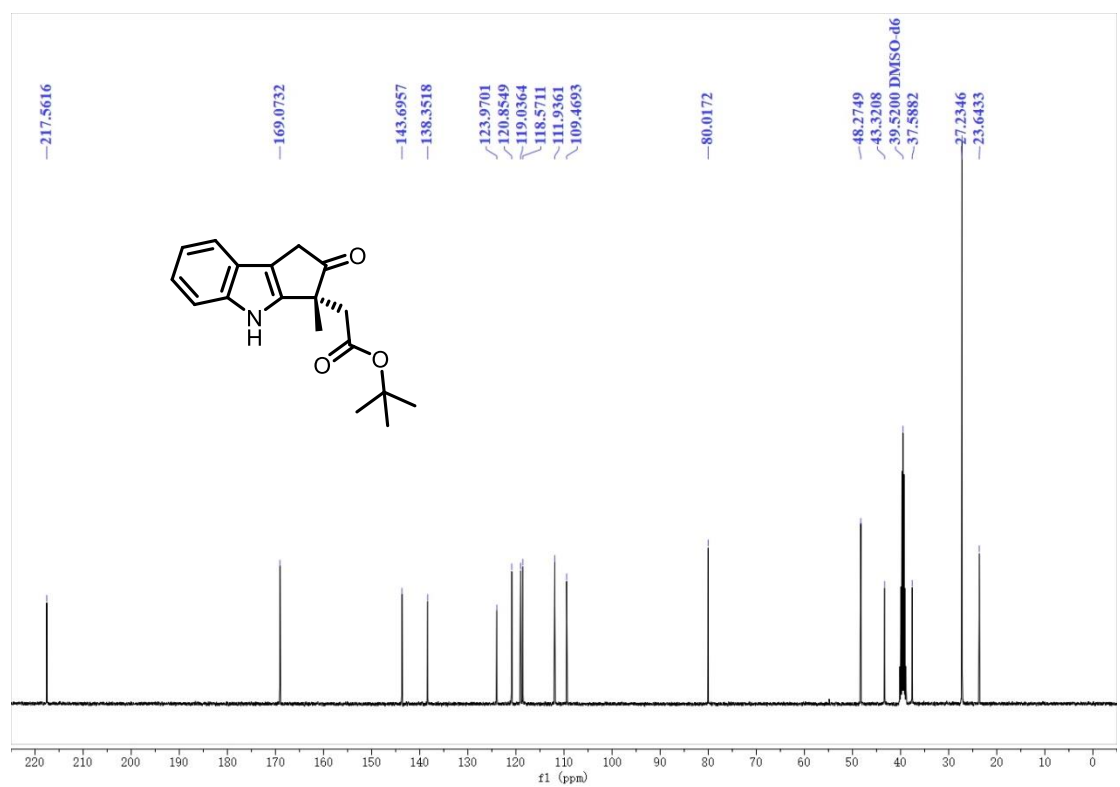
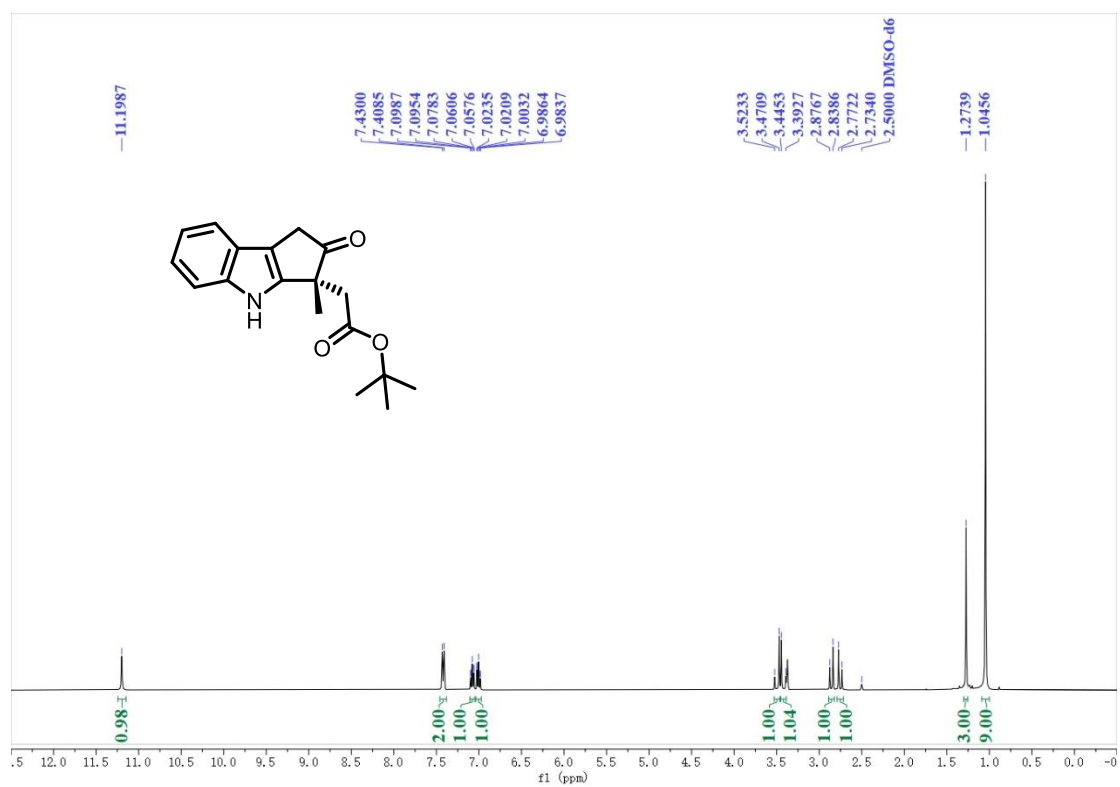
**3qa**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



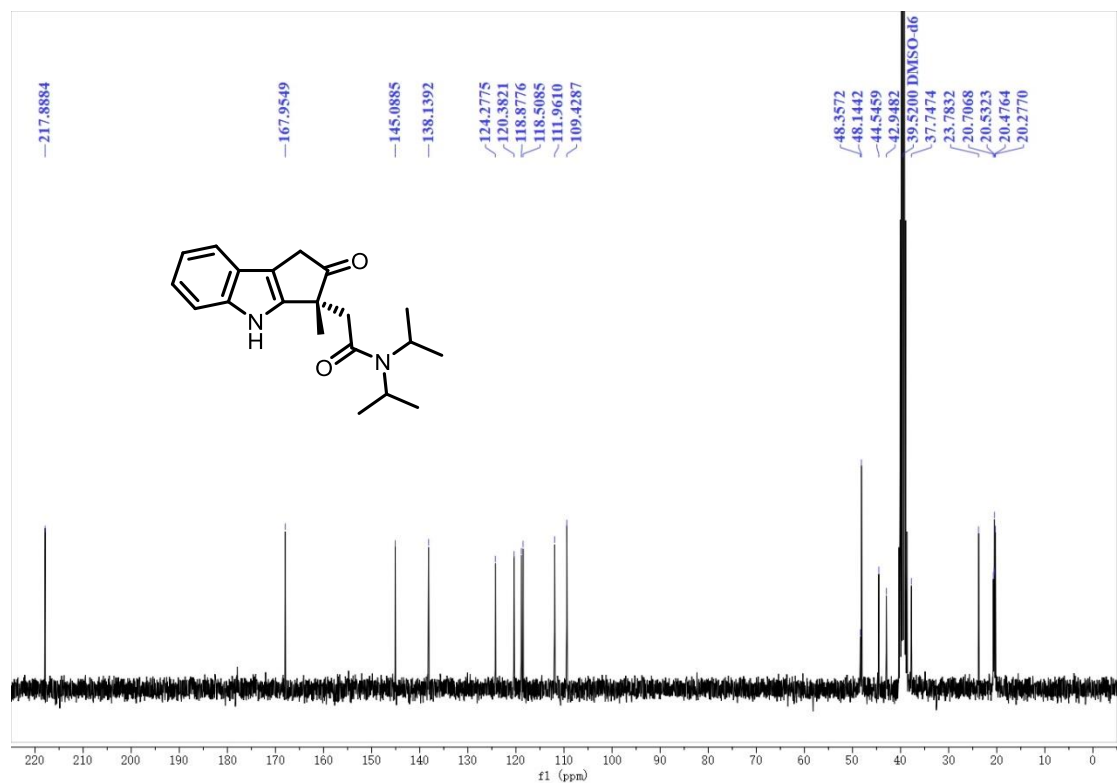
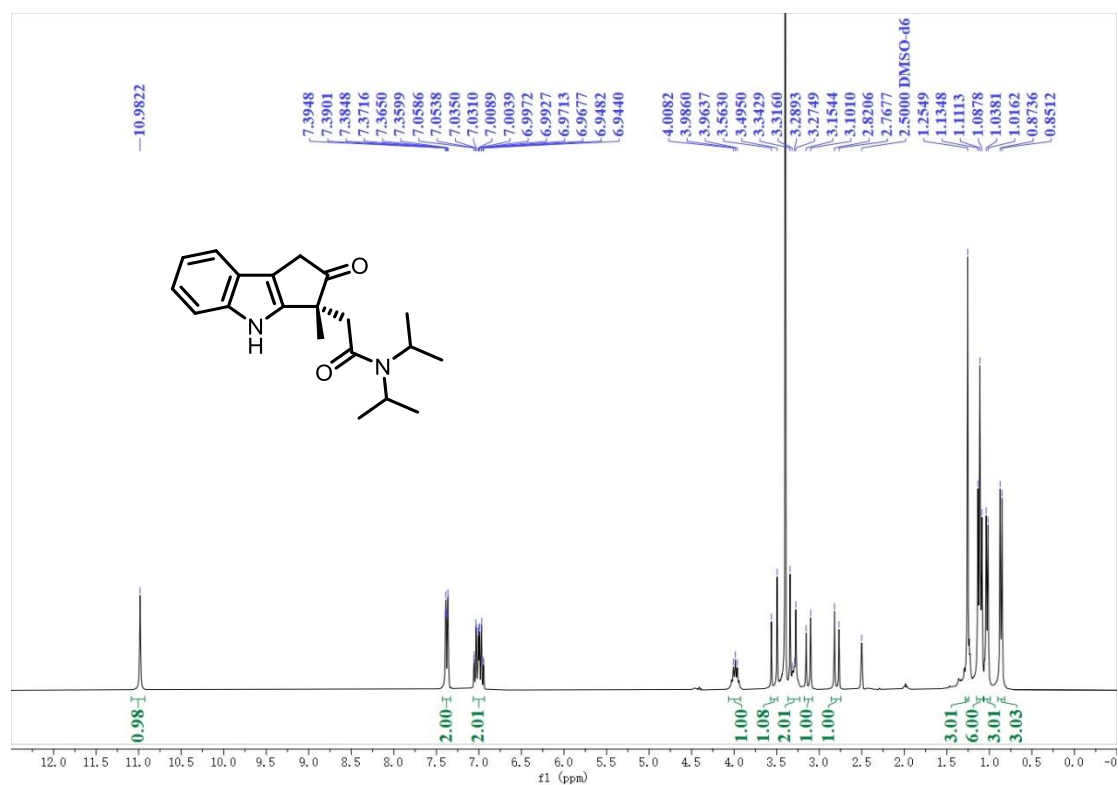
**3ra**  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-}d_6$ )



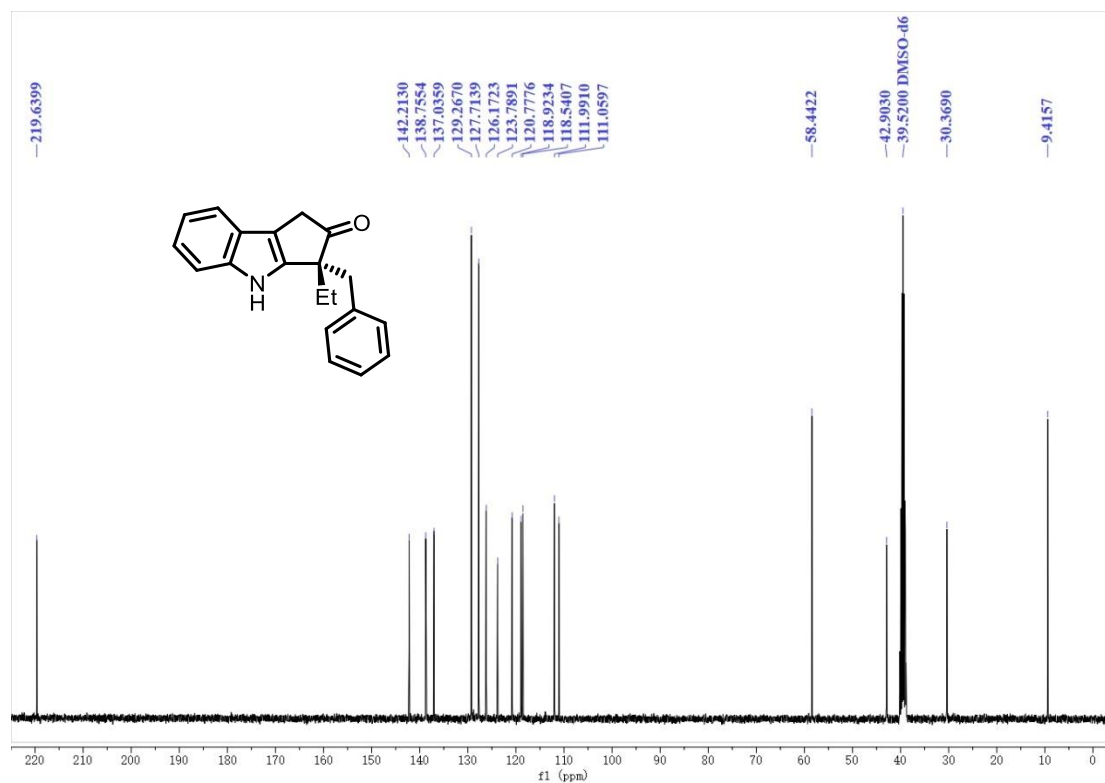
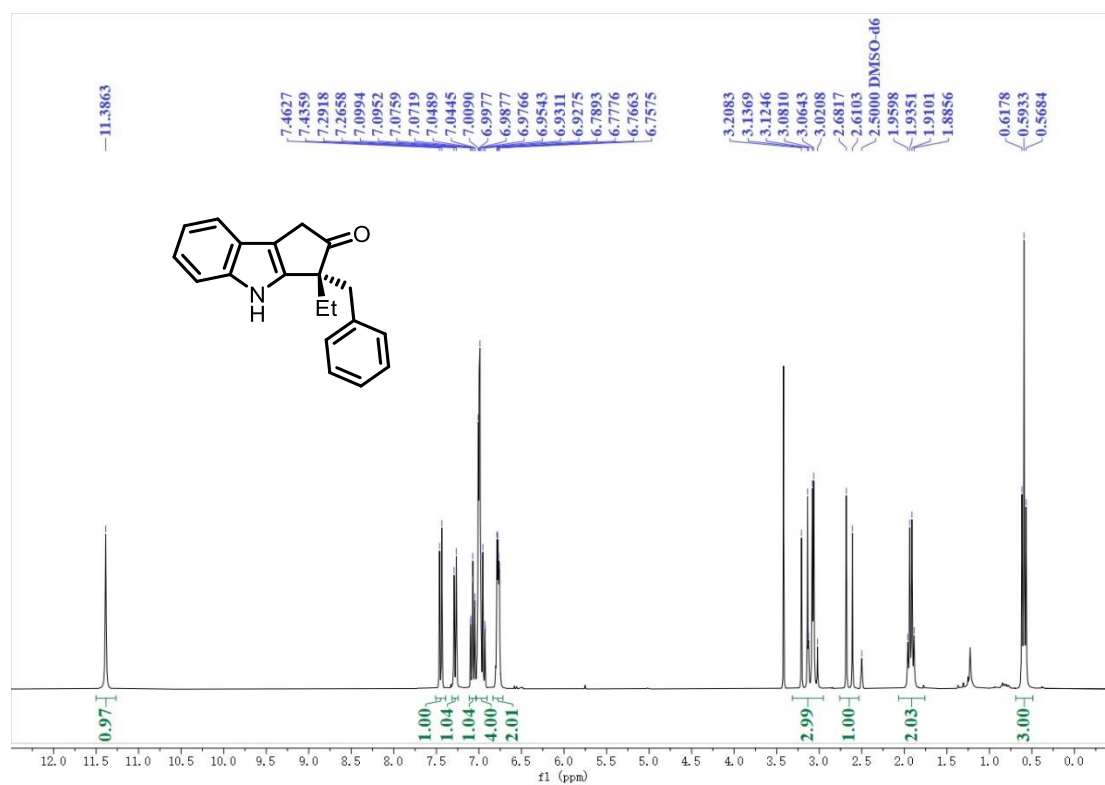
**3sa**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



**3ta**  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-}d_6$ )

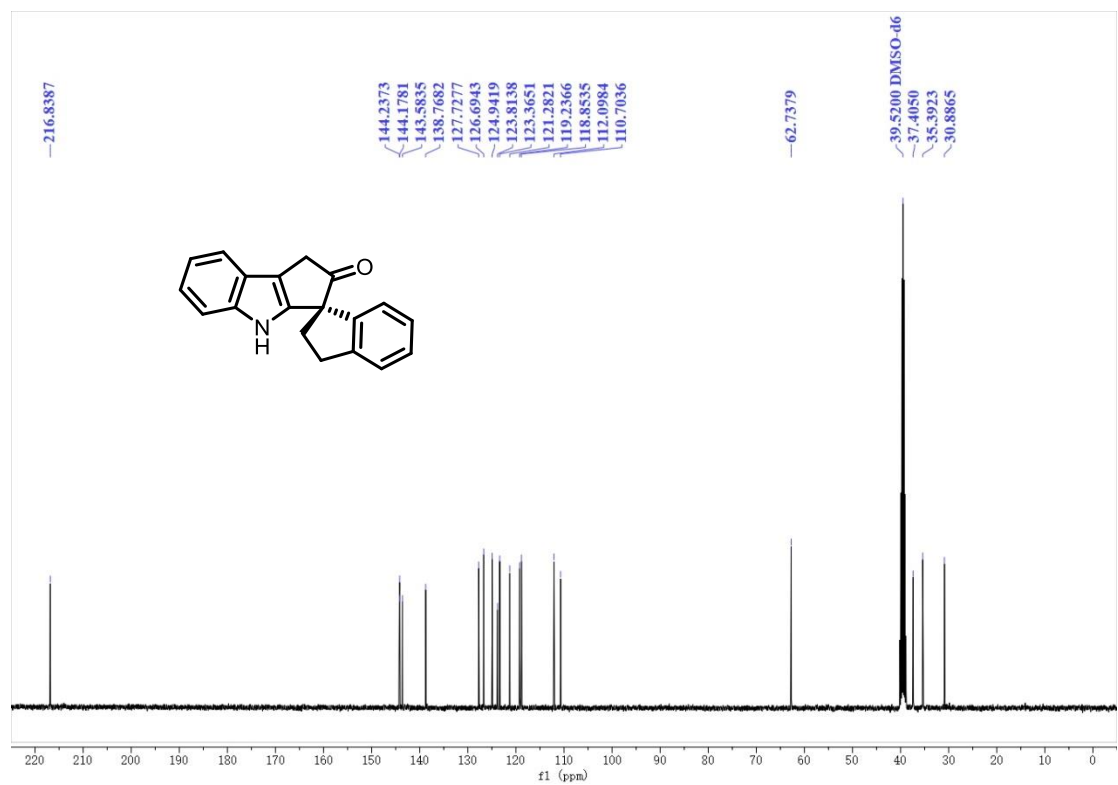
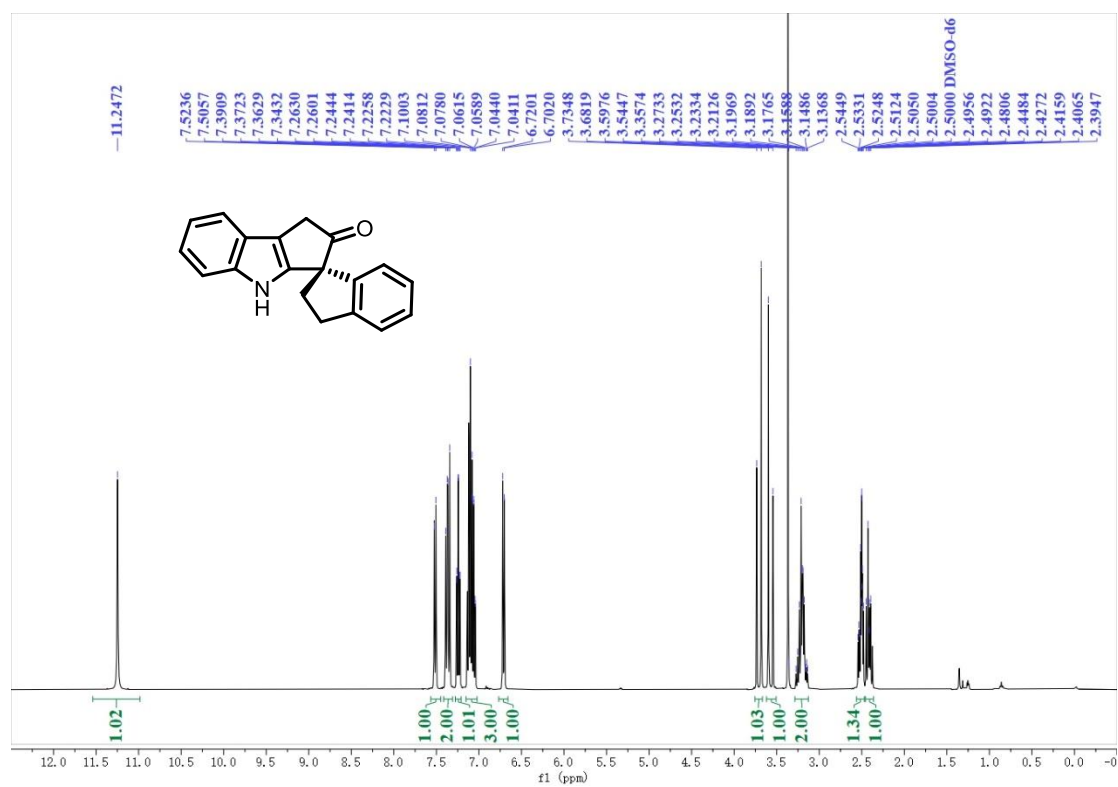


**3ua**  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )

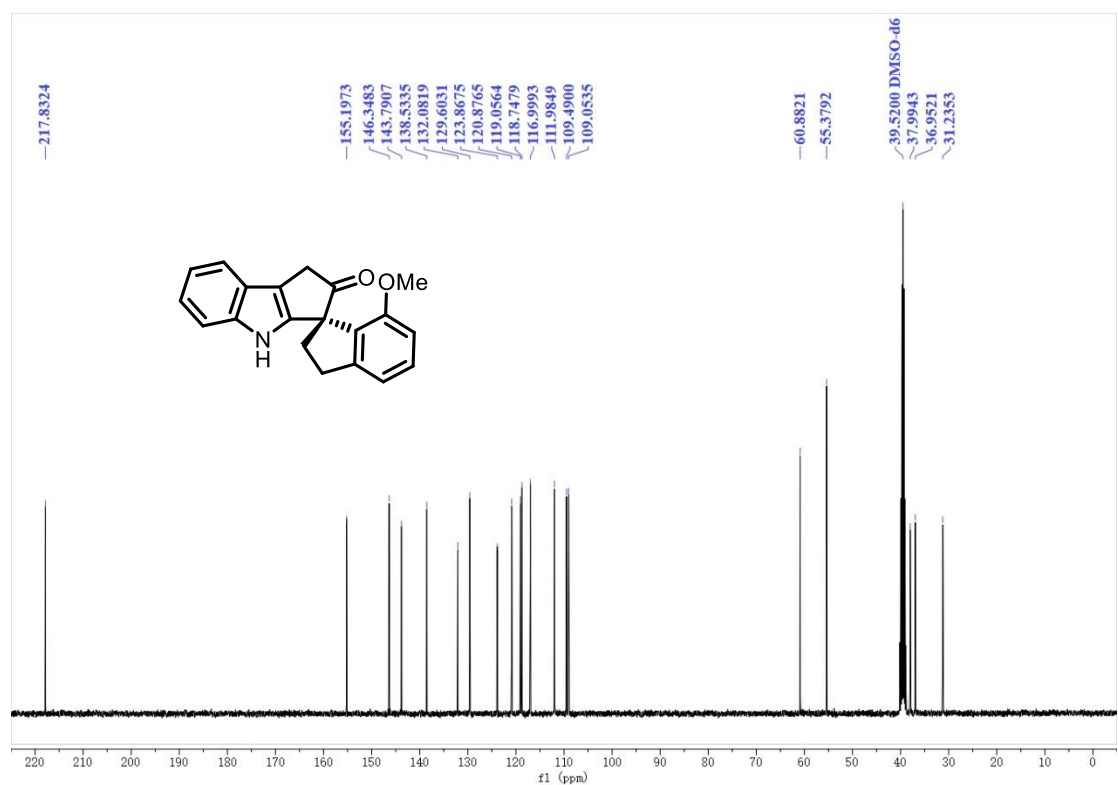
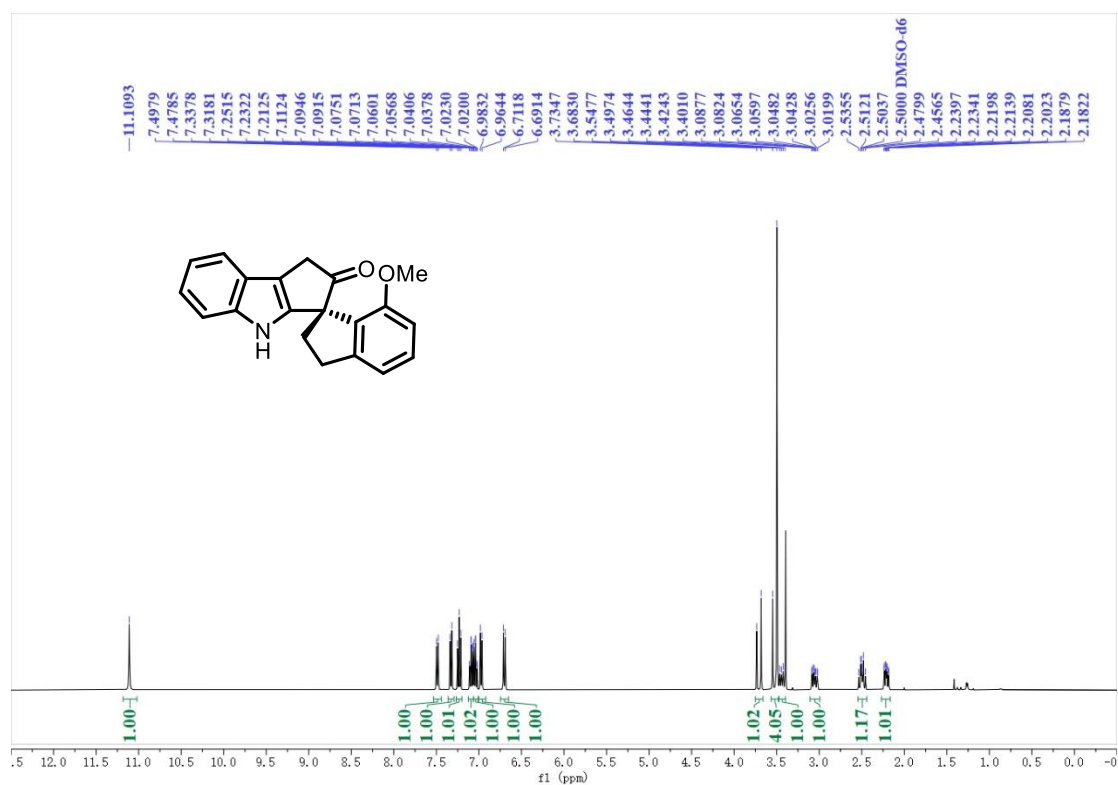




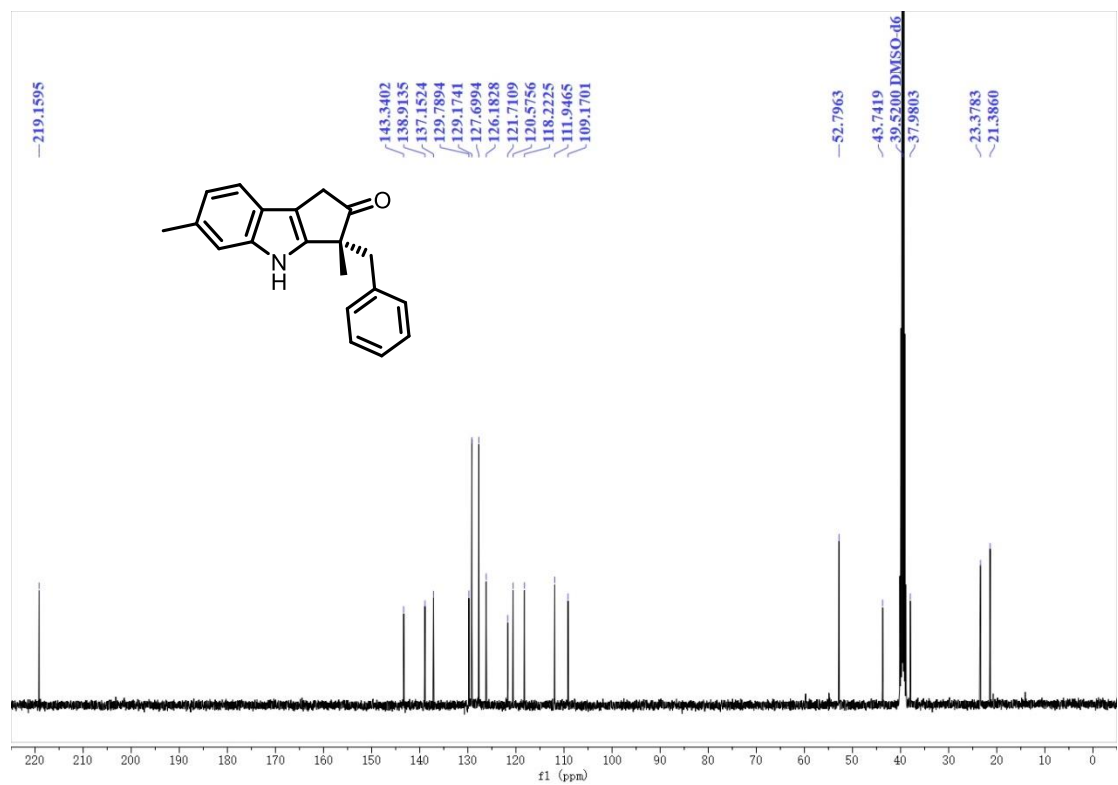
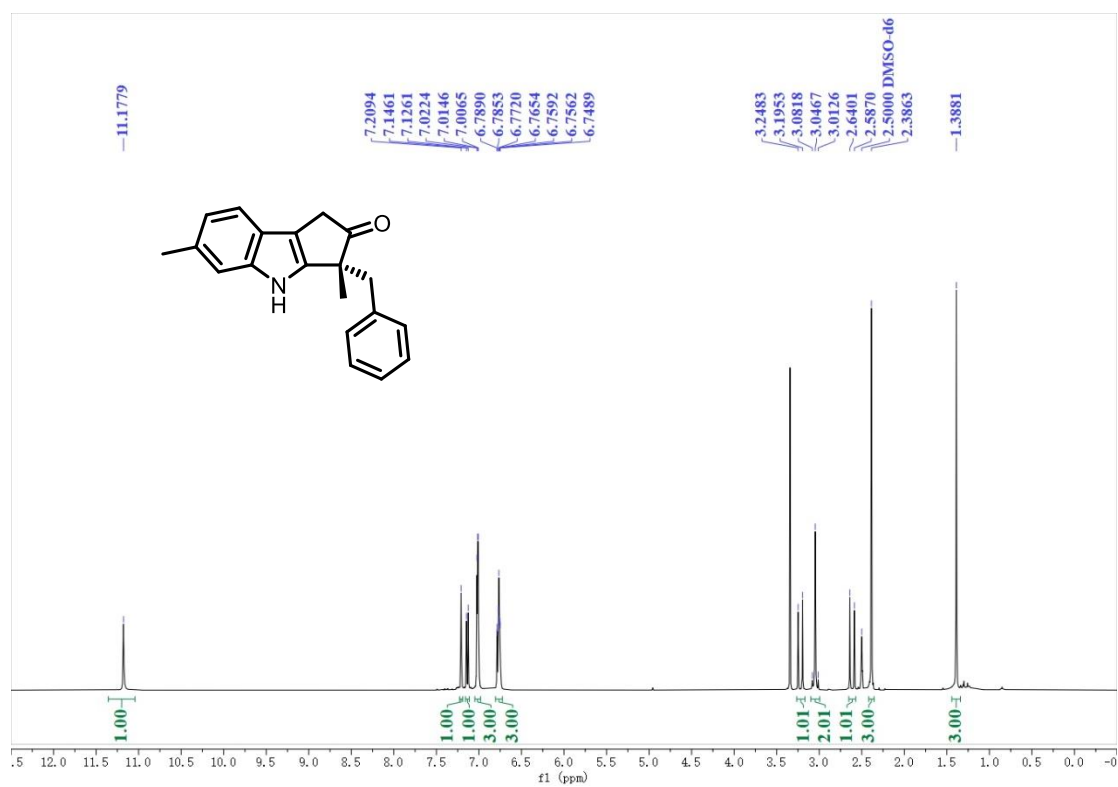
**3va**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



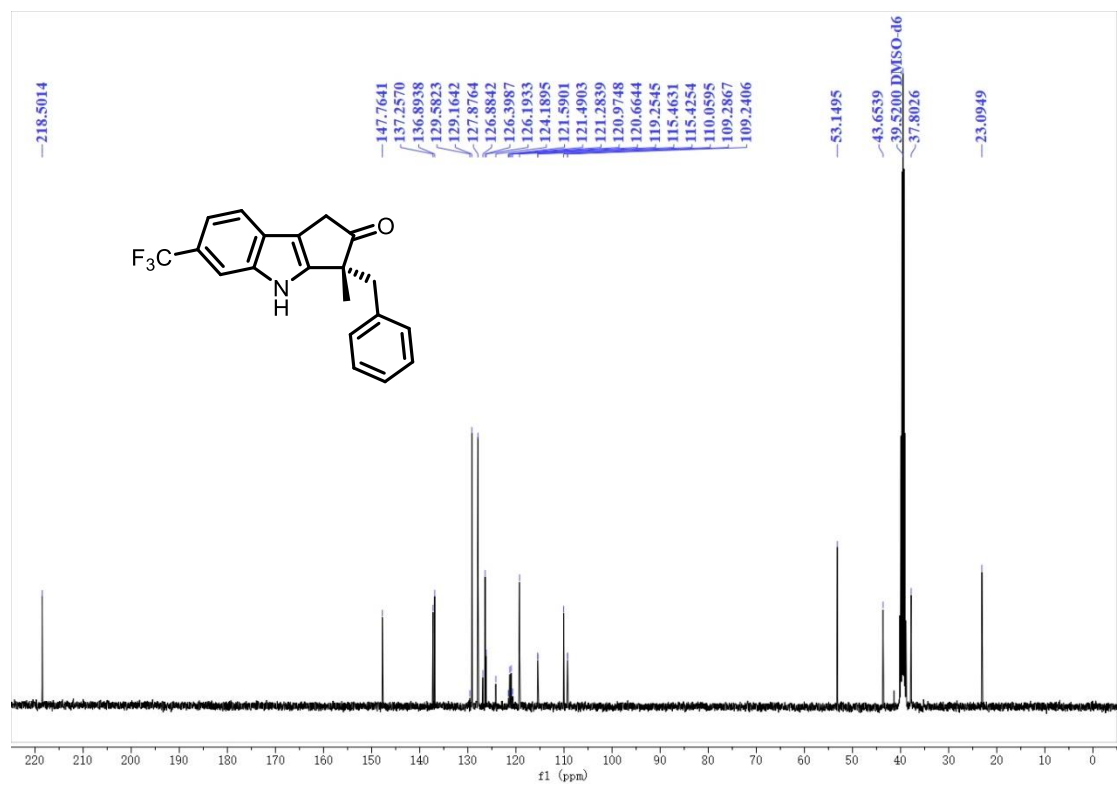
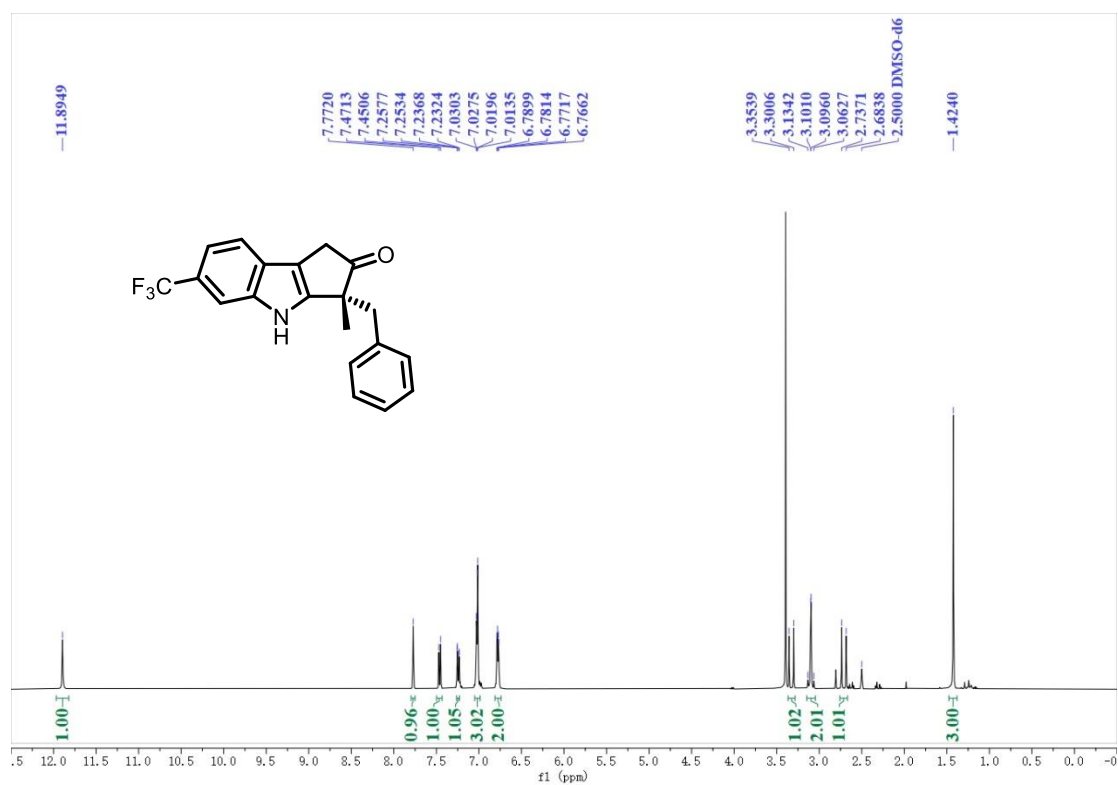
**3wa**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



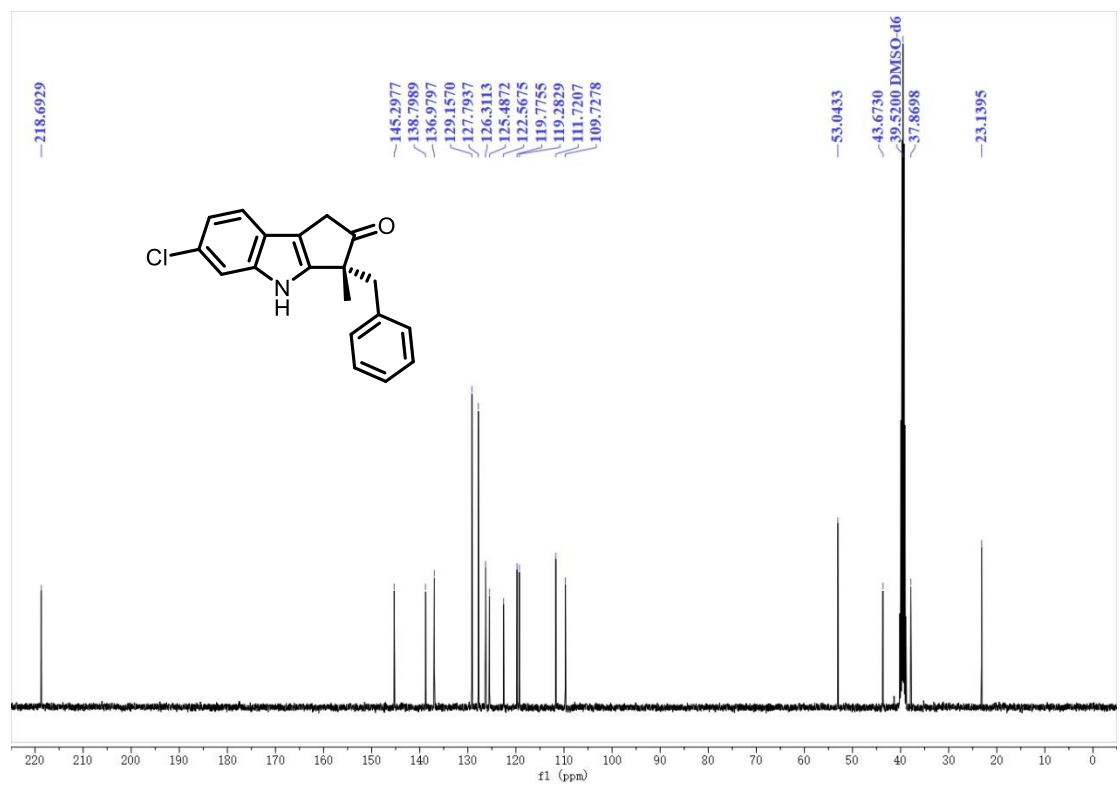
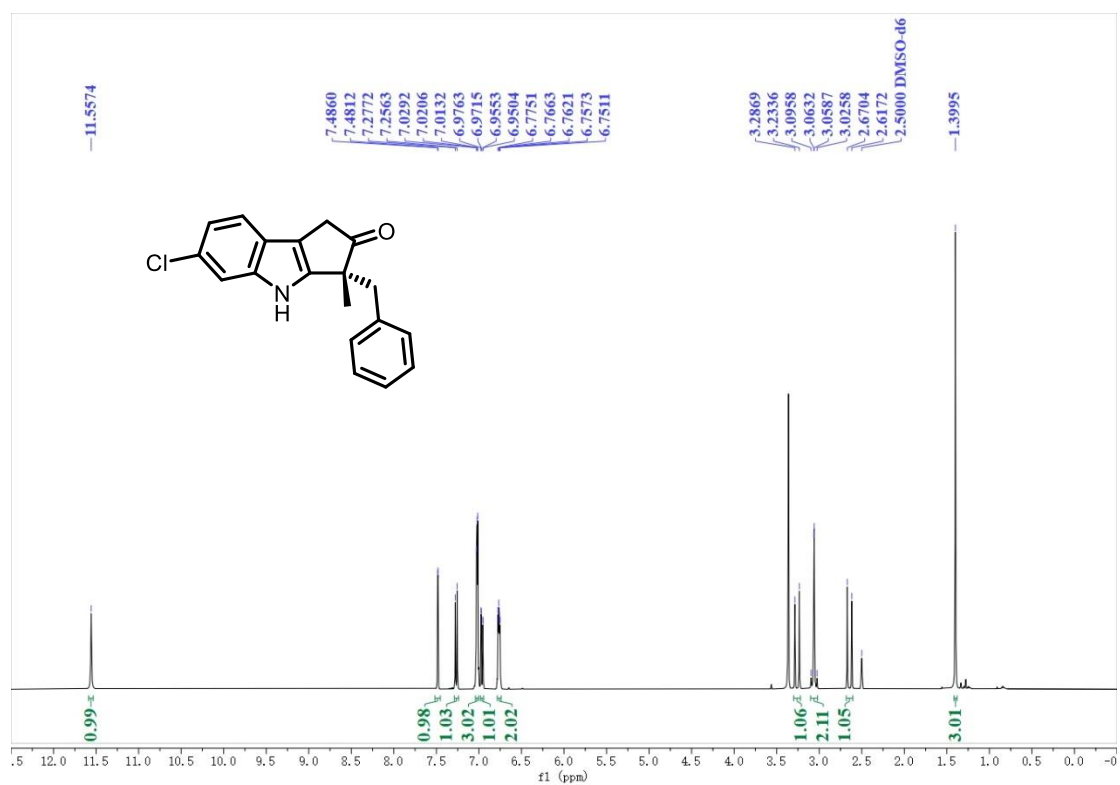
**3ab**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



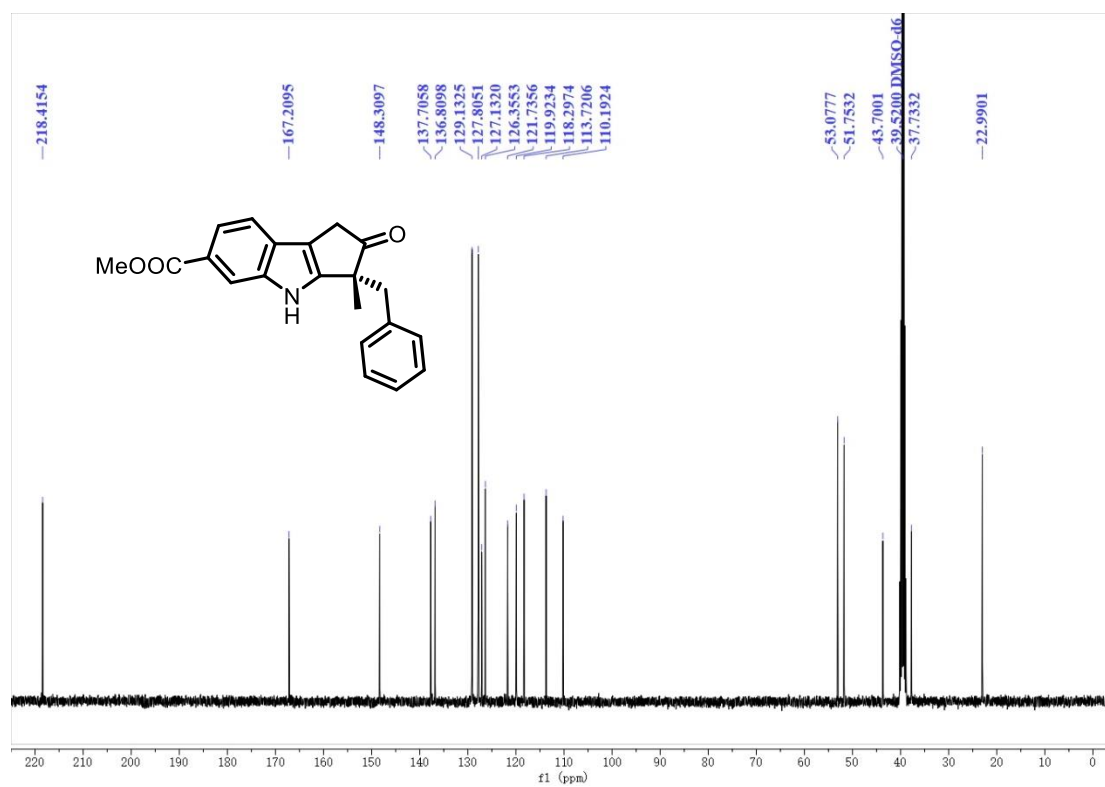
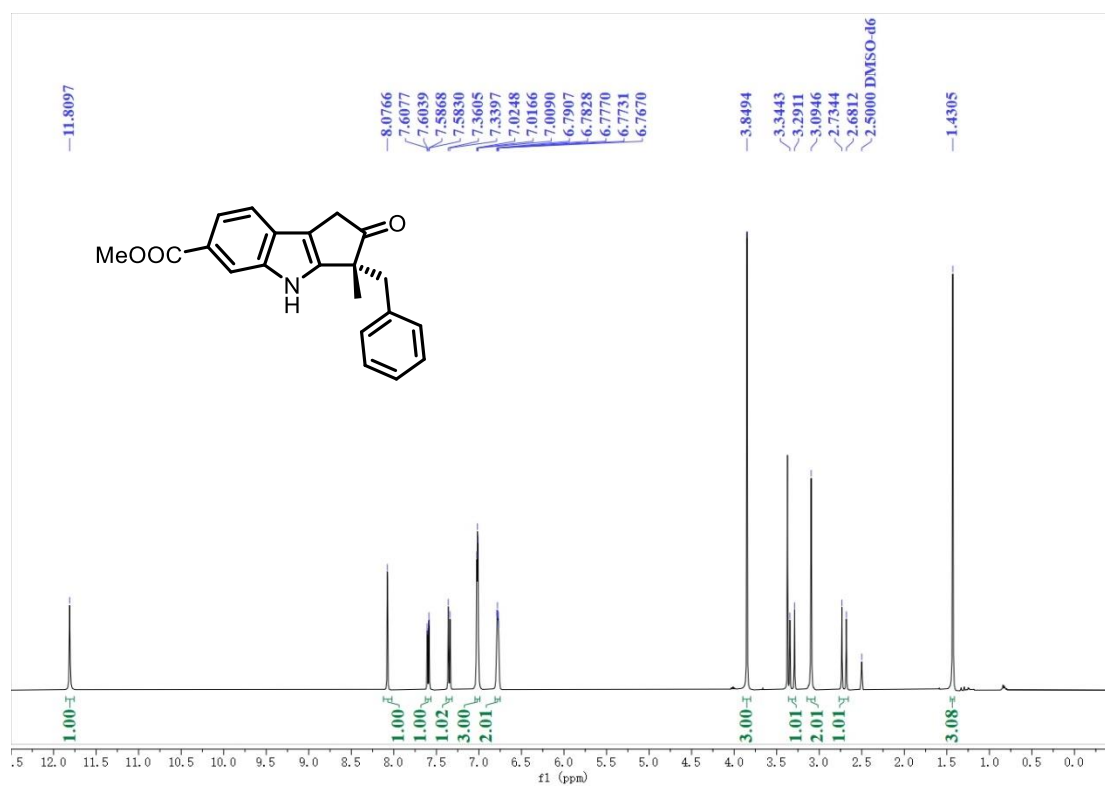
**3ac**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



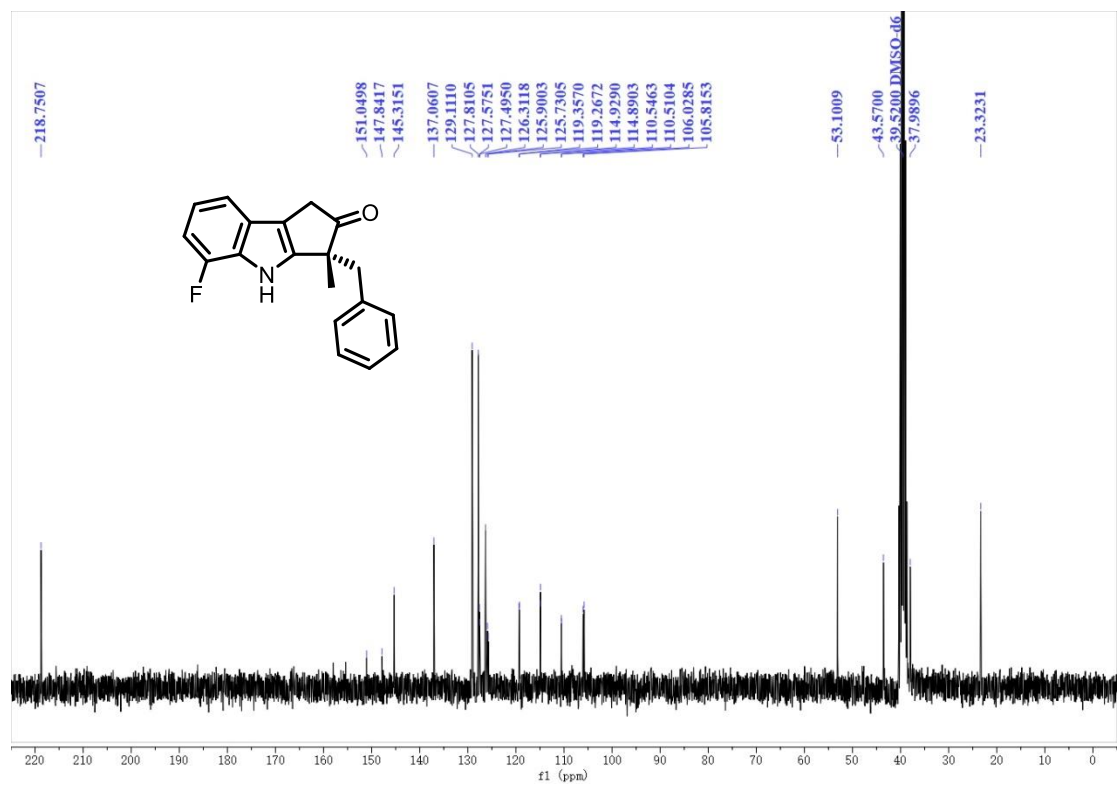
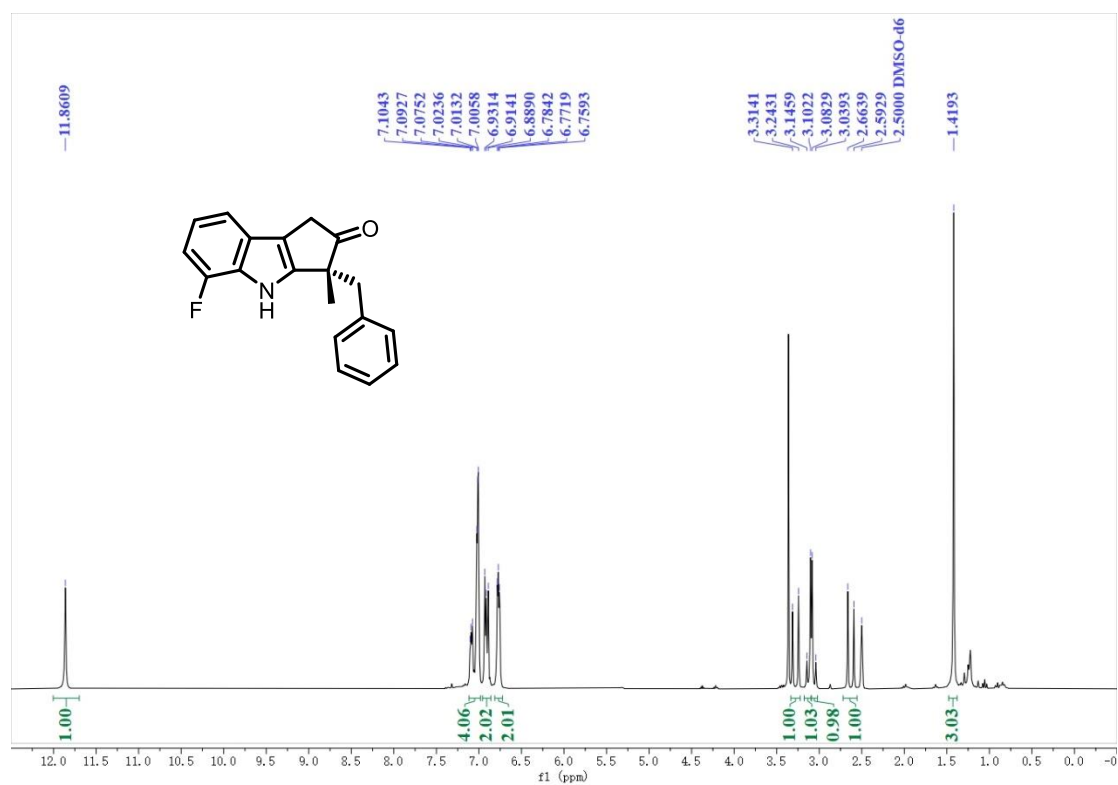
**3ad**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



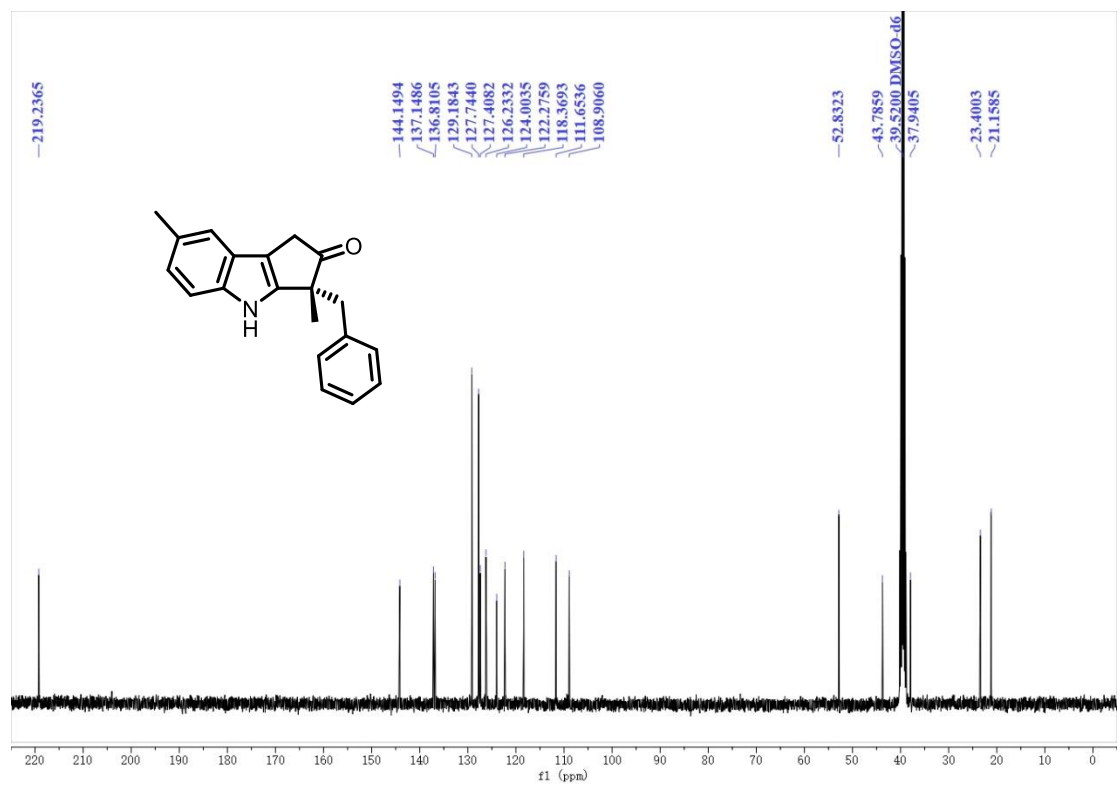
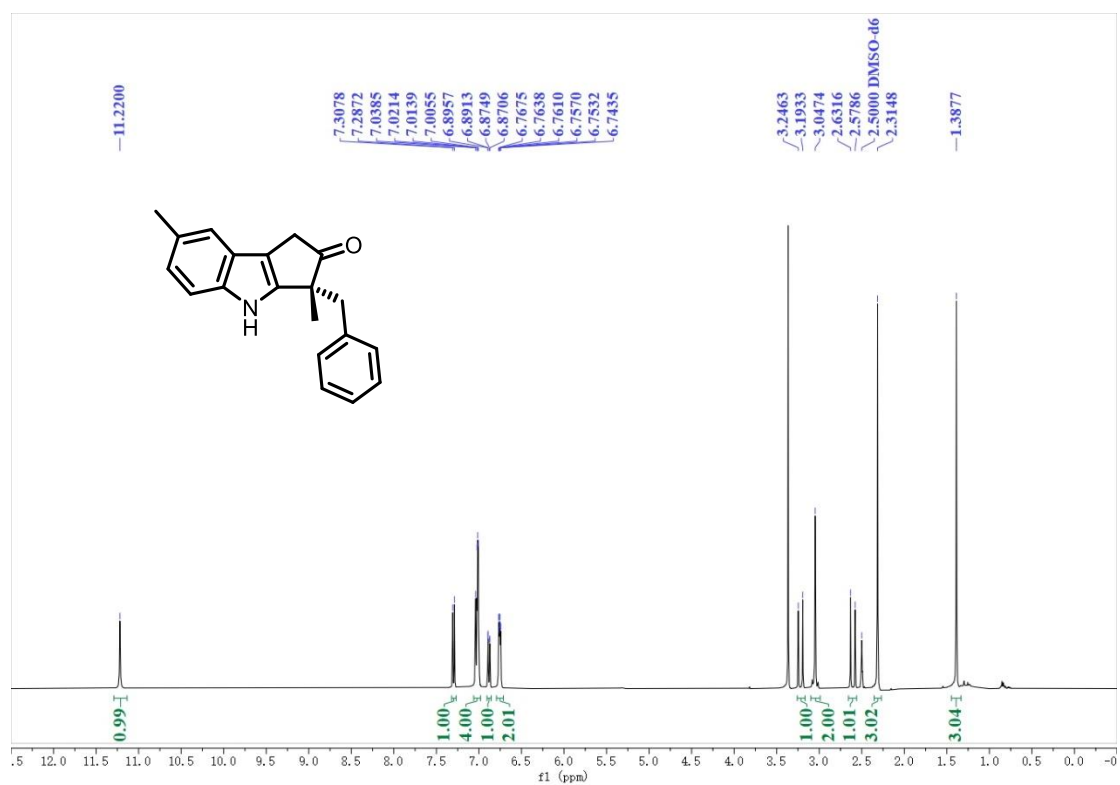
**3ae**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



**3af**  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-}d_6$ )

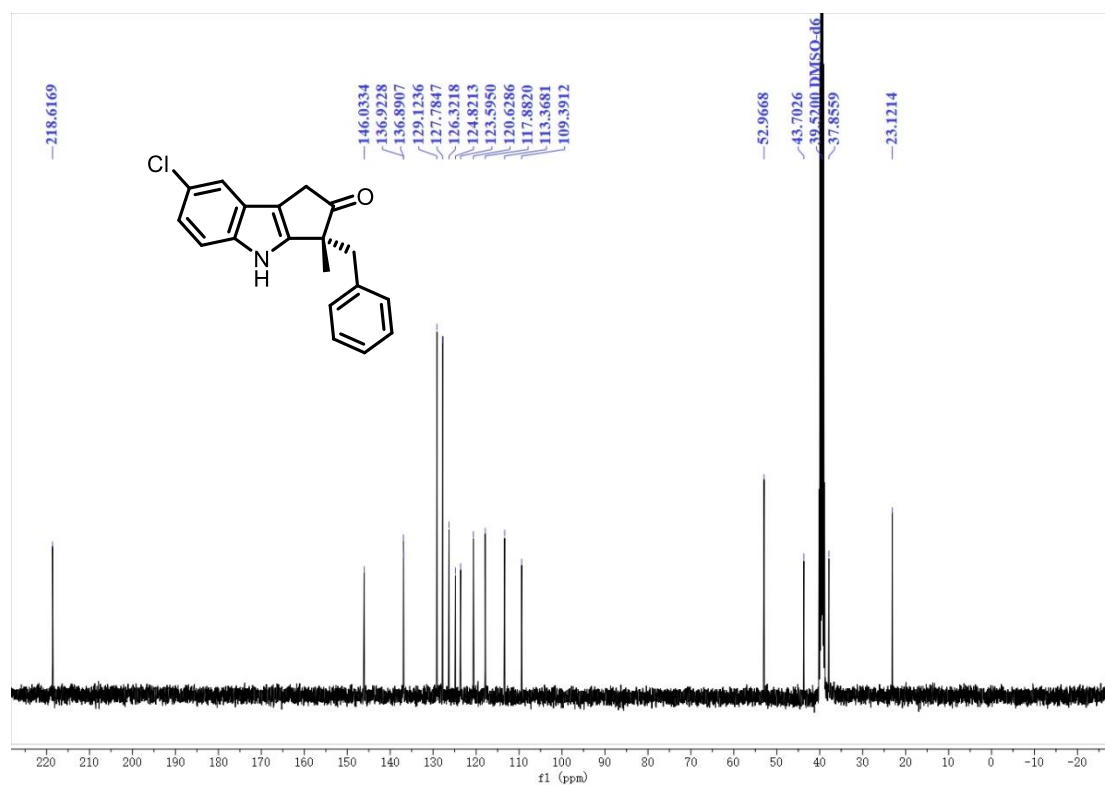
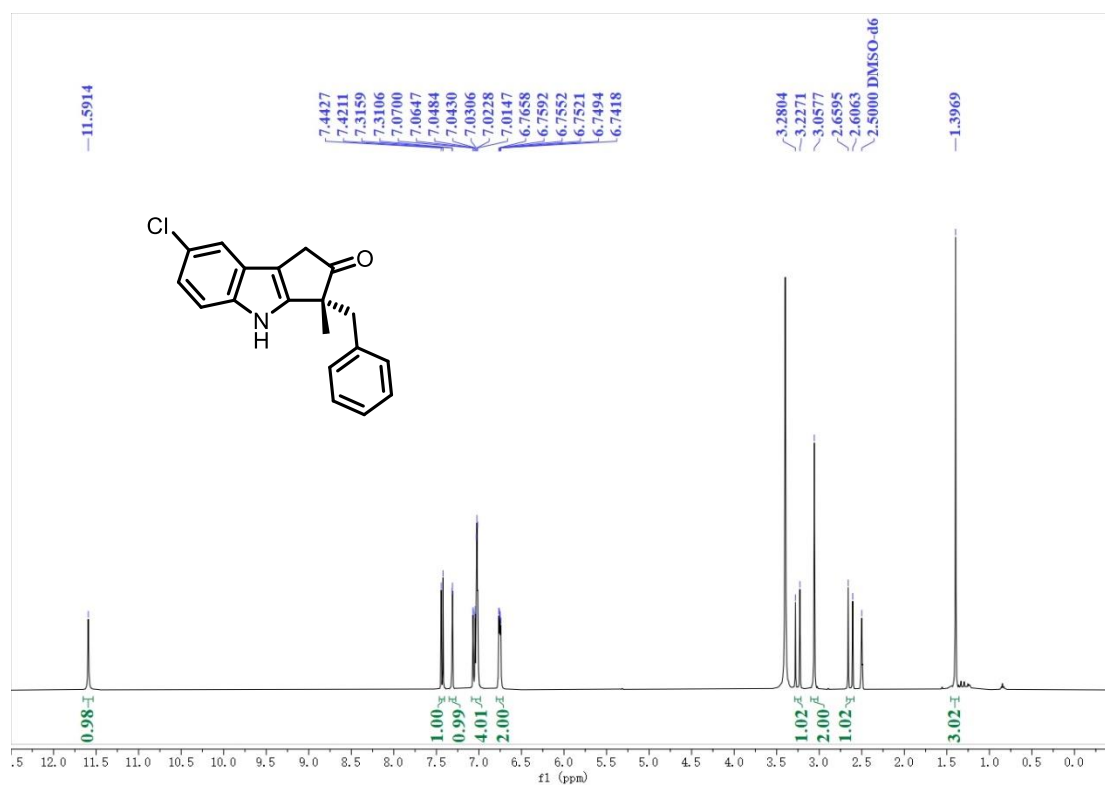


**3ag**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )

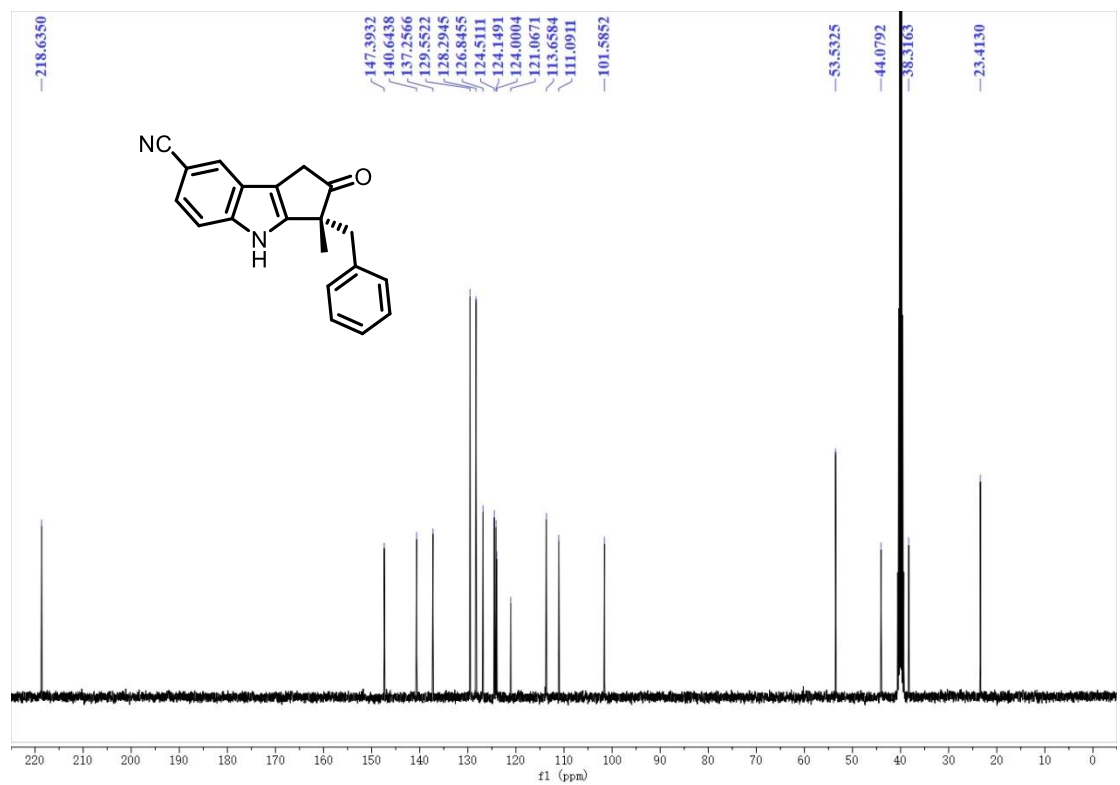
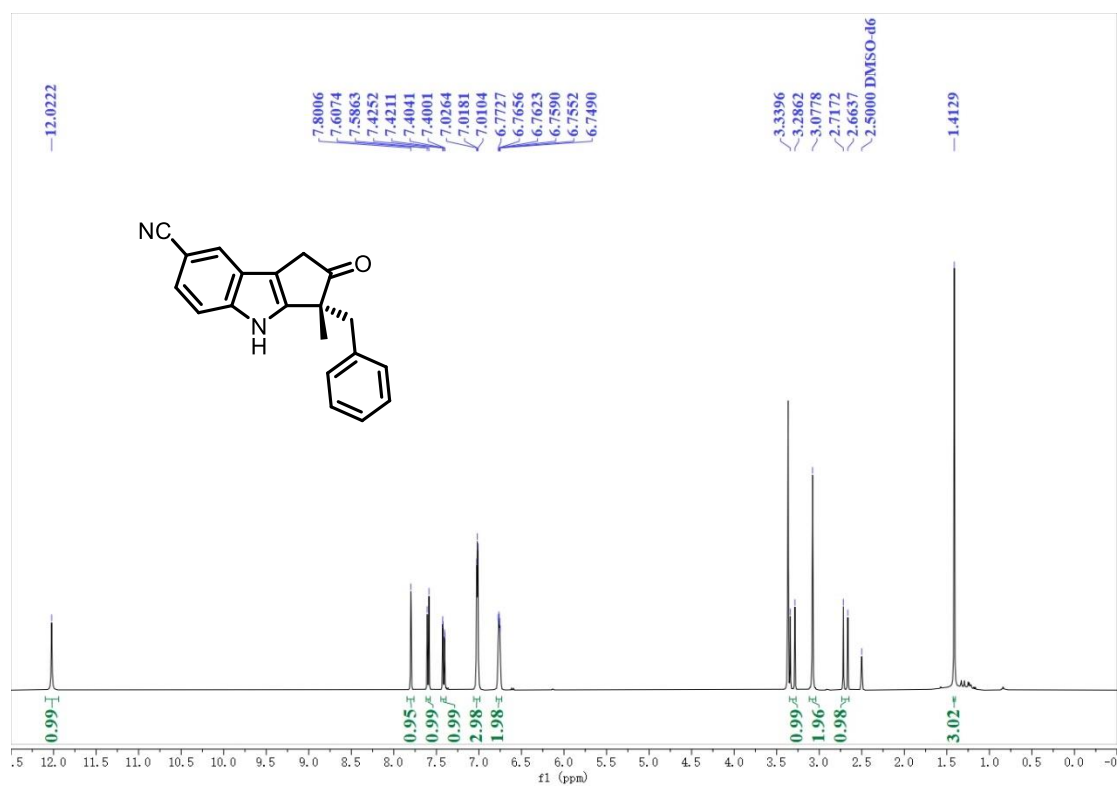




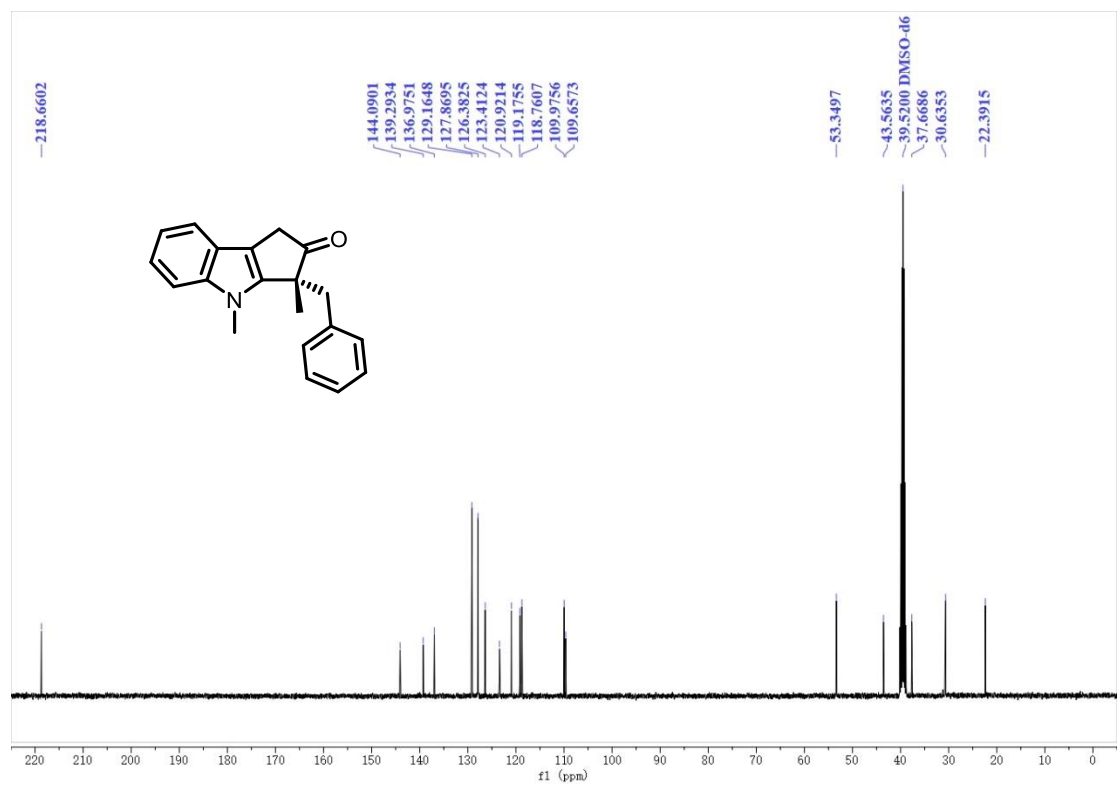
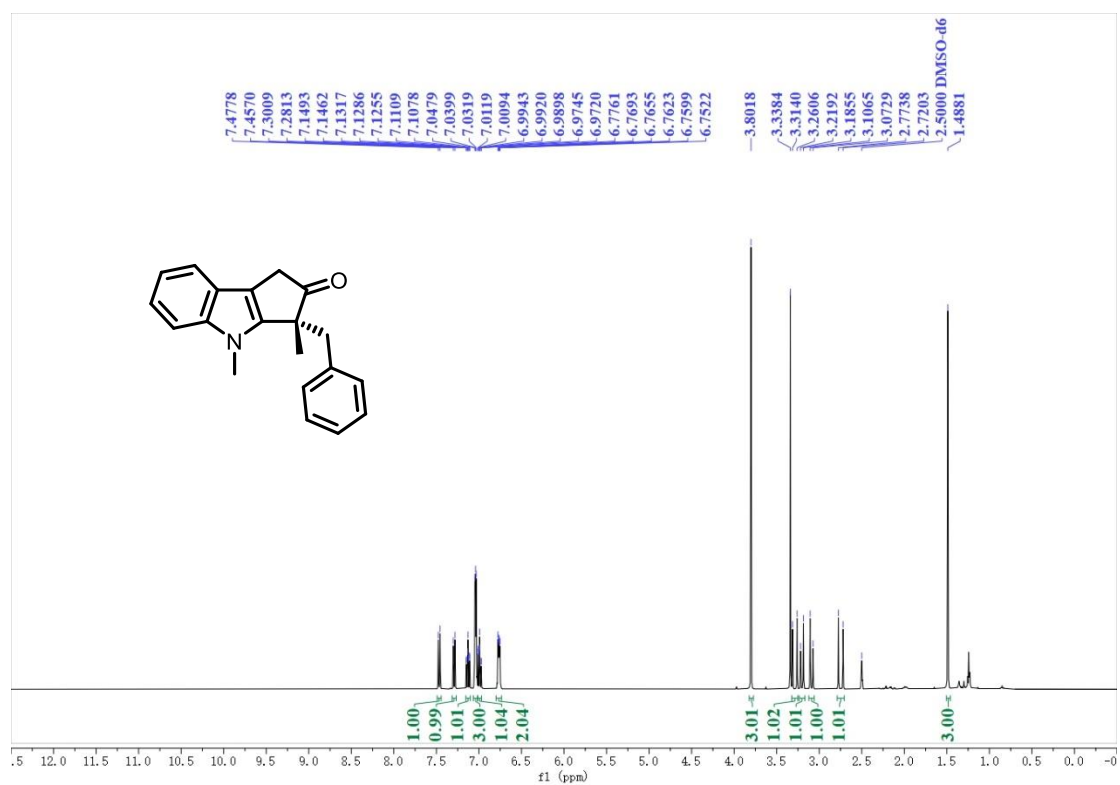
**3ah**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



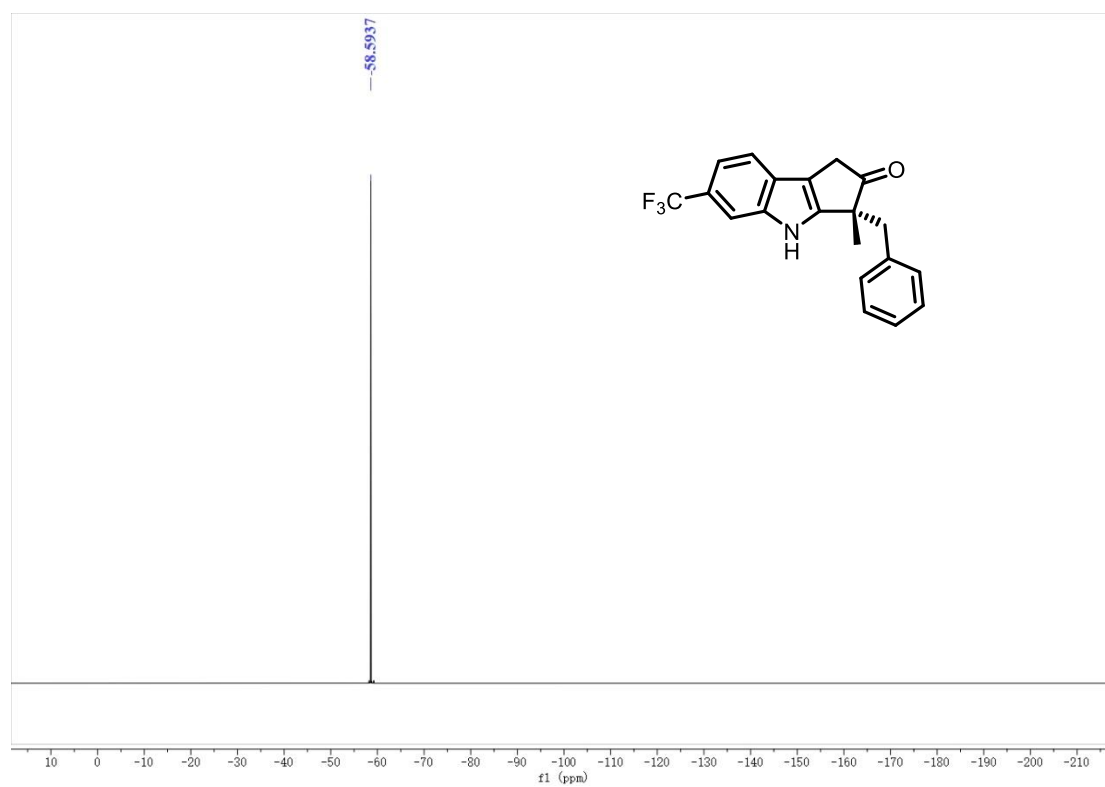
**3ai**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



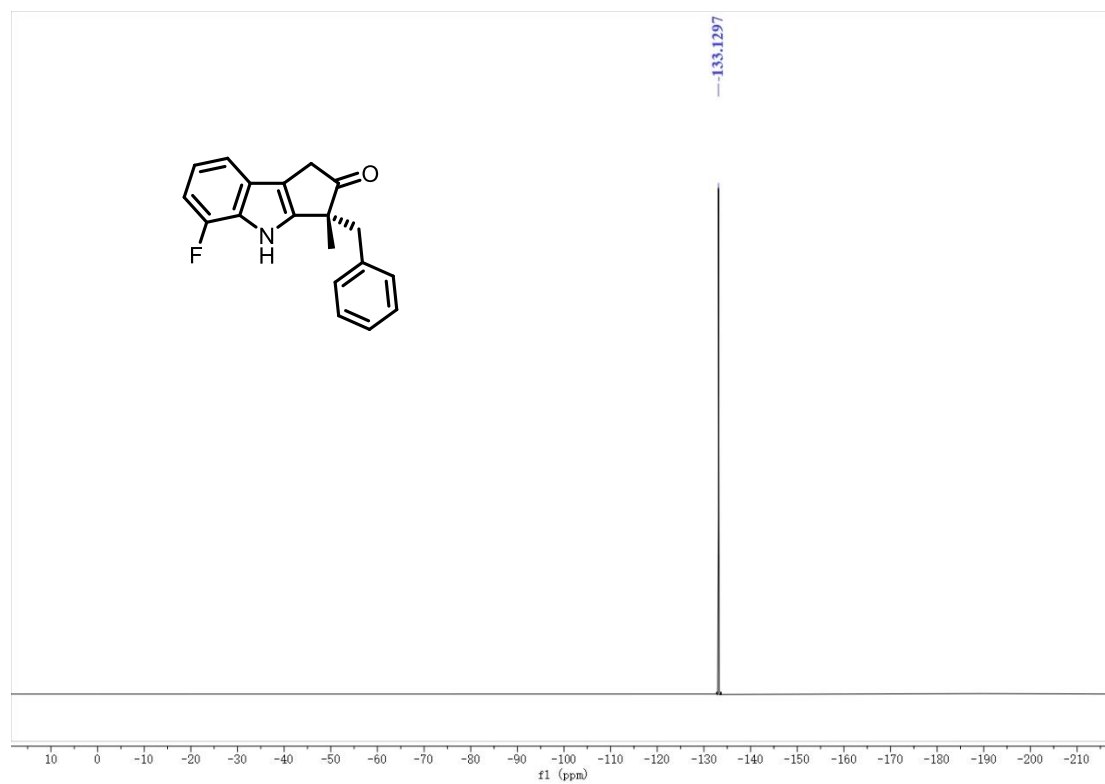
**3aa'**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



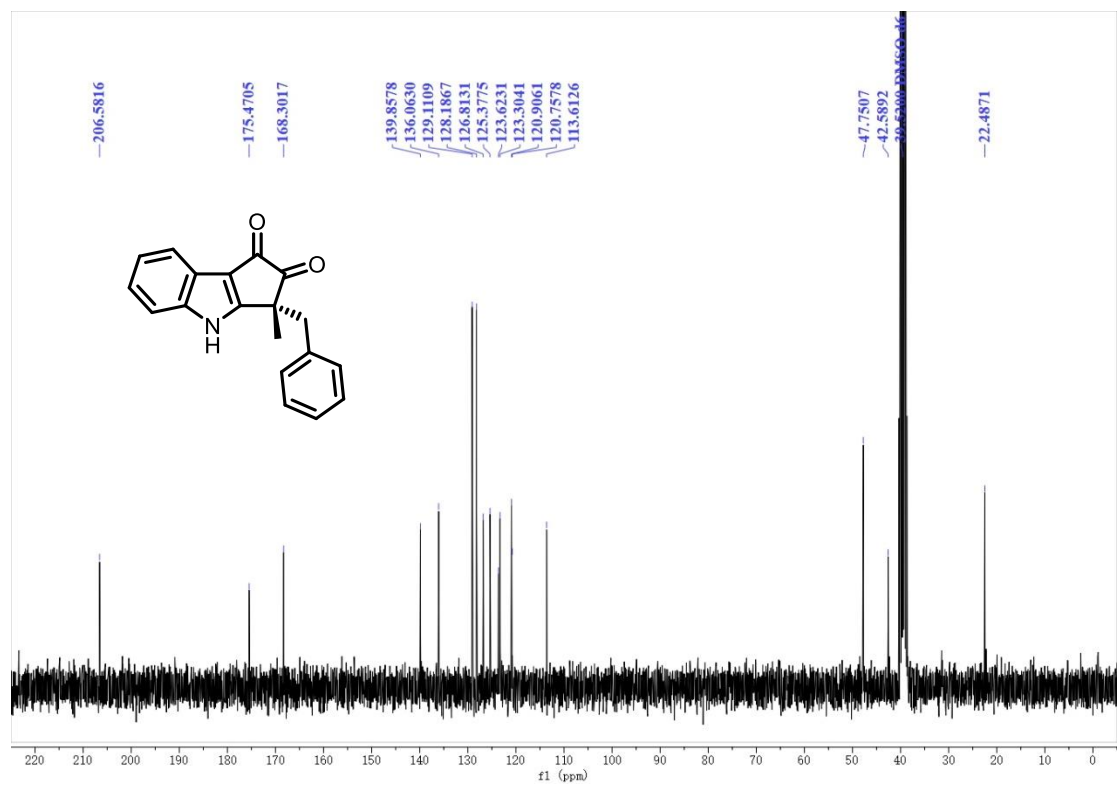
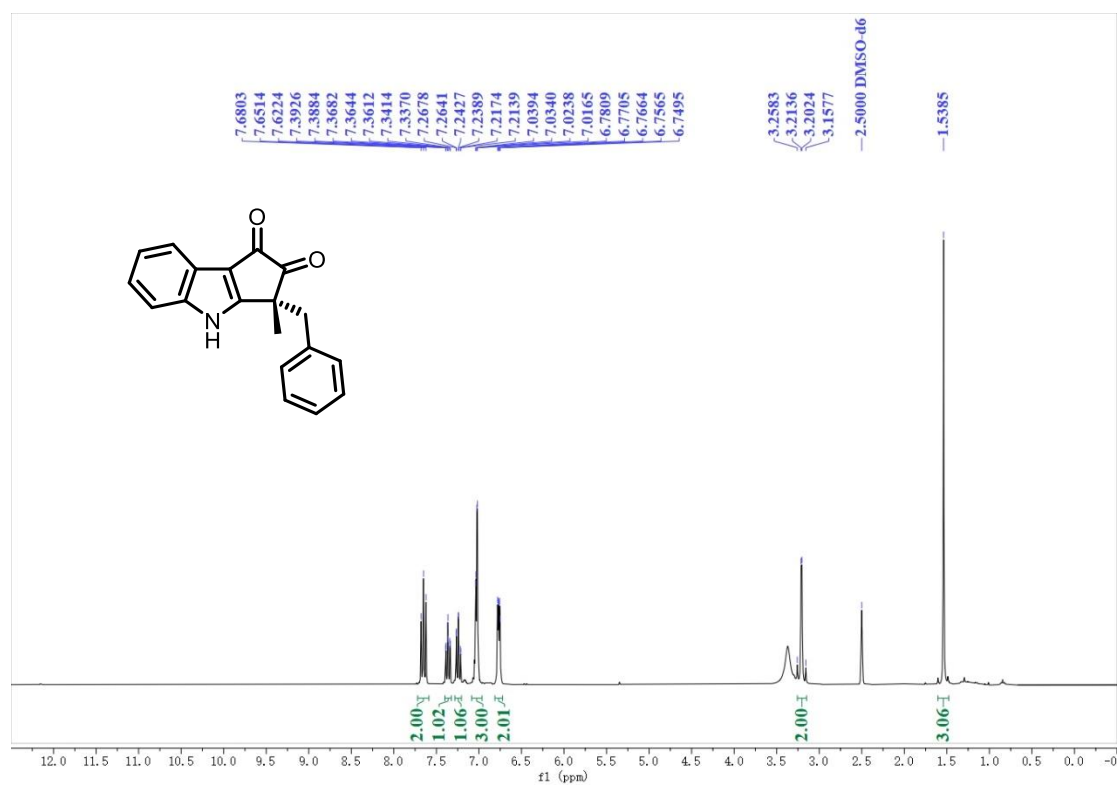
**3ac**  $^{19}\text{F}$  NMR (282 MHz,  $\text{DMSO-}d_6$ )



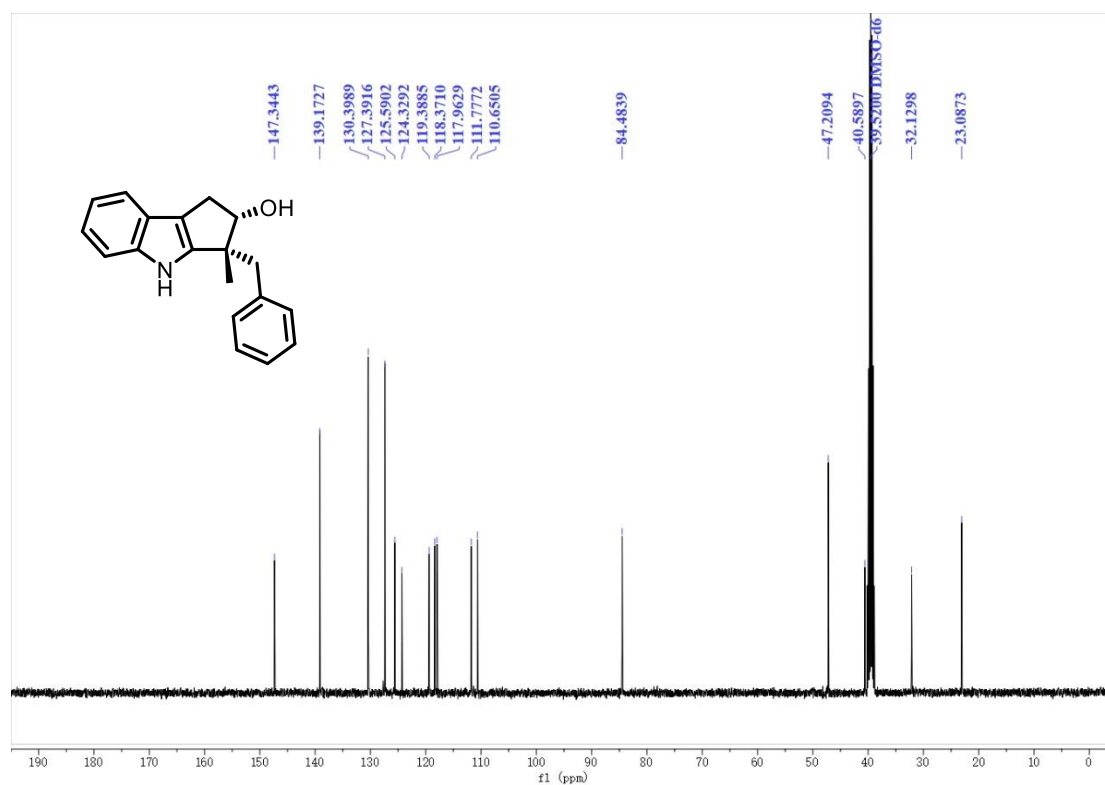
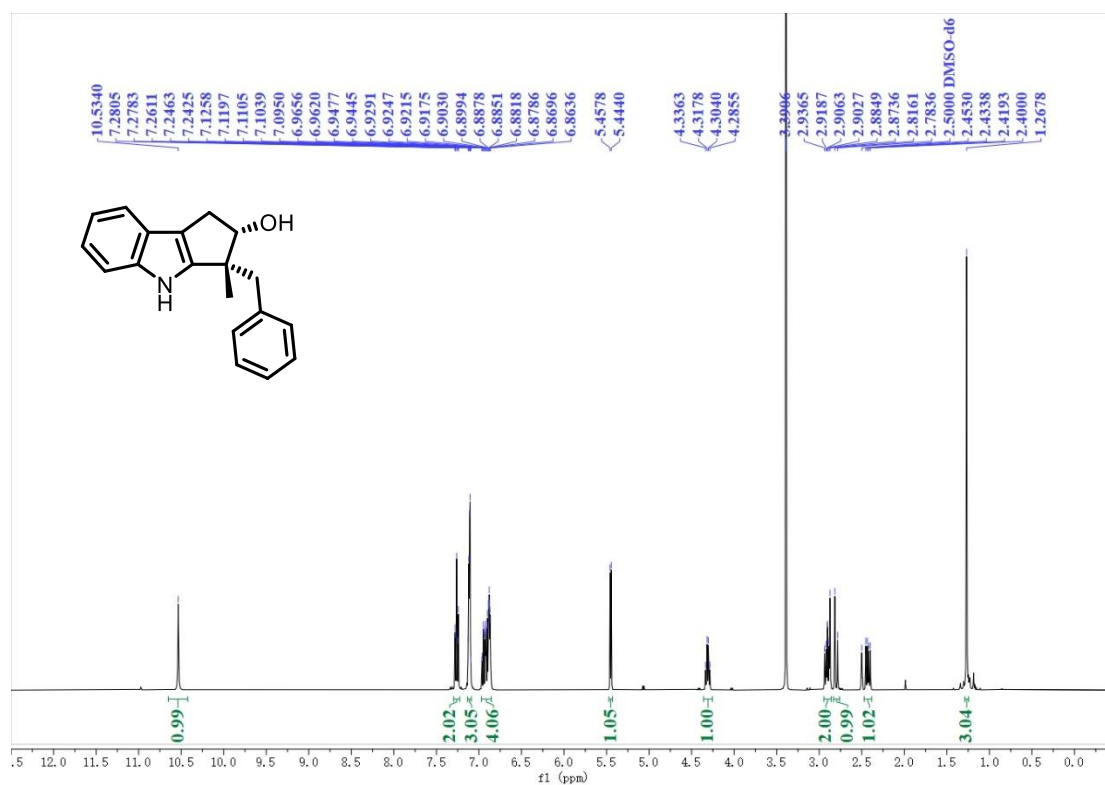
**3af**  $^{19}\text{F}$  NMR (282 MHz,  $\text{DMSO-}d_6$ )



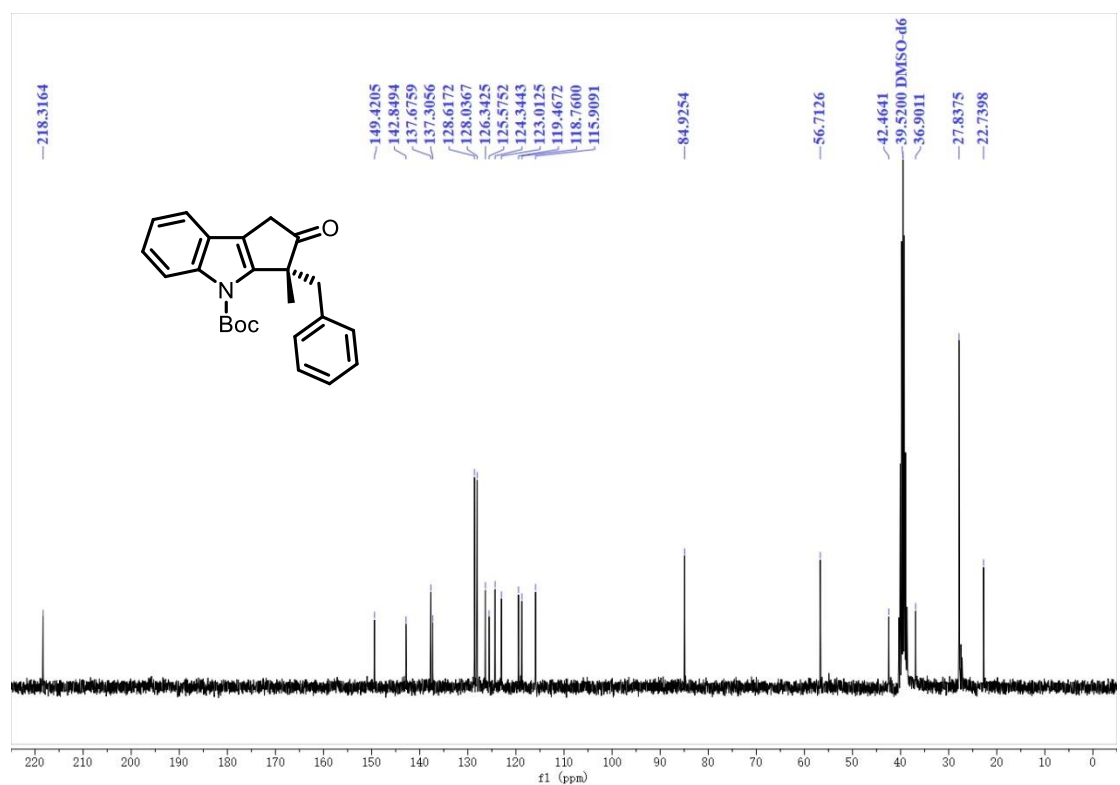
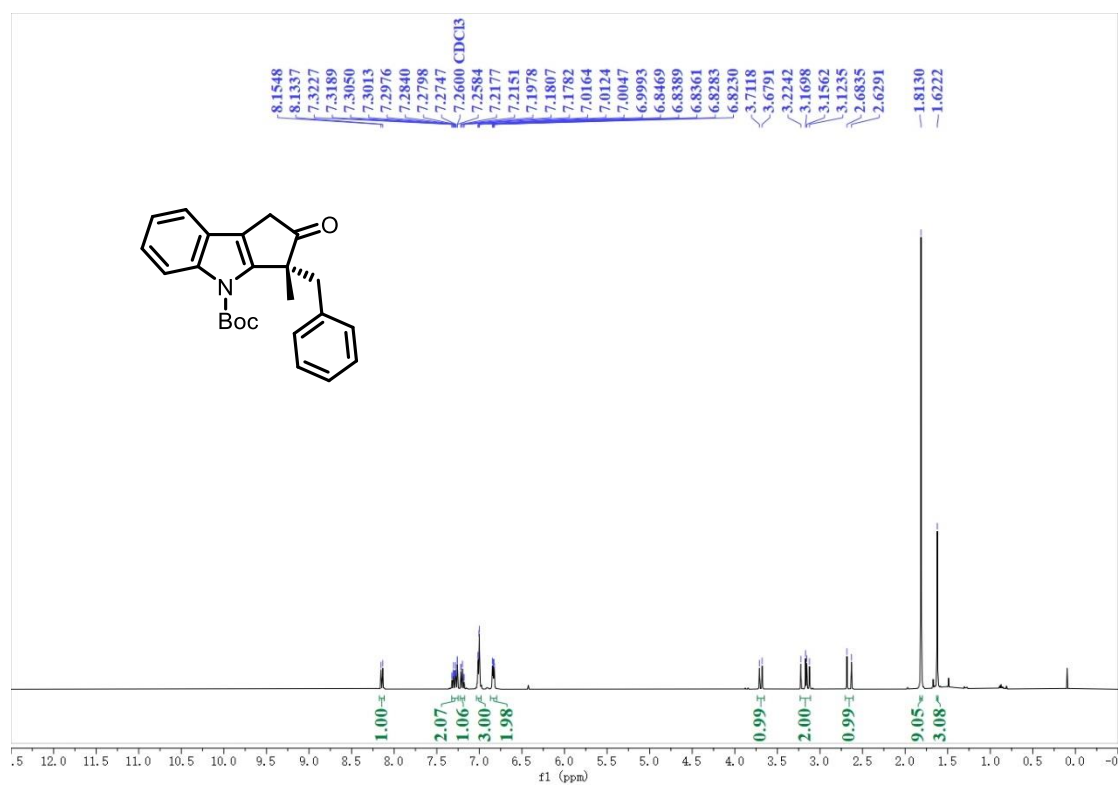
4  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-}d_6$ )



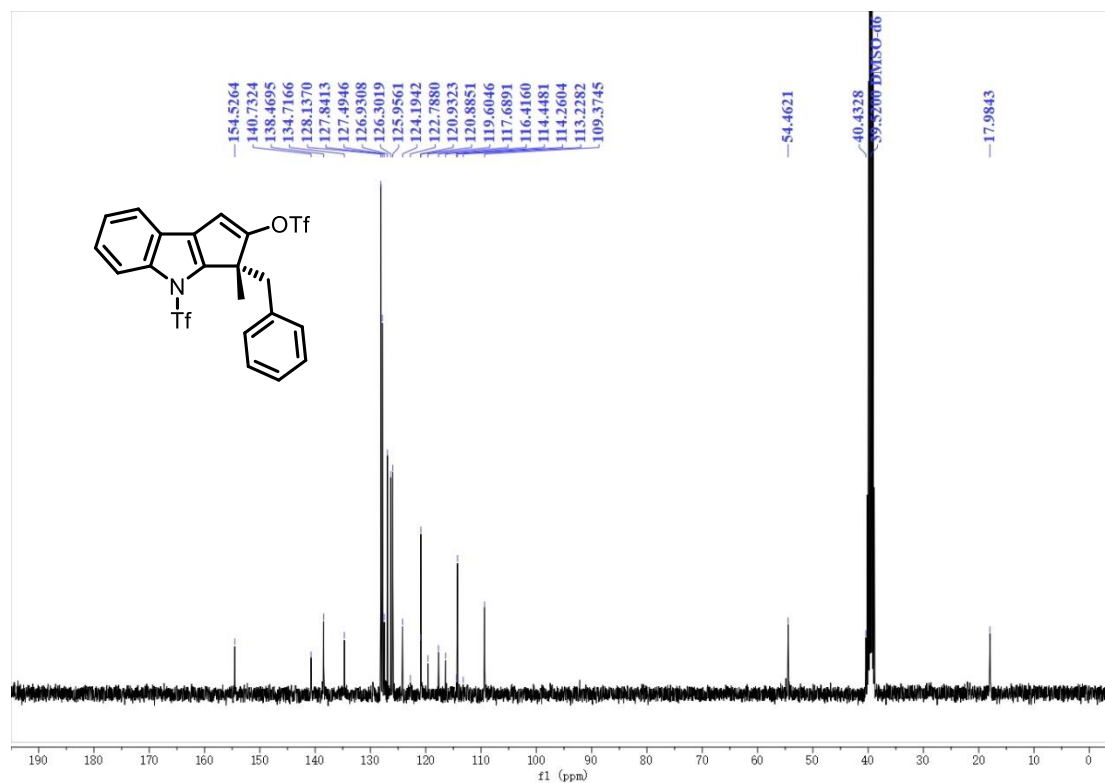
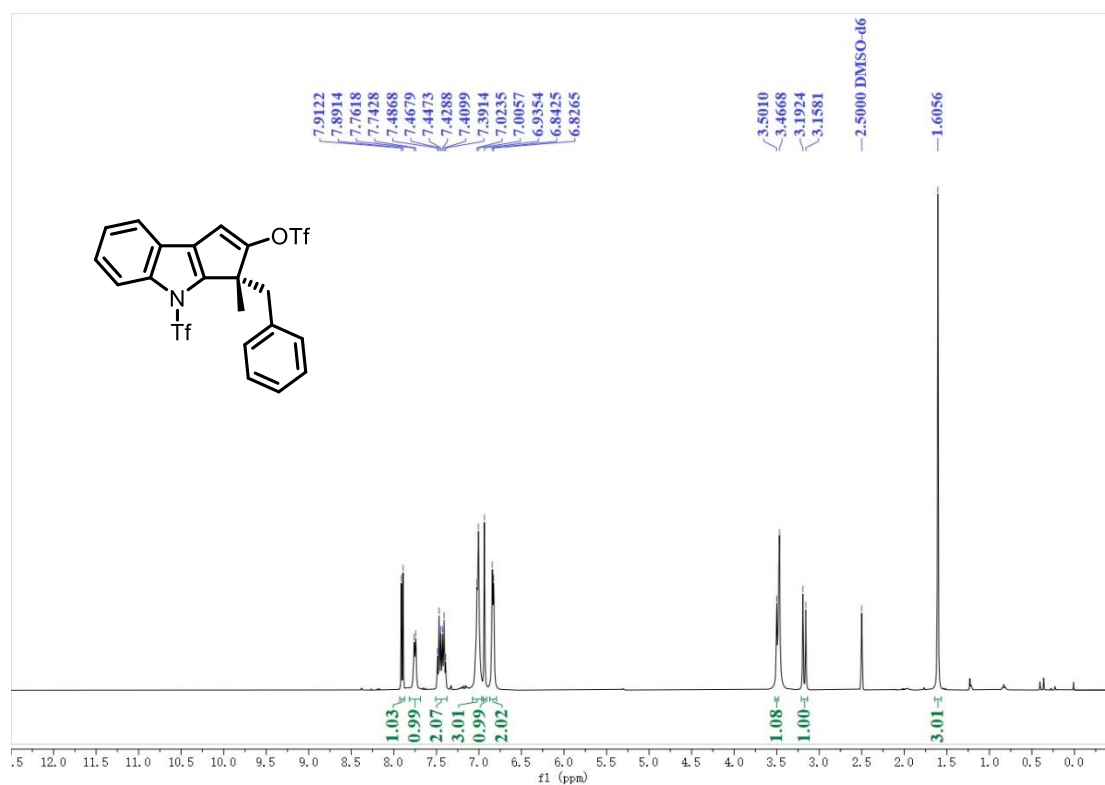
$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



$^1\text{H}$  NMR (400 MHz,  $\text{CHCl}_3\text{-}d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-}d_6$ )

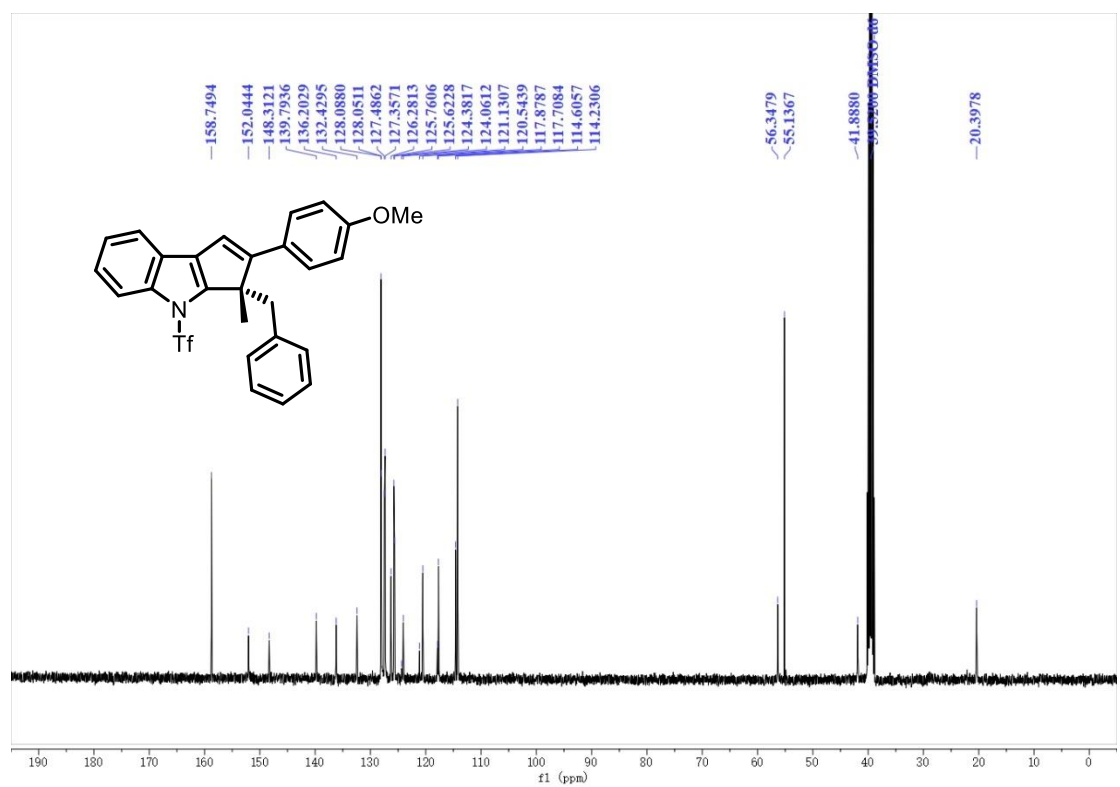
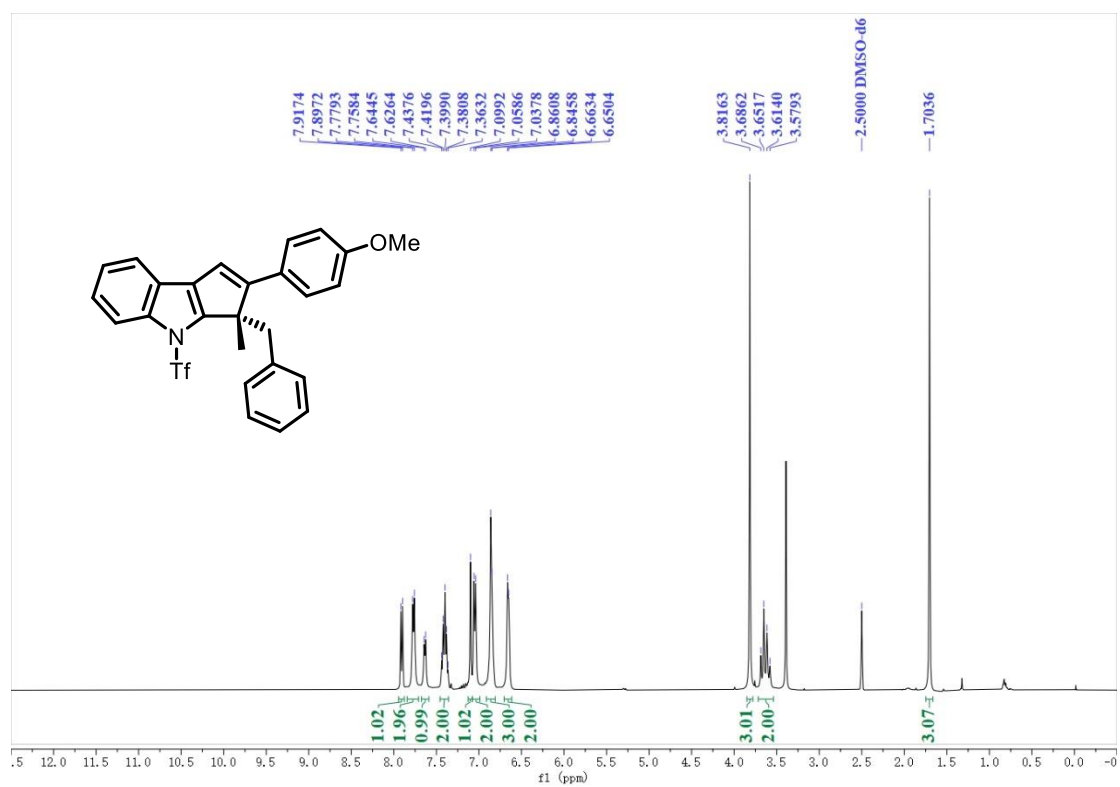


7  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )

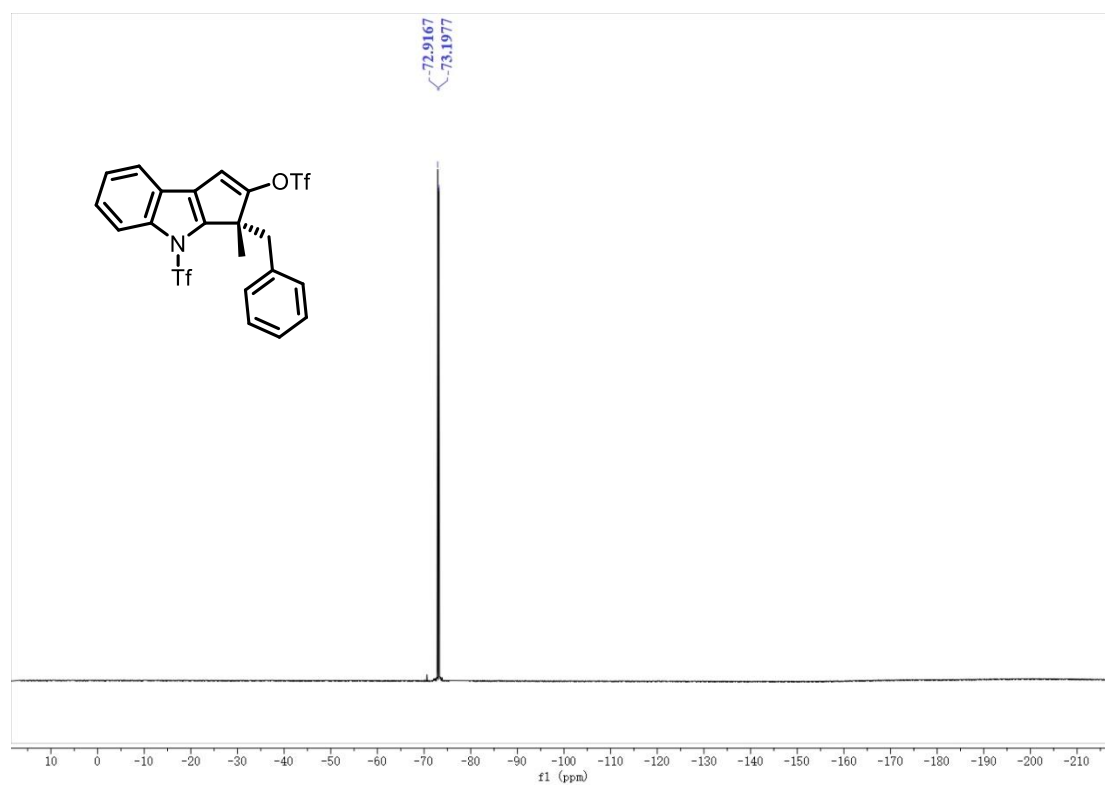




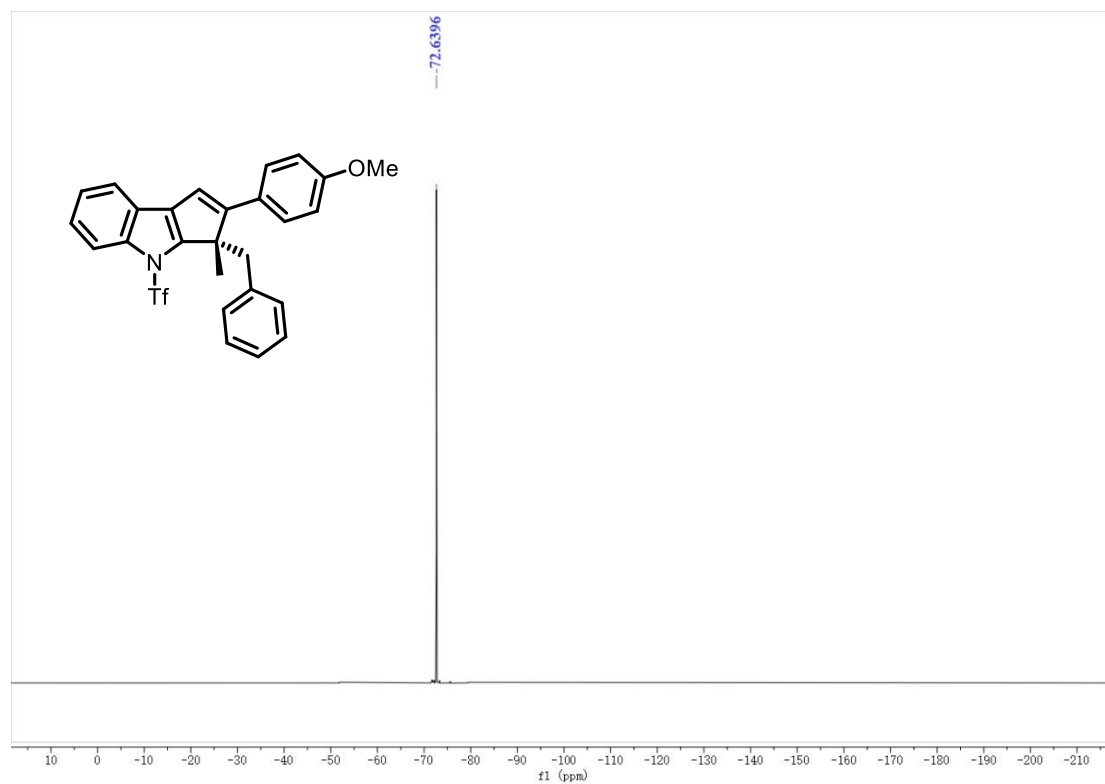
8  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )/ $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )



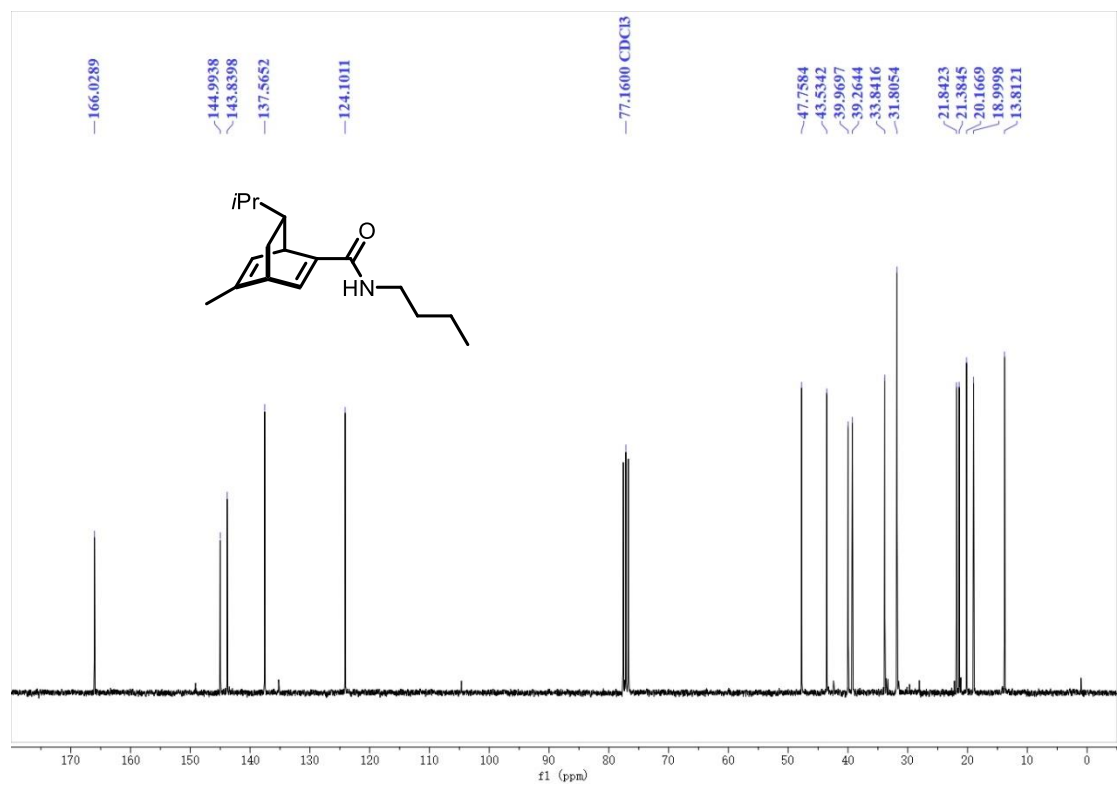
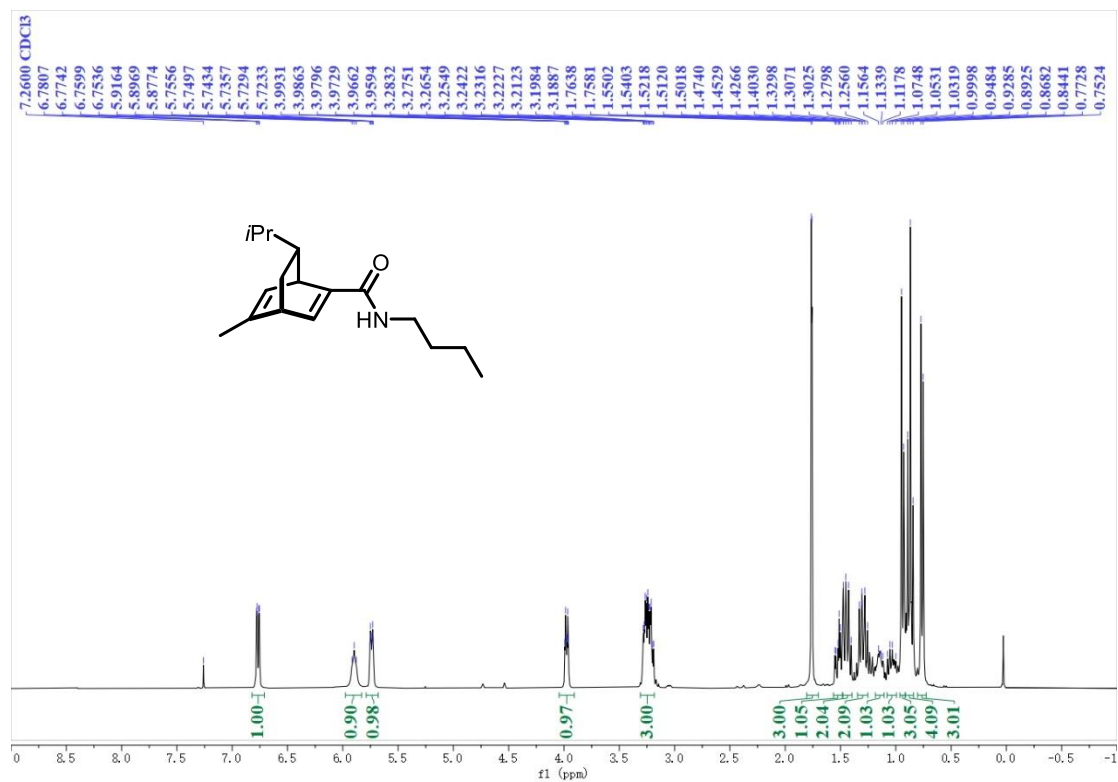
7  $^{19}\text{F}$  NMR (282 MHz,  $\text{DMSO-}d_6$ )



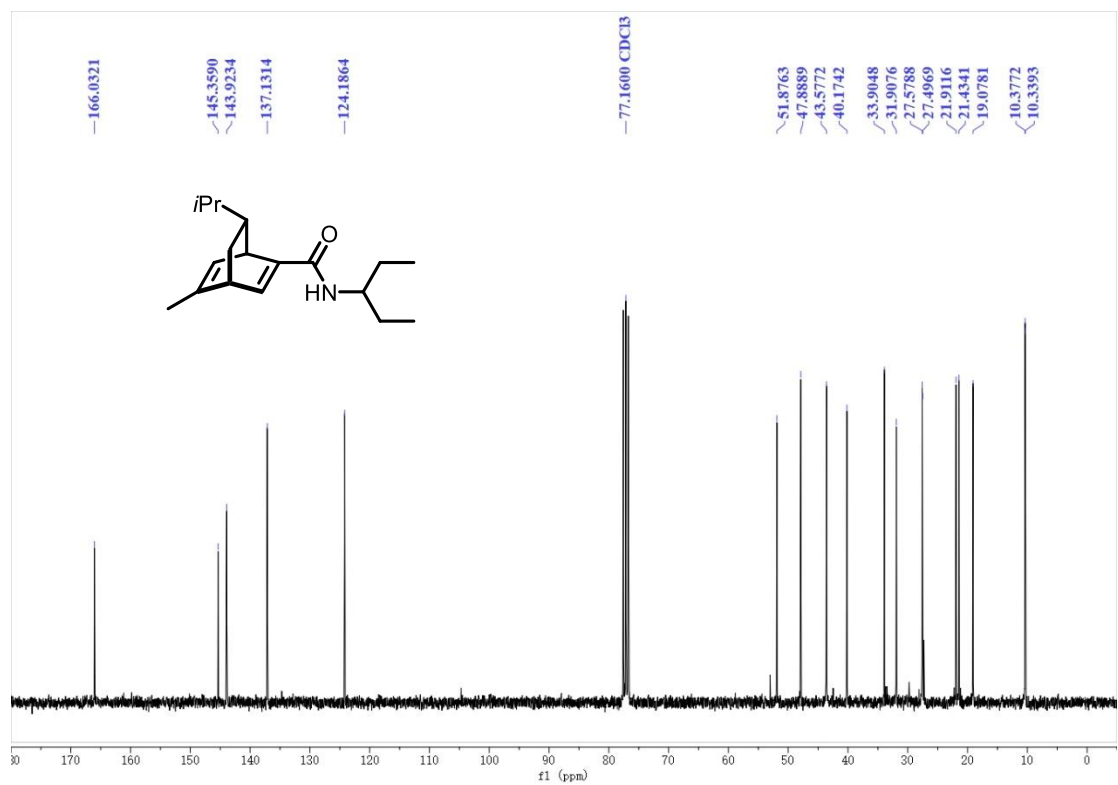
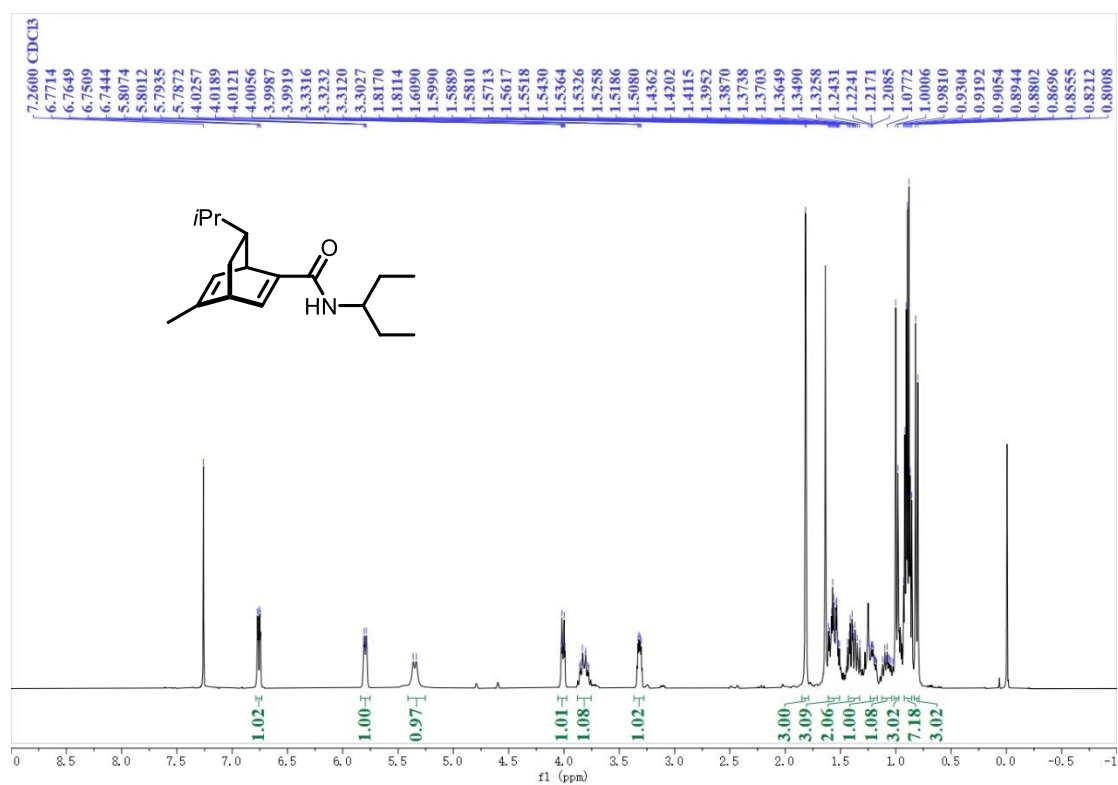
8  $^{19}\text{F}$  NMR (282 MHz,  $\text{DMSO-}d_6$ )



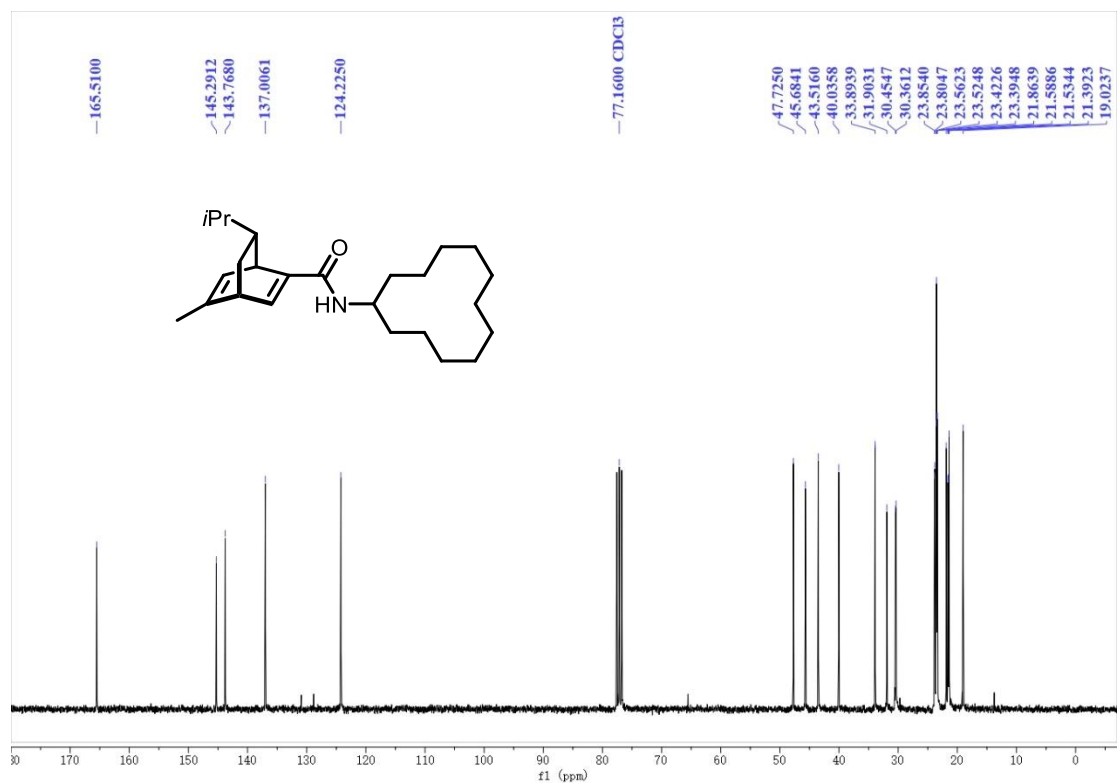
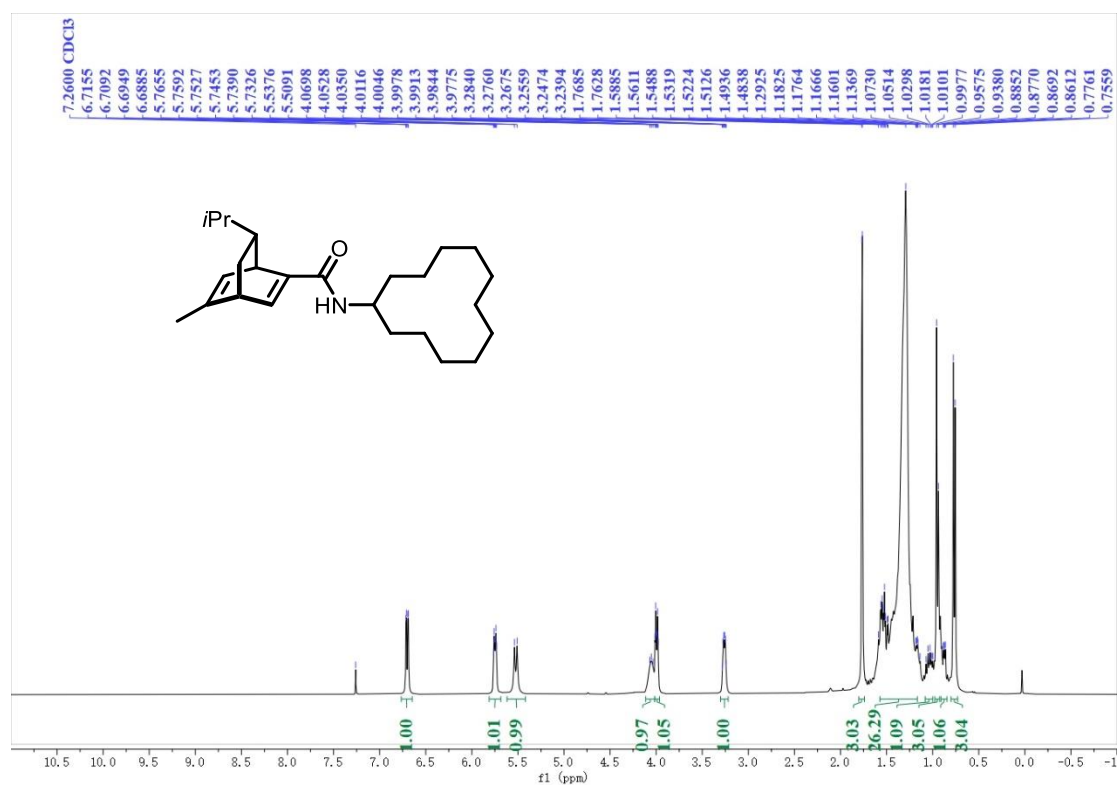
L6  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3-d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3-d$ )



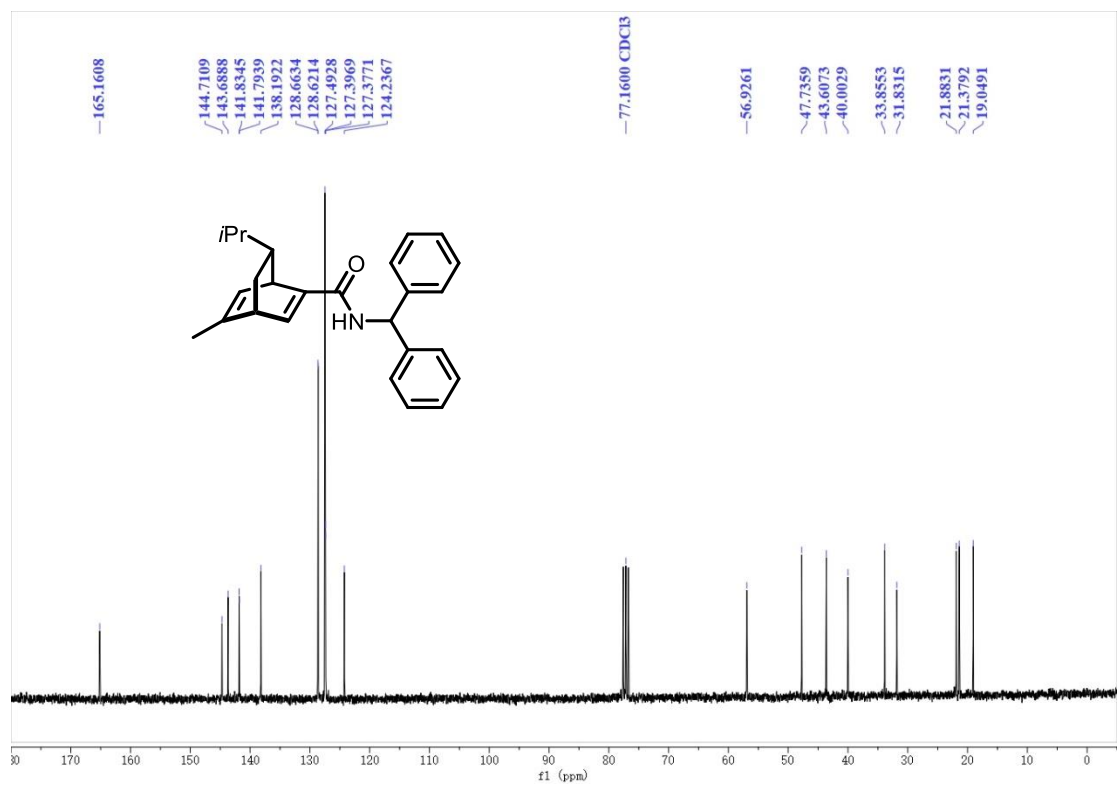
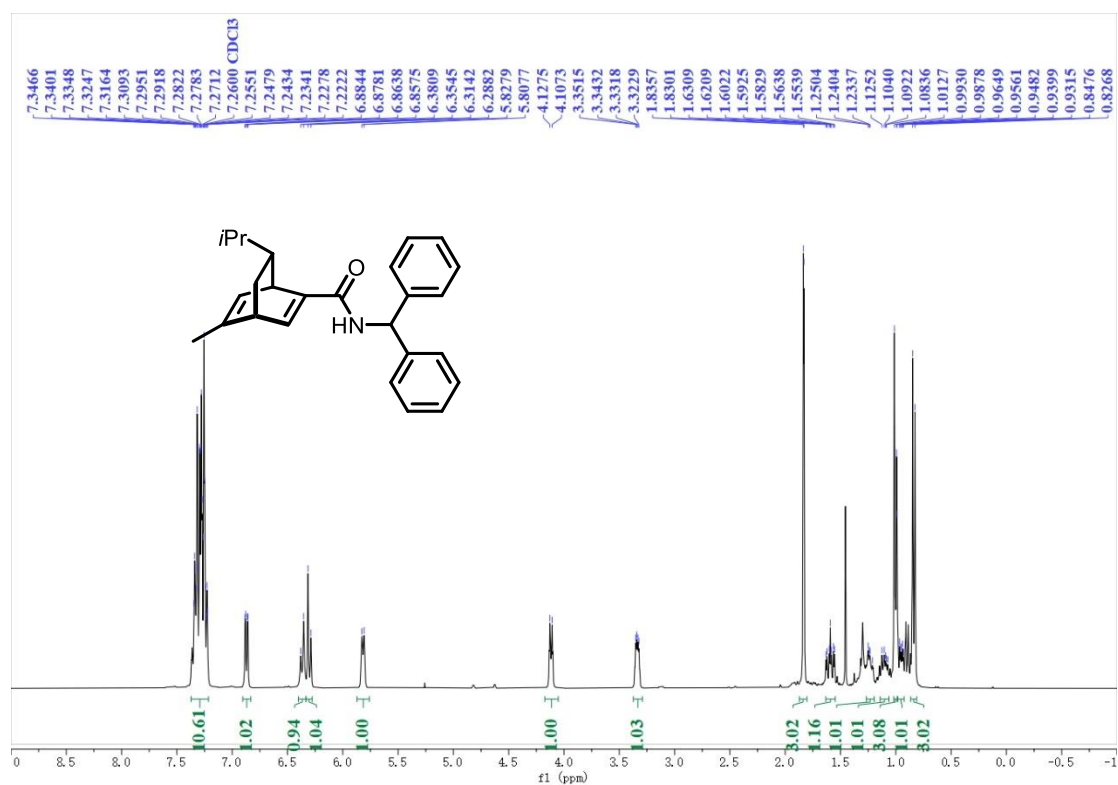
L11  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3-d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3-d$ )



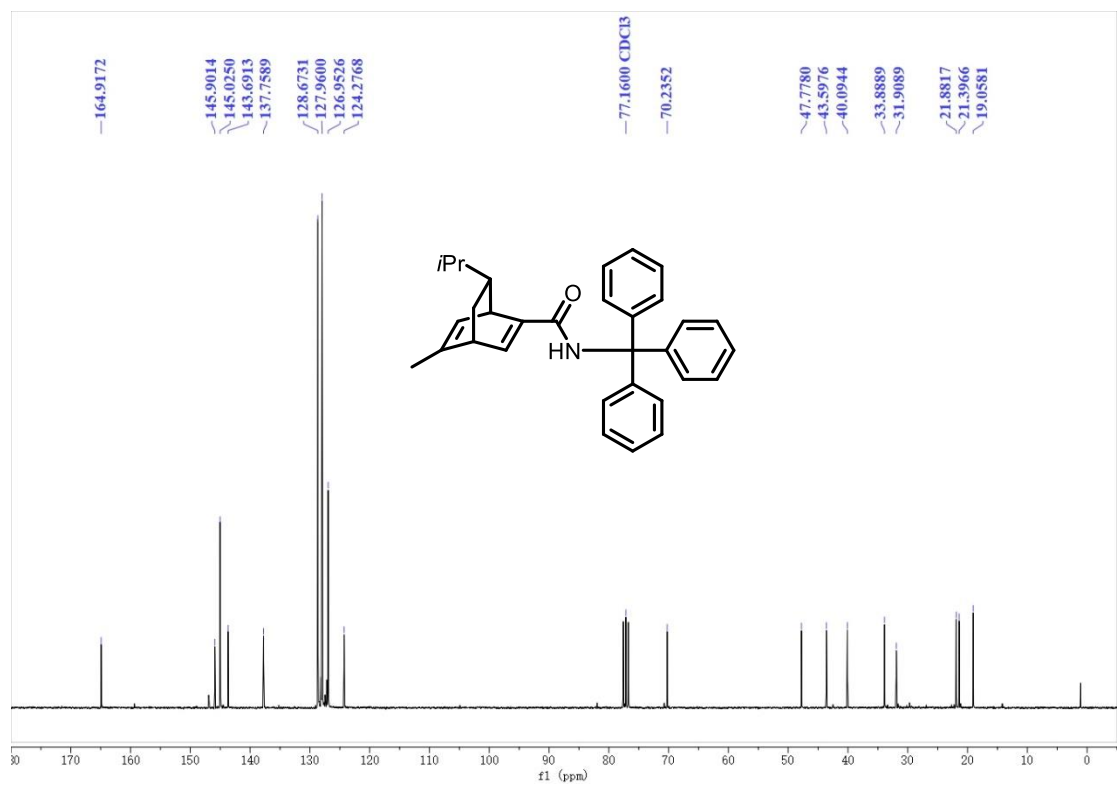
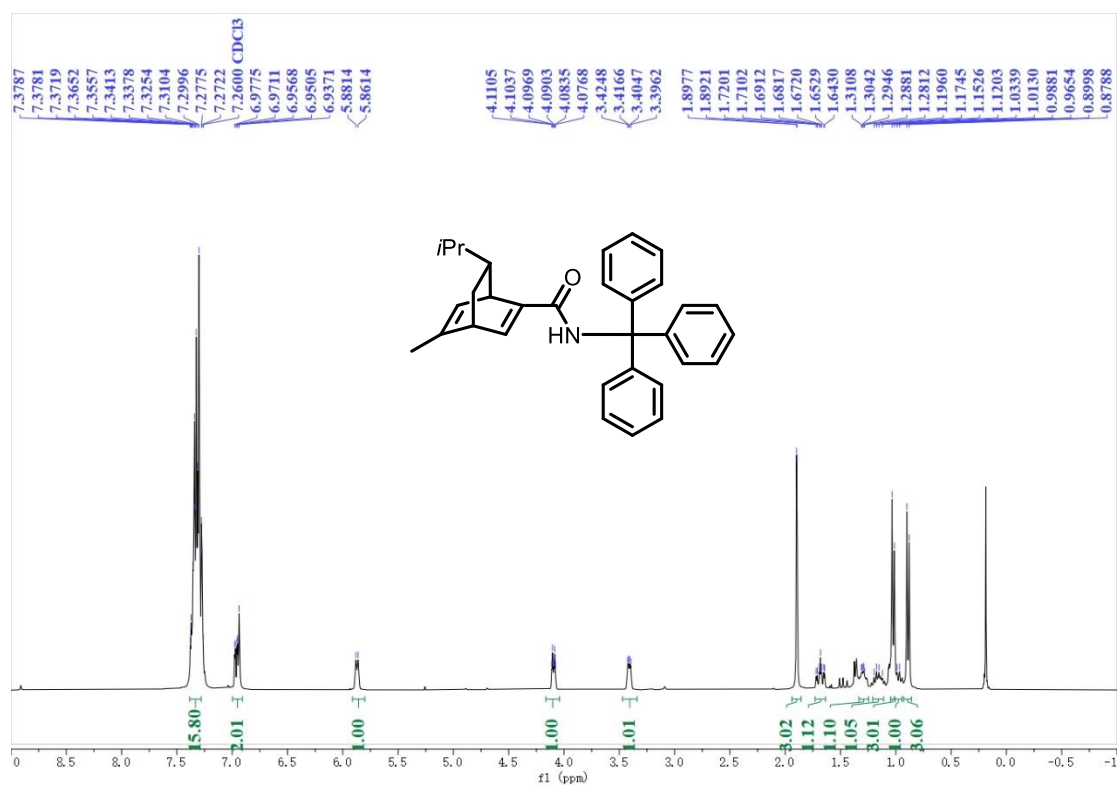
L12  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3-d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3-d$ )



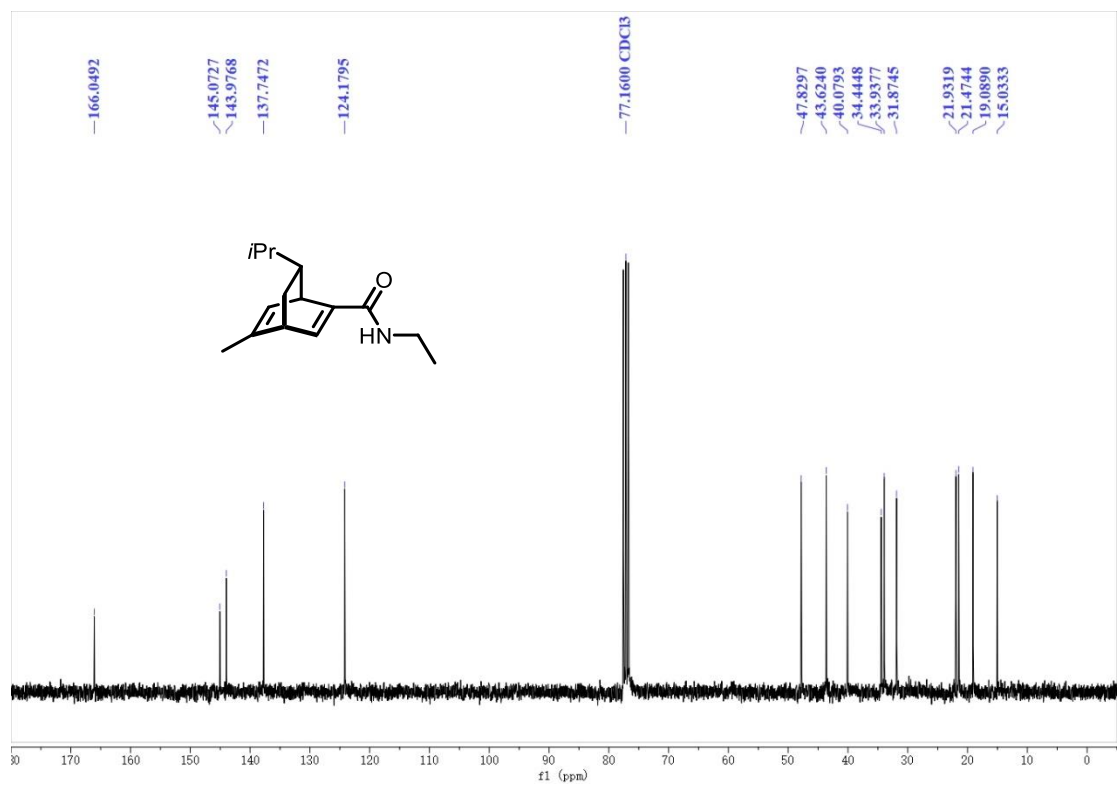
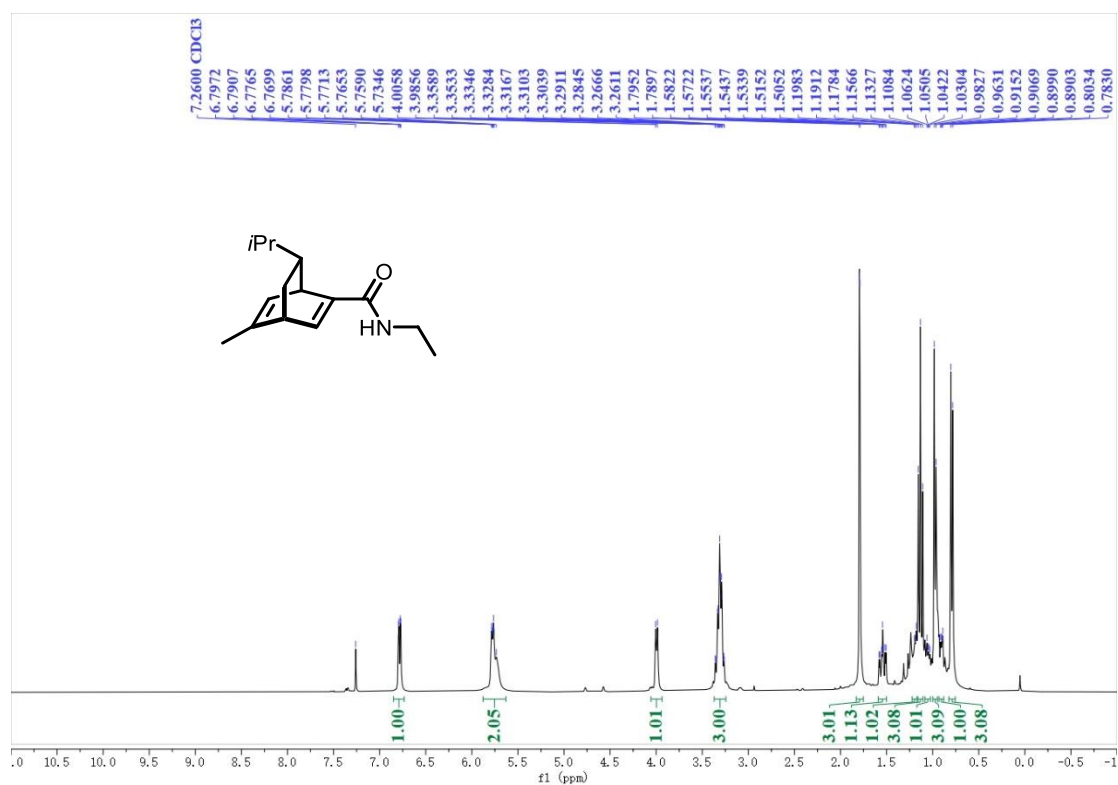
L14  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3\text{-d}$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3\text{-d}$ )



L15  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3-d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3-d$ )

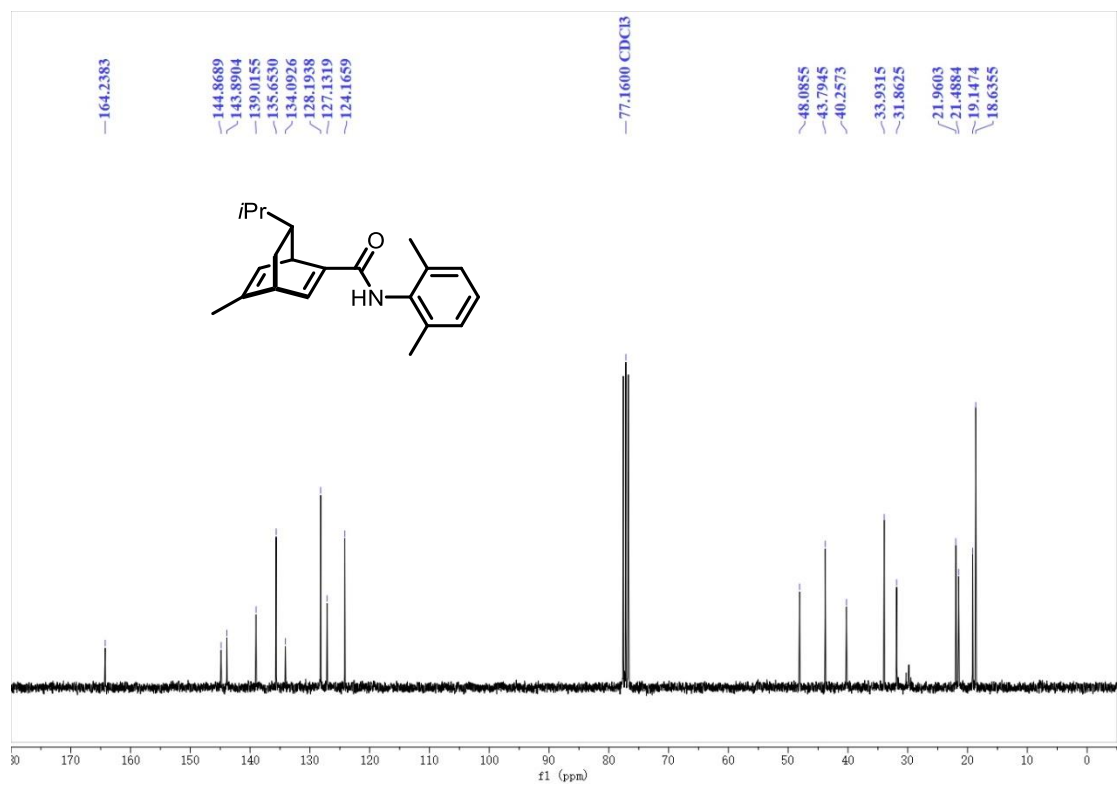
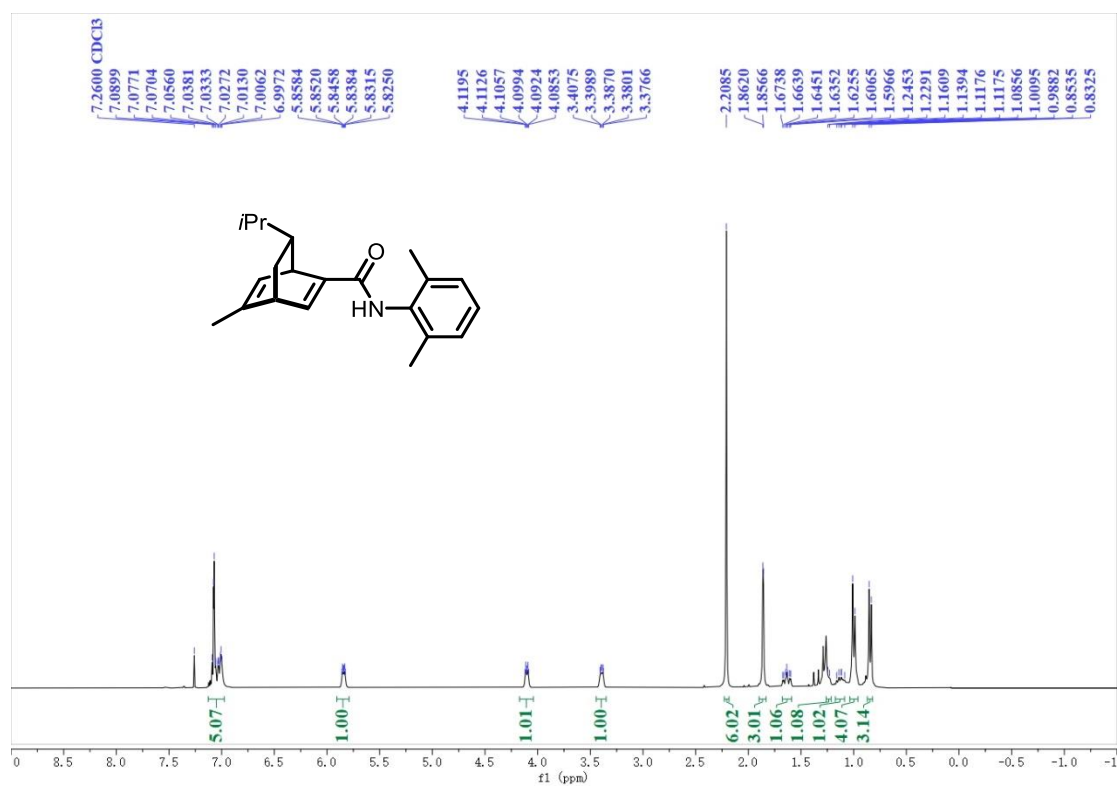


L5  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3\text{-}d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3\text{-}d$ )

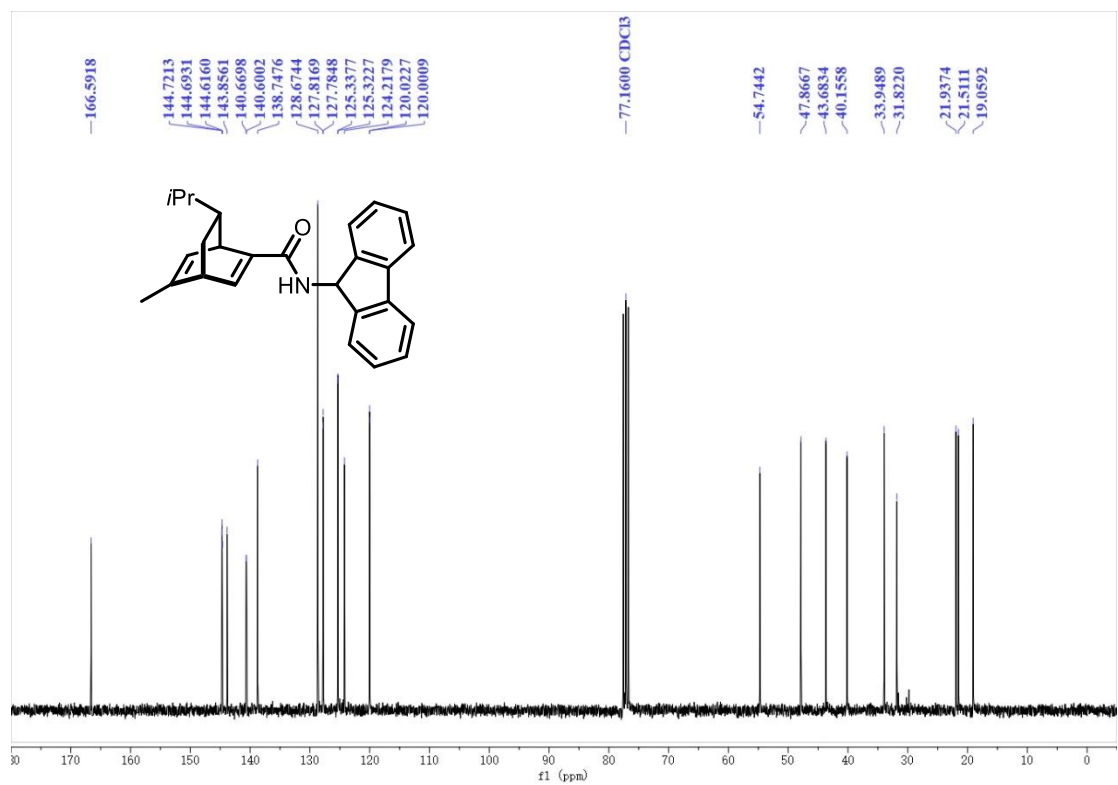
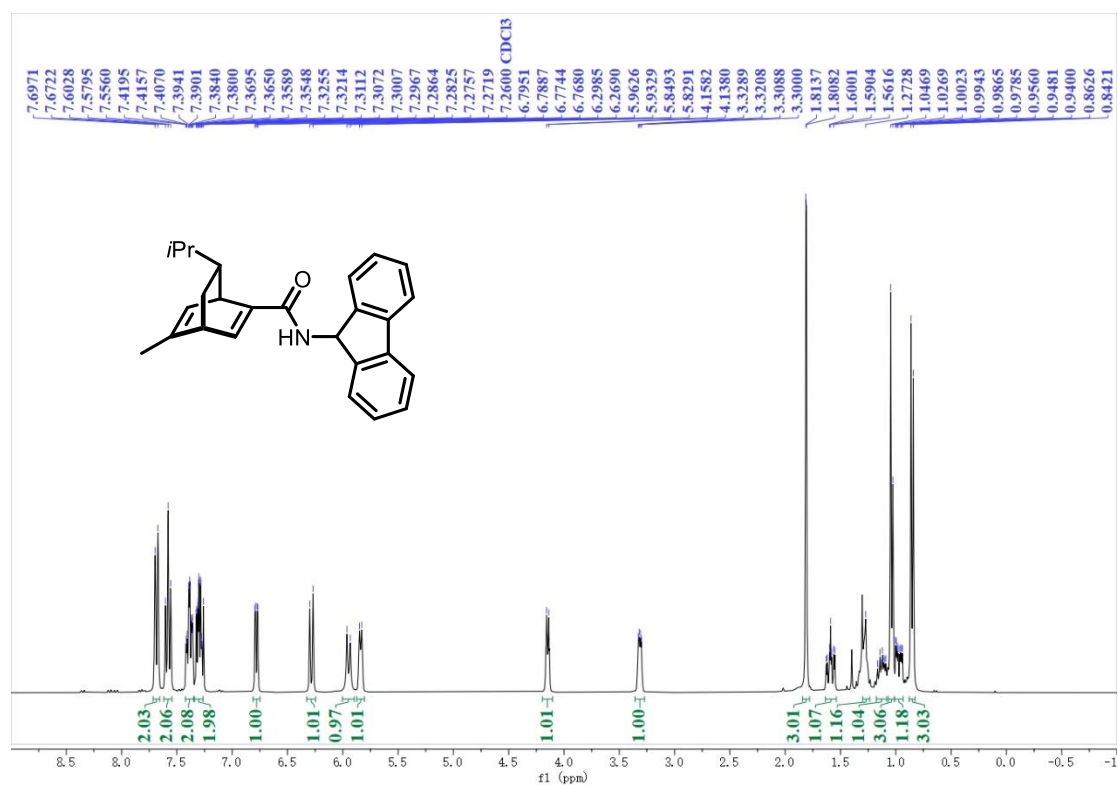




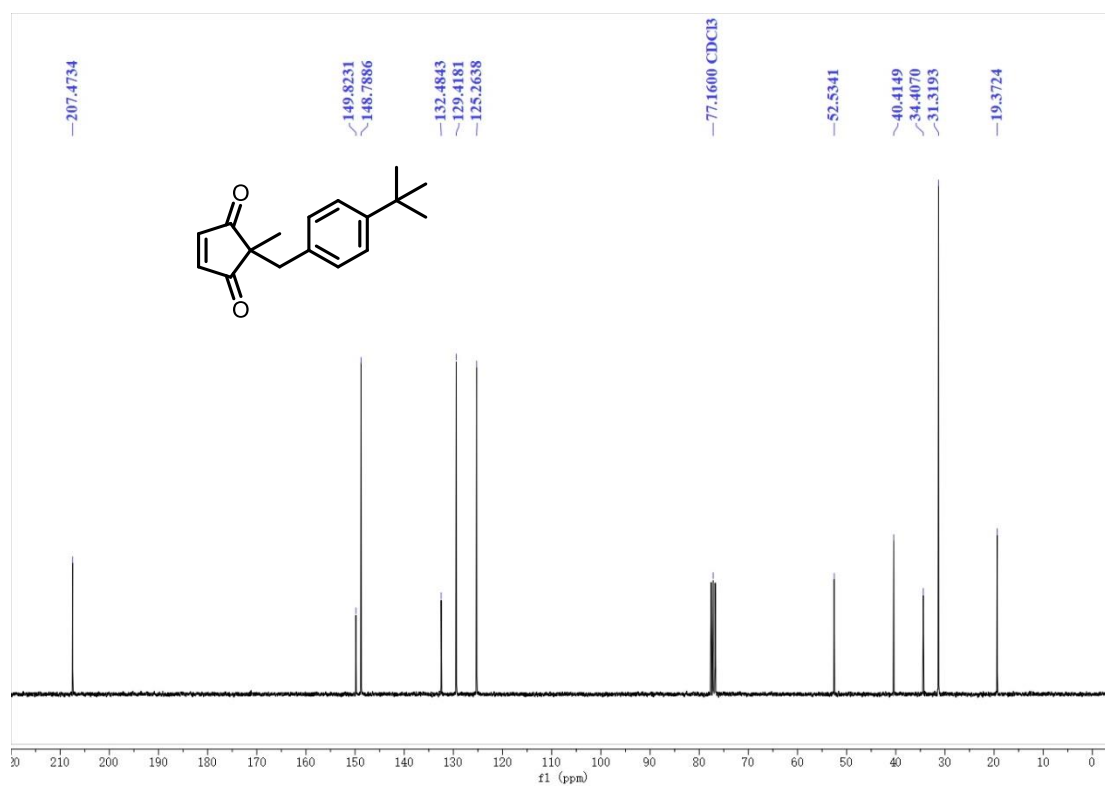
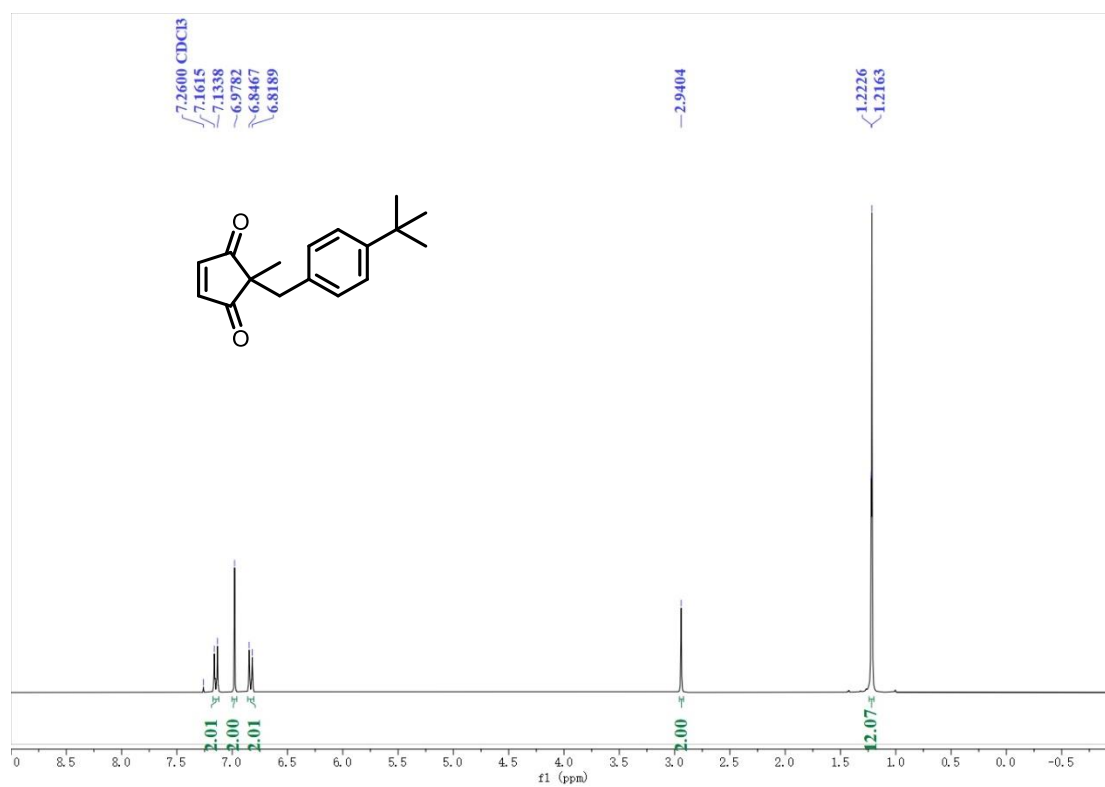
L17  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3-d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3-d$ )



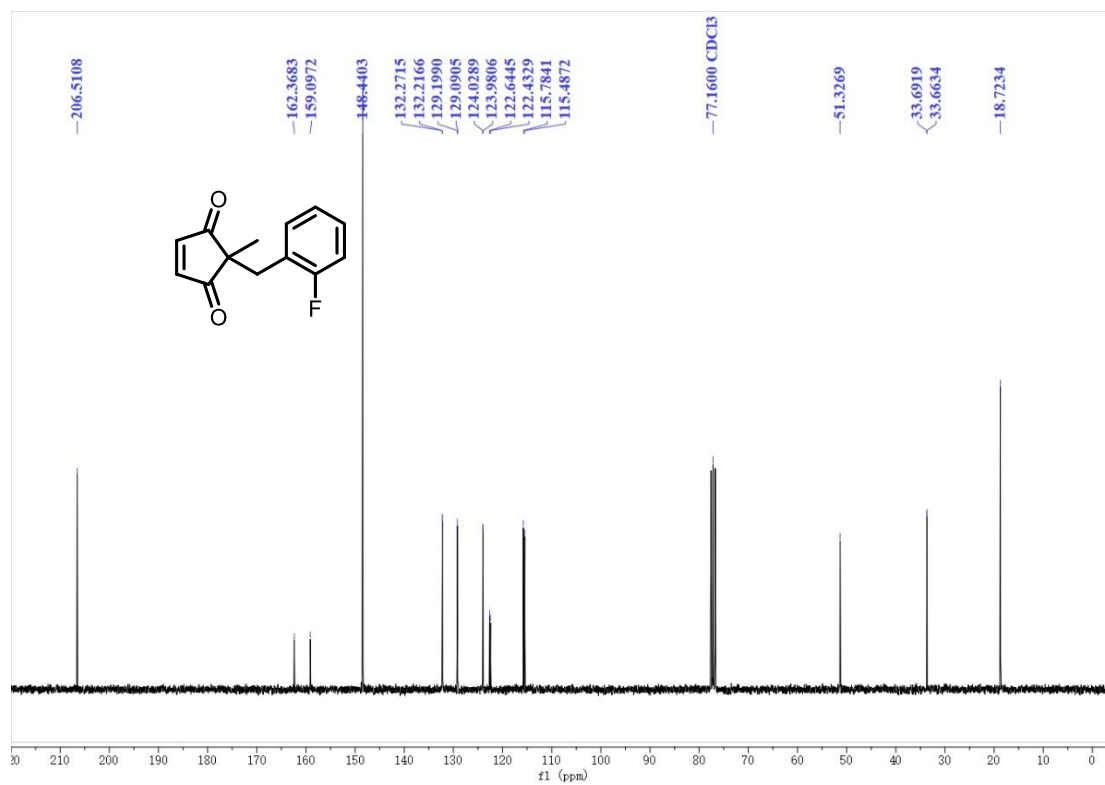
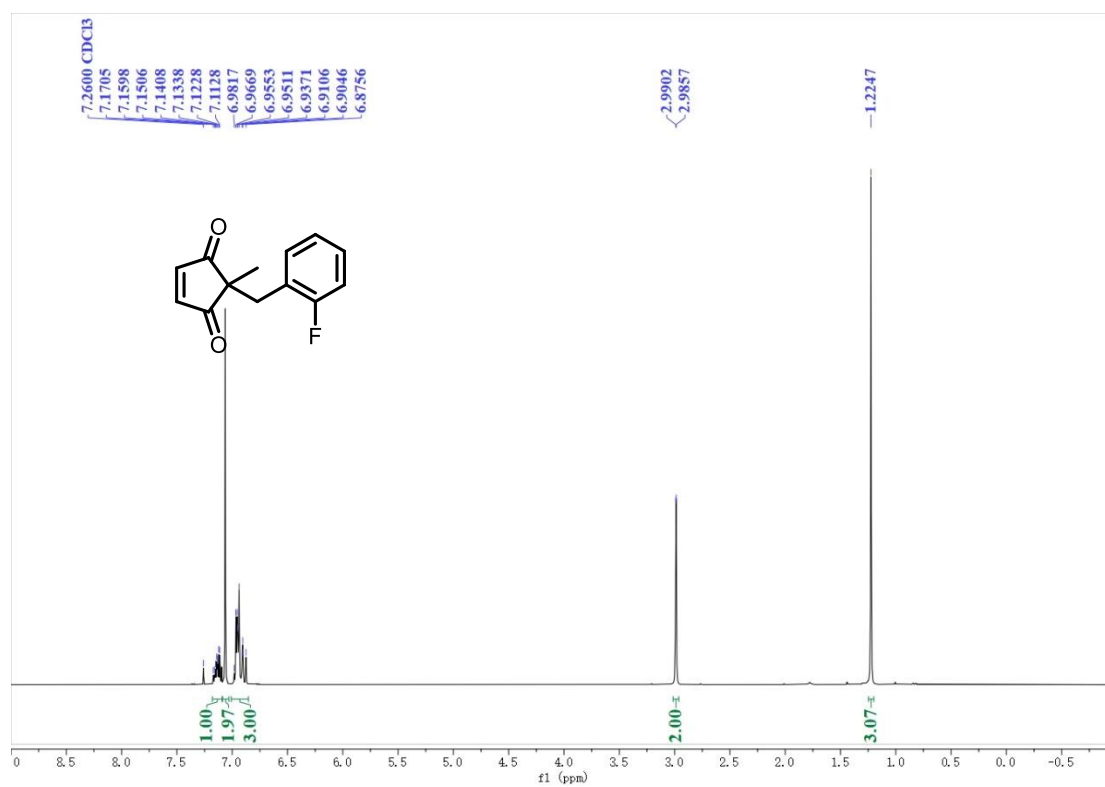
L13  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3-d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3-d$ )



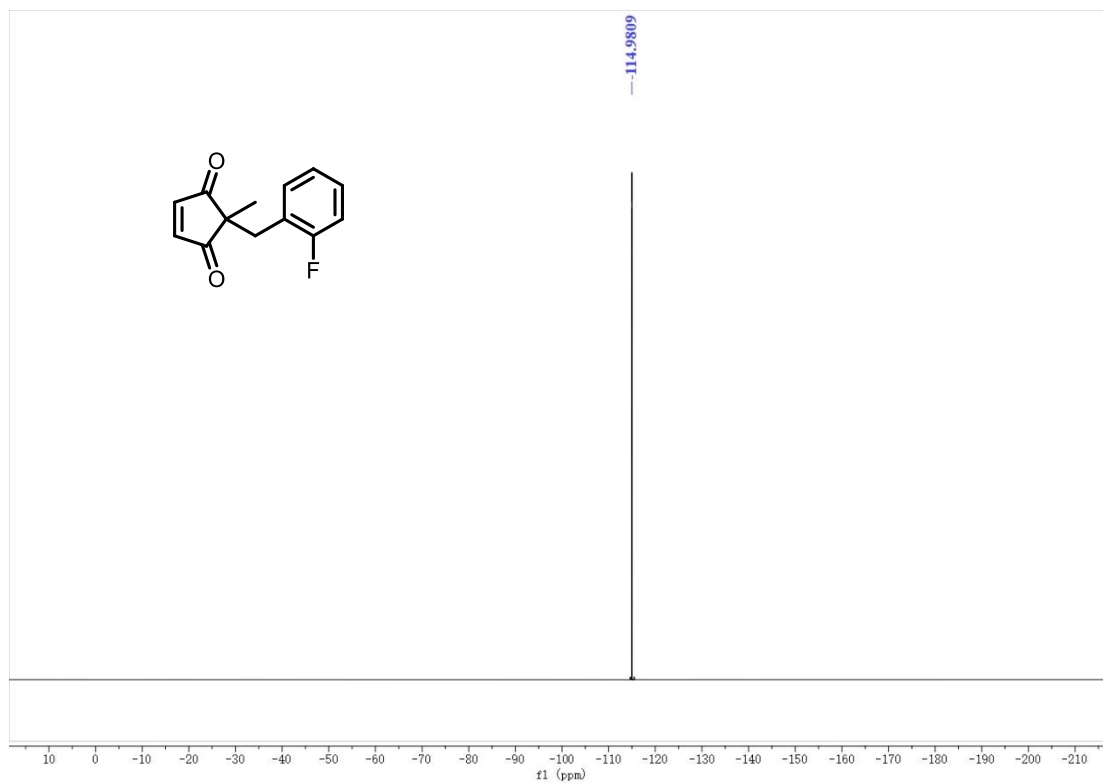
**1c**  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3-d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3-d$ )



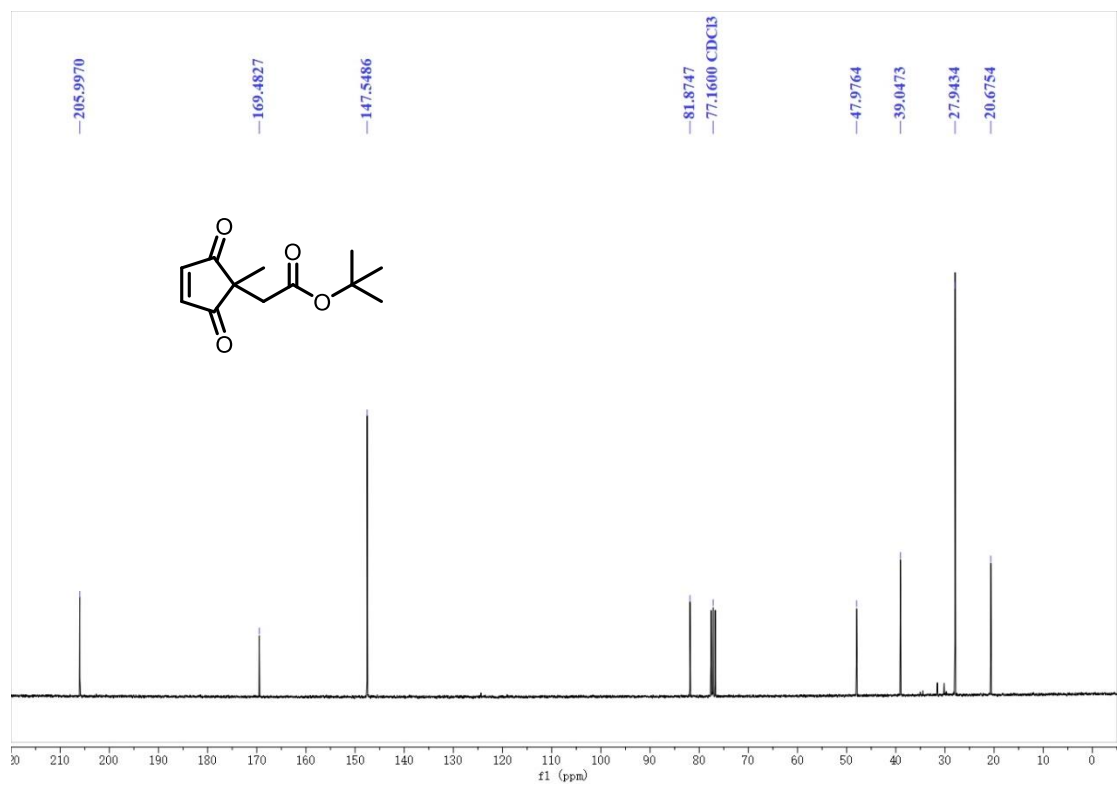
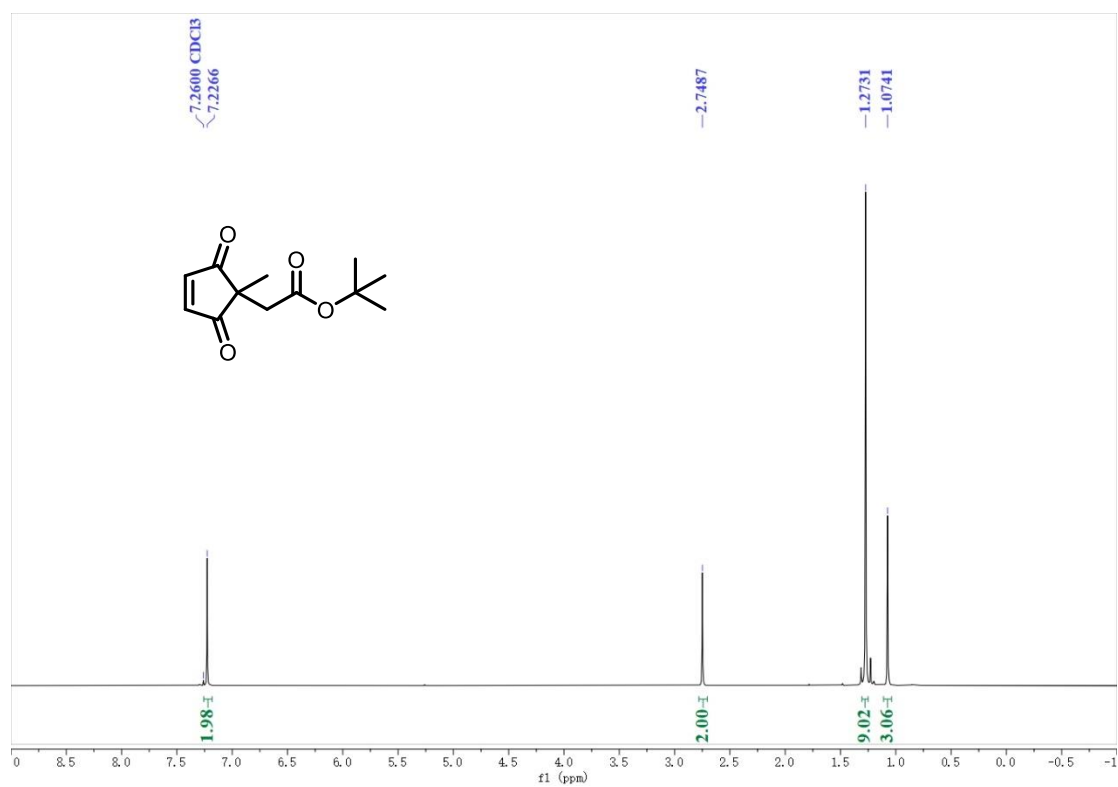
**1j**  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3-d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3-d$ )



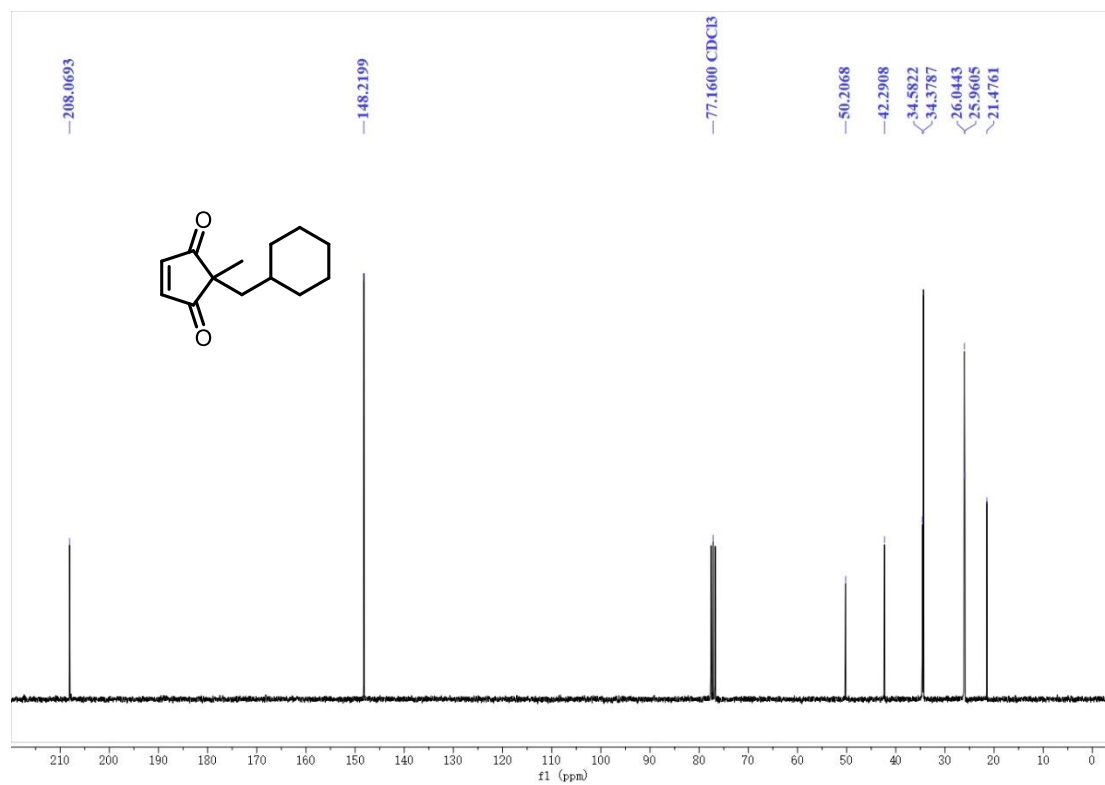
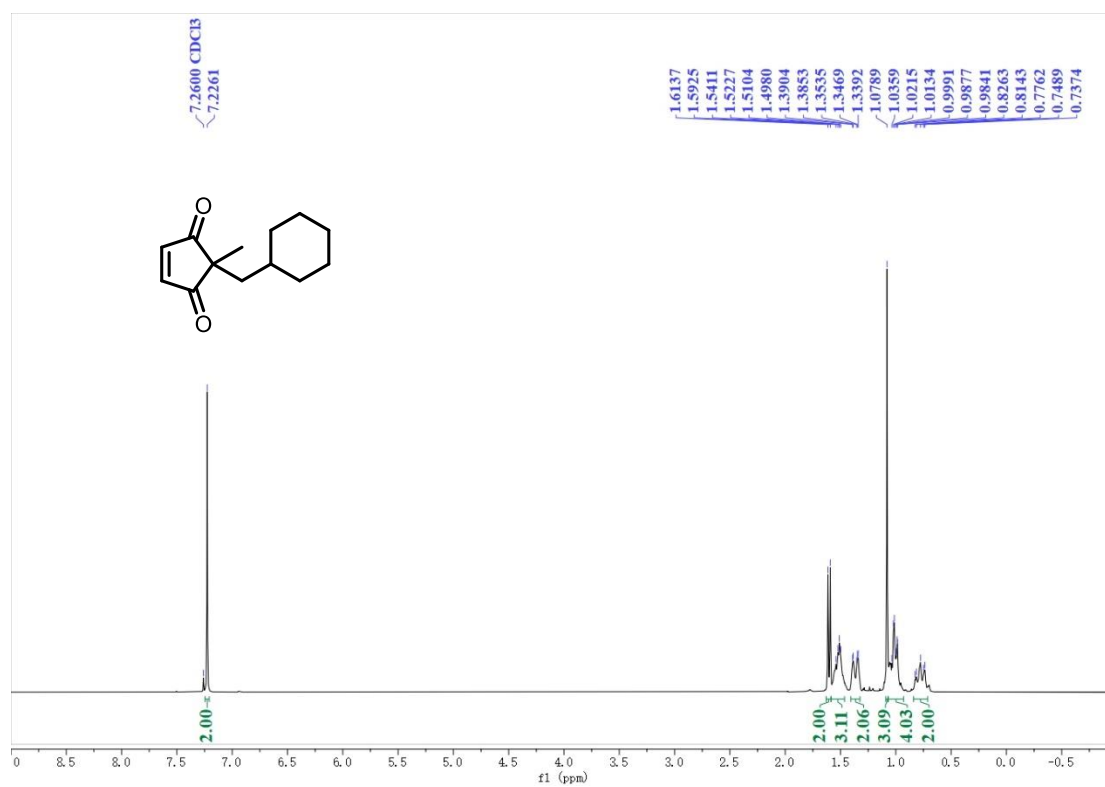
**1j**  $^{19}\text{F}$  NMR (282 MHz,  $\text{CHCl}_3-d$ )



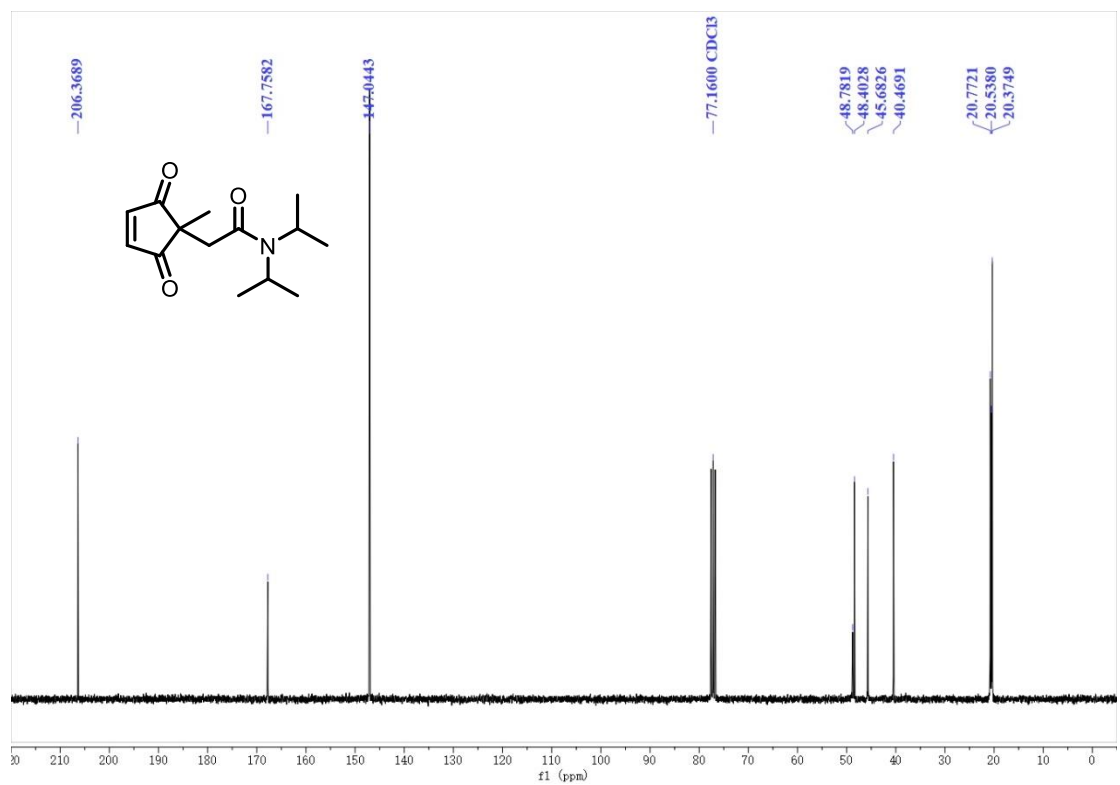
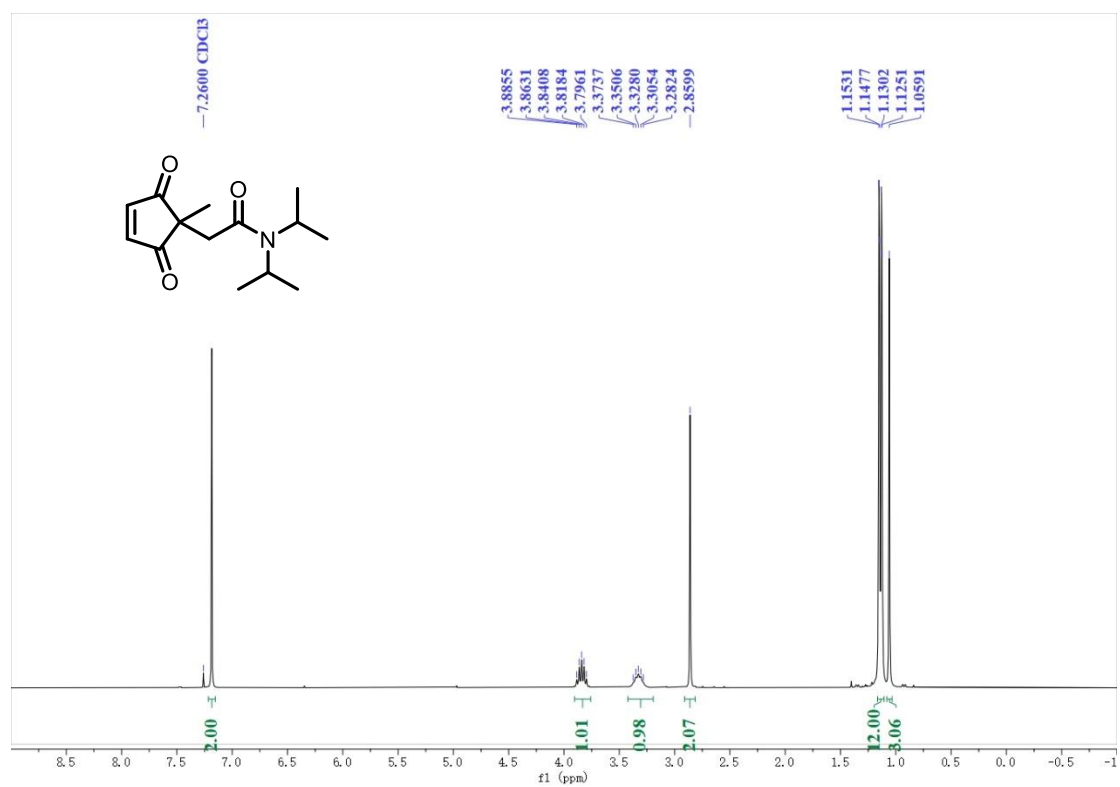
1s  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3-d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3-d$ )



**1p**  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3-d$ ) /  $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3-d$ )

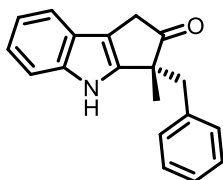


**1t**  $^1\text{H}$  NMR (300 MHz,  $\text{CHCl}_3-d$ )/ $^{13}\text{C}$  NMR (75 MHz,  $\text{CHCl}_3-d$ )

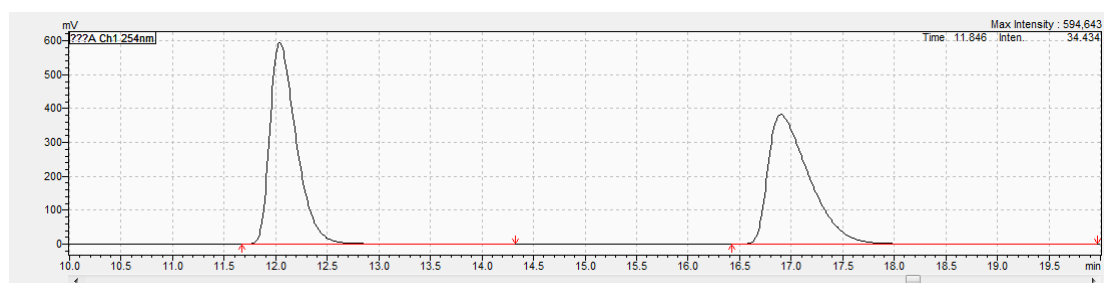




## 10.HPLC Charts

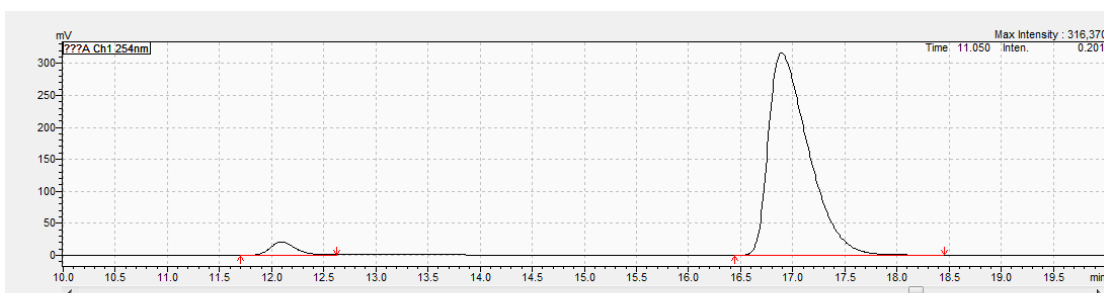


3aa



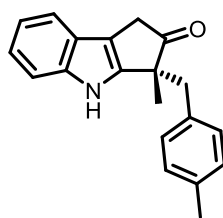
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	12.038	10624513	594660	50.001	50.001
2	16.901	10624134	382594	49.999	49.999
Total		21248647	977254	100.000	100.000

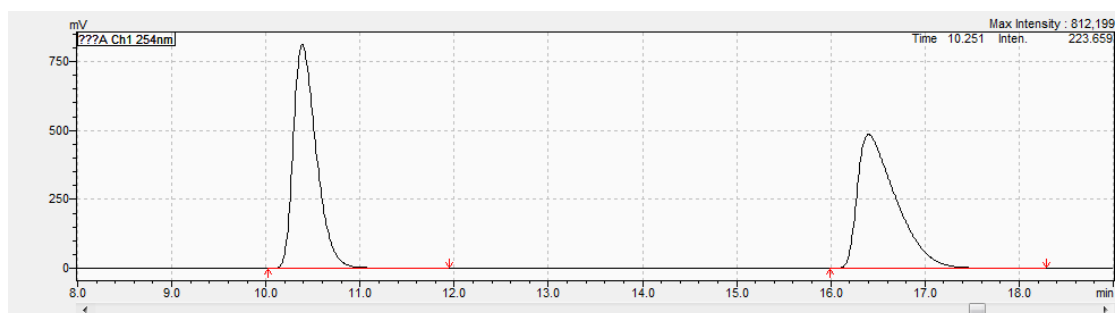


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	12.094	383961	20956	4.130	4.130
2	16.894	8449216	318298	95.870	95.870
Total		8813177	337252	100.000	100.000

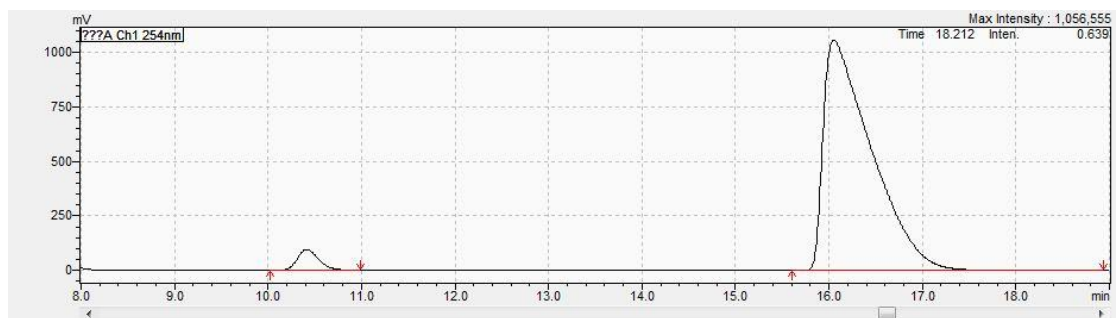


**3ba**



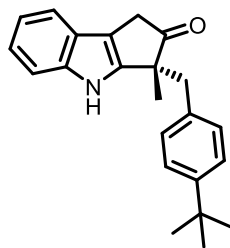
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.386	13781125	812195	49.916	49.916
2	16.400	13827385	486320	50.084	50.084
Total		27608509	1298515	100.000	100.000

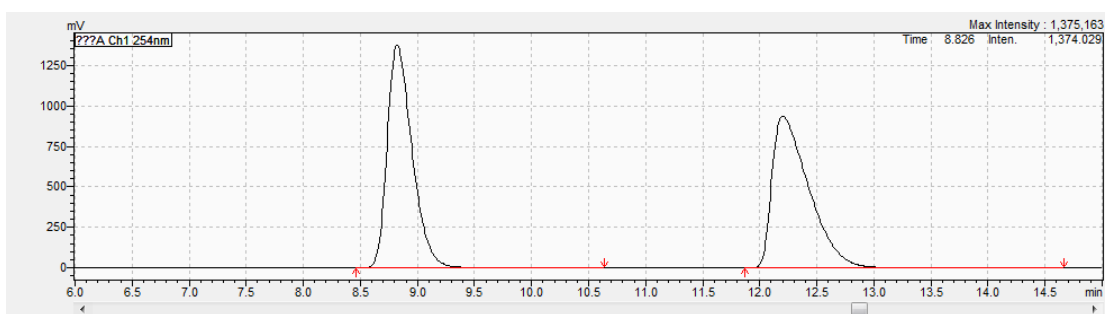


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.412	1569940	95556	3.983	3.983
2	16.052	37849943	1056590	96.017	96.017
Total		39419884	1152146	100.000	100.000



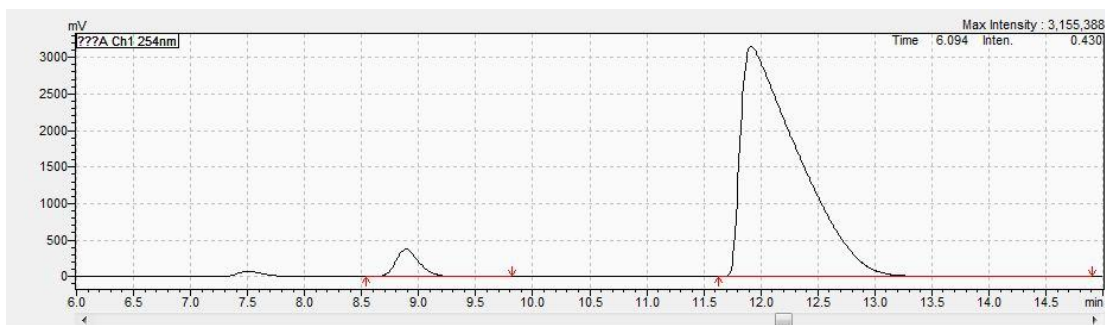
3ca



Results View - Peak Table

Peak Table Compound Group Calibration Curve

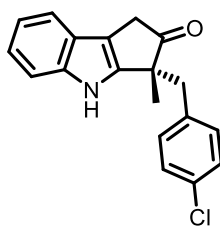
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.822	20928970	1375333	49.880	49.880
2	12.203	21029813	936993	50.120	50.120
Total		41958783	2312327	100.000	100.000



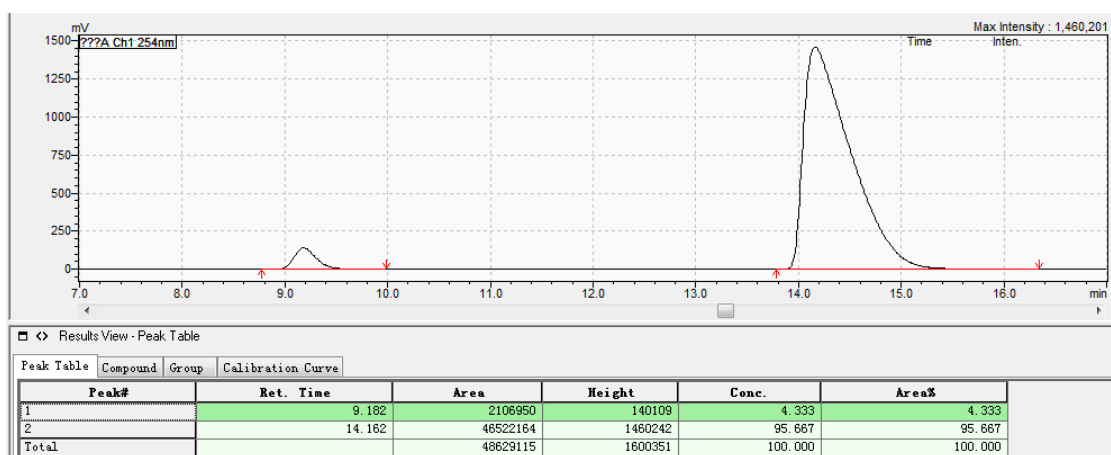
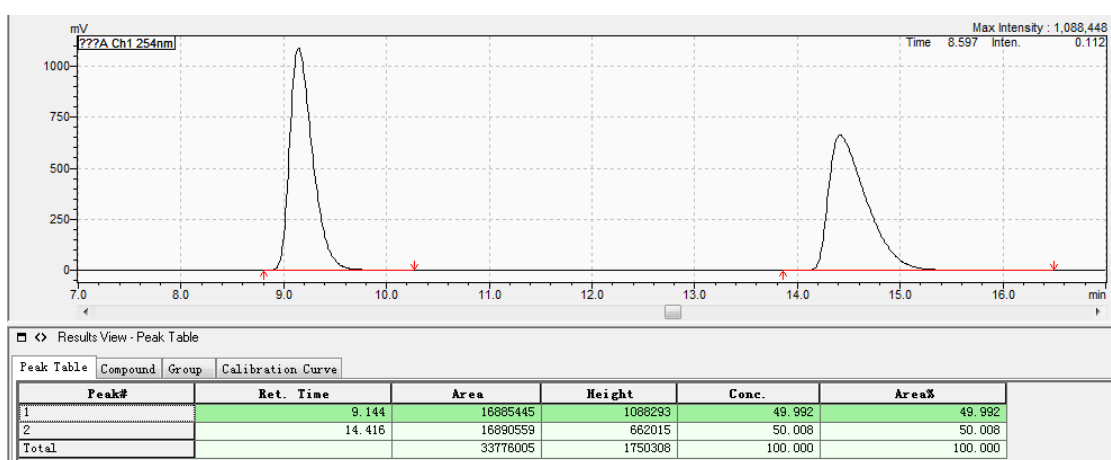
Results View - Peak Table

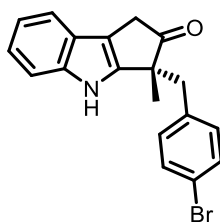
Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.888	5404327	374556	4.659	4.659
2	11.917	110590142	3155298	95.341	95.341
Total		115994469	3529854	100.000	100.000

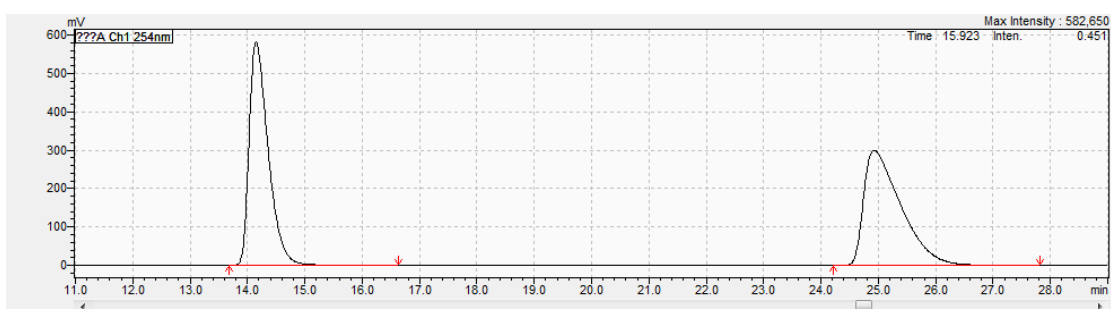


**3da**





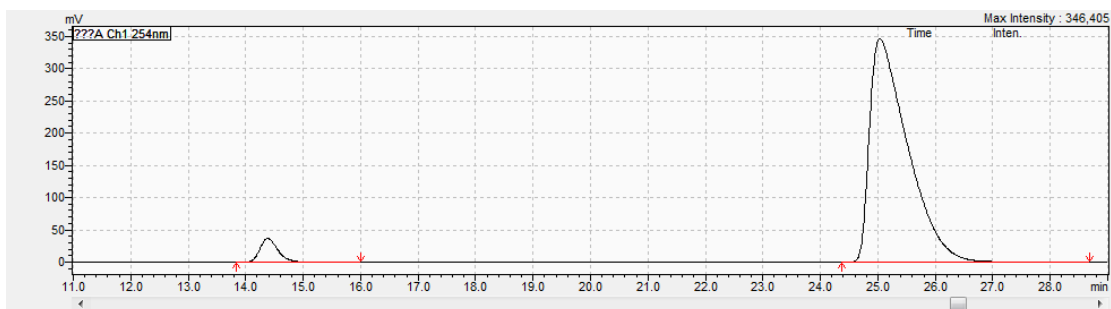
3ea



Results View - Peak Table

Peak Table Compound Group Calibration Curve

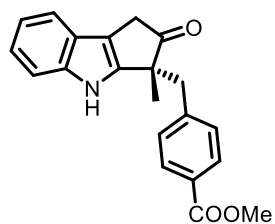
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	14.151	13455291	582673	50.000	50.000
2	24.927	13455262	299933	50.000	50.000
Total		26910574	882606	100.000	100.000



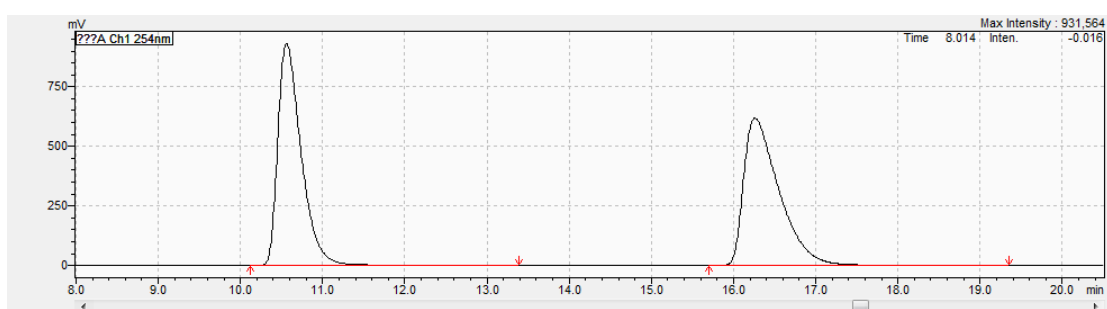
Results View - Peak Table

Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	14.383	814278	37049	4.846	4.846
2	25.035	15988131	346696	95.154	95.154
Total		16802409	383745	100.000	100.000



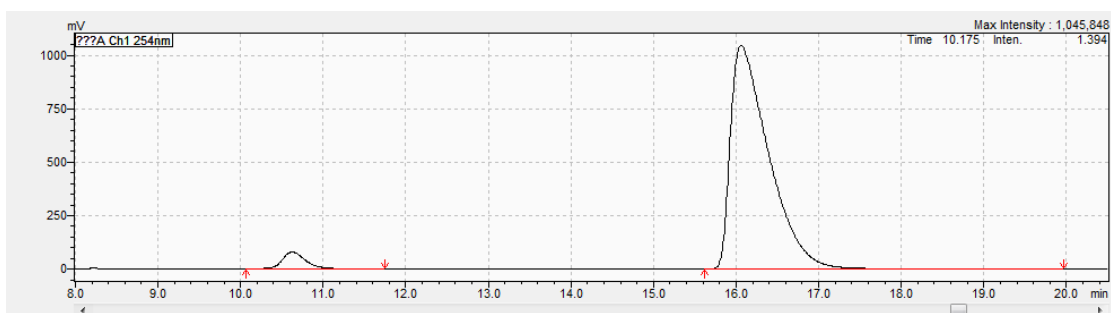
**3fa**



Results View - Peak Table

Peak Table Compound Group Calibration Curve

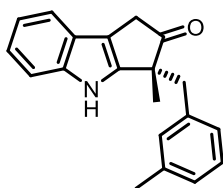
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.560	18438997	931802	49.883	49.883
2	16.259	18525671	618640	50.117	50.117
Total		36964668	1550241	100.000	100.000



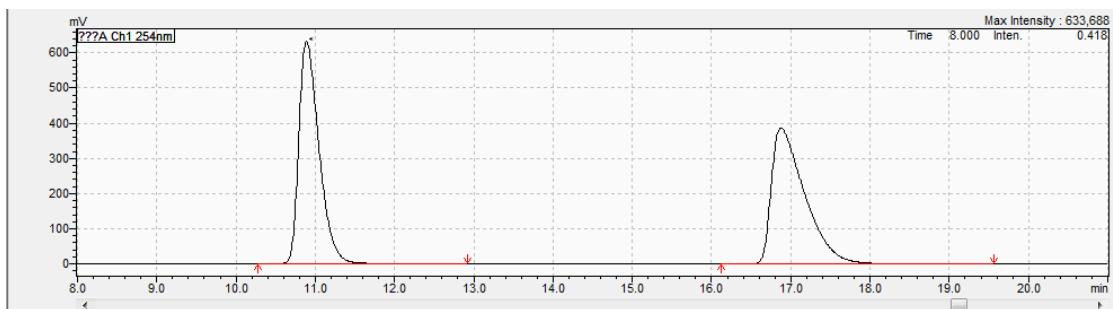
Results View - Peak Table

Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.625	1825806	79874	4.597	4.597
2	16.061	33741781	1045900	95.403	95.403
Total		35367587	1125774	100.000	100.000

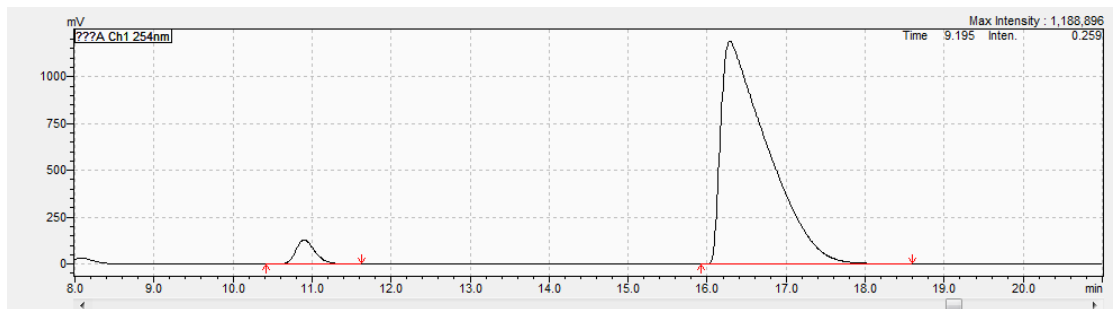


3ga



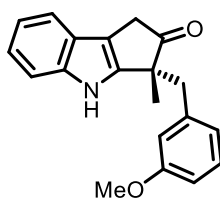
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.890	11258065	633688	49.920	49.920
2	16.878	11293978	386842	50.080	50.080
Total		22552043	1020510	100.000	100.000

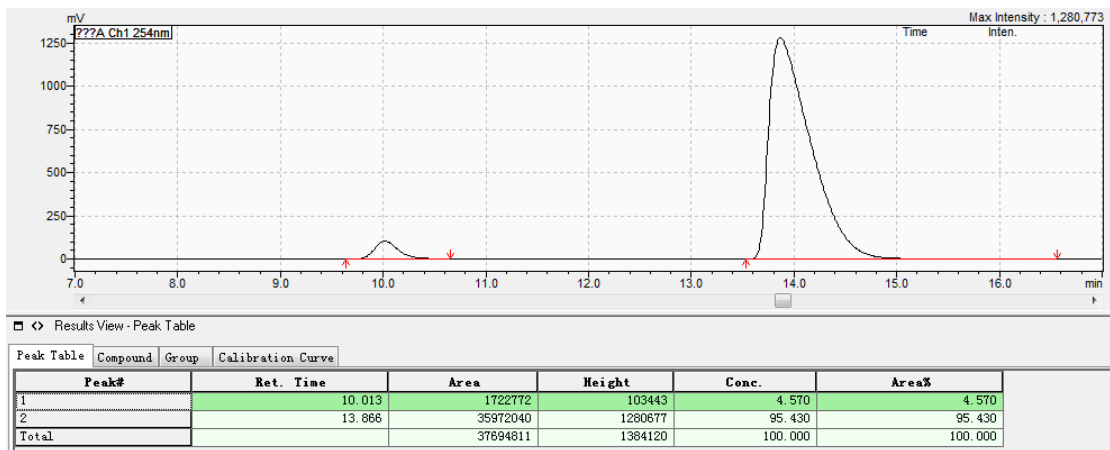
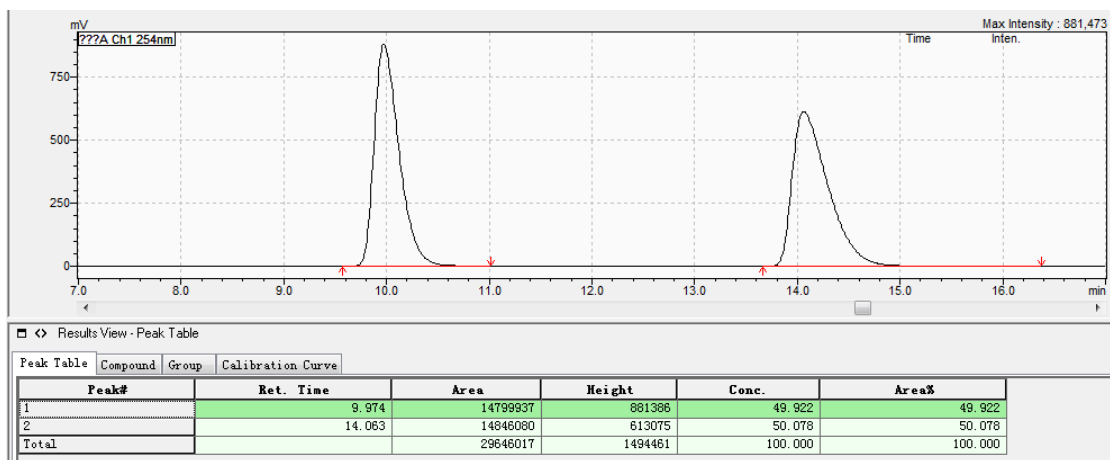


Results View - Peak Table

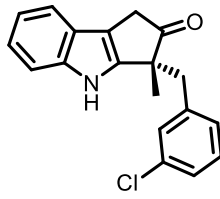
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.699	2175730	128915	4.277	4.277
2	16.287	48694843	1188784	95.723	95.723
Total		50870572	1317699	100.000	100.000



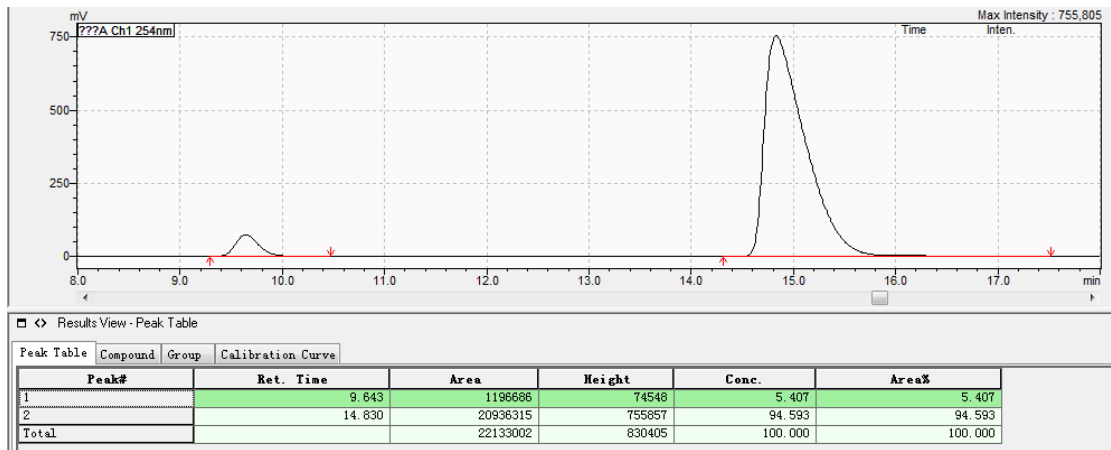
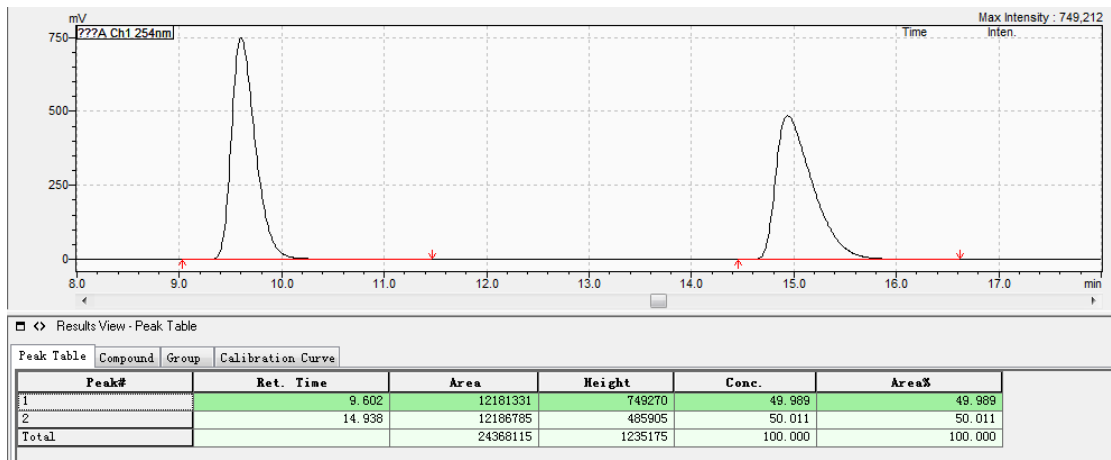
**3ha**

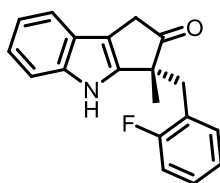




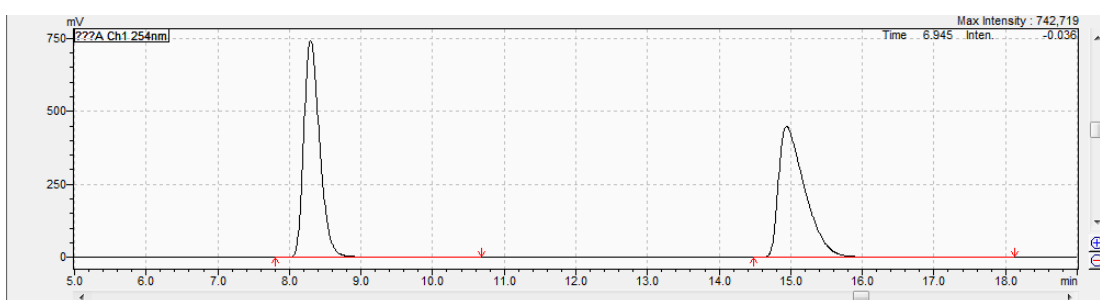


3ia





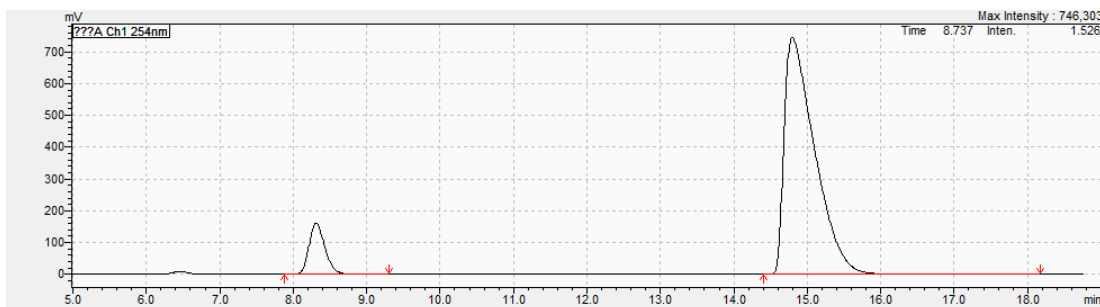
3ja



Results View - Peak Table

Peak Table Compound Group Calibration Curve

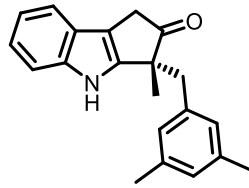
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.295	11442307	742862	49.918	49.918
2	14.943	11479832	447967	50.082	50.082
Total		22922139	1190829	100.000	100.000



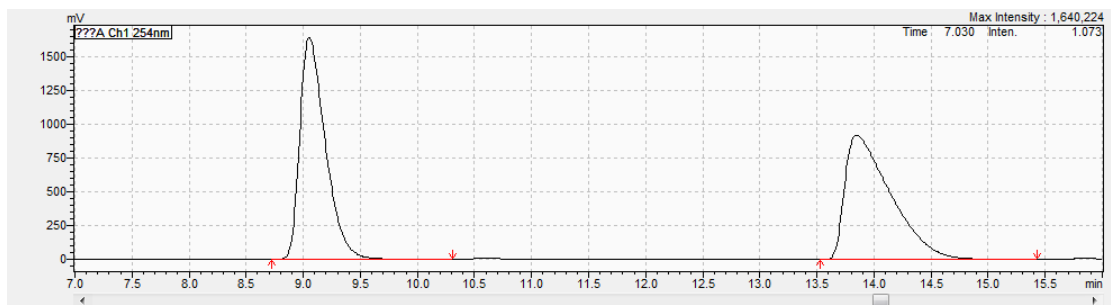
Results View - Peak Table

Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.313	2435907	160557	10.173	10.173
2	14.797	21508869	746484	89.827	89.827
Total		23944776	907040	100.000	100.000

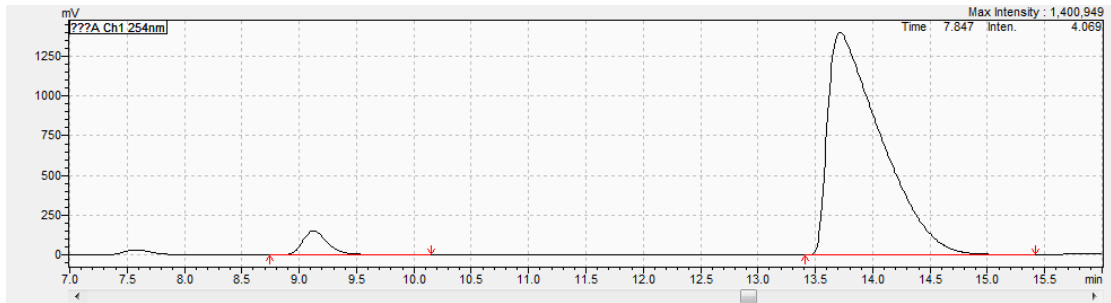


3ka



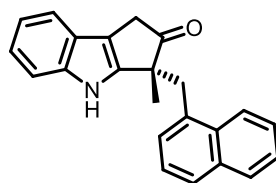
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.053	25577175	1639780	49.965	49.965
2	13.850	25812590	919415	50.035	50.035
Total		51189765	2559196	100.000	100.000

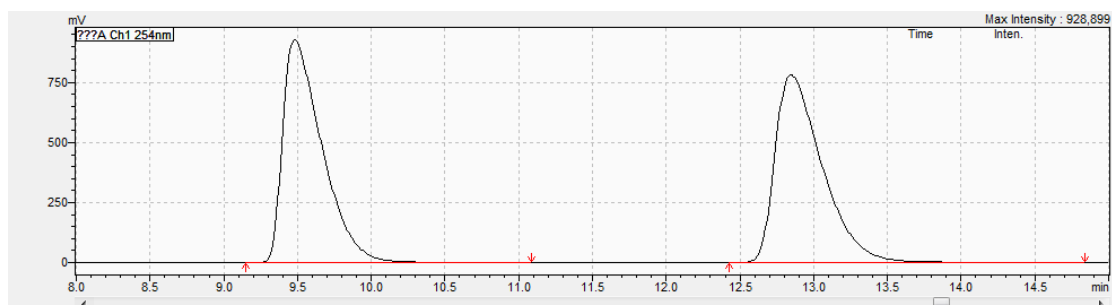


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.124	2354101	152322	4.949	4.949
2	13.715	45212707	1401332	95.051	95.051
Total		47566807	1553655	100.000	100.000

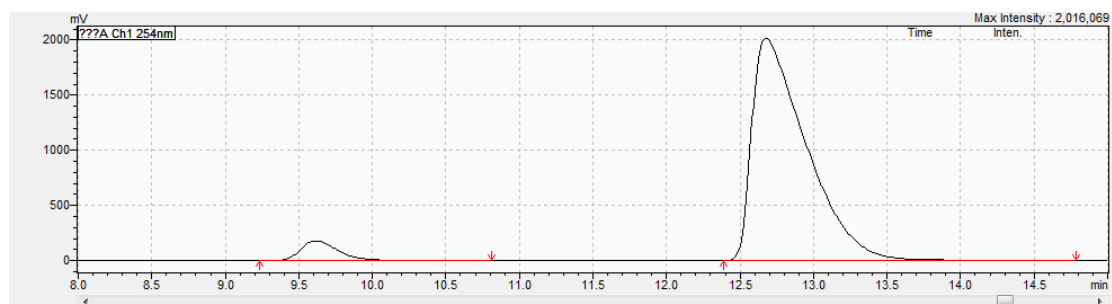


3la



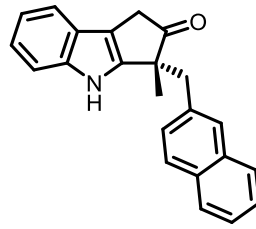
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.482	17239310	929442	49.631	49.631
2	12.846	17495428	783021	50.369	50.369
Total		34734738	1712463	100.000	100.000

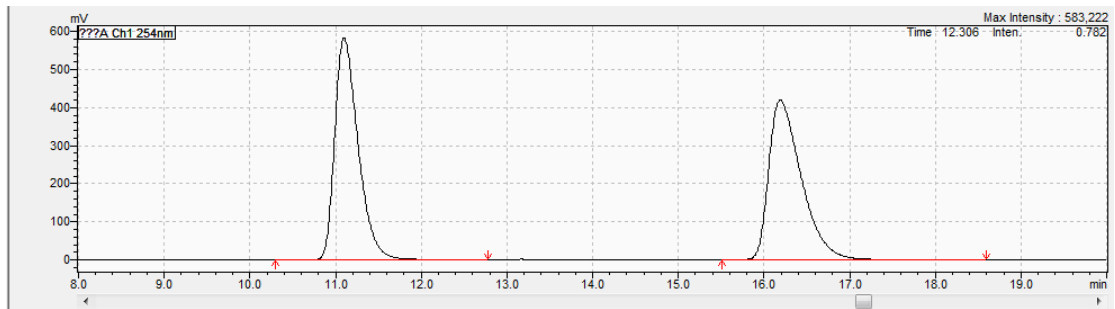


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.617	3138251	178361	5.718	5.718
2	12.678	51709909	2015230	94.282	94.282
Total		54848160	2193591	100.000	100.000



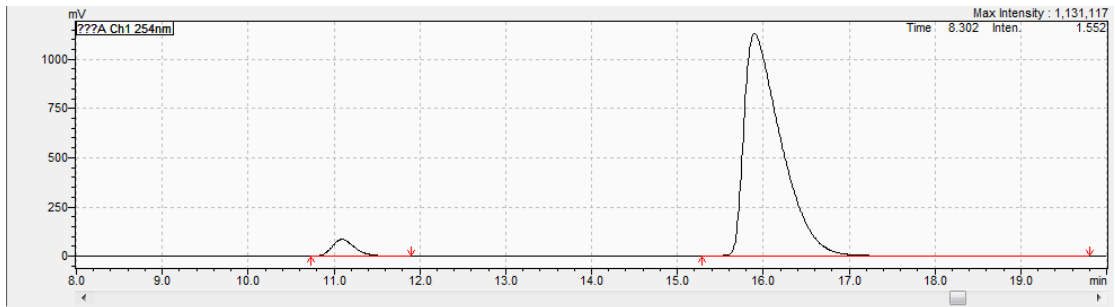
**3ma**



Results View - Peak Table

Peak Table Compound Group Calibration Curve

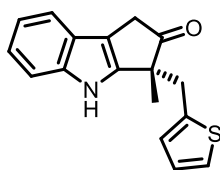
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.099	11110082	583206	49.934	49.934
2	16.191	11139471	420089	50.066	50.066
Total		22249553	1003295	100.000	100.000



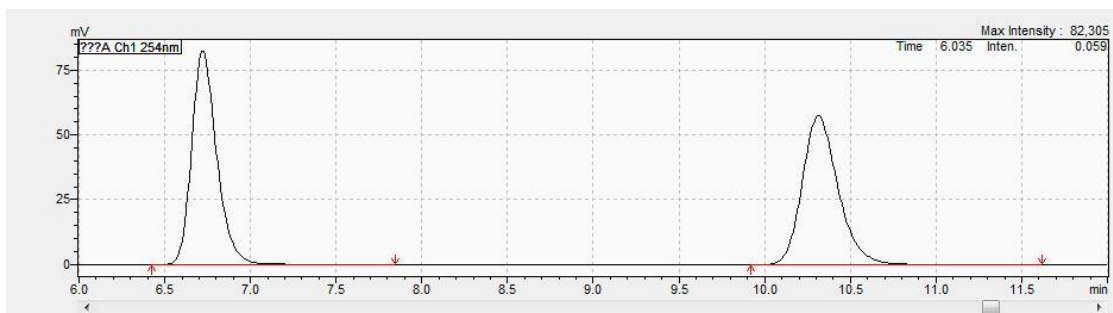
Results View - Peak Table

Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	11.092	1610606	85795	4.530	4.530
2	15.899	33945954	1131127	95.470	95.470
Total		35556561	1216922	100.000	100.000

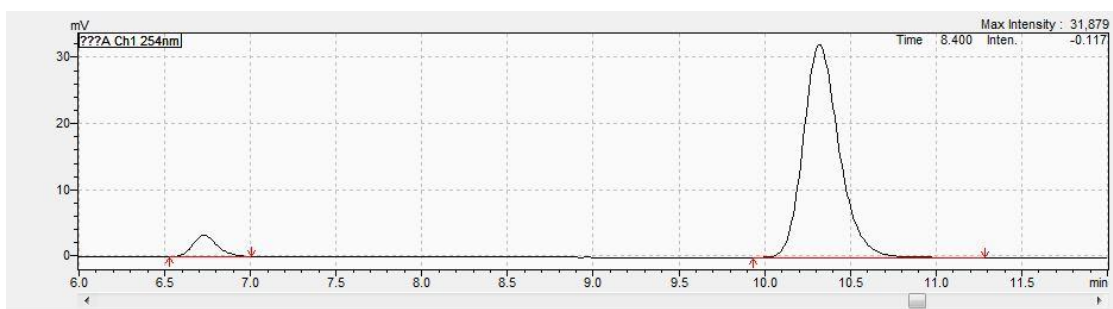


**3na**



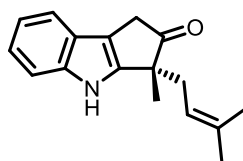
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	6.721	841909	82424	50.117	50.117
2	10.312	837980	57362	49.883	49.883
Total		1679889	139786	100.000	100.000

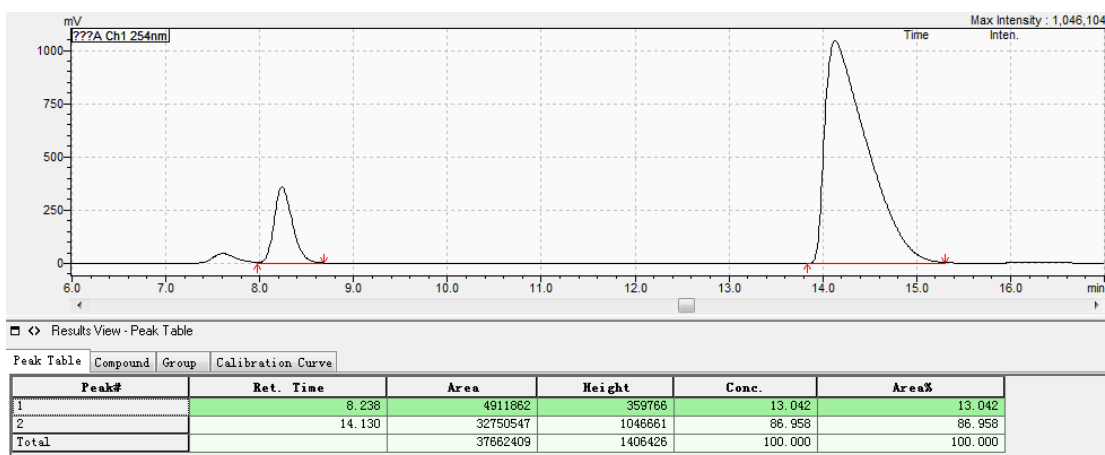
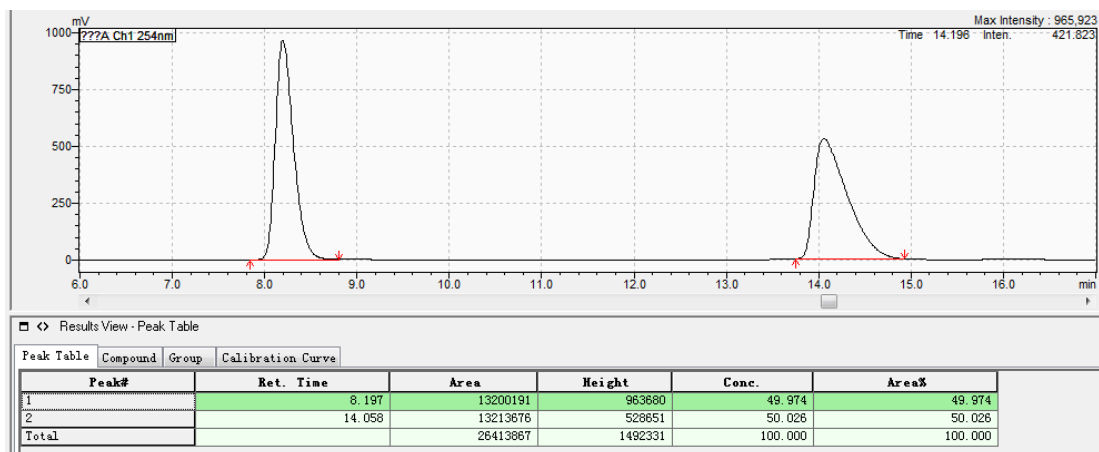


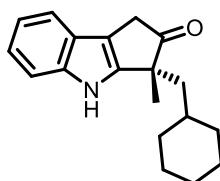
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	6.727	32039	3221	6.410	6.410
2	10.320	487795	32102	93.590	93.590
Total		499834	35324	100.000	100.000

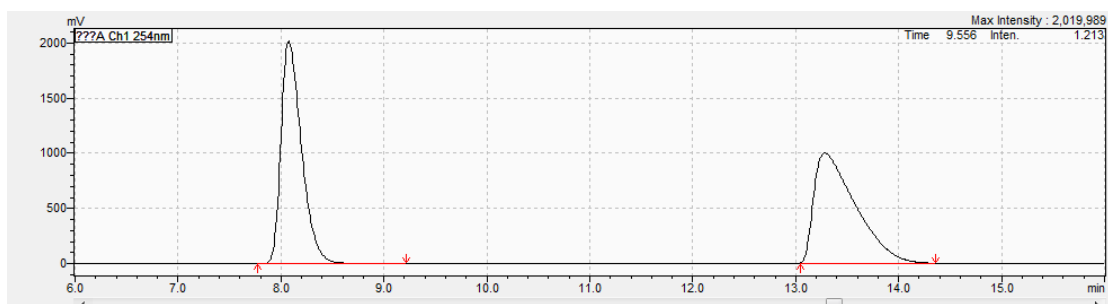


30a



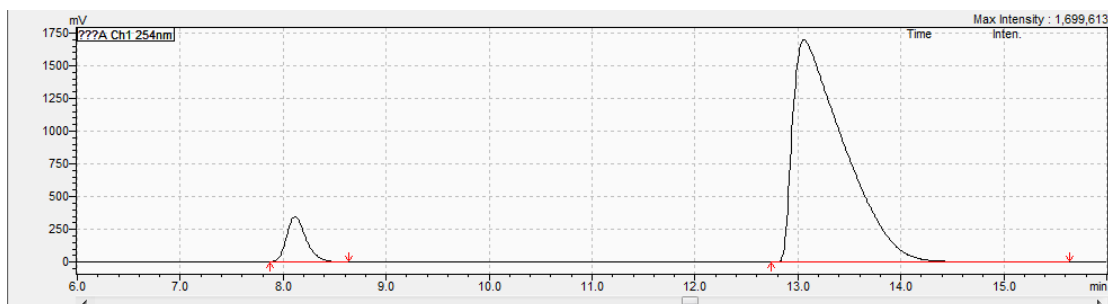


3pa



Results View - Peak Table

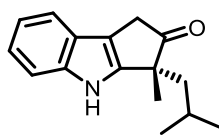
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.076	27957956	2019732	49.996	49.996
2	13.284	27962782	998152	50.004	50.004
Total		55920738	3017884	100.000	100.000



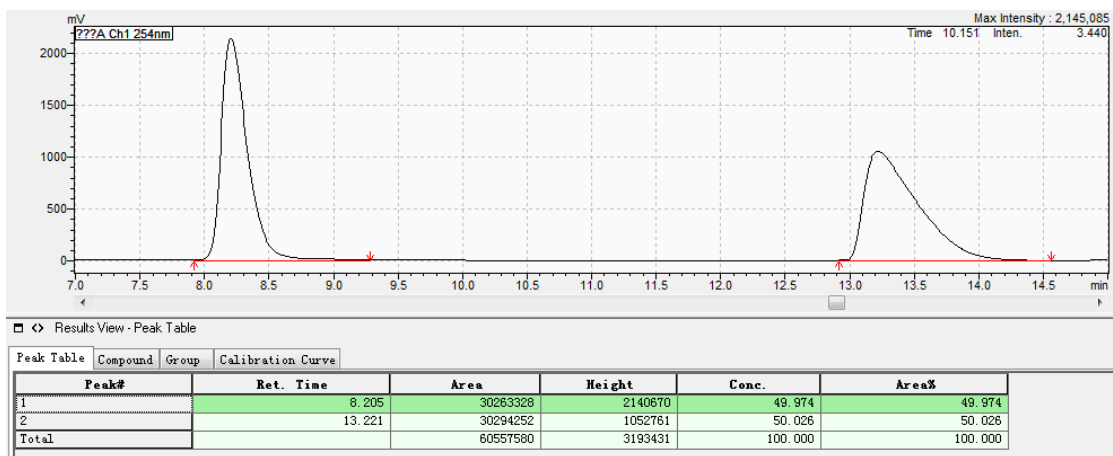
Results View - Peak Table

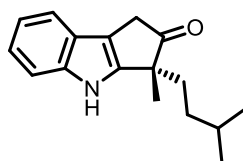
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.114	4572337	345635	7.225	7.225
2	13.060	58710030	1699638	92.775	92.775
Total		63282367	2045273	100.000	100.000



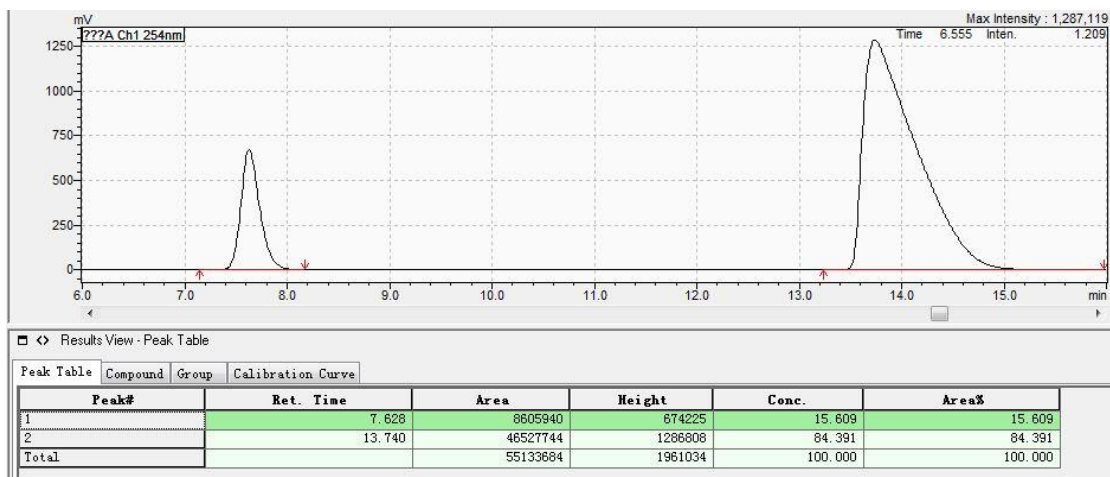
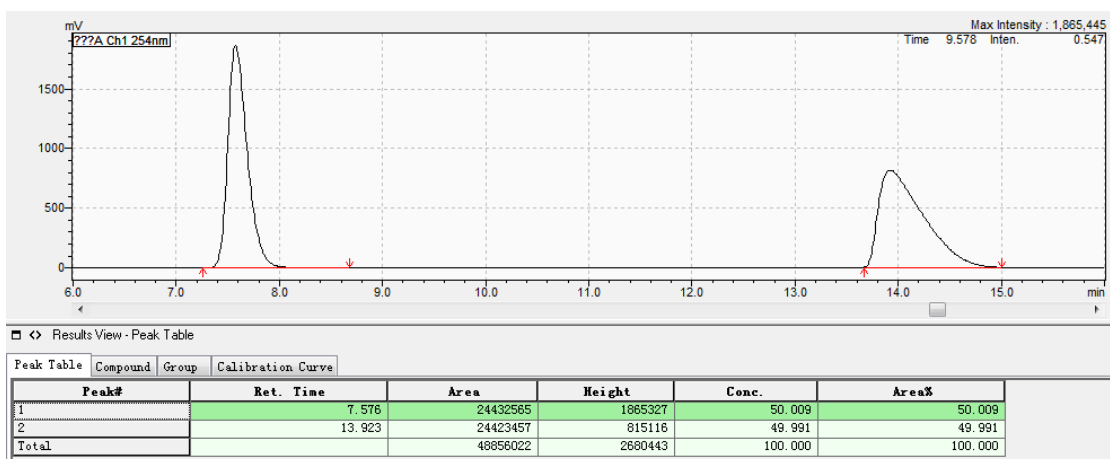


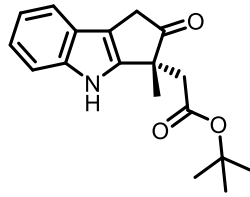
3qa



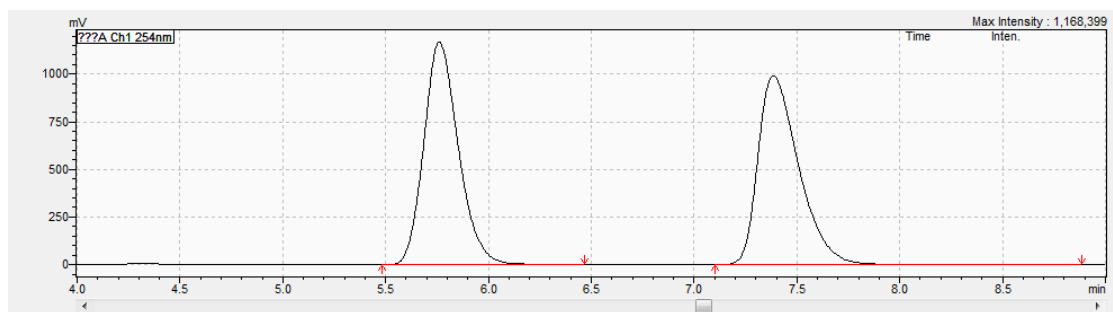


3ra



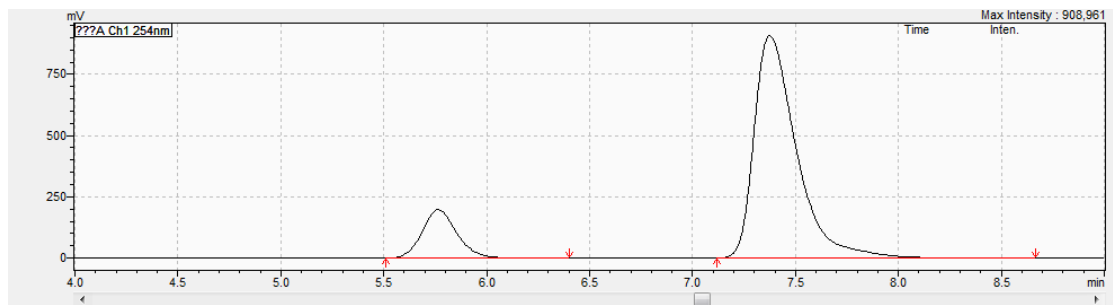


3sa



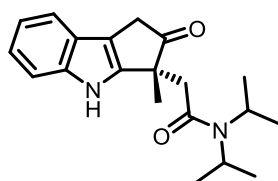
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	5.761	13836170	1187830	50.008	50.008
2	7.385	13631772	991705	49.992	49.992
Total		27267943	2159535	100.000	100.000

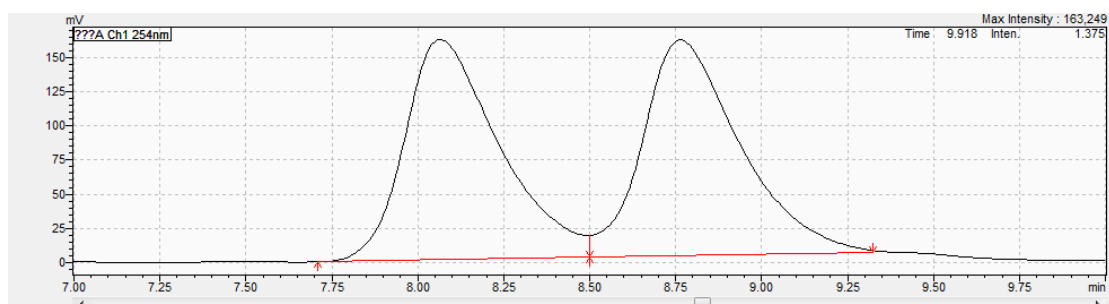


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	5.784	2284346	196740	15.023	15.023
2	7.375	12921780	908659	84.977	84.977
Total		15206127	1105400	100.000	100.000



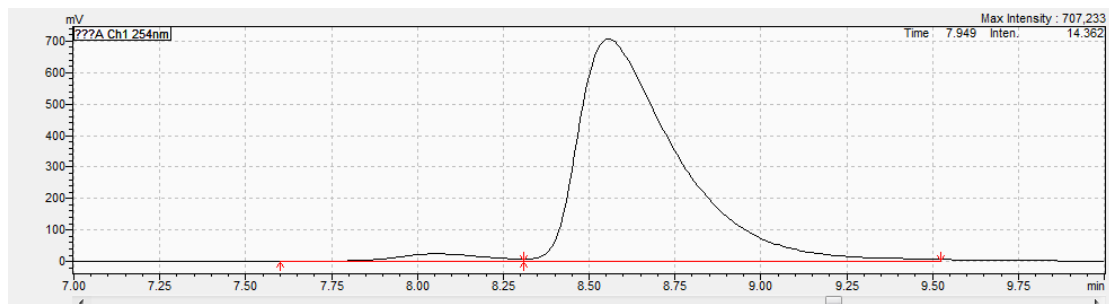
3ta



Results View - Peak Table

Peak Table Compound Group Calibration Curve

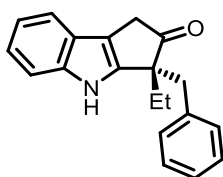
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.065	3094860	161309	49.763	49.763
2	8.764	3124335	158037	50.237	50.237
Total		6219196	319346	100.000	100.000



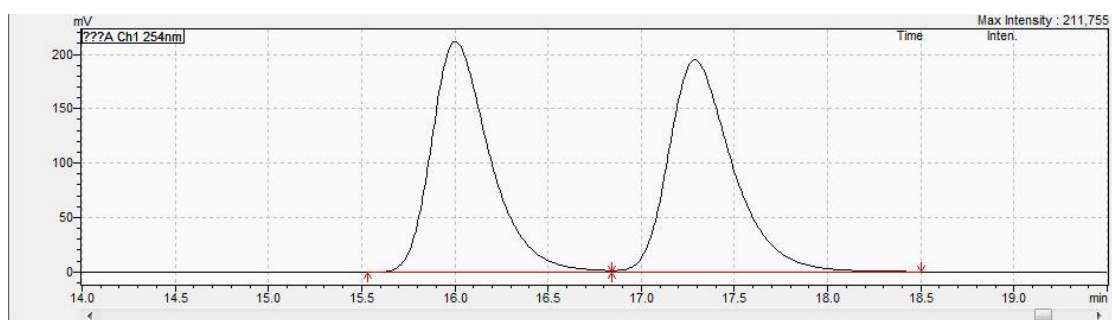
Results View - Peak Table

Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.057	428186	23820	2.978	2.978
2	8.556	13952085	706239	97.022	97.022
Total		14380271	730059	100.000	100.000

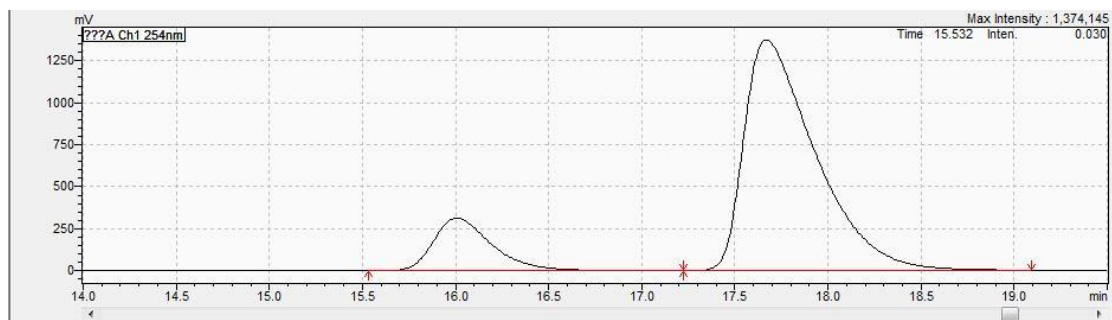


3ua



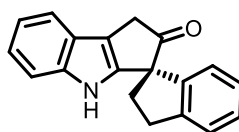
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	16.004	4630872	211999	49.896	49.896
2	17.287	4650182	194681	50.104	50.104
Total		9281055	406680	100.000	100.000

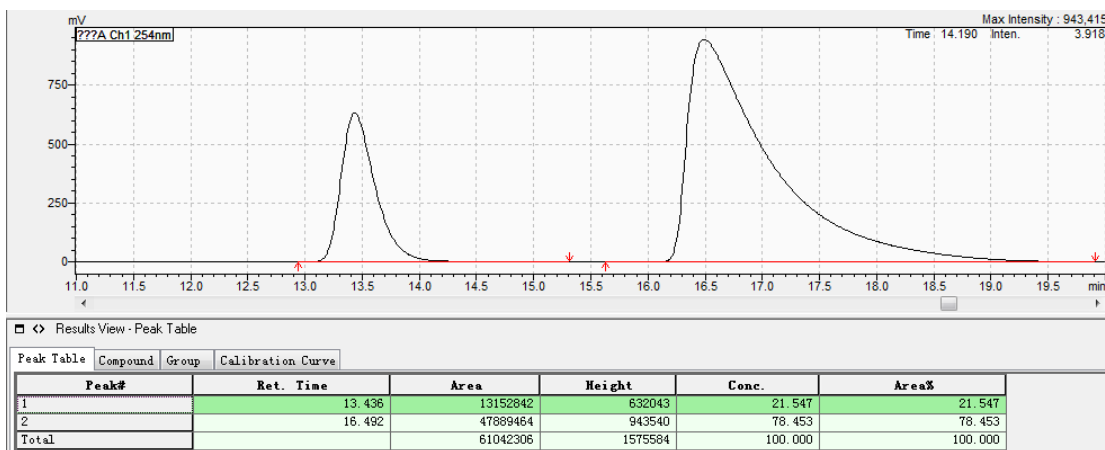
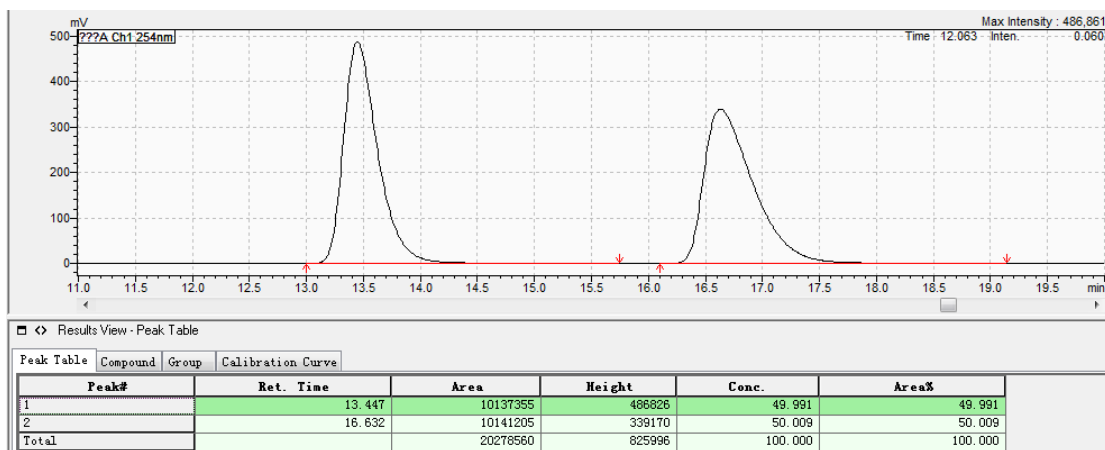


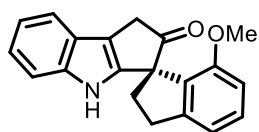
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	16.008	6781977	313854	15.615	15.615
2	17.669	36649665	1373479	84.385	84.385
Total		43431642	1687334	100.000	100.000

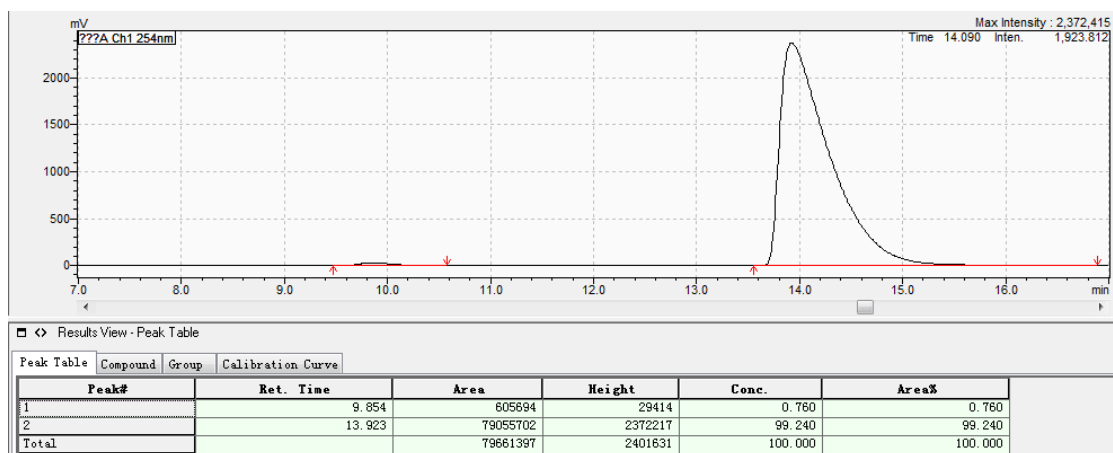
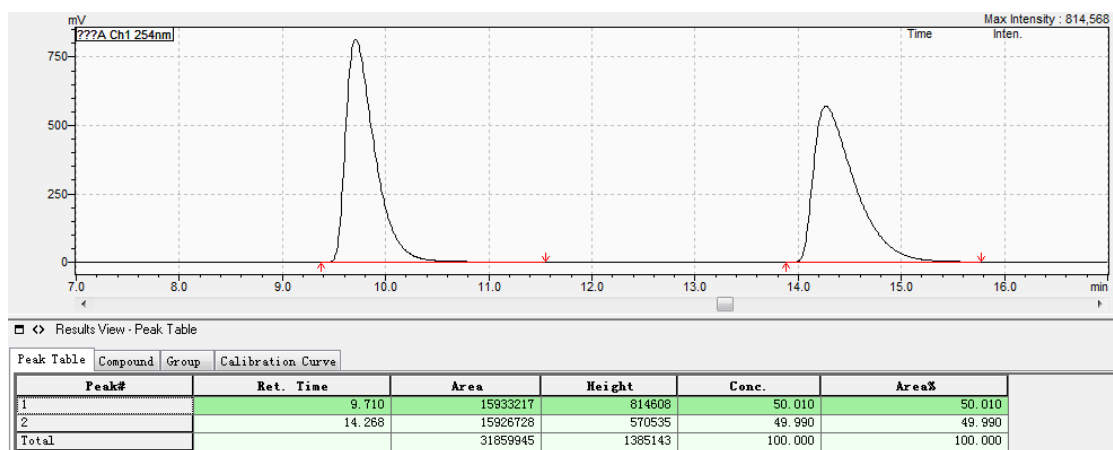


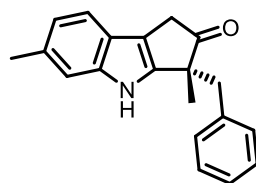
3va



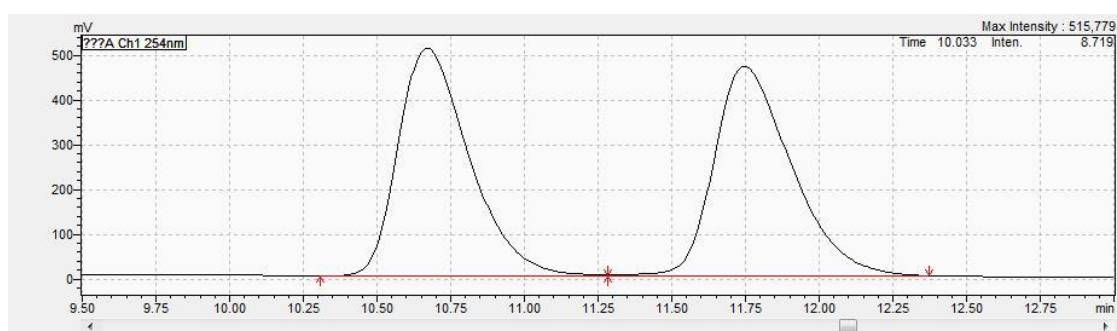


3wa





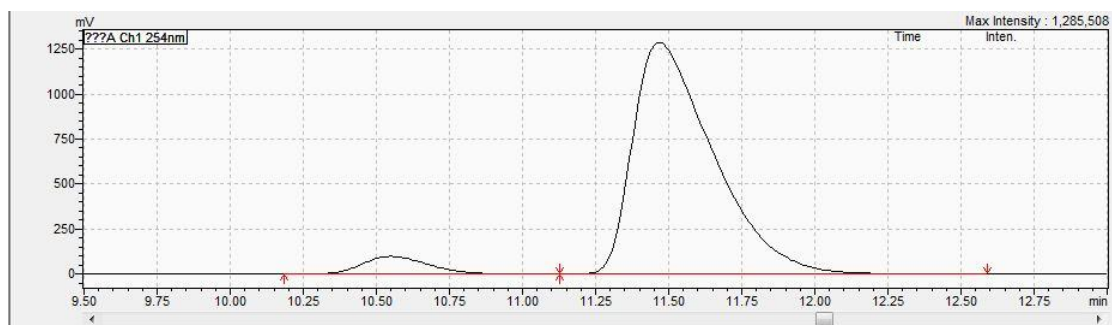
**3ab**



Results View - Peak Table

Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.669	8513331	508544	49.910	49.910
2	11.747	8543949	467522	50.090	50.090
Total		17057280	976066	100.000	100.000

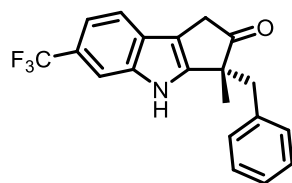


Results View - Peak Table

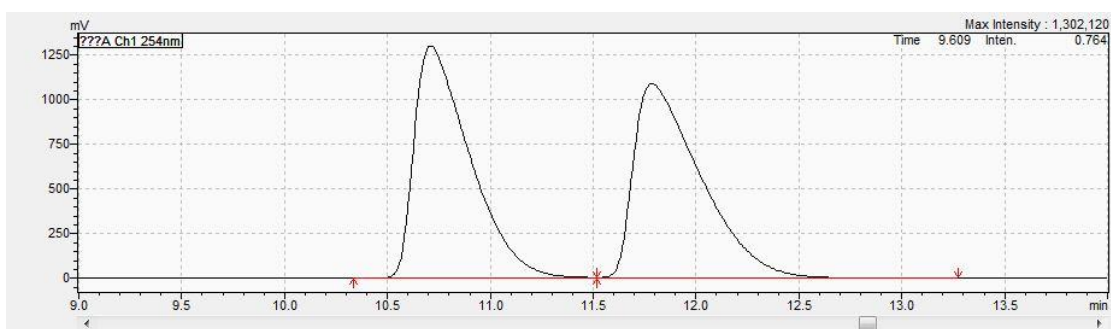
Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.552	1544949	98593	5.916	5.916
2	11.467	24570229	1283976	94.084	94.084
Total		26115178	1382569	100.000	100.000





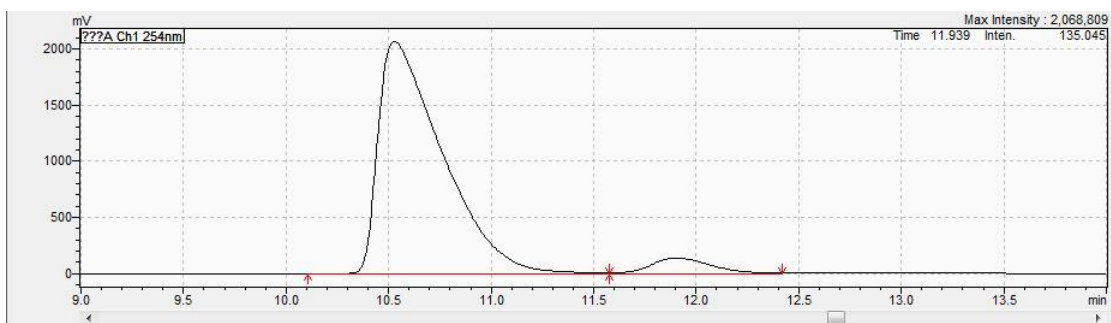
**3ac**



Results View - Peak Table

Peak Table Compound Group Calibration Curve

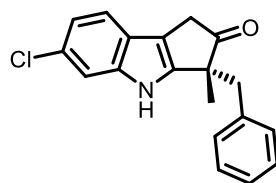
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.710	24580955	1301377	49.900	49.900
2	11.786	24679234	1090882	50.100	50.100
Total		49260189	2392259	100.000	100.000



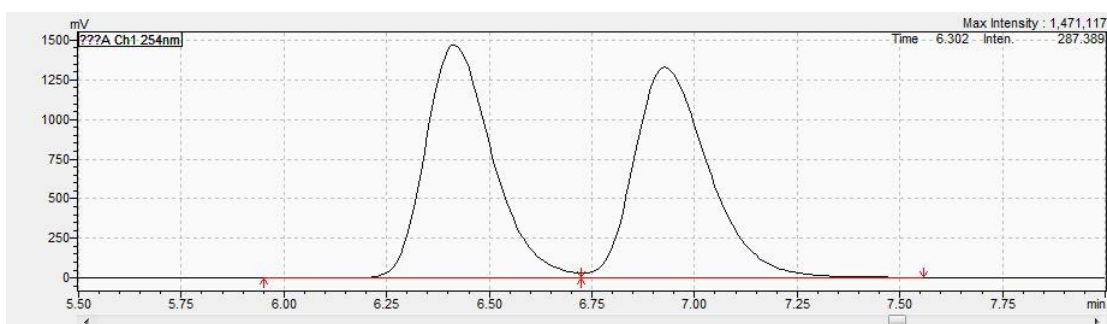
Results View - Peak Table

Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.528	44886380	2068096	94.023	94.023
2	11.903	2853527	139529	5.977	5.977
Total		47739907	2207625	100.000	100.000

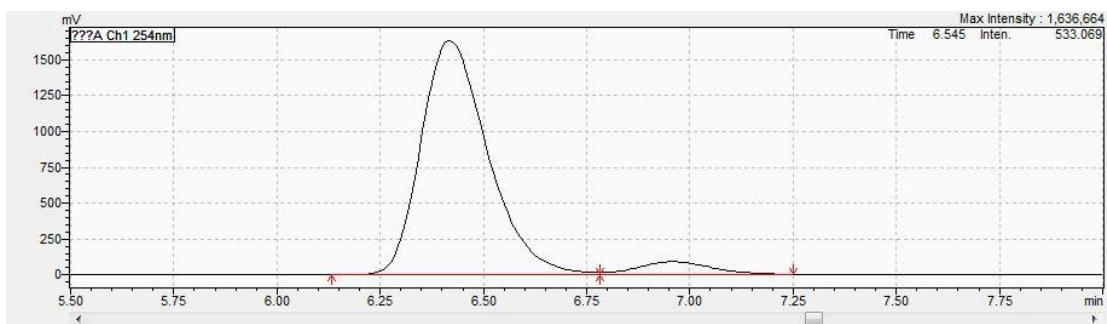


**3ad**



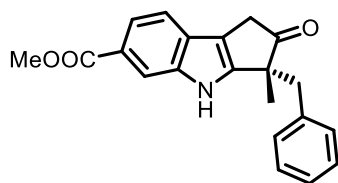
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	6.415	16619033	1469469	49.897	49.897
2	6.929	16687903	1325676	50.103	50.103
Total		33306936	2795144	100.000	100.000

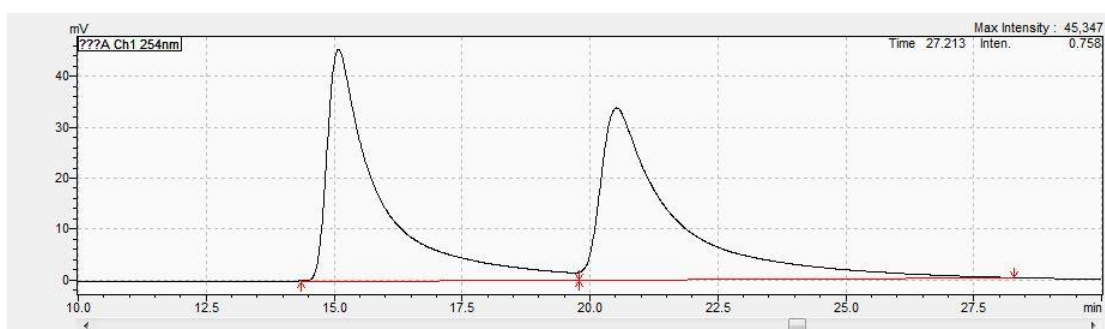


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	6.418	18431811	1835919	94.058	94.058
2	6.957	1164308	90944	5.942	5.942
Total		19596119	1726863	100.000	100.000



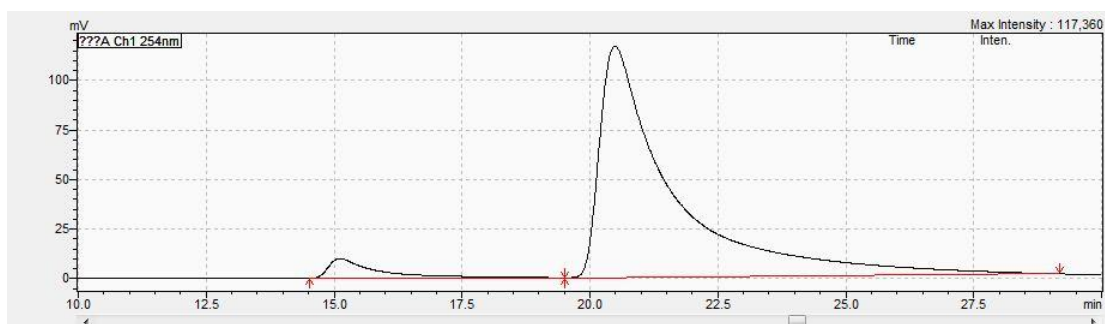
3ae



Results View - Peak Table

Peak Table Compound Group Calibration Curve

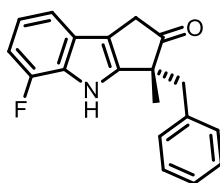
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	15.085	3245918	45548	49.648	49.648
2	20.521	3292009	33768	50.352	50.352
Total		6537928	79315	100.000	100.000



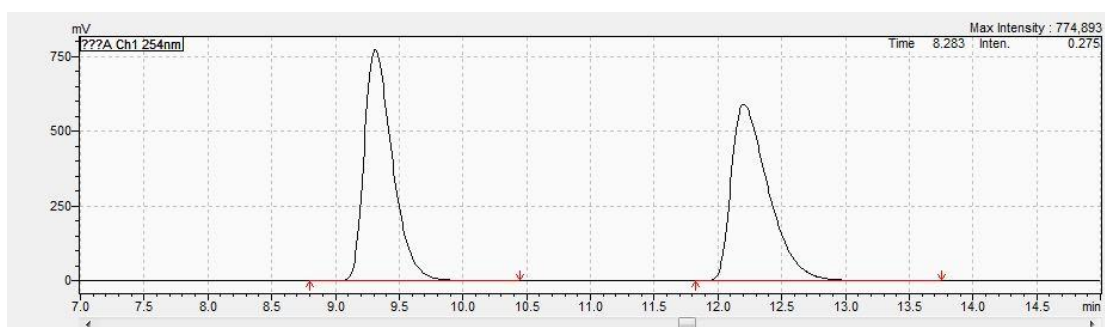
Results View - Peak Table

Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	15.110	659865	10037	5.397	5.397
2	20.490	11566112	116723	94.603	94.603
Total		12225977	126761	100.000	100.000

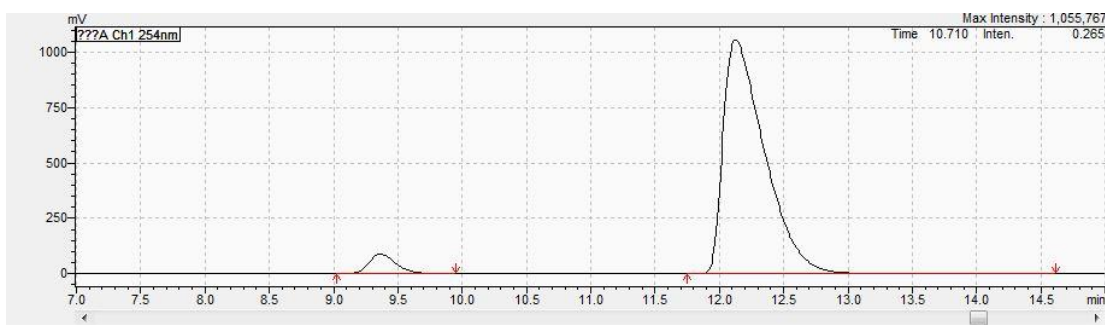


3af



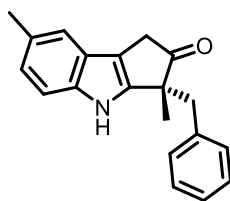
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.311	11964639	774815	49.890	49.890
2	12.203	12017618	590387	50.110	50.110
Total		23982257	1365202	100.000	100.000

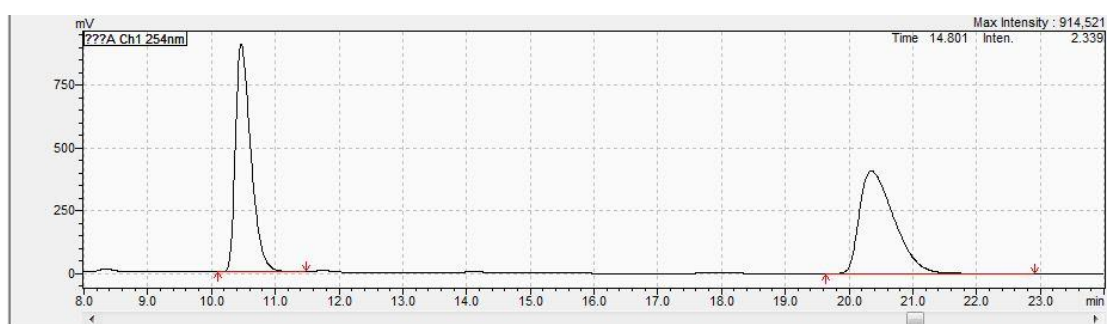


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.365	1317038	89190	5.261	5.261
2	12.126	23716638	1055818	94.739	94.739
Total		25033675	1145009	100.000	100.000

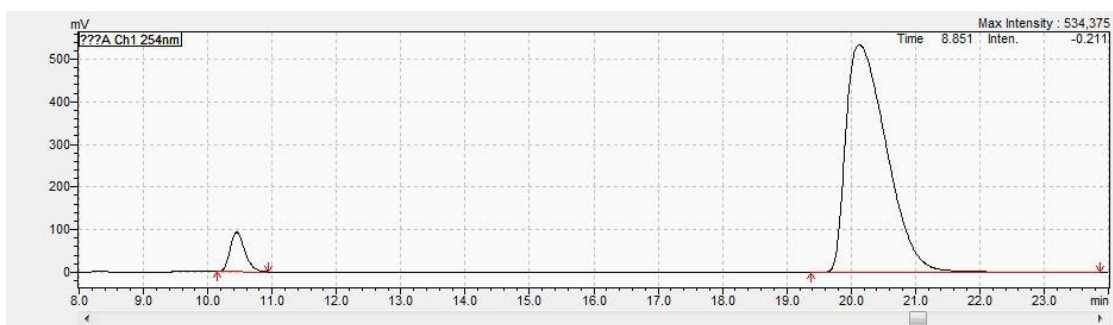


3ag



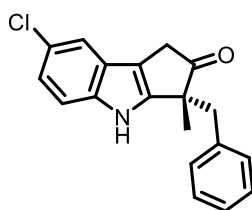
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.467	15342429	907885	50.010	50.010
2	20.350	15336099	408045	49.990	49.990
Total		30678528	1315929	100.000	100.000

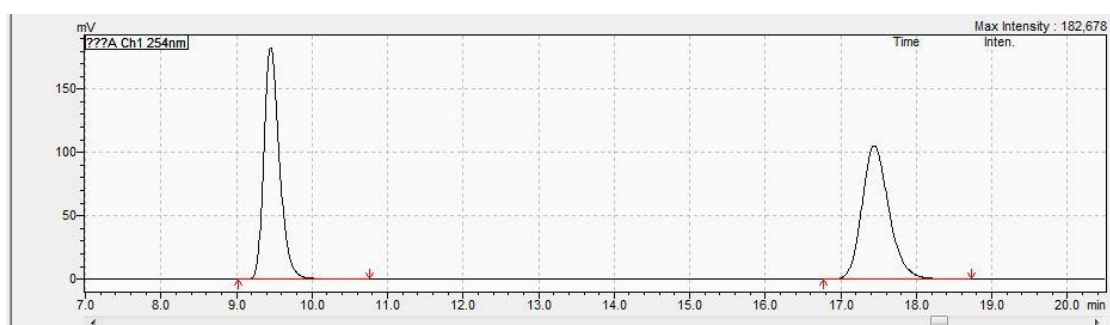


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	10.449	1467734	92682	5.849	5.849
2	20.128	23627610	535687	94.151	94.151
Total		25095344	628369	100.000	100.000

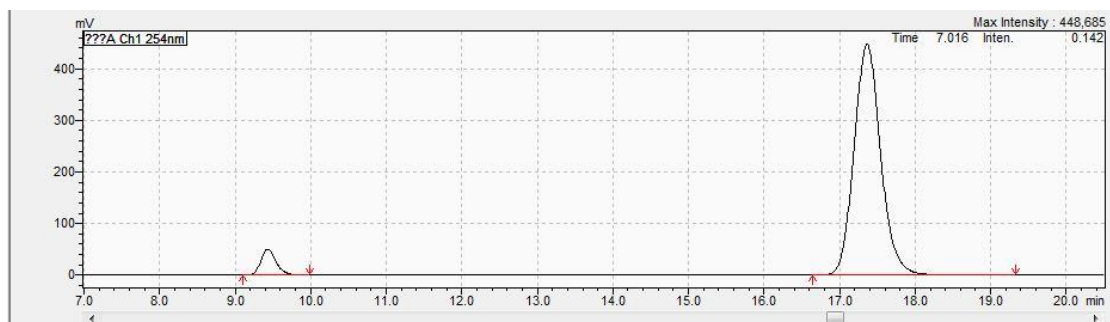


3ah



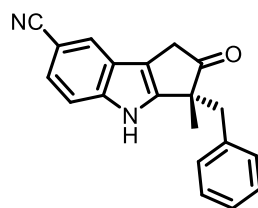
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.452	2622829	182816	49.991	49.991
2	17.443	2623784	105492	50.009	50.009
Total		5246613	288308	100.000	100.000

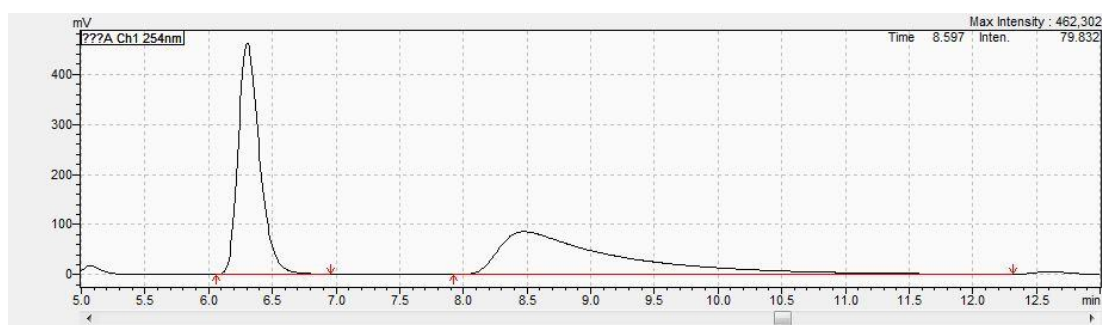


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	9.431	706415	50237	6.033	6.033
2	17.365	11002769	448643	93.967	93.967
Total		11709184	498880	100.000	100.000

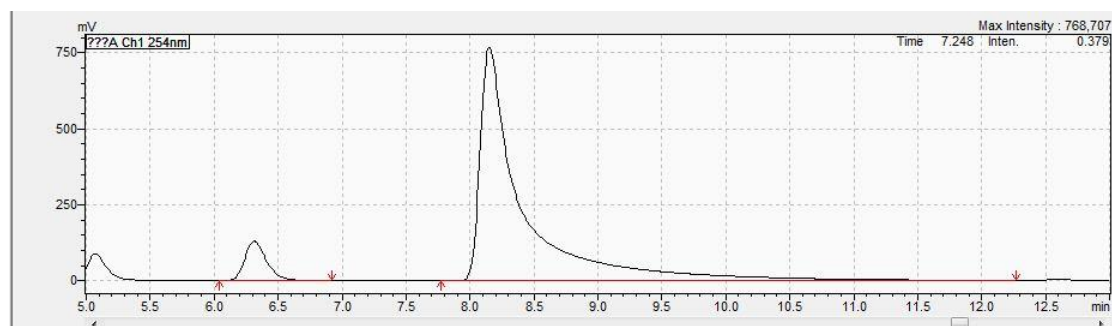


3ai



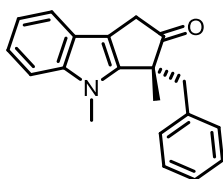
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	6.303	5436135	462020	49.934	49.934
2	8.477	5450462	85413	50.066	50.066
Total		10886597	547433	100.000	100.000

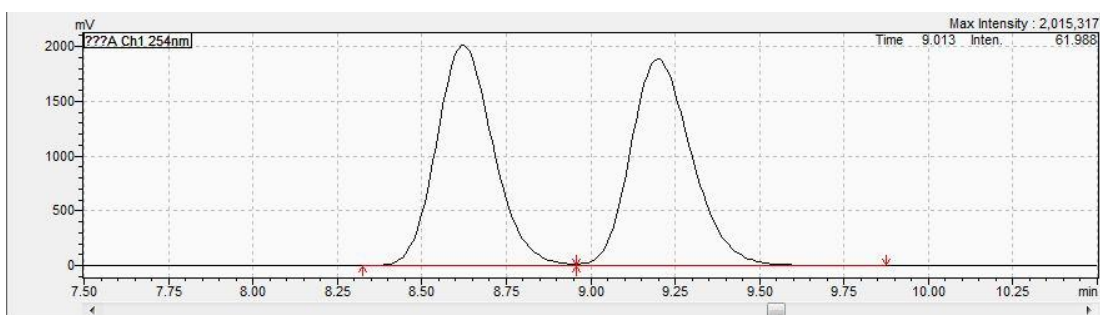


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	6.314	1518824	129302	7.982	7.982
2	8.151	17509818	768545	92.018	92.018
Total		19028642	897847	100.000	100.000



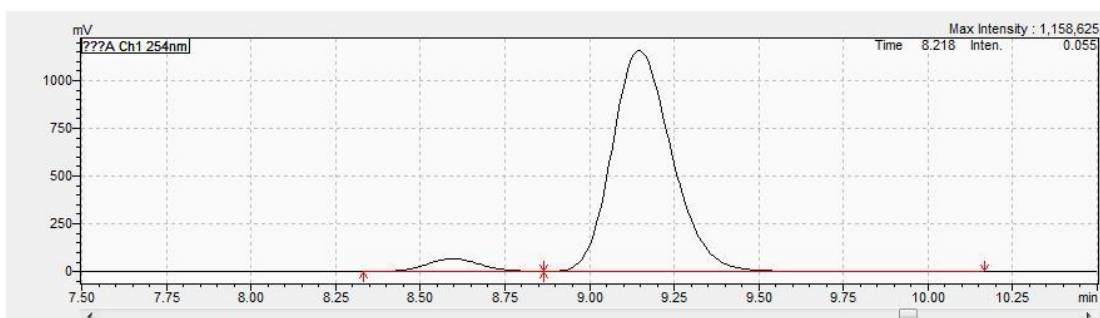
**3aa'**



Results View - Peak Table

Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.622	23618643	2014524	49.828	49.828
2	9.199	23781407	1896805	50.172	50.172
Total		47400050	3901329	100.000	100.000

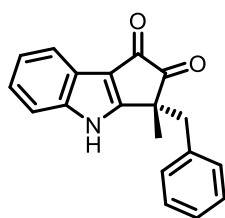


Results View - Peak Table

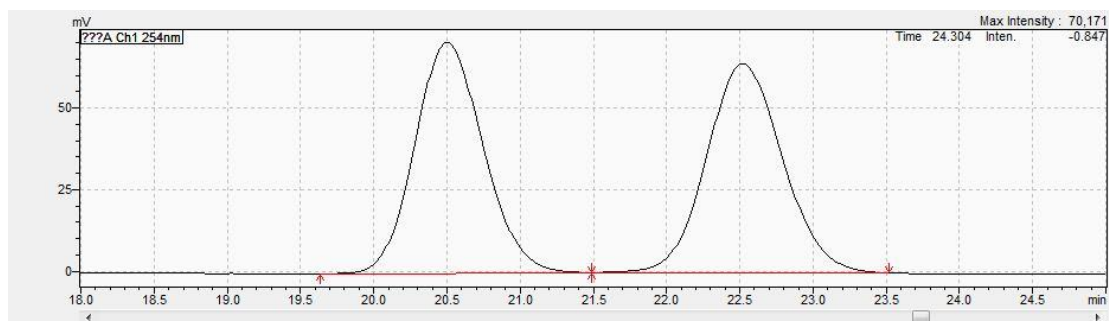
Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.595	758721	67018	5.066	5.066
2	9.146	14219272	1158408	94.934	94.934
Total		14977993	1225426	100.000	100.000



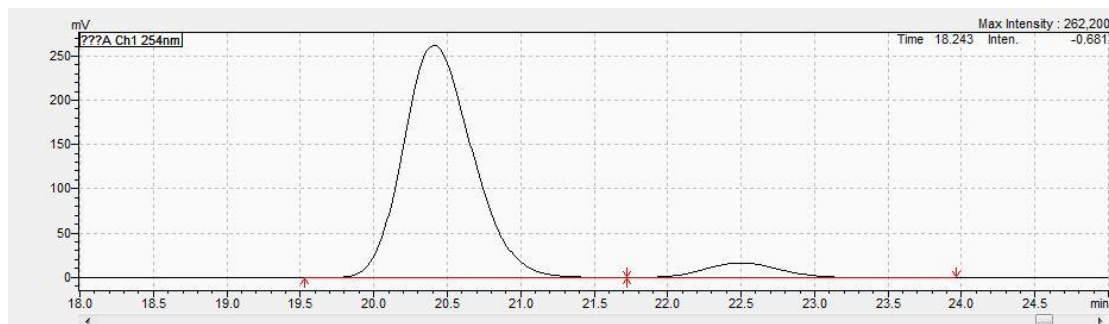


4



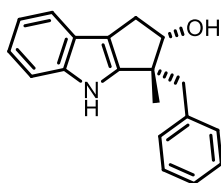
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	20.501	2313382	70867	49.792	49.792
2	22.520	2332700	64223	50.208	50.208
Total		4646082	135090	100.000	100.000

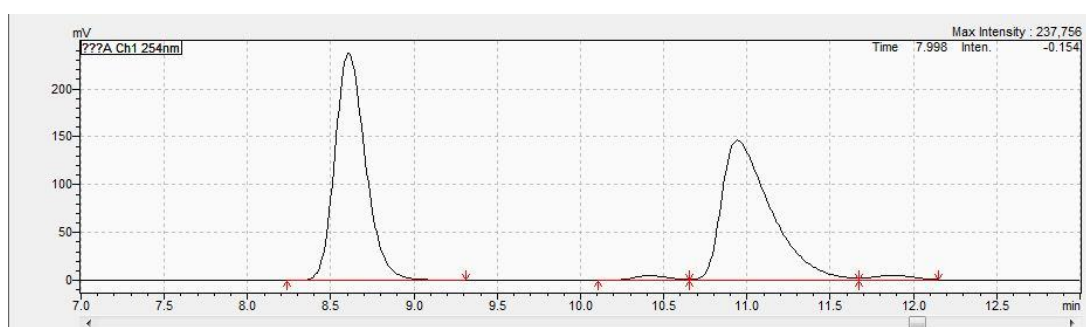


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	20.412	8632331	262854	93.313	93.313
2	22.496	618587	17009	6.687	6.687
Total		9250919	279863	100.000	100.000

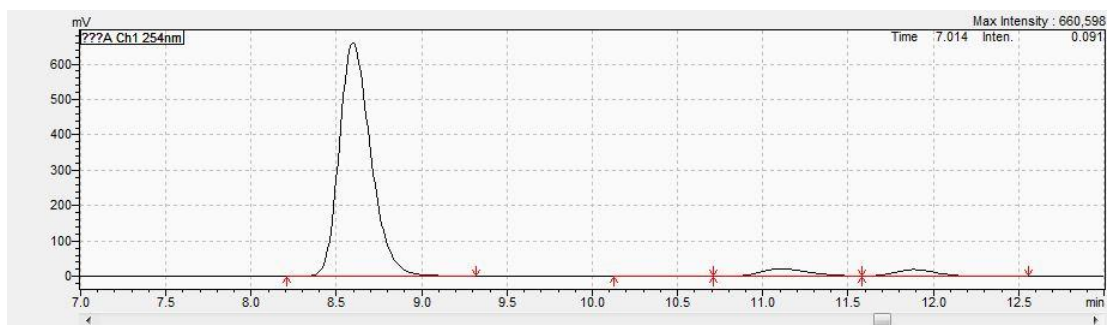


5



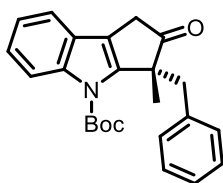
Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.607	3043986	237894	48.871	48.871
2	10.416	75021	4960	1.204	1.204
3	10.942	3028871	146445	48.626	48.626
4	11.877	80877	4809	1.298	1.298
Total		6228555	394108	100.000	100.000

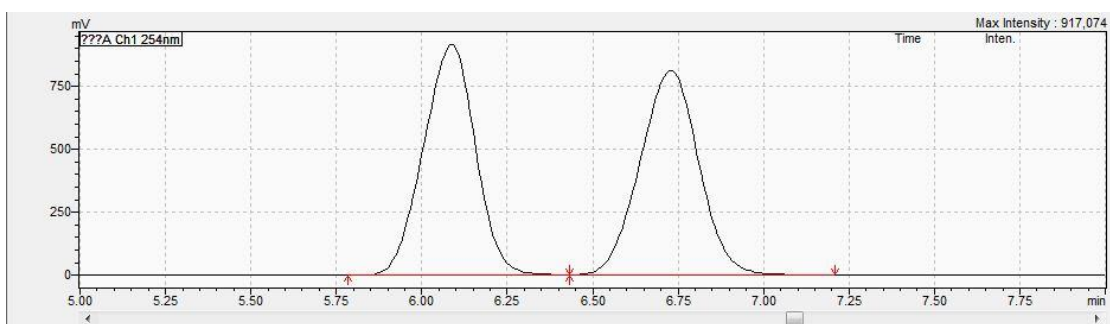


Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	8.597	8533765	660543	91.500	91.500
2	10.422	14334	970	0.154	0.154
3	11.107	440157	21397	4.719	4.719
4	11.868	338291	19487	3.627	3.627
Total		9326548	702398	100.000	100.000



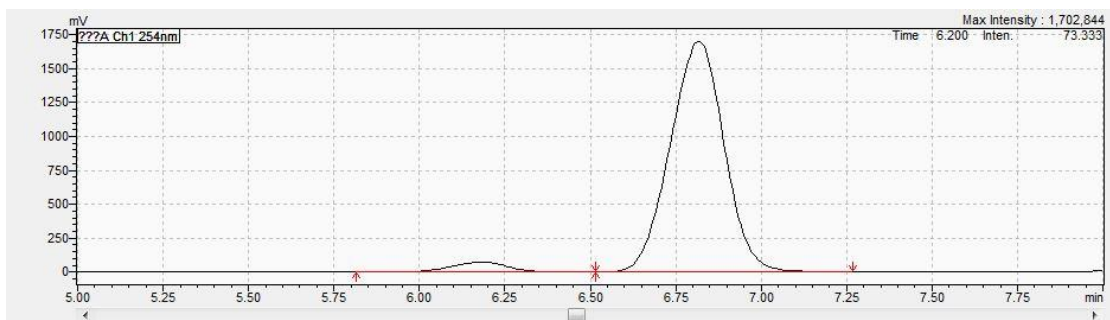
6



Results View - Peak Table

Peak Table Compound Group Calibration Curve

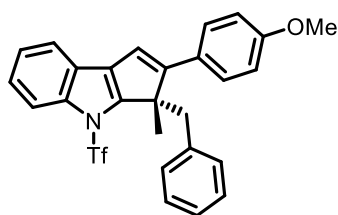
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	6.088	9709901	916621	49.924	49.924
2	6.729	9739633	813481	50.076	50.076
Total		19449533	1730102	100.000	100.000



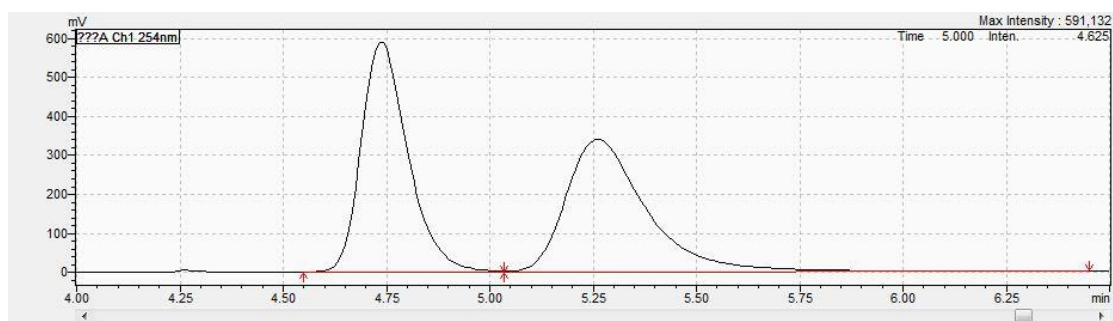
Results View - Peak Table

Peak Table Compound Group Calibration Curve

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	6.184	808858	74184	4.154	4.154
2	6.818	18661477	1701034	95.846	95.846
Total		19470336	1775217	100.000	100.000

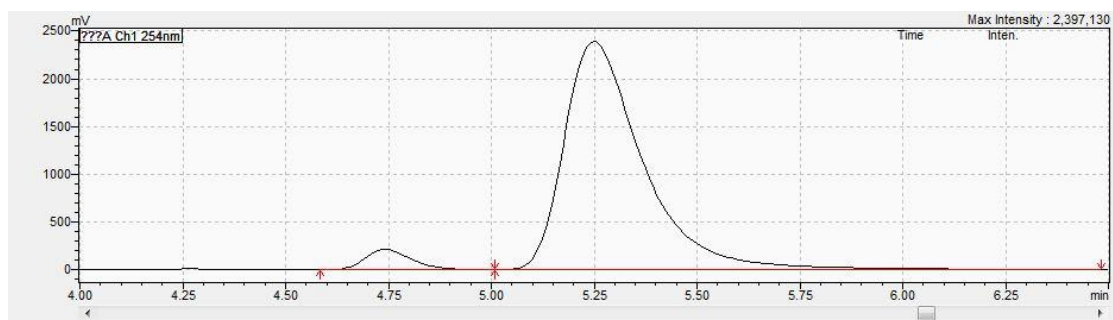


8



Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	4.738	4618004	589291	50.146	50.146
2	5.261	4591082	340715	49.854	49.854
Total		9209086	930007	100.000	100.000



Results View - Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	4.742	1657468	213437	4.956	4.956
2	5.249	31788788	2396122	95.044	95.044
Total		33446256	2609558	100.000	100.000

# 11. Cartesian Coordinates

TS1	-244.19 cm**1 ***imaginary mode***			H	5.27458639665429	-0.54990836192698	-3.59962152089860
H	1.12608260423783	-0.55165120448530	0.98167918222643	H	3.99690474128331	0.70153381333633	-3.60924541058939
C	-0.27744531377416	3.01868026780233	1.52345283730398	H	5.43451171883769	0.89414282627644	-2.56854208851639
C	-0.85012493777562	2.00456587284896	0.54817852394358	H	3.66741895867854	-2.37986483253240	-3.01825547937578
C	0.06758629169983	2.10161293653530	-0.64288196402478	H	2.58240613737697	-2.21175733962244	-1.61048362434985
H	-0.30219362108695	2.05473668516127	-1.66979244873994	H	2.31386637920851	-1.21564081437532	-3.06894386205390
C	1.39006996111804	1.77048836765786	-0.35375050256149	Rh	0.96287955670576	3.97282500533857	-0.06147784218489
C	1.60998145852604	1.53463512400926	1.12716738389917	C	0.31148713158620	5.82798206196497	0.57093589458084
C	1.06761963435712	2.78705973173723	1.78243340290022	C	-0.75024774041864	6.15445947519453	-0.28373118742008
H	1.58505872068042	3.26350565211781	2.61891933490498	C	-1.80599891474768	6.96213251137412	0.14105556019969
C	-0.71477444728561	0.59593780881027	1.17763425757464	C	-1.75077051642776	7.51930327235439	1.41922547183559
H	-1.09768685107649	-0.15277945159375	0.46836708781465	C	-0.66788356515702	7.25942937175856	2.25329080910373
H	-1.36594369797692	0.55922253424454	2.06513135851994	C	0.38516647394946	6.41478021599266	1.85771049911267
C	0.75355995267120	0.30999199039094	1.56428431257336	H	-0.75737945903972	5.76407772841116	-1.30655187905285
C	-1.20799487042115	3.79525878574165	2.39292562791916	H	-2.63891587190583	7.17664287917838	-0.53221380301128
H	-1.83853093032625	3.07851829447610	2.94721709873432	H	-2.54791390880118	8.18224838755554	1.76591410069921
H	-1.87835650005774	4.43853455013305	1.80407699107056	H	-0.62369599207744	7.70994143095945	3.24943206929240
H	-0.66627732701341	4.41226463856287	3.11935801114323	C	4.12090142975979	4.58134797454864	-0.95736906071868
C	0.91998298549191	-0.03707104608748	3.05316301386046	C	3.08559550632265	4.35332404385624	-2.06984001965509
H	0.43473639478157	0.76988847650109	3.63481426811321	C	3.33734676461448	5.37259204718673	0.07259665512959
C	0.20657560837214	-1.34663337742808	3.37735475218628	C	1.83595985729427	5.03484382368071	-1.72598188729185
H	-0.85858433439857	-1.31743742104296	3.10276950208707	C	2.04024828639582	5.82596402870565	-0.53461591511330
H	0.26896449931410	-1.57426794070522	4.45285588313950	H	1.15129695930985	5.32081452064516	-2.52901843209596
H	0.66979629310560	-2.18449314263392	2.82934320626961	H	1.86081560718937	6.90105432574300	-0.47621703126146
C	2.38256104270673	-0.11459125498469	3.48051045796409	O	3.34470672217882	3.76939786252741	-3.10578147183066
H	2.94269918389649	-0.81857254985524	2.84137203891779	O	3.76519087788971	5.69282712395911	1.16796056177962
H	2.46393321856516	-0.47106923855625	4.51899045316812	C	5.21895096948687	5.49536912069324	-1.51663596022561
H	2.88943509887809	0.86065755600796	3.43012786195584	H	5.74478007818457	4.97652819273921	-2.33182003573876
C	2.18084339976146	1.11127426448213	-1.44728448664243	H	4.79561932855510	6.42930408360160	-1.91753671395792
C	3.99969293663337	-0.57889053042395	-1.85050636419724	H	5.94262422803435	5.75074022881776	-0.72968065156835
O	1.82778385698286	1.19178819536422	-2.62043113067300	C	4.67479858326615	3.24151282396355	-0.45382007899707
H	2.66859312699952	1.39458138013638	1.37631016158652	H	3.83127758511112	2.67851643435072	-0.04041739118635
H	-1.89145764159280	2.23645658327527	0.28987659497150	H	5.01365665071783	2.69888077660429	-1.34883913555817
N	3.21250923532972	0.34995113404162	-1.02817732318995	C	5.77902653782479	3.27759458128303	0.56270152795160
H	3.40184358584892	0.32643549623664	-0.03416212787816	C	7.12133802423009	3.35505324703717	0.16900823283277
C	3.08209295165474	-1.66249182554889	-2.42336944664998	C	5.49180109457779	3.19244446096519	1.93147641500901
C	4.71716002176845	0.16644870639871	-2.97745911350980	C	8.14674836488482	3.36683624172810	1.11477111979245
C	5.02700394137071	-1.20887616330059	-0.91291988755130	H	7.36629558259751	3.39643337598293	-0.89603579251411
H	5.65270697196275	-1.92508176231542	-1.46442675606661	C	6.51278790335599	3.20169183911833	2.88004722874167
H	5.68462294147265	-0.43912987486462	-0.47861907483548	H	4.44960911009878	3.11716464987025	2.25350726200315
H	4.53052410031812	-1.74905771000052	-0.09069151834620	C	7.84544453295632	3.29308112423449	2.47480955560281

H	9.18783599889528	3.42545147868086	0.78604908062143	C	4.56094370401100	0.11523448654273	-3.03564894649246
H	6.26733362638025	3.13247339980551	3.94313061838070	C	4.94640704497044	-1.22199882530291	-0.95813460965531
H	8.64785841008006	3.29734968967719	3.21720591123315	H	5.55641044847271	-1.94830152400066	-1.51401430637363
N	1.41002116165678	6.11944217221740	2.72301116968149	H	5.61491358608870	-0.44127748640887	-0.56232729216114
H	2.31589392050171	5.93260139908758	2.28586905015389	H	4.47919715432760	-1.74589787418525	-0.10860368732914
H	1.48382371622352	6.73935044860413	3.52230116154697	H	5.13966140395262	-0.60034006271238	-3.63901722005105
<b>TS2 -240.39 cm**-1 ***imaginary mode***</b>							
H	0.99072802022557	-0.60451063316424	0.95475017190873	H	5.24889485739830	0.88835872982675	-2.66182044120500
C	-0.37572684300968	2.97549065784675	1.53173907861149	H	3.53723304274101	-2.43786796256142	-3.00624919123680
C	-0.95850009887470	1.96860027341099	0.55488485379262	H	2.49753711670121	-2.26413800743437	-1.56567226874185
C	-0.03885887830186	2.06081711581209	-0.63437951588776	H	2.16831971790578	-1.29112301940075	-3.02733835431733
H	-0.40808763972189	2.02207532742246	-1.66176765904857	Rh	0.88329510118414	3.91746275901084	-0.05111637494058
C	1.28144106447406	1.71798614490369	-0.34766032950373	C	0.26621203206376	5.78650382634894	0.56723718801501
C	1.49715882921812	1.47154847511996	1.13251786430319	C	-0.77362104511813	6.12619747115083	-0.30843721057088
C	0.96558310630570	2.72664375514059	1.79284279265131	C	-1.82833160210847	6.94599886932910	0.09654577757691
H	1.48707713751513	3.19656943375090	2.63066057013123	C	-1.79103742166197	7.50138943979397	1.37610127447031
C	-0.83785524843774	0.55738112464360	1.18088961502862	C	-0.72698299265222	7.22990536964680	2.23060807052730
H	-1.23758555656167	-0.18547556977658	0.47468470248751	C	0.32421530320509	6.37371941079952	1.85458878785254
H	-1.48179329673296	0.52887961714425	2.07413091678319	H	-0.76465053046052	5.73612549660111	-1.33155111755011
C	0.62924883301710	0.24974202025547	1.55523213925575	H	-2.64590346652529	7.17052820936041	-0.59208304012838
C	-1.29689166652289	3.76565004181231	2.39902470414212	H	-2.58802631267437	8.17173743608031	1.70876451487317
H	-1.93639857190869	3.05905350794357	2.95615530181288	H	-0.69780768229355	7.67828805213770	3.22827754175432
H	-1.95958870713888	4.41498710066487	1.80806079252155	C	4.06675747083925	4.43388275073766	-0.89001298217168
H	-0.74726701806987	4.37880134414540	3.12295982049615	C	3.04123006149258	4.20506612309319	-2.00682449749230
C	0.79793602953564	-0.12974672150952	3.03581257282629	C	3.28064239402956	5.23578862004493	0.12861544350015
H	0.32660340457765	0.67160425167505	3.63636267483985	C	1.81529779498744	4.94647295642031	-1.69996886937944
C	0.06814749288599	-1.43605151803732	3.33604246730828	C	2.02075518044293	5.73867993746614	-0.50888047637402
H	-0.99796742317855	-1.38655311624461	3.06832256261530	H	1.16167293383730	5.25184115939593	-2.52140354965634
H	0.13348229501294	-1.68782366434945	4.40598513584295	H	1.87162018127120	6.81837105642007	-0.45506166669138
H	0.51689497986428	-2.26817345323299	2.76749929632492	O	3.29499304365294	3.59657567442605	-3.03044795535278
C	2.26135670871099	-0.23663069597175	3.45388156898464	O	3.69149581679518	5.50194858949756	1.24666270324885
H	2.80953321857317	-0.93137110628357	2.79446315191934	C	4.68735906420793	3.18144919711646	-0.30028110255693
H	2.34330000621892	-0.61990835156882	4.48272962316901	H	5.45047389085794	3.45727378504753	0.44176423380202
H	2.77907566392254	0.73357019297714	3.42536629478794	H	3.92911400597341	2.56568009748598	0.19621778056313
C	2.06184296887337	1.05903664930294	-1.44855859600218	H	5.16289614952646	2.58285717911530	-1.08940844255741
C	3.88586542571679	-0.61678347458259	-1.87475137726072	C	5.20298516599707	5.33171354032613	-1.45995252232019
O	1.68132550052773	1.11941444124846	-2.61409038040650	H	5.90663030370488	5.52435530057467	-0.63504404039085
H	2.55352083988005	1.31982293870275	1.38355854319214	H	5.72725650380394	4.72266941748982	-2.21251538314872
H	-1.99737618591975	2.21127451606647	0.29658286717827	C	4.75818164869145	6.63205679491144	-2.07016121192759
N	3.11514061412108	0.31959240942753	-1.04532268673183	C	4.44280515595584	6.71512028763873	-3.43273298299796
H	3.31579748491555	0.29602112665354	-0.05372952556076	C	4.62602524700272	7.78402148805455	-1.28334626277077
C	2.96307979210062	-1.71948780284479	-2.40167856790781	C	4.00018539818198	7.91298894798422	-3.99205446103034
				H	4.54544919528819	5.82573045164047	-4.05980790284607

C	4.18216883667222	8.98347506334386	-1.83926466051030	N	2.31558989354441	0.21210414841671	2.90321599957774
H	4.87886960420503	7.73951877893304	-0.22023142586174	H	1.58350879587495	0.70733899154604	3.39940933079621
C	3.86576767909608	9.05135426089679	-3.19647155749206	C	3.50940285929632	-1.88515123706768	3.36156352113805
H	3.76368915432617	7.95852262563296	-5.05843397278388	C	4.68656674140545	0.33646233513077	3.52954149359216
H	4.09003695284706	9.87225687912383	-1.20955621362132	C	2.90460034509813	-0.27306543314770	5.17646664177533
H	3.52225276469020	9.99163146110763	-3.63530862903890	H	3.65304774280476	-0.71462200270518	5.84980740193370
N	1.32909916930324	6.06667323642977	2.73699660993606	H	2.77807363997310	0.78623274463456	5.45270020995174
H	2.23538745736136	5.84278883238168	2.31831878814376	H	1.94701354822630	-0.79293940895477	5.33671800515681
H	1.40335846108249	6.68599693687817	3.53636937890942	H	5.47753405922837	-0.13140567195123	4.13487937916259
				H	4.99126011626188	0.31444500329321	2.47451362981667
<b>TS3</b>	<b>-244.90 cm**-1 ***imaginary mode***</b>			H	4.58805885605899	1.38689397095067	3.84383188221438
H	-0.57315046637262	-0.86164990843769	0.39217558372812	H	4.26773980701205	-2.35709540262374	4.00429253431169
C	-0.6644726579085	3.01361934297315	0.21062294033685	H	2.55419622807275	-2.41290976459018	3.50673423997127
C	-0.05947258701986	2.09512152463771	-0.83834000313394	H	3.81593472304737	-1.99770049542451	2.31336298295936
C	1.28214400115471	1.73546191048057	-0.25530909736864	Rh	1.27174126690993	3.19314560954316	1.40630442525900
H	2.19360380330789	1.68388158987481	-0.85319726334048	C	0.89452514629825	4.52732573885495	2.94914869084391
C	1.18309987903705	1.10444894871938	0.98164182217570	C	1.32858028774176	3.80040061164219	4.06577193770245
C	-0.25559353499371	0.96990904991007	1.46382891987133	C	0.70801128856719	3.93303880149829	5.31021950871211
C	-0.75518780384190	2.40464526544635	1.45415991176763	C	-0.31296869888621	4.87288031302569	5.44865624437233
H	-1.36864959311228	2.81060616045252	2.26251442765004	C	-0.69077921506920	5.66786103312405	4.37058011217223
C	-0.93323259484863	0.82382474958297	-0.94333110944071	C	-0.08752670440277	5.53703431504109	3.10355941827828
H	-0.49450826883434	0.15189263410667	-1.69588318075540	H	2.16415460390571	3.10072914806669	3.96500748625739
H	-1.92474985492089	1.12166753546796	-1.31948525490110	H	1.04096405249251	3.32895894179142	6.15714819954009
C	-1.05757776463158	0.13032459234507	0.43080498912085	H	-0.80588389971580	5.01235479834403	6.41453785041660
C	-1.40283535814689	4.22992299950082	-0.23073056446059	H	-1.47233485664518	6.42334584597162	4.49494548095017
H	-2.25749331240794	3.91398862917820	-0.85451804113434	C	3.31307969855209	4.74885937052412	-0.58254304539090
H	-0.76661208903674	4.87405973798262	-0.85552470536913	C	2.26822540155774	5.39939621132956	0.31135413298647
H	-1.77154971875767	4.82052351490474	0.61620885467196	C	3.82542521291739	3.59898462899989	0.29749095893585
C	-2.5220849698229	-0.08311320155479	0.84887371844552	C	2.50237606207459	4.96318704807510	1.73112811932717
H	-3.02644487043284	0.89937118627697	0.77659749142055	C	3.31687026923037	3.77101753917200	1.65584367758014
C	-3.21816754156530	-1.04238015178696	-0.11285526190228	H	2.63085104227888	5.76235734451479	2.46451650361643
H	-3.15736378704145	-0.70149056813239	-1.15723991339856	H	3.86419680537552	3.34850018131506	2.50171771988113
H	-4.28388635693019	-1.15009368990397	0.14216755251109	O	1.45811966490820	6.23518193415561	-0.05957116852051
H	-2.75784673913821	-2.04343765034552	-0.06032846034404	O	4.60137496898439	2.74810503048966	-0.10296679026943
C	-2.66599343891166	-0.58351832853088	2.28269500748630	C	4.49258313682728	5.72888372956607	-0.71412780471329
H	-2.08286358954777	-1.50701403988190	2.43849446820440	H	4.17503537981008	6.64926582703281	-1.22328147019597
H	-3.71896202888611	-0.81468498466604	2.50626779209515	H	4.90036153864770	5.99573211543159	0.27293842312285
H	-2.32998552001672	0.15640067542286	3.02418251399281	H	5.29228254167016	5.25805869390682	-1.30485648927259
C	2.33214149519189	0.32828802973402	1.55998359086748	C	2.80009072041220	4.26062224162363	-1.94841070844279
C	3.36230263886247	-0.40649602357703	3.72642820079561	H	3.36356592950988	3.34354751112771	-2.17897911055838
O	3.20340437631166	-0.14617240428543	0.83833593145805	H	1.74376277013164	3.97522937210683	-1.83795751722717
H	-0.30460401246462	0.52230979556292	2.46230702530061	C	2.94361287484863	5.20600381944387	-3.11141112652634
H	0.02695494216292	2.59747158569276	-1.81031397979453	C	2.15026333477720	6.35604263488236	-3.22727514351788

C	3.88192013962526	4.94299831246260	-4.11661378664761	O	3.12591360647037	-0.06924732242880	0.71732715473894
C	2.29377148153448	7.21453567997606	-4.31602961896212	H	-0.31816802229978	0.46856494540471	2.49555427397914
H	1.42769344535592	6.58046265692779	-2.43921656419165	H	-0.26344159178382	2.62676834184016	-1.74667890041524
C	4.02811719412474	5.79931204011428	-5.20887071507619	N	2.32017264197056	0.26434357771853	2.82087766037853
H	4.50625684703532	4.04754692669821	-4.04222663695885	H	1.59783924781616	0.74403125373151	3.34569526461070
C	3.23310837645591	6.93996895936208	-5.31223586343595	C	3.60569587372594	-1.78719255560950	3.23494327631324
H	1.66645892552561	8.10715319356195	-4.38908586265912	C	4.70841524383888	0.47465613191150	3.35376898397105
H	4.76611327553715	5.57126659961959	-5.98266616761047	C	3.01397503373011	-0.19219461413842	5.06962911614955
H	3.34334808851797	7.61289709678004	-6.16661464220752	H	3.80173330614068	-0.60680042678607	5.71466955460382
N	-0.4635733523810	6.33853067201297	2.06620317775977	H	2.86242515385583	0.86289702903078	5.34928769905875
H	-0.98465514047563	7.17541170565609	2.29481243301968	H	2.08095474999670	-0.74311726172601	5.26679005891257
H	0.16030566099077	6.40976718156995	1.26013377273658	H	5.53863366289055	0.03550695318281	3.92720741778876
				H	4.97235040268282	0.46152137283537	2.28752630953112
<b>TS4</b>	<b>-244.50 cm**-1 ***imaginary mode***</b>			H	4.58720335125560	1.52150160586813	3.67219266104608
H	-0.62453782511627	-0.88291929306629	0.40423011605614	H	4.40556984561445	-2.22901321134482	3.84804523889793
C	-0.86112346964290	2.98783210316639	0.31381890760458	H	2.67698920849158	-2.34897123440384	3.41903400347420
C	-0.28475949813798	2.10527929536227	-0.78117254466668	H	3.87446512378386	-1.89176805881246	2.17554434795237
C	1.09566118244379	1.77615756855396	-0.27343311790123	Rh	1.12613127446918	3.20242606819713	1.41721679221196
H	1.97709953847177	1.77261417154379	-0.91791823089532	C	0.78599384699773	4.45068155061355	3.04002220432141
C	1.07796619377052	1.12376890302803	0.95640597854100	C	1.29009808479884	3.69030327710349	4.10366117724924
C	-0.33072858137276	0.93460963053626	1.50439453672577	C	0.71009759654321	3.73484826690172	5.37337862571001
C	-0.87445203668477	2.35354576111426	1.54764030176310	C	-0.34496055311799	4.62008647568053	5.59303312604572
H	-1.45745735834366	2.72586306617332	2.39376314383956	C	-0.79110902972158	5.45216751612894	4.57017838041919
C	-1.12909206412553	0.81365154827718	-0.86637926520376	C	-0.22635520234647	5.41151551020538	3.27986807766865
H	-0.72221184217015	0.17204207543954	-1.66206087521821	H	2.15228310330874	3.03745709424559	3.93773019295206
H	-2.14960182727871	1.09459849540807	-1.17150865653680	H	1.09854649640599	3.10522066632542	6.17707477140124
C	-1.15027188259316	0.08450216468074	0.49413995886326	H	-0.81084907873141	4.68865606122242	6.57972157784741
C	-1.64627438839158	4.19496927594676	-0.06796002654091	H	-1.59839334800426	6.16646891538625	4.75814091301985
H	-2.54153462398547	3.87040922593458	-0.62736063306992	C	3.00798237385072	4.91406299335770	-0.57939471735583
H	-1.06672876778335	4.84565437308403	-0.73978700741404	C	2.04911390240525	5.52519273865178	0.42865937738680
H	-1.95722411289346	4.78062627858334	0.80531041540936	C	3.58998057780709	3.72525446226074	0.19084783070805
C	-2.57897162795932	-0.20706348404834	0.98212095767850	C	2.34845534807501	4.97735027607927	1.79273031052219
H	-3.12898484071664	0.75323374013026	0.96772479841551	C	3.16690434379364	3.80343753327845	1.58697612460721
C	-3.28273051020311	-1.16880429254806	0.02842619970483	H	2.51039109540386	5.71801347866428	2.57829613422022
H	-3.29551395664710	-0.79396250173070	-1.00596578455672	H	3.76685923305509	3.32977089200338	2.36714139100201
H	-4.32650058529678	-1.33534569499544	0.33689663043085	O	1.24740328661564	6.40651949546950	0.16007813879075
H	-2.77441810184334	-2.14780392948765	0.02298774036533	O	4.35150756222216	2.91249904816359	-0.30933856357215
C	-2.62105946334027	-0.75516763205560	2.40497901213658	C	2.35427325845853	4.55940939086927	-1.90306221162460
H	-1.98522727623665	-1.65170748636679	2.49992952141734	H	3.05521333011189	3.97625938917391	-2.51819569975511
H	-3.64773031820480	-1.04565900061726	2.67641993577152	H	1.44408285676591	3.96718155155249	-1.74894623334191
H	-2.28182576345418	-0.02057890178308	3.15027738213773	H	2.08205168286822	5.47234650106691	-2.45215750619934
C	2.27502402969290	0.38002788371393	1.47796653491652	C	4.16463976347275	5.92261199071244	-0.84674170939259
C	3.41990324345824	-0.31396055434911	3.60307569213492	H	4.82218536880842	5.44707510164474	-1.59079018934635



H	3.71650275199585	6.81168049462088	-1.31749515083751	H	2.09070048899803	0.14529782823964	3.43281101308074
C	4.96593865159236	6.31932227567394	0.36195022623910	C	2.12323791567571	1.13055509220897	-1.32649435867789
C	4.58431643041195	7.41011104387211	1.15382696155106	C	4.30204780314221	-0.12509920202402	-1.49445712431416
C	6.09639317092060	5.58291922543405	0.74025865722747	O	1.79332596695653	0.98644446886421	-2.50030879471266
C	5.30701210503765	7.75076817039136	2.29739768342272	H	2.15445092829522	1.00037419904236	1.49396831954948
H	3.71031253302373	8.00251122083406	0.86759062447583	H	-2.10696247914609	2.49219093900828	-0.02801976331049
C	6.82016254288090	5.91960493407655	1.88300114139854	N	3.30110390945938	0.71255983438611	-0.82033826951971
H	6.40742462275817	4.73094437758505	0.13019933169905	H	3.46164797293920	0.88632591096086	0.16330898560926
C	6.42592723117503	7.00407555281108	2.66761049331084	C	3.67169415694552	-1.46915492218959	-1.86992908486297
H	4.99729859322461	8.60840337984047	2.90025590053979	C	4.85585508794503	0.57107729977748	-2.73795483018147
H	7.70060660247918	5.3371357088280	2.15989584739315	C	5.42375618866740	-0.34205235137505	-0.4807377687052
H	6.99447226289745	7.27150531434631	3.56201313864883	H	6.20490279892705	-0.98426186521227	-0.91185620967593
N	-0.67262169252215	6.24681357907665	2.29461918976449	H	5.88516647954179	0.61625504248671	-0.19408271737305
H	-1.20968537401744	7.05164912359221	2.59279961416107	H	5.04052762049878	-0.83167215687533	0.42897583535120
H	-0.05010039976985	6.41277016610159	1.50140421260918	H	5.62160296530539	-0.06436952018157	-3.20790989882173
				H	4.05513264301729	0.76360351925594	-3.46297975772795
<b>TSS</b>	<b>-311.90 cm**<sup>-1</sup></b>	<b>***imaginary mode***</b>		H	5.31593577210586	1.53468617095045	-2.47367244636330
H	0.48269263719537	-0.67286036849949	0.65075455714869	H	4.41819333588222	-2.11816511018028	-2.35223907700446
C	-0.57542283911685	2.97024140309776	1.44630810148862	H	3.29461320688704	-1.98135439185732	-0.97103105623180
C	-1.13708136388274	2.11517727848831	0.32170145320956	H	2.83474413888352	-1.32146293127384	-2.56649612713243
C	-0.07079811092415	2.20253570266828	-0.74321387856546	Rh	0.98020582458012	3.84798026733510	0.10958982593420
H	-0.31851940293694	2.27066058080078	-1.80519888705988	C	0.94493183361029	5.68098201327303	1.19653105861108
C	1.17208032370166	1.72059414994622	-0.32253418614329	C	1.76010121272174	5.73480166587195	2.33571118379486
C	1.16310504242244	1.29960619179213	1.13773474354652	C	1.42743289359870	6.51297081567449	3.44102659564575
C	0.68157764332892	2.54220691722427	1.84936765229174	C	0.26712860069652	7.29082945859980	3.40301037348731
H	1.14378161649846	2.89193677989031	2.77647780295226	C	-0.54990566987269	7.27173987257761	2.27820661015169
C	-1.23841380477504	0.65342614125773	0.81828736455210	C	-0.23401035372232	6.47088768872814	1.16961620857120
H	-1.63513542607788	0.02439710078715	0.00744817497587	H	2.67441185511848	5.13830038304935	2.36800757913979
H	-1.97561575617009	0.62547414962626	1.63624707936658	H	2.07602612669775	6.51995507899309	4.32010488472074
C	0.13609759059397	0.14513497457853	1.30834495858621	H	-0.00409937339257	7.91987312588152	4.25488805519954
C	-1.48509762388449	3.82946917059418	2.25669874722911	H	-1.45918100278986	7.87896875815106	2.24438551712484
H	-2.19800673802736	3.17773210319300	2.79162023245593	C	4.07104891625452	4.92570211435790	-1.00390569617030
H	-2.07452555819396	4.50755620714958	1.62370083901877	C	3.02116452043248	4.36892578513721	-1.97408809770083
H	-0.93352926670986	4.42187979057459	2.99854414360119	C	3.28579033824004	6.00410769944486	-0.27278683245905
C	0.08139170626668	-0.40951029961406	2.74113863592947	C	1.69261049639289	4.84092998702190	-1.59210966322049
H	-0.36371967919665	0.37770438551214	3.37944234364500	C	1.80182546458372	5.84217160739777	-0.54362594590630
C	-0.82278434231155	-1.63768272703722	2.80388817236643	H	0.90649800424816	4.85965710104661	-2.35451554258191
H	-1.83794889587293	-1.42600025935018	2.43612820155669	H	1.26273151575695	6.78559516028427	-0.67796483471955
H	-0.91178451082995	-2.00965695648578	3.83645155210213	O	3.30802904227757	3.70775542626257	-2.95576957339031
H	-0.40766727018682	-2.45348941388892	2.18808331913679	O	3.76926296683446	6.92170125230675	0.34510410245903
C	1.46113693087483	-0.74658891007252	3.29771911464276	C	5.23207387915050	5.53157975447986	-1.78228371505091
H	1.99660943771902	-1.43961642994266	2.62644835188025	H	5.77176493910209	4.74156567935536	-2.32397130706060
H	1.37322189835719	-1.23608576489382	4.27997593337331	H	4.87123546950586	6.26833799966336	-2.51577961220064

H	5.93003746578830	6.03411775325938	-1.09903633135922	C	1.39714649270820	-0.78368138579179	3.20941772421753
C	4.53618713267818	3.79168460467625	-0.05181280734380	H	1.93358097629830	-1.46214295884479	2.52417396835956
H	3.70508222215000	3.53691531113795	0.62990664938399	H	1.29376165853489	-1.30051905851927	4.17602361415119
H	4.69880916672300	2.90670435268071	-0.68277217812545	H	2.03337720239134	0.09786516432046	3.37703822999609
C	5.78930808822331	4.07916194057624	0.72509255097288	C	2.14634424330514	1.20854866915288	-1.33912096776839
C	7.02128848906902	3.59392323632984	0.26639247385960	C	4.35338478762190	0.01226153949257	-1.49748026381931
C	5.77130835903971	4.83735647906630	1.90271909205377	O	1.81832548204149	1.03605453241746	-2.50964202429907
C	8.20218311562761	3.86231149936489	0.95798445806826	H	2.12503382414237	1.00958303457973	1.46691036500140
H	7.05122868349372	2.99539056208795	-0.64872158613856	H	-2.10261694022705	2.56735272478564	-0.08609653857367
C	6.94931420131465	5.10955460593863	2.59646325613007	N	3.33593711367892	0.83385893409454	-0.82894463996168
H	4.82411470184325	5.22732296388402	2.27994840803925	H	3.50150330629846	1.04360839072001	0.14687505901781
C	8.17024869434746	4.62454592104491	2.12569884385242	C	3.74772252781110	-1.34327948665525	-1.87367384144124
H	9.15206786326256	3.47213367560809	0.58297490499229	C	4.90008295404946	0.71705255452698	-2.73918208171732
H	6.91271803821546	5.70406638140461	3.51313231477494	C	5.47475362701981	-0.18929344289693	-0.48070456501790
H	9.09386833027930	4.83687694461432	2.67030906978164	H	6.26218281578711	-0.82647337133668	-0.90793687691762
N	-1.01213971521092	6.50742732439079	0.03315621201741	H	5.92829054891472	0.77400506681091	-0.19895452491345
H	-1.02209308536858	5.66117238169185	-0.52722127981458	H	5.09494672700102	-0.67783733560094	0.43098650040148
H	-1.92742693029016	6.93246027594109	0.12563063037847	H	5.68631308335941	0.09974032706923	-3.19990702803955
				H	4.09982052212376	0.88531810199787	-3.47052374653780
<b>TS6</b>	<b>-312.46 cm**1 ***imaginary mode***</b>			H	5.3249775853451	1.69556121560110	-2.47417402096093
H	0.45437854502394	-0.62684152301975	0.55664142429793	H	4.50858763085013	-1.97968538702615	-2.35034717027674
C	-0.59242148039659	3.00279397383615	1.42333933672271	H	3.37496525398219	-1.86057202247880	-0.97580691840727
C	-1.14099140036293	2.17624395652180	0.27107756975935	H	2.91224525560701	-1.21203678691501	-2.57501201551377
C	-0.05623644409802	2.28007178735352	-0.77377184808058	Rh	0.99300467309518	3.89717046651887	0.13493541761273
H	-0.28593441834567	2.37468802125197	-1.83782357470612	C	0.97056943132751	5.71016493034884	1.25610541149384
C	1.17679310684157	1.78260708487674	-0.34303811689753	C	1.79675384314562	5.72896047980293	2.38931161578984
C	1.14081059470075	1.32675503684187	1.10643690937709	C	1.47159407049449	6.47267959086113	3.52003167957827
C	0.65445144131235	2.55580302426692	1.83840869568370	C	0.31289393506362	7.25443833164896	3.51285175976542
H	1.10153814609472	2.88093398940561	2.78181759747993	C	-0.50924126678039	7.27532420461252	2.39219902464451
C	-1.26048935677296	0.70548126068575	0.73581194524846	C	-0.20304114919321	6.50705016308577	1.25756357716132
H	-1.65355494898862	0.09565613456134	-0.09133536825346	H	2.71753336469855	5.13980995771131	2.39265376255714
H	-2.00700276567106	0.66820817332202	1.54499089994576	H	2.12590641209612	6.45334391895039	4.39471765754175
C	0.10393702696643	0.17547896947084	1.23126464552810	H	0.04883050049710	7.85732911441216	4.38567467118353
C	-1.50835763548882	3.84943817427524	2.24034314337450	H	-1.41559997717442	7.88783287022386	2.38237316293158
H	-2.23469672664028	3.19156556169261	2.74902511647807	C	4.11370743491482	4.99946805288609	-0.82928120123344
H	-2.08242278443349	4.54814936475033	1.61574905217707	C	3.11451415692432	4.39461978357338	-1.82059105666147
H	-0.96306507126215	4.41923202522801	3.00425716944014	C	3.28935578030669	6.09211523512304	-0.16335342509520
C	0.02685970753359	-0.41745964646483	2.64753849414658	C	1.77093074842015	4.89552402307130	-1.53130279066845
H	-0.41731283678683	0.35693710383483	3.30201239276340	C	1.82322819845483	5.90576821605624	-0.48818034349605
C	-0.89035731626481	-1.63723854385678	2.66709549739849	H	1.02327408087828	4.89583589336638	-2.33135664634374
H	-1.89924380650246	-1.40439466813784	2.29498188650651	H	1.26107023595655	6.83406250600221	-0.63429532565579
H	-0.99388089889472	-2.03662684260563	3.68800717084297	O	3.43865733328704	3.67074848712587	-2.74429530088989
H	-0.47741042409410	-2.44008636477339	2.03308141052057	O	3.74311672024928	7.00961570164198	0.47629791271293

C	4.5562300373164	3.97587152969697	0.21955584745885	H	-2.99461655336892	-0.97180190655203	-0.67282861872790
H	5.21388591136129	4.45379722282769	0.96128299372351	H	-3.91815912786461	-1.49828198777167	0.75159820579312
H	3.68779538516139	3.54399907329017	0.74499207809263	H	-2.35829019160428	-2.26535734838647	0.36934869343081
H	5.10324277209498	3.15518456443379	-0.26665804601869	C	-2.11625036304936	-0.77544403978871	2.68549573017690
C	5.34440173785241	5.57654050582087	-1.55411870431576	H	-1.44060998209045	-1.64296118250258	2.77694101331399
H	5.96153162552057	6.08197748170012	-0.79488863589845	H	-3.11293064297884	-1.09325697839412	3.02872565753773
H	5.92499085845590	4.72407616033676	-1.93753934285396	H	-1.76435852707225	0.00060588046189	3.38127091929241
C	5.03844070806667	6.52434570266505	-2.68563577463186	C	2.65440529014020	0.47093328655979	1.43685518868096
C	4.96710518877344	6.05855186705047	-4.00586279498017	C	3.90073461372491	-0.19275374559811	3.51337598368664
C	4.81404241937163	7.88826089725572	-2.45134525610499	O	3.46617026248553	0.00056997733872	0.64555935948167
C	4.66885240988221	6.92299584444862	-5.05793457705145	H	0.13539627180552	0.52707288652889	2.59396234887938
H	5.14125228550095	4.99879852655483	-4.20440386483072	H	-0.12367562198471	2.52488652531009	-1.72461287808084
C	4.51283593369102	8.75587587181808	-3.50145696744991	N	2.77898905585178	0.40608809291865	2.77866498246881
H	4.88091335326908	8.27381805673215	-1.43140685060397	H	2.10413101177444	0.93086648760506	3.32630224693983
C	4.43602445749590	8.27599827003112	-4.80907088294107	C	4.03607124771934	-1.67210244114495	3.14608807856153
H	4.62012821138428	6.53688445420684	-6.07971684350909	C	5.19692079863348	0.56126989988571	3.20308643810029
H	4.34364189570581	9.81635846812108	-3.29655161509009	C	3.56578765865594	-0.05824631441940	4.99649221777995
H	4.20226769518398	8.95525396970906	-5.63307519262708	H	4.37599379378921	-0.48414445563329	5.60548606298373
N	-0.98839869999061	6.58217146812390	0.12761909325071	H	3.44565469398364	1.00013128349474	5.27794908291961
H	-1.00999022418781	5.75242341777424	-0.45671723279973	H	2.63365619969131	-0.59221661672964	5.23881174749701
H	-1.90040079029109	7.00930186755790	0.24063043951956	H	6.04276540413093	0.09647528844533	3.73190073562090
				H	5.40663558812839	0.54543836719163	2.12481651741512
<b>TS7</b>	<b>-317.73 cm**<sub>1</sub> ***imaginary mode***</b>			H	5.12280932598348	1.60906089652659	3.53301984268686
H	-0.23720662549199	-0.91165437683886	0.57277797411620	H	4.84677415767513	-2.13041870521429	3.73227197362471
C	-0.62826839266038	2.93704955921305	0.35463216456259	H	3.10125574009301	-2.20987590153615	3.36741147851371
C	-0.08029932556417	2.03642418817854	-0.74241463473487	H	4.26289736315588	-1.78901812844301	2.07840365047648
C	1.33925041840136	1.78042431403719	-0.29647167936283	Rh	1.40562139289825	3.26905238587638	1.26762371601527
H	2.18308166756505	1.79402974591505	-0.99090147602731	C	0.93561007763362	4.87420169036720	2.58096277234732
C	1.41696162989293	1.17479987558336	0.95956944540867	C	0.14283190570335	5.94797423286837	2.16580744800307
C	0.04944259814277	0.95403728829409	1.58940390774045	C	-0.74502473215864	6.58037732388029	3.03427970597948
C	-0.53829842644348	2.35283383247303	1.61012590170948	C	-0.82735241123913	6.14602167196705	4.35749805809096
H	-1.07554579487093	2.74488155372439	2.47777346432567	C	-0.02601463056038	5.09780298133229	4.80186504171039
C	-0.87864834166799	0.71315746420675	-0.72849164388107	C	0.87294466498009	4.45566600859557	3.93734127810269
H	-0.49703967174218	0.05229002606317	-1.5209958341274	H	0.21379693532287	6.29376947939956	1.13367581426039
H	-1.92522377519561	0.94571158451108	-0.98198154413861	H	-1.36183165935246	7.40887040389135	2.67852844878938
C	-0.79327980666010	0.03909386681554	0.65923312010166	H	-1.51012965028448	6.63432313941152	5.05773547198570
C	-1.48197943731862	4.10612376136812	0.00155569703719	H	-0.07923455764273	4.76592360053287	5.84304950394113
H	-2.36379411116798	3.75016329351064	-0.55949115574094	C	3.45476427672064	5.23703850376469	-0.45346696180004
H	-0.94895558268773	4.81208975853532	-0.65352944902727	C	2.86486496007368	5.91067530309377	0.77897174842794
H	-1.83155259292953	4.64233252364548	0.89317703888867	C	3.87455154664312	3.86339279832928	0.07939353905396
C	-2.17891417586360	-0.28352641688513	1.24283459647436	C	2.78401876542870	4.92580338868478	1.92724459505805
H	-2.76452927787802	0.65557968127466	1.22699636120192	C	3.44138937592969	3.71567118687907	1.46441377093638
C	-2.90283218508530	-1.30600116078149	0.37146611797014	H	3.05939331669093	5.35483825507720	2.89586194622665

H	3.97372347191434	3.02293792429470	2.12236309930378	C	-2.18738672956392	-0.34587785917642	1.25110337457251
O	2.60259028278205	7.08705563247981	0.86822257575617	H	-2.80268370054745	0.57391454428055	1.27728270413924
O	4.52348533340043	3.06845682498497	-0.58270059777205	C	-2.88565478874593	-1.35568523939122	0.34438199728505
C	4.70463855545215	5.99560650434315	-0.89898841167392	H	-2.99803476235167	-0.98272069008605	-0.68468226695225
H	4.44713703562908	7.02246246110157	-1.19244296740475	H	-3.89057888730291	-1.59710884575817	0.72412526290173
H	5.44603345898106	6.04221564501573	-0.08654571044047	H	-2.30942907303385	-2.29527024254865	0.29853666835743
H	5.16435595611569	5.48250316450187	-1.75613952041784	C	-2.09641220476427	-0.89239240670150	2.67219475421858
C	2.43978231908493	5.04823905606797	-1.60601775559433	H	-1.39912947968898	-1.74611345304520	2.72291407618284
H	2.88813181849755	4.30075182917502	-2.27994227025694	H	-3.08118759565202	-1.24815401367652	3.01265857946370
H	1.52580295799656	4.59642966660497	-1.18590452198631	H	-1.75528185567341	-0.13556434596249	3.39396408213815
C	2.10401510129251	6.28723179891519	-2.38505975133252	C	2.60435846019828	0.48539374271271	1.41131932392758
C	1.06302233011189	7.13689781251810	-1.99090084618698	C	3.97406960440207	-0.11738191358293	3.42347979367544
C	2.84123577946478	6.62560162422272	-3.52780150356212	O	3.30275354990889	-0.11144848691812	0.59687286675834
C	0.77486280305858	8.29666317694737	-2.70939100573304	H	0.12853219523833	0.48714720633139	2.61196956733007
H	0.46718846513136	6.88441170940306	-1.11036470458515	H	-0.24395477240818	2.62850643527485	-1.62934683159268
C	2.55809954852554	7.78485960078979	-4.24871092326172	N	2.84758773379463	0.52789129717640	2.73652849018171
H	3.64819824544168	5.96543210140410	-3.85810429924301	H	2.25329337773580	1.1399697864709	3.29123433180804
C	1.52472087536841	8.62759246137324	-3.83885511689730	C	3.89956292089915	-1.63331140999825	3.22545279023581
H	-0.04331345201326	8.94572858186570	-2.38659420467093	C	5.30284308773440	0.43097044378947	2.89517456371002
H	3.14603107316574	8.02874952101826	-5.13761597631988	C	3.83311967865000	0.21589560830650	4.90624620307469
H	1.29948024555411	9.53636479653143	-4.40297510096230	H	4.64084915689366	-0.26525250661758	5.47613167808978
N	1.64327300904584	3.40249533833048	4.40089536093337	H	3.89829463205160	1.30230930708852	5.07404462725923
H	2.50184682477863	3.21657509653358	3.89396491691523	H	2.87010606919313	-0.14300947086212	5.30213139831803
H	1.78608444624993	3.37951927462912	5.40514230599943	H	6.14399449582330	-0.06060273674755	3.40699720856463
<b>TS8</b>	<b>-314.45 cm**<sub>1</sub> ***imaginary mode***</b>			H	5.39415493780766	0.25187972247668	1.81556755384435
H	-0.23521097164301	-0.88798380681824	0.54128687965728	H	5.37627650859760	1.51413762380443	3.07895482935424
C	-0.72683554981514	2.95423835567066	0.46974913370614	H	4.72307701128754	-2.12527107849085	3.76483069062387
C	-0.17457766828336	2.10714321711246	-0.66579991530861	H	2.94696146714497	-2.02486502754515	3.61449336124081
C	1.25605607243251	1.86746343145319	-0.24901655971102	H	3.97488324570684	-1.89000849901155	2.16030544530293
H	2.08730479432510	1.92356748607275	-0.95628631275423	Rh	1.31958608983806	3.29093666109617	1.37508268524517
C	1.36515416153841	1.21884381014578	0.98285158067374	C	0.85410259905449	4.83054968177093	2.76831763447341
C	0.01098851194617	0.94494964739550	1.62410736399114	C	-0.02026417722640	5.86988215685398	2.44238306993516
C	-0.60878150088148	2.32791844676310	1.70153994482577	C	-0.91482762146922	6.38971229681748	3.37682737948102
H	-1.13939722792787	2.67944663262312	2.59039069581086	C	-0.92288805902367	5.87485958663970	4.67268400769527
C	-0.93887116171313	0.76426715486566	-0.69073724098654	C	-0.03220671508292	4.86545329865893	5.02890986630411
H	-0.54924596234653	0.14409876272774	-1.51177959934436	C	0.87940752870077	4.34193422067107	4.10097226594127
H	-1.99423939188190	0.97775857526103	-0.92371725298967	H	-0.01157686558232	6.27749591998211	1.43093789473624
C	-0.81812068780360	0.04169369643303	0.66964752577104	H	-1.59874021772142	7.19234705923725	3.09101442710155
C	-1.59825081780756	4.12413733139647	0.16832393501849	H	-1.61378505894274	6.27148961782453	5.42114467401610
H	-2.47231169387288	3.78119869972980	-0.41255163180323	H	-0.02250377884751	4.47422047277292	6.05059322996802
H	-1.07268738272163	4.86758823640992	-0.45126191052657	C	3.25291046899200	5.25698892111101	-0.41193186347895
H	-1.95908438342409	4.61265597467735	1.08243750968146	C	2.59731187596391	5.91040071899186	0.79804346360970
				C	3.70201452412284	3.89845974046829	0.12509456532668

C	2.66122602076011	4.98638449923835	1.99189887489711	H	-1.90595786799549	3.01969611625304	2.96535484089776
C	3.34722510495251	3.78978005209714	1.53441386566264	H	-1.78553541024883	4.48406062513606	1.96564191089800
H	2.95823950018131	5.47101010137732	2.92772486625174	H	-0.65671989681536	4.23793472860613	3.33074590122173
H	3.91752167381948	3.12143302089141	2.18521484785885	C	0.68637018212486	-0.27066532332870	2.90740173069931
O	2.15698302570210	7.03728236043856	0.80777346613190	H	0.22052512864052	0.50211964184915	3.54851279014080
O	4.32079649477720	3.08506680201595	-0.54739145993105	C	-0.11043851332847	-1.56230751933941	3.07002468956009
C	2.29940244458582	5.14816109016496	-1.59509129196827	H	-1.15976781887891	-1.44573016535571	2.75962328679779
H	2.79032302895937	4.60818169953966	-2.41844231721909	H	-0.10757665273614	-1.89946434060395	4.11831105181837
H	1.38652434485763	4.60118112070916	-1.31466943708699	H	0.33106891503044	-2.36664766259525	2.45745924498666
H	2.01363478848823	6.14994286360665	-1.94897062085734	C	2.12175979166254	-0.47703717200961	3.38099568149163
C	4.50531975970148	6.07290974476808	-0.81843872739507	H	2.66894055674463	-1.14612865018376	2.69530700647493
H	4.94197415784491	5.57092646704877	-1.69547212960165	H	2.13652441591105	-0.93903186169178	4.38034901989237
H	4.15912636885376	7.06807447956227	-1.13840395931276	H	2.68276972629725	0.46680552035842	3.44809454951561
C	5.54329171465548	6.20694293651015	0.26435076643938	C	2.30313755397014	1.08325331502187	-1.2532566689097
C	5.49210403307006	7.26235519357638	1.18498510376155	C	2.78556659795440	0.66379406587197	-3.67802245823835
C	6.57065017563491	5.26193860258741	0.39233734206658	O	3.01998011367875	0.17766733830207	-0.82731603715168
C	6.43544662514948	7.36738366341686	2.20726921217674	H	2.58963347760355	1.19183373736540	1.40429480147791
H	4.70462441819001	8.01520283556800	1.09467470495312	H	-1.86494971720155	2.41259680911327	0.25465638756666
C	7.51485682265297	5.36384754007544	1.41303631140905	N	2.17226528301189	1.38680249918738	-2.55419151633469
H	6.62536759116192	4.43421711178962	-0.31904024291894	H	1.69577982537483	2.25065477820667	-2.78451672114087
C	7.44906303559647	6.41629528904526	2.32679503062305	C	4.31261247981292	0.75543200924975	-3.62457100171128
H	6.38151280301748	8.20190682847187	2.91136191555219	C	2.33540596491166	-0.79891203892090	-3.65465707037342
H	8.31070352505228	4.61830290169501	1.49149182006609	C	2.27462679489205	1.34028094273436	-4.94794094016677
H	8.19103470038800	6.49919063252903	3.12522539181155	H	2.70600953249643	0.85330263501680	-5.83426059070642
N	1.74397715232967	3.32101241419466	4.47989085479970	H	1.17744195149864	1.26984609464331	-5.01545025143282
H	2.64595042470088	3.32247295056245	4.01445148373690	H	2.56021288263401	2.40275816304093	-4.95813949385138
H	1.86407101868523	3.22990555993561	5.48405777801263	H	2.75278027492567	-1.33265768001959	-4.52177921068242
				H	2.67745109162244	-1.29713231166575	-2.73780524955788
<b>TS9</b>	<b>-238.36 cm**-1 ***imaginary mode***</b>			H	1.23742831464376	-0.86466464028394	-3.70245446726439
H	0.96503374905366	-0.58513525534308	0.80388374355845	H	4.75110071784557	0.20759447001718	-4.47249085895632
C	-0.27173826612174	2.98071968407754	1.62469574301437	H	4.63033642865993	1.80611098185726	-3.68279964034265
C	-0.85203721744945	2.09573701873736	0.53486576410516	H	4.69584557358329	0.31941483672835	-2.69211018952170
C	0.12358775152018	2.23350993329083	-0.61136713481784	Rh	1.07136042073469	4.00830119049331	0.17692373759419
H	-0.23161827335016	2.28363466785509	-1.64465312557283	C	0.60997974154212	5.81726696235388	1.05622358357609
C	1.41147200736512	1.80799499375285	-0.28501971001865	C	-0.42688223809257	6.37055784761176	0.29397193381354
C	1.54895838532322	1.43870223042237	1.17291203999016	C	-1.37190682767096	7.22638331805891	0.86215918828363
C	1.04418841952171	2.65046870708770	1.91850547315062	C	-1.22412295965168	7.59435075038713	2.19988000824877
H	1.54637013942629	3.03565543058758	2.80953413354167	C	-0.15957502523905	7.10620556611792	2.95140009824023
C	-0.82605186067336	0.63296441086968	1.04444880467616	C	0.77994448548318	6.21195663682426	2.40665672917993
H	-1.22356838698453	-0.02769321383350	0.25956433474876	H	-0.50789111694359	6.1216727238796	-0.76873159144601
H	-1.51450334924518	0.56407693959253	1.90161896116502	H	-2.19096708960471	7.62037866802176	0.25637483608305
C	0.60627286064290	0.22947026579073	1.45596165647794	H	-1.93279141768095	8.28689478419652	2.66180777362302
C	-1.19633016640348	3.73735327414183	2.51831692968655	H	-0.04103316973189	7.41015265223645	3.99579370104680

C	4.22448964597288	4.41732385165760	-0.82865018546731	H	-1.52694711688870	0.55244535062923	1.99699135677462
C	3.10639114116136	4.46073842401373	-1.87970382983693	C	0.56588687669547	0.17950149753822	1.45682057555334
C	3.55851817622087	5.05065652447441	0.38157895666009	C	-1.12190746188212	3.71310878660576	2.62013757462212
C	1.97667406122071	5.22017457959728	-1.35938956099674	H	-1.82876626864830	3.00552576561630	3.08707292879514
C	2.32409660634110	5.77830535589696	-0.07217770284249	H	-1.71570046645243	4.47858369475634	2.09913469898895
H	1.29062611062544	5.70120145420236	-2.06143851803323	H	-0.53859132490830	4.19167213973099	3.41549260958215
H	2.29170546421038	6.84317329833624	0.16603692400386	C	0.69959000049994	-0.33681516938480	2.89853112779158
O	3.22203668892193	4.00113997597164	-3.00382516147818	H	0.28186266629232	0.44010773921619	3.56717387328807
O	4.02492995300802	5.05124905075799	1.50902828601434	C	-0.11876709727186	-1.61162543255389	3.08572414266112
C	5.31134640605872	5.38470746832000	-1.32767518471078	H	-1.17814914624898	-1.46813294855293	2.82494018531273
H	5.76019093453431	4.97939475014319	-2.24646150416315	H	-0.07563316580049	-1.95959477190734	4.12956369972233
H	4.89085009408705	6.37642069154642	-1.55477672878370	H	0.27574485981204	-2.41928968559578	2.44608189107607
H	6.10049285049424	5.50178627530072	-0.57207320634586	C	2.14960759763744	-0.58142053064372	3.30461404731963
C	4.76156153649276	2.99486815345215	-0.59446730776307	H	2.64912183223184	-1.25707553518427	2.58952163893884
H	4.12184692410659	2.50327097564702	0.15201365915555	H	2.19808627494498	-1.05352801822678	4.29817226052088
H	4.62233044009856	2.45259903550947	-1.53788187953679	H	2.73613822558909	0.34788299475806	3.35480463086781
C	6.20429813119466	2.86095192928618	-0.18634341030850	C	2.16454133265255	1.03874502188417	-1.32368906165870
C	7.15399213471329	2.41694546738708	-1.11488408699439	C	2.57291742355886	0.69182398684619	-3.77219303897692
C	6.63364569181920	3.15184777072103	1.11577551758901	O	2.88365369428244	0.11337844120370	-0.94609949289607
C	8.49480024815143	2.26641869927915	-0.75853184097133	H	2.56342218108642	1.10373855526750	1.32894903736473
H	6.83369555846561	2.17943105544505	-2.13345573689044	H	-1.91139098483629	2.42001594037425	0.37843579375634
C	7.97214182196140	3.00283790454084	1.47585897369573	N	1.98640467014131	1.37543972133778	-2.61039723813104
H	5.90442288974284	3.51365226981332	1.84392074305164	H	1.51175006560416	2.25041639545344	-2.79860416351169
C	8.90885499215496	2.55881554567017	0.54033772217497	C	4.10069936285242	0.77942795607960	-3.74007515755098
H	9.21786991307623	1.91483732491901	-1.49945567673822	C	2.11640308909683	-0.76862451244437	-3.79415638420490
H	8.28775939411673	3.23295569167841	2.49715875638904	C	2.04102138607748	1.41804592219148	-5.00570916833222
H	9.95754941987666	2.43870357083714	0.82465100653367	H	2.44811701022047	0.95954542916610	-5.91832143582616
N	1.78931717043674	5.69731192760342	3.17845139065453	H	0.94190514955398	1.35968049648710	-5.05157441208030
H	2.64295224268436	5.42390963471892	2.68490248149307	H	2.33707061255529	2.47730799422258	-4.98323889573733
H	1.96801754395429	6.19038756499231	4.04592236338118	H	2.51760991907225	-1.27245262045935	-4.68647186301911
<b>TS10</b>	<b>-235.90 cm** -1 ***imaginary mode***</b>			H	2.47121599779069	-1.30056124022407	-2.90130128210876
H	0.87876854289394	-0.63528229850256	0.78175080305473	H	1.01750225609203	-0.82894109250114	-3.82645115827427
C	-0.25019626854712	2.94761840538995	1.68185250790830	H	4.52469212598121	0.28331970404340	-4.62644489678359
C	-0.89395933634497	2.08126824863801	0.61301723993845	H	4.41143673579622	1.83342975861557	-3.73626365302415
C	0.03439138387333	2.20907890008717	-0.57211985456209	H	4.49685587665442	0.28901885976841	-2.84057939771710
H	-0.36337645378939	2.27856121773036	-1.58863297938426	Rh	1.05666047415986	3.95813211211384	0.18776189538469
C	1.32608786655254	1.75715456377367	-0.30528202999450	C	0.63242512678788	5.77214919849480	1.07513674627536
C	1.51897969447547	1.37231262651699	1.14293936170161	C	-0.41799249683150	6.32856977498812	0.33430018083877
C	1.07064956634289	2.58938175646210	1.91707032609365	C	-1.34551302862063	7.19145149614794	0.92084360218075
H	1.61611163499373	2.95817791054304	2.78949688285141	C	-1.16481359745954	7.56431922832854	2.25317800695732
C	-0.87480645647938	0.61462747003689	1.11137667183699	C	-0.08488550745253	7.07418476461773	2.98121326044665
H	-1.31916854239307	-0.03254551593881	0.34048017263207	C	0.83675895304697	6.17241778964443	2.41868932703289
				H	-0.52419825952420	6.07582729084856	-0.72543051469142

H	-2.17657846549000	7.58700508822690	0.33265476994307	H	-1.23859283735638	3.15262578782692	2.07541521748136
H	-1.85944769280911	8.26173347655637	2.72891191574649	C	-0.67393380965487	0.78244316822098	-0.83687084727632
H	0.05945405638534	7.38137542574769	4.02145730738601	H	-0.19880106633708	0.03728096458043	-1.49225089555698
C	4.19725732468653	4.32193991208158	-0.85923107001533	H	-1.66989698711665	0.99067498457705	-1.25892994734526
C	3.08056417414908	4.38304875965849	-1.90528818001374	C	-0.79258861741280	0.27111784647986	0.61478992764550
C	3.55900012725909	4.99235743760080	0.34550885154124	C	-1.27384069344191	4.24450336850788	-0.57842500749787
C	1.95562575326445	5.14492596853260	-1.37458255876549	H	-2.13142718557702	3.83241360264026	-1.13895653631873
C	2.32039031472514	5.71397229858430	-0.09648994027439	H	-0.65600266206073	4.80289294006504	-1.29774844364399
H	1.26685759782437	5.62558467301375	-2.07430211357923	H	-1.63841818695338	4.94323309226112	0.18389758335923
H	2.29525097302055	6.78099952556732	0.13109505093290	C	-2.25351906260428	0.05220764226591	1.04067166456984
O	3.18990787675536	3.94224002485213	-3.03846830527441	H	-2.79705985024517	0.99332413002640	0.83052225084621
O	4.06333748887131	5.01671638081846	1.45653392239142	C	-2.89392728888361	-1.05643536173055	0.20981771556125
C	4.73681993784186	2.93718534499593	-0.54914837953332	H	-2.83098463229147	-0.85557355931261	-0.87026580680435
H	5.57861069374615	3.01800245937275	0.15387102241687	H	-3.95816066553854	-1.17596854204424	0.46593580628823
H	3.97092508675945	2.29977429470577	-0.09276617610029	H	-2.39260010733496	-2.02033705830041	0.40050493848187
H	5.09248111238890	2.44953758543077	-1.46689178365640	C	-2.39900072629904	-0.25430500416931	2.52753594909984
C	5.37315072033578	5.21423755133377	-1.35245763618023	H	-1.77713893247169	-1.11935672467512	2.81431047910873
H	6.14817765380635	5.18178642153758	-0.57124586775404	H	-3.44414155086995	-0.50175528151336	2.77030450277660
H	5.78214106925268	4.72181603966676	-2.24841019607426	H	-2.10735380287871	0.59518649704373	3.16267340352496
C	5.01791516545162	6.64125085384862	-1.66410938172387	C	2.46457320477388	0.71669356730997	1.87059344364251
C	4.58366231875098	7.01107400620570	-2.94366542499965	C	4.90619581924786	0.29402169685181	2.14222598436379
C	5.09130648420016	7.62850598342227	-0.67260430264326	O	2.12944353040103	0.05270457663291	2.85217366649450
C	4.22565234350806	8.32900437482375	-3.22328606295252	H	-0.05651964578660	0.95362612395481	2.58066897590751
H	4.52650097557976	6.25191225406039	-3.72803546576885	H	0.23209566975690	2.46116666410556	-1.91819526741363
C	4.73508722146650	8.94802959412089	-0.94916146244828	N	3.73490618028222	0.85568800409022	1.45309481167359
H	5.43744821921787	7.35810630976772	0.32907495435608	H	3.94270411148783	1.53476997296184	0.71660957404843
C	4.29911817836019	9.30240276792575	-2.22610277921626	C	5.03086565153517	0.90200993887144	3.54228681138744
H	3.89330668869161	8.59918536413544	-4.22912019617775	C	4.79687620068531	-1.23045834329155	2.21898840729491
H	4.80548633488292	9.70507769927708	-0.16372551043225	C	6.13004382270409	0.66911852680940	1.30881591471441
H	4.02446157666156	10.33715713608301	-2.44632417542534	H	7.03879322006500	0.27031086439355	1.78221484336555
N	1.85986702804066	5.65320605333521	3.17017355100097	H	6.05646171306354	0.24987625546657	0.29322708764020
H	2.70364515236302	5.38379715357522	2.65779985284138	H	6.22957285300285	1.76051924149791	1.21938068981296
H	2.05876354453284	6.14940250710045	4.03155230084824	H	5.69655903016779	-1.64532857422484	2.69822870375139
<b>TS11</b>	<b>-242.98 cm**<sup>-1</sup> ***imaginary mode***</b>			H	3.91570682802916	-1.53297031444496	2.79874782693567
H	-0.26655587957512	-0.69502444701082	0.71275980475738	H	4.71621042586024	-1.65907413049762	1.20789188619085
C	-0.50923115333733	3.11610821611831	0.02195642081617	H	5.91854962665612	0.50036599717858	4.05419981368404
C	0.14673898704806	2.09072170362580	-0.88878969809777	H	5.13571845463541	1.99618157276754	3.47621929482385
C	1.49566284821353	1.87853506787244	-0.24505279378427	H	4.14280127075349	0.66980338223670	4.14551024517258
H	2.40821514897857	1.80396538692987	-0.84190100489706	Rh	1.38843952591715	3.53715492677186	1.20051123979092
C	1.39630618461804	1.40467144358440	1.06532611703731	C	0.92625495084196	5.01376630624532	2.58693573918085
C	-0.04154034464291	1.27097083474472	1.53427418431708	C	1.39085806250230	4.41327648105106	3.76321756974719
C	-0.59706660853215	2.66940338997535	1.33404410578333	C	0.75757273226993	4.63091308510551	4.98927224906683
				C	-0.30741368056181	5.52992514661560	5.03861596661176

C	-0.71989506152033	6.20026713587199	3.89096569399270	C	1.27810937319688	1.42512563325276	1.03513089653821
C	-0.10608735780973	5.98090057207524	2.64173472879890	C	-0.11282101283601	1.20635260026897	1.60459536870348
H	2.25775664419808	3.74397892306884	3.72593967112955	C	-0.75054294747178	2.58043510739475	1.49205449923079
H	1.11362051435254	4.1257827955391	5.88968042101479	H	-1.34976250278335	3.01288997823498	2.29740534835555
H	-0.80982567821444	5.73611085834614	5.98748875746130	C	-0.90523855547370	0.75549794666129	-0.72533398762057
H	-1.53814126897418	6.92474162091863	3.94370503826105	H	-0.45450524744299	0.05605031471483	-1.44519088492639
C	3.28321344858363	4.99475940270659	-0.98765535915203	H	-1.94256125376048	0.92804062065400	-1.05409672494958
C	2.26686088619399	5.72900430188580	-0.12510966357245	C	-0.87361491617304	0.19130347071288	0.71072179189611
C	3.81439154420920	3.93601906365253	-0.01863597703820	C	-1.62772505701433	4.18648748487263	-0.31119341947228
C	2.52909877907895	5.41137356310047	1.31969044372330	H	-2.51253840071966	3.76413311429464	-0.81932215037261
C	3.39676138094938	4.25791632132360	1.33845491752084	H	-1.08265638743441	4.78479508268279	-1.05680746118931
H	2.62294787806325	6.26835745028739	1.98936783628813	H	-1.95383056399876	4.85059404416950	0.49829226979900
H	3.98593170395374	3.93705806871138	2.20017615057920	C	-2.27638514352080	-0.14456675439679	1.24237712952125
O	1.45128487533939	6.53119160109269	-0.54687127551248	H	-2.89840296245866	0.76255373299127	1.11807798338276
O	4.52657266416395	3.00199431063541	-0.37612228383665	C	-2.90684551235549	-1.26344937673903	0.41747908249667
C	4.44713350984832	5.96063432659664	-1.26944930444013	H	-2.94597262417483	-1.01785033402667	-0.65444831550822
H	4.09511926716447	6.81377961654390	-1.86615148694874	H	-3.93587943152300	-1.46796342118423	0.75168195511450
H	4.88584017932483	6.34186630729811	-0.33469504077835	H	-2.32767155835108	-2.19603398613027	0.52583714002584
H	5.23248354249337	5.43715325213026	-1.83447662092759	C	-2.27484513181232	-0.51874835799779	2.72107584847204
C	2.72110407389387	4.36497086831980	-2.27281782864021	H	-1.56819461621580	-1.34314352588846	2.91614405308080
H	3.37239883195682	3.50518700424825	-2.49510724388145	H	-3.27463311087679	-0.85553317194707	3.03631405670451
H	1.72219027800501	3.96720146808826	-2.04846736620009	H	-1.99359239423824	0.32535044496668	3.36788964559472
C	2.64753435215561	5.24275547040898	-3.49258896801438	C	2.43480367163397	0.78562611044367	1.75638833477638
C	1.54556822113715	6.07526225295970	-3.72745281136670	C	4.90985376101244	0.53341388480168	1.89549252588687
C	3.68030498291316	5.22629519826315	-4.43901592967063	O	2.20096452717499	0.09489324976339	2.74911073692059
C	1.48318659448261	6.87459813734408	-4.86803980598538	H	-0.03255086434207	0.85929959147037	2.63835616068271
H	0.73338175499010	6.09975161289873	-2.99787672041328	H	-0.16210450115725	2.50715667240932	-1.81636632482416
C	3.62337325681065	6.02599696064607	-5.58044144881098	N	3.66686651621087	1.00485552491453	1.26610993738027
H	4.54089384780019	4.56966733226654	-4.28046683935907	H	3.78577891727488	1.69009115262101	0.51437008049038
C	2.52313633096597	6.85490078130500	-5.79876080149007	C	5.05569078856042	1.13853530335630	3.29521474962028
H	0.61312338733767	7.51559726087742	-5.03403069666208	C	4.92417099967405	-0.99532629406902	1.96301588502100
H	4.44022712349182	5.99557848647997	-6.30654737438518	C	6.06148433856620	1.01147261937476	1.01317592355333
H	2.47267891537610	7.47941938864744	-6.69452568364837	H	7.01844115485550	0.67625470680796	1.43852190986663
N	-0.52704225567843	6.65684521577375	1.53132798125310	H	5.97350638053656	0.60275050623220	-0.00545723291306
H	-1.08902452929148	7.48353979509887	1.69184916918062	H	6.07587346253665	2.10887826525798	0.94066665593783
H	0.11646164652139	6.71945429352492	0.74033623341054	H	5.87482634890914	-1.34128695312237	2.39644471826375
<b>TS12</b>	<b>-242.03 cm**-1</b>	<b>***imaginary mode***</b>		H	4.09737295159613	-1.36740648592888	2.58148037361132
H	-0.27971387228192	-0.73988356313909	0.73025190611919	H	4.82877691613522	-1.42388332227821	0.95318870118977
C	-0.78244410820167	3.06876530597896	0.19326053599930	H	5.99148266383314	0.79385791669774	3.76082714183291
C	-0.15196216218918	2.10232055964834	-0.79652561115291	H	5.08538093502145	2.23765792018854	3.23812548806144
C	1.25198187763337	1.93736710310145	-0.26471861450278	H	4.21531244323057	0.84233784891776	3.93706163115071
H	2.11715845084492	1.93730222052846	-0.93257466618546	Rh	1.18429017935984	3.54508545250665	1.23694746109641
				C	0.77126243847055	4.93498144139498	2.72669406678139



C	1.33476667729830	4.29946540731702	3.84004847881184	C	-0.89662879528984	2.14698839188207	0.41809659204831
C	0.77055366847670	4.42464506988708	5.11181810479961	C	0.12261196965363	2.22526138088102	-0.69780207139782
C	-0.33063998830487	5.26516676703788	5.27254048104444	H	-0.19991257074360	2.31345808739498	-1.73929991366158
C	-0.84215228523862	5.97306931069721	4.18888177373868	C	1.37071235288027	1.71602300798548	-0.32398762844118
C	-0.29574378513357	5.84907171483595	2.89597409376376	C	1.42168234691603	1.29419346669572	1.12818654394844
H	2.22737453206867	3.67647587143749	3.71603123048769	C	0.99379080173608	2.53610130189414	1.86831358133205
H	1.20473793967352	3.89238547737643	5.96100995272339	H	1.49997447762821	2.87564329426495	2.77591868220529
H	-0.78414748154247	5.39589553987606	6.25872620825202	C	-1.00062218121150	0.68266382540169	0.90791018902453
H	-1.68906880178869	6.65170559247080	4.32857632007568	H	-1.42799495517924	0.06558852278230	0.10339382533502
C	2.86000173159852	5.18227627604168	-0.99052427451076	H	-1.71519233588721	0.65698325643370	1.74578828624201
C	1.92750006634590	5.86102342893194	-0.00053476913514	C	0.38303138734068	0.15898263463045	1.35245243514082
C	3.47091543792457	4.06993096680783	-0.14530240286364	C	-1.14515296791920	3.83557275462360	2.38520856024277
C	2.29326789088218	5.44203650264643	1.39062257880274	H	-1.84828007390925	3.17961989691016	2.92789952198834
C	3.17173923672714	4.30452412487611	1.26171959445565	H	-1.74753015014475	4.53561416889864	1.78896886471369
H	2.42571799792718	6.24724605187703	2.11480212675864	H	-0.5625540108732	4.40270218118030	3.12278988292395
H	3.83542042917669	3.94235562900661	2.04897798225001	C	0.37501051318072	-0.36982309913255	2.79599917128352
O	1.08667909947419	6.68682822255609	-0.31457755659959	H	-0.04428805485084	0.43101420044384	3.43500102548440
O	4.15402615051808	3.16604064515588	-0.62194635590193	C	-0.53198206568164	-1.59176632020924	2.91422191281241
C	2.15981318849358	4.71541804517008	-2.25296374454659	H	-1.55785168764597	-1.38283551121621	2.57524703619433
H	2.84883414038221	4.10952047523881	-2.85899313707195	H	-0.58933063408333	-1.94176578416592	3.95674494821721
H	1.27455260034430	4.11175290008803	-2.01532119716681	H	-0.14059807456872	-2.42225410258366	2.30255916879347
H	1.83483131062076	5.57988642628772	-2.84945118316744	C	1.77190411505079	-0.70183547181347	3.31036970937651
C	3.99909505633973	6.17384170348423	-1.38010938010771	H	2.27903167521005	-1.41351557884602	2.63688837058902
H	4.61661982701183	5.65589432238544	-2.13003412698913	H	1.71733467380877	-1.16665617835497	4.30706840245601
H	3.52266679766083	7.03330560598483	-1.87739789913601	H	2.40981213448391	0.18994292957802	3.39809324692497
C	4.86189567163380	6.63696950218532	-0.24002814285328	C	2.35628612849356	1.04186204835710	-1.23763359831599
C	4.51344054943824	7.76164510277038	0.51856597097228	C	2.98873786745428	0.58590952562012	-3.61628937619936
C	6.01323260532957	5.92183017844285	0.11494194010896	O	3.16416828419545	0.24611359625008	-0.75712343560904
C	5.28703020056823	8.15338773571777	1.61132060595846	H	2.43482690347802	0.96886601417809	1.38106993251646
H	3.62418573681482	8.33893913780607	0.24841601546479	H	-1.87378364999873	2.54300985759933	0.11260491247771
C	6.78796563859212	6.30967158283527	1.20682517890196	N	2.23637528503368	1.27267249024083	-2.55492444171328
H	6.30110057469174	5.04542310928670	-0.47184908738359	H	1.66375896338459	2.05547841018802	-2.84688487402252
C	6.42466546104213	7.42564359257155	1.96174166204567	C	4.48669885008256	0.87909987462811	-3.49840349904130
H	5.00159720556289	9.03556087865007	2.19029637351991	C	2.72765979689713	-0.92094617781821	-3.54176533741843
H	7.68317881067915	5.73883394268951	1.46728870708134	C	2.45619463549185	1.12851043934571	-4.9405332342962
H	7.03193218246086	7.73260271112515	2.81709719868518	H	2.98416191787152	0.65346260604297	-5.77997071558445
N	-0.81545622435365	6.55859775838961	1.84776055806363	H	1.38075671919498	0.91451437506798	-5.04605457860564
H	-1.39764681708084	7.35106103247258	2.09007581240274	H	2.60696675344677	2.21606220172450	-4.99971532652301
H	-0.20749756977589	6.70987126214232	1.04102447872313	H	3.26001947157290	-1.43259529095432	-4.35789123271392
				H	3.07394265070993	-1.33259082264289	-2.58474832417819
				H	1.65183476782784	-1.13103855095109	-3.64655635786493
<b>TS13</b>	<b>-304.83 cm**<sup>-1</sup> ***imaginary mode***</b>			H	5.03457487311077	0.36812632519060	-4.30485741682032
H	0.69296366968850	-0.67276568015329	0.69522058729711	H	4.66285805940509	1.96090760754362	-3.57764225748219
C	-0.27586373154938	2.98145431174581	1.52633771567999				

H	4.87439448271132	0.52510222852951	-2.53339194533191	<b>TS14</b>	<b>-307.26 cm**-1 ***imaginary mode***</b>		
Rh	1.21759952707474	3.86534508080303	0.13188011960314	H	2.77174363631844	2.88688228812792	3.59966399980667
C	1.29104191758876	5.63398892476963	1.30703028015825	C	0.55554071683470	1.09197863901139	0.98077209016460
C	2.16615474827690	5.61406622708100	2.40024878507027	C	1.82012816568753	0.50952632229925	1.59130618656812
C	1.92159780043549	6.36508861737371	3.54729239575428	C	2.93066854328298	1.17555794296351	0.80746590462507
C	0.79181251030231	7.18527260960084	3.59729704866975	H	3.81980525009432	0.60894816968605	0.51525581553757
C	-0.07989676210326	7.24094588779611	2.51511626608163	C	2.90909193353872	2.57088629835271	0.92322864189402
C	0.14944996365825	6.47401568427745	1.36243439408587	C	1.73332027437880	3.07347234570048	1.73270087694187
H	3.05734792068575	4.98450780322724	2.35730013805506	C	0.54405784172973	2.47921608078260	1.02286184714721
H	2.61468135033416	6.31705164712890	4.39044539256614	H	-0.36393964969810	3.05601466143443	0.82713780059052
H	0.58843569314295	7.79101840023997	4.48424957722960	C	1.90394342382363	0.95862620649945	3.06950065540561
H	-0.96345698112003	7.88523532646800	2.54947683787046	H	2.83295870448563	0.56664209408749	3.50998549334776
C	4.20410182600058	4.76973731774316	-1.25281147437286	H	1.06915493555203	0.49045727085817	3.61467999865854
C	3.02182258933278	4.45493941078283	-2.17322343129276	C	1.82968796262786	2.49834313792365	3.17338190293679
C	3.60037883554426	5.80276322516009	-0.31002802943670	C	-0.65185164717189	0.23346719889619	0.81376725725431
C	1.78740401718504	4.95152851214078	-1.58353454076511	H	-0.97033750532815	-0.11533332610926	1.81182028802153
C	2.09152246347991	5.83438466724285	-0.47124131499495	H	-0.44127795393978	-0.65910771063475	0.20863089359558
H	0.92217164779527	5.09852501315660	-2.23844671420672	H	-1.48466808200046	0.78541983547847	0.35929699837467
H	1.65519866170370	6.83806034007511	-0.47645648473534	C	0.68081562698929	2.96701245571528	4.08158963731436
O	3.14284895717406	3.92662935818279	-3.26622396451053	H	-0.24083421601043	2.46943994244786	3.72315648021605
O	4.23046136754755	6.55769942801060	0.39037843292954	C	0.92309008850658	2.52704865752335	5.52270795527470
C	5.35753844576478	5.36841923302378	-2.04724200454701	H	1.07167944259668	1.43981431487609	5.60589255127085
H	5.77225051366574	4.61831544008677	-2.73578818593171	H	0.07264186279801	2.79859276360274	6.16736931905410
H	5.01897269614430	6.23065484047508	-2.64125156487876	H	1.82274857392085	3.01895888789316	5.92965628902177
H	6.15481213357429	5.70520308289863	-1.37084940043003	C	0.45663633762440	4.47443576348078	4.02330839156716
C	4.60894736486373	3.46778475647392	-0.50729183545041	H	1.38642843881276	5.01927989787318	4.25964564846382
H	3.79819475756796	3.20352632249512	0.19474149593390	H	-0.30462945357782	4.78112332711508	4.75743234873747
H	4.64605593341995	2.67240479275401	-1.26496083178974	H	0.11317965570841	4.81035946190804	3.0338660078808
C	5.92574931254290	3.51939456234609	0.21156436018935	C	4.09231591644599	3.49774650243413	0.85601051220380
C	7.09051078215742	3.07136692672137	-0.42574475265510	C	6.54234826030473	3.67974718772575	0.37548603787791
C	6.02956537043535	4.01018145138797	1.51895615452751	O	3.98876219027047	4.63438043278230	1.31949124945904
C	8.32617764651457	3.12311910479331	0.21772645804260	H	1.73152832663090	4.16689493042924	1.73275539014642
H	7.02282124668848	2.67111499735445	-1.44148826094515	H	1.84810253653688	-0.58392903374428	1.49754381614535
C	7.26309177016187	4.06383580256868	2.16653709007313	N	5.24219006668725	2.99280165781669	0.38223505273905
H	5.13172011556240	4.35337715177261	2.03726853092260	H	5.19697585637079	2.11444316274841	-0.11950589081726
C	8.41700044622770	3.62345665175177	1.51694943008957	C	6.48392841717482	4.96293110925748	-0.45761278124105
H	9.22224416102179	2.76616503711098	-0.29690382589691	C	6.96145498356584	3.99248764324640	1.81464411294139
H	7.32271716134135	4.44882940279160	3.18788222201430	C	7.53932887047718	2.70413434098534	-0.24641839308537
H	9.38396637324104	3.66376514585132	2.02496258951981	H	8.54120953896994	3.15624144903533	-0.27364704562561
N	-0.67390422684722	6.59805633844635	0.26334430799118	H	7.59759999019352	1.77546479578693	0.34330653915457
H	-0.76381925489942	5.77726786594074	-0.32669400305304	H	7.23987218391619	2.45150008881063	-1.27399727778693
H	-1.55828941137767	7.06849756640298	0.41675748162127	H	7.95095127161342	4.47430478048543	1.81994168269621
				H	6.24050528526265	4.66880437634682	2.29330970178481

H	7.02425969374091	3.06715853348412	2.40816941798637	H	0.98911372375203	-0.62493758800714	-1.85579394053214
H	7.47660241950246	5.43802459613302	-0.48128419802119	H	-0.35167557847115	-1.48879349294331	-2.41843804597671
H	6.17313273208443	4.72612498675517	-1.48442768503412				
H	5.76549799602357	5.67170059262631	-0.02465598218298	<b>TS15</b>	<b>-316.60 cm**-1 ***imaginary mode***</b>		
Rh	1.68582001329875	1.89597036081719	-0.76577907239547	H	-0.14175786097764	-0.76361643620343	0.88520551299734
C	-0.03319948437750	1.78181798032490	-2.01238162374132	C	-0.68001179162374	3.03175038344021	0.33502008087381
C	-0.83378773082192	2.93272933647624	-2.00843911262765	C	-0.07080525057104	2.06673325130888	-0.66846985731358
C	-2.20950796810061	2.86573438966917	-2.21116032934560	C	1.34708831403242	1.90435567357715	-0.16995003823323
C	-2.80256511904529	1.62560685664159	-2.46286821211590	H	2.19060730709737	1.89617563158916	-0.86643759000176
C	-2.02485562252509	0.47372836623452	-2.50491527052575	C	1.41700999435279	1.39353073116866	1.13126527002563
C	-0.63955646934118	0.52939477644263	-2.28287095034242	C	0.04487356713432	1.18673621411381	1.74367855132062
H	-0.36958768833380	3.90668167904715	-1.83155443066458	C	-0.59292114367406	2.55812011790413	1.63581259016366
H	-2.81152896850245	3.77703482262198	-2.18509548945473	H	-1.16374044719735	3.00232838140024	2.45608933739399
H	-3.87964642809357	1.55469821011669	-2.63557530561018	C	-0.81660433528691	0.71657853758244	-0.56364634260952
H	-2.48534761923463	-0.49714832845373	-2.70952564450694	H	-0.38587795450093	0.01039946527314	-1.28910966143878
C	2.98777630939902	3.94768272566788	-3.20786733398659	H	-1.86401810207093	0.88300042502307	-0.86216933724669
C	3.81445602122544	2.79382859764008	-2.63835738996524	C	-0.74039595508267	0.16488755734078	0.87725153396525
C	1.70293215436435	3.24104297620692	-3.62534285928540	C	-1.55887831818333	4.14025136708727	-0.13079771955443
C	2.95733379319495	1.63583401689493	-2.42058018412323	H	-2.42596628840815	3.71216785636864	-0.66354448296721
C	1.65119906223360	1.85497168132417	-3.01559161627795	H	-1.03424472864919	4.79477496553053	-0.84344124413597
H	3.42533259052790	0.64828218353567	-2.35007986110191	H	-1.92771401225584	4.74741981651871	0.70584156893947
H	1.24318479495272	1.07739660996842	-3.67013498474120	C	-2.12430745792942	-0.17395545936127	1.45433617932713
O	5.02083225531282	2.84212847811166	-2.46431372393908	H	-2.75358925607181	0.73028172632104	1.34597493931152
O	0.87876166736057	3.69226807497363	-4.38276522450468	C	-2.77626731066804	-1.30028551924027	0.65692234309593
C	2.67608579634740	4.98884034237592	-2.12672026059866	H	-2.85301787283264	-1.06065323805215	-0.41427756353017
H	2.04509823474039	5.78742611529908	-2.54544982435740	H	-3.79211836927822	-1.50876519452856	1.02704748303027
H	2.14567769736460	4.53365160506201	-1.27318593550448	H	-2.18839918099540	-2.22904408690225	0.75055846012847
H	3.61106297054576	5.43232719151483	-1.75419939220562	C	-2.07267055441059	-0.54091664604404	2.93411215828964
C	3.68830343598050	4.62913684445504	-4.39727615636788	H	-1.35536649412674	-1.36057317984385	3.10977362461148
H	2.98171928826556	5.36683736687852	-4.80869167397541	H	-3.05960691673644	-0.88160405107693	3.28370607164891
H	4.54491197290805	5.18807436376782	-3.99184556095158	H	-1.77511325531465	0.30740325739754	3.56794652381224
C	4.16406369132261	3.70604519692643	-5.48910284521795	C	2.57678743081112	0.66987048662922	1.76066486280551
C	5.48796209420255	3.24604893880046	-5.50691265904714	C	5.00537593543989	0.10942386344279	1.58686407434000
C	3.30317055357643	3.28756076491952	-6.51333686469647	O	2.37921261301567	0.00450651596482	2.77863726789418
C	5.93737405520827	2.38748361133530	-6.50886258903858	H	0.15174340304516	0.84637178353295	2.77732916570896
H	6.17179607961202	3.56635634847022	-4.71770870944864	H	-0.10206871772412	2.47076855960729	-1.68865964375996
C	3.74867915884786	2.42601229573271	-7.51603803086439	N	3.76600480650843	0.76203678519593	1.13950988076526
H	2.27191785988753	3.64809043695558	-6.52610182811591	H	3.88672920452123	1.48498711261903	0.42365486531008
C	5.06721222781960	1.97082803794834	-7.51677931843947	C	5.44214604470358	0.66683989868169	2.94487737470884
H	6.97563529858906	2.04458484758163	-6.50394492399743	C	4.80917944798894	-1.40642576493854	1.66200651891427
H	3.06177603155548	2.11484296037798	-8.30755991161456	C	6.06756684828177	0.42638562732033	0.53502589207746
H	5.41827986415614	1.29947736515702	-8.30483261939372	H	7.02479619980506	-0.03432230550177	0.81901346091442
N	0.13779133693836	-0.60153229780833	-2.40778210231921	H	5.77298006974315	0.03107241978259	-0.44980829077537

H	6.21645483061817	1.51188565684011	0.43797350560816	H	3.28779154533511	8.08577917663546	-5.24211323809357
H	5.75666474853098	-1.89078766392143	1.94317866679673	H	1.33839309754575	9.53087838304379	-4.66607864398493
H	4.04472099474625	-1.66797948410171	2.40448293051888	N	1.39885282774612	4.09485675026185	4.36039301996823
H	4.49737023120263	-1.80090988975108	0.68238880904381	H	1.66813935937885	3.29119248109043	3.80035120755803
H	6.37536575337479	0.18337391591101	3.27224563362033	H	1.12132131472407	3.84242294527540	5.30229711984691
H	5.62284635700879	1.75089372593778	2.87627648850177				
H	4.66998150743881	0.48584840316772	3.70502459284992	<b>TS15'</b>	<b>-314.28 cm** -1 ***imaginary mode***</b>		
Rh	1.32585984716164	3.52139945638107	1.25180331614369	H	-0.06399479243601	-0.81426325478058	0.90232879719447
C	0.76381575655533	5.27396384443286	2.33299839344126	C	-0.65622235374523	2.97014049002594	0.32578493346226
C	0.02089934707934	6.29841538810263	1.73932303231200	C	-0.03554628889985	2.00534319844071	-0.67078958470328
C	-0.87743023572570	7.07168536851059	2.47232430722572	C	1.38313124485569	1.86655146003506	-0.16923415309154
C	-1.02582125080845	6.82955238495319	3.83859223675812	H	2.22939727823917	1.84944739619671	-0.86121649671769
C	-0.29080032765115	5.82170088558232	4.45648667805623	C	1.46035281082258	1.36546758022214	1.13477557606814
C	0.61541578550767	5.03700420359476	3.72701231360295	C	0.09200189752703	1.14396189943196	1.74904375644554
H	0.14434725471525	6.50041064201884	0.67502513313064	C	-0.56320096983838	2.50649644651088	1.62997823613410
H	-1.45047159758417	7.85985896352593	1.97853435416923	H	-1.14096984485698	2.94873995311600	2.44645337690113
H	-1.71926785315859	7.43006484398352	4.43322741979476	C	-0.76137769093204	0.64550262698317	-0.55649345767051
H	-0.40743141813882	5.62957667056342	5.52714725660119	H	-0.32030375568891	-0.05949530534007	-1.27690823911259
C	3.41637159584910	5.35102655673898	-0.54510381025225	H	-1.81108971686290	0.79443826934996	-0.85619781222643
C	2.81701614556516	6.14397613199792	0.61074640816661	C	-0.67728342649496	0.10460823155027	0.88838006919550
C	3.74746195528361	4.01023836034353	0.10661430840222	C	-1.54641554420715	4.06619623031377	-0.14774117705970
C	2.65973920638084	5.25651340537774	1.82806850239789	H	-2.40750175029187	3.62761788454870	-0.68171465394082
C	3.33584807619641	4.01576067561524	1.50166508336317	H	-1.02458845608200	4.72312875511006	-0.86051095562472
H	2.87114538797264	5.74478995453726	2.78364208710136	H	-1.92310093943056	4.67413696750967	0.68484731892795
H	3.82566432740222	3.37284275540788	2.23733043072010	C	-2.05605454851592	-0.25325725281201	1.46607525802654
O	2.59835646345117	7.33132594254749	0.59351829875572	H	-2.69881533741089	0.64124868854652	1.35562227911039
O	4.31480811580535	3.10255770103960	-0.49827391344727	C	-2.69142177933914	-1.39129108359562	0.67172384248925
C	4.72086140254476	6.01259391477958	-0.99251334559493	H	-2.77287302681736	-1.15548830461679	-0.39996214500497
H	4.52573335874885	7.02818129606972	-1.36305341672388	H	-3.70367522534454	-1.61430779265586	1.04323043635887
H	5.43283878697365	6.08005286270999	-0.15562705274154	H	-2.08948289352497	-2.31083559977057	0.76694442655862
H	5.18397878061408	5.41952296306049	-1.79432574488375	C	-1.99875422175875	-0.61590376611348	2.94665325049639
C	2.43215308524613	5.12835307886942	-1.71762256740578	H	-1.27067073721841	-1.42572103948707	3.12380423074941
H	2.89218420497351	4.35553195127830	-2.35380479056632	H	-2.98088914196407	-0.96879649246733	3.29767466708371
H	1.50317590495328	4.69789842003524	-1.30693380976719	H	-1.71191829747940	0.23771734387886	3.57829986234788
C	2.11789914453246	6.34295004151836	-2.54309023787847	C	2.63308758638602	0.64813397764968	1.74421771834675
C	1.01882137573638	7.15595934749020	-2.24126571850410	C	5.05982669839553	0.09194574226892	1.50960173153075
C	2.92205557720104	6.69320032812529	-3.63621281740333	O	2.45747665289105	-0.02767869505656	2.75892609821427
C	0.73836298559772	8.29393102043940	-2.99601698831291	H	0.20160811202583	0.81259612557789	2.78556751780606
H	0.36850465543807	6.88849049041772	-1.40519246400696	H	-0.07278455311901	2.40172004489256	-1.69393744073669
C	2.64744835489543	7.83144715563789	-4.39331000293456	N	3.81144506373672	0.75348574377308	1.10244337613661
H	3.77319669805315	6.05952988392139	-3.90044465329800	H	3.91664875509411	1.48693136970965	0.39592161294889
C	1.55595194514417	8.63916560629746	-4.07254814502570	C	5.53262959909781	0.62970553183062	2.86335533513479
H	-0.12607247207307	8.91348107367624	-2.74347871443789	C	4.86096597283277	-1.42424137416230	1.56984565274411

C	6.09516428530045	0.42029440625056	0.43473945598933	H	2.18432276229845	3.00514919669671	-2.60890196035721
H	7.05832818567832	-0.04597097487989	0.68793192092318	C	3.88142301849328	4.02325341422549	-5.37753121748600
H	5.77415570324836	0.03810176920474	-0.54704565483239	H	4.65064436734555	6.01879751775472	-5.68997451926823
H	6.24417000005862	1.50672890273058	0.34794212518815	H	2.98277269788639	2.14739084392587	-4.78953808213152
H	5.81277812213373	-1.91423442710295	1.82539310373409	H	4.23404334383784	3.64743466773333	-6.34152262352435
H	4.11144372126685	-1.69326182892237	2.32486009394937	N	1.17045288666847	4.17709870622117	4.34590090652837
H	4.52818095273978	-1.80595836000435	0.59206402305943	H	1.47293305170694	3.35083894328455	3.83776910031753
H	6.47289795508579	0.13981187564186	3.15955158331213	H	0.80662337213494	3.96556243980381	5.26800535948717
H	5.71357040107673	1.71429169736511	2.80493221491334				
H	4.78004531577767	0.43933646886523	3.64071179209786	<b>TS15"</b>	<b>-315.07 cm**</b>	<b>-1 ***imaginary mode***</b>	
Rh	1.34238272337852	3.49400936462172	1.23118146854230	H	1.82621924925504	-1.71424685730889	0.76672147757647
C	0.75651981312656	5.28873311247955	2.23098036814057	C	-0.13842172002419	1.58971088587308	0.28573908588328
C	0.10310166420816	6.30985174545895	1.53226296943140	C	0.75862811751162	0.93487573229874	-0.75149687650553
C	-0.83514456925961	7.13411869783100	2.14959935918595	C	2.14848938365564	1.32965864290999	-0.30587263433012
C	-1.11346816545961	6.95195722613350	3.50540596291990	H	2.90465365587636	1.63890643152203	-1.03322688619921
C	-0.46758514253181	5.95237679496132	4.22722030815903	C	2.45774685548037	0.87619360743717	0.98257114658566
C	0.47514872148897	5.11382441223482	3.61300186539642	C	1.29140456888736	0.16399377559911	1.63966498176873
H	0.32505882007292	6.46345578181257	0.47391316542584	C	0.17721732714069	1.18806868765986	1.57416910166571
H	-1.33767724876436	7.91641657811200	1.57621067037278	H	-0.48986187363704	1.37500728535041	2.42060224883120
H	-1.83891283811846	7.59527546321100	4.01036191267360	C	0.59630571974780	-0.59892666056068	-0.6438507553456
H	-0.68501479746006	5.80931737312119	5.28976396656549	H	1.24541055780653	-1.08171887052355	-1.38981630653943
C	3.54385130870469	5.45103254039080	-0.41270965430968	H	-0.44207479360829	-0.85014152094887	-0.91355401921550
C	2.96199761730699	6.17278336036775	0.80085793997447	C	0.92163760256511	-1.08024914593227	0.78724792694836
C	3.80098445620603	4.04735369786333	0.13059063755338	C	-1.40437649334821	2.25961570831116	-0.12128659307005
C	2.69046942051142	5.19089514496409	1.91591051027854	H	-2.04809028849141	1.52926510987157	-0.6423965866877
C	3.34368127258716	3.96130171790838	1.51426228265997	H	-1.21517707483525	3.08325702540299	-0.82497153171852
H	2.85330392963651	5.57392329800789	2.92770263544247	H	-1.95244771542081	2.65161613548962	0.74540706001289
H	3.80906457132454	3.26192510358457	2.21367001593533	C	-0.21272900269915	-1.91576750300480	1.40147593639013
O	2.81584040178893	7.36769214622114	0.87770416214128	H	-1.14176652844750	-1.32027090250327	1.31358084573748
O	4.36915190384618	3.16393462005924	-0.50575859608578	C	-0.40794883422724	-3.21081287598018	0.61763075887928
C	4.87990280949645	6.09461746808704	-0.78340313102751	H	-0.59399097618188	-3.02514373710209	-0.45095456390848
H	4.72416873651849	7.13965188198180	-1.08812943309482	H	-1.26076883280805	-3.78565075827954	1.01113791429493
H	5.56880252524980	6.08345030725554	0.07527845211427	H	0.48957729086230	-3.84779965085132	0.69450471363668
H	5.35041572178239	5.54545586322410	-1.61007126353670	C	0.01378921618772	-2.22435883002142	2.87800100440690
C	2.50670343359937	5.51024831282668	-1.56115516308006	H	0.99424579794377	-2.70622967992689	3.03218923404829
H	1.60786792373847	4.95727341477748	-1.23714071646187	H	-0.75861648476831	-2.91386712011784	3.25278066884762
H	2.21811650979896	6.56876406765363	-1.66490141984899	H	-0.01941661003715	-1.32213100176224	3.50642649217579
C	2.97537287479656	4.99010977271035	-2.89189126006901	C	3.82913584901478	0.60122388938399	1.53479110039489
C	3.66293500770569	5.82640277861496	-3.78197114966248	C	6.28687098795909	0.92382634568680	1.23855236221492
C	2.73540655614777	3.66657922844997	-3.27937355455816	O	3.93676822184091	-0.13405105399404	2.51799036679210
C	4.11594681681702	5.34892910475017	-5.01139758917948	H	1.55886493606399	-0.11119790290667	2.66375031734902
H	3.84112620155911	6.86996510621229	-3.50866901830139	H	0.53706847058619	1.29775429993362	-1.76146835830953
C	3.18319879781295	3.18458351870227	-4.50833345012073	N	4.87631459074692	1.13626070795454	0.88141265523361

H	4.69890338791209	1.88836145947582	0.20915946540516	C	-0.45856257567610	4.92158545188845	-2.78191094658776
C	6.57954585232047	1.50442948159158	2.62494798534060	H	0.35738994416709	6.60621073416762	-1.70677243159063
C	6.62331457285257	-0.56883697930677	1.19663310269987	C	1.12744490306826	3.23770265542116	-3.46037706941392
C	7.12057000772160	1.65363217323494	0.18648723455891	H	3.18163171478407	3.58965951491281	-2.89293029784637
H	8.19083919600645	1.52124020718160	0.40132701981624	C	-0.18305502774738	3.71492656958431	-3.42522018291836
H	6.91830391058681	1.25285332152729	-0.81924696407307	H	-1.48134784170463	5.30611655857361	-2.75016326381665
H	6.89522526878711	2.73002516118676	0.17811720865172	H	1.35412178223278	2.29614088720845	-3.96741809769648
H	7.69195074773872	-0.71671527172300	1.41441498768342	H	-0.98809816829355	3.14830186555264	-3.89991440650866
H	6.03215892061603	-1.12624696106360	1.93408257134752	N	1.05114643942118	3.40528027597848	4.2555477544560
H	6.41485871634502	-0.97904040185857	0.19626422509594	H	1.64168913524005	2.72937694978293	3.77893165187304
H	7.64089801470973	1.36337047306048	2.88130821006809	H	0.74354388126309	3.08715274441513	5.16751175296206
H	6.36106871228065	2.58357521698078	2.64419713956960				
H	5.96574202177804	1.00644523661637	3.38799544019925	<b>TS16</b>	<b>-316.21 cm**-1</b>	<b>***imaginary mode***</b>	
Rh	1.56865292444052	2.81485153364241	1.12718843542954	H	-0.04433385814162	-0.81725855824097	0.91659848987355
C	0.36879088088278	4.27837059556997	2.10003914374679	C	-0.86205210934563	2.94947730327419	0.53257977110843
C	-0.56784795102182	4.99552496273578	1.34899803346686	C	-0.23091683182561	2.06947372967245	-0.53334122716703
C	-1.76500138289345	5.44039493831779	1.90640623017192	C	1.21532679654441	1.99485936745610	-0.10137879852875
C	-2.02467133947181	5.18664804716639	3.25384726587527	H	2.02551345977543	2.07775479765904	-0.83165970983885
C	-1.10196757033288	4.48729835751171	4.02774642176171	C	1.38083539037690	1.44084261482787	1.17384067896062
C	0.10225636287227	4.02857087053257	3.47311065652791	C	0.05573014877532	1.11302768254301	1.83552992337879
H	-0.36190933003513	5.20179174537847	0.29731781220579	C	-0.67884036282478	2.43912037853820	1.80897267340050
H	-2.48469025166143	5.98657088471606	1.29206036457975	H	-1.24230253321227	2.81172910297456	2.66913224429184
H	-2.95315648128063	5.53743622447535	3.71225541798205	C	-0.86695992936367	0.66298193487078	-0.45332402106666
H	-1.30520948217079	4.28806340674471	5.08402021614104	H	-0.40605632949573	0.01863019495449	-1.21685908048800
C	3.35277013987924	5.71548841756806	-0.17142565910673	H	-1.93338236174904	0.75575474465601	-0.71362748609930
C	2.22366620872613	5.95019877368955	0.82465348396288	C	-0.69875171251978	0.07154606915357	0.96397973498827
C	3.81332055433547	4.30341822387856	0.15117619975261	C	-1.84368728696850	4.00246141038325	0.15172724707091
C	2.23644951242721	4.84878471845901	1.86950852090203	H	-2.69810186512671	3.52827985234179	-0.36240680661075
C	3.27723034032659	3.92472816717154	1.45791652397786	H	-1.40572561668379	4.72611936704092	-0.55268779126739
H	2.22417968295160	5.19726355859097	2.90798584514508	H	-2.22096111935183	4.54530506058250	1.02796288949155
H	3.90586170744049	3.37226979971947	2.16315411571430	C	-2.03659625758204	-0.37192736203367	1.57764909854183
O	1.51581727587399	6.92679234071611	0.83079548907090	H	-2.72554794739731	0.49261318804209	1.51857906235437
O	4.58423202183160	3.66134243646231	-0.55288464748431	C	-2.64361791152598	-1.51504429836504	0.76831462684655
C	4.51121513239034	6.63958959464572	0.26299217013336	H	-2.77443346718891	-1.25053644281398	-0.29181078816266
H	4.20415827884440	7.69001321522289	0.15386358135277	H	-3.63010250217781	-1.80003677294496	1.16590147822906
H	4.80082418693942	6.46589269207857	1.31043021792471	H	-1.99420734328869	-2.40572279627381	0.81244783939458
H	5.38680598358514	6.45295949192265	-0.37613359641814	C	-1.90997678161196	-0.77629192052973	3.04275690407511
C	3.00946227116209	5.99957077342194	-1.63275739995373	H	-1.14366742383027	-1.56000977981288	3.16952261967233
H	2.76340769866394	7.06975714061739	-1.71158911531094	H	-2.86344339538574	-1.18085909268097	3.41650485281377
H	3.92975679381819	5.83837543476095	-2.21529807095453	H	-1.63603294990888	0.06961010202381	3.69027800409320
C	1.89334639166637	5.18297698764296	-2.22255741023594	C	2.61944758047353	0.78653941890052	1.72240813708308
C	0.57303230920894	5.64924447442135	-2.18952266592559	C	5.08235087453349	0.46877014717832	1.45597370504561
C	2.15482518359317	3.96262962886916	-2.85855452637458	O	2.51861767998846	0.05671718262399	2.71037763850426

H	0.23216570219687	0.74245353633247	2.84931922113421	C	5.52130779454535	6.28090321289071	0.17102451582935
H	-0.33685652255344	2.50592168436050	-1.53489767865875	C	5.62947522170473	7.18826063737740	1.23370992285913
N	3.77324873716264	1.01705635221420	1.07159410198485	C	6.47263687869895	5.25615789974523	0.07276237341280
H	3.79496622318205	1.75946225358513	0.36447702809954	C	6.64800293974302	7.06441040818162	2.17907595573535
C	5.48739077407591	0.96868124201646	2.84591701752525	H	4.90817117044987	8.00500880775871	1.31958329825331
C	5.04177573789062	-1.06091133876258	1.42402501416404	C	7.49165610198602	5.12941035730618	1.01568678597453
C	6.08814425927649	0.97046916088131	0.42101761427047	H	6.40385445824193	4.54253343606405	-0.75179912642058
H	7.08912453760755	0.57918429316644	0.65380840199928	C	7.58046589984801	6.03185596030495	2.07611782358465
H	5.81267328027200	0.63318507005453	-0.59045203077457	H	6.71630440350455	7.78368868920172	2.99947521596900
H	6.13663216590000	2.06946842575172	0.41557509849541	H	8.22216315518096	4.32166014872487	0.91917050655889
H	6.03436696529095	-1.46745134631310	1.67090843032334	H	8.37941756094483	5.93543505436896	2.81589727174433
H	4.31184577038282	-1.44738177252549	2.14708346996743	N	1.15531973672764	4.12099221197232	4.51183522525357
H	4.76367139253617	-1.41568345725704	0.41936849321385	H	1.48992800320049	3.34041413838462	3.95428267107550
H	6.47144876337456	0.56085953445862	3.12337720310253	H	0.86842326444589	3.84649044962135	5.44458431871231
H	5.55790276953739	2.06761093527376	2.85604672460469				
H	4.75342843933905	0.65526484242129	3.60053448322469	<b>TS16*</b>	<b>-318.77 cm**-1</b>	<b>***imaginary mode***</b>	
Rh	1.14984672803502	3.55422474553218	1.37345159589758	H	-0.17715322128574	-0.79458981742522	0.86973201057292
C	0.51359048709623	5.27020100665517	2.47301118491574	C	-0.79978805781525	3.00667951205049	0.47352477552486
C	-0.26267114693569	6.25862308739918	1.85924813886507	C	-0.20668840655859	2.09188174455823	-0.58522285842418
C	-1.21956837888011	6.98150700332532	2.56847479834871	C	1.23042281393038	1.94218276373652	-0.14339980562352
C	-1.39221102334783	6.72825651551737	3.93031401609266	H	2.05020621434105	1.98366294235790	-0.86628480940778
C	-0.62214837872498	5.76013012908740	4.56833454144171	C	1.35737104597420	1.38891912310220	1.13583965177542
C	0.34213553950655	5.02444143327687	3.86212333923807	C	0.01233489699172	1.12951919103120	1.78787476280094
H	-0.12551171011156	6.46487166267248	0.79559071270925	C	-0.65728911489162	2.49008903938615	1.75248545770172
H	-1.82078100460536	7.73935925421489	2.06084792476431	H	-1.20597857698666	2.89341846594058	2.60812127668667
H	-2.13266789291490	7.29009265388385	4.50581021277409	C	-0.92025015431974	0.72299294644651	-0.50439803723585
H	-0.75786748350204	5.56011868584962	5.63528468048214	H	-0.49695226732464	0.05208386544300	-1.26676951260619
C	3.09778804729774	5.64469203446682	-0.36130552038420	H	-1.97959866995743	0.87607445793532	-0.76536924893260
C	2.53551783975586	6.32282508943538	0.88308830132384	C	-0.78740949463059	0.12524606285830	0.91376896346444
C	3.45630448367967	4.25257205070877	0.14702205377344	C	-1.71277654396468	4.11377384144917	0.07542665523414
C	2.42191142871405	5.32691625061035	2.01288491253084	H	-2.57449988215782	3.69064886802944	-0.46982519087239
C	3.13240702468298	4.14500840911592	1.56322894118902	H	-1.21378285871637	4.8177793961932	-0.60848858296209
H	2.62659797163848	5.72640335901861	3.01071651761668	H	-2.08850211046229	4.66776507954474	0.94529735562344
H	3.68206504121902	3.47090618038991	2.22422699870962	C	-2.14811942510089	-0.24955571417207	1.52303367886155
O	2.28914176573651	7.50166684143743	0.96801223360081	H	-2.79221892507272	0.64861593184265	1.46028445420521
O	3.98478714768621	3.39794726214201	-0.56265118685008	C	-2.80978623337222	-1.36093914402567	0.71269175066225
C	2.07153249283480	5.61633641734363	-1.48999566217147	H	-2.92312775818724	-1.09092971712310	-0.34803223700357
H	2.48332417131537	5.06804649046271	-2.35022787279851	H	-3.81094680701324	-1.59424850932728	1.10722220656625
H	1.14474755484859	5.11322115455923	-1.16936013186271	H	-2.20722563269667	-2.28377142350865	0.76008073321584
H	1.82464634314505	6.64038895495745	-1.80728814379854	C	-2.04792777186773	-0.65766546867203	2.9891799606849
C	4.38811800442415	6.36752128468394	-0.81816440244511	H	-1.32122535707426	-1.47749602075615	3.12006795594557
H	4.69310120861080	5.91832385185921	-1.77509025683533	H	-3.02171434587686	-1.01455960353514	3.35897302220104
H	4.12117570014042	7.41849736755876	-1.00991092833486	H	-1.73627168362900	0.17465088999118	3.63724486237676

C	2.56073605186567	0.69039363712663	1.71007890530058	C	4.41455258096528	6.26095530197002	-0.89816796184402
C	5.00905619447704	0.26012977322017	1.47089213230929	H	4.05598983924612	7.27087039279928	-1.15271860420694
O	2.41765271907357	-0.01236748109433	2.71217859944474	H	5.03080520794057	6.35849233003018	0.01020489842225
H	0.16338850179027	0.75468478283721	2.80404754248291	C	5.26141682770510	5.72107103047813	-2.01642735920217
H	-0.28303820465860	2.53048299086687	-1.58855759436040	C	6.37676527803704	4.91718419484122	-1.74709137391077
N	3.72798282932406	0.85572077614546	1.06447143758682	C	4.96975519040570	6.02647274269028	-3.35236882812963
H	3.79340707874378	1.59857679774056	0.36007706460192	C	7.16929295926932	4.41979233471005	-2.77990566555065
C	5.43280406624673	0.78673407826223	2.84534571877621	H	6.62613204219467	4.67900895518860	-0.70961970071043
C	4.90094683957391	-1.26642878863000	1.48835546632763	C	5.75792456970470	5.52790204126228	-4.38991004894677
C	6.03720194741929	0.68047237785481	0.42118314254918	H	4.11841332633777	6.67293812365573	-3.58208658399646
H	7.02153477628382	0.25955439587503	0.67239397127399	C	6.85967404360400	4.72029162085657	-4.10723625272061
H	5.74988025145566	0.31491413833985	-0.57713309711908	H	8.03641774952056	3.79595469135165	-2.54693112215730
H	6.12785220582911	1.77561206594640	0.37081697235396	H	5.51462770304375	5.77933429949814	-5.42566912164926
H	5.87633644992721	-1.70682307728818	1.74544118832936	H	7.48118717190269	4.33298742980723	-4.91884735660317
H	4.15840156826975	-1.59869092805481	2.22514792933429	N	1.56582915482147	3.92838970467867	4.44140570983259
H	4.60404248679444	-1.64060466919518	0.49621856761512	H	1.81733749038060	3.16772029609891	3.81682107134464
H	6.39882707487704	0.34812772493199	3.13888843725143	H	1.38434495613873	3.61077857423642	5.38700949743453
H	5.54711147742064	1.88161318153003	2.82053945013358				
H	4.68550032408140	0.52744696854029	3.60746250069059				
Rh	1.22771596352950	3.50780168309622	1.34004431481275	<b>TS16"</b>	<b>-315.30 cm**-1</b>	<b>***imaginary mode***</b>	
C	0.67917841150199	5.17610001500984	2.55034102995969	H	-0.12754711038470	-0.81967605910859	0.87373342427664
C	-0.17643609332094	6.17853209639368	2.08448161338181	C	-0.85672449421057	2.96580015035055	0.50525310116054
C	-1.05243795731506	6.84573442563125	2.93909340529975	C	-0.24736962129895	2.07424924114255	-0.56406839511724
C	-1.06173301083658	6.51910245441101	4.29589282813445	C	1.19659038635490	1.96112221480902	-0.13454531146030
C	-0.21020280522910	5.53282843798293	4.78567202108399	H	2.00834196589893	2.02459846585698	-0.86543301374571
C	0.67382089457878	4.85262031637313	3.93445750967062	C	1.34904486930341	1.40287647109678	1.14012409612577
H	-0.15948948684956	6.44931967821372	1.02780164364465	C	0.01691874052838	1.10370227098885	1.80130124493866
H	-1.71687426668362	7.61875118051832	2.54599737846034	C	-0.68827923316462	2.44592923576303	1.77972393243254
H	-1.73636305035523	7.03639367243909	4.98324288163959	H	-1.24112687485652	2.82907348511109	2.64199967201241
H	-0.21825275213090	5.27417422884529	5.84870728291885	C	-0.92044063691457	0.68474567777739	-0.48702649755195
C	3.14508633323060	5.43612950121110	-0.53789241687652	H	-0.48122590800529	0.03120798681504	-1.25546782162138
C	2.49416207556811	6.16172226171235	0.63696074359114	H	-1.98521631080601	0.80782312646066	-0.74159655473866
C	3.54541743243831	4.09846676177490	0.07013663933470	C	-0.76192216303919	0.08319932420908	0.92700077161714
C	2.51792983562966	5.28981469186280	1.87112227160923	C	-1.80752809618257	4.04702383031214	0.12495387684952
C	3.23036853846798	4.08480967243312	1.49258438421639	H	-2.66662374041953	3.59989550561411	-0.40519152442634
H	2.77463532241965	5.80263244548239	2.80249531015152	H	-1.34265555377153	4.76681704646898	-0.56634171319844
H	3.79522922912835	3.46243601087387	2.19072930822366	H	-2.18294650865185	4.58884155169905	1.00265379771803
O	2.09401288388147	7.30049400860175	0.59280964174888	C	-2.10758199915328	-0.33218666053722	1.54313600821905
O	4.07861691501310	3.19769370907404	-0.57594152628598	H	-2.77690661996249	0.54797418104390	1.48960062739927
C	2.18705585183583	5.28771840480250	-1.71157849347038	C	-2.74313321074052	-1.45760792601979	0.73114804793822
H	2.65487135348871	4.69953348854937	-2.51358510745349	H	-2.87129442758469	-1.18539846216738	-0.32734356515028
H	1.26828805208900	4.77028563276281	-1.39292581051946	H	-3.73457485383088	-1.72139525683129	1.13097570627903
H	1.91230792763150	6.27538516605779	-2.11071564498359	H	-2.11425606898815	-2.36316139711186	0.76934129810384
				C	-1.98577875567871	-0.74503412966959	3.00630955335230



H	-1.23649731979567	-1.54583319787658	3.12786487489504	H	2.49866206386269	4.82923609382439	-2.46737980368334
H	-2.94687762105064	-1.12998380759852	3.38114386788981	H	1.15125010384250	4.83831842328456	-1.29430686979467
H	-1.69178041556048	0.09202648209833	3.65651603558894	H	1.73702744517226	6.37507904918257	-1.98958875985604
C	2.57271958475129	0.72509768223951	1.69500168489822	C	4.37513018256641	6.19645938582377	-0.92348563061292
C	5.02512038099946	0.34001749974539	1.42331428371645	H	5.04456554074768	6.23316520471651	-0.04905344492531
O	2.45547421309505	0.00942788061256	2.69122688412243	H	4.83372162832553	5.50492759823953	-1.64769423898451
H	0.18612078689027	0.72659451941875	2.81378783197056	C	4.26877163745152	7.56678339432254	-1.52918306791197
H	-0.34370377754610	2.51667097039382	-1.56400423113163	C	4.01065082464937	7.72674047338056	-2.89729445295695
N	3.72973437951173	0.91941338733765	1.03884843939227	C	4.46150039760573	8.71466672397282	-0.75021496915926
H	3.77299609550978	1.66509377740037	0.33684532692368	C	3.93364519724381	8.99662286241765	-3.46837576826712
C	5.45455936745657	0.85366199033472	2.80081332102682	H	3.88287032916355	6.84149150037747	-3.52623675814702
C	4.94272597400268	-1.18821127111795	1.41934910872038	C	4.39065605128516	9.98592079149896	-1.31776403215973
C	6.03463739671482	0.79307542128991	0.36954908666075	H	4.67527681978528	8.60707730219303	0.31655020984451
H	7.02958736073351	0.38955350816664	0.60704416533003	C	4.12250761531402	10.13172279813565	-2.67955003730213
H	5.74573371700386	0.43299757129629	-0.63031667449548	H	3.73585228923131	9.09953078941090	-4.53866696770399
H	6.10189816879845	1.89038107498128	0.33164541335866	H	4.55135587085158	10.86901361334003	-0.69369159714694
H	5.92774225038471	-1.61575850113116	1.66096952719895	H	4.07044455918571	11.12766699440345	-3.12698187809579
H	4.21275371423817	-1.54349792148657	2.15799674407683	N	1.44015917095133	3.95577474941008	4.46768110358666
H	4.64299668461476	-1.55293516472439	0.42453487418001	H	1.71334756187595	3.19608295256083	3.85086702330891
H	6.43214465414304	0.42924268182341	3.07629318031814	H	1.24576304892308	3.64081178324679	5.41159459004199
H	5.54750679662486	1.95082262167939	2.79161072033831				
H	4.72115890867924	0.56857821243043	3.56713086191903	TS17	-257.48 cm**-1	***imaginary mode***	
Rh	1.16582180897099	3.51701612310515	1.35581548569161	H	1.41074483976829	-0.15093613202128	-0.62642997607787
C	0.57911412805517	5.18148033231451	2.55306741621594	C	0.56486507417953	3.52585594915734	0.26960335738839
C	-0.27686105511132	6.17147850386118	2.06226585221570	C	1.65144964507869	3.07438210685375	-0.69897714311143
C	-1.17578259793018	6.83671969849404	2.89428695994695	C	2.78381972845794	2.65328906558774	0.21921574527353
C	-1.20728665737697	6.52142441441309	4.25356962020819	H	3.81775195013799	2.92618544658170	-0.00786586915795
C	-0.35607347102887	5.54750842323804	4.76814020118872	C	2.41622740897468	1.64576080880688	1.10635623539722
C	0.54966633079789	4.86853252309548	3.93906849921414	C	0.96889585631239	1.23032302294764	0.95201677082095
H	-0.24411030832322	6.43163789850841	1.00295011700743	C	0.21784106644856	2.52092780176628	1.16720648738376
H	-1.84079385120387	7.59922391993544	2.48209384874187	H	-0.69833356019113	2.57475665314925	1.75966274952640
H	-1.89969090310736	7.03793229652540	4.92363127860247	C	1.14065886013516	1.83823446389835	-1.47405451212287
H	-0.38202618990405	5.29788136921318	5.83302265396107	H	1.92353678899817	1.50633838167689	-2.17202689951346
C	3.04661076119381	5.51584505086778	-0.48856053167910	H	0.27883965751964	2.15160399789244	-2.08458774403084
C	2.42864874139850	6.22402470527557	0.70973768275462	C	0.73697010856334	0.71434433034077	-0.49468503901083
C	3.46224696676835	4.16581793081085	0.09198772703310	C	-0.24725162760591	4.75013608026377	0.00253919630279
C	2.44027972504786	5.31081661163816	1.91719273499982	H	-0.86497856596373	4.59229198494586	-0.89879220090349
C	3.15713651007336	4.11816670191595	1.51326460853366	H	0.39387994240043	5.62294855737932	-0.19162129411833
H	2.68156392703223	5.78885739932356	2.87081340828301	H	-0.91533077796330	4.97301147665921	0.84635806204529
H	3.72886641551624	3.48374917961798	2.19481262441357	C	-0.70082738457979	0.22040327488379	-0.72709059985904
O	2.02507168198641	7.36214464574981	0.70646178944722	H	-1.35896594612376	1.11037982099126	-0.70765288165021
O	4.02993457198474	3.30348970184367	-0.57733294648756	C	-0.82721235607778	-0.42911439701296	-2.10273389115497
C	2.04755117248539	5.38359908512371	-1.63093824912774	H	-0.51524626473133	0.24744250315134	-2.91258863418928

H	-1.86677465571786	-0.73237580717596	-2.30223402355357	O	-1.24936197776103	4.37487829345034	3.48563758023396
H	-0.19736631173898	-1.33288952875296	-2.16142097687469	C	0.10156537371772	3.64638901842201	6.15439612078360
C	-1.17840353397685	-0.74408755831992	0.35415129274621	H	0.52539851647304	2.97382603483605	6.91311290056347
H	-0.48349778932832	-1.59488323607846	0.45645233555967	H	0.50794495277069	4.65630633534340	6.31748042064819
H	-2.16837796465668	-1.15229546536351	0.09778228949030	H	-0.98975627041833	3.68824176619238	6.28671876905473
H	-1.26787222340241	-0.26286494294650	1.33937041751097	C	-0.20210596118910	1.76574550705014	4.45257477181715
C	3.32683403526507	0.69128885642548	1.82038740951342	H	-1.28219696311745	1.95306565239801	4.33793854647909
C	5.71692209994987	0.08777021023654	2.25751585606263	H	0.16981993749430	1.41607444539175	3.48158630153243
O	2.85181962058094	-0.31214710362693	2.35488185550342	C	0.01134773941682	0.67732021789944	5.46939500504782
H	0.72906092626065	0.46257681026490	1.69322177882958	C	1.03531638879956	-0.26554252604273	5.30343351392701
H	1.95232904638073	3.88519893957517	-1.37459079401464	C	-0.82962783659670	0.55615158421554	6.58381387998387
N	4.63925153773607	0.96366181014592	1.77776455604175	C	1.22527861024153	-1.28437548852304	6.23640438816210
H	4.92222792318365	1.84110181489528	1.35884872355102	H	1.68457607413606	-0.20489230129319	4.42562394414946
C	5.55731902990874	-0.21739378808438	3.74892652399391	C	-0.64025444800660	-0.46009132495538	7.52045669221480
C	5.71123010003551	-1.20896441770010	1.44304124991586	H	-1.65314748309882	1.26362688242665	6.71485922858075
C	7.02199700391950	0.84274522126629	2.01893120852059	C	0.39217567184347	-1.38315657429590	7.35187782569800
H	7.87642480838177	0.22570526328444	2.33121831052966	H	2.02826340752242	-2.01157163988615	6.08712549038943
H	7.14586859215604	1.08526456628454	0.95149685460759	H	-1.30902014966186	-0.53635926115239	8.38207467016009
H	7.03961238555914	1.77935325945952	2.59500993455800	H	0.54005307295904	-2.18365838407266	8.08155388001010
H	6.52681762629478	-1.86950068356543	1.77425665736479	N	5.16981583610700	3.26644182429170	3.87992024158041
H	4.75780628340389	-1.74015125141783	1.56987214063816	H	4.35931479426062	2.89529642024824	4.37856396124358
H	5.85304710187199	-0.99103509609089	0.37325290794864	H	6.07657026804948	3.16141741693045	4.31244500013738
H	6.41319913693744	-0.81409132233622	4.09885424023691	H	0.91271858116955	6.04633026665532	2.97521555379725
H	5.52034799749310	0.71530099911474	4.32758176223704				
H	4.63475765313723	-0.78204936462856	3.93518847345636	<b>TS18</b>	<b>-257.76 cm**-1 ***imaginary mode***</b>		
Rh	1.94319991947819	3.65717799567219	1.93898833600878	H	1.39623422262816	-0.13588945297027	-0.69153579407668
C	3.74230921593306	4.60237308503493	2.43763523880655	C	0.56384125221047	3.53286994242941	0.25107595410069
C	3.62975646062205	5.71654421564588	1.59683465380694	C	1.66497729695268	3.09175299602444	-0.70604372900763
C	4.75478981021378	6.33817756490593	1.04994777501549	C	2.78001728786212	2.65043795173045	0.22325107125175
C	6.01671269060347	5.87491772052562	1.42452012048773	H	3.81817838174620	2.92610487927807	0.01990647048317
C	6.14431649015058	4.83921314887039	2.34350829327298	C	2.39479141349235	1.62967073191823	1.08583941440622
C	5.01766517534835	4.20425955945083	2.90977657785907	C	0.94754113331629	1.22514382301041	0.90394902477744
H	2.63557862819503	6.10278103156130	1.34076640724011	C	0.19891985408958	2.51555533879071	1.12864247877166
H	4.64099207994383	7.18279626570281	0.36695325689384	H	-0.72609626649013	2.56224950121788	1.70775946679810
H	6.91777320373784	6.34637473381954	1.02295795415990	C	1.16203306436597	1.87046008960991	-1.50921236824828
H	7.13701926292923	4.51402815203109	2.66885780429951	H	1.95646529891316	1.54366211987660	-2.19648057371098
C	0.42842171959165	3.13730969156063	4.73964272204249	H	0.31456137541734	2.19850887170040	-2.13187284614395
C	1.93777433001890	3.22349488616661	4.56884864507977	C	0.73146738860976	0.73549792369424	-0.55457946115229
C	-0.07200280951694	4.21327892664634	3.76576196896793	C	-0.23938228404210	4.76308217364505	-0.01639768404613
C	2.28468853177198	4.53437163254752	3.91194552450347	H	-0.84192370615824	4.61730085147846	-0.92997503831496
C	1.06270539721462	5.02042844218957	3.32037458563129	H	0.40906139294753	5.63485403358601	-0.19023523109461
H	3.01769679378449	5.15385376562627	4.43414621300511	H	-0.92075134266842	4.97993335758932	0.81814906815567
O	2.73283755149534	2.41841532374799	5.02667625311295	C	-0.70957250735645	0.26498843372000	-0.81571038620279

H	-1.35565439907397	1.16363072226705	-0.79081535536090	C	1.00745948205403	5.01670095872000	3.28496306995528
C	-0.82602731859546	-0.36016949225035	-2.20347536602399	H	2.92537706503729	5.14036800530792	4.46402631591335
H	-0.49413868220237	0.32517221365829	-2.99786906679120	O	2.57598435933047	2.40359618656809	5.06799450186151
H	-1.86694763585449	-0.64550895189227	-2.42151291147744	O	-1.31678904274688	4.39884077799841	3.36860511729966
H	-0.20791667813404	-1.27151920930550	-2.26868701873351	C	-0.25134916222664	1.75281578965620	4.41281964356431
C	-1.21635437838996	-0.70986633915253	0.24249241660272	H	-1.34726251052634	1.80013934635345	4.33076405426651
H	-0.53590362210018	-1.57283033883642	0.33962288831874	H	0.15372200789605	1.32529268042069	3.48764249192673
H	-2.20892486371784	-1.09827313491435	-0.03392476429479	H	0.00690097805355	1.07899302434999	5.24230589407793
H	-1.31167435482763	-0.24331607778260	1.23415102269429	C	-0.12932294357975	3.58726128961519	6.10331405425255
C	3.29039524249876	0.66173132952260	1.80060206192143	H	-1.22935668931183	3.54074791941941	6.12222316572682
C	5.67199107894968	0.03166355845401	2.24574870920576	H	0.24812178401381	2.82704991184666	6.80470075045052
O	2.80168871915622	-0.34144492785761	2.32106841870328	C	0.33744294071048	4.95280999440492	6.52173531172662
H	0.69375734526427	0.44652807239726	1.62894004089808	C	1.57101520852203	5.11989056095050	7.16399440066898
H	1.98039462843200	3.91191459610043	-1.36353733286189	C	-0.43156619618359	6.09060563367547	6.24516114542669
N	4.60629367005313	0.923797979151897	1.77010727948207	C	2.02903877435391	6.38998733045584	7.51317596188848
H	4.89941347746329	1.80745923904840	1.37185474781709	H	2.17929256785149	4.24023119167801	7.39300628916806
C	5.49134524969203	-0.30504080277813	3.72780313851947	C	0.02335339835093	7.36181309902257	6.59188055109161
C	5.66797171466782	-1.24736827312687	1.40338311286857	H	-1.39840556335041	5.97468537252989	5.74823260956542
C	6.98503903520820	0.78240622168987	2.04148096721510	C	1.25729092690520	7.51599584759320	7.22524644706647
H	7.83111819713351	0.15171082225845	2.34933409099257	H	2.99252906349672	6.49999596767045	8.01765070027300
H	7.12437273719640	1.04983090473168	0.98189326534633	H	-0.59178867661271	8.23764241790909	6.36914277529510
H	7.00305274448493	1.70480963021846	2.64038638205419	H	1.61359204200333	8.51213150771872	7.49987898522737
H	6.47349000785771	-1.92196446534695	1.73092988494829	N	5.06209586479620	3.16594394381638	3.96445657993431
H	4.70861773517038	-1.77326410944622	1.50607018459055	H	4.22977860169311	2.82341190350085	4.44690950226296
H	5.82564699494968	-1.00741935959306	0.34055141002479	H	5.95484156413358	3.03250685087401	4.41790938524024
H	6.33272275439854	-0.92488063278903	4.07263228526646	H	0.87973486463458	6.04046614629028	2.92523627897865
H	5.46402147463513	0.61485852188806	4.32729726118391				
H	4.55619357535983	-0.85614565229240	3.88913714765288	<b>TS19</b>	<b>-323.42 cm**<sup>-1</sup> ***imaginary mode***</b>		
Rh	1.91113191487919	3.63468894877558	1.94305618218394	H	0.48090456916868	0.01309357678885	-0.32069712135036
C	3.70932702080668	4.55030077286851	2.49622239276137	C	0.85427480992677	3.85076499426481	0.04936974518041
C	3.64992579227111	5.67044463846220	1.65755999115823	C	1.67322661393015	2.97409327012039	-0.88484263280026
C	4.80561823779957	6.26450838226521	1.14499800443540	C	2.70857134701234	2.37462703608457	0.03893496338384
C	6.04429323171089	5.76675616946517	1.55146528009256	H	3.75510478071007	2.30255620426711	-0.27025912483985
C	6.11902486274315	4.72427919207681	2.46860212315689	C	2.14222149522762	1.62465648366742	1.07326481271213
C	4.96087454434235	4.11619692269219	2.99961420488711	C	0.62540038007990	1.65257250174323	1.05255626869954
H	2.67393215516149	6.08331535334491	1.37551715652879	C	0.31468044380967	3.13059726954037	1.11245012061110
H	4.73291632839699	7.11431831079068	0.46279615193036	H	-0.49243715373081	3.52969425614879	1.73366480404109
H	6.96824844409354	6.21553976711318	1.17681614969279	C	0.75983777957390	1.86028964708602	-1.44341796295633
H	7.09368363019941	4.37143211710398	2.81870263880396	H	1.34786083287725	1.21277928419027	-2.11101271679986
C	0.30328809101439	3.14226378896846	4.67368909800632	H	-0.01643773225772	2.33748259789599	-2.06259448915182
C	1.81811613247612	3.22526329727127	4.57420181925796	C	0.11921628260982	1.05666606561171	-0.28960117849268
C	-0.15052564510109	4.22214069498789	3.68834856822350	C	0.37344078289196	5.18065122189902	-0.42108503721578
C	2.20476120439554	4.52387152274892	3.92211988826214	H	-0.32257331404581	5.02568356880803	-1.26447540461267

H	1.20126586155414	5.79934850744409	-0.79720211754749	C	1.70666303469273	6.59620578515229	2.33968372764944
H	-0.15080598938062	5.73337049117044	0.36790559849983	C	4.01265079094026	6.30508839319175	2.85915847884036
C	-1.41520983965129	1.01696273951351	-0.38682822893587	C	1.87324534577876	5.29369490156731	2.97605108175573
H	-1.76404761516699	2.06423207726985	-0.47070673118991	C	3.27320344619955	5.04075230588143	3.26581818348362
C	-1.85366395291715	0.27287509010618	-1.64526546859204	H	1.05510237427751	4.91170299808591	3.59735797703931
H	-1.42102241158496	0.70860362192348	-2.55838350587726	O	0.65572205034384	7.15669615527443	2.07860113161763
H	-2.94946495089460	0.29128660023151	-1.75309506011822	O	5.14274416453304	6.56720148766444	3.18973455093970
H	-1.53902051737190	-0.78344724882551	-1.59730394837655	C	3.08877374551174	8.62561599984016	2.77273675449793
C	-2.07184668455479	0.39764856093482	0.84276600403985	H	2.37500259406070	9.28737823096027	2.26121640218313
H	-1.66857667639792	-0.61060750958935	1.03772259962369	H	2.79913488886534	8.55807394272489	3.83236100686697
H	-3.15826537342999	0.29843740819475	0.69299430328943	H	4.09197557132925	9.06927860056364	2.71530313278307
H	-1.91952902722252	1.00091718062172	1.74967260348399	C	3.36461352127678	7.32828432877137	0.59566523204766
C	2.77511161473200	0.50680960350255	1.84906676817615	H	3.46083219955501	6.30627952189573	0.19381951687513
C	4.80831362947469	-0.93798093332199	2.05824811327919	H	2.45997884341394	7.76283585320885	0.14206176684103
O	2.08389345520792	-0.16327244063046	2.61780982220703	C	4.55699591937058	8.16104951835698	0.21373495834277
H	0.23981719783355	1.10032480090145	1.91416571685883	C	4.38459512824361	9.50135584022318	-0.15692142317066
H	2.13102282202140	3.56482500798629	-1.68880968083198	C	5.85670475908900	7.63873421100243	0.22817282769201
N	4.07343667432658	0.25476855352599	1.60974827833677	C	5.47597181344199	10.30085722430171	-0.49463568856122
H	4.55342273531709	0.86107195292662	0.95612797099401	H	3.37533500593292	9.92214267252595	-0.18322005292225
C	4.85525139292634	-1.01957070526914	3.58492883076534	C	6.95070213095627	8.43385966636033	-0.11059411461601
C	4.14139333629450	-2.19039450192613	1.48165147160618	H	6.01913505839065	6.59682311637014	0.51123269640214
C	6.22440448119541	-0.80433168576805	1.50498039102944	C	6.76527896377856	9.76908082929619	-0.47103982541769
H	6.82693018077306	-1.67637476242831	1.79671184808070	H	5.31701976191409	11.34360652354375	-0.78205013693834
H	6.21307131427066	-0.74862537502780	0.40471158201986	H	7.95635791324887	8.00561680532683	-0.09496015022131
H	6.71079296903994	0.10175336847425	1.89613760507972	H	7.62302547145495	10.39167716081535	-0.73824029674091
H	4.70265781708511	-3.08879139496941	1.77970973817743	N	3.82581480779692	2.38577126394508	4.47387835693108
H	3.11026162680550	-2.28527437423693	1.84871550567265	H	2.85942686463918	2.29393256126496	4.17766968692522
H	4.11983577709837	-2.14242816111509	0.38198153507090	H	4.11748741327138	1.64983449092763	5.10588819151957
H	5.38758842456203	-1.93328427751943	3.88937664044220	H	3.53249552000683	4.67198479322184	4.26486761785965
H	5.39093270679961	-0.15713703591345	4.00287928140123				
H	3.84157495831936	-1.04493603676445	4.00459772257755	<b>TS20</b>	<b>-323.36 cm**-1 ***imaginary mode***</b>		
Rh	2.31341833327371	3.69575175779779	1.70001476580323	H	0.54838518668124	0.06533702694885	-0.34904402825050
C	4.30563306691798	3.62530977241411	2.45686735495137	C	0.77783607547179	3.90051370860560	0.12673918446468
C	5.25528614153772	4.00649878140861	1.49255465296061	C	1.62981347610136	3.08435872196546	-0.83244775941628
C	6.57516810164033	3.57466473725187	1.54070638925940	C	2.69136654959168	2.49879666994941	0.07060695452254
C	6.98942259704081	2.78644661058402	2.61887804240979	H	3.73859481457478	2.47462596572881	-0.24361772241977
C	6.07627265504575	2.39344327450161	3.58909576870977	C	2.15868366358743	1.69709361180126	1.08405129505177
C	4.72318048411016	2.76197643452089	3.50258151424364	C	0.64249049216756	1.66919870760624	1.07019314294794
H	4.94391460179380	4.66819406142118	0.68045415342329	C	0.27715941533964	3.13140521501577	1.17397526789832
H	7.28149749021833	3.87856247301579	0.76469058492642	H	-0.54242842336886	3.48052370877169	1.80886348496716
H	8.03350812994632	2.47433381681279	2.70495007488276	C	0.75818041225052	1.95171329042029	-1.41997945453370
H	6.40336125853426	1.78107845884605	4.43372032993127	H	1.36917203780965	1.34490945894577	-2.10492468764382
C	3.07537649277808	7.24691001962172	2.11618510234251	H	-0.03710470628286	2.41501518340998	-2.02538468520990

C	0.15096106734016	1.09448163061051	-0.28679611370369	H	7.98551200526797	2.58912840000732	2.79619659006282
C	0.22027803573725	5.21008370703015	-0.31553075944732	H	6.33675875470563	1.83306269606763	4.48170106820618
H	-0.46920107039621	5.02755485134694	-1.15872045362762	C	2.94670968793975	7.26346661787824	2.12792346128278
H	1.00551753265047	5.88590038338088	-0.68339480929956	C	1.58777117697337	6.61663049415066	2.40213720709467
H	-0.33297721381998	5.71475120258048	0.48546102663600	C	3.89811948912149	6.37748574890976	2.92075756933974
C	-1.38154361717473	1.00568571173542	-0.37881437107812	C	1.78260806787785	5.33015749190801	3.06526281811622
H	-1.76580795082945	2.04254590479504	-0.43359501074718	C	3.18945139303752	5.10734810857938	3.35205945212233
C	-1.80179061422456	0.28096708620644	-1.65455870343324	H	0.97276974310581	4.93690700229241	3.6895954798997
H	-1.38721484924339	0.75415788056520	-2.55734661267233	O	0.52399399970225	7.15368790497265	2.14236790264216
H	-2.89808771888277	0.26763137259881	-1.75786460214035	O	5.02556610563222	6.67456998068916	3.22914953714390
H	-1.45382418222301	-0.76573876606054	-1.63561913531511	C	3.28452862424356	7.21133288021215	0.63522742935251
C	-2.01109668025865	0.33358751329454	0.83712206417599	H	4.30080889157260	7.59564247617691	0.46122434295578
H	-1.57269951809495	-0.66469604496392	1.00603536605133	H	3.22315694981880	6.18328680865131	0.24535250513856
H	-3.09410512565396	0.20076586912150	0.68878549660677	H	2.56967561337650	7.83271100274778	0.07546181521843
H	-1.87568152886287	0.91913950932964	1.75822506827777	C	2.98643680511964	8.72297671209426	2.61913401151839
C	2.83059304479698	0.57491265611857	1.81914220460420	H	4.00082165750225	9.10507620090205	2.42686340449482
C	4.89546726943332	-0.83106182106078	1.95187132708414	H	2.29200091575903	9.29186745575898	1.98264360915699
O	2.16544926816846	-0.13631051557740	2.57383978732820	C	2.62703017530699	8.92853720366825	4.06803010004958
H	0.28153602800319	1.07847714554186	1.91663464726751	C	1.30068017896674	9.17790909070208	4.44751292833588
H	2.06148829393337	3.71487379355876	-1.62065055535371	C	3.60572283931444	8.87885932515658	5.07038517794913
N	4.13160038609649	0.362541115250962	1.55701110222403	C	0.96028521320356	9.36227903225785	5.78691580084773
H	4.58607859357876	0.99601924757062	0.91075414708572	H	0.52769868418870	9.22231337443193	3.67678188924238
C	4.94631529765950	-0.97983896686568	3.47348377309596	C	3.26848064648368	9.06250667624680	6.41123153962743
C	4.25561808392304	-2.07156807213422	1.32097628555365	H	4.64645077410702	8.69715269751486	4.79200983323971
C	6.30706744390449	-0.64154685752098	1.40402055750259	C	1.94330655814707	9.30251230651925	6.77519410607197
H	6.92982750157367	-1.51068041568857	1.65959155609190	H	-0.08006733764261	9.55862186747602	6.05998921066878
H	6.29288006187018	-0.54165335663283	0.30683143422098	H	4.04844549235892	9.02433745102285	7.17643173571712
H	6.77292356494761	0.25925027428012	1.83102527669161	H	1.67806544362221	9.44968560089762	7.82542835126156
H	4.83643351692572	-2.96999657121479	1.57893300846882	N	3.75646549249574	2.41541464880443	4.50348183622489
H	3.22733908261415	-2.20453873759439	1.68446331119237	H	2.79327560334275	2.33459844423235	4.19421725232244
H	4.23144267058502	-1.97622263325720	0.22440184174254	H	4.04341857229505	1.65579076071941	5.10928085645984
H	5.51069537580617	-1.88710682729246	3.73679244225896	H	3.46382506230064	4.74841573912658	4.35052191230449
H	5.45002957135039	-0.11844825048654	3.93153227219204				
H	3.93418634240890	-1.05964454113041	3.88927472689566	<b>TS21</b>	<b>-331.69 cm**-1 ***imaginary mode***</b>		
Rh	2.25815612291662	3.75642484594146	1.76782118670111	H	1.33682553641201	-0.07508675061550	-0.73622967587926
C	4.25241990477598	3.72059812155954	2.53122715162196	C	0.68568168061491	3.57137858306515	0.42687008334277
C	5.21387283611895	4.14500232988468	1.59640642415063	C	1.75256044866841	3.14048762646307	-0.57181356492671
C	6.53557484139846	3.71877179889071	1.64978820647292	C	2.86134582885265	2.61592336688240	0.32046486295284
C	6.94047342218306	2.89713084477740	2.70616739957686	H	3.90606159152216	2.86967759550627	0.12003322716110
C	6.01760205832709	2.46891226031785	3.65159586617931	C	2.4507774286641	1.55067481208061	1.12002982187913
C	4.66308568866409	2.82993064583352	3.55690085642840	C	0.98469790050666	1.21266056055626	0.94386149324852
H	4.91731516938656	4.84287607895129	0.80930372606375	C	0.29760617067448	2.51995012622426	1.25803607731947
H	7.25199820941467	4.05536158920352	0.89697428183647	H	-0.60771550291804	2.57066101850964	1.86976642118305

C	1.18799263126566	1.98535404618399	-1.43063028167654	C	4.61463121495453	5.01312972572079	2.12853228581323
H	1.95834001016162	1.66264528399164	-2.14670527757664	H	4.24298353829145	2.39844949357624	4.29589384034024
H	0.34774513076803	2.38308100584890	-2.02170409710405	H	6.70154793263688	2.56663216530974	4.35112582980994
C	0.71907180527215	0.81823349296289	-0.53365434458692	H	7.85136074454772	4.32142682464423	2.98274572720726
C	-0.09844410367138	4.82396489902955	0.21286749406860	H	6.51536577227127	5.85295310497979	1.55994182873032
H	-0.69133832058433	4.73091379242621	-0.71378224585685	C	0.72657143752071	3.44368097695950	5.09784853611627
H	0.56099437722033	5.69686283082693	0.09046417104528	C	2.18157993849979	3.89805321211741	5.12355381104534
H	-0.78819745447108	5.00802672223764	1.04827968741223	C	0.13817190846026	4.27632726136657	3.95275898709681
C	-0.74810747553986	0.43339476730613	-0.78971745417401	C	2.48384124458505	4.77839145726412	3.92455625730027
H	-1.34844575451291	1.35843386359974	-0.69342192061228	C	1.20508687601757	5.00960000204430	3.28001818303826
C	-0.92609117613649	-0.09880475371983	-2.20909987841844	H	3.13275119113758	5.62899289284056	4.15373155138325
H	-0.57784997563774	0.61734177654060	-2.96852475255645	O	2.95427828980579	3.68268650387599	6.02667274873094
H	-1.98461796200931	-0.31901038069262	-2.41784221067190	O	-1.05726491850519	4.32236059184652	3.70145693674599
H	-0.35637566704201	-1.03356408155803	-2.34538325701536	C	0.04392992925282	3.82496294179005	6.40930358666180
C	-1.27930125601627	-0.57844034325593	0.22066758876740	H	0.51426633070844	3.30189581245439	7.25316705802250
H	-0.63837123248515	-1.47587032001444	0.25319917342072	H	0.11532399611355	4.90834590736340	6.59034006528630
H	-2.29429086307242	-0.90420389857084	-0.05550899283450	H	-1.02024753674967	3.55139141057351	6.36599617476179
H	-1.33288229284457	-0.16685762634653	1.23930136533832	C	0.56502858371923	1.93906113670255	4.76862038844752
C	3.30876572722264	0.51849970267746	1.78586079764788	H	-0.50824744925298	1.78341642404000	4.57323990896382
C	5.65181011156588	-0.30167314949844	2.11408005129242	H	1.09769972764869	1.73873178532496	3.82275303520862
O	2.77786098338322	-0.43497863134258	2.35737845156336	C	1.04119448694036	0.98024795015478	5.82082325545125
H	0.71068947488605	0.41158994308833	1.63639393966278	C	2.34001071715398	0.45975618794647	5.77316147232159
H	2.08762693649277	3.98116792543970	-1.19260838309959	C	0.19938613375909	0.57231805882203	6.86416825687336
N	4.63932414255945	0.66844121158013	1.67338986843683	C	2.79338994532194	-0.43108645057144	6.74421627816086
H	4.97941486344621	1.49941219981085	1.20587267214827	H	2.99619179008603	0.73907872216285	4.94621963390855
C	5.56946452320403	-0.52935730037388	3.62555587436724	C	0.64843930432373	-0.31759811633388	7.83957595173797
C	5.45320647440425	-1.62455945061827	1.36830346261293	H	-0.82597806266405	0.95005011194186	6.90543050952800
C	7.00923181720744	0.29206999796564	1.74666125533383	C	1.94917867297005	-0.81966185204700	7.78518382763430
H	7.81310372239798	-0.39493277275910	2.04696544645171	H	3.80966429044318	-0.82936057070671	6.68223200184295
H	7.08404404628534	0.45268224076614	0.65930104351031	H	-0.02503182037185	-0.62652283533178	8.64348042623818
H	7.16876317893735	1.25530823884374	2.25353606275692	H	2.30014421179306	-1.52054891356200	8.54702866104343
H	6.22906754325175	-2.34516774445737	1.66779940435347	N	3.90850987996678	5.88145107612385	1.32914828392390
H	4.46859559820702	-2.05419948981724	1.59651804157026	H	4.35505036381743	6.75829550706329	1.08787812239287
H	5.52693176600251	-1.46751600381881	0.28111702335105	H	2.90675836424783	5.94626122684686	1.46580681947468
H	6.35241750456457	-1.23669028329221	3.93777989546136	H	0.96610905421936	5.91383494276586	2.71296296061455
H	5.71682576541136	0.41218071599583	4.17279355636387				
H	4.59106502290917	-0.94423439482119	3.90030326954563	TS22	-331.82 cm**-1	***imaginary mode***	
Rh	2.03636326264532	3.48890905139133	2.10744345296234	H	1.34509230849211	-0.03526526751519	-0.83015103265479
C	3.95500042353770	4.01737978409448	2.90540873413050	C	0.67614955080948	3.58853061003420	0.39357415967486
C	4.73573114008359	3.15266472875922	3.68211273343568	C	1.74910378119981	3.18189294726768	-0.60980617476661
C	6.12395970556715	3.24653873853562	3.72124792177646	C	2.86037924338823	2.65272005989101	0.27765203020340
C	6.76272648939013	4.22466653799273	2.95757912886324	H	3.90354936113043	2.92256909507397	0.090143359175972
C	6.01731288490271	5.08700760231994	2.16159286539468	C	2.45425817606997	1.57211256715618	1.05878211752917

C	0.99190212943623	1.22478218261693	0.87211535970054	C	6.10532331451836	3.20116153011464	3.64493366584760
C	0.29588120341956	2.52131645994159	1.20858130619641	C	6.74520878472281	4.19837980846498	2.90711167721106
H	-0.60580359754006	2.55570274095875	1.82667836595634	C	6.00079919567234	5.09357416240570	2.14726354433009
C	1.19605995931059	2.03716086316687	-1.48909355820415	C	4.59739018934753	5.03224370430128	2.12551701941217
H	1.97280710963090	1.72899904677447	-2.20468785239729	H	4.21889107164584	2.34641669183622	4.20607697284949
H	0.35737873849316	2.43849367686910	-2.07993158552545	H	6.68487159478317	2.49542347422431	4.24369426960078
C	0.72807406313567	0.85483322858963	-0.61168005265323	H	7.83499890125346	4.28364263867592	2.92399599859658
C	-0.11674666839779	4.83839799832080	0.19655704819994	H	6.50041728811220	5.87366732790097	1.56538519766971
H	-0.69948859759304	4.75911890966176	-0.73780674059305	C	0.79380973366730	3.34256544275104	5.08943062394332
H	0.53617902110270	5.71932092129136	0.09845815250490	C	2.22180491000624	3.87670612190090	5.10817904449436
H	-0.81728721545379	4.99999928882569	1.02755054961675	C	0.14890957189833	4.14499007930051	3.95492676745895
C	-0.74016696575505	0.47640544035248	-0.87271152751470	C	2.46533267256980	4.77007653147039	3.90961974596237
H	-1.33779454901081	1.40192741612484	-0.76518245084674	C	1.16502869802945	4.95744319729106	3.29338926195367
C	-0.92006313096711	-0.03740792437154	-2.29845406273909	H	3.09324974555194	5.64111974651749	4.12035466855338
H	-0.56736892672058	0.68611092313661	-3.04880581151486	O	3.02138015891373	3.66937679201804	5.98948627469393
H	-1.97975762722551	-0.24890183974031	-2.51035699392492	O	-1.04813248738532	4.11518328679594	3.70274549591520
H	-0.35575794904342	-0.97372009547948	-2.44612637098109	C	0.78370723211727	1.83949122211165	4.80818587182791
C	-1.27549927444388	-0.54541342297155	0.12528278046596	H	-0.25311956228497	1.49590825278582	4.67436491204316
H	-0.63822818492404	-1.44576063296506	0.14776612970675	H	1.34824095032557	1.60143397436972	3.89220082145941
H	-2.29163270008492	-0.86387222186295	-0.15522779975418	H	1.23503380227899	1.29197581245967	5.64927668756516
H	-1.32823257119135	-0.14543780156484	1.14853930908862	C	0.07858312850305	3.62773600952185	6.42638807352772
C	3.30880350018560	0.54682491633284	1.73939105319990	H	-0.92731732568686	3.18776443907182	6.35089011330437
C	5.64233501054169	-0.32152846949306	2.01149136969716	H	0.62244664040102	3.07932833742433	7.21089022884620
O	2.77580531413468	-0.36389388334218	2.37604482025219	C	-0.02975799136458	5.08351555613014	6.79659301276392
H	0.72262665554990	0.41148587716296	1.55180379740978	C	0.98592117604145	5.72047368066351	7.52274379316642
H	2.07910006297102	4.03551433494176	-1.21557894535227	C	-1.14884165113936	5.83819190570945	6.41813829701563
N	4.63702519817857	0.65652569360240	1.57109671528724	C	0.89020082443466	7.07188795748920	7.85422620881413
H	4.97437725101679	1.43825854861002	1.02363109302651	H	1.86006580299126	5.14500641993497	7.83733177068679
C	5.58838278399145	-0.51996058049497	3.52790917658625	C	-1.24836873499690	7.18890647519116	6.74912968122995
C	5.40240717171218	-1.65436281120922	1.29569597450897	H	-1.95030413837260	5.35477926043014	5.85436176506632
C	7.00129490682365	0.24372411419090	1.60748629695244	C	-0.22724853009348	7.81206493515300	7.46730109180712
H	7.80031937963380	-0.45002559178132	1.90523471548222	H	1.69115009571571	7.54779821986364	8.42616968081827
H	7.05862035201052	0.38394794674102	0.51615732731121	H	-2.13291159477284	7.75694462465071	6.44852482990443
H	7.18370358280362	1.21333085885903	2.09469448392480	H	-0.30616231533121	8.86974579784162	7.73193564281663
H	6.16702895642813	-2.38725635777662	1.59441406898973	N	3.89002129186956	5.92844274588708	1.35873279397675
H	4.41294382684955	-2.05655397327700	1.55272851765008	H	4.34237326971863	6.80729650211923	1.13625982880710
H	5.45728219906469	-1.52069857433169	0.20430979967515	H	2.89093227398850	6.00042407123019	1.51041161975433
H	6.35728307478874	-1.24559948463708	3.83295785765692	H	0.87441644873366	5.85776508795215	2.74486056084452
H	5.77996745293076	0.42557289215427	4.05332254665133				
H	4.60433143336662	-0.89811445391518	3.83279020323555	<b>EB1</b>			
Rh	2.02292224529190	3.49122969321713	2.07427291073324	H	-0.01838514184427	-0.98725859356865	0.45093968065355
C	3.93737987923265	4.01957041674960	2.87877466309984	C	-0.87168860327878	2.75520983972144	0.95089347217810
C	4.71564849884176	3.12171827415223	3.61950110294896	C	-1.31668898358777	1.89649268284865	-0.21662927547319

C	-0.09699865442237	1.82859763836975	-1.09718440885063	Rh	0.96886333714741	3.50232676503157	-0.05407009907902
H	-0.16854342385797	1.90707584189299	-2.18337895905194	C	1.12157940086200	4.97339584426286	1.39213117410353
C	1.01805428959194	1.30116934468163	-0.47039669842190	C	0.31915400538482	6.11743018989851	1.39752360119514
C	0.74982094959601	0.94336419190791	0.98139680319901	C	0.41187733523450	7.09901083395155	2.38775152319636
C	0.26470503056592	2.24315113327934	1.57719823459721	C	1.35336566316093	6.94637014974527	3.40454140279646
H	0.56645728341927	2.55661924744637	2.57737981546161	C	2.15558716196304	5.81049909371337	3.43685789531117
C	-1.62505325542667	0.47832467737387	0.32392386659758	C	2.04035878998934	4.80732054769591	2.45548308203747
H	-1.96275254604410	-0.15541394093891	-0.50918374778668	H	-0.40871544270887	6.26357586339790	0.59332041006597
H	-2.46834644274371	0.56112874492872	1.02769733438447	H	-0.23436859482312	7.97985406748966	2.35059536100451
C	-0.38546199267642	-0.11814127062673	1.02574726337124	H	1.46448313590305	7.70972836205449	4.17963095175829
C	-1.83359720379402	3.71151876137750	1.56526083947345	H	2.88542815985365	5.67569778990059	4.24168242218981
H	-2.72185928470053	3.14264482012882	1.89205634254824	C	4.00043808122578	4.69329657332320	-1.44416270124330
H	-2.17911247691556	4.46124629566123	0.83791303040464	C	3.10948506334504	3.73296400989862	-2.23529820407183
H	-1.40303233199093	4.22465530106079	2.43332886064701	C	2.98681051845865	5.66960029086294	-0.84557676886453
C	-0.69319920878556	-0.60208225606822	2.45276444451157	C	1.68619889995275	4.06773503505805	-2.00010603863133
H	-1.16689213635837	0.24176374626323	2.99010322863320	C	1.61376341413850	5.21620082347321	-1.18820170386978
C	-1.68927152224023	-1.75807861789944	2.41904858073690	H	0.93905562324906	3.77017606204153	-2.73821358268689
H	-2.61869828246214	-1.4919495323578	1.89336457446033	H	0.79368530225686	5.93578294288252	-1.18820343673701
H	-1.96044271668784	-2.07366657174141	3.43849739459682	O	3.52725003101562	2.89909352181492	-3.00821978042867
H	-1.25139580901955	-2.62926817063637	1.90311945785199	O	3.27303841110009	6.70615335003828	-0.28680339877607
C	0.55858539126839	-1.0096269902277	3.22348785085904	C	4.90357478177214	5.44583177495517	-2.42207122836975
H	1.13720825266005	-1.76476417934546	2.66435886118198	H	5.59389031709031	4.74275252518595	-2.91084943457920
H	0.28698804839538	-1.45177022768991	4.19453660731756	H	4.31097860435900	5.94896347097166	-3.20141072474784
H	1.22434104969084	-0.15811798548231	3.42813215317024	H	5.48726953659300	6.20660724870697	-1.88551877605368
C	2.14331479385641	0.65744248613751	-1.23480240525024	C	4.81875837360807	3.89779868381282	-0.40652567484811
C	4.45883041421583	-0.27632370534217	-0.90697367554346	H	4.12385967083644	3.45035660843421	0.31797454158052
O	1.94966270559632	0.19985073874004	-2.35586598044120	H	5.28341178051475	3.06403216315523	-0.95433243676492
H	1.65270893610152	0.57788342350877	1.48156792441626	C	5.88883270202848	4.66531959483978	0.31844769835254
H	-2.18069298009151	2.33131702720202	-0.73481542247896	C	7.22091433855500	4.58101801332938	-0.10580714360097
N	3.30626389136698	0.56939387819492	-0.56119443185948	C	5.59249883849179	5.47087115194546	1.42585007272004
H	3.32457303308889	0.97892623980803	0.36453325394816	C	8.23070878420771	5.28487239667700	0.55041335329060
C	4.02484578353105	-1.74494606223387	-0.88441118200468	H	7.46864768870177	3.94739677393146	-0.96242183299075
C	5.02877813284691	0.09213126681704	-2.27657394681782	C	6.59895871433619	6.17382844227360	2.08571751175328
C	5.50992862351969	-0.02783982760521	0.17260951717112	H	4.56132802982891	5.55189708833714	1.77314124233053
H	6.38832106365185	-0.66446171778697	-0.00475303603534	C	7.92191222077916	6.08601305565698	1.64952738257346
H	5.84001489267804	1.02236992395240	0.16833372555603	H	9.26407692293410	5.20296116661727	0.20317092940669
H	5.11195602847213	-0.26515403907532	1.17233725948137	H	6.34674525875043	6.79536784531900	2.94909737666562
H	5.92838645454250	-0.51043165764497	-2.47329729871303	H	8.71065317178866	6.63714709218406	2.16820305668376
H	4.29293231986479	-0.09625727573811	-3.06829691327226	N	2.79131363331927	3.64834869710679	2.59597818159481
H	5.29696499241868	1.15696975406046	-2.31360020721368	H	2.86230143568469	3.07535270252304	1.76370726564938
H	4.87950267378385	-2.39910065560933	-1.11403530750811	H	3.66801546660052	3.73382385981124	3.09721385764000
H	3.63571200952828	-2.01641923362111	0.10929529328086	<b>EB2</b>			
H	3.23800386032773	-1.92690609416644	-1.63024137036853	H	0.28955097420246	-0.76797791672489	0.45455041201269



C	-0.83734033917109	2.89522227756898	0.97564470498882	H	3.72282844119419	-1.83173026707632	-0.01749716013283
C	-1.19479058229593	2.03128828834179	-0.21704799154721	H	3.38172533902798	-1.60140851898268	-1.75587264719986
C	0.04281309709121	2.06574922494322	-1.07521347695046	Rh	0.96543018435817	3.78987612427288	-0.01839706317410
H	-0.01351005817064	2.14797906341087	-2.16234204128084	C	0.83411136639443	5.30911226243196	1.37553325471675
C	1.17662705661962	1.58926863922718	-0.43760460145879	C	-0.12402346687544	6.31981586833051	1.27490426824249
C	0.91164719512297	1.20933617059391	1.00709299977672	C	-0.27852498004812	7.30457060304043	2.25466164442074
C	0.32811520864010	2.46532935215653	1.60440457497728	C	0.56196018209927	7.28771385031763	3.36704904527947
H	0.60390186730573	2.80224368294430	2.60504798137262	C	1.53060384759912	6.29605529203650	3.48873994832478
C	-1.40950830391191	0.58437126669044	0.29193536721769	C	1.68396386531196	5.30322720381024	2.50344809991767
H	-1.67138565816392	-0.05861832577164	-0.56125654640621	H	-0.77963487124557	6.35116978640909	0.39846450442514
H	-2.27874934415234	0.58869190496941	0.96842554161146	H	-1.04114139334307	8.07952490845769	2.14105792931656
C	-0.14940204250433	0.07146148842720	1.02310574833831	H	0.46987647452677	8.05142694145434	4.14437986189861
C	-1.88842687687759	3.74197369719571	1.60416896553938	H	2.19354935764774	6.27977052032854	4.35967654538858
H	-2.71755454110602	3.07809336557712	1.90699722181607	C	4.11294458302279	4.87755898299695	-1.14865243155471
H	-2.30134640891014	4.47482660079940	0.89601209902173	C	3.23857077066682	4.00765567727697	-2.04845209916495
H	-1.51700928727805	4.26811711991712	2.49129262261699	C	3.10283198354001	5.82708194839424	-0.50470841665669
C	-0.45439617689061	-0.44013537533434	2.44088330481084	C	1.81999633657248	4.40040734267254	-1.88466544042404
H	-0.98644288049402	0.37056366971711	2.97470478915706	C	1.74745613244108	5.51675252465571	-1.02492854577357
C	-1.37944838110045	-1.65277083431452	2.38289587057690	H	1.10714669448892	4.17041187519347	-2.67989352535642
H	-2.31414099696726	-1.43681644773577	1.84406445197397	H	0.98240054377668	6.29283607859255	-1.06114183479642
H	-1.64760859083828	-1.99170751661277	3.39560060185248	O	3.66815908975148	3.20898743241711	-2.85261949157996
H	-0.88303965724731	-2.4926337745090	1.86800498002238	O	3.40248621153481	6.72944531864005	0.24744140078189
C	0.80630964224357	-0.78020029829296	3.22991581043441	C	4.90291740714477	4.07246360381987	-0.12572928957806
H	1.43425291804231	-1.49908726182600	2.67629436731205	H	5.35217464428485	4.75122237930023	0.61418400047997
H	0.54542822907766	-1.24143553521130	4.19493189007592	H	4.26205129911954	3.35053138615452	0.39857354099421
H	1.42046440267332	0.10599957670050	3.44783899420000	H	5.70651759615035	3.50740168339679	-0.61999813798899
C	2.31209436234042	0.96457274844436	-1.20257803972243	C	5.08626722801454	5.70247563666864	-2.02645981261483
C	4.60010806319553	-0.03053315302138	-0.86789671378619	H	5.70286889874936	6.30802432094307	-1.34453086011187
O	2.14424026831058	0.56928327879731	-2.35108265693376	H	5.74983391038921	4.98307190659855	-2.53070402798495
H	1.82543716348381	0.90250566360355	1.52555936785659	C	4.41556940942005	6.58914196538366	-3.04212460195100
H	-2.07849363423498	2.41249695981077	-0.74413329728043	C	4.09329466028176	6.10630349709673	-4.31787771736971
N	3.44948627809765	0.80689749453979	-0.49856968563932	C	4.06974202192271	7.90937838213547	-2.72346227037643
H	3.44744371121174	1.15907306649560	0.45077398588241	C	3.43491440020320	6.91462281571490	-5.24388458968749
C	4.14653084075042	-1.48936240826679	-0.97450508813328	H	4.36295987370390	5.08170589582754	-4.58569782337199
C	5.22351318755029	0.43605329469795	-2.18321359951007	C	3.41187100772059	8.72043102794844	-3.64744326800552
C	5.61495395764516	0.11591143077191	0.26346817681927	H	4.31973640182722	8.30321361652786	-1.73516929410829
H	6.49239266687374	-0.51607483777449	0.06592057252271	C	3.08896086358148	8.22451764083976	-4.91078080193217
H	5.95489849216708	1.15890443534437	0.35353672394411	H	3.19489565405423	6.51941900971170	-6.23452680299692
H	5.17906162560861	-0.19489491730802	1.22654212466976	H	3.15382091374907	9.74845654972440	-3.37975350760884
H	6.11732459409566	-0.16791395976017	-2.40136057989690	H	2.57525452750168	8.85980350096362	-5.63694127023910
H	4.51018376809019	0.33117058439805	-3.01008609321579	N	2.63016014983565	4.30391451890152	2.68499213106988
H	5.51361503706865	1.49410955010570	-2.12254010511618	H	2.87201481099014	3.80227017879988	1.83690423638120
H	5.00012687981642	-2.13616669786042	-1.22770767437050	H	3.44635688190262	4.56497475494774	3.22739172994953

				H	4.91570809657601	0.44365125078077	3.01108587811534
<b>EB3</b>				H	4.18494612026581	1.45306903381700	4.29208047063406
H	-0.51849150701179	-0.89277075985813	0.39028446752327	H	4.23654951589054	-2.31677332108224	4.34705689245369
C	-0.41019793518155	2.97354375535808	0.11148020204595	H	2.63067128118032	-2.52014980668893	3.59395401849884
C	0.17254896175997	1.98508617024943	-0.88714675155200	H	4.00700560494766	-1.93514584385560	2.61684637458101
C	1.46314850787217	1.53635111710475	-0.25730915456688	Rh	1.41271964039810	3.18660020909753	1.39225647404524
H	2.40543742220194	1.46694952693326	-0.80259049864231	C	0.68994647762719	4.30755527971434	2.93602107321377
C	1.29737467162281	0.98218585887905	0.99422893592261	C	0.88149883287689	3.59059613073415	4.12088480251541
C	-0.15740036939382	0.94532443345274	1.43352432985740	C	0.40554083873174	4.04337869527661	5.35605934226802
C	-0.58329093563839	2.39902132123272	1.37223842148043	C	-0.27437537683632	5.25918964887688	5.40615590230766
H	-1.25505203256870	2.82549275365401	2.11870047118504	C	-0.44434641781091	6.00524339444376	4.24394915556645
C	-0.79148418574521	0.77707072300193	-0.98083110283298	C	0.04068519621727	5.55923160724445	2.99772478981149
H	-0.39895164387201	0.06614382271121	-1.72229935282201	H	1.41777185224421	2.63485809092307	4.09071271307737
H	-1.7562969506026	1.14318469835089	-1.36601256472211	H	0.56719122310437	3.44846666549867	6.25863549697935
C	-0.9694937296849	0.11556245088452	0.40072727796196	H	-0.66203315722538	5.64047580606952	6.35492780281287
C	-1.10929872153116	4.18687921420345	-0.39298459680486	H	-0.95552208341669	6.97261242474240	4.28599172888788
H	-2.01213048142923	3.87065785044542	-0.94533208716654	C	3.60724294207731	4.60771742555055	-0.79319123596630
H	-0.47465790679313	4.73765945207789	-1.10241044958305	C	2.75852954959460	5.36932576891062	0.21302895455421
H	-1.39581556041125	4.86548986838990	0.41996615492202	C	4.02351089540246	3.35690637175804	-0.00811716438025
C	-2.44885814005292	-0.03807125697436	0.79137242970678	C	2.88352250831191	4.71742981350762	1.53917585592601
H	-2.91805229950957	0.95958036561070	0.69414450352971	C	3.55415557997206	3.48118884722823	1.38696073351674
C	-3.15514283761222	-0.98693719526115	-0.17337879528626	H	2.83157332476841	5.30606564169716	2.45512729267771
H	-3.06256039347450	-0.66081994804206	-1.22011410838138	H	4.03520152615088	2.91635594600084	2.18962784639455
H	-4.22851648707644	-1.05788724105138	0.06112584853109	O	2.13798311917087	6.39003161735972	-0.02993734041103
H	-2.72742650142381	-2.00098570560891	-0.09948299943624	O	4.71123390725251	2.47313508332508	-0.47787520862404
C	-2.64153156559669	-0.51270115828044	2.22810709223380	C	4.88540034757064	5.42153967594106	-1.04166146553729
H	-2.09263768721530	-1.45205173591222	2.41100892919139	H	4.64115899474149	6.38245976409881	-1.51524044475898
H	-3.70647403887487	-0.70676641453258	2.42868751173265	H	5.41628127826334	5.62320050001977	-0.09849919221855
H	-2.30115693549645	0.22707383685198	2.96786417840289	H	5.55818805075661	4.85783273796565	-1.70455187985370
C	2.41559993414343	0.27161620011244	1.70629933232626	C	2.88830348879517	4.22677451950290	-2.09917884720599
C	3.18829709902249	-0.45487400344851	3.98295811927744	H	3.47963747339914	3.41140823611498	-2.54563343325946
O	3.42365262703088	-0.08214453617036	1.10649612108699	H	1.90545117238463	3.81169364302424	-1.83815078107177
H	-0.27776924280798	0.53505802955681	2.44107789880662	C	2.71317662845549	5.32371490089649	-3.11399936049604
H	0.32261739144983	2.44393463923702	-1.87188117736308	C	1.58543153666737	6.15428733699009	-3.10108496107934
N	2.21720815529428	0.09390680387719	3.02724015970860	C	3.67611630975718	5.52965263040490	-4.11043798583474
H	1.34445568572885	0.42591986607108	3.41833037351314	C	1.42949628694092	7.16673082429947	-4.04644158442189
C	3.53759752543870	-1.89629444024801	3.60851087059438	H	0.82285779382347	6.00802738014458	-2.33357585319816
C	4.44255413418709	0.42247878067906	4.00215603919263	C	3.52685278763565	6.54343916648898	-5.05689911007876
C	2.50971230522477	-0.42074659793642	5.34995141521075	H	4.55549632379573	4.88029241977328	-4.14694621593257
H	3.19089396399696	-0.81401815731552	6.11781371251308	C	2.40236275500223	7.36812436271361	-5.02684262226446
H	2.23755413892037	0.61009034733362	5.62865718585656	H	0.53970868676630	7.80139651989206	-4.01915936290011
H	1.59634217426521	-1.03634284895440	5.35222052238382	H	4.29095611978582	6.68532600456174	-5.82578667198630
H	5.16802951408459	0.02948200587443	4.73006098274270	H	2.28042861791279	8.16121958496515	-5.76918709967313

N	-0.15965479913790	6.33382472547209	1.86770500438952	H	2.57468071833668	0.61647617584232	5.50012099704458
H	-0.39441271986549	7.30027036793447	2.06784196818141	H	1.96132542254515	-1.03562823497802	5.19436948133237
H	0.57898337549583	6.27794857768973	1.16613430691217	H	5.42870399800858	0.18827287930912	4.31193709334554
				H	5.00203600958562	0.69180741665639	2.65204887409747
<b>EB4</b>				H	4.36135112529867	1.59481378632183	4.05474561090020
H	-0.50025533881178	-0.86650671800380	0.34872122981316	H	4.54722177718637	-2.16435351380125	3.89755250619686
C	-0.75575703384944	3.00285220361826	0.35486422131881	H	2.88741777805521	-2.39550842605387	3.28272559980176
C	-0.15379133526722	2.14465907713512	-0.74620449184967	H	4.14719818101391	-1.71306511806365	2.21583035409010
C	1.20999498687688	1.77324715224594	-0.23324561511227	Rh	1.11837712963691	3.29727001874248	1.54397232563218
H	2.11398116385904	1.83028470252879	-0.84105323397790	C	0.40681850611982	4.25101457515172	3.19638550383243
C	1.17998230626982	1.12331186820897	0.98122417185517	C	0.75517175537567	3.49110979984423	4.31678279889443
C	-0.23375965982878	0.92199013039930	1.50589951667952	C	0.32259224681023	3.81645724416981	5.60678840853987
C	-0.79524938135112	2.33004686707531	1.57752929225615	C	-0.47178401782829	4.94865776426254	5.77954782028952
H	-1.45487014850600	2.63611152251343	2.39107418504267	C	-0.79620103513518	5.74093742651265	4.68236814160483
C	-1.01213379569228	0.86241717217396	-0.87231933141401	C	-0.35616770663165	5.42340960151577	3.38103379889351
H	-0.61136861826783	0.24534683030282	-1.68956890943793	H	1.38565946080426	2.60333451868288	4.18883043689184
H	-2.02924031656465	1.16587747091214	-1.16648478458802	H	0.60712225342326	3.19055659119327	6.45639239978587
C	-1.03657707105545	0.09240243669902	0.46320523889956	H	-0.82882425796782	5.23028272493540	6.77402924277286
C	-1.58687131284526	4.17815709264184	-0.02545104195666	H	-1.39670976576495	6.64610262110592	4.82026331869740
H	-2.47599504855115	3.81720172915530	-0.57266737657207	C	3.02907735853733	5.00508074894751	-0.66854266627470
H	-1.03617950820376	4.84317431031492	-0.70737893902795	C	2.14754662038075	5.62235470009789	0.40481489790342
H	-1.90604284613106	4.75909722763926	0.84852771281096	C	3.60841180263401	3.77335549537069	0.03328800871731
C	-2.46700741204464	-0.22425000950260	0.93096168066375	C	2.43394812549644	4.95856909155483	1.69642170202335
H	-3.02377929724482	0.73212539160486	0.94639924882333	C	3.21667209348856	3.80331560059948	1.45613385289532
C	-3.15747915222855	-1.15467357190969	-0.06299369651378	H	2.37652465425782	5.50919571002065	2.63496963458041
H	-3.16993937789692	-0.73992389255279	-1.08199256104587	H	3.79842021222503	3.26235794015818	2.20691565528531
H	-4.20089660985937	-1.34167444712123	0.23457112835012	O	1.38391620247294	6.55580874414921	0.21499726279717
H	-2.64065812528496	-2.12824326238472	-0.10414446836870	O	4.35011859334938	2.97914377500166	-0.51099627396510
C	-2.51727793028719	-0.82338928067153	2.33270350771028	C	2.29927129057379	4.70195668246987	-1.96454352494102
H	-1.88103811322059	-1.72201561895449	2.40007697797985	H	2.96464312145108	4.16015844815886	-2.65255972053226
H	-3.54552697745195	-1.12476876454181	2.58540365549168	H	1.40485205670095	4.09205293866241	-1.78705859420965
H	-2.18600139499928	-0.11563517414174	3.10699972426499	H	1.98293555480616	5.63837456558319	-2.44652010551326
C	2.40056092120029	0.46232873481354	1.56155041624973	C	4.20550185015865	5.98286928944825	-0.95799633535380
C	3.4055774332734	-0.33018320171739	3.72325755136004	H	4.84761246165487	5.48518581681602	-1.70106993797535
O	3.36785464814656	0.19279280031923	0.85961110787306	H	3.77275350743934	6.87782700668751	-1.43144885290090
H	-0.24661702535703	0.43174084980535	2.48484445814044	C	5.01352960540733	6.36878259937774	0.25075016695838
H	-0.11299117712154	2.68250614821247	-1.70108509015299	C	4.64262211652251	7.46324836840487	1.04320713017774
N	2.33309034871596	0.22310685098974	2.88589831899195	C	6.12596783811468	5.61090393648464	0.63846011408168
H	1.48296757026275	0.49252325782397	3.36506874939656	C	5.35540803312626	7.78385358658366	2.19807477322331
C	3.76948132652655	-1.73770016638309	3.24651820292808	H	3.78202980157376	8.07168390331829	0.75147109957260
C	4.62517420285954	0.59391460057986	3.67911871195816	C	6.84057374628064	5.92827163869624	1.79313566744553
C	2.85166198128716	-0.38900802464158	5.14462089054095	H	6.43110283678627	4.75731533785762	0.02761942785219
H	3.61065107998265	-0.79597999822082	5.82767463581136	C	6.45491050857915	7.01398391233295	2.57959204349470

H	5.05222256086313	8.64294551285131	2.80225733840876	C	4.67385260527609	0.39450793048057	-3.05449469284387
H	7.70635647718020	5.32480734390872	2.07821972192506	C	5.30016007557696	-0.55151588376292	-0.82917441280548
H	7.01462068032766	7.26439656822021	3.48443618810072	H	6.00817039585606	-1.24733217473893	-1.30125532098368
N	-0.70444484086370	6.24120491975509	2.32094528200587	H	5.84317676979686	0.37278974002322	-0.57472083277174
H	-1.01268660320056	7.16765103095061	2.59566748022591	H	4.93683925587066	-1.01205659566122	0.10372783659929
H	-0.02506266858884	6.28954792921614	1.56099231167314	H	5.37310166997082	-0.29425876013643	-3.55238144892881
<b>EBS</b>							
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C	-0.48051669822671	2.98357774887621	1.44304519862477	H	4.05703468431924	-2.25131815281762	-2.63460657726058
C	-1.07783287513520	2.13705941576661	0.33677282456547	H	3.03340471653290	-2.03398513309702	-1.18751835486127
C	-0.06161699624855	2.23636799584614	-0.76884759621790	H	2.52741407935467	-1.34023215416049	-2.75473699730308
H	-0.35659341671742	2.34417579319042	-1.81469591727597	Rh	1.04170284814309	3.93342396427567	0.09256477788164
C	1.19302001836013	1.74756279515835	-0.42484452652638	C	0.91856213625263	5.50637438194194	1.41741878072841
C	1.26620485641390	1.33808821725208	1.03461573469739	C	1.79907564779854	5.58276819975716	2.49643949986542
C	0.80909151734983	2.57266794459747	1.77298648828018	C	1.68878345895057	6.57337789128953	3.47902161874357
H	1.29448541709252	2.89678525069729	2.69641841953976	C	0.66569860333509	7.51396611405459	3.37889405550028
C	-1.14179016044629	0.67086711467876	0.83107255323013	C	-0.22930730125914	7.45614866560765	2.31266451342115
H	-1.56046143868746	0.04226181523083	0.03141416936990	C	-0.11728447399149	6.46240096263451	1.32570753875635
H	-1.84848518444408	0.63017902402397	1.67479875733987	H	2.60265042933095	4.84677023411356	2.59069483823633
C	0.25638293272042	0.17791853198331	1.26660394403924	H	2.39770705431151	6.60237628267038	4.31073438552713
C	-1.38670872240672	3.75753165095391	2.34017325822656	H	0.55512396502383	8.29631928862541	4.13488201497990
H	-2.06729001493512	3.03667107375331	2.82646210908570	H	-1.03895847623306	8.18880860591444	2.23516446929229
H	-2.01092540208450	4.46708957288011	1.77977815831398	C	4.07117443950366	4.86170395110213	-1.00501671614933
H	-0.83585695039761	4.29733803834361	3.11973080789734	C	3.19821285288018	4.11671775278037	-2.01757829767257
C	0.27311973043460	-0.35550628349899	2.70885697507935	C	3.12307143223114	5.97231056409745	-0.54950433555027
H	-0.15704558405858	0.43311913017718	3.35557088546224	C	1.77934525209859	4.50880104138230	-1.83416424643392
C	-0.60653453313064	-1.59724524636987	2.82851433644422	C	1.74709766775295	5.65216140083170	-1.00820299329777
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H	-0.64444408336148	-1.95376231104374	3.86955426310784	H	0.97572043888837	6.42409505066458	-1.02929101398416
H	-0.20362839168386	-2.41553934145859	2.20804658413578	O	3.63576237392379	3.40390523932666	-2.89221408459275
C	1.68110010216065	-0.66268021086853	3.20894038026100	O	3.45600471094092	6.98944741238358	0.01978861710298
H	2.19907783757205	-1.35526408383081	2.52367948171833	C	5.31069739434514	5.43167246216535	-1.67979081784449
H	1.64296909839842	-1.14163210923404	4.19949373031755	H	5.95922608995588	4.61564824266005	-2.03008966586846
H	2.30117185862584	0.24064275873216	3.30773112201953	H	5.03871841218545	6.05414209177158	-2.54540213803691
C	2.06894887472818	1.14737106944846	-1.48949427144920	H	5.87556464764118	6.05156474832064	-0.97040353046466
C	4.14101632172755	-0.25584148535104	-1.77872738365792	C	4.43156159708382	3.86602311943662	0.13160544060045
O	1.67245811109496	1.05994063218378	-2.64741693027784	H	3.52305713783013	3.68121006223931	0.73595269503915
H	2.27723760703407	1.05221549747991	1.34333577537220	H	4.67857612664014	2.90940337465607	-0.35242202225161
H	-2.06477516683749	2.50710353804296	0.03127809345145	C	5.58432198735474	4.26381972317643	1.01170909659915
N	3.24318545665551	0.65227405054951	-1.05093893279236	C	6.79562119258614	3.56749165304590	0.91472195455044
H	3.45053390275607	0.77582589160818	-0.06855400328763	C	5.49452688836811	5.31664824254581	1.93311258642377
C	3.39180304434666	-1.54953028241057	-2.10918809019244	C	7.88902213169648	3.90847605027531	1.71128006968427
				H	6.88000129986322	2.74132242421422	0.20212996551478

C	6.58567281052178	5.66124072348360	2.72910311087549	N	3.24831192328506	0.60707330514338	-0.99807354920717
H	4.56609398675220	5.88345541041859	2.01822902818425	H	3.47484654104929	0.80672291108630	-0.03240258285093
C	7.78751825678219	4.95918982390386	2.62216480266630	C	3.34168162343177	-1.63709191879490	-1.97089715957204
H	8.82401395759718	3.34966644903405	1.61846895978021	C	4.70139018617835	0.22808123901043	-2.96565070683726
H	6.49551156873604	6.48610458329286	3.44104564942992	C	5.25958379318797	-0.65587462272215	-0.69639095173308
H	8.64136691077686	5.23035531016756	3.24841935229723	H	5.95523991436458	-1.38621514640422	-1.13353446019554
N	-0.99502817109464	6.45347843620383	0.24868740881760	H	5.82532224628794	0.25965168645920	-0.46131883418592
H	-1.12419219363072	5.54268657525760	-0.18264187563205	H	4.86645175822754	-1.07629283512972	0.24325590511695
H	-1.87354472436983	6.93807332634090	0.39548065001541	H	5.37645427287445	-0.50464967408541	-3.43339740500965
				H	3.89718841633793	0.47536370121724	-3.66980714085309
<b>EB6</b>				H	5.26320544656684	1.14869483960122	-2.75624750081895
H	0.53767946430695	-0.62026101508416	0.62636309825993	H	3.99363513550121	-2.37947444667098	-2.45557080504040
C	-0.48523595874917	3.03542016046442	1.38378037492351	H	2.95150705204683	-2.07312766132656	-1.03799371836954
C	-1.07494041558715	2.17987991074298	0.28039819033733	H	2.49602285494351	-1.42675141208690	-2.64017100431757
C	-0.03831868483575	2.24417866406221	-0.80876346548264	Rh	1.07227010911908	3.94235781508230	0.03908262483750
H	-0.31457157631760	2.33336582906320	-1.86148113221802	C	0.94137778030150	5.53650230887353	1.33381402993177
C	1.20281362825705	1.74414209639698	-0.43351727121098	C	1.81316527711277	5.62850716708368	2.41900958236000
C	1.24450734575527	1.36043005108379	1.03393001561495	C	1.68601467763035	6.62997685920188	3.38827095108752
C	0.79311552935151	2.61412530339459	1.74225232492102	C	0.66194031845638	7.56688833163008	3.26396585304764
H	1.26871285364183	2.94981825452921	2.66670833601506	C	-0.21761673325714	7.49749727361460	2.18569381393153
C	-1.16940927200643	0.72325752431859	0.79737453113427	C	-0.09193828768546	6.49122688654254	1.21346019592928
H	-1.58184656674972	0.08718259622316	0.00038666697812	H	2.62490347616259	4.90203241551639	2.52339834112771
H	-1.89218586833191	0.70629434120520	1.62812895624872	H	2.38387904864582	6.67283962979189	4.22864280987576
C	0.21328394879065	0.21919311887788	1.26755696458464	H	0.54033334112032	8.35759965325667	4.00954839176679
C	-1.39632457546399	3.83139524515230	2.25653253152139	H	-1.02525083851338	8.22994914022347	2.08764072049933
H	-2.08892168385264	3.12324016582100	2.74458094872699	C	4.13042055958733	4.84994036615080	-0.97722919791375
H	-2.00775808252953	4.53778624138863	1.67835941334522	C	3.29879525899927	4.03239962458031	-1.96389270300059
H	-0.85116648840839	4.37786657621503	3.03549689678911	C	3.15397792872849	5.95479309299180	-0.57177798168774
C	0.19550998294187	-0.28920085021124	2.71893317028476	C	1.87776163322421	4.45426449196981	-1.87683883235158
H	-0.23363627860259	0.51686276152020	3.34454716669117	C	1.80813587836525	5.62931157185741	-1.09884757046537
C	-0.70591505399784	-1.51477934410064	2.84370311704343	H	1.17718872224884	4.17153059309017	-2.66598217566923
H	-1.73069875034910	-1.31575871123149	2.49600853726337	H	1.03460189561391	6.39619414421713	-1.17192896452932
H	-0.76774726449579	-1.85284447346672	3.88975780285311	O	3.75889923186604	3.23534492834698	-2.75060987179841
H	-0.30556144572761	-2.34987726910429	2.24433075341727	O	3.46154358335252	6.95281017197285	0.04400797497732
C	1.58936919021553	-0.60950211075840	3.24955256721786	C	4.51699122966790	3.99546251545220	0.23228417096058
H	2.10841375071725	-1.32163767866260	2.58542622050907	H	5.00880119345489	4.62114264968245	0.99211059843918
H	1.52633998962058	-1.07055231556526	4.24731432528078	H	3.62710425514327	3.52802339948453	0.68758416228928
H	2.22154232799944	0.28588100770147	3.34368673813403	H	5.20822906520981	3.19600705233037	-0.07426807506098
C	2.08325071065883	1.09488965311020	-1.46550444779173	C	5.39105367836530	5.43190635982779	-1.64201339639548
C	4.12722610945349	-0.35618971423747	-1.67605995444749	H	5.91523470124037	6.02576834797645	-0.87738273434159
O	1.69016309854862	0.95479584085101	-2.61993131019942	H	6.04259392160406	4.58522815529955	-1.90695127592919
H	2.24529313919862	1.06246521600929	1.36290198179749	C	5.13103975169376	6.27991349889988	-2.85988247931326
H	-2.05071579250281	2.55898310006348	-0.04909759173681	C	5.11597827870277	5.71291576628314	-4.14167980045586

C	4.88581989303674	7.65502587469462	-2.74017468767169	O	3.65016165331654	0.07425843986241	0.84756864700290
C	4.85140963012019	6.49156847250031	-5.26776844108338	H	0.15878665783418	0.52719380045674	2.59566222332864
H	5.31042988938491	4.64372716788928	-4.25288040266486	H	0.09508265618128	2.41563760112998	-1.77452464528748
C	4.62059856323085	8.43661319583493	-3.86415046733463	N	2.72806889289125	0.36858419398712	2.91023965102320
H	4.90294739123766	8.11572705990315	-1.74972411898511	H	1.93627003347718	0.77526628637327	3.39677100117807
C	4.59869123435433	7.85696549167350	-5.13299409128982	C	4.07096631726441	-1.62903190980852	3.39826826172839
H	4.84634688657882	6.02823538273992	-6.25800183226811	C	5.07552633474424	0.67588433611058	3.56453290574847
H	4.43460921935457	9.50763300361591	-3.74735945276318	C	3.32398983303383	-0.05704483419060	5.19412558535794
H	4.39189584649493	8.46877109532071	-6.01492424923652	H	4.09078840203270	-0.44717495877958	5.87831973134964
N	-0.95344777071745	6.46730705490592	0.12280196867967	H	3.12342121795619	0.99102570279270	5.46719111341875
H	-1.07646069986120	5.54849545184013	-0.29340675160010	H	2.40135038633216	-0.63989665421219	5.34198456656046
H	-1.83593497460800	6.94956709678137	0.25359110113754	H	5.88049946116889	0.29499393904775	4.21070694242155
<b>EB7</b>							
H	-0.18351747371401	-0.95244163294447	0.60342401546041	H	4.86276448616685	-2.03394335577080	4.04622989516797
C	-0.47531995601776	2.89267732655001	0.27274177612711	H	3.15969776302182	-2.22796364463465	3.54876230044214
C	0.09131939651114	1.95410373625431	-0.77902203699276	H	4.38787597457982	-1.72766555983341	2.35163367874902
C	1.48368351691963	1.65833411400521	-0.28460252523962	Rh	1.51125408202099	3.29339192921576	1.25831132683606
H	2.35097693608780	1.64962011102117	-0.94648782346847	C	0.71698928617949	4.72073794561272	2.50697034818735
C	1.50802910439482	1.10526856276507	0.98659209287101	C	0.09990636188786	5.89842825130294	2.09316459260092
C	0.12337797585031	0.93103954176277	1.57936819501694	C	-0.56133224377250	6.74655366942725	2.98997905443990
C	-0.42629579120028	2.33973920152510	1.55033114261324	C	-0.58906915753109	6.41555339857566	4.34221081861695
H	-1.01128755610331	2.74490082163320	2.37797093328554	C	0.05013270762824	5.25896965957089	4.78613931609373
C	-0.74622471994350	0.65416641177366	-0.75639736042187	C	0.71295606666933	4.40859495951381	3.88698797095438
H	-0.35934832317187	-0.03370418409016	-1.52247674169561	H	0.12718570385773	6.17510406161960	1.03776713239506
H	-1.77794129814616	0.90971480838980	-1.04554323085530	H	-1.04414354897898	7.65802953216541	2.62785757186202
C	-0.71639627456688	0.01410389360551	0.64809404990862	H	-1.09766988825789	7.06217131208993	5.06257703716678
C	-1.36023437658701	4.01458544609793	-0.14484007025675	H	0.04793966666691	5.00335403972932	5.85072366410274
H	-2.21041720592886	3.58834359455807	-0.70580308017129	C	3.49893417134082	5.10594218847710	-0.73912469236075
H	-0.84520209219769	4.70840197613326	-0.82527968498967	C	3.07579190182272	5.68316562282968	0.61098934155654
H	-1.75465197952276	4.57207854879540	0.71301140679272	C	3.88278798127091	3.66839200053348	-0.38728121676187
C	-2.12667090150584	-0.25648868487653	1.19980780909951	C	3.15841396112543	4.61924606539442	1.64263174722405
H	-2.68852957937369	0.69485595274928	1.13671892936525	C	3.63047773599557	3.42808324727119	1.05142245996389
C	-2.84743325105070	-1.28813532008493	0.33637920819693	H	3.26172763581527	4.88931183138833	2.69447148684295
H	-2.89428357801230	-0.98648622307391	-0.72071642441609	H	4.14047987474588	2.61859589790000	1.57661916936985
H	-3.87987220611842	-1.44136554856423	0.68673219173475	O	2.81468824979628	6.85024387719446	0.81443265070141
H	-2.32921025750035	-2.26072726740914	0.38429518810969	O	4.36529021627256	2.88410297005471	-1.17954400688584
C	-2.11951741250907	-0.70598751267676	2.65763090076009	C	4.74514075183647	5.84584942254259	-1.22761052074056
H	-1.46275342033756	-1.58150786015974	2.79601708971076	H	4.51353787088932	6.90671424437545	-1.39479271604425
H	-3.13243685137618	-0.99665135636280	2.97624223630861	H	5.55604048518873	5.78189946548140	-0.48577527050526
H	-1.77750094807520	0.08456265672321	3.34205013195119	H	5.10161149592550	5.40389875167897	-2.16950739432561
C	2.73236402295946	0.45786350608120	1.56559928352093	C	2.37477307279691	5.07759699345448	-1.79860773898604
C	3.80940002196835	-0.16360192857211	3.75069695125202	H	2.73872533306689	4.42606402957390	-2.60938253259279

H	1.49898348758966	4.57987202704789	-1.35195956864346	H	-1.79859598136066	0.03880907950274	3.36548525451277
C	1.97479266258416	6.41158967392540	-2.36385082046222	C	2.80624603490310	0.44377484726864	1.73194955214931
C	0.94508708132622	7.16363729917636	-1.78541238090444	C	3.83352026531314	-0.31657927821767	3.89451258285713
C	2.62584081372429	6.93507878003374	-3.48875788216741	O	3.77646813008630	0.17873621178948	1.02769685145119
C	0.58117754469024	8.40434812226864	-2.30553811336617	H	0.18074782005553	0.45667760829973	2.70442245740969
H	0.42090633291672	6.76836848854978	-0.91332782166712	H	0.23766602328454	2.41080195555136	-1.63930387940431
C	2.26985645625846	8.17853977535300	-4.01058524234864	N	2.75456852043617	0.22893345177462	3.05984819257211
H	3.42077024807625	6.35483644276773	-3.96527411251072	H	1.91517718958618	0.52171503310376	3.54537455534716
C	1.24610443469802	8.91905223845044	-3.41901379778658	C	4.18118763005828	-1.73481996509217	3.43782077368324
H	-0.22844021824633	8.97184056263965	-1.83926934317033	C	5.06124105230374	0.59504122738119	3.82235696306781
H	2.79155438004603	8.56806992716808	-4.88877935069531	C	3.29453794941752	-0.34682415301527	5.32233890129692
H	0.96240599562755	9.89170089418097	-3.82930669514219	H	4.05604812857951	-0.75147055388725	6.00391108093309
N	1.31271896039226	3.23662675456064	4.35147184082858	H	3.03144157921004	0.66690277355253	5.66459291140867
H	2.14727609843099	2.97340661570714	3.83422306795372	H	2.39801766582490	-0.98304222666486	5.39038287161842
H	1.50137244499519	3.23446175620869	5.34938246735241	H	5.85504217509941	0.21013455486382	4.47990866598217
<b>EB8</b>				H	5.45088009411237	0.64410578954807	2.79653566988591
H	-0.08659647232228	-1.00671420946917	0.69399677533325	H	4.80268629164270	1.61376983111929	4.15066828143023
C	-0.42234088611738	2.83877510259652	0.39095006711059	H	4.96691765296077	-2.15442548344560	4.08379597530069
C	0.20773526813947	1.93296842073148	-0.65196935429275	H	3.29607649098756	-2.38647462058641	3.49990138543061
C	1.58621665924946	1.66198153902972	-0.10952656040014	H	4.54311319179037	-1.73104465946281	2.40112712439446
H	2.47926414567366	1.68229445653660	-0.73587922112285	Rh	1.52145118706762	3.27920304439232	1.44120038335131
C	1.57884395212347	1.08241987493695	1.14971082495581	C	0.62462074897526	4.73752004236234	2.58068940566661
C	0.17935311717361	0.87395383852974	1.69272890029592	C	0.05043855671748	5.89546974379869	2.06130641125882
C	-0.39635321309871	2.27209397132604	1.66355376762562	C	-0.66971304039637	6.79022838001452	2.86181649566380
H	-1.01944223081083	2.65309287965770	2.47496988344144	C	-0.79962180820601	6.52849552023198	4.22377408840367
C	-0.59054586053878	0.60827078281882	-0.68108965664971	C	-0.21123659189084	5.39071737016274	4.77245147262155
H	-0.13705204889862	-0.06136531976643	-1.42656365545122	C	0.50574748014208	4.4891106903815	3.96816211043525
H	-1.61153164439138	0.83168487078709	-1.02835876853431	H	0.16422775527846	6.12133560789964	0.99786155726899
C	-0.61897761109384	-0.03940392167661	0.72060906841838	H	-1.11459149105465	7.68609936775591	2.42067258071041
C	-1.33516252228160	3.93203050027185	-0.04252388980887	H	-1.35239586212078	7.21545573719885	4.87075279729095
H	-2.14816916692061	3.48049404267642	-0.63783812531817	H	-0.29950008785088	5.18819895302197	5.84472174376243
H	-0.82558610287184	4.65689945237504	-0.69481541860449	C	3.51719562402700	5.28342375475792	-0.31950047488344
H	-1.77888418259921	4.46129264828673	0.80890027345270	C	3.10801983227291	5.72184689563706	1.08550068602514
C	-2.05255757811353	-0.30811844152693	1.21081734672575	C	3.86170330035550	3.80851003086374	-0.13096581472446
H	-2.61034822783994	0.64336996157992	1.12028181579962	C	3.17323187729888	4.55793250314385	1.99612331992183
C	-2.73645702320155	-1.34104048575000	0.31949559653871	C	3.63761440765442	3.43169693455993	1.28496662852328
H	-2.73350397145740	-1.04379800552208	-0.73989475931127	H	3.24439874749347	4.70318934675073	3.07547524181372
H	-3.78462673512728	-1.48853338763096	0.62243595764677	H	4.14293749645001	2.56620979280338	1.71589342653142
H	-2.22489363459396	-2.31532651768288	0.39518291841429	O	2.83513837413955	6.86393033692121	1.39038704296429
C	-2.11086230660943	-0.75336096386134	2.66880832712445	O	4.29625650522646	3.09149040147116	-1.01113035826643
H	-1.46243899804626	-1.62943557143226	2.83906194855349	C	2.38863170902159	5.48111758197102	-1.32486681657965
H	-3.13747816041142	-1.04168970532207	2.94256788930341	H	2.70368214459190	5.13669084864110	-2.32091190976372
				H	1.49475673606814	4.91199114351731	-1.02580559147901

H	2.12085834579277	6.54654268211566	-1.38471007185591	C	2.16651334642221	-0.28132370408918	3.43214878598517
C	4.77914199006113	6.06134599032971	-0.75815718156278	H	2.73181681705258	-0.98525817888538	2.79829931404052
H	5.04424493409481	5.71437220786953	-1.76863304439006	H	2.18079550883779	-0.67304944523397	4.46101850205378
H	4.49770620096425	7.12330867848198	-0.82945480810215	H	2.70863556942392	0.67580011348284	3.43911158871226
C	5.95158650554589	5.89324765452475	0.17256423716649	C	2.30571111264368	1.04608575442933	-1.34207116418898
C	6.12730739009919	6.74572342838493	1.27125131704717	C	2.78114316203741	0.67533609097212	-3.77750113767211
C	6.86973937056677	4.85075310032582	-0.01382860432733	O	3.02240790107724	0.13967208127552	-0.92041748254253
C	7.18090362054923	6.55397970856301	2.16463959090887	H	2.63373745198829	1.23910901270504	1.32487701028102
H	5.42528994635656	7.56862636751901	1.42716331010978	H	-1.83804544899229	2.39922186819812	0.19186008462522
C	7.92415625445428	4.65624202269506	0.87763857048372	N	2.17217751917959	1.37259600113517	-2.63556020681194
H	6.75146880838066	4.18155901678224	-0.86966394474409	H	1.67660761338580	2.22974096147491	-2.84940562517318
C	8.08134697134309	5.50549608694215	1.97325642466077	C	4.30789085992743	0.75888342875838	-3.71652433059317
H	7.30160449289287	7.23105678234272	3.01447681701668	C	2.31974897659380	-0.78342525017365	-3.78964876005999
H	8.62957599799742	3.83763189915884	0.71195995853185	C	2.27440245349930	1.39087307417232	-5.02768281516487
H	8.90829552418860	5.35503217236565	2.67206561749495	H	2.69904031946241	0.92465586525229	-5.92807938045715
N	1.04277317988427	3.33399200725481	4.53019178417897	H	1.17634969233474	1.33280526639306	-5.09428146026293
H	1.85356275074189	2.97224736019362	4.03631126705073	H	2.56993862641570	2.45050934896565	-5.00925927458813
H	1.20942188551978	3.38237808435185	5.53019645124181	H	2.73585617165005	-1.30069548795860	-4.66710631979717
<b>EB9</b>							
H	1.02141069327529	-0.57826125991515	0.85557467971280	H	1.22143670954930	-0.83892269992092	-3.84209513073903
C	-0.26069762975631	2.98903574936847	1.57164243655159	H	4.74637532951154	0.23988799325185	-4.58214584478376
C	-0.82233887132134	2.09785148490616	0.47772610947914	H	4.62791145465791	1.81018023184085	-3.73578821209048
C	0.14040809828222	2.17715806699227	-0.68380638823675	H	4.68661955982410	0.28894271796698	-2.79873819310427
H	-0.22542202691606	2.25012664748534	-1.71140302334183	Rh	1.01139589529894	4.13234757202960	0.20882183465335
C	1.40834133282218	1.75221142144185	-0.36874693917761	C	0.23200094316264	5.70883878140737	1.16722297609952
C	1.58871797561900	1.47553918236701	1.10163076294586	C	-0.83303422836766	6.26538759153333	0.46232174079856
C	1.07817947646264	2.69235894226488	1.83715590290749	C	-1.62018544205377	7.28603808684725	1.01057117881370
H	1.56378824397918	3.04235804415798	2.75146804554518	C	-1.30428477645357	7.77059293509843	2.27840350919408
C	-0.77974091046579	0.63893067717039	1.01275225928822	C	-0.21284292014487	7.25262787432778	2.97326592556355
H	-1.15123723013409	-0.03932202966811	0.23055170148449	C	0.58023689779348	6.22424969809983	2.43373612906156
H	-1.48184763734442	0.57361159956088	1.85810847953999	H	-1.07738319988968	5.88430042057156	-0.53702576101596
C	0.65180962991468	0.27105520250039	1.45461491919389	H	-2.46241243438400	7.69448471884033	0.44660433828091
C	-1.21421155799143	3.59531663859068	2.55038423463228	H	-1.89854747332541	8.57029765119336	2.72894709420941
H	-1.78404117158989	2.77832820256160	3.02632525982287	H	0.04608668501114	7.64994357503629	3.96002076602038
H	-1.93593246702679	4.26611678218869	2.06376074346840	C	4.30956992847122	4.34627607805127	-0.83875757299928
H	-0.68820774648977	4.14836214340060	3.33773413160456	C	3.18467228986999	4.41518243495112	-1.88766496870112
C	0.73133023175413	-0.13448429166713	2.93667482496023	C	3.66941350867246	5.00488937129463	0.37260540400293
H	0.24608338421462	0.66629957970580	3.52651013574530	C	2.07512792882708	5.21865386416243	-1.35881090615694
C	-0.04307285759251	-1.42774148350799	3.17525181738034	C	2.42774009946840	5.68284730785708	-0.06768314295541
H	-1.09269175116793	-1.34834459727322	2.85436094840711	H	1.37991076174317	5.71660955606444	-2.04048602550867
H	-0.03947957634951	-1.69742574804011	4.24282616969176	H	2.15573569160566	6.65093841425012	0.35264601333020
H	0.41506447624596	-2.26118843761148	2.61646809577635	O	3.28370187694473	3.96592645362030	-3.01336430390642
				O	4.12475219989957	5.01476074149717	1.50351007942782



C	5.41092759657419	5.29113393950219	-1.35004003350125	H	-1.15619263608871	-1.33915836997434	2.91757892218967
H	5.84160019965761	4.88153317665267	-2.27553937620665	H	-0.08247539455399	-1.68221840916592	4.29197670797445
H	5.00889034428258	6.29278842886815	-1.56700139099880	H	0.33290732155235	-2.27869973789309	2.66686160054700
H	6.20960773907878	5.38878626687914	-0.60176799736176	C	2.12972549567439	-0.31432353494337	3.41496281956976
C	4.81910621207560	2.91404576546146	-0.60935460189816	H	2.67155567904162	-1.03558829425810	2.78003708293126
H	4.15829733491934	2.41940635821110	0.11648296268279	H	2.15904037919487	-0.69180904455731	4.44885251314729
H	4.70032552681880	2.38195918733849	-1.56159905474434	H	2.68601026389338	0.63448399902408	3.39724436296704
C	6.24989626696020	2.76701231875145	-0.16495938632726	C	2.18539495746873	0.93830808348596	-1.38313490657186
C	7.22349488028953	2.34458169910479	-1.07831824809041	C	2.57495028364133	0.48527392539552	-3.81743024676326
C	6.64471589280816	3.03328782121611	1.15316959757679	O	2.91849891940063	0.04497367826672	-0.95981033225948
C	8.55587935197877	2.19427384206278	-0.69204351109765	H	2.58034875244674	1.15964146910904	1.26887698951738
H	6.92925634922635	2.12654740458187	-2.10913106668451	H	-1.89471525578364	2.39314465502528	0.22903786838195
C	7.97471945511394	2.88404628299057	1.54300340614288	N	2.00470627130507	1.22141804542304	-2.68055654362889
H	5.89726567503205	3.37997811264430	1.86981439831887	H	1.49634322273113	2.06792840914983	-2.90591259144796
C	8.93634796532636	2.46391975641092	0.62200441187084	C	4.10135392168832	0.59015089993087	-3.81822407659842
H	9.29894548088031	1.86166205579465	-1.42173919235478	C	2.13222472261880	-0.97809900318653	-3.75343656227821
H	8.26376315515343	3.09623231109118	2.57598130069394	C	2.00913790429167	1.14320884849227	-5.07366100876658
H	9.97862598018765	2.34507956852574	0.92936368585466	H	2.40111644983864	0.64307735901041	-5.97067100884503
N	1.63791078149137	5.69789932765641	3.15647211320469	H	0.90999776169081	1.07221833788860	-5.09176953053519
H	2.43147073743631	5.37579679305699	2.60118508657768	H	2.29326598570111	2.20551262582877	-5.11408342037606
H	1.94751233069855	6.28440003237517	3.92435163227473	H	2.51880169430961	-1.52423867531094	-4.62693159385053
<b>EB10</b>							
H	0.92213027464705	-0.63429639817377	0.86716874718614	H	4.51438430999796	0.05105842732399	-4.68424804563966
C	-0.27151060056249	2.97016640175082	1.55964922895195	H	4.40291318938446	1.64530841686102	-3.87742977967879
C	-0.87831728699392	2.07507922967523	0.49357856599163	H	4.52006666727503	0.15321722259071	-2.90138691984467
C	0.05723705004141	2.12333697873037	-0.69133794041504	Rh	0.99806563650421	4.05514766388790	0.14088472377860
H	-0.33412416771332	2.18869575307090	-1.70993343241165	C	0.29805659699764	5.66902748244828	1.10301704645961
C	1.32454232204011	1.67640255385688	-0.40065935798609	C	-0.78433611871463	6.24319527323468	0.43913743124479
C	1.53444635707191	1.41230274664677	1.06879712917117	C	-1.52296535842537	7.28800081280577	1.00907466978556
C	1.06609219210094	2.64860367269226	1.79878944414254	C	-1.14111743619345	7.77830867122431	2.25638067866291
H	1.58124069465684	3.00803645473344	2.69302920510812	C	-0.03195334644584	7.24292959093733	2.90866960884416
C	-0.85073900015472	0.62193118815814	1.04460544349315	C	0.71365757790851	6.19180175866786	2.34584244318388
H	-1.25096145295779	-0.05725626978445	0.27742881066181	H	-1.08258751640356	5.85620210336509	-0.54311373657860
H	-1.53633458757076	0.57765155698353	1.90484791103940	H	-2.38007159701179	7.70941365191591	0.47791952491245
C	0.58315326570704	0.23205164456868	1.46002623646801	H	-1.69757734012068	8.59562417392695	2.72337104763416
C	-1.18721429055830	3.61927419778808	2.54615179886965	H	0.27910837766782	7.64496759349887	3.87825662416476
H	-1.76708083323610	2.82639877305346	3.05003297909917	C	4.26953149829597	4.22676456680754	-1.06443308373358
H	-1.90179228777638	4.29876528200685	2.06115946057199	C	3.10595795399890	4.26268102883326	-2.06494493679927
H	-0.63074896990950	4.17434327516877	3.31072031030357	C	3.67858498343609	4.91401918841606	0.15590654868047
C	0.68715493918364	-0.15236987516088	2.94628599655386	C	2.01069837553239	5.06773296467535	-1.50507591271090
H	0.22651389635470	0.66494440240352	3.53314259076721	C	2.41775949053109	5.57758599761412	-0.24709027331717
C	-0.10208525860051	-1.42949962083463	3.22042936213499	H	1.28649969565943	5.54288292308787	-2.17284471562557

H	2.17085313764244	6.56275072877275	0.14771248846646	C	-2.20639680906148	0.03466397617703	1.04839354959576
O	3.16063434793037	3.80029281176390	-3.18937705875134	H	-2.75242276240183	0.97778146164213	0.85513349277016
O	4.19674551656106	4.94766189180413	1.25876862738533	C	-2.85545551523233	-1.06391294221157	0.21066494695457
C	4.84486241832667	2.85501647692367	-0.76679516332797	H	-2.80623649554636	-0.84872359818300	-0.86733872009210
H	5.67745240042990	2.95717224427377	-0.05554581512977	H	-3.91621562943210	-1.18755530894181	0.47864417396866
H	4.09908788636149	2.18593125657915	-0.32142291408189	H	-2.35107634894013	-2.02967280947001	0.38263049891361
H	5.22488477229187	2.38683806788568	-1.68500495413551	C	-2.33495189680924	-0.29017379509207	2.53290041148834
C	5.40111383970393	5.14012379568118	-1.6257771921969	H	-1.71016254607325	-1.15868416351291	2.80198543317938
H	6.23912210469887	5.08041274978017	-0.91442041311700	H	-3.37739532695593	-0.54099837087596	2.78337187274283
H	5.73169574998559	4.68377346630607	-2.57196624428641	H	-2.03722949972409	0.55152185007122	3.17558745723326
C	5.01584755155260	6.57762782752246	-1.84410018042360	C	2.50838531154843	0.71093809809566	1.90053598448619
C	4.46435118710885	7.00100251910937	-3.06025736453435	C	4.93970237387949	0.26485051990574	2.20824688263966
C	5.16452895630922	7.51744884273361	-0.81552365516442	O	2.16014740599319	0.11476483040781	2.91938251750872
C	4.06131339721587	8.32378509678086	-3.23969556612507	H	-0.00187272472916	0.93222366573731	2.57574729486484
H	4.34884483291483	6.28210820327749	-3.87570673381216	H	0.29629737518577	2.44744752349105	-1.91711836091289
C	4.76193614811282	8.84083089313210	-0.99120209447070	N	3.78037009055568	0.81115422913262	1.48489555711520
H	5.60082760552883	7.20467116564827	0.13713873850517	H	3.99808300409292	1.39705192557050	0.6764888950127
C	4.20594781812015	9.24795727918031	-2.20428171317932	C	5.03994440262561	0.89792873883690	3.59898068648164
H	3.63467631126805	8.63614630996733	-4.19651273833577	C	4.82317833315325	-1.25738990131804	2.31282545431811
H	4.88849452089424	9.55939723160825	-0.17711878016181	C	6.17782262391510	0.62640766879072	1.39106535712672
H	3.89256902803796	10.28560656418320	-2.34499640547550	H	7.07685818349381	0.23246754471061	1.88630363224934
N	1.79391289231350	5.65158267984286	3.02486643235724	H	6.12272020479185	0.19418537373954	0.37989574944565
H	2.55737321340890	5.31959570926345	2.43397644076037	H	6.28335054409099	1.71669825672574	1.29157127946428
H	2.14725552722152	6.24031893339980	3.77201619573919	H	5.70600154576353	-1.66597115755837	2.82737439808345
<b>EB11</b>				H	3.92453119254442	-1.54350963695150	2.87464449753212
H	-0.22283670399095	-0.71014757950190	0.69026305156089	H	4.76928209424340	-1.70731652495512	1.30938046441680
C	-0.45574127153404	3.10129651231645	0.02102997111486	H	5.91899663800718	0.50235673671687	4.12982541398226
C	0.20084804088077	2.07670323226304	-0.88900282324504	H	5.15002367941892	1.99039210441909	3.51774549699219
C	1.54036264913154	1.80609763342038	-0.25281121865531	H	4.14281159541501	0.67746338071534	4.19238144548679
H	2.45313765633171	1.74901658301910	-0.84853525927083	Rh	1.36774076259152	3.59584183966700	1.22426868583094
C	1.44541610587044	1.36059884114890	1.05166740694476	C	0.56790962455824	4.81167812016933	2.6479472973600
C	0.01064592082054	1.24998745089520	1.52989463340440	C	0.77422689468439	4.19979921878138	3.88735575789809
C	-0.55180886167711	2.64222433982664	1.33452800669366	C	0.28349686943649	4.74582552614560	5.07823055047489
H	-1.24354845722095	3.08240481838112	2.05426028946611	C	-0.42929952607341	5.94266733102052	5.02038718061515
C	-0.64863880589408	0.78184788878230	-0.83957784289725	C	-0.62368823290780	6.57764440501614	3.79777001470850
H	-0.19906320964496	0.03722635255177	-1.51252009209120	C	-0.12560933033730	6.03846103087788	2.59363108156787
H	-1.64652336371670	1.01786828346047	-1.24158166850808	H	1.32685648013526	3.25213009910550	3.93539686136658
C	-0.75023941871491	0.25658426824038	0.60730683981023	H	0.45596714869017	4.23730938205430	6.03002735647532
C	-1.26827720028899	4.19985044408996	-0.56960821882442	H	-0.82845680229498	6.39510988065536	5.93244005992412
H	-2.14019161126107	3.75884268223544	-1.08473975582340	H	-1.16749335589857	7.52699113579561	3.75589267549397
H	-0.69524768918015	4.75684463082006	-1.32494071897563	C	3.47185989050238	4.87769978989427	-1.11757598469048
H	-1.61586551868342	4.90510369253457	0.19529829349546	C	2.54203672098515	5.70294264678396	-0.23707993557900
				C	3.90419621479333	3.75583056670500	-0.17376593845163

C	2.69852309341515	5.25871474383470	1.16962115995023	H	-2.61675518205573	3.68466190199505	-0.66270476381087
C	3.46651260691041	4.07063519029678	1.19413504723484	H	-1.24835369596994	4.77006182109650	-0.97346477314409
H	2.59544634499319	5.96548783664651	1.99272896499037	H	-2.03766315234343	4.79398735602602	0.62720124286817
H	3.98112621857092	3.65930567415579	2.06554825293092	C	-2.19485871607778	-0.21643567885733	1.22861341451394
O	1.84053747783461	6.61835780177114	-0.62915341269385	H	-2.8433209517898	0.67772939613432	1.15749946612468
O	4.55929434797270	2.78844306087690	-0.53239170379094	C	-2.81867340197986	-1.31649410102843	0.37391412574510
C	4.72417621037914	5.72630682710366	-1.39274115057097	H	-2.89615762787260	-1.02642451216229	-0.68473832482411
H	4.45889042363652	6.61254947915134	-1.98583656112116	H	-3.83163387789218	-1.56283398457122	0.72817883416474
H	5.19058229210247	6.06182221976129	-0.45384688725067	H	-2.21227352048621	-2.23650411340813	0.42537649387510
H	5.45987538724344	5.13020520938643	-1.95246040382179	C	-2.14525635903821	-0.64921950709998	2.69015762149811
C	2.84260529580493	4.31707698957992	-2.40383585098500	H	-1.41760905175673	-1.46585936740087	2.83404736347913
H	3.52194595893894	3.52452217565791	-2.75596226576694	H	-3.12946179579481	-1.01951037574135	3.01646648733767
H	1.89174440912019	3.83457750521910	-2.13871506327263	H	-1.86520539304667	0.17429901745552	3.36345790690922
C	2.60122602590542	5.29878450031523	-3.51803375181679	C	2.49995713826713	0.87676783374991	1.740209202923890
C	1.36433027358179	5.94039480109540	-3.65845833567753	C	4.98255993281392	0.72481560946670	1.88102907495603
C	3.60386608662505	5.57960550382641	-4.45535231710398	O	2.29538269348268	0.22970494220841	2.76702471072269
C	1.13956537497375	6.84725057931091	-4.69270011495761	H	0.04667044893599	0.80193001999215	2.61176233478633
H	0.56770425360476	5.72491689315666	-2.94339486994119	H	-0.18355174302071	2.59079500687483	-1.78047631752068
C	3.38560579065019	6.48927663474810	-5.48993761647952	N	3.71958269875606	1.11770760567622	1.23401569686699
H	4.56919719407175	5.07191715308908	-4.37709230074824	H	3.81162810625530	1.72934490714632	0.41975979320821
C	2.15227402497281	7.12961451903967	-5.61041225816085	C	5.09699860672901	1.38686490740595	3.25757231234642
H	0.16529434426152	7.33466315104626	-4.78436354917766	C	5.06118100168969	-0.79824475072827	2.00492611796669
H	4.18215348253422	6.69359857754196	-6.21027305846293	C	6.11266551705884	1.22266063644595	0.98239116037941
H	1.97739034338408	7.84038582386457	-6.42228663792416	H	7.08208183594013	0.94172586826778	1.41842816099941
N	-0.35758244137752	6.69676536043404	1.39942795015005	H	6.04381652824814	0.77750986770262	-0.02230400503336
H	-0.60937277669512	7.67379431442383	1.50431950394526	H	6.08379875173156	2.31734468574248	0.87603823796419
H	0.35273509936244	6.57647191304405	0.67776184442382	H	6.02286696874402	-1.08712550259363	2.45530915509079
<b>EB12</b>				H	4.24766535737253	-1.18117057139615	2.63453919072689
H	-0.19634397724944	-0.73872447840185	0.63947811003756	H	4.98955092103061	-1.26792618060897	1.01172081250541
C	-0.80380778812914	3.07043447548028	0.25246161195632	H	6.04324002274922	1.09535996705106	3.73780178848334
C	-0.15822682828553	2.15468166731154	-0.77450196460302	H	5.08751679725479	2.48351649261970	3.16100941685502
C	1.25042499140304	1.96219309005776	-0.27517175074877	H	4.26635141845615	1.08352046946464	3.90840454762007
H	2.10588636912363	2.03207697794829	-0.94867050411825	Rh	1.07040439863215	3.64491195384211	1.33256125282996
C	1.31195705245192	1.44170764964399	1.00284574038593	C	0.31192093482888	4.68390384788122	2.91138258138959
C	-0.06159680650152	1.17776420858944	1.59102938143435	C	0.67946983847401	4.00747398907587	4.07810333788508
C	-0.75099759503178	2.52668164036817	1.53613080695256	C	0.26247796799961	4.42755684980691	5.34556840853736
H	-1.40795616318533	2.86268194518747	2.33975438793350	C	-0.54198953716023	5.56197507540215	5.44302403351394
C	-0.89998691606019	0.79571043355318	-0.73538129299463	C	-0.89886376344814	6.26105114962193	4.29395331420530
H	-0.46651251019867	0.13256297122527	-1.49814228522773	C	-0.47557699204697	5.84943363679625	3.01350717761852
H	-1.94824366582537	0.97449954143080	-1.02291723418287	H	1.30410759368483	3.10758429617308	4.00450014749465
C	-0.81524442534539	0.17558775535788	0.67412688149829	H	0.56230584104968	3.87040420569797	6.23662992161077
C	-1.72555649250062	4.14707552891234	-0.20231553845683	H	-0.88656347855964	5.91534023860433	6.41883443598632
				H	-1.51403255951308	7.16343118514277	4.37222265044883

C	2.82569051636079	5.24476788242737	-1.08308915781707	H	-1.73615219529056	0.73232412996016	1.46709806800066
C	1.93635961302419	5.93498065374572	-0.05812623739607	C	0.32715060421996	0.16149646509543	0.99464969868799
C	3.42086438939666	4.09492278563379	-0.27992847481147	C	-1.03582275225465	3.74719564799970	2.39145265111301
C	2.26353948276446	5.41149937381411	1.28644564414774	H	-1.77106550030192	3.04486187021293	2.82177701629428
C	3.11161444771622	4.28721478216052	1.14490990403377	H	-1.60231843401885	4.55234204255753	1.90409741617132
H	2.18913394482445	6.04426850145414	2.17025686584932	H	-0.43790429120482	4.16865356723040	3.20852756078948
H	3.73837010396296	3.85927349647223	1.92966591525104	C	0.31102735492485	-0.49256441459515	2.38632330164893
O	1.13090111543306	6.80979997797906	-0.32805038630279	H	-0.06254160459463	0.26693143642309	3.09975640313532
O	4.09207453751707	3.20099058355502	-0.77678002980215	C	-0.65206064165945	-1.67620385465040	2.40931831054083
C	2.08978887521221	4.81703402690866	-2.33947880890673	H	-1.66925957205646	-1.39109412862753	2.10127305641560
H	2.75734061136326	4.22756681607704	-2.98448137834079	H	-0.71739263760678	-2.11142555194067	3.41863273220239
H	1.20701681157783	4.21000049807822	-2.09768052212540	H	-0.30476148799357	-2.46815521704641	1.72443807118704
H	1.75247386028722	5.70226918110217	-2.89729761992600	C	1.69587377671891	-0.93327178907843	2.84857931489687
C	3.98865270582270	6.20995515223354	-1.46459111490239	H	2.16051400532892	-1.60895477635437	2.11047836190976
H	4.59980087216774	5.68436402373330	-2.21450249516298	H	1.62905252315534	-1.47846026372353	3.80281797792634
H	3.53254210144008	7.08328324194702	-1.95651722579216	H	2.37738337780160	-0.08387403527025	3.00291327656950
C	4.84817619860611	6.64297928458647	-0.30907353190907	C	2.35399925274725	1.18561177184046	-1.51836284839122
C	4.51011780142438	7.76469208673963	0.45862707487601	C	2.49517652186427	0.11620217364433	-3.79212202282960
C	5.97356800508228	5.89485558901690	0.06027992326518	O	3.46102616425244	0.83014142057016	-1.12076081449566
C	5.26695028705362	8.12047825948230	1.57477418760738	H	2.42160949356739	0.87841374419060	1.06568748958807
H	3.64001226482581	8.36575600998736	0.17927941244917	H	-1.81794288756906	2.75250610887650	-0.01050345614425
C	6.73128630962667	6.24649373271283	1.17676996199971	N	1.88441136854372	0.96776452228319	-2.75993761626505
H	6.25585843452825	5.02103196785680	-0.53312949998233	H	0.90999199890057	1.19674524292364	-2.91440434746799
C	6.37721563211495	7.35879571604099	1.94090489287279	C	3.95228544623735	0.49115083177202	-4.05881580525001
H	4.98894594128145	9.00012773964388	2.16118794220680	C	2.39634261754377	-1.34607339044014	-3.34528646430426
H	7.6050927388845	5.64928775913953	1.44902485165742	C	1.67483283828433	0.33878334047884	-5.06098893629787
H	6.97026152626227	7.63650513487836	2.81601226318428	H	2.05238772853268	-0.29952551581193	-5.87254478824455
N	-0.86796128615457	6.56922021712815	1.89831007065071	H	0.61404083532699	0.08883229855258	-4.89662690087387
H	-1.18803250580372	7.50964354885481	2.10330410061643	H	1.74018991384209	1.38882606417024	-5.38541921542702
H	-0.21572860321560	6.56695215497518	1.11451155822327	H	2.82872089034232	-2.01203659918593	-4.10762179978798
<b>RB13</b>				H	2.94508610394299	-1.49615233540940	-2.40388792709169
H	0.58289884138935	-0.62424847608112	0.26108134687035	H	1.34551793322183	-1.63519991426594	-3.18824908729970
C	-0.19670923856804	2.98531187179928	1.42143632980221	H	4.32895641705423	-0.11244585128698	-4.89834933199394
C	-0.86104716442823	2.28351981268053	0.25166941367029	H	4.03745391603367	1.55530725353070	-4.31313594230807
C	0.15433756423682	2.40356814994215	-0.85930218816574	H	4.57472864330889	0.30031489991501	-3.17645048033324
H	-0.16099328596290	2.66351472327345	-1.87356271753901	Rh	1.37188054872782	3.93906684595016	0.13771986779980
C	1.36892870407013	1.79711724374327	-0.56150235240922	C	1.45891244802431	5.36952811996062	1.62205234147255
C	1.41846559517878	1.25990637000076	0.85286345084013	C	2.39651282522270	5.23401805009506	2.64675446515009
C	1.05983956302884	2.45205833430432	1.70155506620642	C	2.44887719966243	6.11585710164657	3.73218607451958
H	1.57620478564612	2.66180265477041	2.64085743176703	C	1.52992852680060	7.16088575533439	3.79927137572245
C	-1.03399332034130	0.79066784339470	0.62056398543473	C	0.57734165469237	7.31250662513993	2.79422322259675
H	-1.50527049874197	0.26583343945106	-0.22358300344262	C	0.52739989865265	6.42893086432599	1.70283018812107
				H	3.11412052507782	4.40922263766002	2.61602040485798

H	3.19998428281211	5.97840140143592	4.51450900595399	H	1.53345920177719	2.65763893642549	2.64340803742772
H	1.54494768625849	7.86118281849755	4.63897562332569	C	-1.11097836855067	0.88374666069828	0.57514213820978
H	-0.15201210677925	8.12696100723859	2.84778537388695	H	-1.58418251493666	0.37340503869397	-0.27675987185473
C	4.37242905038190	4.83706446440344	-1.14294316499142	H	-1.83417743959940	0.86018173637171	1.40541674972267
C	3.37170015221017	4.20470906329786	-2.11276387421658	C	0.21310839637873	0.20053448437349	0.98569087223149
C	3.52582633583097	5.94037656676409	-0.50787412033855	C	-1.02875559967902	3.83588562025830	2.33923705094161
C	2.00049530782450	4.65379418366812	-1.77451700980312	H	-1.79011628020650	3.15605929220720	2.76039357957902
C	2.09954084902736	5.71825360683371	-0.85534802666656	H	-1.56482969459604	4.65516324545369	1.84121218859891
H	1.19473052178903	4.51870930065551	-2.50021400776903	H	-0.43118137632986	4.24195696808651	3.16423316362077
H	1.37505562273435	6.52713717203766	-0.7460552733730	C	0.13807366896521	-0.44028779256289	2.38135588818925
O	3.68086430527277	3.53196295152011	-3.07060961904984	H	-0.21540176498000	0.34107986463159	3.08134501405417
O	3.96041680735075	6.89236814730413	0.1039249891324	C	-0.87772077326415	-1.57936559890134	2.39336363591600
C	5.55457807273008	5.42028435635157	-1.90522670419829	H	-1.87479648695207	-1.25195772204281	2.0623633597170
H	6.13020247666504	4.61455570401133	-2.38339089246039	H	-0.98307255762079	-2.00254030705162	3.40443713659038
H	5.21536074500596	6.11593953780900	-2.68745271196749	H	-0.55256092087428	-2.39205346595110	1.72203282560858
H	6.21379669393451	5.96692507271898	-1.21728719404445	C	1.49176889081306	-0.93986186390489	2.87505791531233
C	4.81407233993146	3.75842503729264	-0.11730542868334	H	1.94091169895372	-1.63902554887698	2.14935493424759
H	3.95389522556467	3.52653487005033	0.53754976901966	H	1.37987024684852	-1.47771955988732	3.82923434512697
H	5.01682287696566	2.83937178222931	-0.68652058046494	H	2.20811906682424	-0.12192249657816	3.04170038684814
C	6.02403353412924	4.11156186802778	0.70328528714658	C	2.31662632862875	1.10536150606782	-1.49987853132063
C	7.26128840066640	3.52607067923477	0.40617992702706	C	2.42870750751130	0.00090972387727	-3.75589858998233
C	5.95906527919620	5.02351410161107	1.76555543656875	O	3.40364628194484	0.70366653642707	-1.09393489892059
C	8.40334647816083	3.84277512387605	1.14206760027604	H	2.33490768920594	0.82739647203900	1.09679142758113
H	7.32682430182858	2.80815819908071	-0.41653007774507	H	-1.79718886481348	2.87447792271777	-0.08053896407553
C	7.09802244400934	5.34312684185060	2.50279751462773	N	1.83609623372046	0.88184504574417	-2.73829840617046
H	5.00748167647579	5.49560396481639	2.01330766615956	H	0.87702023948041	1.16043874682473	-2.94000134810592
C	8.32572398541342	4.75559317470378	2.19344816940120	C	3.80874602796793	0.49825566303621	-4.18196305869404
H	9.35813907315911	3.37225829585473	0.89272827393566	C	2.51686563123371	-1.42565411725443	-3.20492554266984
H	7.02499689303241	6.05653242056740	3.32815766809109	C	1.48021875594513	0.03694646783685	-4.95209004276219
H	9.21801334764420	5.00599316654611	2.77309407830328	H	1.85925150517232	-0.61336846051480	-5.75331799687813
N	-0.40531596044309	6.63180771121059	0.69251770215300	H	0.47541156620589	-0.31719752998306	-4.67033185807385
H	-0.65133504711544	5.79265459420562	0.17561294050112	H	1.39224061504209	1.05989232277104	-5.35039099203863
H	-1.22116930139532	7.17474711701681	0.95362943195230	H	2.92713466021670	-2.10321862190953	-3.96894996988250
<b>EB14</b>							
H	0.45188503511264	-0.60121614727756	0.26386062634097	H	1.51802618890643	-1.79078163871802	-2.91882953630905
C	-0.19931079097419	3.04341924752752	1.38532944590634	H	4.22180280961387	-0.17799775354933	-4.94573726271534
C	-0.86701808693816	2.36608928499489	0.20357336814674	H	3.74068849932121	1.51152600210033	-4.60011131340078
C	0.17708452108426	2.43965428055606	-0.88361428819118	H	4.49204105896762	0.53222784879077	-3.32464302524461
H	-0.10276608688828	2.71077365749250	-1.90561365334377	Rh	1.44274339715053	3.92012963534460	0.12668078359193
C	1.35614928693426	1.77750148728748	-0.55941265787917	C	1.48734547055174	5.38757872932030	1.57543826245402
C	1.35384760388856	1.25029026915607	0.85966933498419	C	2.38312809151418	5.29054238725585	2.64052592200992
C	1.02840440573678	2.46216766386681	1.69449282549495	C	2.38244567340413	6.20791694834049	3.69732406350377
				C	1.46131550142357	7.25311872600491	3.68677173263374

C	0.55795444456591	7.37230514706744	2.63301792221977	C	1.49904391733512	1.44360198865835	1.14874696942643
C	0.55718027559373	6.45043881844529	1.57321609765910	C	0.12144767842327	1.22231205834679	1.73502862096189
H	3.11428162997644	4.47690510451189	2.65857428695131	C	-0.52339460103666	2.58788861550467	1.64760084560340
H	3.09758354225374	6.10129764618166	4.51725570490701	H	-1.15659857037744	2.97700296460509	2.44826758214347
H	1.43868566467926	7.98140040917263	4.50224605291684	C	-0.69018621588656	0.79944964497445	-0.59770652713227
H	-0.17025808250726	8.18959178681379	2.62331360477657	H	-0.22921626534763	0.11224978282009	-1.32232679026974
C	4.55101041023668	4.74803183117708	-0.85315420447426	H	-1.72777388392561	0.96560483025949	-0.92798455702682
C	3.66614618374071	4.01826231708271	-1.86012456954503	C	-0.65582967092546	0.22325536404019	0.83441814031612
C	3.63335714856600	5.86936469301232	-0.36631218818261	C	-1.54028726310700	4.13384708965288	-0.12481886189364
C	2.27277897770389	4.51949520275390	-1.74759686020784	H	-2.34963282803304	3.63313907821540	-0.68481718643056
C	2.26927559159308	5.64451510936451	-0.89771733005292	H	-1.05474465770703	4.83340969196957	-0.82136324185666
H	1.56253606041686	4.32627695055794	-2.55519297454402	H	-1.98432085326200	4.69704349259881	0.70435813675732
H	1.53254346337051	6.45006971701009	-0.90530753580973	C	-2.05993152614651	-0.09592146437779	1.37555329081322
O	4.07164705477070	3.22145581499050	-2.67572733794288	H	-2.67296657409447	0.81757137042909	1.25381039796788
O	3.99627356689665	6.80976177323001	0.30739820667502	C	-2.70860006264025	-1.20839572488058	0.55632499708382
C	4.93567329282842	3.81787344148572	0.29824656157970	H	-2.75028259646167	-0.96465367172019	-0.51591902521591
H	5.48956458897028	4.37770012941420	1.06654839273778	H	-3.73837160612287	-1.39822001661368	0.89663074884665
H	4.04005065437220	3.37428054776774	0.76487871022276	H	-2.14110334832180	-2.14807234080692	0.66423274372292
H	5.56817689423550	2.99962778866841	-0.07621864237572	C	-2.05424102445128	-0.46785625275634	2.85498042522902
C	5.81277802950600	5.31861073959005	-1.52785681707130	H	-1.35652598028967	-1.30024662635043	3.04780326366205
H	6.36685374861061	5.87735986517520	-0.75781270340627	H	-3.05637757992120	-0.79241415917562	3.17531674753903
H	6.43685707686956	4.46523094139511	-1.83365153441962	H	-1.76087205388163	0.37375844005351	3.49975799145683
C	5.54119874080273	6.20524453851697	-2.71544430923104	C	2.64795235079513	0.72659362819094	1.80571462109553
C	5.49760467665449	5.67271323584150	-4.01139836746134	C	5.05299537897859	0.06888870055766	1.62248052867942
C	5.30620664250430	7.57776049152822	-2.55378572670334	O	2.44909114710153	0.13751191965288	2.86780336609297
C	5.21427916783812	6.48193986725821	-5.11085515846920	H	0.21387786072038	0.86107083261899	2.76307607053968
H	5.68351413245543	4.60564043274493	-4.15383183266151	H	0.04340246013738	2.58152713585865	-1.66728434458413
C	5.02171241468502	8.38998374614290	-3.65131075124525	N	3.82666986324346	0.73796092598991	1.16071041736753
H	5.34695727325806	8.01229539278706	-1.55219266320146	H	3.93817978056165	1.35445299240299	0.35540265262100
C	4.97073567613034	7.84429868737440	-4.93429615704439	C	5.51608081629056	0.66181882869349	2.95604678251014
H	5.18632100217143	6.04517345965851	-6.11271477436610	C	4.80912779534681	-1.43573882184111	1.75508977108513
H	4.84333440960860	9.45832989928906	-3.50264405204610	C	6.11119900698267	0.32263331124468	0.55091267635199
H	4.74840915304949	8.48025039769552	-5.79512204465663	H	7.05879333268552	-0.15355712315208	0.84072996782444
N	-0.32620360448590	6.61492202772800	0.51182508641703	H	5.79640594284698	-0.09618266477282	-0.41784330705252
H	-0.54643430792867	5.75311137057164	0.02062318713271	H	6.28898294761494	1.40051707129425	0.41935395069364
H	-1.15640100498251	7.16061457956529	0.71612796903041	H	5.74042694711699	-1.93970835181005	2.05468663445654
<b>EB15</b>							
H	-0.07335273954783	-0.71514251762379	0.84270982241042	H	4.03848156221432	-1.64275627690817	2.50884768485888
C	-0.59300343391306	3.08890527467172	0.35023892844470	H	4.48173557010584	-1.85708520659631	0.79206643198450
C	0.05226105612555	2.15678798774278	-0.65561902570057	H	6.43305427711429	0.15653727749222	3.29513803679415
C	1.45413184491550	1.97472967122411	-0.13270702300631	H	5.73725376702674	1.73499638393869	2.84698673296815
H	2.30511734939996	1.99447419581659	-0.81628820992339	H	4.74316943824563	0.53761406064074	3.72648084146292
				Rh	1.35309319806567	3.65134494916476	1.36577309740974
				C	0.41703128641299	5.16158924732021	2.39921492671219

C	-0.17418356895701	6.27840501530358	1.81700039173006	C	-0.08050768102723	2.14850026385607	-0.53729319223258
C	-0.87706233606016	7.22409516393890	2.57318242206450	C	1.34350112179177	2.01069315120405	-0.06665472436157
C	-0.97742773942777	7.05082652961848	3.95169377857109	H	2.16982138569011	2.09789302197708	-0.77419793815225
C	-0.37870773046210	5.94894830599935	4.56015523677753	C	1.45614628630345	1.44139852674251	1.19365117132279
C	0.32799907941842	5.00099191675870	3.80197159002739	C	0.11013160612327	1.14193073185041	1.81781736276673
H	-0.08501492266894	6.43118850260253	0.73977160028372	C	-0.59321833434296	2.48119246144062	1.79664346182814
H	-1.33430502760628	8.08771721087762	2.08343093372773	H	-1.21696545168033	2.81585456282169	2.62885014337603
H	-1.52124868419299	7.77572197456442	4.56382615835135	C	-0.76221233926288	0.75907272522640	-0.50032272413440
H	-0.44987720114823	5.81213708543203	5.64394369739869	H	-0.29276559923825	0.11488797951286	-1.25828410587448
C	3.45101090451140	5.27646213518674	-0.62175420811034	H	-1.81500669243273	0.88909689760137	-0.79683140245773
C	2.89196800663329	6.02321870531419	0.59099630403625	C	-0.66096303505297	0.14282787006090	0.91199890411962
C	3.83037850456611	3.92086647279369	-0.03164628434113	C	-1.73714635331243	4.03429103214356	0.10849282803527
C	2.89043779640959	5.11308728190185	1.76383233506335	H	-2.53321652473794	3.51668611124438	-0.45511720092479
C	3.46848221764661	3.88190929074757	1.39655636064364	H	-1.30234641498345	4.78623821103616	-0.56735874274882
H	2.86662600522083	5.51654030348288	2.77588493097234	H	-2.18945447829316	4.54068311157491	0.96924299471453
H	3.93048351416138	3.17409181241612	2.08642742257331	C	-2.03572572916813	-0.23885075987094	1.48732592319957
O	2.58507189767530	7.19579067904867	0.60035149644935	H	-2.68309463603760	0.65578881298781	1.41038585129843
O	4.37202316344176	3.02969062433585	-0.66638619492054	C	-2.67303250643291	-1.35027197724202	0.65786903672871
C	4.71909332577868	5.97565743890712	-1.11212101713158	H	-2.75874989351374	-1.07893049747030	-0.40511456162476
H	4.48208780715083	6.99638451307783	-1.44206029401767	H	-3.68403678914321	-1.58465412146970	1.02559471720838
H	5.47001710090167	6.03688559667846	-0.30954728089224	H	-2.07106465897458	-2.27244355789912	0.72043563159469
H	5.15503793089270	5.41902300213104	-1.95444338724862	C	-1.97164216039954	-0.64921200040664	2.95493651376803
C	2.40902971357346	5.06934010386906	-1.74547829803323	H	-1.24533060213708	-1.46615159585202	3.10373695167601
H	2.82296981925917	4.30015239107868	-2.41705542182050	H	-2.95353965706459	-1.01099741479444	3.29736205252360
H	1.49833425593128	4.64779323082346	-1.28915328577774	H	-1.68199466397566	0.18335316477372	3.61296110020397
C	2.05735537596687	6.29439494758210	-2.54134421610313	C	2.66489013669603	0.77761803959787	1.79655721454272
C	0.98289422512989	7.11251899952897	-2.17214741972811	C	5.11104201675387	0.31894654984588	1.54851308187934
C	2.79904906253562	6.64491084971575	-3.67717194249669	O	2.53747257806060	0.15695366469717	2.85141060093797
C	0.66453553869309	8.25384167163453	-2.90647811639762	H	0.25248886800896	0.75308019039482	2.83011590404387
H	0.38562556376964	6.84909938250991	-1.29661207348824	H	-0.14052297039573	2.60404385047506	-1.53362086429814
C	2.48717997587334	7.78738287142708	-4.41346214494279	N	3.82102791003196	0.88188206934819	1.11865118151797
H	3.63049960233832	6.00824783658480	-3.99193920376771	H	3.86220928461744	1.51776860973977	0.32103642997419
C	1.41963629203110	8.59855083877091	-4.02816470420591	C	5.54530246628644	0.92988962719226	2.88436783809445
H	-0.18053990317684	8.87683019744884	-2.60200301009789	C	5.00592137168971	-1.20349308288506	1.65953953402615
H	3.07894268930079	8.04212342289209	-5.29664297297572	C	6.12417711480268	0.68628804566977	0.46628987984531
H	1.17162960659571	9.49304425316563	-4.60539482086203	H	7.11326686474092	0.28459729395561	0.72903968606845
N	0.98281968662457	3.94821049907453	4.43024615867465	H	5.82861260268381	0.26658135911759	-0.50804160181805
H	1.10129489011147	3.12196472682377	3.84993959084179	H	6.20992461597809	1.77848322277980	0.36114926884946
H	0.64264734530416	3.71543675385585	5.35722686716238	H	5.98370490644641	-1.62723297371791	1.93414430249513
<b>EB16</b>				H	4.27105053031574	-1.48989581855810	2.42312251427851
H	-0.04735444521076	-0.77468134359633	0.87165290412424	H	4.69857264438234	-1.63734401160780	0.69548361463880
C	-0.72917313191735	3.01963501920781	0.51930195788848	H	6.50607759736139	0.49684477916364	3.20141670605298
				H	5.67986534065436	2.01877253777318	2.78906826158016

H	4.79914768641826	0.73245151634822	3.66580052878888	<b>CRI</b>			
Rh	1.22196503881038	3.63466834567640	1.49211745842903	H	0.88665006377124	-0.65896259091283	0.74249507924078
C	0.24470490516391	5.07302844948552	2.58479981101943	C	-0.52051279811227	2.85831248184093	1.55861393801347
C	-0.40429522392815	6.17361734524474	2.03335665019837	C	-1.07334209083808	1.91981437960418	0.50213561529278
C	-1.14062750658683	7.06715038212703	2.82097037092946	C	-0.12477181505342	2.12671464615372	-0.64983581417377
C	-1.21396677950593	6.85777512381650	4.19622088557454	H	-0.47183405067357	2.09897318734643	-1.68599826984609
C	-0.55638131856155	5.77222221167329	4.77238885437427	C	1.21073691410462	1.77486727670309	-0.34112582719371
C	0.18376090273628	4.87550733978338	3.98383325068087	C	1.36708771481995	1.39135599538618	1.12190139793863
H	-0.33514403458133	6.35527403020290	0.95804421229830	C	0.80906744394895	2.59929646392488	1.84054612204665
H	-1.64469572466383	7.91961767793092	2.35807620406530	H	1.30961002492472	3.02565119088333	2.71533498162857
H	-1.78322622661426	7.54223288169536	4.83142817246648	C	-0.95827055050237	0.46611973021880	1.02154556006523
H	-0.60583070853368	5.60900522208180	5.85373187984058	H	-1.33586805185459	-0.22408563016970	0.25210301657778
C	3.19334235049388	5.45730235915690	-0.46133150376181	H	-1.62303129851842	0.36364895880149	1.89431407886313
C	2.61954762550388	6.09981057181725	0.80263536969095	C	0.50150674359783	0.13460028599127	1.40895290406222
C	3.60604100497694	4.07289241967321	0.02142113099728	C	-1.45932574102865	3.56700817274512	2.47256132001178
C	2.71883607661077	5.13782331180838	1.92355253470061	H	-2.00025811248414	2.80473718599614	3.06167465199089
C	3.32499316558989	3.95269600092669	1.46348584373274	H	-2.21132375495835	4.15124225405540	1.92634090562069
H	2.71052535454045	5.48080300691118	2.95797873401342	H	-0.93329517743008	4.22843087416048	3.17240423793729
H	3.83955957371335	3.22565608926639	2.09207190374894	C	0.62975518593869	-0.38298273873294	2.85128904575339
O	2.21031095499531	7.24020951216295	0.86070876503246	H	0.14433244284723	0.36151479896128	3.51116607229575
O	4.11949575455757	3.22334709462919	-0.69101633499094	C	-0.10836972577889	-1.70932830661954	3.01198287348148
C	2.16453268687513	5.40430187425858	-1.58336614695827	H	-1.16703160775928	-1.63348579570286	2.72193252770693
H	2.58011365974880	4.88110092050155	-2.45711004658276	H	-0.07164737790965	-2.05879147128553	4.05563973460831
H	1.25497582228200	4.87696484940814	-1.25488848135320	H	0.35528225537132	-2.48711246505391	2.38156951866406
H	1.88420420143096	6.42544125957766	-1.88087324446032	C	2.08136702521723	-0.53554228339714	3.29643755227710
C	4.45520150195248	6.23581502983886	-0.90652316237571	H	2.64343294143457	-1.17261465586019	2.59191635342660
H	4.83076463438484	5.75925733789343	-1.82506801994247	H	2.13441493832521	-1.01075450966194	4.28828804162003
H	4.13251766159518	7.25641994087255	-1.16438462532384	H	2.60499636288350	0.42914633130980	3.36856585290106
C	5.53700693619226	6.27444680329286	0.14065471769427	C	2.02813735423977	1.12463156097771	-1.42276393639722
C	5.55748202194344	7.27949542678940	1.11682705949367	C	4.05083759243698	-0.34492103221145	-1.77421257505380
C	6.51512740408242	5.27219806741762	0.19590757362136	O	1.61685592197503	1.05371391393875	-2.57764040806408
C	6.51922396433349	7.27583760517913	2.12677106942709	H	2.41468121792397	1.23155372947817	1.40356466078349
H	4.80739994175512	8.07379091375939	1.08333847487800	H	-2.11043555989233	2.17076811846590	0.24194846003489
C	7.47657674494294	5.26424607923519	1.20589182874860	N	3.17754430788889	0.55048146698387	-1.00534963579905
H	6.51878343571711	4.48616263433042	-0.56346006832226	H	3.39555292655717	0.63025325488527	-0.02098364417664
C	7.47917069716570	6.26477373728741	2.17827631131537	C	3.27329384450822	-1.59847638067914	-2.18407610027633
H	6.51992193421751	8.07048022229674	2.87752929755161	C	4.61245432865249	0.36401978496631	-3.00691913682048
H	8.23030654097115	4.47270175929964	1.23000344263421	C	5.19373055692199	-0.72720796280361	-0.83534832809053
H	8.23268139284613	6.26101979868411	2.97006799774920	H	5.88604986661464	-1.41506477299084	-1.34137720847758
N	0.89677862442660	3.84205574388137	4.58007262471474	H	5.75997899698821	0.16452724929778	-0.52246198505589
H	1.05154001929972	3.03569466025695	3.98072018428858	H	4.80878223979630	-1.23007093211524	0.06656509253486
H	0.5798527201747	3.57167011387813	5.50516321479783	H	5.29649638308108	-0.31112875462852	-3.54307015751525
				H	3.80236089997186	0.66293648736754	-3.68353405100235



H	5.16946034272135	1.26774176872059	-2.71745685479031	H	3.28352620244883	6.77163401802626	1.71289518049097
H	3.92728732555153	-2.28790564797270	-2.73941853781998	H	2.54821178057210	6.89915151764116	3.24432896013155
H	2.89339565726554	-2.12313550409529	-1.29350178206396				
H	2.42164827532440	-1.33163803455692	-2.82508445280543				
Rh	0.86968193735866	3.84245003260023	0.01602693237551	<b>CR2</b>			
C	1.05292095447517	6.11787406410907	0.36988537747175	H	0.83964476399169	-0.62985029338238	0.83367287050451
C	-0.28764220222517	6.11164466204171	-0.11009641461383	C	-0.49669773683936	2.92030783178918	1.65408522590192
C	-1.37837604046336	6.40535478300498	0.70351165465751	C	-1.10385328923542	1.94381349964482	0.66084783843890
C	-1.14815063507756	6.71782632153361	2.04074243736451	C	-0.20043186236434	2.12288064947516	-0.53201134749675
C	0.14120194089711	6.72279238585051	2.55145093455620	H	-0.58697484592789	2.09782675738532	-1.55432486258225
C	1.26627081622307	6.45102452762690	1.74780028532126	C	1.15019501001048	1.77937158339119	-0.27830594156857
H	-0.45568593615752	5.99068915560973	-1.18123922285065	C	1.36212320818691	1.41148270376799	1.18246180766144
H	-2.38730052892441	6.41112496180808	0.28704785828047	C	0.84325322586666	2.64597361428842	1.88820538115875
H	-1.98441863897726	6.96003907509624	2.70170907218473	H	1.39204082715343	3.10118865796824	2.71880968071917
H	0.31230084716590	6.97745585650505	3.60086952874922	C	-0.97425792934016	0.50845447936350	1.22045128159583
C	4.15756907658074	4.68770042547791	-1.15615684737399	H	-1.41214975100572	-0.20387906292387	0.50502310879027
C	3.01268803399923	4.270151331312445	-2.09155608795007	H	-1.58056377048771	0.44929842070888	2.13870515715747
C	3.59552566597111	5.90401782811988	-0.46420114060918	C	0.50248198039042	0.16564598920193	1.52328600443819
C	1.75706763004129	4.85077598749531	-1.62842365381073	C	-1.37108189774239	3.71244229384354	2.56406322711088
C	2.10241719435788	6.05656276214718	-0.75469212196777	H	-1.90564279835713	3.01739029645114	3.23591406059529
H	1.02538489134631	4.99658001752149	-2.43350098861830	H	-2.12861214029128	4.28391143902503	2.01129885054876
H	2.06642597388416	7.02300881846197	-1.29967378464196	H	-0.79135512326505	4.40898991017423	3.18480548032143
O	3.20342337509379	3.59613470293329	-3.09061019597020	C	0.71204136178553	-0.35853001689448	2.95333416443042
O	4.26952982690628	6.69857451358496	0.15852000681457	H	0.28917445994910	0.39473267571730	3.64553955616856
C	5.43737562468108	4.98741183582850	-1.91800693473092	C	-0.04409439429227	-1.66850111910637	3.15884833057338
H	5.80318302790617	4.07271307204983	-2.40605074135045	H	-1.11865293978600	-1.56666480737579	2.94562502387781
H	5.25985054771105	5.74291306335004	-2.69791613691110	H	0.05897162491876	-2.02656367005365	4.19508513018157
H	6.21570701124932	5.36395292998968	-1.24043657085273	H	0.35545194372701	-2.45194864767135	2.49250375916778
C	4.34507546656839	3.55443553196247	-0.10350315122444	C	2.18613524484582	-0.54666535726490	3.30117435630510
H	3.39967026396707	3.44438560878471	0.45887996433408	H	2.68653001338106	-1.19161594723274	2.55822620023885
H	4.46895514314733	2.62864768728042	-0.68202667688222	H	2.29340272338261	-1.02960734118843	4.28487432884751
C	5.49541063430020	3.70854637476428	0.84661687311292	H	2.73566541224390	0.40531505628957	3.34423290954741
C	6.75838635782392	3.20164560024739	0.51011415295873	C	1.90915074134357	1.13861274067443	-1.40536805100371
C	5.33748764148088	4.33527062735771	2.08926588776984	C	3.76272436611114	-0.50015609214002	-1.87590621578127
C	7.83774601147450	3.32844822561434	1.38325643503676	O	1.49001692260191	1.18164731858849	-2.55942459134149
H	6.89149871173600	2.69327655596542	-0.44902463203984	H	2.41968377397934	1.25012223928722	1.42408384292448
C	6.41474139619208	4.46208174225111	2.96575810973538	H	-2.14893623327380	2.19386681604051	0.43423712498214
H	4.35773911101702	4.73032117682285	2.37198398030607	N	3.00355771702964	0.43770783899137	-1.03851843651842
C	7.66959069710675	3.96321803484037	2.61452829035305	H	3.22762386676154	0.41884581631569	-0.05249887997588
H	8.81415982510793	2.92448533385751	1.10291746665843	C	2.84338172352411	-1.62787514282241	-2.35460625164487
H	6.27221581789686	4.95226698874122	3.93253979323994	C	4.39139747519291	0.21924233767581	-3.06950553184501
H	8.51337837390118	4.06160728122422	3.30247651770152	C	4.86086153378634	-1.07288647760149	-0.98218042936163
N	2.50831814199161	6.49969303634054	2.31414456250408	H	5.46182484077962	-1.80419177840916	-1.54150127713353
				H	5.53187087520157	-0.27568804372661	-0.62542888137180

H	4.42842105952864	-1.58328844071142	-0.10632973580807	H	4.69483182969112	9.96981158236309	-1.12159499890725
H	4.97418723631815	-0.49592334281081	-3.66969206064509	H	3.67242763411764	10.11108632385704	-3.39264077146554
H	3.61520818579527	0.66928659272797	-3.70083805336182	N	1.76909669225453	6.92610374884793	2.49328472705909
H	5.06430080839397	1.02054406197262	-2.73020146488950	H	2.69257304728921	6.59345181985856	2.21047513876334
H	3.40947534441207	-2.34683128381103	-2.96622912329554	H	1.62887427403446	7.26949229374575	3.43336967063959
H	2.41471006377943	-2.16674560909232	-1.49520452920166				
H	2.02117105756496	-1.22316477349265	-2.96027363345946	<b>CR3</b>			
Rh	0.80230483509851	3.84838115198660	0.06457201313953	H	-0.50788071151435	-1.05733541178630	0.51504685941720
C	0.78662125841217	6.10814095861016	0.40450697720098	C	-0.60645305942990	2.80767702526766	0.15229413420175
C	-0.42389850827526	6.00397749986685	-0.34283733048525	C	0.02106253284452	1.83324064642638	-0.83639866073425
C	-1.67042359149462	6.35008442123593	0.17395677159998	C	1.34832473944217	1.52830318248475	-0.17613329484542
C	-1.73742274919709	6.86643326638338	1.46653232861448	H	2.27473991741335	1.42602831703731	-0.74739883846156
C	-0.58655275682546	7.02155081645932	2.22003041149309	C	1.19723808303643	0.95516482230786	1.10188659572251
C	0.69152554593537	6.67393353257917	1.72592767849558	C	-0.26090864831543	0.82258711521538	1.51691254786304
H	-0.37326960256818	5.74445856923194	-1.39873069800866	C	-0.74180094519495	2.25710584380505	1.41895469694967
H	-2.56409082517805	6.25293959862685	-0.44506499533084	H	-1.35926821394969	2.71500574997316	2.19573979573701
H	-2.69981893586956	7.15907518600014	1.89528149452600	C	-0.84295174187638	0.55802131452681	-0.90988240097643
H	-0.64399841251397	7.43873132236098	3.22894774137401	H	-0.38061642086613	-0.14921255415101	-1.61509618217162
C	4.12408009873647	4.54663956709029	-0.76423855689856	H	-1.82485526815053	0.83037167714002	-1.32920362487452
C	3.07295110371350	4.23863775689513	-1.83281902902334	C	-1.00893051371031	-0.07279268549444	0.49238428426663
C	3.38108388537938	5.43891080056737	0.20516641543288	C	-1.29764942724975	4.03777662497341	-0.33701107311746
C	1.82456304253698	4.89905237974278	-1.50157804953622	H	-2.13110084964007	3.74697144883412	-1.00044204205005
C	2.08515816070112	5.95739261708765	-0.43098621931172	H	-0.62380348968257	4.67259519553416	-0.93273309518368
H	1.20935174044184	5.15561150434710	-2.37035944859575	H	-1.70432670178530	4.63241811558410	0.49147834113064
H	2.36839835220211	6.95649693181045	-0.83292944736290	C	-2.48566927439073	-0.29946810887811	0.85691472295199
O	3.33274177322738	3.58508075720714	-2.83342615546955	H	-3.00428884670144	0.66934605761000	0.72417669321653
O	3.83651505104669	5.72124684083112	1.29638720236303	C	-3.12281405459742	-1.31060739023325	-0.09280603159943
C	4.68604727584957	3.31447512979568	-0.06939132294213	H	-3.02706728969030	-1.00966635023776	-1.14679097638921
H	5.43823524577538	3.61338501194909	0.67486064249247	H	-4.19552159367529	-1.43351624494444	0.12354043514713
H	3.88974215772741	2.76072217614745	0.44546516176185	H	-2.64356812089629	-2.29814607159997	0.01736112565698
H	5.15773020798132	2.64779198634245	-0.80493550109095	C	-2.68188928611018	-0.74549355593950	2.30213649439449
C	5.28609111723117	5.34095563605628	-1.41970447264884	H	-2.09330148744274	-1.65352225289572	2.51788869913951
H	6.06591206645538	5.48368226996694	-0.65596608174338	H	-3.73992025195461	-0.98409725465682	2.49226823328891
H	5.69504343978322	4.68559582981040	-2.20450908699452	H	-2.38517635823409	0.02792976837021	3.02585898950452
C	4.88632842339907	6.67071702913778	-1.99666906855373	C	2.27840354164694	0.14601740141647	1.75486888054038
C	4.32406524381884	6.76584276610649	-3.27676826936015	C	3.29540506795773	-0.36400281132882	3.99559297975910
C	5.01731455334305	7.83988818989040	-1.23574531329822	O	3.02961844878825	-0.56969711085479	1.09792282937250
C	3.88934509638986	7.99346633595767	-3.77456182131765	H	-0.34604620179517	0.42719051065656	2.53536435758212
H	4.22132605438105	5.86313355969829	-3.88405088042700	H	0.15018248210230	2.29261242901067	-1.82563950607318
C	4.58419455713997	9.06929500135537	-1.73129485072518	N	2.32198913380964	0.26575984161728	3.09693062712769
H	5.45962378212294	7.78147579072669	-0.23714191245566	H	1.71393874720953	0.97116948422000	3.49914848448292
C	4.01353670259534	9.14896927524641	-3.00191716640113	C	3.20036109631856	-1.88701321380215	3.88467256340320
H	3.45223492338093	8.04824484117196	-4.77507783050325	C	4.70923161947341	0.11613459786596	3.65587809574978

C	2.92340801141714	0.07757377981049	5.40850356533840	H	3.84053741733089	4.76305871777004	-3.96200604095878
H	3.62416433097160	-0.35431082093350	6.13722668578834	C	2.08181610595159	7.65686469804716	-4.33303086959281
H	2.96829968112806	1.17489078446029	5.49956756585543	H	0.69290116293021	8.45323313343244	-2.88097494611493
H	1.90584210096704	-0.25345698868750	5.66895019323759	H	3.50141176018326	6.60997787626126	-5.58256280232169
H	5.44432391654269	-0.36455295684951	4.31899071305923	H	1.92732073750525	8.46897216244714	-5.04826060989803
H	4.96196914922700	-0.12874848040205	2.61518042160586	N	0.73009962010424	6.90262527666307	1.17397652538214
H	4.78829003683379	1.20627353634538	3.78799036916380	H	0.01030366804254	7.61281159560555	1.12720262478342
H	3.90215006185817	-2.36011650670482	4.58804599905560	H	1.67174889226041	7.23025631393864	0.97822386825227
H	2.18178310699490	-2.22639622851923	4.12865368401081				
H	3.44493268342187	-2.21713900567085	2.86633450363997	<b>CR4</b>			
Rh	1.30478986997367	3.03556646185798	1.28710564127417	H	-0.61821435913396	-0.92958484191032	0.35036163518394
C	1.59320468678730	4.97945574164421	2.42510541920251	C	-0.94823422118267	2.93180848859151	0.61161810655180
C	1.33952654683963	4.05707145271479	3.48540291561061	C	-0.40498104371533	2.15807591969897	-0.58383667946510
C	0.11899916531140	4.00753691091530	4.16046571122321	C	1.00972004241367	1.85439776158053	-0.13496241996346
C	-0.89147112325296	4.88953918956528	3.78301941494280	H	1.86466626726467	1.90176694580004	-0.81429315952556
C	-0.67095378935041	5.82454210267855	2.78198652012115	C	1.04085630111083	1.09554932239701	1.05167524880047
C	0.56503759759366	5.92618684657099	2.10986200584496	C	-0.34747960482755	0.79317542846157	1.59918235235203
H	2.16704669303919	3.45206850988110	3.86044158492773	C	-0.90703599399431	2.19021002916848	1.78632152425708
H	-0.02608941860565	3.29550470880246	4.97520415662714	H	-1.44287005137252	2.48723324499379	2.69163339558869
H	-1.86082896508914	4.86627011826545	4.28773354040136	C	-1.20656095623682	0.85292249632515	-0.75666234648461
H	-1.45755131168845	6.53515666029379	2.51452264400277	H	-0.80008413513101	0.29294068089616	-1.61245456555444
C	3.82740828395492	4.65223725765818	-0.47362689196564	H	-2.24487016594854	1.11817698184818	-1.01293093698670
C	3.40158383283688	5.64952463892294	0.58164537009743	C	-1.16723128575151	0.01057538089509	0.53906690900397
C	3.97893355035898	3.34899640514993	0.32381292914031	C	-1.71646357423857	4.19462274332987	0.40830252357877
C	3.04489742009350	4.95457806713527	1.90136490336832	H	-2.59331152913697	3.99682718780342	-0.23277957150459
C	3.35374056144012	3.48776995917765	1.62143516735063	H	-1.10538431685739	4.95271943487514	-0.10713618740677
H	3.70610914998998	5.43824182064579	2.64791555751045	H	-2.06492494179761	4.61317319812319	1.36160309863110
H	3.75778661515209	2.85795147862741	2.42156860613883	C	-2.57524029198400	-0.36790217186862	1.02867883681117
O	3.44203249348824	6.85201511369890	0.42879098242499	H	-3.15481574750170	0.57220002541656	1.10584252511907
O	4.55271700739929	2.36922404162114	-0.14089374609998	C	-3.27148737783198	-1.26904231896326	0.01190653378765
C	5.14250736491928	5.05148392837429	-1.12790379851736	H	-3.31797881867526	-0.81065408873549	-0.98727157159397
H	5.04188247088302	6.01438889557218	-1.64703191772104	H	-4.30305811962346	-1.49396858254736	0.32492979190467
H	5.94242071272813	5.14249995851517	-0.37774843010872	H	-2.73435818751424	-2.22769489559081	-0.08555751918743
H	5.43865373131690	4.28132409485675	-1.85447297231164	C	-2.57344561918805	-1.03267936960557	2.40133211160989
C	2.69171267446871	4.44453810551412	-1.51641849639751	H	-1.92045701329074	-1.92205483396551	2.40887058394494
H	2.95182357771865	3.52133678076294	-2.05816010416115	H	-3.58827033542464	-1.36516512473663	2.67003036008711
H	1.75777654258014	4.23447185759971	-0.96607196918711	H	-2.22984193925459	-0.35537011310280	3.19702606046967
C	2.47557846643038	5.56368583980895	-2.49336667502053	C	2.25457218481437	0.33938359222599	1.50531188607527
C	1.58774446626827	6.60951071002325	-2.20966354163430	C	3.49145717991394	-0.32386247472393	3.59310787567142
C	3.15554874457974	5.58008255582135	-3.71866915392352	O	3.04397294886662	-0.16091975152465	0.70967187154841
C	1.39222022935757	7.64745773523832	-3.11997044074929	H	-0.28800977168490	0.24215758064097	2.54423485497615
H	1.04683558174203	6.60850439986532	-1.25945810466820	H	-0.42821472198185	2.76681143489704	-1.49774032048379
C	2.96346870792158	6.61710173395436	-4.63084355170094	N	2.37341523706105	0.26309617963159	2.84791002962172

H	1.72215316540500	0.82890592981355	3.38180686726777	C	5.81044002999633	7.87761696916283	2.19421867124225
C	3.63599500452704	-1.80566322440386	3.24169991961181	H	4.37652234515293	8.27501158638877	0.63069822213419
C	4.78237955432858	0.43799078568043	3.27981909207648	C	6.87545146716719	5.71542450862102	2.12427211338347
C	3.14485528703078	-0.17418338127641	5.07239436805506	H	6.27955810203962	4.41834916858793	0.50545989690992
H	3.95007525083619	-0.59042781674040	5.69450914474172	C	6.70799765160506	6.95808797250187	2.73700318515893
H	3.01898625648725	0.88750025917747	5.34027174813792	H	5.67970700765422	8.85728471105533	2.66123848138115
H	2.21145691474161	-0.70714041113756	5.31232350961520	H	7.58267917802674	4.99150708015781	2.53766164442057
H	5.62915466152161	-0.00154376446501	3.82841674452547	H	7.28119298120682	7.21160597546605	3.63249008057389
H	5.00319743832065	0.40017601940987	2.20403192773187	N	-0.14042273541998	6.88131375790474	2.30604925722956
H	4.68760403039616	1.49299133584863	3.58012579927753	H	-1.03611573848641	7.34559642935917	2.36713750251738
H	4.44816306286033	-2.25406186248627	3.83352888901125	H	0.51854584493988	7.16426528767258	1.58081584200859
H	2.70358522764324	-2.34619056243974	3.46680525399621				
H	3.86387013706579	-1.93099795530959	2.17515753720208	<b>CR5</b>			
Rh	1.04811530642635	3.13254263617948	1.53393587864816	H	0.17918476415436	-0.72589456040531	0.50822245579418
C	1.23471043792352	4.93249708188213	2.87031290149592	C	-0.90226307658425	2.87840083302454	1.43982743152416
C	1.38656724864473	3.85798379455321	3.80333037950599	C	-1.30407839587438	2.13420252776544	0.17646228814319
C	0.39361026432914	3.49598379345104	4.71344722686061	C	-0.07921358004780	2.29568477126005	-0.69323692538099
C	-0.79522260231761	4.22541053821828	4.73068607358028	H	-0.16163738533518	2.43402954760942	-1.77500262609908
C	-0.95744099973367	5.31848721214398	3.89673918876276	C	1.07743803662814	1.73314089385327	-0.11376377198707
C	0.04781468587089	5.73768555948519	2.99156331140256	C	0.81494174137169	1.17322255373775	1.27689115307041
H	2.35458022609520	3.36447234368754	3.88657331665578	C	0.25332997565952	2.36972067151368	2.01198123155778
H	0.56389487709113	2.66762019200203	5.40382403940213	H	0.56830403921029	2.63031576506219	3.02587457360777
H	-1.60003366775325	3.95343347477719	5.41895299100430	C	-1.51610923633681	0.64232038947915	0.51726695304490
H	-1.87676962220116	5.90857783302193	3.94181449377324	H	-1.78693690563399	0.09945908871029	-0.40107077034437
C	3.11821558566170	5.12392994335130	-0.43159814493224	H	-2.37813987613210	0.56312762454690	1.19936519272280
C	2.32600341132316	5.86645607970420	0.62450027044046	C	-0.24983505079144	0.04606385130945	1.17273417338343
C	3.52724198120551	3.83082625888320	0.27047959346585	C	-1.91076462088202	3.73764926440662	2.12509915200690
C	2.49115549769824	5.21605387250288	2.00446038613332	H	-2.78865873814273	3.11518805787374	2.37347062207350
C	3.05607724619288	3.84582670658255	1.63340544456809	H	-2.26596509332001	4.54922730736808	1.47162325017280
H	3.19389317456387	5.88359436097556	2.54957148943510	H	-1.52143893484798	4.17145319577272	3.05293705701154
H	3.66224772820735	3.28648877921913	2.35262533990618	C	-0.55066324169466	-0.62787445420781	2.52193130659313
O	1.72036477620669	6.88835207915621	0.36992179390390	H	-1.09374404336511	0.11179649564880	3.14094871308795
O	4.18624559562157	2.96195954277890	-0.29603437791382	C	-1.45994210393115	-1.83836908563617	2.32535683918829
C	2.31234094330470	4.89781989398533	-1.70352162503604	H	-2.39272640888821	-1.57855642301146	1.80237660094021
H	2.90790005756688	4.30766522421495	-2.41512117088635	H	-1.73334088985984	-2.28877084291068	3.29236304029705
H	1.38335114146832	4.35045803139454	-1.48824092636841	H	-0.94769537890500	-2.61207820353586	1.72853173697175
H	2.05201893322014	5.85900194715358	-2.17011473164820	C	0.70999138092960	-1.03931980490045	3.27577332103631
C	4.39838014711637	5.93688144482463	-0.76532018316580	H	1.35054525166241	-1.68413305068499	2.64985705753065
H	4.98224408063232	5.32050006590202	-1.46673738726761	H	0.45044877391250	-1.60912632963268	4.18167337935830
H	4.08251816217984	6.84791556799198	-1.29651195950717	H	1.31171063160583	-0.17522949395910	3.59419001622196
C	5.23286997311556	6.30386167643492	0.43201080861593	C	2.14842080917182	1.09551436626971	-0.95485908014451
C	5.08015366840304	7.55107869404731	1.05143524483174	C	4.44342981255300	0.08307523845505	-0.79381695073974
C	6.14604427872491	5.39317461262016	0.98101485870444	O	1.87934376704030	0.63953424688034	-2.06293747372148

H	1.73722594692382	0.80251802091728	1.73795749561227	C	6.20892085038295	4.38528447086487	0.24873803344648
H	-2.20084641005006	2.57441051723741	-0.28006319128886	C	7.36908758583798	4.10255273368176	-0.48513701763860
N	3.35376802904943	0.97117679196857	-0.36214526679857	C	6.34601260392278	5.02062362999276	1.48954248402397
H	3.44463856555810	1.37925391611344	0.56065773604219	C	8.62839648309274	4.45710738651108	-0.00301295607166
C	3.94844035286649	-1.36673629019823	-0.77190749534842	H	7.27953641017171	3.59014695946213	-1.44720635086305
C	4.93658682027370	0.45367425509892	-2.19356688030744	C	7.60303404937974	5.37668608310683	1.97568331841029
C	5.57516394980887	0.25637097504020	0.21651339929062	H	5.45672250321212	5.23976793813736	2.08511111066412
H	6.41153844841792	-0.40972331870413	-0.03948437555267	C	8.74921199714404	5.09953683364735	1.22946884149033
H	5.95196812498695	1.29051803032560	0.22142453313541	H	9.52040125006547	4.22471884947217	-0.59073636415074
H	5.23699343515697	0.00381647931080	1.23429876534796	H	7.68801925997733	5.87088480174436	2.94712695016391
H	5.75082960535152	-0.22409002881265	-2.49105539805912	H	9.73512161823819	5.37621807572735	1.61184233395520
H	4.12048488476202	0.37548955755039	-2.92264090145482	N	-0.58202407638126	7.18803188751599	0.31232280715950
H	5.32205068746064	1.48379969190163	-2.21665232396704	H	-0.42958756249672	6.91447081839200	-0.64973862016772
H	4.75751726603940	-2.05311159684673	-1.06424221297633	H	-1.53909179428745	7.44443687346095	0.52118950266350
H	3.60863852415283	-1.64045095525958	0.23919140090888				
H	3.11030073566352	-1.49896990772185	-1.47029814565974	<b>CR6</b>			
Rh	0.88201116744713	3.76906192560129	0.41097232558583	H	-0.19279515846200	-0.74124787485064	0.33755280227181
C	1.39220521450882	5.95690333957671	1.01806660307231	C	-0.95111563625569	2.91519337010152	1.35535996491246
C	2.08860757074652	5.32546454083752	2.07499104971435	C	-1.29390584986745	2.25627476182967	0.02804749325663
C	1.60230270545094	5.32812590115172	3.38256236465157	C	0.03433112905458	2.28546597098087	-0.69430529161163
C	0.40186535920144	5.98383307915960	3.64876521606212	H	0.09406934237060	2.46316052370317	-1.77188770081441
C	-0.32615139034710	6.58211810217467	2.62772619322688	C	1.04261172113685	1.58149915403954	-0.00293756230223
C	0.12879069364319	6.56350951244615	1.29737985782468	C	0.54934181748947	1.00960714531791	1.31970989297496
H	3.07260110145270	4.89575754800265	1.88167035134355	C	0.05201273617127	2.24510825427251	2.03882478344460
H	2.16916334271207	4.84447595672960	4.17989192157531	H	0.27893530212209	2.44026925815686	3.09022378023863
H	0.01201027432345	6.01900225892200	4.66949931735751	C	-1.72838154046010	0.79884819222563	0.29163039072615
H	-1.27732355629294	7.07353427299697	2.84765595324767	H	-1.99110431493916	0.32041377525375	-0.6641146524109
C	4.13792475770760	5.05629164036472	-1.16395408825075	H	-2.64702723104203	0.81880343735118	0.90058449385205
C	2.90651978823496	4.38803159056619	-1.79791385326653	C	-0.61098782251361	0.01994896914674	1.02115224444046
C	3.54547358976422	6.16751307005420	-0.31892990867637	C	-1.90892702780884	3.89950683821508	1.93976459446199
C	1.68639964588836	4.89206203949027	-1.19081861112478	H	-2.89953008200145	3.41881406967658	2.02347853606388
C	2.01925556435123	6.11612562799772	-0.36104284552900	H	-2.0334543282034	4.77854008857614	1.28802965965743
H	0.82839970022931	4.93991075266325	-1.87757778157121	H	-1.60082118778131	4.23584688828521	2.93642237440504
H	1.69614084826535	7.07820724227681	-0.80048364404921	C	-1.12282621092883	-0.72353851358407	2.26467805801232
O	3.01011691403676	3.57926310552131	-2.71049320844641	H	-1.61985314352652	0.02342086684604	2.91309070425525
O	4.17803277768030	7.00368683869358	0.28163083860104	C	-2.15995701480036	-1.77314809041931	1.87227447500531
C	5.03977798638521	5.62862457047358	-2.25305133520357	H	-3.00440297733598	-1.33741807210300	1.31760799442935
H	5.41563158104996	4.81245267041798	-2.88700126210367	H	-2.56910771295543	-2.27711157205161	2.76188862739701
H	4.48361177384251	6.33194920365206	-2.89168778349190	H	-1.70331434709971	-2.54609852802479	1.23087149636556
H	5.89258266646006	6.16110900285450	-1.80976421766476	C	0.00066598860228	-1.37482159009555	3.06479053610269
C	4.86452967268709	3.99797994458592	-0.29530584921405	H	0.60124001998823	-2.04385580686843	2.42462628302983
H	4.19481730443877	3.68913191770448	0.52257628977665	H	-0.40970654304253	-1.98242158247948	3.88634881559286
H	4.97358385607561	3.11854403638265	-0.94437933563947	H	0.68202506592931	-0.63623953655051	3.51203611358775

C	2.15017358720389	0.84425458513584	-0.69806168652683	C	5.22109204775441	5.51238573029519	-2.12389152375795
C	4.39177552338775	-0.19613346230103	-0.27327571199152	H	6.12781690567159	5.99501131526387	-1.72692070832073
O	1.93836199844324	0.27302111385650	-1.76483788133266	H	5.53329720836310	4.74222628267942	-2.8459164383929
H	1.36612989788368	0.51858119669799	1.86082054747019	C	4.34118564036358	6.53344306951534	-2.79499471543183
H	-2.07099997922281	2.81809057640901	-0.50762035528023	C	3.49234313342090	6.17018173130576	-3.84922736080912
N	3.30350306856044	0.75534412362673	-0.00782669020276	C	4.31497789676769	7.86021383202235	-2.34528912813887
H	3.34766371521688	1.27886947641288	0.85959658794299	C	2.63269439895515	7.10254493992324	-4.42833455285602
C	3.85146924566416	-1.62650858028786	-0.17467770918055	H	3.50359623957941	5.13925452598189	-4.21145449615282
C	5.00509748062832	0.04311761031994	-1.65458874309388	C	3.45526590537009	8.79523907191834	-2.92133194169684
C	5.44455964150968	0.03065794992519	0.80844716853143	H	4.97793499357227	8.16282714389178	-1.53001843539703
H	6.27078864801670	-0.68376318349043	0.68408627075994	C	2.60746913130920	8.41778372556421	-3.96299047909776
H	5.85816204185929	1.04842104767276	0.75051624669652	H	1.97868831956707	6.79989876034533	-5.25049301036479
H	5.01366532334037	-0.11484193287325	1.81195572740948	H	3.45089540448130	9.82550397306986	-2.55586410529793
H	5.8553055986708	-0.63837266940102	-1.80728445464351	H	1.93334978800941	9.14901019161384	-4.41655868634091
H	4.26217916381770	-0.13235257894240	-2.44315240378151	N	0.00673587431421	7.14990894538634	0.76323962051096
H	5.36232902521494	1.07830860844488	-1.74671102531645	H	0.13901586652763	6.96066215024280	-0.22198444905192
H	4.65878617722271	-2.35181222749776	-0.35769229262955	H	-0.92543458673406	7.47071048343305	0.99488804927093
H	3.43630800548890	-1.81506207482607	0.82780091137490				
H	3.06006441134226	-1.79221820372441	-0.91866679776403				
Rh	1.03397892645404	3.59773250549400	0.56999923448910	<b>CR7</b>			
C	1.81914095445129	5.63132434746626	1.33491821033228	H	-0.25314176009006	-0.89108587305946	0.68296302897244
C	2.42879994258378	4.81424820824654	2.31876234068625	C	-0.75579372272153	2.93842064646899	0.33787292193789
C	1.92601838250918	4.73228139790957	3.61750764001378	C	-0.16024396710999	2.01541830093410	-0.71455317886133
C	0.79634265088507	5.47922641117665	3.94841714540493	C	1.25430256998408	1.84053402832013	-0.21258460383422
C	0.15595605361532	6.26354940198016	2.99761040788985	H	2.11418720642843	1.82514748158334	-0.88742118979166
C	0.62999077463620	6.34367805362818	1.67504385549397	C	1.30375216890134	1.26438680853956	1.07505442513024
H	3.36561096557570	4.30577958313424	2.08029920581874	C	-0.08067414832619	1.00977826547528	1.65580364802238
H	2.42428416119361	4.10726878240181	4.36067035326921	C	-0.69514141693900	2.39760527369551	1.61505454685934
H	0.39437574386019	5.44233800379776	4.96431648937065	H	-1.25868750922754	2.81103395463906	2.45622983058816
H	-0.73948861180227	6.82995945979864	3.26580581808678	C	-0.91385659510899	0.66940824791189	-0.68446997043330
C	4.53745242710529	4.76415941366150	-0.95063642219684	H	-0.48543312236450	-0.00197235434493	-1.44396191429037
C	3.27824403589049	4.07274524498037	-1.49391675946032	H	-1.95955424886606	0.85631954455953	-0.97805569321075
C	3.99843406805440	5.77273469357177	0.04721470381931	C	-0.85167840924810	0.03702145237359	0.72491013895568
C	2.08381318411496	4.66394133339809	-0.91107655528723	C	-1.61026682560846	4.08202572105538	-0.09743168697158
C	2.47850225994626	5.82792860753973	-0.02483371949740	H	-2.44587459712206	3.69095134149572	-0.70398631451085
H	1.27181342357282	4.81395397164532	-1.63844194224713	H	-1.04963458599982	4.78026624494018	-0.73866855693259
H	2.23043905020756	6.82688919428092	-0.42758284463016	H	-2.02706445204801	4.63524558525395	0.75238559301063
O	3.33503514588359	3.20643922126536	-2.35719792988041	C	-2.24211166161557	-0.33872370976219	1.26350782528620
O	4.67803348790517	6.43545425171133	0.79484696312219	H	-2.87019192659918	0.57121328750123	1.20948426183526
C	5.52618143620805	3.81485820743659	-0.28889756385405	C	-2.88656757353330	-1.40900252893080	0.38642615316267
H	6.35937534248299	4.38607589614124	0.14637538640303	H	-2.95385036163203	-1.09860181723334	-0.66703109988176
H	5.04244269608746	3.23663445284440	0.51185563512643	H	-3.90587003072687	-1.64135228586353	0.73227580849743
H	5.93034632661726	3.10846360192830	-1.02770564845768	H	-2.29974728307668	-2.34254045383646	0.42285422207345
				C	-2.20947635749010	-0.80479812699270	2.71568228671979

H	-1.49971937686516	-1.63988935253485	2.84427617034039	H	4.70457155464961	6.89690491939044	-1.45440268058837
H	-3.20239188308931	-1.16241711631243	3.02988124107647	H	5.66223165383422	5.84203551208711	-0.38361577926881
H	-1.91577169015708	-0.00331367920882	3.40952364191911	H	5.14843549391228	5.24197398951469	-1.98088419720005
C	2.51687495515676	0.53750870918893	1.57773075298960	C	2.40367388305171	5.22270609153737	-1.55372168949035
C	3.73201974055298	-0.11518402905286	3.67629175838593	H	2.72052922142867	4.45372000765997	-2.27683211575777
O	3.30886621209565	0.00348197783888	0.80586559607127	H	1.51250470442255	4.82343523264566	-1.03956915570742
H	-0.01653893750799	0.61815475682525	2.67706259831565	C	2.05381771310014	6.49010483461744	-2.27842453940927
H	-0.19089999472095	2.47364067847743	-1.71207339584227	C	0.98447151374773	7.29206184371791	-1.86000187124350
N	2.63856053684645	0.50882345196430	2.92138415362382	C	2.78090340430285	6.89297273982255	-3.40761306738319
H	1.99451019248137	1.09096440865062	3.44573852329781	C	0.66233036706072	8.47013005664065	-2.53317976885833
C	3.82261616893983	-1.60458370528971	3.33594745232576	H	0.38297779437269	6.98093282088882	-1.00185390934710
C	5.05421719579205	0.59193013204964	3.36485649228936	C	2.46555830798115	8.07152325285752	-4.08193665618970
C	3.38886451837354	0.04931336214870	5.15444248090751	H	3.60021510516140	6.26623046886606	-3.76908924315038
H	4.17495085535978	-0.40158107386689	5.77684801442047	C	1.40691784111227	8.86803980804577	-3.64365315780811
H	3.30925518182705	1.11404109696688	5.42355216895588	H	-0.17930452128592	9.07795330785385	-2.19087512358735
H	2.43351057889384	-0.44383613897158	5.39261684514262	H	3.04582053069433	8.36600638757457	-4.96039715575203
H	5.87890744702385	0.12382664391694	3.92352339742181	H	1.15583606216830	9.79068584881245	-4.17324480799513
H	5.28027919072157	0.53303994389546	2.29126665427806	N	2.53597298743355	3.93922177210885	4.46792952376660
H	5.00195297212757	1.65285208408647	3.65470284297540	H	3.34087943510079	3.63185706995269	3.93882631120708
H	4.61186709366094	-2.07795806581929	3.93922347263174	H	2.31921653561698	3.35550703714121	5.26629596902634
H	2.86851555963125	-2.1073480627524	3.55771766461669				
H	4.05500514901645	-1.74792696071977	2.27303314426142	<b>CR8</b>			
Rh	1.25593441332718	3.32741732607774	1.26443592978151	H	-0.25550173630629	-0.90333189661784	0.71715711101875
C	1.67131496808832	5.17622371558793	2.55381172698511	C	-0.90333996069236	2.91192193207619	0.43902420121262
C	0.56895383184534	5.85261121658868	1.98781349313617	C	-0.32457259845244	2.02397296621311	-0.65139520495828
C	-0.66755595418304	5.91942767139653	2.62834768522328	C	1.11749769415950	1.89717738903498	-0.21755840979941
C	-0.83549248674406	5.26242390358185	3.84530725591267	H	1.94639089675897	1.92149313345349	-0.93030116780559
C	0.21293210784599	4.55227042806379	4.41618305012241	C	1.24712039173134	1.30597976514287	1.05910086790715
C	1.48329163844968	4.50838633317220	3.80860845655240	C	-0.09952934287805	0.99326087901440	1.70027397303012
H	0.71032893366252	6.40100037750424	1.05684897072728	C	-0.76327960689588	2.35826549038149	1.70359225525345
H	-1.48783891227360	6.47704283164236	2.17365967757875	H	-1.29694902800689	2.74289844837401	2.57695828320958
H	-1.79923629842804	5.29661930788841	4.35997436136524	C	-1.02233965934394	0.64788547175914	-0.60513057890177
H	0.07737990953969	4.04405509936129	5.37453356239563	H	-0.59578688869593	0.00186206447390	-1.38745596840920
C	3.55833895276094	5.30682665595906	-0.51923012361003	H	-2.08551034021243	0.79297358003779	-0.85677868752726
C	3.18595312367344	6.10194995062310	0.71914892043603	C	-0.87993888273208	0.00501468922825	0.79410954098430
C	3.79179232440310	3.89070797210462	0.02449152290908	C	-1.80445265333049	4.04050080932201	0.06403536036025
C	3.06949754689689	5.19051297934711	1.94195216189213	H	-2.64416186870308	3.64591789468444	-0.53441403711413
C	3.32568329820094	3.79519352097751	1.39425428555776	H	-1.28171816454108	4.77799691426681	-0.56585564627147
H	3.80459215208270	5.55649745265099	2.68603519072843	H	-2.21411500441525	4.55268448233756	0.94304795764851
H	3.83470071013622	3.04402648715321	2.01073775003254	C	-2.23514416493158	-0.41679970460565	1.38601930614288
O	3.04924944759398	7.30231908037286	0.75619015173497	H	-2.89513469104910	0.47139881981733	1.35506369197533
O	4.30757727262489	3.01569600342899	-0.66325943231541	C	-2.87503227441530	-1.51005750184062	0.53418745044329
C	4.84628889701814	5.85913325843098	-1.12239844336542	H	-2.99213392016390	-1.20412154856281	-0.51626696469452

H	-3.87214797167140	-1.77695179470731	0.91784646078488	O	2.94022427647574	7.33534253727262	1.00611926454816
H	-2.25518807486548	-2.42261568353105	0.54899204101211	O	4.03652712296551	3.10796489716041	-0.76272966979091
C	-2.13321851063980	-0.87832343891372	2.83626439260910	C	2.66608014092118	5.73222094176042	-1.52647531740334
H	-1.39724135317183	-1.69412969700596	2.93918584440284	H	3.01158416452338	5.18978230956340	-2.41898863551235
H	-3.10337431375644	-1.26165330362330	3.18911439903912	H	1.64406034274352	5.39411146756952	-1.29088165898814
H	-1.8345533871572	-0.06740427165212	3.51683874203349	H	2.63649537931232	6.80875305173213	-1.75150378760344
C	2.46863958471222	0.53497224958145	1.47183462969764	C	5.05101379912958	5.90959045347315	-0.69466396412471
C	4.00397878316094	0.04296695824576	3.38695618968274	H	5.38637921042304	5.30527465066625	-1.55188005818627
O	3.00639242829300	-0.24072601153100	0.68411342750663	H	5.00829014899304	6.96205841290153	-1.01490194628867
H	0.03662095513875	0.59785057227048	2.71336809064570	C	6.00246562661659	5.76005097146278	0.46445435867794
H	-0.41996650477867	2.49149707098062	-1.64056830707157	C	6.24474917332765	6.83585948246678	1.32880286719992
N	2.86511422685060	0.71726795378179	2.74745169535923	C	6.61617925867057	4.53083591845662	0.74439572789294
H	2.44317756208029	1.49566432574409	3.25279496802190	C	7.06294941779702	6.68696708484937	2.44847893932984
C	3.77130516535575	-1.46960426410418	3.39447885291826	H	5.77862002150220	7.80310204524856	1.12227189725176
C	5.30406970527113	0.38730425297251	2.65322360294162	C	7.43229731406991	4.37777505377128	1.86426374696502
C	4.07469249951787	0.55505899163649	4.82266675180074	H	6.44213459610516	3.68241483467072	0.07830065942290
H	4.89420586666057	0.05424574885921	5.35780859692346	C	7.65585318843821	5.45469067191438	2.72332577973528
H	4.26227700902600	1.63858213120200	4.84587428973185	H	7.23819701097660	7.53998800430221	3.10931173718728
H	3.13584152207340	0.35243640322583	5.36162095418689	H	7.89926715439381	3.40980261140885	2.06522418696294
H	6.15687866460873	-0.11086619147589	3.13900176882428	H	8.29604174776363	5.33533466434475	3.60121783602023
H	5.25417973594331	0.05893124640942	1.60651728565842	N	2.42736895373971	3.62848437719859	4.42205161757730
H	5.48392318621641	1.47376773310822	2.67227556642854	H	3.37817549358203	3.89687402060779	4.19617741815379
H	4.61009432338048	-1.97741928229014	3.89416584450426	H	2.31082022042139	3.37051942548738	5.39515012739629
H	2.84570883910604	-1.71183890824978	3.93936525086213				
H	3.68607575461532	-1.85485409733636	2.37000443114002	<b>CR9</b>			
Rh	1.14153929487202	3.35264331034325	1.28097180265478	H	0.86711178475527	-0.58668190331236	0.78062729012967
C	1.61598577603900	5.12110426498993	2.66561985940778	C	-0.47547141419354	2.94876777397244	1.61317425162803
C	0.51489967767093	5.81408555814912	2.11592266599390	C	-1.01983622179873	2.03514438588136	0.52881311600636
C	-0.72572747391221	5.84977839442020	2.75603722255512	C	-0.02348391805921	2.24596128855495	-0.58475936335708
C	-0.89886693914382	5.14379303581836	3.94264879569134	H	-0.35426334314902	2.27115659388506	-1.62780649989405
C	0.14431893088952	4.39578906120803	4.47744280509763	C	1.29261384689013	1.86472510529543	-0.22743052404213
C	1.40992344562289	4.36663007233971	3.86556246370659	C	1.38646330691825	1.43506992637787	1.22299708676066
H	0.65837685932172	6.40137912821996	1.20768033078298	C	0.83577549461625	2.63958260790112	1.94844008271493
H	-1.54412624069066	6.42717441688895	2.32304805859424	H	1.31496718452176	3.04522207254964	2.84507392846905
H	-1.86142870227154	5.16429473608136	4.45989162926165	C	-0.96139240395708	0.57258789706803	1.02687881041420
H	0.00196801630535	3.83506488035615	5.40501561729547	H	-1.33555737805101	-0.09518282453102	0.23602592838428
C	3.60904303311958	5.45421042619709	-0.36194721240181	H	-1.65562214033384	0.47826369216234	1.87751628815686
C	3.15056555458050	6.14920697303159	0.90880689943205	C	0.47612683193440	0.19734138922943	1.45193312132733
C	3.64322414995047	3.97044368004743	0.02065065756747	C	-1.41382343103627	3.72188977476217	2.47358731334452
C	3.01173520093945	5.14764430655491	2.04983534778086	H	-2.02478659287499	3.00854397770202	3.05469495637477
C	3.21176817739296	3.79622538499228	1.38961155357316	H	-2.10383704647131	4.33843045091941	1.88127513859032
H	3.77148153104410	5.43106723572232	2.80626655426035	H	-0.87924757277080	4.37038301128480	3.17981014276941
H	3.69325434408256	2.98764540476174	1.94766080897369	C	0.54372846403758	-0.35205415479744	2.88611904338450



H	0.05084865909938	0.38769278679173	3.54611926135343	C	2.43154261967615	5.93221630846229	-0.02769410197010
C	-0.22528108776647	-1.66645636303485	2.99316363001924	H	1.35300766648046	5.60635790598417	-2.00663972039305
H	-1.27268023472224	-1.56412323658096	2.67138255530739	H	2.85287205006734	6.93895319807938	-0.25074412000578
H	-0.22912015563387	-2.04025822512879	4.02910405192489	O	3.27075882041129	3.99726725278904	-2.93791559864630
H	0.24382557695561	-2.43890894539150	2.36018021631503	O	4.05272369830081	4.93555725539351	1.55646768028375
C	1.97574968974522	-0.54413087829631	3.37598826086197	C	5.34778576849997	5.45181701028565	-1.31912437226294
H	2.54719638081833	-1.17841467966936	2.67699967533002	H	5.78394393309436	5.04044954363109	-2.24135947753886
H	1.98620673295647	-1.03894515713263	4.35970254719641	H	4.90440820809293	6.43104049242888	-1.55515086530658
H	2.51544728885699	0.40840302555908	3.48188934481068	H	6.15042994810009	5.59616812712098	-0.58239613661327
C	2.20804846080851	1.15283442148510	-1.18372738653407	C	4.85683020593864	3.05547228126361	-0.54981948278685
C	2.69003172721966	0.70988076684733	-3.60410993733644	H	4.23116270403116	2.55578938625729	0.20403783800969
O	2.94862560326735	0.26730304871925	-0.75357691567825	H	4.71322971995303	2.50827015872173	-1.49006546293841
H	2.42804035017168	1.21947698587923	1.48138815504936	C	6.30760563398800	2.95040345643511	-0.16319754297200
H	-2.03853964818770	2.32074859582220	0.23413401898384	C	7.25268615643104	2.54072480745841	-1.11229176752949
N	2.07031588596080	1.43845492168257	-2.48905144592917	C	6.75243632423050	3.23964002506890	1.13403933902266
H	1.59892411053949	2.30412960074672	-2.72386453931038	C	8.60334365162090	2.42484711759427	-0.78163131141049
C	4.21628503250276	0.81867605300919	-3.56038243911207	H	6.92044604267175	2.30329795399587	-2.12725216167419
C	2.25719394009226	-0.75792185569747	-3.55933164469050	C	8.10081238555502	3.12471215730167	1.46888288222737
C	2.16468525805230	1.36241233772614	-4.88059693540255	H	6.02581180783053	3.57037478465890	1.87893352726015
H	2.59385313220513	0.86670827506737	-5.76323020895490	C	9.03268523463980	2.71706469435126	0.51244321078590
H	1.06762069501566	1.28160428368976	-4.93891934516221	H	9.32221832218974	2.10072841777827	-1.53895073394216
H	2.44093424265874	2.42715914166833	-4.90772296817491	H	8.42784895626641	3.35310269941005	2.48700368712653
H	2.68041718738100	-1.30038010319214	-4.41827232570586	H	10.08943740962238	2.62495209213016	0.77655854135414
H	2.60586274162422	-1.23745087845752	-2.63498274146569	N	2.35114312537639	6.42919932532489	3.00636313911458
H	1.15997519753440	-0.83789937130384	-3.60499413914763	H	3.15716837482300	5.90941422990285	2.65494783682002
H	4.65679822505357	0.27497680224542	-4.41007194291897	H	2.28195686552717	6.59220195412815	4.00219860799215
H	4.51716248368323	1.87388912245215	-3.61805172770429				
H	4.60824587638807	0.38848020822546	-2.62891510411483	<b>CR10</b>			
Rh	0.95428515650001	3.93119550014940	0.19338833391305	H	0.69632913021482	-0.67300599255445	0.77045210260580
C	1.18732340478680	6.10744549506056	0.87730868925865	C	-0.56388705816515	2.88835480485107	1.61430142594215
C	-0.04746104402152	6.29119916971627	0.19094476445508	C	-1.11498061318722	2.00598949449654	0.50893585554582
C	-1.21115332987378	6.72415312582795	0.82106362763062	C	-0.09810971968167	2.20067698359688	-0.5887051061780
C	-1.15982162990216	7.03652829377759	2.17750330653042	H	-0.41596755216880	2.24183976419847	-1.63523846805089
C	0.02405635062675	6.90249463037583	2.88379401764244	C	1.19969662378953	1.77882034691688	-0.21400633833176
C	1.21757934365058	6.45620046569769	2.27462028710907	C	1.26245288017599	1.33457780089220	1.23362075790332
H	-0.07426490410817	6.18098394449344	-0.89137369325391	C	0.73340528136385	2.54418150234516	1.96692533852286
H	-2.13049394201859	6.84576657031708	0.24557437834337	H	1.20664009424834	2.92465092268172	2.87762391469591
H	-2.05393391569481	7.39226626377285	2.69661449071242	C	-1.10382546765000	0.53613597326748	0.98886835686887
H	0.05992390491324	7.15922105402601	3.94598508787231	H	-1.47910507497915	-0.11165565177151	0.18202332007842
C	4.29083786005626	4.46766049049354	-0.78920534319673	H	-1.81681251165119	0.44872729646538	1.82456301964314
C	3.14998973890953	4.46396401328291	-1.81228892330399	C	0.31505029836138	0.11989147464195	1.43755008455227
C	3.63173214285882	5.08413775530120	0.42569865967131	C	-1.50423373301798	3.66200105339811	2.47150552927564
C	1.99913703698036	5.13671433096141	-1.25786480125654	H	-2.15937308874464	2.94663593724015	2.99984866984668

H	-2.15330708114993	4.32543190222800	1.88281491481593	C	3.02017931883816	4.38035236169634	-1.94031857460426
H	-0.97368031474702	4.26033895968965	3.22233870178492	C	3.80174064135002	5.25142146385124	0.14179554804625
C	0.33964812940668	-0.43577685116903	2.87080706058745	C	1.90637111851605	5.01267695700614	-1.27152273791434
H	-0.14826230453561	0.31460656916037	3.52237328768266	C	2.43943062486147	5.88248176914499	-0.13327907816010
C	-0.46358208863417	-1.73102369360659	2.95807898664292	H	1.17100131817803	5.44058936898235	-1.96267085827744
H	-1.50144256833975	-1.60231137695315	2.61539374823715	H	2.70957544512984	6.91387268856459	-0.45326633127470
H	-0.49782138546029	-2.10716758319505	3.99262088977519	O	3.02808301888082	3.88236772675587	-3.06110443099804
H	-0.00072411851094	-2.51325171067985	2.3325564838202	O	4.49023529861692	5.37229698909109	1.13486599362044
C	1.75556835087014	-0.66430742359404	3.39036803346530	C	4.88071672053443	3.14433436283359	-0.68302114711833
H	2.32540531486808	-1.31265537581707	2.70305214684802	H	5.73833875239899	3.30937990042274	-0.01472966985671
H	1.73288291276564	-1.15951183005353	4.37372074409365	H	4.15041975629211	2.51096237879566	-0.16096854341979
H	2.31667136483645	0.27438024931667	3.50827359291863	H	5.22714004529820	2.60825730495306	-1.57669963477095
C	2.12723212649041	1.06312538470101	-1.15604619757611	C	5.34263122155026	5.32696147033984	-1.83198063134969
C	2.60597261449575	0.56639788014283	-3.56606732991716	H	6.26156364479687	5.31944423565168	-1.22602140233643
O	2.89769446333904	0.21170446872023	-0.70775155250261	H	5.55197390838142	4.78805369073966	-2.76933282400482
H	2.29424669316778	1.08688824558733	1.50145703701602	C	4.92956749520011	6.74484914446008	-2.11614312973165
H	-2.12137459719635	2.32304081424821	0.20397678225361	C	4.12623763003533	7.05784944131299	-3.22098824153826
N	1.97030014012878	1.30574214058287	-2.46773859784979	C	5.29593748659530	7.77680262366184	-1.24215729139272
H	1.48392157877241	2.15700275375854	-2.72407821156629	C	3.68896805950784	8.36399817938929	-3.43691556752020
C	4.12632424552059	0.73778704462781	-3.54133182760237	H	3.83846020621592	6.26387447274983	-3.91440748098835
C	2.23138193185581	-0.91482413729020	-3.47063696849183	C	4.86060749816062	9.08428141339491	-1.45590113810444
C	2.04131545574989	1.15484493464399	-4.85715031853505	H	5.92738697763143	7.54836203844727	-0.37885947021693
H	2.48294627431614	0.64857708259217	-5.72761485124586	C	4.05102832243918	9.38103716835831	-2.55254584100045
H	0.94823873751193	1.02549917481394	-4.90104981372464	H	3.06275615003783	8.58968094575127	-4.30407664060759
H	2.27103840855306	2.22879519835135	-4.92213415346746	H	5.15684033844415	9.87558088118540	-0.76237495880639
H	2.66669605297608	-1.46653443974982	-4.3175377757180	H	3.70841079139031	10.40507722388247	-2.72170831135168
H	2.60688403020223	-1.35212848961023	-2.53604750974566	N	2.61849780697375	5.85353855943774	3.00937200740845
H	1.13765244775732	-1.03791885756900	-3.50209591398882	H	3.48706091819783	5.74770324714952	2.48225628664073
H	4.58272176407599	0.18013761405288	-4.37351759893772	H	2.67880863246698	6.10597949189959	3.98675523859374
H	4.38202633162685	1.80173289631202	-3.64097718795779				
H	4.54106440646054	0.36079602119294	-2.59653571709583	<b>CR11</b>			
Rh	0.92199339989449	3.84604695106776	0.22207321692341	H	-0.16139495900495	-0.83886494630103	0.87835658241504
C	1.31994269840672	5.99216360993885	0.92952995378721	C	-0.54841230544490	2.93979480701789	0.09626126842269
C	0.04900871335782	6.32239947381900	0.37594792172927	C	0.13925517230616	1.90650974845058	-0.78484998096876
C	-1.02823118664822	6.75242671959812	1.14092618943781	C	1.48998842569375	1.77147368414416	-0.11206684317233
C	-0.85432501861535	6.88881520069707	2.51815666532660	H	2.40640445293307	1.67634839448712	-0.70206385197169
C	0.35812667855870	6.57464018467559	3.10601504218408	C	1.38778835552681	1.32655533488296	1.22529620240844
C	1.47141940998054	6.13209729961835	2.35419953495931	C	-0.05094976194881	1.14777456568655	1.66422580101842
H	-0.06041409086439	6.33449278284158	-0.70795444087411	C	-0.62927035749103	2.52689702843382	1.41895063887088
H	-1.97533723360022	7.00615248366893	0.66164175711242	H	-1.27051594525783	3.02586254044962	2.15000391270769
H	-1.67702594003485	7.24051576155923	3.14646978155790	C	-0.63828121035132	0.57734931649340	-0.70720225193529
H	0.48677563551629	6.68279684971509	4.18639691355958	H	-0.14124429243265	-0.16913548157492	-1.34529827708617
C	4.27794726104633	4.48685845678931	-1.07748804987593	H	-1.64187888853627	0.74156524244336	-1.13183778800575

C	-0.74097347398089	0.09387979069660	0.75684541688813	H	-1.89699470751351	5.42340746000477	3.94622713361610
C	-1.33249528251023	4.05303692358610	-0.51592081293348	H	-1.63561721725249	6.87812520888805	1.96994260364482
H	-2.15239080987035	3.62815722679816	-1.12155476127287	C	3.67618993682500	4.99371647585448	-0.88581557108116
H	-0.71655396980554	4.65985105264659	-1.19704942837249	C	3.23514532848502	6.09318655674716	0.05723178247054
H	-1.76950571227787	4.70993097809885	0.24734043579907	C	3.88998934694113	3.80342667695733	0.04997565794333
C	-2.19004721078573	-0.21064461296463	1.16924881049095	C	2.96087491827028	5.55217919170591	1.46449409155016
H	-2.78939687103536	0.69250947877333	0.94426274795318	C	3.37051220027225	4.08828874037032	1.36109407108071
C	-2.75047629285062	-1.36565050717440	0.34299446357068	H	3.59537786369261	6.16991284211567	2.12958721842563
H	-2.69051681662004	-1.17113502949393	-0.73838928219771	H	3.83789404987842	3.58225626168171	2.21176022510261
H	-3.80697297091077	-1.55307429494550	0.59076816779829	O	3.20277538640448	7.26642931323005	-0.24567680730892
H	-2.18906976974962	-2.29329291592352	0.54666155873788	O	4.43125785760106	2.76363961344093	-0.34386965470810
C	-2.33323128399340	-0.51337047600499	2.65707154985225	C	4.97402531161756	5.36208611092669	-1.59504397246360
H	-1.66298291739205	-1.33675670776657	2.95738916652390	H	4.83459187401992	6.26301220074424	-2.20784701826298
H	-3.36393039199487	-0.82213920890056	2.89170689596362	H	5.77549265062255	5.55715951251985	-0.86662236422406
H	-2.09863649770129	0.35734745778840	3.28693731280011	H	5.29012679936343	4.53192500875416	-2.24260964483393
C	2.45456012007564	0.65686594093648	2.04296165170634	C	2.53879718715905	4.63161774371703	-1.88243751205705
C	4.89300175802664	0.23356301328030	2.31720063193178	H	2.83227695312761	3.66794442397633	-2.32820936393738
O	2.12629605160639	0.02599181502743	3.05129257983402	H	1.62270855186843	4.44399249034625	-1.29679139424973
H	-0.08108240004896	0.85557664243767	2.71780411620042	C	2.26056557386988	5.62836529150522	-2.97042891322663
H	0.23429932128153	2.25944432153677	-1.8205699919716	C	1.29272112346250	6.62753251416164	-2.80559547214873
N	3.72282919041351	0.77350567146213	1.61187255781976	C	2.95647869480567	5.56872506294224	-4.18559923202156
H	3.92613550684970	1.42430134531860	0.84258879891654	C	1.03405297949061	7.54653897490779	-3.82184784867093
C	5.00453897870504	0.85361496834536	3.71365260601103	H	0.73913256843102	6.68533277193008	-1.86448099770633
C	4.79710580721132	-1.29127986425907	2.41016317323693	C	2.70269031786336	6.48774733472651	-5.20285396108490
C	6.12142278089848	0.61263667987277	1.49222520845574	H	3.70233820363506	4.78368614194515	-4.33790511808562
H	7.02926726036792	0.22347154133969	1.97558637356600	C	1.74042111209445	7.48234347957100	-5.02333372451248
H	6.06054257401514	0.18876586547736	0.47785819021994	H	0.27206826846540	8.31682309250768	-3.67521643517868
H	6.21508473193734	1.70452083273763	1.39877476690830	H	3.25481898148098	6.42232106222735	-6.14412242760747
H	5.68971849754129	-1.69484695408911	2.91211524908261	H	1.53649045748362	8.20125782751824	-5.82111825119386
H	3.90645121176644	-1.59234663219795	2.97664064676677	N	0.49944257536619	7.22454109236099	0.54894479252374
H	4.73858330186964	-1.73265812117035	1.40298181549785	H	-0.27407692487794	7.86595431635744	0.42715720057398
H	5.89251045995680	0.46302197644610	4.23372953246264	H	1.40906352507537	7.59236817534166	0.28684578191085
H	5.10158415784503	1.94806883948663	3.64052261631166				
H	4.11424100460853	0.61890838047151	4.31207868392390	<b>CR12</b>			
Rh	1.35263481920757	3.43345346799912	1.15873921608436	H	-0.06670563263508	-0.82434912642258	0.79851796790053
C	1.51741459051675	5.53919465601581	2.01189414349034	C	-1.04052099122426	2.92285077058925	0.54731772449939
C	1.34407361514803	4.74462815014166	3.18590330062141	C	-0.34090280628233	2.10724808110894	-0.53003961495689
C	0.13849731526692	4.69564863425722	3.88583605841817	C	1.08994837608244	2.10359633235025	-0.03511633355832
C	-0.93792690977631	5.45081127595338	3.42247830738192	H	1.92825314316724	2.21717835055080	-0.72841885751847
C	-0.79703634043133	6.26378122437815	2.30837000434551	C	1.22218715670006	1.50162160525107	1.23718395517119
C	0.42059811133317	6.36472480220649	1.60202653415999	C	-0.11135834765127	1.06274348884884	1.80825881980241
H	2.21520668124988	4.24691515090729	3.61569203549522	C	-0.89479115792515	2.36072306323244	1.80870320869699
H	0.05394157992810	4.08310134142634	4.78530720170212	H	-1.49791918497974	2.67788075997455	2.66357602341749

C	-0.91133763064608	0.6747693329071	-0.53776654229696	C	-0.40295817404682	6.21651499669396	2.30672137042849
H	-0.39260181620879	0.08697657258699	-1.31048628078237	H	1.98507501216125	4.31312457349202	3.86975607007328
H	-1.97090008876017	0.72780217087061	-0.83627845417887	H	0.07368466671661	3.68652722842908	5.28745742017399
C	-0.76908511425417	0.02656233337110	0.85767992071738	H	-2.17206777892929	4.72366759981967	4.84059765685302
C	-2.02705560472498	3.97689318015594	0.17017179530825	H	-2.44034851614059	6.32943546018902	2.98866242077911
H	-2.81227267445332	3.53129970227571	-0.46535235346173	C	2.77983220707159	5.67826818463411	-0.65960220806466
H	-1.55667994082964	4.78126682364423	-0.41727984212978	C	2.19324485942207	6.56335929401763	0.42237841659651
H	-2.50273684398586	4.42163724176711	1.05378718926676	C	3.19200213765274	4.41877863633917	0.09328209820764
C	-2.10661436252213	-0.51868184480456	1.38448765089498	C	2.20536441382502	5.87097184956480	1.78400045479881
H	-2.83762369188829	0.31133199382429	1.33661476636907	C	2.80696323281210	4.50471637061498	1.47631161797806
C	-2.61406868490526	-1.64738047708907	0.49025081892557	H	2.83327063320458	6.52585077448296	2.42106527829628
H	-2.71419819365016	-1.33411883440685	-0.55986011705202	H	3.44037167463173	3.99767058610222	2.21132417882283
H	-3.59891059623688	-2.00744761668652	0.82681067960433	O	1.83388956099380	7.70329142258825	0.21825538631750
H	-1.91783136373336	-2.50284425855823	0.51777151925897	O	3.78551329803201	3.49374271012412	-0.47682674974509
C	-2.02622458838173	-0.99434844620889	2.83107977593247	C	1.73231309985588	5.40048520339149	-1.73747887258489
H	-1.23117506935921	-1.74973169584718	2.95279936496554	H	2.14804200038365	4.70532443600463	-2.48175305106356
H	-2.97576909413960	-1.45914536461585	3.13949231818333	H	0.83094742359192	4.94153617943863	-1.30223424728509
H	-1.81872565205701	-0.17270603207958	3.53209020351118	H	1.44692812871109	6.33549494807763	-2.24152549360830
C	2.46472704455297	0.91026021175033	1.83931547589334	C	4.02545453575902	6.34926513248423	-1.28147958218737
C	4.95379785478528	0.83013844750956	1.78992074023625	H	4.38259596564862	5.68546305606016	-2.08307853667596
O	2.35186046196151	0.11712605661626	2.77832329565480	H	3.69589607039110	7.29246505883092	-1.74410970884380
H	0.03577256529347	0.65448819644447	2.81236207499575	C	5.13234613622946	6.60635254909691	-0.29316500615945
H	-0.42829885966444	2.58268001027737	-1.51617619220800	C	5.16619755213760	7.78600700887661	0.46290854079418
N	3.64167350175798	1.27473158877444	1.30230847110345	C	6.13202226657456	5.64815894620020	-0.07709641517449
H	3.65486656889729	2.02659473623684	0.59946734238443	C	6.16201258156083	7.99575949335129	1.41726539460465
C	5.15855757461278	1.26540867768378	3.24433117113483	H	4.40194876257273	8.55034819252413	0.29987130673718
C	5.07662033442195	-0.69013121955309	1.65738782745781	C	7.12870318472304	5.85486701038264	0.87545676026542
C	6.00621244451661	1.50279882180036	0.91018456600557	H	6.11640811390996	4.72351576515096	-0.65870225605206
H	7.01126020927688	1.18949050182786	1.22819284086690	C	7.14499432008242	7.02890691438790	1.62960705216364
H	5.87552262796659	1.22264398840252	-0.14661161044554	H	6.17174267525782	8.92363527538085	1.99520576892614
H	5.94273114952447	2.59877636613552	0.98318128113140	H	7.89837634970615	5.09350364990170	1.02826828619161
H	6.07115914704313	-1.02151942921382	1.99332017645456	H	7.92593172098128	7.19311747077606	2.37659006723974
H	4.31202236816994	-1.19550466562608	2.26190714844449	N	-0.63752897349581	7.12737912617773	1.32650367648588
H	4.94918947046411	-0.99200825012420	0.60607587097085	H	-1.52690373366953	7.60925255693570	1.35327984504268
H	6.15415384971209	0.95607685907986	3.59765733393079	H	0.14368168674098	7.65763098538143	0.95178153568754
H	5.08878356382723	2.36131691938625	3.32883025219639				
H	4.39838963050722	0.81345224749236	3.89503775431465	<b>CR13</b>			
Rh	0.89509217218920	3.57149449995593	1.44366345285914	H	0.45613435116951	-0.64887280673397	0.66132667917024
C	0.86819122439693	5.58103244309970	2.50403800595940	C	-0.61196364139390	2.97342414274211	1.53279457399786
C	0.99254508431398	4.68536621578813	3.60992147035019	C	-1.05661489646116	2.19156212980711	0.30718549174311
C	-0.07375695175679	4.36939417498031	4.44882269413630	C	0.13508436118536	2.34194349167273	-0.61451301750311
C	-1.31555578646509	4.95608015898744	4.20242675024719	H	-0.01536415170731	2.46706410362154	-1.69139148347786
C	-1.47103622988030	5.85347465941015	3.15958959341505	C	1.31527625248587	1.79043913333332	-0.05987342127237

C	1.10515994091201	1.27415486275075	1.34925160613080	C	2.13309258952736	5.26485838914653	3.39553239720373
C	0.56651762854858	2.48422690008959	2.07624237692365	C	0.97381074527017	5.94249997172773	3.77071313664333
H	0.91929708693807	2.77578336082538	3.06887344824054	C	0.19388868160559	6.60043023156074	2.82861741952668
C	-1.24861045761543	0.70934997475570	0.69492167325140	C	0.55496040107925	6.62267329831491	1.46869934880240
H	-1.55174257483375	0.14106098443245	-0.19771848498422	H	3.47197025531454	4.83849515511224	1.77572771175479
H	-2.08481385426517	0.64639326908925	1.41010390279744	H	2.74205266593573	4.73934236214479	4.13303207576666
C	0.04533039215591	0.13919958647263	1.31840569034420	H	0.66052555467459	5.95090997213889	4.81805380253651
C	-1.59253904984653	3.86547996461835	2.21709601996080	H	-0.72085906597707	7.11475020810504	3.13382393489055
H	-2.47614313780710	3.26574847128821	2.49835287278919	C	4.19950020038195	4.95970534742916	-1.42391582715664
H	-1.94772891043836	4.66581173870161	1.54918310152520	C	2.84996282532040	4.52360534275646	-2.01143951507004
H	-1.17736948862060	4.31701106710833	3.12515507323645	C	3.81416938881644	6.06288685057405	-0.45491577812006
C	-0.19858362793793	-0.49704330630237	2.69668339340268	C	1.76635526378541	5.04532231353325	-1.20772946065553
H	-0.71560074227306	0.25965180057641	3.31766073356275	C	2.29405378795995	6.17006114340158	-0.34067246758633
C	-1.11447162416389	-1.71204224086460	2.57313271713310	H	0.82335364502256	5.19494934508125	-1.75431678984633
H	-2.06981899973098	-1.46501411231824	2.08599613170175	H	2.03760558802476	7.18788371485726	-0.69316414724509
H	-1.34401259151017	-2.13719602155769	3.56279983237739	O	2.76343289982848	3.84020974030382	-3.02683487126763
H	-0.62917009347827	-2.50127375055473	1.97403230292381	O	4.59025901346742	6.78569039356247	0.12337696462743
C	1.09452963404455	-0.88632460648616	3.40566642722530	C	5.13164093044047	5.48121689956728	-2.50993028085009
H	1.70617830297760	-1.54968327573321	2.77064188799014	H	5.38212559979316	4.67295649226801	-3.21212994531020
H	0.87713965010475	-1.42768321574467	4.33969445405550	H	4.65206376557501	6.29291666532683	-3.07781043291011
H	1.70904668227721	-0.01251391608447	3.66735585276302	H	6.06011989706795	5.86897444152331	-2.06861461898106
C	2.43203818566157	1.12059080519543	-0.81831803376171	C	4.79623512284865	3.74090854474346	-0.66307415159575
C	3.20827409007173	0.42860234651529	-3.10206341032030	H	4.10915480010940	3.45822406437304	0.15076983856691
O	3.27058900290214	0.45685415019165	-0.20665430519394	H	4.78082029059567	2.90907729278755	-1.37902727024622
H	2.05837089788560	0.92170635918337	1.75384826704234	C	6.19282197733736	3.91050812787574	-0.13664228490185
H	-1.97053067389322	2.61584866365344	-0.12998486352290	C	7.29240952784472	3.58348281818134	-0.94250253862852
N	2.37280691048595	1.1859999447295	-2.16019755696487	C	6.43890295892006	4.38102403067202	1.15940175903876
H	1.82086949070329	1.93610425499856	-2.56298312801100	C	8.59707611119419	3.73460065078346	-0.47481363972530
C	4.67635405302189	0.84961818678068	-3.01429590844138	H	7.11888670979401	3.19546003560282	-1.94996486057892
C	3.06379220233578	-1.07008165186795	-2.82478748517572	C	7.74150788604051	4.53293349172587	1.63236579545074
C	2.66714786374937	0.74142642941185	-4.49588225915614	H	5.60048794247493	4.62897576793179	1.81412516194539
H	3.25166002459329	0.20428263152179	-5.25676659441080	C	8.82639849759751	4.21392777571781	0.81531099741748
H	1.61464640853058	0.42961455422305	-4.58599974353912	H	9.43930264600057	3.47004918660738	-1.11958379906376
H	2.73301046225831	1.82023604380821	-4.70215878599328	H	7.90942417404691	4.89976728208226	2.64838645858738
H	3.64317082107468	-1.64416681278487	-3.56362799968403	H	9.84795033100506	4.33102611267667	1.18612765347989
H	3.42845821815902	-1.31929816749042	-1.81986069758102	N	-0.19494483386537	7.31780177287850	0.56544237210214
H	2.00802354616602	-1.37318782354699	-2.90064779792810	H	-0.10908626810482	7.10315249789926	-0.41931670665650
H	5.28070462706465	0.26155935418825	-3.72158664483438	H	-1.12348121607327	7.60366430265563	0.84998154980745
H	4.77956009546544	1.91408248922127	-3.26885124833981				
H	5.06587206423775	0.68535762805308	-2.00036984322224	<b>CR14</b>			
Rh	1.11364486993192	3.85169665187206	0.42380945452603	H	-0.00319529531023	-0.60137029656224	0.39234833001602
C	1.76944754751809	5.97940424390070	1.07533768015058	C	-0.75243843454431	3.05403865162232	1.44125332156675
C	2.52051416610077	5.29067700588020	2.05661158617612	C	-1.12528852526640	2.40680453664837	0.11459097012218

C	0.18660838472476	2.46524424572280	-0.63963964936069	Rh	1.19799369465512	3.76152569994042	0.63148082711760
H	0.21680043921079	2.69304086755877	-1.70984620073488	C	2.13380803303413	5.68091550237758	1.50446532712688
C	1.21432361357633	1.75625152389132	0.02535453105981	C	2.69806027865449	4.77805501385845	2.43862769879570
C	0.75778978360739	1.16033862571293	1.34671717816208	C	2.20037342073195	4.66605898524812	3.73752365588923
C	0.27004075421513	2.38128078424344	2.09492050812542	C	1.11618165798360	5.45747994775245	4.11446265022191
H	0.52092597403386	2.56525903974151	3.14261584043187	C	0.51444061024763	6.32260174506200	3.20913220188368
C	-1.53961903431919	0.94268708492894	0.36426197105628	C	0.99127250315680	6.44625763565180	1.89095654084965
H	-1.80431620007790	0.47371116268913	-0.59581320012307	H	3.59869050927987	4.22464935482036	2.16450593031196
H	-2.45368755607162	0.94294516866219	0.98009469356939	H	2.66509192513179	3.97691417535355	4.44495906504237
C	-0.40601801241942	0.16880073419736	1.07567891526838	H	0.71891121963605	5.39271394806449	5.13084900954073
C	-1.68654024610962	4.04280132504147	2.05637502407497	H	-0.34512681204537	6.92575660430067	3.51237600146322
H	-2.67866280717648	3.57209957470350	2.17180139831212	C	4.62789944971584	4.77944105220201	-1.07772353090009
H	-1.82292652753882	4.92424918902144	1.40985140969130	C	3.26373462272200	4.32317747405820	-1.61214312731484
H	-1.34189571442250	4.37618607179586	3.04226905964752	C	4.27493773808214	5.65070504651931	0.11562175656526
C	-0.89587155802092	-0.55534801927467	2.34002922503342	C	2.19441034728212	4.91667435062888	-0.83098584304698
H	-1.38433746998747	0.20342297334788	2.98118924720443	C	2.77709834044829	5.91788969552373	0.14604588171713
C	-1.93756201032530	-1.61342139605879	1.98484207638196	H	1.32230954983333	5.21625104122528	-1.43277528904164
H	-2.79038194863387	-1.18966999519322	1.43369301587443	H	2.65888873595921	6.97853685383116	-0.14827324463066
H	-2.33330570673720	-2.09838964389126	2.89092973207788	O	3.15156408604504	3.62204712322079	-2.61083142259319
H	-1.48994077823305	-2.39959438245557	1.35328921200951	O	5.07119336946165	6.07605173500295	0.91876528987735
C	0.23983002833869	-1.18836553829045	3.13709027450508	C	5.54965626701522	3.63481319177492	-0.67842246479507
H	0.82769272950055	-1.87550634038333	2.50470050043159	H	6.44949744183910	4.03530659262862	-0.18837169631993
H	-0.15823676626723	-1.77304424347861	3.98105085224470	H	5.04409320940360	2.94069904785149	0.00836835177096
H	0.93005993086978	-0.43982054068048	3.55286103722174	H	5.85438446006646	3.06691020002061	-1.56894787598976
C	2.42246643295620	1.11297450716659	-0.58690802664252	C	5.30450619628167	5.65626557846773	-2.16448823023677
C	3.17301033126310	-0.16620031513920	-2.61973575493327	H	6.28895517455905	5.96343027772247	-1.77795261989575
O	3.44723779879578	0.93770268890810	0.07296298042503	H	5.47028290146968	5.00334488155583	-3.03543382563915
H	1.60271582521479	0.67557452217277	1.84739146726920	C	4.50414758059494	6.86756656815886	-2.56483564200959
H	-1.91911287379223	2.96997978615210	-0.39450017107856	C	3.52477646960234	6.78567291308283	-3.56420300735842
N	2.24445906877471	0.66394833898554	-1.84113833091708	C	4.68410046107617	8.09201850019688	-1.90784382157880
H	1.33347659827925	0.82762441087000	-2.25161724428431	C	2.73821014325711	7.89046943532084	-3.88708365966417
C	4.54222986612458	0.50409532274488	-2.73935327919675	H	3.37418940696663	5.83791390971843	-4.08687071546589
C	3.30217746560238	-1.53844146400165	-1.95260497434557	C	3.89822754977358	9.19914703699440	-2.22749763757445
C	2.55137674265889	-0.31220062607530	-4.00666386141971	H	5.44872011339003	8.17560073724582	-1.13050865190257
H	3.18308699818459	-0.95221049036742	-4.63908286471151	C	2.91868215855104	9.10052955641959	-3.21596564733395
H	1.55202097288842	-0.77245021897936	-3.94496290836981	H	1.97922430660963	7.80542597711164	-4.66944932579457
H	2.45454866920379	0.66978785257032	-4.49556626788894	H	4.05390948475360	10.14532033590477	-1.70267014600402
H	3.99163761362773	-2.17891701623721	-2.52351673648656	H	2.30214381115819	9.96708140022311	-3.46839775891782
H	3.69143859131785	-1.43197553439479	-0.93009858721379	N	0.42343796518437	7.34308495146545	1.02946356193878
H	2.32256757283065	-2.03910215877586	-1.90473536311034	H	0.55311367569624	7.21403665429640	0.03431183826066
H	5.18511109134042	-0.08757681592717	-3.40845390588883	H	-0.48595517727039	7.71125955399769	1.27982513869033
H	4.43466813361676	1.52026321240791	-3.14389415005262				
H	5.02441481450249	0.57830995985834	-1.75652775807957				

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H	-0.26789052325780	-0.72070365878085	0.90584706305241	H	6.10045879439835	0.41413518290722	3.59116637638103
C	-0.79367211665750	3.07229155322711	0.29334527662343	H	5.31197229712467	1.94441984583877	3.12982566681606
C	-0.15916393095322	2.09475041715454	-0.68253419311359	H	4.35647040848802	0.64504586120016	3.89967484132640
C	1.24580263583921	1.97681551007177	-0.13532056884972	Rh	1.19424710307379	3.55255111270582	1.24199607615699
H	2.10883624831158	1.93940952334260	-0.80672886527868	C	1.53995697869663	5.51381246304426	2.38453967500545
C	1.27103683604827	1.47138306750459	1.18602655361122	C	0.45170124366808	6.14841225441038	1.74599905758910
C	-0.12087898547971	1.24177972992561	1.74333109411609	C	-0.80480704647636	6.23871923959796	2.34069949637308
C	-0.74928461814985	2.61526846084584	1.60326863338303	C	-1.00749861258782	5.64659493271166	3.5865596973892
H	-1.33531979445313	3.07486788843594	2.40428715280725	C	0.02699059959196	4.98316101640672	4.23187701884213
C	-0.88992594861328	0.73895928871989	-0.58875448047450	C	1.32008267900926	4.92328198042968	3.67318522267847
H	-0.42042955847218	0.02881654824095	-1.28634476832608	H	0.61975043830818	6.64153762074743	0.78876099521234
H	-1.92691684244149	0.88377808652036	-0.93258229262292	H	-1.61479600669531	6.76028520496391	1.82851980733461
C	-0.86701632690168	0.20664571637687	0.86199734540316	H	-1.98895982372203	5.69664232807504	4.06513822734698
C	-1.65393939063659	4.17354306504491	-0.22936161625553	H	-0.13621440164741	4.52951771799378	5.21299262093807
H	-2.46933422663599	3.73352898367742	-0.82994513500187	C	3.48582313555537	5.37644905966688	-0.63835390059907
H	-1.08974917433303	4.84264899754707	-0.89782036827570	C	3.09486277927682	6.29049533893266	0.51250466247893
H	-2.09780438981995	4.76801385879728	0.57761673354718	C	3.67464928496160	4.01816776050992	0.03967019725764
C	-2.27294667433322	-0.13167945296971	1.38473076241539	C	2.95796084240571	5.50561559103137	1.81727049063906
H	-2.90159591953598	0.76687864978666	1.23383694280580	C	3.25091796808855	4.07226985568463	1.41525612909678
C	-2.88485772748143	-1.27490903684154	0.57926629340578	H	3.66371154684373	5.95524926923936	2.54309393567633
H	-2.91222089135279	-1.05556934374612	-0.49869535631949	H	3.73645971171839	3.37852055048804	2.10934803284635
H	-3.91644803063399	-1.48045242616369	0.90521244060611	O	2.96097977903495	7.48791305675194	0.42620880375096
H	-2.29973455672687	-2.19996678516892	0.71706169506456	O	4.13139464537743	3.04552536306499	-0.57286670038637
C	-2.28636482816651	-0.47310268769219	2.87149660224850	C	4.80971294485803	5.84809936746984	-1.23686829428289
H	-1.57399367466693	-1.28567706777964	3.09394454569303	H	4.70354007560567	6.85989093954481	-1.65186149689164
H	-3.28655790810029	-0.81338087701398	3.18212267025017	H	5.60016321445671	5.87126305886056	-0.47104584655701
H	-2.02123507426055	0.38783928238403	3.50273607982423	H	5.12408423190429	5.16079801376003	-2.03557191522151
C	2.41276097618203	0.76253827712681	1.85743015967991	C	2.36749536929639	5.23473372197554	-1.70346159161787
C	4.85615066177697	0.27005399183125	1.81375546218063	H	2.69968019013848	4.42458440348303	-2.37241917337006
O	2.19379644216460	0.11414542422181	2.88359473319561	H	1.45893722291838	4.87217673168047	-1.19288720557950
H	-0.04841749020946	0.91123109500709	2.78348054875478	C	2.04599169704095	6.46096524251655	-2.50821173786532
H	-0.16644049512347	2.48894712903048	-1.70750297736076	C	0.96529920255605	7.28306271481680	-2.16551169459063
N	3.62226579574837	0.86056290394991	1.27693188116589	C	2.80842091510890	6.80487972032053	-3.63344303102894
H	3.74762112945019	1.54005751645697	0.51699696263153	C	0.66569504054024	8.42488069988267	-2.90748451666996
C	5.17241650021308	0.85387652124342	3.19472998232961	H	0.33766979369775	7.01694323810581	-1.31116020564986
C	4.72273193677835	-1.25303734877566	1.88962898198728	C	2.51547620682229	7.94746789368411	-4.37673531197083
C	5.97554597572860	0.63138599607790	0.83948006593906	H	3.63782185498572	6.16091705644534	-3.93746323198384
H	6.92904346234428	0.21448416054300	1.19473674181934	C	1.44517761514927	8.76560755455985	-4.01292526409208
H	5.77115750119177	0.22290298945840	-0.16251454788110	H	-0.18499064983396	9.04949142411315	-2.62254010250983
H	6.08239350710403	1.72231671452217	0.74766655354608	H	3.12337240864054	8.19628140633880	-5.25063202852227
H	5.66626108234419	-1.69647512645331	2.24280953534826	H	1.21276112922133	9.66000050300260	-4.59670631066581
H	3.91751485198939	-1.54092366959217	2.57763414535150	N	2.35357066502551	4.41137939239753	4.40258664232615
H	4.49812154926612	-1.66630191022409	0.89405292521345	H	3.20117863660547	4.12758258806863	3.93130453419173

H	2.12017536055398	3.85092679363056	5.21294923280116	H	5.83550755022813	-1.40513955420676	1.88712760470772
				H	4.11790987730046	-1.33350747928418	2.37746948823323
<b>CR16</b>				H	4.55170432407193	-1.42422254750011	0.64809559639787
H	-0.17297370991635	-0.74796559974123	0.89889233501723	H	6.28780429457081	0.71095173615780	3.21355083604582
C	-1.00590803490417	3.01970243159559	0.52219832764465	H	5.40495424706918	2.21041177416407	2.83023694684713
C	-0.35335840645150	2.14624532557380	-0.53696138653125	H	4.56969495453346	0.87188878193671	3.67199116999224
C	1.08455845944726	2.10754897329474	-0.07212617096472	Rh	0.99955467229801	3.60060437402865	1.38933049108977
H	1.90939632387293	2.17441379307075	-0.78773478847077	C	1.29533832105537	5.52080040680081	2.61185951837964
C	1.22065228960416	1.53657795300410	1.21574695720701	C	0.16870181938681	6.09638379629567	1.98275723871684
C	-0.11728284587063	1.17680629511395	1.83290265660233	C	-1.08354614529393	6.11866860088457	2.59671222963178
C	-0.85161732795576	2.50405429313664	1.80114534079074	C	-1.24071556034800	5.50946682127406	3.83970401181839
H	-1.42327746358171	2.87758379362188	2.65575813294943	C	-0.16882102007072	4.88253118322276	4.46248564890635
C	-0.97476139864570	0.73455911921052	-0.48107545761533	C	1.11618004945112	4.88852510082849	3.88561276230656
H	-0.48866824806352	0.09909753035004	-1.23692036669685	H	0.29623208682686	6.60331388431747	1.02494497052696
H	-2.03575571799740	0.81524407251352	-0.76788588234117	H	-1.92535382374267	6.60302512152958	2.09983506629751
C	-0.83683323454116	0.13461347712436	0.93668486359410	H	-2.21674369401094	5.51048195766053	4.33178856138735
C	-1.97985159826160	4.06980736476246	0.10518779701584	H	-0.29928120111862	4.40390533133100	5.43659033951806
H	-2.77219480545941	3.59917334158798	-0.50296415276860	C	3.25796991372721	5.71409431338695	-0.40654026562029
H	-1.50301730189091	4.83513903878617	-0.52737240617854	C	2.80067363837024	6.50094687583515	0.81283733524613
H	-2.44806393353414	4.56240450489424	0.96527907742058	C	3.41850142139889	4.28956179589165	0.12296822850245
C	-2.18548267010048	-0.33073465335963	1.50999675834624	C	2.70741928456911	5.60032400732909	2.03786397655223
H	-2.88314513782640	0.52599766672839	1.43994270816733	C	3.02928098095757	4.21518743836084	1.50912485301445
C	-2.75721197115193	-1.47433169962368	0.67567251800585	H	3.40945450578612	6.00063104577420	2.79491215162767
H	-2.86259905113105	-1.20319667333128	-0.38562100018043	H	3.55790871719466	3.48764307870789	2.13404330705810
H	-3.75053897670080	-1.77503043260325	1.04395314582965	O	2.55250015306078	7.68322604694314	0.81021091928825
H	-2.09851772938408	-2.35768440084281	0.73039088675438	O	3.85400737615185	3.37792230789842	-0.59126280224119
C	-2.09477832124533	-0.74671526623982	2.97450519204068	C	2.23195139446119	5.80186879195521	-1.53247851725020
H	-1.32511610106394	-1.52480523154535	3.11529332246931	H	2.57382514301494	5.20791059373324	-2.39289810437179
H	-3.05417579130455	-1.16326269828357	3.31918196371953	H	1.25630167007242	5.40820619278700	-1.20495777786962
H	-1.84541917083070	0.09600133782299	3.63584594114980	H	2.10230130035215	6.84725704579210	-1.84974191158558
C	2.44606449897205	0.88276564569567	1.78928575932283	C	4.63149847681865	6.24646448556303	-0.87799076633192
C	4.90218883370660	0.52251429515074	1.54828856820922	H	4.93959376599317	5.62952457531298	-1.73605349687600
O	2.33943677833732	0.20418694278233	2.81367413391530	H	4.48325549891637	7.27660492660590	-1.23731285918814
H	0.03832245099287	0.80129601951629	2.84860554502131	C	5.68756347935288	6.21486517170285	0.19584087296778
H	-0.44779724831969	2.58935358479371	-1.53728484214340	C	5.87794341602695	7.30969492803178	1.04961186650359
N	3.60181111779659	1.06013839979923	1.12387364624876	C	6.46801034746663	5.06898398947197	0.39978678402136
H	3.63565031017557	1.78375639804978	0.39479682933908	C	6.81013433165152	7.25548063615932	2.08598042001883
C	5.31288297533127	1.11509016325873	2.90039241455253	H	5.28551607368099	8.21617186113768	0.89997184950471
C	4.84450490749050	-1.00525585067850	1.62343131859359	C	7.39827887630162	5.00980826399845	1.43625803244975
C	5.91519956118210	0.93528619248031	0.48226308189801	H	6.33475724684386	4.21124120367255	-0.26333246765567
H	6.91264829339148	0.55472184466579	0.74581705803314	C	7.57028907754624	6.10308758615040	2.28624334142345
H	5.63804286547349	0.52684435431171	-0.50214411148811	H	6.94426320867360	8.12117092127469	2.73995618820789
H	5.97151478188927	2.02993584984254	0.39607926556334	H	7.99385260692047	4.10401870421706	1.57851117973671



H	8.30013285424040	6.05971910420409	3.09880264757938	C	-0.84692225782622	7.06203641715675	2.52785218060383
N	2.18432110462701	4.39743960972258	4.58262779553083	C	-0.97718830364682	6.80508140687110	3.89327040746939
H	3.01843959570782	4.13213951384003	4.07634841577190	C	-0.24048094020877	5.78508232600227	4.48886512263133
H	1.98228446637677	3.80395880880872	5.37803289863903	C	0.65024104657052	5.00327636589473	3.73767902939540
<b>TS23 -315.32 cm**-1 ***imaginary mode***</b>				H	0.14618622071193	6.50572012053248	0.70951390188077
H	-0.15578286691190	-0.76135784031699	0.83808800031208	H	-1.42171430827545	7.85963420978420	2.05157649245753
C	-0.67901703785857	3.04110070757334	0.3284468353789	H	-1.65786991326772	7.40316097313069	4.50484328766827
C	-0.07750465960216	2.08211851087877	-0.68631763642999	H	-0.34347111320666	5.58104221411331	5.55873174926947
C	1.34123182367054	1.90878925343790	-0.19361539816460	C	3.41702331814461	5.33557128438440	-0.56284819168337
H	2.18463028935477	1.90348116177609	-0.89016327929524	C	2.82301073579946	6.12905112713257	0.59623128453789
C	1.40972558568552	1.38861673800833	1.10374822509387	C	3.75663922408297	3.99759808274129	0.09009057360503
C	0.03977112988466	1.17866256785157	1.71761915787400	C	2.67369387246729	5.24283228090767	1.81529568789804
C	-0.59115861620607	2.55479831766721	1.62472481860509	C	3.34599330472447	4.00198087314324	1.48540351658680
H	-1.15712533657219	2.99412018341775	2.45092100247526	H	2.89199475631307	5.73202391933756	2.76869095161273
C	-0.83211921679769	0.73622159735033	-0.59118336891920	H	3.83835188735545	3.35948907978167	2.22003524732201
H	-0.41150301629225	0.03425911248495	-1.32656979938369	O	2.60263913681420	7.31604418694223	0.57913151032936
H	-1.87991650351905	0.91415739583098	-0.88156108419352	O	4.33101933749016	3.09212780018644	-0.51264543933435
C	-0.75192290013652	0.16879033340014	0.84338633655402	C	4.71447458493579	6.00034272904679	-1.02514307747562
C	-1.55502223433767	4.15728977491200	-0.12421167225428	H	4.51173641256020	7.01441656708945	-1.39571355442281
H	-2.42543080422916	3.73730930979054	-0.65795223393508	H	5.43570636926444	6.07184407404439	-0.19662743000158
H	-1.03044900226402	4.81646204971547	-0.83244650444117	H	5.17023756724071	5.40740674092979	-1.83129179896854
H	-1.91913668153799	4.75794095245579	0.71921471798398	C	2.42242603669219	5.10903369189988	-1.72630372447805
C	-2.13407090947321	-0.17248382570565	1.42302553067032	H	2.87530439889357	4.33352806578834	-2.36433073829456
H	-2.75995382495576	0.73597809759632	1.33154581504157	H	1.49644860490828	4.68172617140822	-1.30583007214948
C	-2.79556120241853	-1.28428855292978	0.61322430356263	C	2.10281080810930	6.32178364098556	-2.55266957916032
H	-2.87973089068645	-1.02793374166147	-0.45353017519060	C	1.01762012750753	7.14700490519990	-2.23393470897586
H	-3.80926691634788	-1.49513636794680	0.98783765381263	C	2.88901252410595	6.65866057699925	-3.66286726435634
H	-2.21010774749887	-2.21628167838359	0.68805726868026	C	0.73354220242343	8.28364321202650	-2.98929296709288
C	-2.07529296787243	-0.56136620605361	2.89691417666394	H	0.38142793593881	6.89095221606150	-1.38360906423421
H	-1.36242124333367	-1.38832079451006	3.05577167302548	C	2.61040608862024	7.79532592269057	-4.42097992519510
H	-3.06214855846668	-0.90076648589744	3.24792245024890	H	3.72933642720119	6.01586944863064	-3.93953109185311
H	-1.76809111947990	0.27548962484578	3.54125859538741	C	1.53314067686885	8.61519107904260	-4.08355992348790
C	2.57843260539012	0.69545667220926	1.73785738700220	H	-0.11966031790425	8.91299370272874	-2.72314999175218
C	4.95445344171885	0.24278055444663	1.73729261785861	H	3.23652498978089	8.03903498007972	-5.28340563374510
O	2.41497530028865	0.02333278738624	2.75666794628732	H	1.31254477944387	9.50584868863625	-4.67756576543308
H	0.14921075862156	0.82851648068884	2.74791231109656	N	1.43584870664738	4.04825603954159	4.34920303260652
H	-0.11026664644205	2.49592851292175	-1.70252256750729	H	1.68960335572769	3.24830926172562	3.77668782300532
N	3.77697468612390	0.82212555116444	1.14279098796842	H	1.16910147515621	3.78708399146927	5.29188323113875
H	3.92424199983191	1.53540200800293	0.42080831446348	H	5.80616674438114	0.39901213174864	1.06288947230812
Rh	1.33005335182636	3.51542644221636	1.24183788948675	H	4.82284903005811	-0.83804359420635	1.89628166482482
C	0.78087327264140	5.25646876822892	2.34467066715127	H	5.19179522768732	0.69757480290608	2.71482819060207
C	0.035822238791110	6.29166459263116	1.77300083321172	<b>TS24 -316.02 cm**-1 ***imaginary mode***</b>			

H	-0.09067115954148	-0.81918570503686	0.85925507365810	H	-2.08232873455749	7.26023230090341	4.58924187050770
C	-0.85526135126884	2.96321880012186	0.53009950799151	H	-0.72311523458968	5.49989063559758	5.68987720999416
C	-0.22473842124563	2.09141689553375	-0.54341111379148	C	3.11272077145470	5.57605570498327	-0.32814879740824
C	1.21539643529046	1.98934870909752	-0.09729202875602	C	2.55591251319812	6.27145738197327	0.90965800682232
H	2.03540587904495	2.06975294100572	-0.81691571520713	C	3.49970429325049	4.20115008331982	0.20772200929207
C	1.35623924230866	1.41440528551464	1.17147456341022	C	2.43656818847433	5.28797170565321	2.05053569963383
C	0.02121754074793	1.09278281860313	1.81324973408997	C	3.14724528337474	4.10042460863617	1.61665986741734
C	-0.69339486432055	2.43007102150412	1.80030210434799	H	2.63893026250707	5.6984902540357	3.04419387985439
H	-1.26138909620072	2.7962552377180	2.66004292632781	H	3.68495426741979	3.42796145799969	2.28985451824482
C	-0.88290194640859	0.69357590033874	-0.49200264375402	O	2.31345808366111	7.45184791686462	0.98219933448593
H	-0.42590709603617	0.05481840347541	-1.26253659921827	O	4.06459054965987	3.35047187673655	-0.47964061165334
H	-1.94550411403234	0.80772744481503	-0.75942193092037	C	2.06010315459413	5.49634796312931	-1.43226844192823
C	-0.73610703037915	0.07563354168102	0.91632646528987	H	2.46225482668153	4.93150220216576	-2.28637808832653
C	-1.82203297732439	4.03210168300189	0.15531668885151	H	1.15076344813994	4.98621479411083	-1.07545795393068
H	-2.67599549006401	3.57328509842085	-0.37324745068601	H	1.78719375182565	6.50671320797548	-1.77145803129660
H	-1.37077675562207	4.76101667831897	-0.53496658787945	C	4.37037276894335	6.31296185649744	-0.84232752581813
H	-2.20248740784531	4.56610881690800	1.03557777233947	H	4.66627480204732	5.82930702993401	-1.78519415092805
C	-2.08419748050708	-0.36455735935099	1.50924143815870	H	4.06714822121772	7.34520551515530	-1.07686770436120
H	-2.76329071593137	0.50841460512023	1.46152622013104	C	5.53290121033389	6.31260661732944	0.11583509625952
C	-2.69611234271700	-1.48464909706010	0.67201014891207	C	5.64782946114444	7.28526900017279	1.11847035284050
H	-2.81622427120296	-1.19697972634657	-0.38332869346155	C	6.51906501068304	5.31957087515212	0.03681537271734
H	-3.68828564182930	-1.76807473488123	1.05629649040343	C	6.71089950208077	7.26010725020873	2.02132137400691
H	-2.05563134866330	-2.38237376248348	0.70242914657531	H	4.89718688332653	8.07663328479611	1.18742660768956
C	-1.97460215977660	-0.79947543682590	2.96695271380268	C	7.58348592392666	5.29263077836170	0.93657761984703
H	-1.21907084758920	-1.59509302254165	3.08406089448452	H	6.44393513798198	4.55511836369067	-0.74039647163055
H	-2.93595912755661	-1.19959384921104	3.32486323531317	C	7.68215711470930	6.26241887500980	1.93477257025183
H	-1.69559107671909	0.02981053843405	3.63349453372243	H	6.78449057345088	8.03038794352121	2.79356834758385
C	2.58388256292173	0.75987462158772	1.72995224219992	H	8.34356197796439	4.51097276905351	0.85453380674400
C	4.98424293930415	0.46627477007588	1.63207348846463	H	8.51788197712496	6.24468075223308	2.63918124178184
O	2.49598011474894	0.02288286483855	2.71275136369020	N	1.16764913384820	4.05270879098601	4.53968393341433
H	0.18259748210117	0.70463319197778	2.82312481602040	H	1.48799042388311	3.27353668041629	3.97191841644680
H	-0.31387564470422	2.54534281274409	-1.53879873843314	H	0.88222701128668	3.77142252257216	5.47091574452736
N	3.75149607749994	0.99579363566984	1.10765087537015	H	5.80904540125438	0.77844012612480	0.97882204613875
H	3.82460482285909	1.74773774533651	0.41323799025766	H	5.18786337571238	0.82993011350576	2.65390529728914
Rh	1.15516945476462	3.52727999694029	1.40108543333042	H	4.96125636269159	-0.63371743426593	1.66968760616332
C	0.52915143432861	5.23478652724230	2.51801338374821				
C	-0.23951465033587	6.23844127119941	1.91990425620149	TS25	-313.03 cm**-1 ***imaginary mode***		
C	-1.18384670732568	6.96404602139339	2.64311113634552	H	0.11226140816162	-0.63177707720291	0.08762183228673
C	-1.35194681335008	6.69656474767595	4.00279022354647	C	-0.81026052346127	3.11080561157812	0.48712792651856
C	-0.59052293821876	5.71129608298144	4.62473490822930	C	-0.06414001443514	2.50527402721470	-0.69065651032909
C	0.36162227212001	4.97316715047378	3.90479540617072	C	1.34416008693531	2.35830359706238	-0.16343223068659
H	-0.10455457793951	6.4544667195830	0.85837238890314	H	2.20510013395653	2.61532146622090	-0.78697777073565
H	-1.77868748209037	7.73501038006813	2.14789250914629	C	1.42116555526372	1.53560636532674	0.96669362960180

C	0.06070861840666	1.04199974338040	1.41964881796489	C	3.0464333474933	4.13539895369749	2.1031087114859
C	-0.71791012658182	2.32643028213571	1.62672144497958	H	2.36048619871262	5.47869732150683	3.70754447963104
H	-1.36131237815390	2.48415528156635	2.49679886037005	H	3.57649724976030	3.39536711112162	2.70728532621486
C	-0.65137864790634	1.10568293855926	-0.98393729757101	O	1.94628195823246	7.47340076440272	1.89805254858460
H	-0.10528206439300	0.66073747118050	-1.82914958481114	O	4.18760617284340	3.80507227593576	0.00875182537658
H	-1.69598741821927	1.23407243268532	-1.30921834343045	C	4.29415140197716	6.77783605479987	0.21975048845383
C	-0.57758706819282	0.21108264299577	0.27333458775812	H	4.00221242090295	7.82524258125708	0.06301821042254
C	-1.79026376781331	4.21043743802117	0.26950595840776	H	4.95085548255464	6.72817666376670	1.10212364157702
H	-2.59037468677760	3.84865064785540	-0.39983690002793	H	4.86314632287602	6.42961261540271	-0.65442156160368
H	-1.32371734416558	5.07561680006137	-0.22599545788713	C	2.15432159497365	5.85266009919787	-0.84171105631106
H	-2.24756905162776	4.54053470640124	1.21114957065230	H	2.71796065237017	5.27350735883010	-1.59051340812820
C	-1.94340874690162	-0.38433018783344	0.65114166583646	H	1.25389615839124	5.26654327073993	-0.59146066884694
H	-2.65756191051933	0.45847634848947	0.72112662879691	C	1.75748647486247	7.17820253690518	-1.42450004842772
C	-2.43308362116406	-1.33027305699028	-0.44203801192792	C	0.56052129613721	7.80269535472792	-1.05295804341980
H	-2.48122083579262	-0.83912590646583	-1.42557943243700	C	2.57725968803232	7.81770719907127	-2.36416354708842
H	-3.43845132440681	-1.71511346076456	-0.21066276186370	C	0.19703167936103	9.03548198813028	-1.59348165126455
H	-1.75505857019412	-2.19566072101481	-0.53375317578636	H	-0.09851439428262	7.31018581390467	-0.33349507752914
C	-1.92407627249077	-1.10186104291612	1.99716211260563	C	2.21989629589584	9.05184976469121	-2.90541725544117
H	-1.13796414796619	-1.87571123693938	2.01859300541788	H	3.50600956724877	7.33472652637060	-2.67986983098414
H	-2.88765483877894	-1.60115436558806	2.18318593327698	C	1.02826633504348	9.66669098942734	-2.51962247004475
H	-1.74280849699731	-0.41530826304384	2.83719663242883	H	-0.74361336200603	9.50406951765855	-1.29274582952898
C	2.63451175601299	0.83669778594017	1.50228916427119	H	2.87317477366161	9.53279419435371	-3.63832869863574
C	5.11104230850987	0.62095862219495	1.30313661859209	H	0.74438645569086	10.63211409944801	-2.9464663201634
O	2.51876476656740	0.04571251957665	2.43283152371769	N	1.08610939394617	3.31430784679322	4.77001338083326
H	0.16870816994462	0.45889687435628	2.33859606063770	H	1.44664881175615	2.70585417814749	4.04044790649083
H	-0.10639351444870	3.15478158423002	-1.57460552086338	H	0.82983948964235	2.80652451207461	5.60918458323749
N	3.80110810015448	1.10169482871397	0.86919112708381	C	6.08868242476400	0.75264046517917	0.12468130714763
H	3.85672339070406	1.98901696688931	0.35560617679115	C	7.4624833096247	0.59074213237064	0.34906071267735
Rh	1.10489416322455	3.53424614408522	1.62319517555064	C	5.64546380932601	0.93409367676769	-1.18751840425127
C	0.33370466310899	4.88961450596002	3.07782625408228	C	8.36844968681349	0.62783740646875	-0.70603391451920
C	-0.51169632633282	5.94746929660494	2.73184363698211	H	7.83144958179954	0.43242694672481	1.36495672366203
C	-1.49984416240843	6.40664116253590	3.60104876333208	C	6.55324755485931	0.96876320658651	-2.24825998419470
C	-1.63592870870464	5.80791867119367	4.85426643746630	H	4.58035288102609	1.03999803295046	-1.39763986185135
C	-0.79618781906418	4.76231415029933	5.22781134952937	C	7.91726187648835	0.81896055226314	-2.01394169855582
C	0.20233870352161	4.29264061644298	4.36091975168696	H	9.43575111525271	0.50391551385545	-0.50567239219343
H	-0.39862818286410	6.42693520681926	1.75844268960082	H	6.18300784589618	1.11286631188439	-3.26657721597232
H	-2.15314362198431	7.22930738874284	3.30134126006927	H	8.62744583139389	0.84663564256957	-2.84423936656566
H	-2.40133176778906	6.15768485227065	5.55206868360055	C	5.09270085859103	-0.88644697792464	1.57954022778035
H	-0.90155898381437	4.29297082679739	6.21044179749304	C	5.93939828021087	-1.46440343028556	2.52794671685309
C	3.05425136990816	5.90385232432366	0.41478481267710	C	4.32758625014595	-1.72701704135746	0.76215656849918
C	2.31729080905120	6.34613212537064	1.67409425949027	C	6.00163634744842	-2.85155966592319	2.67490607762590
C	3.50665588225993	4.48985266118006	0.77016105982658	H	6.56324151138731	-0.83179428724008	3.16220176264834
C	2.23349481690501	5.19871932236599	2.65816765470452	C	4.38606470693890	-3.10918138127632	0.90897477214230

H	3.68127206737962	-1.28932441531690	-0.00214377501788	H	-2.78489726891986	-1.56562170303213	2.81298701257095
C	5.22279040732141	-3.68013364299669	1.87065103663579	H	-1.61734150547534	-0.31611928117263	3.28223296020844
H	6.66815011078869	-3.28355901829179	3.42593291041200	C	2.66886511457878	0.78253401219921	1.57538561597675
H	3.77494940736159	-3.74734719686334	0.26527536181950	C	5.12551641484519	0.55871576629041	1.34341218259344
H	5.27003842419507	-4.76585738196751	1.98677808822009	O	2.58865741631431	-0.04585121811710	2.47722992182197
C	5.52142446835637	1.49208971787542	2.49839009173282	H	0.25231794837157	0.51198340967874	2.60857579556323
C	6.26359406065074	2.66352218170274	2.30980852984481	H	-0.23955632685706	2.78196343258085	-1.54679777925770
C	5.00674760709460	1.22749917508429	3.77522311397934	N	3.82407118771125	1.08434945933853	0.93899991270104
C	6.49464585278342	3.54273153448972	3.36675844462901	H	3.86197921230707	1.95311069984149	0.38827120056386
H	6.65125813750654	2.90759811990131	1.32019409854772	Rh	1.08460103091326	3.51896551349748	1.53194541804483
C	5.23436694088994	2.10744532041022	4.83208486700080	C	0.31583771510272	5.10093598896827	2.73776401205292
H	4.40258281822867	0.33393340945744	3.93125843351261	C	-0.40864106999309	6.14531833143816	2.15283878932073
C	5.98134527107142	3.26901827541685	4.63357053885295	C	-1.43661193977766	6.79321925055443	2.83390073707652
H	7.07583419564293	4.45219851224835	3.19358126561834	C	-1.73515334982961	6.40586000935576	4.14130507894365
H	4.82159440739545	1.88268142866310	5.81893076670111	C	-1.01860386481145	5.38058281321315	4.75203810971241
H	6.16057017844863	3.95848347534093	5.46242934814785	C	0.01743922590193	4.71985498673077	4.07357196876761
<b>TS26 -311.50 cm** -1 ***imaginary mode***</b>							
H	0.11703939916551	-0.81256210382753	0.49561459550999	H	-2.53288981405272	6.90702093899359	4.69588684013615
C	-0.86359069412611	2.93855715703269	0.53463528005376	H	-1.25318515431170	5.07727384798370	5.77660918897000
C	-0.14918409758670	2.22876932824287	-0.60311125346778	C	3.05515923660914	5.85030548947145	0.19129167301171
C	1.28139526096326	2.16911040555500	-0.12018245114712	C	2.46031134750226	6.36983420996193	1.49744352884359
H	2.11333878864031	2.38318005055152	-0.79710841016961	C	3.44009043827203	4.42147169445829	0.55435313911614
C	1.42650428887129	1.46159863091377	1.07983056423643	C	2.26143633823290	5.22737203260622	2.46705565357622
C	0.09612455640183	0.99610189840907	1.64020391519648	C	3.03044845354394	4.12766519533518	1.92040056279406
C	-0.70232053679819	2.28028368131341	1.74470525526730	H	2.37477476603155	5.48510791383804	3.52409422157221
H	-1.32051865407137	2.51061867629145	2.61716647039850	H	3.55190322881813	3.38453690303057	2.52745734443918
C	-0.71221365461088	0.79369403802348	-0.72385430422595	O	2.25110085207018	7.53221771679518	1.74446854004529
H	-0.18512355741367	0.27068598513307	-1.53581037681674	O	4.03980924675318	3.67335936917329	-0.21654898661694
H	-1.76965820173022	0.86658890531482	-1.02381931246735	C	2.01759357348599	5.90422827241897	-0.92987498724800
C	-0.57542704089940	0.03953646419862	0.61808804847083	H	2.44391277282524	5.46953625110868	-1.84610239915725
C	-1.88375580523920	3.98446142972873	0.24757464439443	H	1.11499040174546	5.32970378939955	-0.66447832254858
H	-2.69728227651076	3.53802574773440	-0.35078649828338	H	1.72835918843770	6.94616760498551	-1.13290582290740
H	-1.45950553356762	4.80741876478386	-0.34744666994658	C	4.31234897062426	6.65547740255944	-0.20816768402914
H	-2.31337392866996	4.39794950936033	1.16923709810896	H	4.55459804939924	6.39368021233638	-1.24852378838129
C	-1.91729257011819	-0.52161550345746	1.11685074335019	H	4.03058244345078	7.72028941250307	-0.19277513618114
H	-2.63764778676893	0.31881423692071	1.12673564523793	C	5.52139165093126	6.41296609282726	0.65776485400497
C	-2.44394243052706	-1.58334933753935	0.15542822837893	C	5.67266940873235	7.04478794529968	1.89941935592948
H	-2.54454510333959	-1.20106536043203	-0.87149130099792	C	6.51950122827827	5.52255328769898	0.23920805649241
H	-3.43218123346507	-1.94962747604954	0.47441679432418	C	6.78724380834354	6.79016798252253	2.69914057544952
H	-1.75983410144428	-2.44831391195354	0.12433472182665	H	4.91372618009921	7.75436506935888	2.23913178501788
C	-1.83334317790953	-1.08917678019809	2.53021745154846	C	7.63462594733343	5.26595144055953	1.03491852771225
H	-1.04315242393074	-1.85607582793482	2.59965883196771	H	6.41232475631589	5.01602459788579	-0.72314990958677

C	7.77215754372618	5.89997955324722	2.27016296472815	C	0.99551643877470	2.02405035392220	-0.48155150529984
H	6.89018891181098	7.29679654997701	3.66232666213134	C	0.54038175386651	1.72098560493476	0.93756566579366
H	8.39903214642799	4.56567601974974	0.68770980231142	C	-0.88973378718642	1.24286155662633	0.90766001611486
H	8.64651161025647	5.70344428772880	2.89590597807209	H	-1.62934431604218	1.63573991355086	1.59387776443949
N	0.77803264214894	3.76080374389000	4.70628682840698	C	-1.09851713472822	0.23445769887292	0.05939564063118
H	1.17170054292314	3.03794434805089	4.11040931142176	C	0.14795132081329	-0.20390162044247	-0.67729229224159
H	0.41320598201067	3.39894069166717	5.58006537221946	C	0.78619635168937	1.00729092773613	-1.31379524264925
C	6.15809809686230	0.97235510435545	0.28151094463066	H	1.07737959664728	1.01042740054506	-2.35654954452312
C	7.51324919924700	1.0888862053392	0.61154717935936	C	1.39299501779036	0.48666399676167	1.39685193008997
C	5.78293769830071	1.13275672405756	-1.05605728275948	H	1.1418422303622	0.23475132685150	2.42779708682312
C	8.46319767654922	1.38646178041195	-0.36316616295114	H	2.44537648200759	0.77542952140697	1.37994284974892
H	7.83602885214410	0.95373386345854	1.64548278468221	C	1.13518434717508	-0.70754608688680	0.4451793053859
C	6.73137863563363	1.43383672292945	-2.03276020024375	C	1.6509777576819	3.32659194988276	-0.79768950373139
H	4.73733800326416	1.02057032986587	-1.34780489472318	H	2.53889658139147	3.48104862816895	-0.17552444366306
C	8.07621221718505	1.56736941248456	-1.69121555965866	H	0.97783499359359	4.16657301763443	-0.59742248194599
H	9.51474775573242	1.47891050804603	-0.07961997855786	H	1.95621647229961	3.37534174820860	-1.84368483194282
H	6.41248101434419	1.56276758911596	-3.07024799269266	C	2.43827347461023	-1.31528715129194	-0.10294476303143
H	8.81980631377792	1.80571572614892	-2.45586511653172	H	3.02097626234046	-0.50174405169006	-0.55009479695855
C	5.15345291677700	-0.97459929800645	1.29049619136729	C	3.26460312377922	-1.92176360366382	1.03669159899842
C	6.16393502825995	-1.68761591565480	1.94503759772972	H	3.48652980882044	-1.19227000307779	1.81723788549130
C	4.26127336669533	-1.67919071219137	0.47680415802386	H	4.21526311325561	-2.30964812586971	0.66443045221289
C	6.26102312321400	-3.07212823510953	1.81470072830770	H	2.72625233289865	-2.75262330697554	1.50203839298319
H	6.89138122204032	-1.15966017470878	2.56499166829330	C	2.18813733061116	-2.37292009127129	-1.18052955377957
C	4.35618084901327	-3.06336214390820	0.34459568923867	H	1.50700148091213	-3.14755244562270	-0.81748997420947
H	3.48424106824546	-1.13795681032750	-0.06622230753346	H	3.12443438353956	-2.85857649323324	-1.46422320182485
C	5.35399297505861	-3.76878861170566	1.01683648424592	H	1.75382376758805	-1.94624565170548	-2.08493833675210
H	7.05540257299730	-3.60833196494238	2.34040365812317	C	-2.34527607758513	-0.55424952299943	-0.09058346239784
H	3.64247317973934	-3.59390028067233	-0.29114970476548	C	-4.79028283796578	-0.56838919611608	0.04371723493111
H	5.42766796413919	-4.85451815404570	0.91538996093450	O	-2.32262886013110	-1.73104287947027	-0.43143698910351
C	5.45041919888940	1.15244142125223	2.72231231126320	H	-0.08506778797841	-0.99771650981891	-1.37771067770806
C	5.90757956629422	2.47432427426473	2.80497389286360	H	0.68745613589335	2.56587083991790	1.60927832732349
C	5.17363020747744	0.47073901827752	3.91102175373557	N	-3.50912172799483	0.09425285150551	0.19678287896337
C	6.10143510461341	3.09272887602995	4.03774530258915	H	-3.48520999578056	1.09713069281613	0.25517604028450
H	6.10929577681717	3.03813415945294	1.89175695136619	H	-5.56099549630321	0.03399595869994	0.52293900306980
C	5.36785102290227	1.08665848524906	5.14793213534933	H	-5.05305053384522	-0.71655277047956	-1.00782419365939
H	4.78912525928588	-0.54791065962258	3.87190716854671	H	-4.75333167105722	-1.54678393129523	0.51956992630826
C	5.83516332343463	2.3980008247947	5.21781044555764				
H	6.46082541896673	4.12411816240516	4.06857554763190		<b>Ligand R=Et</b>		
H	5.14758278233063	0.53340839031521	6.06464937830430	H	0.70217874143319	-1.56085621370522	0.87332340524497
H	5.98942812161849	2.87798604727513	6.18760318988902	C	1.58066775358704	1.96508049971792	-0.35518252456693
				C	0.98217955800132	1.64321205315782	1.00539128531664
				C	-0.48333514505598	1.32767560296013	0.83558376654543
<b>Ligand R=Me</b>				H	-1.23143086447991	1.76802919562047	1.48295473352024
H	0.60672145019608	-1.49782678613234	0.98507186767575				

C	-0.72504273964722	0.39174950149991	-0.08379939425872	C	0.83980766445100	-0.12320718349726	-0.74099400729998
C	0.52625898197023	-0.14610446573141	-0.74296210727051	C	1.56216160525773	1.10674393019988	-1.23490054260097
C	1.33829979995552	1.01797962751178	-1.25772535248241	H	1.90847633416680	1.18623485945374	-2.25758035183435
H	1.71093609266023	1.04216932481128	-2.27393033163257	C	1.99622743455479	0.32944190920269	1.44659352825824
C	1.65866672880026	0.30250931334072	1.45783036056752	H	1.68123922625475	0.00387598054700	2.43868465823087
H	1.29724097883622	0.03055074590887	2.45020701453279	H	3.05937539352730	0.56924861940161	1.50516284371833
H	2.73335161509170	0.47458576714849	1.53893743667628	C	1.73729904762744	-0.76766960857812	0.38455715666021
C	1.35572761595900	-0.80911056426906	0.42280305310351	C	2.48174980448346	3.33629974512023	-0.47751676751485
C	2.38005082420436	3.20940823458510	-0.55002612760747	H	2.83766811044890	3.46278466350536	-1.50073833528615
H	1.77623891805795	4.10082889085258	-0.35071365882677	H	3.34424566413256	3.40232707300828	0.19423676606893
H	2.76501289939033	3.27928340762138	-1.56817059231692	H	1.82971695622844	4.18176143493960	-0.23483909911946
H	3.23041330935316	3.24610579211431	0.13923267664841	C	3.03731195797704	-1.39714456780984	-0.14530730024048
C	2.62687259217451	-1.53168067962971	-0.05760596725620	H	3.67876452730061	-0.58277187663100	-0.50141517083620
H	3.32447734794073	-0.76774614469984	-0.41971140682751	C	3.77414370366745	-2.12974991052371	0.98141097652022
C	3.29284814105034	-2.27439493572174	1.10587848196041	H	3.99103443820557	-1.47447769752871	1.82639556660514
H	3.53077915786346	-1.60935174782694	1.93751332437612	H	4.72243633910407	-2.53821612647711	0.62543762131871
H	4.2220944818143	-2.74893676773391	0.78348374295459	H	3.17213847780686	-2.96398421027499	1.35327168999337
H	2.63402484590749	-3.06035257515633	1.48677149506365	C	2.79235272256121	-2.35893589892688	-1.31071219300729
C	2.35099127393226	-2.50998880266824	-1.20214482622803	H	2.05702586299078	-3.12141763093307	-1.03933513188284
H	2.03453143580567	-2.00215258888990	-2.11347469748924	H	3.71760819146448	-2.87029846574587	-1.58541214410610
H	1.56636752352036	-3.22030737301121	-0.92730120799756	H	2.42544885007211	-1.84622054515767	-2.20010819049972
H	3.25023617261978	-3.08207740491894	-1.44109043737087	C	-1.69085768132500	-0.41792568395657	-0.30720213946714
C	-2.03118432932735	-0.24654886863153	-0.37672596447186	C	-4.15851521774042	-0.35637535133627	-0.18785132691433
C	-4.48032565362779	0.00566571685033	-0.37224398093915	O	-1.68312079323527	-1.57237076281422	-0.72245476283818
O	-2.10205335236661	-1.41115442622699	-0.75448009066666	H	0.61430085092357	-0.84381496473018	-1.51862960145005
H	0.27112233289971	-0.87587747188756	-1.50267990864350	H	1.36672688220885	2.41327755691720	1.80424612956995
H	1.16089562121294	2.43328382428127	1.73376122452081	N	-2.84215873359381	0.26263389600167	-0.06524477994755
N	-3.13454774903720	0.52933554032117	-0.19855822990749	H	-2.78038584940137	1.22493056872419	0.22031013708254
H	-3.00533435733622	1.49550320625836	0.04405071625429	C	-4.51340538394519	-1.15184290495134	1.06872336679517
C	-5.01985082499301	-0.68153883633512	0.87904511669566	C	-5.19318784871187	0.71637163743545	-0.50563075829301
H	-5.12565869986834	0.83597286627077	-0.66527769754271	H	-4.08731827429136	-1.05290212714762	-1.02525900741099
H	-4.45069430217527	-0.70329161115020	-1.20002259219323	H	-4.59157711542690	-0.49102833626111	1.93618077132175
H	-4.37820403750819	-1.51867099813233	1.15531904425606	H	-5.46981472868883	-1.66413446029010	0.94206133159770
H	-5.06595212917153	0.01266082465901	1.72106207335764	H	-3.74801652579080	-1.90134539723696	1.26902812449713
H	-6.02624293294458	-1.06634384916551	0.69868289490126	H	-6.18025746073937	0.26815394058858	-0.62589953645053
<b>Ligand R=iPr</b>				H	-5.26023421494198	1.44828150359702	0.30535358858645
H	1.14117827397628	-1.57075067584562	0.82594011195321	H	-4.94268805141128	1.24477063841848	-1.42708576250777
C	1.76525376114310	2.03893741613975	-0.30745076626396	<b>Ligand R=nBu</b>			
C	1.22203665405993	1.63640690860588	1.05444680632755	H	1.13324212206770	-1.57077537183655	0.73257956531227
C	-0.22329613969981	1.22921479027401	0.90880264032589	C	2.32675499160816	1.96796394094468	-0.13727199086562
H	-0.98109036530580	1.59609299618213	1.58987073146944	C	1.46634731769592	1.61148891930360	1.06496010019362
C	-0.42661670034601	0.30821371839148	-0.03465113112890	C	0.05437491800211	1.35365933809666	0.60124159428371

H	-0.79293616681587	1.79358371185081	1.11235603002128	<b>Ligand R=tBu</b>			
C	-0.02918157515542	0.46496979384272	-0.39009389930923	H	-1.39255343746208	-1.49854872704645	-0.97109814933641
C	1.312180692229698	-0.08714747172123	-0.82078296136545	C	-2.03857686142655	1.99834434031747	0.46242219488392
C	2.23827549214186	1.06870087796115	-1.11382286485958	C	-1.54351524982428	1.71534903840166	-0.94712728852978
H	2.80187806464890	1.12171190855978	-2.03669764110192	C	-0.08535990183861	1.33311847944362	-0.89157730960532
C	2.00829750160315	0.23131512153031	1.57595224515309	H	0.63663930539138	1.76893293227954	-1.57073182059587
H	1.45597950681620	-0.06919428151667	2.46701095931374	C	0.17676217350880	0.34725949675727	-0.03206358153473
H	3.05119319880407	0.36331556659031	1.86952198228272	C	-1.04959695400586	-0.16758808591892	0.6889241359694
C	1.88218792139126	-0.82568762989882	0.45116476539608	C	-1.77590099921843	1.00339989099439	1.30585802086996
C	3.18420726171648	3.1885706558389	-0.11117735499390	H	-2.08211724754690	0.99532942809422	2.34430511437701
H	3.88539736580811	3.16039223512280	0.72963529438666	C	-2.30636195165954	0.42461201820114	-1.40847878792328
H	2.57918566851690	4.09236356016277	0.01518842438257	H	-2.02561725650970	0.18331573723763	-2.43432613676516
H	3.76124272514440	3.28990589878382	-1.03118114628307	H	-3.37582035609011	0.64267998364631	-1.40666091739771
C	3.20331237369832	-1.57167441311985	0.19383345518094	C	-1.98260669998138	-0.74367594906519	-0.44475435208075
H	3.97970151087362	-0.81826929524550	0.01727394769203	C	-2.78112812573083	3.25799148420120	0.75836145737569
C	3.60211435414320	-2.39062839172732	1.42625322862713	H	-3.66928345370177	3.34878408381224	0.12408498526379
H	3.69350192749546	-1.77219212003139	2.32064772909138	H	-2.16131847674362	4.13807798606780	0.55797784395840
H	4.56062861896581	-2.88987549455105	1.26857896842215	H	-3.10174288302588	3.29635217497741	1.80017997525995
H	2.85502842198286	-3.16299258215133	1.63092783666999	C	-3.25021037913646	-1.43584011547489	0.08652712818503
C	3.13730749112435	-2.48381588456890	-1.03298511624452	H	-3.89674672229449	-0.66053505621426	0.51339076162524
H	2.29926439788761	-3.18245433943093	-0.95815709175173	C	-4.00789036354497	-2.11107184726761	-1.06225977228926
H	4.05382098913187	-3.07132293687962	-1.12185223627723	H	-4.26279778040094	-1.40738446752827	-1.85626125187127
H	3.01847305419303	-1.92139887353053	-1.95935080418356	H	-4.93688760386519	-2.56102708842421	-0.70548111782660
C	-1.26975743642809	-0.11651541155574	-0.95775179816201	H	-3.40168518413258	-2.90681137510463	-1.50480446009603
C	-3.66825584098801	0.21058305835832	-1.40431930382141	C	-2.94908792363065	-2.46278785137337	1.18064623484134
O	-1.29209447358666	-1.25712684946188	-1.40807863693000	H	-2.20604625135362	-3.18975132630718	0.84123446119359
H	1.19152006100284	-0.77507791578413	-1.64971978447910	H	-3.85447655523966	-3.01163176355765	1.44916324325934
H	1.51921995383664	2.36479237358363	1.85007312227440	H	-2.56692624917029	-1.99768180652863	2.08973257850556
N	-2.37148471289360	0.68085838867377	-0.94152290778803	C	1.46949117968626	-0.36604668557692	0.13186680836515
H	-2.26715551820126	1.63189775933404	-0.63728579741995	C	3.97527635148097	-0.10507430030734	-0.02811537077004
C	-4.43243533885215	-0.59879728190332	-0.35618633427493	O	1.49595671984491	-1.55613744524190	0.43005514724457
H	-4.24833401788394	1.08629797091272	-1.70484728979605	H	-0.77749216919845	-0.94029683569529	1.39885509309617
H	-3.50237022385701	-0.40371743142494	-2.29002900036728	H	-1.73550984836051	2.54392702688820	-1.62783263295328
C	-4.78322959550347	0.19242128280757	0.90141934457639	N	2.58385345445748	0.38164233232900	-0.08709060854211
H	-5.35038885005272	-0.97418454021337	-0.82131295799105	H	2.44719083401968	1.37312542430862	-0.18401132473636
H	-3.83462537641926	-1.47541516961281	-0.09313137755253	C	4.30142883577971	-0.61243434321242	1.38284287267978
C	-5.54973372752306	-0.63782778654912	1.92852822708478	C	4.18443142655432	-1.21748350719301	-1.06259622649234
H	-3.86393732939638	0.57297542630593	1.35680165496485	C	4.86235593150314	1.09398297133905	-0.37121910324471
H	-5.37767298241608	1.07091677571526	0.62396176426177	H	5.91302770368290	0.80452134674435	-0.34386108210207
H	-4.96490127642741	-1.50452559093940	2.24629142333638	H	4.64129984532311	1.46990304376535	-1.37295082584512
H	-5.78849604640578	-0.05233296001225	2.81883199597646	H	4.72000370869244	1.90629660511405	0.34645697124105
H	-6.48961241379159	-1.00963550035792	1.51257554693377	H	5.22435124812027	-1.54986034702276	-1.04561039986179
				H	3.54170427645113	-2.06851814732731	-0.84764778748227

H	3.95659525301495	-0.85257850367914	-2.06604453186547	C	-4.35544208204960	1.34258908590573	-1.83228371395968
H	5.33911725535924	-0.94933783324489	1.42912976527033	H	-5.64976705758919	0.10971049773835	-0.62433591448523
H	4.16646062066957	0.18489236222476	2.11669266997583	H	-4.71021251993995	1.26008429304993	0.29709333494925
H	3.65139042155303	-1.44368602883306	1.64856227867912	H	-5.09988793411223	2.12130766124091	-2.00831154764430
<b>Ligand R=CHE2</b>							
H	1.78554457096258	-1.72287167025837	0.51099772594154	H	-5.02098912822585	-1.96439022204309	0.56398920680423
C	2.13928573366302	2.07267216178613	0.08241697758407	H	-3.33930441620854	-2.28420957981160	0.93861571489145
C	1.66350881421254	1.38478047993050	1.35242311395885	C	-4.25994145599441	-0.83127889264439	2.23780109575409
C	0.24129643113683	0.92122624319125	1.15716309631776	H	-4.52118142154588	-1.57539778946820	2.99224779761120
H	-0.51801352036193	1.10952579538320	1.90596303089511	H	-3.33622125958452	-0.34781119183239	2.56400172163893
C	0.06533950328482	0.18370808267194	0.05985719404231	H	-5.05151890791641	-0.07914390574214	2.23367703726055
C	1.33401585473109	-0.02475005899283	-0.73832389693789	<b>Ligand R=Cy</b>			
C	1.96321908846419	1.32246252162652	-1.00235078187847	H	-2.16294845032705	-1.42525515463190	-1.13190042165471
H	2.27263344366070	1.61653001526370	-1.99731698087981	C	-2.69084141230938	1.92565294983009	0.65634867891634
C	2.52591781836357	0.08094737548070	1.47469759059261	C	-2.27802712044424	1.77394635751350	-0.79941918736640
H	2.25682267235198	-0.44815404560580	2.38957088991741	C	-0.82288110013027	1.38201479581010	-0.86090983858829
H	3.57366858529762	0.37317371452786	1.56403411907744	H	-0.13365789855488	1.87852575618719	-1.53226456824995
C	2.30817313536609	-0.80644996561109	0.22408720581793	C	-0.52327801180495	0.31836530756912	-0.11375954000725
C	2.77093187888702	3.42256572408598	0.15087906272893	C	-1.71293978544624	-0.25726212319160	0.62232878519850
H	3.08163384192379	3.76717602912259	-0.83623514515669	C	-2.39122166920025	0.85468104233855	1.38686744636361
H	3.65197029945558	3.41416153924509	0.80145215690933	H	-2.63802295213444	0.75045024678083	2.43587820151159
H	2.07918601699875	4.16080104790982	0.56958158148525	C	-3.07829163669833	0.53625080197633	-1.33580217729902
C	3.63411531876256	-1.21929109002943	-0.44010730755786	H	-2.85688187486283	0.39061715035948	-2.39371956401784
H	4.21073001083124	-0.30514084941489	-0.62223176295960	H	-4.14351605535963	0.75946527759570	-1.25413963822414
C	4.44495225932848	-2.11598291431943	0.50156230155565	C	-2.71434857964734	-0.71920700742582	-0.50520607983972
H	4.64292941547068	-1.63516551085700	1.46105545147865	C	-3.39926727980520	3.15744266593191	1.11126067156349
H	5.40757056598619	-2.37779505566254	0.05681336172393	H	-4.32004745889065	3.31697541785402	0.54011630021997
H	3.90743392094365	-3.04759909289397	0.70149869196900	H	-2.77923092082430	4.04732988533015	0.96085862707949
C	3.42829248108532	-1.93001340793932	-1.77971887245656	H	-3.66131594264442	3.09913118564071	2.16845578991499
H	2.75417781662019	-2.78388435976882	-1.66934523024375	C	-3.95779254336727	-1.44985533791391	0.03141999063669
H	4.37968319014913	-2.30365534639629	-2.16477791513849	H	-4.56592525142543	-0.71496680933603	0.57133977880351
H	3.00593667541263	-1.26887343973274	-2.53686484262945	C	-4.79393891865685	-2.00212313184608	-1.12808692498749
C	-1.17091207860449	-0.53584688593279	-0.33507695386472	H	-5.70328241598977	-2.48132971564819	-0.75892391527431
C	-3.64594287604077	-0.53721831505461	-0.25385810503043	H	-4.22708371271641	-2.75224073989321	-1.68747441978010
O	-1.12291198535317	-1.59823119388036	-0.94641583145908	H	-5.09167614612602	-1.22127403143498	-1.82978117343008
H	1.12912216891963	-0.59806408291754	-1.63529897338303	C	-3.60512892407003	-2.58069193822964	1.00010290608420
H	1.78337558033118	2.01321370932974	2.23411561667435	H	-3.15748209765685	-2.20843282314136	1.92184539902724
N	-2.34175928372177	0.05421383431498	0.02387284118167	H	-4.50066123481109	-3.14284505805542	1.27403441748867
H	-2.29915212942940	0.96388229104009	0.44991640475830	H	-2.89823083928908	-3.27973830999174	0.5447225591368
C	-4.08447746704942	-1.48834656184266	0.87073818733139	C	0.77514734358114	-0.39822445275309	-0.0748566604072
C	-4.66028496900793	0.56903536228629	-0.55134885511731	O	0.83073161253058	-1.60654611425308	0.12847019714055
H	-3.51075391191085	-1.14117730615435	-1.15371110613699				



H	-1.40911439645386	-1.09374008182239	1.24140157953602	C	3.85439534791821	0.60171122533839	-2.17113240744542
H	-2.49879470765202	2.66369461647756	-1.38789720846342	C	3.84162688798085	-0.93405374956176	-2.11371038674416
N	1.88245932635508	0.36126388805483	-0.30064070560101	C	5.16311934810515	-1.56221659494604	-1.65234414530814
H	1.77780422047704	1.36178562799697	-0.26829303200470	C	5.54980625175772	-1.24197262712354	-0.20247916419628
C	5.18499609751007	-0.86643321767397	1.19021226561960	C	4.59714576927971	-1.81313612712703	0.85354504483272
C	3.75947545711363	-0.31153079069085	1.17142953558705	C	4.78332645821029	-1.19599168886947	2.24647545420497
C	3.22905917246517	-0.19039432236699	-0.26186579848593	C	4.28365413302627	0.25120413828618	2.34996052083316
C	4.16315439093367	0.65331456870647	-1.12853331061492	H	-4.39613878599131	2.03807398187591	-1.87162496125767
C	5.59271470851390	0.10742422266890	-1.10432753136922	H	-1.90644829065233	1.91348580797659	-1.98774635158460
C	6.12370165613429	-0.02291508088754	0.32501106163461	H	-2.31853285287677	-0.72574493047291	1.33275638236103
H	5.17437746641234	-1.89598752030811	0.81534283947999	H	-4.01823281155246	0.90056331998252	2.23480093995924
H	5.55399073938114	-0.91453986152606	2.21774598586152	H	-4.09967875894719	-0.39154256718629	-2.43706403888549
H	3.74340826861656	0.68129030861919	1.63695323111793	H	-5.44656141426789	-0.18566881367436	-1.32618281054988
H	3.08582338638419	-0.94961480885685	1.74536145382957	H	-2.93978294329454	-1.68384446973525	-0.90258997190464
H	3.15758022179232	-1.19551000441702	-0.68354803682668	H	-6.33408414782490	2.51458130680893	-0.00653880917383
H	3.78104910102998	0.68784352060809	-2.15188235319318	H	-5.64536452143266	2.79215676401799	1.60020523666183
H	4.16463761240131	1.68474900471481	-0.75243103610257	H	-5.05651597372692	3.70224510386456	0.19977031980327
H	5.60712166525721	-0.87656717829162	-1.58599115620249	H	-5.45284061907057	-1.35378362948365	0.75682175970810
H	6.24644117320914	0.75272710606906	-1.69652824166495	H	-3.13835233563539	-3.32518491716796	1.10300555896392
H	6.22127768927379	0.97601701367279	0.76601504466378	H	-3.68975995276306	-2.13720335516728	2.28400800843104
H	7.12606984792655	-0.45876542371892	0.31502126209653	H	-4.71802008223902	-3.50420403327236	1.87200705723145
<b>Ligand R=Cy12</b>							
C	-4.38421031153280	1.66697653405907	0.27815208272833	H	-4.55395925271417	-3.59980064599997	-1.11789702754252
C	-3.93947125069536	1.36731799919094	-1.14485047595236	H	2.04865871515602	0.07420675424756	-0.27312492131260
C	-2.43285136988604	1.38309000857522	-1.20425513548027	H	0.05786307931600	2.16238318844538	-0.81090635259071
C	-1.85355802609138	0.60003775568780	-0.29308835422444	H	2.20415751039990	3.07898665885691	0.16094306646545
C	-2.83979599856000	-0.13240755026891	0.59027665102778	H	3.61977044465357	2.06439674034325	0.22705950392895
C	-3.80409852960701	0.87223578633101	1.17386363858016	H	1.15667750947310	1.78827656148716	2.01653878519518
C	-4.36068509883000	-0.11915965573926	-1.41373691512989	H	2.66945825994460	2.53570113473057	2.48235071691750
C	-3.66788691399971	-1.05066176847543	-0.38844035049896	H	2.30781765519862	-0.40075445099109	1.71977502036457
C	-5.40683499447244	2.72162316382644	0.53819642229912	H	2.37545024730513	0.19690945990185	3.34703386267182
C	-4.66276242756236	-1.98072847963543	0.32776298716992	H	2.49213187904534	2.28354911353263	-2.31516598769217
C	-4.01343859328534	-2.77682567716035	1.46253572387244	H	1.77213710772505	0.73277594525622	-2.72101983975533
C	-5.30884094519485	-2.94420817532456	-0.67373010641486	H	4.50411269159169	1.00150002821680	-1.38988066388610
C	-0.40867030205305	0.27997168759465	-0.19581625206698	H	4.30162016658444	0.92268926678720	-3.11603486790704
C	1.89192975809145	1.09590812025643	-0.60812426976145	H	3.58931265935837	-1.32138577522519	-3.10517747933033
O	-0.02838012791380	-0.81209294448340	0.21710078077848	H	3.03790866007949	-1.27471837132097	-1.45806353720060
N	0.44504790688864	1.25775408394736	-0.59991559764778	H	5.96947716744835	-1.23065846146904	-2.31561427660336
C	2.54077514719483	2.06102930271173	0.39031283696788	H	5.09720594884318	-2.64862795168630	-1.77296760460031
C	2.23813260135264	1.74431390778094	1.86010564159243	H	5.62424318678133	-0.15830924174312	-0.08409167688884
C	2.75353277667432	0.38079194779213	2.33707809355754	H	6.55724763830921	-1.62499591781199	-0.01111988228425
C	2.46118440772555	1.22594304836313	-0.202944730399650	H	4.74384544135209	-2.89607646650897	0.91195149497268

H	3.55993082636308	-1.67472569259236	0.54168463107044	C	-5.66587004960847	-0.73786516950238	1.49959428597427
H	5.84419498111897	-1.23534599820573	2.51612737738253	C	-5.93733562791662	0.44613583836606	0.82825298884650
H	4.25708561625955	-1.80775249882895	2.98644955536629	C	-5.07285332337378	0.89516290505629	-0.16534111050305
H	4.71622161731871	0.83137003234589	1.53157831650916	C	-3.93478283430469	0.16804832851457	-0.49988487244492
H	4.67207993091841	0.70695037014308	3.26572218936305	C	-3.67020435535279	-1.02332193354289	0.17843490099682
				C	-4.52942995533494	-1.47193455211874	1.17083356878519
<b>Ligand R=CH2Ph</b>							
H	1.65922895776630	-1.72877053887796	0.31770384988980	H	-6.33619640750918	-1.09062673458650	2.27324378036818
C	2.95461483936814	1.88125400943611	0.37561244876430	H	-6.81983207138551	1.02249327285129	1.07655202272998
C	2.00752913306872	1.28487878180709	1.40506731509927	H	-5.28864052136164	1.82054005382305	-0.68769388972447
C	0.62731272523111	1.18449499819299	0.80541866459327	H	-2.79020073428742	-1.59851005905799	-0.08244007362715
H	-0.24788912972814	1.51565351007401	1.35051021860133	H	-4.31675629707335	-2.39961795865854	1.68753203858354
C	0.59976851779614	0.55018228263914	-0.36768391385590	<b>Ligand R=CHPh2</b>			
C	1.95858527805680	0.07152173398611	-0.82972052347106	H	-3.06032921533056	1.32899185598339	-0.90417204710501
C	2.92004282587155	1.23473253613342	-0.78681426542786	C	-3.46307887764370	-1.61239266688716	1.52491917513922
H	3.54790630805059	1.48073578472168	-1.63373880889497	C	-2.94277515655926	-0.23536216181252	1.90618909144333
C	2.48886388811358	-0.19318290953009	1.61560795870255	C	-1.52528650643663	-0.09259971927331	1.41222240228234
H	1.86633625855557	-0.67302017286929	2.37155480163983	H	-0.74551059621187	0.30064210897510	2.05275966650640
H	3.50892250237219	-0.16681121605734	2.00278718132589	C	-1.38128217006788	-0.37086702347489	0.11532215040114
C	2.43165913361792	-0.95664157675459	0.26888504378871	C	-2.67319093954732	-0.76358086372954	-0.56707670243779
C	3.83013050824782	3.03314679467882	0.73967480830179	C	-3.31980859685973	-1.87259104011838	0.22785833226694
H	4.46603355487436	2.78851849242640	1.59710235024488	H	-3.66024495827831	-2.78409650599882	-0.24683301054830
H	3.23465599553599	3.90502947762554	1.02941913014960	C	-3.79127889741220	0.78470191918521	1.06964654266784
H	4.47574396783423	3.32132724031737	-0.09080372520371	H	-3.49004021086775	1.80157422406097	1.32343325180723
C	3.76121419190242	-1.65460060611956	-0.06827259195928	H	-4.83778373029763	0.67313531679549	1.35878364135994
H	4.55565695580179	-0.90231638754331	-0.00399613588732	C	-3.60511984097209	0.50183309484723	-0.44146559508589
C	4.05807859824229	-2.75420475820567	0.95708953633787	C	-4.09034635523350	-2.48823204484898	2.55699586573996
H	4.07429002427542	-2.37137300567053	1.97876721435331	H	-4.94666772330127	-1.99388551830698	3.02790358919282
H	5.02674963243845	-3.21904500158023	0.76113250511843	H	-3.38168308084507	-2.71863304564925	3.35913046262708
H	3.29696227534149	-3.53832157887874	0.90799651451580	H	-4.43557313882080	-3.42858092120205	2.12560617008623
C	3.77789057118156	-2.24584495103532	-1.47986177547600	C	-4.94585844603101	0.35917941146482	-1.18346948923485
H	2.92408540044059	-2.91095788103695	-1.63607172547373	H	-5.54032788477808	-0.39230760226303	-0.65122313222256
H	4.68806545393520	-2.82806926748691	-1.63964219298678	C	-5.71356655361643	1.68518642631054	-1.15427030430821
H	3.74378356806906	-1.47483508406288	-2.25008066234574	H	-5.87896404267881	2.04301905252672	-0.13675376870050
C	-0.61295102600026	0.14059562599180	-1.11443330035093	H	-6.68971952817793	1.58073698837848	-1.63288218954610
C	-2.98561066546856	0.65974325117849	-1.56739031452434	H	-5.16037672645642	2.45994386933782	-1.69307626482987
O	-0.64597978678502	-0.90801166442022	-1.74989454877040	C	-4.77374093577364	-0.10568352557940	-2.63158435634300
H	1.88715329973108	-0.40365550071889	-1.80144771335819	H	-4.08413919742737	0.54794890338124	-3.17289123196297
H	2.01821297646941	1.83396985584598	2.34577525258750	H	-5.73214149730438	-0.08605720974586	-3.15503612322209
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H	-2.82629201368103	-0.10984452677256	-2.32228013285888	C	2.28747582532518	0.12984946619118	-0.60803279697980
H	-3.40418399461345	1.53755105716937	-2.06308300267426	O	-0.23458444781505	0.17617322736143	-1.87656761530914

H	-2.49474336544661	-1.01352737568751	-1.60662744588923	H	-4.16296338996146	4.24358029426490	0.45098884716254
H	-3.03796817552705	-0.03680421842800	2.97296346766665	H	-5.10719290142183	3.41045858947161	1.69605378063369
N	1.02348716727415	-0.33188269293263	-0.04930157468860	H	-5.67620818076571	3.46231606180524	0.02042935108388
H	0.99019752065493	-0.52778406792148	0.93756168565990	C	-5.27385123908323	-1.33305706102936	-0.00661404123479
H	2.06131883697180	0.33929683545956	-1.65465230027438	H	-5.91791061981244	-0.55705892750032	0.42270993169818
C	5.38873323473468	-2.87766125452210	-0.56534436239975	C	-6.03538322965223	-2.00497718203004	-1.15482927713303
C	4.07829127291710	-3.23228814339957	-0.27923284767025	H	-6.29208989388254	-1.29942115196855	-1.94659138318217
C	3.07443352721206	-2.26877379289658	-0.27996276597645	H	-6.96369559682846	-2.45482085336596	-0.79628576062368
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C	4.68765955401922	-0.59156833017326	-0.85327825829602	C	-4.97180370882412	-2.36216615819859	1.08517131319215
C	5.68909055444462	-1.55093201884346	-0.85683694216918	H	-4.23185142625786	-3.09077254067542	0.74253285901403
H	6.17063429721089	-3.62644100119200	-0.56390948150463	H	-5.87772501594153	-2.90899075796458	1.35581818016576
H	3.83038828063785	-4.26273216427747	-0.05687264977342	H	-4.58510892604997	-1.89959519684015	1.99354690067590
H	2.05328008669535	-2.55776184651020	-0.07248518482152	C	-0.55570987403093	-0.26789998059654	0.05468312566483
H	4.93353527587011	0.43984608248969	-1.07206838779213	C	1.95488202232002	0.02923436165116	-0.02728046621400
H	6.70744352121992	-1.26250077085090	-1.08562610331899	O	-0.52307547066846	-1.42997919105150	0.43382871333058
C	3.25051042978121	3.85292590529621	1.34371123811849	H	-2.80011098300615	-0.83630538252665	1.30495455792836
C	3.58888423367114	2.64602587629898	1.94649027612501	H	-3.74958033274804	2.64110364282029	-1.73170542982116
C	3.30878631089155	1.44560129200317	1.30769470783265	N	0.55971188233474	0.45663851513892	-0.25168567878160
C	2.68359061632920	1.43491791827423	0.06164254450072	H	0.42535896621693	1.44070524144276	-0.40467660141371
C	2.34658587542064	2.64689956526146	-0.53478978140182	C	4.30664290578853	3.64933503390936	-0.50005888086381
C	2.63015101937178	3.85025463802573	0.10054205428182	C	4.42971394532164	2.90072499902544	0.66071248953929
H	3.47428498781981	4.78953326904685	1.83856459774046	C	3.67589211339379	1.74382581419106	0.83848749414627
H	4.07774271860958	2.64087540456931	2.91280099625010	C	2.79118703424246	1.31854094446087	-0.14526339413422
H	3.59420057468568	0.50985781099867	1.77315848584011	C	2.68816618198879	2.06911841441198	-1.31987364227463
H	1.85218228362067	2.64466010675192	-1.49859604921431	C	3.42993631291708	3.22686113029899	-1.49414613428888
H	2.36663644379641	4.78581220219729	-0.37676677662326	H	4.89209222476992	4.54986667697120	-0.63508736260929
<b>Ligand R=CPh3</b>				H	5.11534511038896	3.21324527567798	1.43834953682601
H	-3.41780184210237	-1.39891771721997	-1.06544863090483	H	3.78526890973820	1.17298738697321	1.74845811082497
C	-4.05300715772346	2.10321775984199	0.36080941725575	H	2.04178385428327	1.72503984744803	-2.11777073475438
C	-3.56035044215953	1.81392404423951	-1.04869089500498	H	3.33496797458211	3.79297617383958	-2.41229499482079
C	-2.10364106479639	1.42749282584797	-0.99260225420433	C	3.39419477339729	-2.68802328725482	-3.09219811315183
H	-1.38155848114668	1.86500791322283	-1.67063152605573	C	2.03038537248463	-2.53572459313286	-2.88712666514369
C	-1.84475953868379	0.44397582363939	-0.12905170453338	C	1.55501393436430	-1.66655514995629	-1.91083898801946
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C	-3.79437174977624	1.10939150382502	1.20670771605324	C	3.80680740107036	-1.08657286732178	-1.34414659221807
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C	-4.32874114478585	0.52472463947039	-1.50486726693020	H	3.76185996255145	-3.36547920030039	-3.85254678187262
H	-4.05295490883932	0.28017767754659	-2.53130528062734	H	1.32499529437359	-3.09874414707505	-3.48558288817028
H	-5.39724647052578	0.74694518300496	-1.49967483761269	H	0.49188049315249	-1.58396652344920	-1.75630105563107
C	-4.00621272819813	-0.64227819091735	-0.53926419986135	H	4.51155941960201	-0.51572203587387	-0.75450418184340
C	-4.78797374241999	3.36785022183399	0.65399621494440	H	5.35092610043928	-2.05996693926263	-2.46283738057166
				C	2.30643984369225	-1.59384336800917	3.98148171126845

C	2.88052039406240	-2.26729726171876	2.91427295852170	N	-2.07846909170016	0.47478719366533	0.03517613874449
C	2.76468545906410	-1.76759571321402	1.62085485461061	H	-1.87955334240183	1.45431105211847	0.15266005202486
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C	1.49778095571317	0.08089094952940	2.45512298211996	C	-5.27596294530245	-1.41108550378721	-0.11898169472276
C	1.60870316481545	-0.41411894864866	3.74406035918228	C	-3.90745455707917	-1.17236267209539	-0.1286335323318
H	2.39234986110615	-1.98564288190610	4.98711094957311	C	-3.43972282092677	0.13561375428705	0.02262653874722
H	3.41558829447656	-3.19394619759192	3.08030186462520	C	-4.35864082457653	1.17843761916256	0.18030012574181
H	3.20280639596904	-2.31910003578556	0.80299509325420	C	-5.71986193635710	0.92368081655293	0.18752665352157
H	0.94762652293610	0.99722304365506	2.28499976007491	H	-7.25238253521611	-0.57846905225036	0.04192057439521
H	1.14648717038967	0.11930554991033	4.56537018492695	H	-5.62856124093134	-2.42808983061797	-0.23742022098345
<b>Ligand R=Ph</b>							
H	1.84019609991967	-1.49310790284040	1.01935207039268	H	-6.41489295514884	1.74463038352869	0.31059714108548
C	2.58037153485720	1.94355311069179	-0.51482030484619	<b>Ligand R=Ph(Me)2</b>			
C	2.06138854843230	1.71616495900496	0.89659262907465	H	-2.14969018185345	-1.70986461381898	-0.50493275589217
C	0.59634171291152	1.36604567198533	0.83200858163082	C	-2.89539939418299	2.02424458033759	-0.04963126380981
H	-0.12175371221373	1.84118253668615	1.48903212900014	C	-2.42685578195919	1.38116429481315	-1.34581819702663
C	0.32303656065221	0.35887059022633	-0.00056529748905	C	-0.95511579049658	1.07184051035924	-1.23936122378461
C	1.54695439112129	-0.20695716142391	-0.68632070532082	H	-0.26769286719739	1.32691379160933	-2.0359332930672
C	2.30647284178352	0.92829743747949	-1.32976561763971	C	-0.63429858711883	0.36674823045904	-0.15214687636038
H	2.62467360048803	0.88025936530856	-2.36336980308899	C	-1.82086157013199	0.03186905239292	0.72349007127768
C	2.78754188168753	0.42363937768710	1.40950521732563	C	-2.57616069819860	1.30464319612812	1.02295922828708
H	2.48637769279933	0.22104664683563	2.43781601752741	H	-2.85580861311807	1.57089099165672	2.03437309975098
H	3.86121295062920	0.61871135912638	1.41720404281423	C	-3.15213194545965	-0.00840250280491	-1.41047411049441
C	2.45211032672905	-0.76689643584191	0.47764281438395	H	-2.89225890424666	-0.51194346372268	-2.34225312441340
C	3.35253721938749	3.17790857478472	-0.84006555417656	H	-4.22821632147295	0.17234667070660	-1.42769962738910
H	4.23398683434181	3.27081333173269	-0.19695606089107	C	-2.75670491103223	-0.86068533110770	-0.17903457662293
H	2.74823575565631	4.07606521333014	-0.67617821458290	C	-3.67060934535227	3.29866920175016	-0.08264804679049
H	3.68720268999251	3.17653854683036	-1.87807344581787	H	-4.57928685095023	3.19177092874525	-0.68442278725446
C	3.71202769025772	-1.50058972384396	-0.01544963346526	H	-3.96230535966798	3.61380968784217	0.91992742575663
H	4.38077059715754	-0.75130975039121	-0.45436948911870	H	-3.08552534854094	4.10394615210532	-0.53873177033872
C	4.43883020374864	-2.15850615099533	1.16284797188839	C	-3.97845351916327	-1.42606405971872	0.56548371547785
H	4.69773319991027	-1.43808088541780	1.94043602746904	H	-4.63813533854354	-0.58462523743494	0.80720685745905
H	5.36287845991876	-2.63743217891178	0.83217589730140	C	-4.75272910411356	-2.39455386690248	-0.33516260805468
H	3.80999359455030	-2.92865852372561	1.61880797365831	H	-5.06641038530135	-1.92636610486589	-1.26943796015279
C	3.40513114062466	-2.55047324196989	-1.08569606247300	H	-5.64867542348818	-2.76257924493258	0.16934660089727
H	2.64394282303924	-3.25439785359584	-0.73792886442603	H	-4.13506559627217	-3.26104389259382	-0.58904199984612
H	4.30319415738104	-3.12333158186431	-1.32681826332311	C	-3.59925935985185	-2.12682142161548	1.87205235430230
H	3.04483512033942	-2.10241606771954	-2.01212076908458	H	-2.85149301096028	-2.90521902502390	1.69621848885589
C	-0.98103920968112	-0.32625790768672	-0.16705073958983	H	-4.47526233291125	-2.60190334584749	2.31910118464396
O	-1.04286447276941	-1.51231553092469	-0.45597502169189	H	-3.19134439702042	-1.43477156657604	2.60899329515874
H	1.26725803876391	-0.99455207699787	-1.37651982940849	C	0.68902947819120	-0.21561953306043	0.16924989195240
H	2.26212155264157	2.56131235174998	1.55368179339770				

O	0.79804673205009	-1.21695585881481	0.85997527154731	C	-5.41797821882448	-2.04135347873904	0.96339396138190
H	-1.50033098969036	-0.50703214541311	1.60752959727439	H	-5.74302115281675	-2.07259684777717	-0.07781896091360
H	-2.66647577467236	1.98591288135753	-2.21946616664748	H	-6.31193576180022	-2.05419925527881	1.59068050894167
N	1.76566942330919	0.44175765511056	-0.37780754796378	H	-4.85842505560177	-2.95962521828514	1.16414584921402
H	1.58615492002470	1.38390254814125	-0.68335409791429	C	-4.16562041358117	-0.80383416478678	2.74416745771113
C	5.79634636338420	-0.52293880078553	0.23819112904204	H	-3.46581990358935	-1.61382648110188	2.96784766877909
C	4.95264899800503	-1.44224493671748	-0.36465889419096	H	-5.04770990422204	-0.94230180430296	3.37312320237995
C	3.60729081533078	-1.15520196032269	-0.58752423137703	H	-3.69526064833428	0.13334815053311	3.04272036875982
C	3.12269742908437	0.08782538903088	-0.16225360704580	C	0.16405125228771	-0.25858091049275	0.24795303135866
C	3.96144444618218	1.03151379732175	0.44728248225039	O	0.26321228055744	-0.93728324528403	1.25891612416257
C	5.30157745262350	0.71147776358136	0.63344602461893	H	-1.97515471410970	0.29517579646563	1.70760412982904
H	6.83992053550632	-0.76488633569813	0.39487315777883	H	-3.19768131594224	0.75958974761621	-2.82206258024283
H	5.34175551756067	-2.40086132820968	-0.68590343028809	N	1.24420383131198	0.13864086239449	-0.49722710260461
C	2.72746596979719	-2.15218586545262	-1.28289845225943	H	1.07287648764470	0.87401114986725	-1.16223795913177
C	3.41933148598042	2.35886592433112	0.90239529927606	C	5.23992244432904	-0.54097053765767	0.55623892501200
H	5.95743908028983	1.43342829560716	1.10474458217970	C	4.48297253791721	-1.57160189664211	0.01929591988182
H	3.33060843060299	-2.89612017397465	-1.80324252427213	C	3.14974686443095	-1.37612188744993	-0.32871291439889
H	2.07879609026772	-2.66120727858219	-0.56810436100640	C	2.59796416804213	-0.10643965306281	-0.11508320286540
H	2.07719565759719	-1.66337213338228	-2.01126567390284	C	3.33608009697771	0.93985352883492	0.45341391743927
H	4.18590383576576	2.92639002068847	1.42869488322069	C	4.67087624767170	0.70327792946897	0.77184863281820
H	3.07966888728218	2.97569297304328	0.06326007989342	H	6.27697810951075	-0.71271765867442	0.81688702076442
H	2.56682628413312	2.23224216026019	1.57363652350406	H	4.94038809115497	-2.53943877737321	-0.12995668321629
<b>Ligand R=Ph(iPr)<sub>2</sub></b>				C	2.32517972088287	-2.47816375829475	-0.96818469349561
H	-2.79718711689769	-1.71308647946813	0.44562424199282	C	2.69663505362262	2.29541940213629	0.68817306076979
C	-3.31991741894803	1.83203359376140	-0.92565907830766	H	5.26846405182270	1.49154391723531	1.20874507329154
C	-2.9450177226685	0.62441475931085	-1.77109864079949	C	2.29386797362022	-2.30103662040548	-2.49430638719156
C	-1.48566999411302	0.31137492649817	-1.55881623208542	C	2.79339783157285	-3.88674233056563	-0.59880877414653
H	-0.82032921722203	0.12235792251139	-2.39166560150745	H	1.30545035895151	-2.37862685824811	-0.59733632498619
C	-1.15002634866108	0.18141558992142	-0.27414491350440	C	2.82373393352746	3.17919281188796	-0.56303461786843
C	-2.30864221408988	0.37418554408124	0.67895641056687	H	1.63336776724509	2.12315237284946	0.86789834844186
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