

## Supporting Information

### An Unusual Four-Step Cascade Reaction for Accessing to Furo[3,4-c]pyridine-1,4-diones via Rhodium Catalysis

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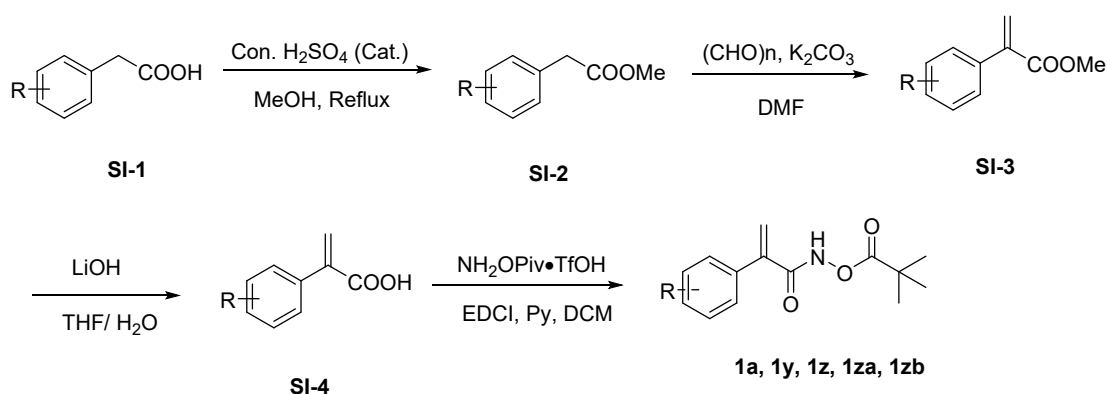
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## General Information

The chemical reagents were purchased from commercial sources and used directly without purification. Analytical thin-layer chromatography (TLC): HSGF 254 (0.15-0.2 mm thickness). Detection was conducted under UV light at 254 nm. Preparative thin layer chromatography was HSGF 254 (0.4-0.5 mm thickness). Yields refer to isolated compounds.  $^1\text{H}$ ,  $^{13}\text{C}$ , and  $^{19}\text{F}$  NMR spectra were collected on a Bruker 500 MHz instrument in chloroform-*d* or DMSO-*d*<sub>6</sub>. Chemical shifts ( $\delta$ ) are expressed as parts per million (ppm). Proton coupling patterns were recorded as singlet (s), broad (br), doublet (d), triplet (t), quartet (q), and multiplet (m). HRMS (high-resolution mass) were measured on a spectrometer with an electrospray ionization (ESI) source.

## Preparation of Starting Materials

General procedure A for the preparation of **1a**, **1o**, **1p**, **1q**, **1r**, **1s**, **1t**, **1u**.<sup>1</sup>



**Step 1:** To a solution of aryl acetic acids **SI-1** (7.3 mmol) in MeOH (20 mL), some drops of concentrated sulfuric acid were added. The reaction was refluxed for 8 hours, then it was cooled to room temperature. The solvent was concentrated under reduced pressure, and the residue was dissolved in EtOAc (30 mL), washed with H<sub>2</sub>O (30 mL) and brine (30 mL), dried with Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The crude product was used for the next step without further purification.

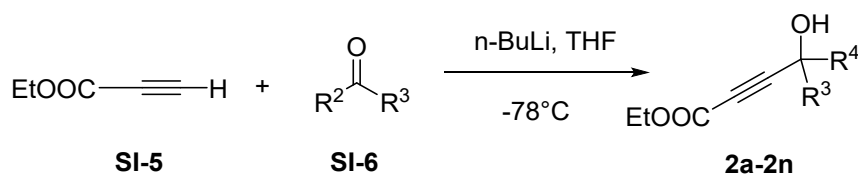
**Step 2:** A mixture of ester **SI-2** (7.0 mmol), paraformaldehyde (1.5 eq) and K<sub>2</sub>CO<sub>3</sub> (1 eq) in DMF (10 mL) was heated at 80°C for 1-3 h. The mixture was cooled to room temperature, water (30 mL) and Et<sub>2</sub>O (30 mL) were added, and the organic layer was separated. The collected organic layers were washed with brine (10 mL), dried with Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure. The

resulting crude product was purified by column chromatography eluting with PE/EtOAc from 50:1 to 20:1.

**Step 3:** A 50 mL RBF was charged with methyl acrylate **SI-3** (7.0 mmol), LiOH (5 eq) and THF/H<sub>2</sub>O (1:1, 0.25 M) sequentially. The reaction flask was subjected to an 80°C preheated oil bath and stirred overnight, at which time the resulting mixture was cooled to room temperature and extracted with Et<sub>2</sub>O. The aqueous phase was acidified with 2N HCl and extracted with EtOAc (30 mL x 2). The combined organic layers were concentrated under vacuum. The crude product was used for the next step without further purification.

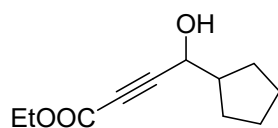
**Step 4:** To a solution of acrylic acid **SI-4** (2.0 mmol) in DCM (20 mL) was added pyridine (7.1 eq), EDCI (2eq) and NH<sub>2</sub>OPiv.TfOH (1.2 eq), and stirred at room temperature overnight. The mixture was washed with 2N HCl (20 mL), saturated aq. NaHCO<sub>3</sub> (20 mL) and brine (20 mL), dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure to give the crude products, which was purified by column chromatography eluting with PE/EtOAc from 20:1 to 5:1.

General procedure B for the preparation of **2a-2n**.<sup>2</sup>



To a solution of ethyl propiolate **SI-5** (0.3 mL, 3 mmol) in THF (15 mL) was added dropwise a solution of n-BuLi (1.6 M in hexane, 2.1 mL, 3.3 mmol) at -78 °C. After stirring for 0.5 h, **SI-6** (3.3 mmol) was added to the solution, and the resulting mixture was stirred at that temperature for additional 3 h. The reaction was then quenched with sat. aq. NH<sub>4</sub>Cl, and the product was extracted with EtOAc. The combined organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub> and evaporated. The crude mixture was purified by silica gel column chromatography (hexane/EtOAc = 5:1).

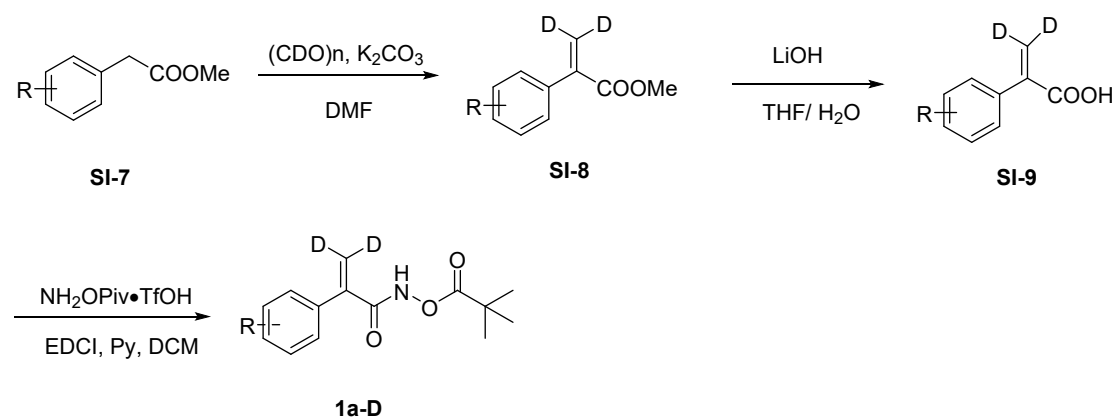
Characterization Data of **2k**



<sup>1</sup>H NMR (500 MHz, Chloroform-*d*) δ 4.33 (d, *J* = 7.2 Hz, 1H), 4.22 (m, 2H), 2.44 – 2.36 (m, 1H), 2.22

(h,  $J = 8.0$  Hz, 1H), 1.80 (m, 2H), 1.69 – 1.51 (m, 4H), 1.48 – 1.38 (m, 2H), 1.29 (t,  $J = 7.2$  Hz, 3H).

#### Preparation of **1a-D**<sup>1</sup>

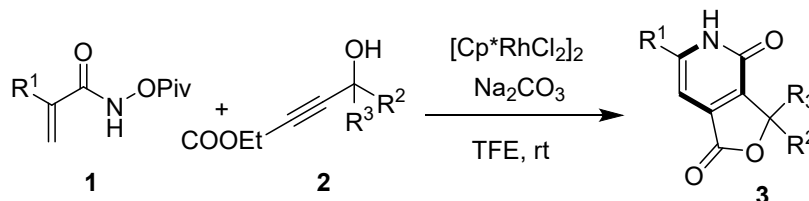


**Step 1:** A mixture of ester **SI-7** (7.0 mmol), D-paraformaldehyde (1.5 eq) and  $\text{K}_2\text{CO}_3$  (1 eq) in DMF (10 mL) was heated at 80°C for 1-3 h. The mixture was cooled at room temperature, water (30 mL) and Et<sub>2</sub>O (30 mL) were added, and the organic layer was separated. The collected organic layers were washed with brine (10 mL), dried with  $\text{Na}_2\text{SO}_4$  and concentrated under reduced pressure. The resulting crude product was purified by column chromatography eluting with PE/EtOAc from 50:1 to 20:1.

**Step 2:** A 50 mL RBF was charged with methyl acrylate **SI-8** (7.0 mmol), LiOH (5 eq) and THF/H<sub>2</sub>O (1:1, 0.25 M) sequentially. The reaction flask was subjected to an 80°C preheated oil bath and stirred overnight, at which time the resulting mixture was cooled to room temperature and extracted with Et<sub>2</sub>O. The aqueous phase was acidified with 2N HCl and extracted with EtOAc (30 mL x 2). The combined organic layers were concentrated under vacuum. The crude product was used for the next step without further purification.

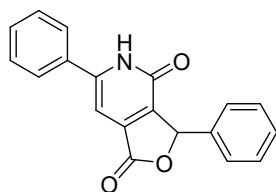
**Step 3:** To a solution of acrylic acid **SI-9** (2.0 mmol) in DCM (20 mL) was added pyridine (7.1 eq), EDCI (2eq) and  $\text{NH}_2\text{OPiv}\cdot\text{TfOH}$  (1.2 eq), and stirred at room temperature overnight. The mixture was washed with 2N HCl (20 mL), saturated aq.  $\text{NaHCO}_3$  (20 mL) and brine (20 mL), dried over  $\text{Na}_2\text{SO}_4$  and concentrated under reduced pressure to give the crude product, which was purified by column chromatography eluting with PE/EtOAc from 20:1 to 5:1.

### General Procedure for the Synthesis of Furo[3,4-c]pyridine-1,4-diones **3**

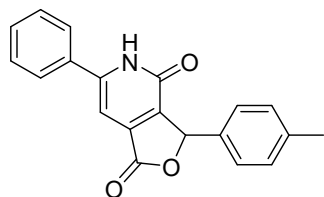


In an 8 mL reaction tube, the mixture of **1** (0.2 mmol), **2** (0.24 mmol), [Cp\*RhCl<sub>2</sub>]<sub>2</sub> (3.0 mol%) and Na<sub>2</sub>CO<sub>3</sub> (1.0 eq.) was added TFE (1.0 mL). Then the resulting mixture was stirred for 6 ~ 12 h. When the reaction was finished, the desired product precipitated out as a solid, and the product was simply collected by filtration. After that, the rest reaction mixture was subjected to flash chromatography on silica gel (dichloromethane/methanol) to provide the desired products **3**.

### Characterization Data of Products **3**

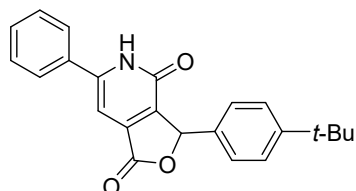


**3,6-diphenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3a)**: white solid (47mg, yield 78%), <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 12.45 (s, 1H), 7.81 (s, 2H), 7.52 (dd, *J* = 5.1, 2.0 Hz, 3H), 7.43 – 7.40 (m, 3H), 7.38 (dd, *J* = 6.8, 3.0 Hz, 2H), 6.86 (s, 1H), 6.59 (s, 1H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 169.21, 158.50, 134.57, 130.26, 129.14, 128.78, 128.60, 127.50, 127.31, 81.60. HRMS (ESI) *m/z* calculated for C<sub>19</sub>H<sub>14</sub>NO<sub>3</sub><sup>+</sup> [M+H]<sup>+</sup> 304.0968, found: 304.0964.

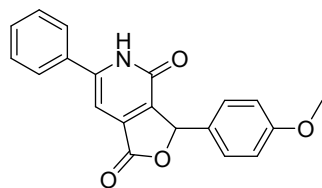


**6-phenyl-3-(p-tolyl)-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3b)**: white solid (37mg, yield 58%), <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 12.44 (s, 1H), 7.88 – 7.70 (m, 2H), 7.52 (dd, *J* = 5.1, 2.0 Hz, 3H),

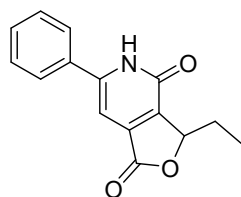
7.29 – 7.17 (m, 4H), 6.98 – 6.74 (s, 1H), 6.54 (s, 1H), 2.32 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, DMSO)  $\delta$  169.82, 159.08, 139.23, 137.16, 132.16, 130.82, 129.72, 129.36, 128.06, 127.87, 82.17, 31.16, 21.28. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{20}\text{H}_{16}\text{NO}_3^+$   $[\text{M}+\text{H}]^+$  318.1125, found: 318.1121.



**3-(4-(tert-butyl)phenyl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3c):** white solid (43mg, yield 60%),  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ )  $\delta$  12.42 (s, 1H), 7.80 (dd,  $J = 6.6, 3.0$  Hz, 2H), 7.50 (dd,  $J = 5.0, 1.9$  Hz, 3H), 7.44 – 7.39 (m, 2H), 7.32 – 7.22 (m, 2H), 6.87 (s, 1H), 6.54 (s, 1H), 1.26 (s, 9H).  $^{13}\text{C}$  NMR (126 MHz, DMSO)  $\delta$  169.80, 159.11, 152.25, 137.17, 132.18, 130.83, 129.36, 127.88, 127.83, 126.00, 82.09, 62.43, 34.89, 31.50. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{23}\text{H}_{22}\text{NO}_3^{2+}$   $[\text{M}+\text{H}]^+$  360.1589, found: 360.1591.

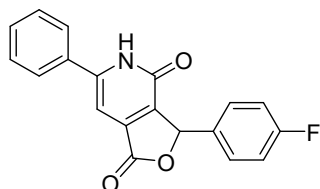


**3-(4-methoxyphenyl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3d):** white solid (38mg, yield 57%),  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ )  $\delta$  7.87 – 7.78 (m, 2H), 7.50 (m, 3H), 7.32 – 7.24 (m, 2H), 6.98 – 6.93 (m, 2H), 6.87 (s, 1H), 6.50 (d,  $J = 3.3$  Hz, 1H), 3.76 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz, DMSO)  $\delta$  169.85, 162.48, 160.41, 159.27, 137.21, 130.76, 129.61, 129.35, 129.29, 127.85, 127.11, 127.02, 114.56, 113.69, 82.12, 55.69. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{20}\text{H}_{16}\text{NO}_4^{2+}$   $[\text{M}+\text{H}]^+$  334.1068, found: 334.1070.

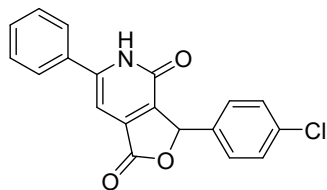


**3-ethyl-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3e):** white solid (26mg, yield 50%),  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ )  $\delta$  12.42 (s, 1H), 7.78 (dd,  $J = 6.5, 3.0$  Hz, 2H), 7.49 (dd,  $J = 5.0, 1.9$  Hz,

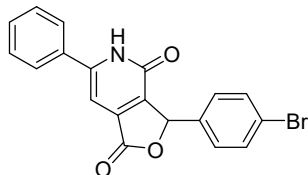
3H), 6.77 (s, 1H), 5.53 (dd,  $J = 7.2, 3.4$  Hz, 1H), 2.22 (m, 1H), 1.77 (m, 1H), 0.88 (t,  $J = 7.4$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz, DMSO)  $\delta$  169.75, 159.44, 150.15, 137.32, 133.27, 130.75, 129.35, 127.81, 97.97, 82.27, 24.94, 9.13. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{15}\text{H}_{14}\text{NO}_3^{2+} [\text{M}+\text{H}]^+$  256.0963, found: 256.0989.



**3-(4-fluorophenyl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3f)** : white solid (40mg, yield 62%),  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ )  $\delta$  7.83 (dd,  $J = 6.6, 2.9$  Hz, 2H), 7.50 (m, 4H), 7.48 – 7.38 (m, 2H), 7.24 (m, 2H), 6.88 (s, 1H), 6.58 (d,  $J = 3.7$  Hz, 1H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{DMSO}-d_6$ )  $\delta$  199.02, 174.52, 168.68, 166.73, 164.14, 155.93, 143.34, 141.89, 138.29, 136.30, 135.52, 135.20, 135.13, 134.09, 132.61, 131.94, 120.89, 120.72, 120.25, 120.07, 102.76, 86.13. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{19}\text{H}_{13}\text{FNO}_3^+ [\text{M}+\text{H}]^+$  322.0874, found: 322.0871.

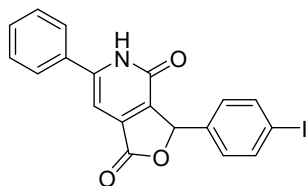


**3-(4-chlorophenyl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3g)**: white solid (48mg, yield 71%),  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ )  $\delta$  12.46 (s, 1H), 7.89 – 7.79 (m, 2H), 7.52 (dd,  $J = 5.2, 1.9$  Hz, 3H), 7.50 – 7.46 (m, 2H), 7.46 – 7.41 (m, 2H), 6.89 (s, 1H), 6.62 (s, 1H).  $^{13}\text{C}$  NMR (126 MHz, DMSO)  $\delta$  168.57, 157.98, 136.10, 133.26, 133.10, 129.80, 128.94, 128.29, 128.13, 126.82, 126.41, 80.12. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{19}\text{H}_{13}\text{ClNO}_3^+ [\text{M}+\text{H}]^+$  338.0578, found: 338.0574.

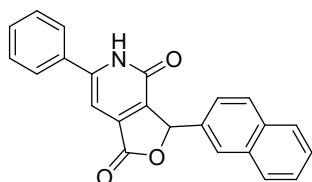


**3-(4-bromophenyl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3h)**: white solid (55mg, yield 72%),  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ )  $\delta$  7.91 – 7.84 (m, 2H), 7.61 – 7.55 (m, 2H), 7.45 (m, 3H), 7.35 (d,  $J = 8.5$  Hz, 2H), 6.85 (s, 1H), 6.47 (d,  $J = 1.9$  Hz, 1H).  $^{13}\text{C}$  NMR (126 MHz, DMSO)  $\delta$  136.91, 134.70, 130.80, 130.50, 129.49, 129.11, 128.66, 128.23, 127.94, 126.43, 126.12, 121.38, 95.27, 80.58.

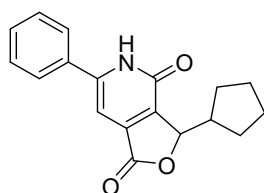
HRMS (ESI)  $m/z$  calculated for  $C_{19}H_{13}BrNO_3^+ [M+H]^+$  382.0073, found: 382.0080.



**3-(4-iodophenyl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3i):** white solid (65mg, yield 76%),  $^1H$  NMR (500 MHz,  $DMSO-d_6$ )  $\delta$  7.87 – 7.80 (m, 2H), 7.79 – 7.72 (m, 2H), 7.54 – 7.45 (m, 3H), 7.20 (d,  $J = 8.1$  Hz, 2H), 6.87 (s, 1H), 6.69 – 6.34 (m, 1H).  $^{13}C$  NMR (126 MHz,  $DMSO$ )  $\delta$  136.64, 136.39, 135.14, 134.66, 129.35, 129.13, 128.58, 128.23, 127.91, 126.40, 126.12, 94.55, 80.79, 30.09. HRMS (ESI)  $m/z$  calculated for  $C_{19}H_{13}INO_3^+ [M+H]^+$  429.9929, found: 429.9929.

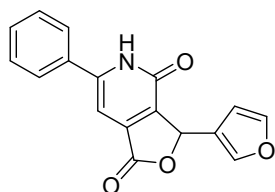


**3-(naphthalen-2-yl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3j):** white solid (42mg, yield 59%),  $^1H$  NMR (500 MHz,  $DMSO-d_6$ )  $\delta$  7.97 – 7.91 (m, 4H), 7.88 (dd,  $J = 9.6, 7.4$  Hz, 2H), 7.54 – 7.48 (m, 2H), 7.45 – 7.33 (m, 4H), 6.89 (s, 1H), 6.57 (s, 1H).  $^{13}C$  NMR (126 MHz,  $DMSO$ )  $\delta$  195.68, 167.16, 162.75, 150.84, 136.27, 135.12, 134.58, 132.77, 130.05, 129.77, 129.34, 129.08, 128.26, 128.03, 127.64, 127.58, 127.21, 126.93, 124.97, 106.20, 82.72. HRMS (ESI)  $m/z$  calculated for  $C_{23}H_{16}NO_3^{2+} [M+H]^+$  354.1119, found: 354.1123.

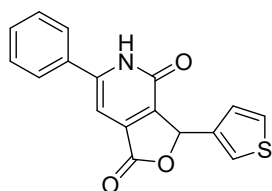


**3-cyclopentyl-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3k):** white solid (10mg, yield 17%),  $^1H$  NMR (500 MHz,  $DMSO-d_6$ )  $\delta$  12.44 (s, 1H), 7.81 (dd,  $J = 6.5, 3.0$  Hz, 2H), 7.51 (dd,  $J = 5.0, 1.9$  Hz, 3H), 6.80 (s, 1H), 5.65 (d,  $J = 3.3$  Hz, 1H), 2.78 (m, 1H), 1.92 (m,  $J = 11.0, 7.7, 3.9$  Hz, 1H), 1.70 – 1.58 (m, 2H), 1.58 – 1.42 (m, 2H), 1.32 (m, 1H), 0.98 (m, 1H).  $^{13}C$  NMR (126 MHz,  $DMSO$ )  $\delta$  169.92, 159.38, 150.05, 137.36, 133.20, 130.76, 129.35, 127.80, 97.83, 83.18, 29.28, 25.89, 25.67, 25.03. HRMS (ESI)  $m/z$  calculated for  $C_{18}H_{18}NO_3^+ [M+H]^+$  296.1281, found: 296.1279.

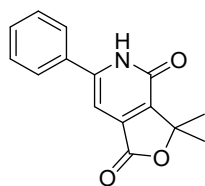




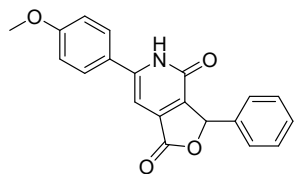
**3-(furan-3-yl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3l):** white solid (36mg, yield 61%),  $^1\text{H NMR}$  (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.93 – 7.82 (m, 3H), 7.69 – 7.62 (m, 1H), 7.48 – 7.41 (m, 3H), 6.83 (s, 1H), 6.50 (d,  $J = 1.7$  Hz, 1H), 6.47 – 6.41 (m, 1H).  $^{13}\text{C NMR}$  (126 MHz,  $\text{CDCl}_3$ )  $\delta$  194.30, 174.30, 171.56, 164.00, 155.61, 152.94, 149.31, 147.53, 142.07, 138.11, 135.56, 132.59, 131.88, 125.38, 114.37, 102.80, 79.95. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{17}\text{H}_{11}\text{NNaO}_4^+$   $[\text{M}+\text{Na}]^+$  316.0580, found: 316.0580.



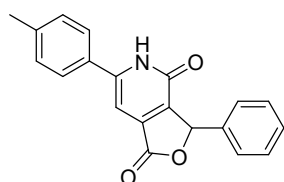
**6-phenyl-3-(thiophen-3-yl)-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3m):** white solid (36mg, yield 58%),  $^1\text{H NMR}$  (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.94 – 7.83 (m, 2H), 7.65 (d,  $J = 2.9$  Hz, 1H), 7.53 (m, 1H), 7.49 – 7.43 (m, 3H), 7.13 (dd,  $J = 5.0, 1.2$  Hz, 1H), 6.83 (s, 1H), 6.55 (d,  $J = 3.0$  Hz, 1H).  $^{13}\text{C NMR}$  (126 MHz,  $\text{DMSO}$ )  $\delta$  188.61, 165.27, 143.35, 135.98, 135.01, 131.11, 129.69, 128.84, 128.27, 128.21, 126.77, 126.46, 126.04, 125.81, 125.33, 125.04, 76.92. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{17}\text{H}_{12}\text{NO}_3\text{S}^+$   $[\text{M}+\text{H}]^+$  310.0532, found: 310.0532.



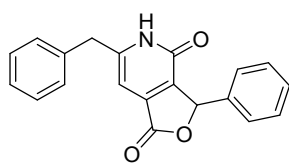
**3,3-dimethyl-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3n):** white solid (19mg, yield 38%),  $^1\text{H NMR}$  (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  12.43 (s, 1H), 7.76 (dd,  $J = 6.7, 2.9$  Hz, 2H), 7.49 (dd,  $J = 5.0, 1.9$  Hz, 3H), 6.74 (s, 1H), 1.63 (s, 6H).  $^{13}\text{C NMR}$  (126 MHz,  $\text{DMSO}$ )  $\delta$  168.67, 159.08, 150.29, 143.53, 136.28, 133.35, 130.72, 129.35, 127.83, 98.01, 86.14, 24.84. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{15}\text{H}_{14}\text{NO}_3^+$   $[\text{M}+\text{H}]^+$  256.0968, found: 256.0990.



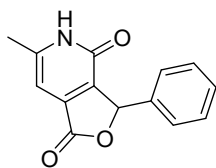
**6-(4-methoxyphenyl)-3-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3o):** white solid (55mg, yield 83%),  $^1\text{H NMR}$  (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.94 – 7.86 (m, 2H), 7.36 – 7.27 (m, 5H), 6.97 – 6.88 (m, 2H), 6.70 (s, 1H), 6.28 (s, 1H), 3.79 (s, 3H).  $^{13}\text{C NMR}$  (126 MHz, DMSO)  $\delta$  171.71, 159.39, 136.99, 134.19, 129.74, 128.91, 128.21, 128.10, 127.99, 127.85, 127.34, 126.40, 113.45, 93.22, 82.42, 55.02. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{20}\text{H}_{16}\text{NO}_4^+$   $[\text{M}+\text{H}]^+$  334.1074, found: 334.1079.



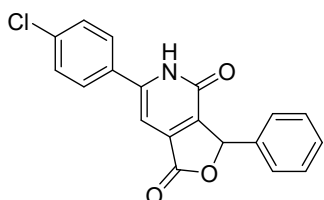
**3-phenyl-6-(p-tolyl)-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3p):** white solid (43mg, yield 68%),  $^1\text{H NMR}$  (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  12.33 (s, 1H), 7.79 (d,  $J = 8.3$  Hz, 2H), 7.44 – 7.39 (m, 3H), 7.37 (dd,  $J = 6.8, 3.0$  Hz, 2H), 7.10 – 7.01 (m, 2H), 6.82 (s, 1H), 6.57 (s, 1H), 3.83 (s, 3H).  $^{13}\text{C NMR}$  (126 MHz, DMSO)  $\delta$  169.32, 160.89, 158.54, 136.62, 134.71, 129.11, 128.80, 128.59, 128.24, 127.49, 114.19, 81.59, 55.31. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{20}\text{H}_{15}\text{KNO}_3^+$   $[\text{M}+\text{K}]^+$  356.0684, found: 356.0688.



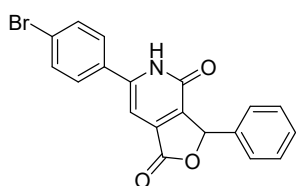
**6-benzyl-3-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3q):** white solid (43mg, yield 68%),  $^1\text{H NMR}$  (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  12.43 (s, 1H), 7.40 – 7.30 (m, 9H), 7.29 – 7.24 (m, 1H), 6.48 (s, 1H), 6.37 (s, 1H), 3.94 (s, 2H).  $^{13}\text{C NMR}$  (126 MHz, DMSO)  $\delta$  169.90, 158.94, 153.02, 138.56, 137.59, 136.98, 135.16, 129.63, 129.48, 129.13, 127.96, 127.40, 98.00, 82.15, 38.41. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{20}\text{H}_{16}\text{NO}_3^+$   $[\text{M}+\text{H}]^+$  318.1125, found: 318.1121.



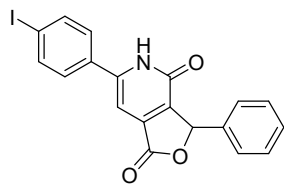
**6-methyl-3-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3r):** white solid (10mg, yield 20%),  $^1\text{H NMR}$  (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  12.22 (s, 1H), 7.41 – 7.35 (m, 3H), 7.30 (m, 2H), 6.47 (s, 1H), 6.41 (d,  $J = 15.2$  Hz, 1H), 2.28 (s, 3H).  $^{13}\text{C NMR}$  (126 MHz,  $\text{DMSO}$ )  $\delta$  169.98, 158.89, 150.18, 137.94, 136.97, 135.33, 129.63, 129.38, 129.12, 128.34, 127.95, 98.11, 82.11, 19.22. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{14}\text{H}_{12}\text{NO}_3^+$   $[\text{M}+\text{H}]^+$  242.0812, found: 242.0810.



**6-(4-chlorophenyl)-3-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3s):** white solid (42mg, yield 63%),  $^1\text{H NMR}$  (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  12.49 (s, 1H), 7.85 (s, 2H), 7.58 (d,  $J = 8.5$  Hz, 2H), 7.45 – 7.40 (m, 3H), 7.37 (dd,  $J = 6.8, 3.1$  Hz, 2H), 6.91 (s, 1H), 6.60 (s, 1H).  $^{13}\text{C NMR}$  (126 MHz,  $\text{DMSO}$ )  $\delta$  169.11, 158.45, 136.57, 135.05, 134.49, 129.22, 129.16, 128.74, 128.60, 127.51, 81.60. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{19}\text{H}_{12}\text{ClKNO}_3^+$   $[\text{M}+\text{K}]^+$  376.0137, found: 376.0138.



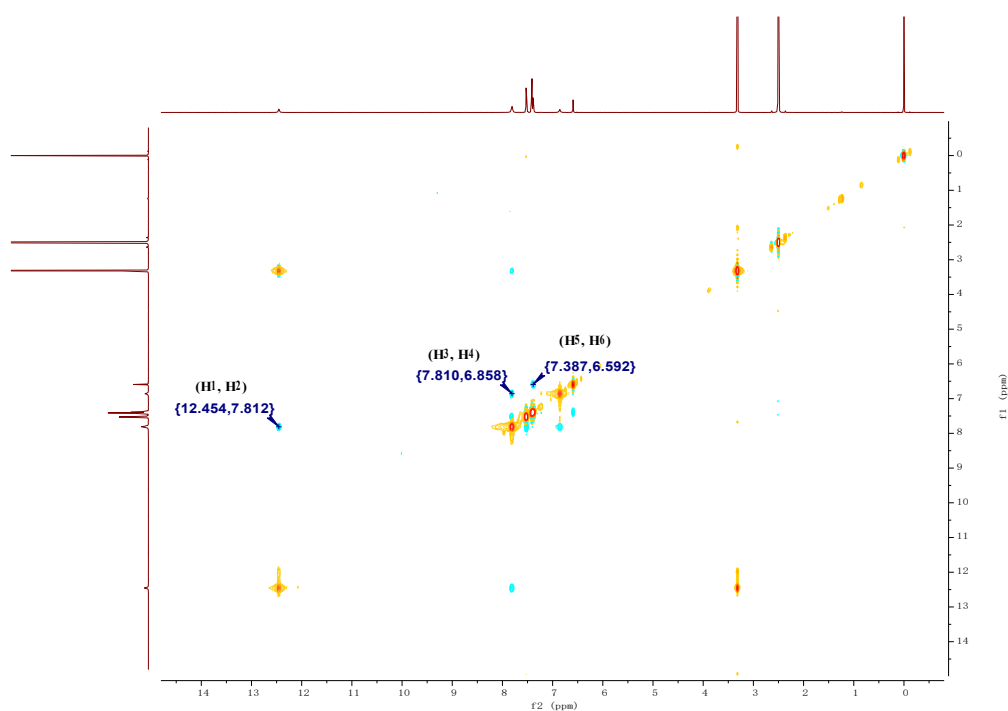
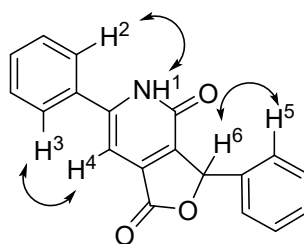
**6-(4-bromophenyl)-3-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3t):** white solid (46mg, yield 60%),  $^1\text{H NMR}$  (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  12.49 (s, 1H), 7.88 – 7.68 (m, 4H), 7.43 – 7.35 (m, 5H), 6.91 (s, 1H), 6.59 (s, 1H).  $^{13}\text{C NMR}$  (126 MHz,  $\text{DMSO}$ )  $\delta$  169.10, 158.45, 134.48, 131.67, 129.42, 129.16, 128.60, 127.51, 123.85, 81.60. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{19}\text{H}_{13}\text{BrNO}_3^+$   $[\text{M}+\text{H}]^+$  382.0073, found: 382.0071.



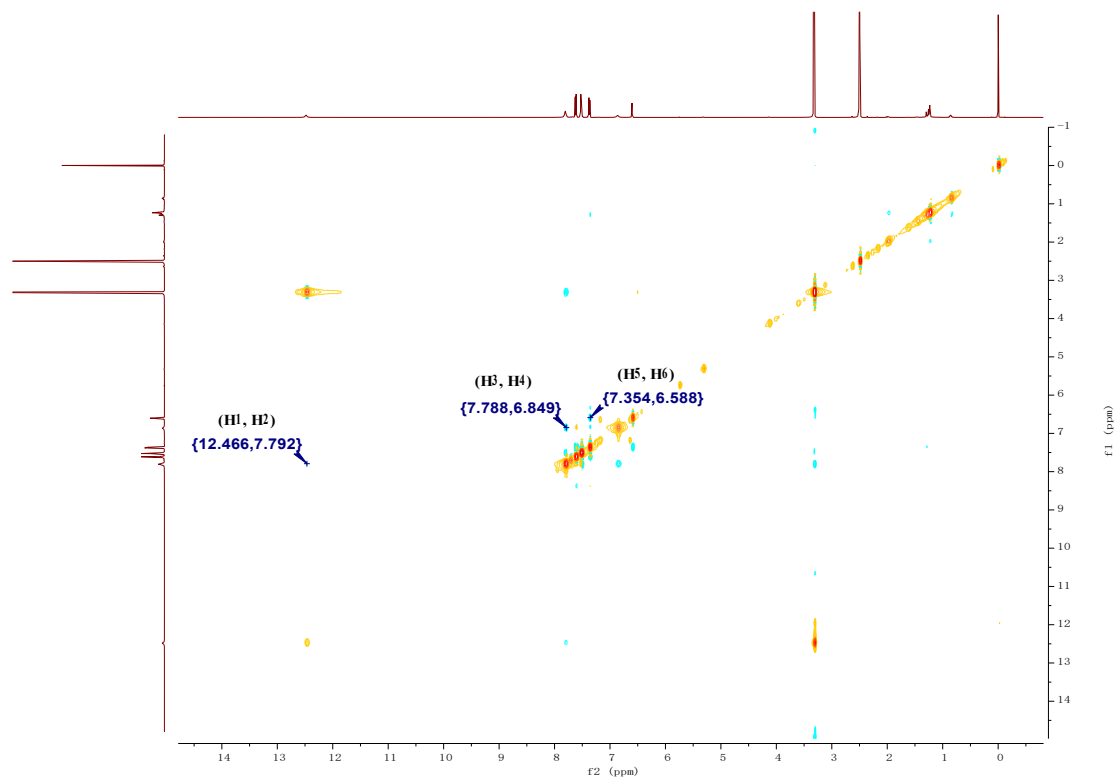
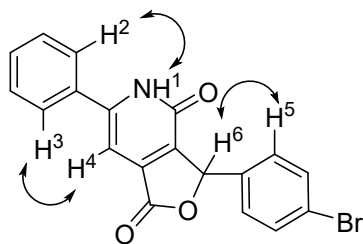
**6-(4-iodophenyl)-3-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3u):** white solid (46mg, yield 60%),  $^1\text{H NMR}$  (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  12.46 (s, 1H), 7.94 – 7.81 (m, 2H), 7.68 – 7.56 (m, 2H), 7.48 – 7.33 (m, 5H), 6.91 (s, 1H), 6.58 (s, 1H).  $^{13}\text{C NMR}$  (126 MHz,  $\text{DMSO}$ )  $\delta$  169.13, 158.49, 137.53, 136.59, 134.49, 129.29, 129.16, 128.61, 127.52, 97.50, 81.62. HRMS (ESI)  $m/z$  calculated for  $\text{C}_{19}\text{H}_{13}\text{INO}_3^+$   $[\text{M}+\text{H}]^+$  429.9935, found: 429.9932.

### NOESY Experiments for Product 3a, 3h, 3n, 3p, 3q

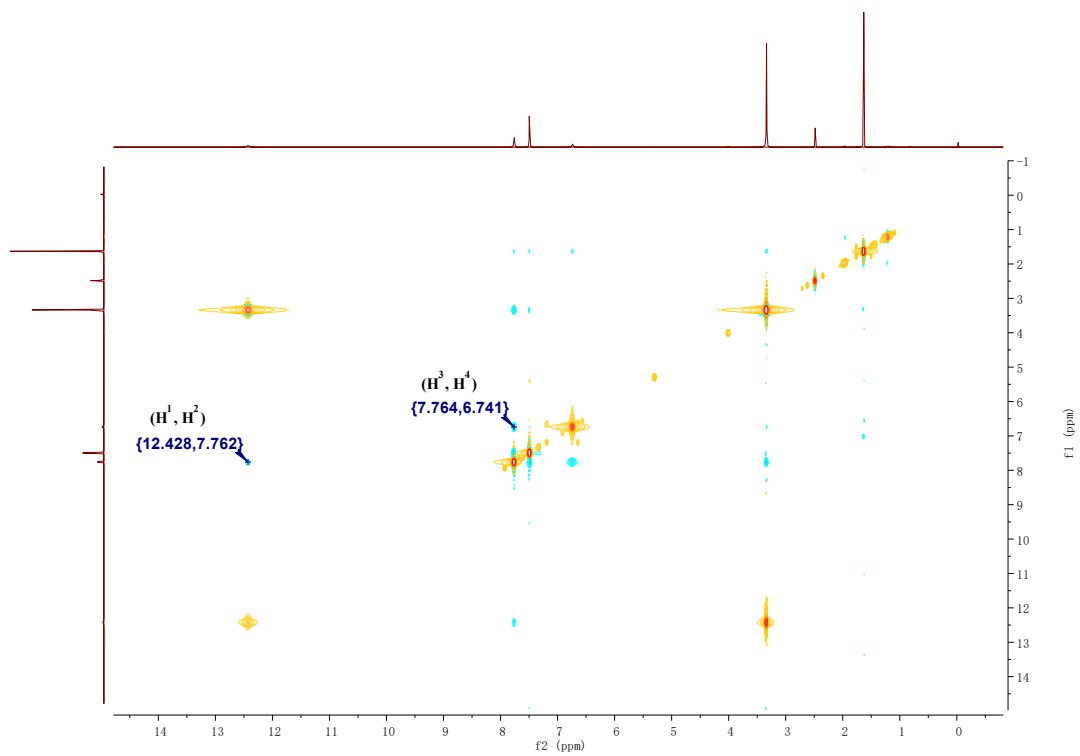
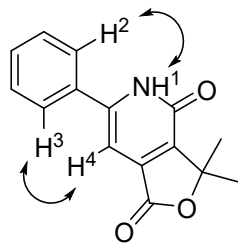
#### 1) NOESY spectra of product 3a



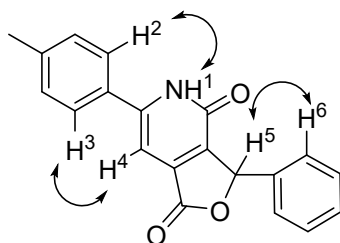
2) NOESY spectra of product **3h**

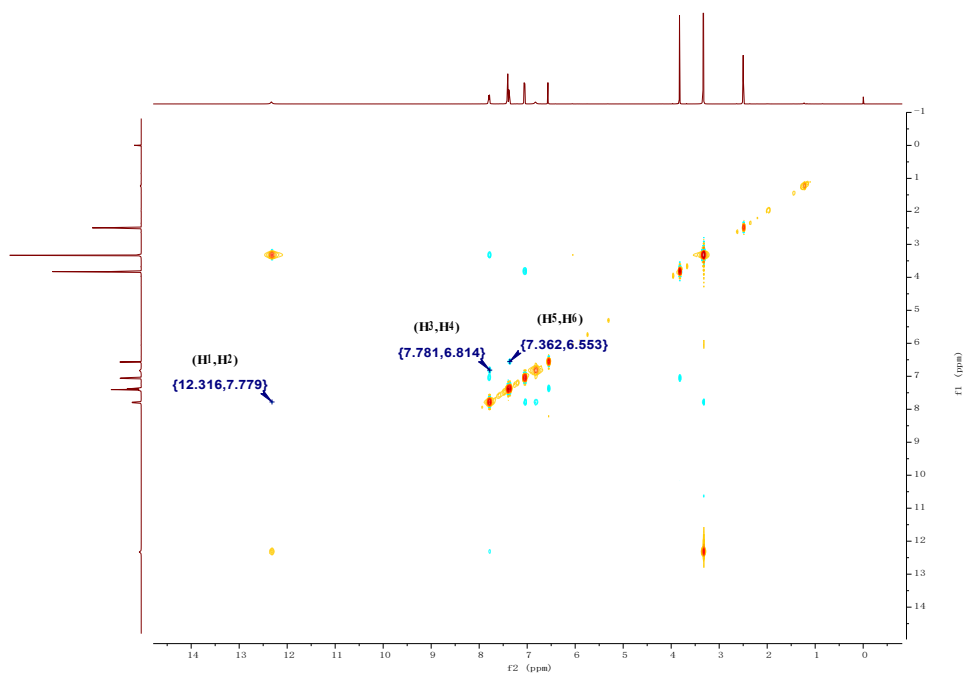


3) NOESY spectra of product **3n**

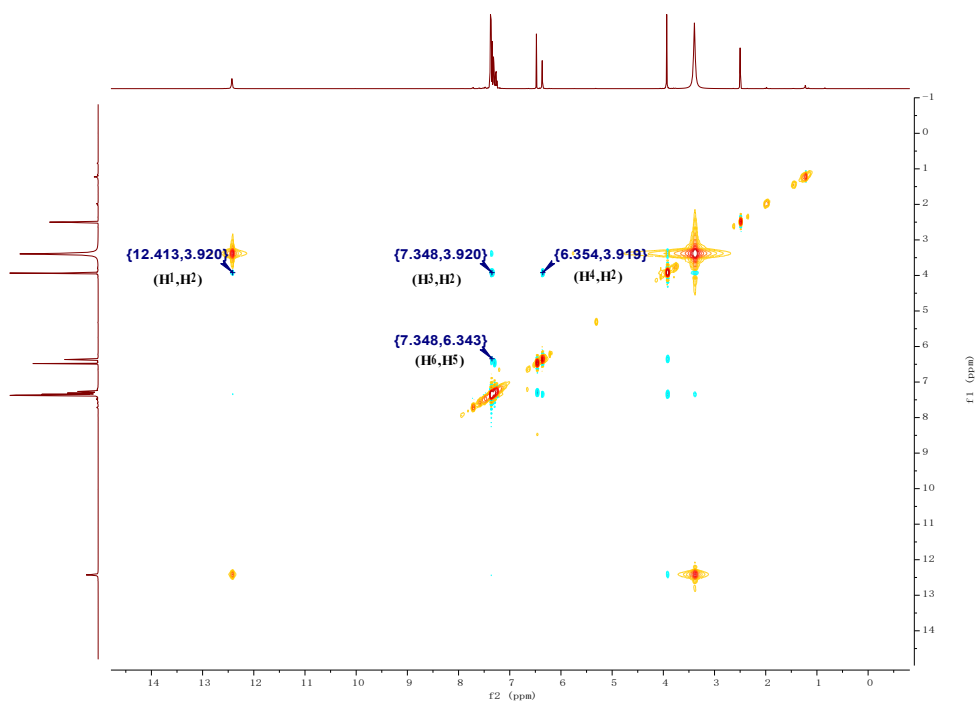
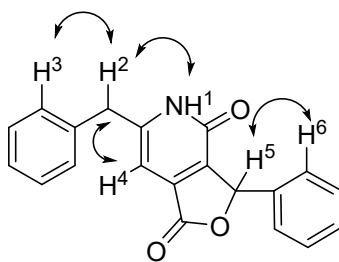


4) NOESY spectra of product **3p**



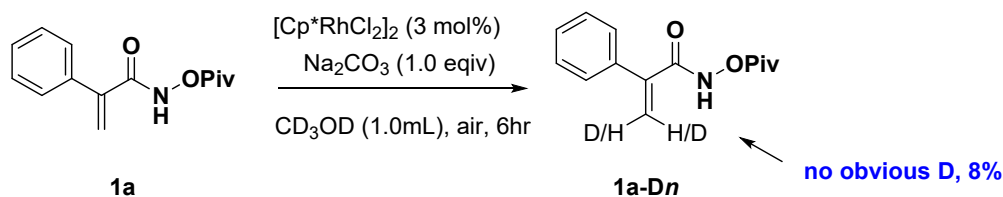


5) NOESY spectra of product 3q

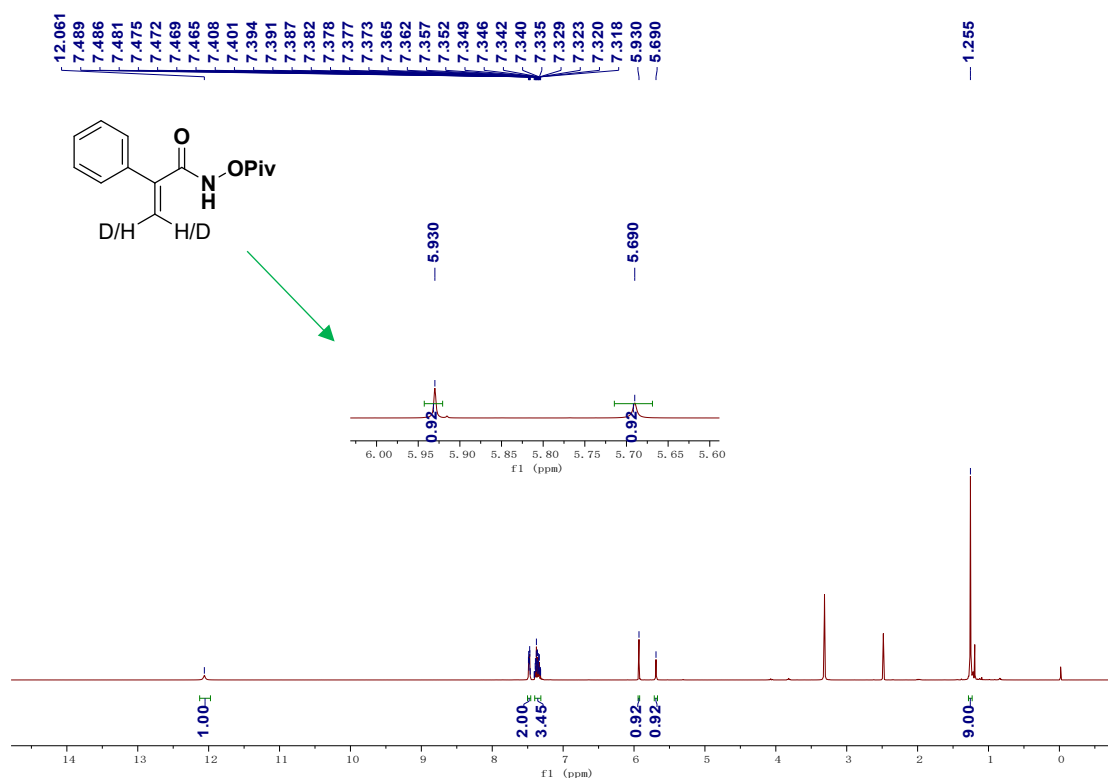


## Mechanistic Experiments

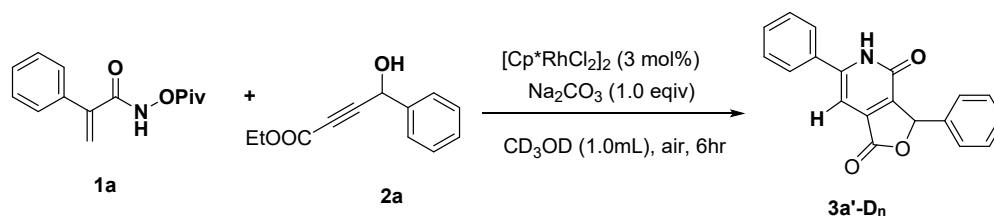
### Deuterium Incorporation Experiment A



To a mixture of **1a** (49.5 mg, 0.2 mmol, 1.0 eq.),  $[\text{Cp}^*\text{RhCl}_2]_2$  (3.7 mg, 0.006 mmol, 3 mol%) and  $\text{Na}_2\text{CO}_3$  (21.2 mg, 0.2 mmol, 1.0 eq.) in a 10 mL reaction tube was added  $\text{CD}_3\text{OD}$  (1.0 mL). Then the resulting mixture was stirred at the temperature for 6.0 h. After removal of the solvents under vacuum, the residue obtained was directly used for  $^1\text{H}$  NMR analysis. The reaction of **1a** (49.5 mg, 0.2 mmol, 1.0 eq.) without **2a** provided the product **1a-D<sub>n</sub>**. Found no obvious H/D exchange occurred at the olefinic bond of the **1a** (8% D).



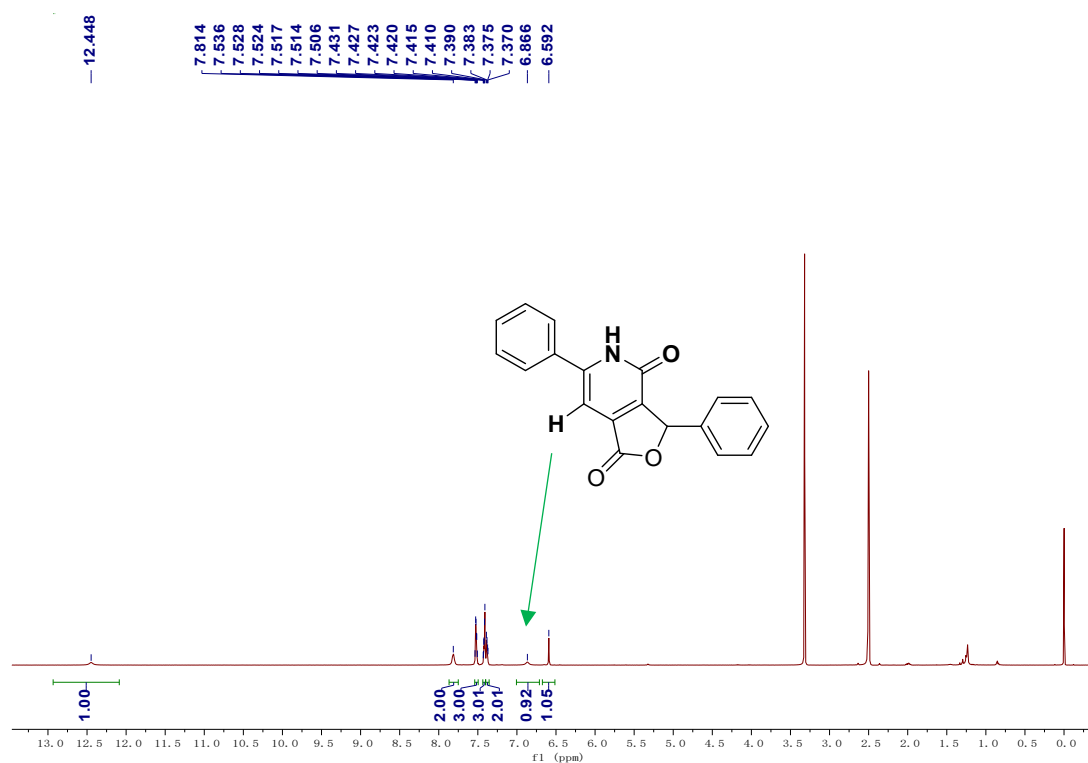
### Deuterium Incorporation Experiment B





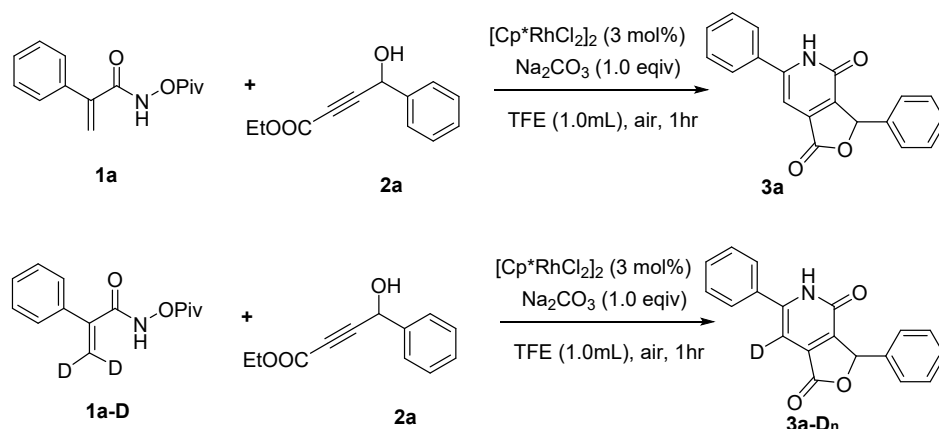
To a mixture of **1a** (49.5 mg, 0.2 mmol, 1.0 eq.), **2a** (49.0 mg, 0.24 mmol, 1.2 eq.), [Cp\*RhCl<sub>2</sub>]<sub>2</sub> (3.7 mg, 0.006 mmol, 3 mmol%) and Na<sub>2</sub>CO<sub>3</sub> (21.2 mg, 0.2mmol, 1.0 eq.) in a 10 mL reaction tube was added CD<sub>3</sub>OD (1.0 mL). Then the resulting mixture was stirred at the temperature for 6.0 h. After removal of the solvents under vacuum, the residue obtained was directly used for <sup>1</sup>H NMR analysis.

The reaction of **1a** (49.5 mg, 0.2 mmol, 1.0 eq.) with **2a** (51.7 mg, 0.3 mmol, 1.5 eq.) provided the product **3a-D<sub>n</sub>**, found almost no deuterium incorporation at the hydrogen of the olefinic bond.



## Determination of the KIE

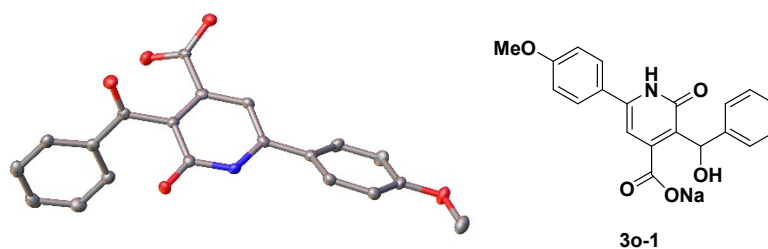
Two parallel reactions for KIE value measurement



To a mixture of **1a** (49.5 mg, 0.2 mmol, 1.0 eq.), **2a** (49.0 mg, 0.24 mmol, 1.2 eq.),  $[\text{Cp}^*\text{RhCl}_2]_2$  (3.7 mg, 0.006 mmol, 3 mol%) and  $\text{Na}_2\text{CO}_3$  (21.2 mg, 0.2 mmol, 1.0 eq.) in a 10 mL reaction tube was added TFE (1.0 mL). Then the resulting mixture was stirred at the temperature for 1.0 h. The reaction was finished to provide the product **3a** (29.0 mg, 48% yield).

To a mixture of **1a-D** (49.8 mg, 0.2 mmol, 1.0 eq.), **2a** (49.0 mg, 0.24 mmol, 1.2 eq.),  $[\text{Cp}^*\text{RhCl}_2]_2$  (3.7 mg, 0.006 mmol, 3 mol%) and  $\text{Na}_2\text{CO}_3$  (21.2 mg, 0.2 mmol, 1.0 eq.) in a 10 mL reaction tube was added EA (1.0 mL). Then the resulting mixture was stirred at the temperature for 1.0 h. The reaction was finished to provide the product **3a-D<sub>n</sub>** (30 mg, 49% yield). The ratio of **3aa/3aa-D<sub>n</sub>** was 0.98 (0.48/0.49)

#### X-ray data of compound 3o-1 (3o-1 is a lactone ring-opening structure of 3o, CCDC 2281784)



**Table S1.** Crystal data and structure refinement for compound **3o-1**.<sup>a</sup>

Identification code	<b>3o-1</b>
Empirical formula	$\text{C}_{43}\text{H}_{43}\text{N}_3\text{Na}_2\text{O}_{15}$
Formula weight	887.8
Temperature/K	150
Crystal system	orthorhombic
Space group	P n a 21
a/Å	12.0888(6)
b/Å	11.2367(5)

c/Å	29.9061(11)
$\alpha$ /°	90
$\beta$ /°	90
$\gamma$ /°	90
Volume/Å <sup>3</sup>	4062.4(3)
Z	4
$\rho_{\text{calc}}$ /cm <sup>3</sup>	1.452
$\mu$ /mm <sup>-1</sup>	0.707
F(000)	1861.9
Crystal size/mm <sup>3</sup>	0.01 × 0.01 × 0.02
Radiation	Ga K $\alpha$ ( $\lambda$ = 1.34050)
2 $\Theta$ range for data collection/°	2.5630 to 60.3280
Index ranges	-15 ≤ h ≤ 15, -14 ≤ k ≤ 14, -37 ≤ l ≤ 38
Reflections collected	7034
Data/restraints/parameters	3689/1/581
Goodness-of-fit on F <sup>2</sup>	1.0430
Final R indexes [ $I \geq 2\sigma(I)$ ]	R <sub>1</sub> = 0.0374, wR <sub>2</sub> = 0.0935
Final R indexes [all data]	R <sub>1</sub> = 0.0450, wR <sub>2</sub> = 0.0886
Largest diff. peak/hole / e Å <sup>-3</sup>	0.5323/-0.2566

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<sup>a</sup>Note: We got the crystal structure of **3o** derivative (**3o-1**), in which the lactone ring of **3o** was open and formed sodium carboxylate salt. We provided the X-ray crystallography data of ring-opening structure of **3o** in the revised SI (**3o-1**, CCDC number: 2281784).

## Computational Mechanistic Studies

### Computational details:

Density functional theory (DFT)<sup>3</sup> calculations were performed by using Gaussian 09 quantum chemical package.<sup>4</sup> Unless otherwise specified, geometry optimizations were performed using B3LYP<sup>5</sup> functional with Grimme D3 correction (EmpiricalDispersion=GD3BJ).<sup>6</sup> Herein, the Stuttgart/Dresden effective core potential (SDD)<sup>7</sup> was used for Rh in conjunction with a standard 6-31G(d,p) basis set<sup>8</sup> for all other atoms. This level of theory is denoted as B3LYP-D3(BJ)/6-31G(d,p) SDD or B3D3/BS1. Frequency analysis was conducted at the same level of theory to verify the stationary points to be real minima or saddle points and to obtain the thermodynamic energy corrections. Intrinsic reaction coordinate (IRC) calculations<sup>9</sup> were carried out to confirm that all transition state structures connect the corresponding reactants and products. Solvent effects in 2,2,2-

TriFluoroEthanol (TFE) were estimated by using the SMD<sup>10</sup> solvation method at the M06<sup>11</sup> level of theory with Grimme D3 correction (EmpiricalDispersion=GD3). Herein, SDD was used for Rh and 6-31G(d,p) basis set was used for hydrogen atoms meanwhile the 6-311++G(d,p) basis set was used for all other atoms. This level of theory is denoted as M06-D3 SMD/6-311++G(d,p) SDD or M06D3 SMD/BS2. If not noted, the energies presented in this paper are the (M06D3 SMD/BS2)-calculated single point energies with (B3D3/BS1)-calculated thermodynamic corrections which were calculated under standard conditions (1 atm and 298.15 K) (denoted as  $\Delta G_{\text{sol}}(\text{M06-D3 SMD/6-311++G(d,p) SDD//B3LYP-D3(BJ)/6-31G(d,p) SDD})$  or  $\Delta G$  for clarity). The 3D diagrams of optimized structures are illustrated using CYLView.<sup>12</sup>

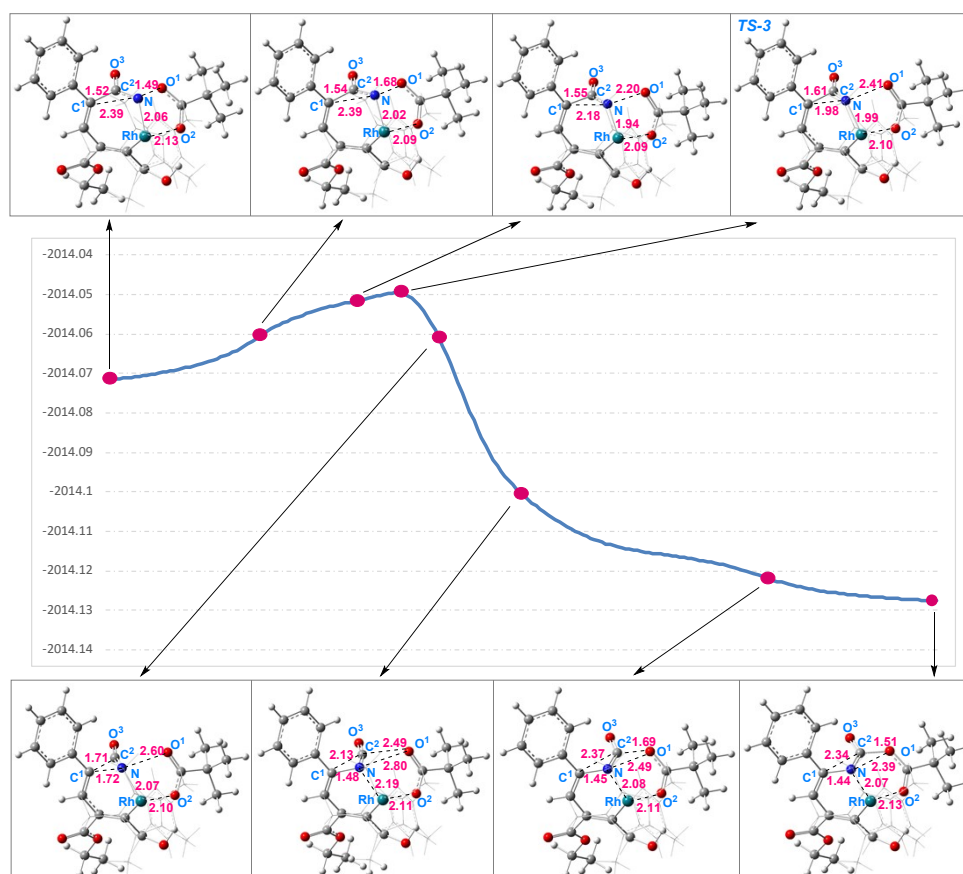


Figure S1. the geometry change along the intrinsic reaction coordinate (IRC) corresponding with TS-3

### Various energy values for the reported species and imaginary frequencies for the transition states

Table S1. Energy, enthalpy and free energy corrections of the structures calculated at B3LYP-

D3(BJ)/6-31G(d,p) SDD, single point energies at the M06-D3 SMD/6-311++G(d,p) SDD//B3LYP-D3(BJ)/6-31G(d,p) SDD level (in Hartree) and imaginary frequencies (in cm<sup>-1</sup>) of the transition states.

Structures	corr. to ZPE	corr. to <i>E</i>	corr. to <i>H</i>	corr. to <i>G</i>	SP <sub>SMD</sub>	Imaginary frequency
2a	0.214498	0.229484	0.230428	0.168075	-689.843664	—
HOAc	0.062006	0.066586	0.067531	0.034715	-229.036865	—
Cp*Rh(OAc)(OPiv)	0.411727	0.439702	0.440646	0.353085	-1075.268944	—
EtOH	0.080204	0.084486	0.085431	0.054825	-154.989869	—
PC	0.277946	0.295268	0.296212	0.230832	-1011.893720	—
INT-0	0.488166	0.520121	0.521066	0.424395	-1323.081328	—
INT-1	0.707712	0.754282	0.755227	0.628139	-2012.978727	—
TS-1	0.706370	0.752772	0.753717	0.624637	-2012.964423	-399.06
INT-2	0.708800	0.755092	0.628979	0.628979	-2013.018542	—
TS-2	0.708598	0.754161	0.755105	0.630803	-2013.008086	-154.74
INT-3	0.710213	0.755844	0.756789	0.632762	-2013.020534	—
TS-3	0.705707	0.751987	0.752931	0.626506	-2013.001913	-351.79
INT-4	0.709984	0.755898	0.756842	0.630809	-2013.078182	—
TS-4	0.708570	0.754396	0.755340	0.628693	-2013.068435	-72.34
INT-5	0.708211	0.755185	0.756129	0.625890	-2013.074173	—
TS-5	0.707436	0.753902	0.754846	0.626496	-2013.058696	-185.80
INT-6	0.708875	0.755476	0.756420	0.628902	-2013.076463	—
TS-6	0.707316	0.753907	0.754851	0.626586	-2013.070315	-150.62
INT-7	0.707545	0.754081	0.755025	0.627403	-2013.074825	—
TS-7	0.706020	0.751719	0.752664	0.625949	-2013.046231	-519.05
INT-8	0.709339	0.754750	0.755694	0.629940	-2013.110663	—
INT-9	0.708422	0.754301	0.755245	0.628233	-2013.091863	—
TS-8	0.704990	0.750457	0.751401	0.625790	-2013.091180	-764.10
INT-10	0.709555	0.756011	0.756955	0.627792	-2013.111598	—
TS-9	0.710534	0.755072	0.756016	0.633649	-2013.095321	-74.44
INT-4i	0.706854	0.753665	0.754610	0.626552	-2012.987038	—
TS-4i	0.706320	0.752467	0.753411	0.627132	-2012.987810	-49.24
TS-3ii	0.708815	0.753929	0.754873	0.630447	-2012.986325	-357.43
INT-4ii	0.710463	0.755790	0.756734	0.632688	-2013.022200	—
TS-5i	0.706841	0.753023	0.753967	0.627137	-2013.039625	-452.56
INT-6i	0.711634	0.757295	0.758240	0.632457	-2013.137003	—
INT-10i	0.360804	0.383523	0.384467	0.306322	-1166.892244	—
TS-9i	0.355709	0.377634	0.378578	0.302891	-1166.817638	-1126.96

**Cartesian coordinates of the optimized structures**

2a

C -1.77733700 0.70427000 -0.19881900

C	-0.86514300	0.08268800	0.29888200
C	0.21289500	-0.68609500	0.93737300
O	0.25586400	-0.46028600	2.34224500
H	-0.65375000	-0.45801100	2.66728300
H	0.02775300	-1.75197100	0.72442000
C	1.55794700	-0.30736000	0.33329600
C	2.33597400	0.69411400	0.91759100
C	1.99736500	-0.93883300	-0.83254900
C	3.55206600	1.05560600	0.33807700
H	1.98752100	1.16844600	1.82747000
C	3.21001600	-0.57161400	-1.41404300
H	1.38909100	-1.71698500	-1.28626700
C	3.99043200	0.42685200	-0.82847000
H	4.15804400	1.83021600	0.79858500
H	3.54708000	-1.06777400	-2.31905000
H	4.93732900	0.71075700	-1.27771600
C	-2.83359200	1.42338500	-0.87396400
O	-3.12195700	1.27509600	-2.04378700
O	-3.45345200	2.27407200	-0.03284500
C	-4.52803600	3.04686800	-0.61972800
C	-5.08169100	3.94386200	0.46866500
H	-5.28174500	2.35793200	-1.01334900
H	-4.12962200	3.61687100	-1.46447100
H	-5.89991600	4.54993800	0.06824600
H	-5.46684000	3.35178300	1.30345800
H	-4.30802500	4.61591300	0.84997100

#### HOAc

C	-0.09230100	0.12513500	-0.00000800
O	-0.64460700	1.20202200	-0.00003500
O	-0.77806500	-1.04599300	-0.00001400
H	-1.71910600	-0.80340100	-0.00004500
C	1.39615600	-0.10987700	0.00004900
H	1.68113500	-0.69192000	0.88127100
H	1.68119400	-0.69199000	-0.88110800
H	1.91502700	0.84752600	0.00003000

#### Cp\*Rh(OAc)(OPiv)

Rh	-0.65129200	0.22273500	0.06702300
C	-1.52749800	-1.37448400	-1.10742300
C	-1.13011000	-1.90473100	0.16483300
C	-1.82682100	-1.17681000	1.19154100
C	-2.72368600	-0.23264200	0.53679100
C	-2.53599900	-0.34861900	-0.86962600

C	0.02498300	2.65084100	-0.09569600
O	-0.43609400	2.17903700	0.99455200
O	-0.00695800	1.91488400	-1.13485300
O	1.34649400	0.10731200	0.54028500
C	2.16817200	-0.49329700	-0.27495500
O	1.84682200	-1.14834400	-1.26986700
C	-3.63538200	0.70747000	1.25765800
H	-4.50280900	0.16765800	1.65574300
H	-3.11727000	1.18237400	2.09436600
H	-3.99920100	1.49741500	0.59869800
C	-3.22229000	0.43651300	-1.94148500
H	-4.00435700	-0.16741500	-2.41676400
H	-3.68660000	1.33935500	-1.54090200
H	-2.51271700	0.73963900	-2.71474800
C	-1.73377900	-1.39985900	2.66720500
H	-1.87413300	-0.46440200	3.21374500
H	-2.50367700	-2.10622900	3.00215800
H	-0.75886800	-1.80548400	2.94365800
C	-0.13621600	-3.00000000	0.37854200
H	0.31964600	-2.92944000	1.36803600
H	-0.63477700	-3.97413500	0.30243600
H	0.65736000	-2.94068000	-0.36610900
C	-1.03790900	-1.84207100	-2.43946100
H	0.04725600	-1.95396100	-2.41219300
H	-1.49946900	-2.80255300	-2.70030200
H	-1.28653700	-1.12365600	-3.22307500
C	0.64440400	4.01835800	-0.14263300
H	1.71502100	3.91481800	0.06366600
H	0.52740500	4.45728000	-1.13506800
H	0.20598200	4.66411000	0.62011100
C	3.64777700	-0.31203600	0.13499900
C	3.96133800	1.19614200	0.17508100
C	3.84377900	-0.91829000	1.53792100
C	4.55792200	-1.01616000	-0.87750000
H	3.79740500	1.65467800	-0.80614100
H	3.32234000	1.70218200	0.90254000
H	5.00868300	1.35870400	0.45396500
H	3.61289800	-1.98970800	1.53670800
H	4.88441400	-0.80049000	1.86029000
H	3.19352300	-0.42700800	2.26550700
H	5.60737200	-0.89776800	-0.58517300
H	4.32977200	-2.08356500	-0.93361600
H	4.42528300	-0.59986100	-1.87925700

**EtOH**

O	-1.14924500	-0.39882500	-0.00001600
C	-0.08763600	0.54861000	-0.00001300
C	1.22150600	-0.22229200	0.00000100
H	-0.13631700	1.20151600	0.88679900
H	-0.13635700	1.20155600	-0.88679600
H	2.07370400	0.46449500	0.00011200
H	1.28652500	-0.86048500	0.88602100
H	1.28668200	-0.86040900	-0.88605700
H	-1.98349800	0.08602200	0.00012200

**PC**

N	1.21389500	-1.08020300	-0.54016300
C	1.92731900	0.02983000	-0.14689400
C	1.28678900	1.24526900	-0.09548900
C	-0.14096600	-1.14414400	-0.92829700
O	-0.63114000	-2.20661000	-1.30261700
C	-0.08120300	1.25490400	-0.44553700
C	-0.77958900	0.14574500	-0.81955300
C	-2.21249000	0.52037000	-1.09827200
O	-2.21987400	1.95732100	-0.93638800
H	-2.48424700	0.30772200	-2.13915900
C	-3.21285400	-0.13323300	-0.15760000
C	-3.80567800	0.58835000	0.88077700
C	-3.52379500	-1.48667400	-0.33146200
C	-4.70495400	-0.04180800	1.74261800
H	-3.57753500	1.64084600	1.00122300
C	-4.41961500	-2.11108400	0.53438100
H	-3.03675100	-2.05052500	-1.11942800
C	-5.01369000	-1.39113000	1.57293700
H	-5.16673100	0.52677200	2.54435400
H	-4.65332400	-3.16250900	0.39645800
H	-5.71448100	-1.87919100	2.24371500
C	3.35455200	-0.16353500	0.17140900
C	4.13431300	-1.09234700	-0.53651300
C	3.95439500	0.59137100	1.19142400
C	5.48243400	-1.26181000	-0.22895100
H	3.69840800	-1.65648600	-1.35604400
C	5.30252100	0.42104500	1.49411300
H	3.35211600	1.29175300	1.76027000
C	6.07001600	-0.50692500	0.78703600
H	6.07596800	-1.97616700	-0.79066600
H	5.75214600	1.00580800	2.29038100
H	7.12022900	-0.64044500	1.02652700



H	1.81114900	2.15645200	0.15639400
C	-1.00094200	2.42225300	-0.51512500
O	-0.78027700	3.58176200	-0.27565700
H	1.67673200	-1.98108400	-0.54160400

**INT-0**

N	0.01654200	0.73713200	0.79908100
C	2.21403700	0.04810700	0.21266500
C	1.55462400	-1.11307800	0.02194600
C	-2.60105800	-1.28127100	-0.50124900
C	-1.56454600	-1.73930000	-1.43037100
C	-0.93030700	-2.91111900	-0.86156500
C	-1.43667500	-3.05773100	0.45665600
C	-2.49870900	-2.06138900	0.65914300
Rh	-0.45467500	-1.09113200	0.26294300
C	1.30571300	1.21358800	0.52613400
O	1.60617600	2.39660900	0.52680900
C	-3.30264200	-1.93269800	1.91369000
H	-4.04654900	-2.73618300	1.98148400
H	-2.66536500	-2.00035100	2.79987800
H	-3.83142200	-0.97863300	1.95269700
C	-3.55751900	-0.16449800	-0.77384400
H	-4.43155000	-0.53255900	-1.32529900
H	-3.91457000	0.29008500	0.15314700
H	-3.08325200	0.61415700	-1.37191400
C	-1.34191200	-1.17428800	-2.79571300
H	-2.14829600	-1.48512800	-3.47261100
H	-1.32038800	-0.08279000	-2.75645400
H	-0.39474100	-1.51757100	-3.21557000
C	0.09728600	-3.76598700	-1.53370300
H	-0.38087100	-4.53591600	-2.15043000
H	0.74456800	-3.17014600	-2.18121100
H	0.73404900	-4.27047900	-0.80331000
C	-1.06812500	-4.11322600	1.45045000
H	-1.77592800	-4.95094700	1.40626600
H	-0.06823100	-4.50784900	1.25992000
H	-1.08542900	-3.71949300	2.46986100
O	-0.91648500	1.79566200	0.94213100
C	-1.30080900	2.38531000	-0.22682100
O	-1.02615300	1.95432800	-1.32538800
C	-2.08547900	3.66650000	0.05260800
C	-3.05303500	3.48276800	1.23548700
H	-2.51925900	3.22111900	2.15058100
H	-3.60005100	4.41562100	1.40590100

H	-3.78749600	2.69686500	1.02866800
C	-1.03353700	4.74753200	0.39486700
H	-0.35024400	4.90331800	-0.44442000
H	-1.53913500	5.69411200	0.61280600
H	-0.43677400	4.45133500	1.25983600
C	-2.85757100	4.05908500	-1.21377900
H	-2.18497100	4.15469000	-2.06828200
H	-3.61522300	3.30946700	-1.46432800
H	-3.36514600	5.01561800	-1.05525500
C	3.67664800	0.22811900	0.12283000
C	4.25206700	1.41732500	-0.35903700
C	4.53239800	-0.82450000	0.49448100
C	5.63561100	1.53453100	-0.47965300
H	3.60582000	2.24194400	-0.62958600
C	5.91358600	-0.70513400	0.36858000
H	4.10300900	-1.73393500	0.90393900
C	6.47274700	0.47666000	-0.12197200
H	6.06165800	2.45914400	-0.85877000
H	6.55521300	-1.52991700	0.66579100
H	7.55035600	0.57417300	-0.21622100
H	2.08975800	-2.01336200	-0.28250300

**INT-1**

N	0.70835100	0.20643100	0.77214300
C	-1.52376900	0.63955200	1.27668700
C	-1.65154800	-0.62931400	0.85269200
C	0.56535900	-2.90658900	1.66442400
C	-0.59102400	-3.48690200	1.03021500
C	-0.24750300	-3.77220400	-0.33071100
C	1.16074200	-3.47135900	-0.51569500
C	1.65724700	-2.94014600	0.69943900
Rh	-0.03319500	-1.56278200	0.04315200
C	-0.13293700	1.20265300	1.18774800
O	0.21275200	2.35185600	1.46145800
C	3.06777900	-2.52804100	0.97853800
H	3.64382400	-3.38524600	1.34917000
H	3.55983300	-2.16547200	0.07323000
H	3.10556600	-1.74675800	1.73810700
C	0.68815200	-2.45324600	3.08579600
H	1.20523100	-3.20821100	3.69060800
H	1.24778200	-1.51611600	3.14232900
H	-0.29585500	-2.28203600	3.52647600
C	-1.92053300	-3.74920300	1.66293600
H	-1.97062300	-4.78218600	2.02698000

H	-2.09574900	-3.08443300	2.51094900
H	-2.73288800	-3.60701700	0.94571700
C	-1.15000500	-4.39645600	-1.34929000
H	-1.13434000	-5.48954300	-1.25852900
H	-2.17714700	-4.04779700	-1.23305300
H	-0.83153600	-4.14191500	-2.36233900
C	1.94879600	-3.70209000	-1.76699500
H	2.48689200	-4.65627600	-1.71154900
H	1.29478200	-3.74234600	-2.64088800
H	2.66693700	-2.89702500	-1.92883000
O	2.01054600	0.69086000	0.46839500
C	2.79136100	0.93705500	1.57827300
O	2.55686600	0.47839000	2.66965000
C	3.95442300	1.85711600	1.21601900
C	4.75226400	1.27494700	0.03124900
H	4.15960000	1.24863200	-0.88466900
H	5.62598400	1.90692900	-0.15664900
H	5.11395800	0.26355100	0.24776500
C	3.36538700	3.22991800	0.82230900
H	2.76193400	3.64362200	1.63334800
H	4.18533000	3.92145800	0.60021400
H	2.72540300	3.14477800	-0.05570700
C	4.86111100	1.99107000	2.44629800
H	4.30540500	2.38406800	3.30038000
H	5.28070200	1.02387600	2.73805500
H	5.68687600	2.67297500	2.22088200
C	-1.08014100	-0.91834100	-1.72529000
C	0.12109200	-0.60789100	-1.89814800
C	1.29475100	0.02176800	-2.55435600
O	2.52650600	-0.47920800	-2.04714000
H	2.57351000	-0.15023500	-1.13121700
H	1.27292300	-0.28816400	-3.60725100
C	1.24714400	1.55014800	-2.48614800
C	0.19405400	2.25864500	-1.90711700
C	2.34416900	2.25047500	-3.00556600
C	0.24423100	3.65140800	-1.82869800
H	-0.65896500	1.73162100	-1.49999200
C	2.38700000	3.64077000	-2.93936600
H	3.16885400	1.69600400	-3.44256200
C	1.33663600	4.34558900	-2.34455000
H	-0.56593600	4.18518500	-1.34299700
H	3.24314800	4.17411500	-3.34184800
H	1.37639200	5.42858900	-2.27752300
C	-2.64526600	1.46445900	1.77327700

C	-2.44543100	2.50225900	2.69913400
C	-3.95310100	1.21852000	1.31638700
C	-3.52490400	3.25547300	3.15886500
H	-1.43942700	2.71790400	3.03430400
C	-5.02914900	1.96964700	1.78180300
H	-4.12071300	0.43596000	0.58302200
C	-4.81927600	2.99407700	2.70766200
H	-3.35159700	4.05287400	3.87589300
H	-6.03017200	1.76212100	1.41403400
H	-5.65567800	3.58603700	3.06748500
H	-2.59584500	-1.16704400	0.87460900
C	-2.52248700	-0.87907100	-1.93309000
O	-3.29115700	-1.79019600	-1.68872700
O	-2.88388100	0.33278200	-2.38697400
C	-4.30405000	0.59505400	-2.52444900
C	-4.50776900	2.08286400	-2.32024300
H	-4.84340100	-0.00568600	-1.78903100
H	-4.60954800	0.26616400	-3.52331400
H	-5.56333900	2.33372000	-2.46464500
H	-4.21849100	2.37236700	-1.30657000
H	-3.91418900	2.65958700	-3.03476600

**TS-1**

N	1.09431000	-0.19415400	0.80184800
C	-0.80243800	-1.26002000	1.63439400
C	-1.00354300	-1.60241400	0.33189000
C	2.16103400	-2.53822100	-1.26267700
C	0.97546500	-3.10770200	-1.80236700
C	0.50993400	-2.24877100	-2.87271200
C	1.47161400	-1.18778100	-3.04475900
C	2.46324500	-1.33085000	-2.02988300
Rh	0.52066200	-1.05300700	-1.00250800
C	0.23614000	-0.20925300	1.87040700
O	0.30823000	0.52912600	2.85645000
C	3.67251000	-0.46752600	-1.84484800
H	4.48449000	-0.80167600	-2.50295700
H	3.45048500	0.57436200	-2.08717800
H	4.03300500	-0.51634500	-0.81647300
C	2.99132000	-3.05896400	-0.13219200
H	3.91947500	-3.50414200	-0.51115900
H	3.25017700	-2.25454400	0.56102100
H	2.45544700	-3.82779600	0.42826100
C	0.28861000	-4.35755300	-1.34785000
H	0.60227700	-5.21400000	-1.95664800

H	0.51898900	-4.58198200	-0.30467000
H	-0.79695900	-4.26781500	-1.43902800
C	-0.69842500	-2.50648100	-3.72065400
H	-0.49696600	-3.29253400	-4.45854500
H	-1.54902000	-2.82443400	-3.11260800
H	-0.99906700	-1.60901500	-4.26538700
C	1.43361600	-0.10683900	-4.08124200
H	2.07183900	-0.36939900	-4.93365000
H	0.42011500	0.04219500	-4.46117900
H	1.77859500	0.84138900	-3.66465200
O	1.89502900	0.99300300	0.82864200
C	3.11395200	0.84148400	1.43602700
O	3.60725100	-0.23188700	1.68939600
C	3.71408400	2.19778600	1.80196700
C	3.28635600	3.31783800	0.83878700
H	2.20891400	3.49076900	0.86251200
H	3.78273900	4.24797100	1.13287300
H	3.57789100	3.10027300	-0.19383800
C	3.17856200	2.50006200	3.22342700
H	3.54855100	1.76052300	3.93896600
H	3.52014900	3.49162700	3.53818100
H	2.08682400	2.46791700	3.24163800
C	5.24362400	2.06573100	1.82221800
H	5.55459300	1.24253500	2.46799000
H	5.63649000	1.87563800	0.81775100
H	5.69020000	2.99412800	2.19121900
C	-1.46861600	-0.14325300	-0.84637000
C	-0.54462100	0.69393800	-1.18235900
C	-0.19959500	2.06943800	-1.62749400
O	1.20955200	2.27497400	-1.65747200
H	1.55827400	1.94124000	-0.81324200
H	-0.53265000	2.18876400	-2.66637600
C	-0.94356600	3.08198700	-0.76847900
C	-0.79191400	3.08470300	0.62462400
C	-1.80618800	4.00156200	-1.36695600
C	-1.49710500	4.00212400	1.40057900
H	-0.14327000	2.36582300	1.11292600
C	-2.51392400	4.91953700	-0.58900900
H	-1.93078400	3.99466200	-2.44668600
C	-2.36071700	4.92045900	0.79754800
H	-1.37810900	3.98876100	2.47963000
H	-3.18313500	5.62983300	-1.06578800
H	-2.91214600	5.63104100	1.40616100
C	-1.56656000	-1.82989900	2.75073400

C	-1.02821400	-1.87122400	4.05006700
C	-2.85382100	-2.35970300	2.53709100
C	-1.74626100	-2.45154500	5.09255400
H	-0.05388100	-1.43500500	4.23115400
C	-3.56606800	-2.93777400	3.58324900
H	-3.30315200	-2.29184700	1.55096300
C	-3.01364000	-2.99123300	4.86531400
H	-1.31436600	-2.48000000	6.08868000
H	-4.55965400	-3.33697100	3.40085900
H	-3.57170900	-3.43940000	5.68210500
H	-1.70257500	-2.37969400	0.04926500
C	-2.89862800	-0.33007800	-1.12763200
O	-3.49218300	-1.39152900	-1.19130600
O	-3.46666500	0.87347400	-1.32431900
C	-4.89459700	0.88389400	-1.54877500
C	-5.30432900	2.33703200	-1.68046100
H	-5.38443500	0.38934900	-0.70433900
H	-5.11631100	0.30331200	-2.44980200
H	-6.38713000	2.40730200	-1.82161900
H	-5.02673200	2.89828400	-0.78462600
H	-4.81094000	2.80308700	-2.53787200

**INT-2**

N	0.52277500	1.11393100	0.70697600
C	1.29875400	-0.88966900	1.44225400
C	0.73951300	-1.96639300	0.75591100
C	2.82600600	0.81830600	-1.75158600
C	3.15847900	-0.54873100	-1.66445300
C	2.14646300	-1.31478100	-2.38779400
C	1.23800100	-0.38675900	-2.98862300
C	1.59909700	0.92816500	-2.53496100
Rh	1.06006300	-0.26962000	-0.76342200
C	0.39839000	0.30639400	1.79424300
O	-0.27010800	0.41874900	2.80871500
C	0.96166800	2.21818800	-2.94530700
H	1.45573900	2.61774600	-3.84043100
H	-0.09569500	2.07416700	-3.17127200
H	1.05322700	2.96467700	-2.15333800
C	3.54214800	1.97767900	-1.13261000
H	4.04076100	2.57987700	-1.90180800
H	2.84075600	2.62248800	-0.59610500
H	4.30185700	1.63961200	-0.42530400
C	4.33027900	-1.15634100	-0.96273700
H	5.09839400	-1.44805700	-1.68926200

H	4.77768100	-0.46563400	-0.24772700
H	4.04106100	-2.05287900	-0.40912800
C	2.17626000	-2.79606400	-2.60896900
H	2.76714000	-3.05034500	-3.49796900
H	2.62348300	-3.31456800	-1.75710200
H	1.16922200	-3.19499900	-2.75141200
C	0.13090200	-0.71775400	-3.93922900
H	0.49189500	-0.65013000	-4.97311800
H	-0.23481600	-1.73527100	-3.78197200
H	-0.70469000	-0.02882200	-3.81367500
O	-0.56507800	2.04327900	0.61317400
C	-0.18769600	3.35113000	0.50872700
O	0.95097400	3.71574800	0.32629500
C	-1.40840600	4.25312700	0.69815600
C	-2.58839000	3.76997200	-0.16835500
H	-2.93623900	2.78051100	0.13355800
H	-3.42306800	4.46962500	-0.05915600
H	-2.32079800	3.73592700	-1.22976000
C	-1.79534200	4.16418100	2.19305800
H	-0.98548100	4.53289800	2.83026500
H	-2.68205800	4.77914300	2.37726200
H	-2.01340900	3.13225700	2.47743500
C	-1.02035200	5.68873000	0.32472900
H	-0.16439000	6.02995500	0.91095300
H	-0.75151400	5.76231300	-0.73327700
H	-1.86508100	6.35850200	0.51245500
C	-0.68427200	-1.98094400	0.30642200
C	-0.85444500	-0.97059500	-0.56548200
C	-2.08212600	-0.41602500	-1.23357200
O	-1.79686600	0.83505500	-1.87761500
H	-1.44778300	1.41225400	-1.18063100
H	-2.36458700	-1.09258000	-2.04900400
C	-3.29704300	-0.23552100	-0.32887200
C	-3.19243100	0.04433400	1.03759200
C	-4.56390800	-0.25343500	-0.92272700
C	-4.34060300	0.28597500	1.79426500
H	-2.22813800	0.07241800	1.52857300
C	-5.71066700	-0.01062400	-0.16819600
H	-4.64874700	-0.46082300	-1.98615200
C	-5.60167000	0.25697900	1.19829100
H	-4.24141700	0.49545200	2.85519000
H	-6.68664300	-0.03364700	-0.64460100
H	-6.49231900	0.44258600	1.79138000
C	2.67912200	-0.89621700	1.97578000

C	3.35787800	0.32060900	2.16127600
C	3.33320200	-2.09336500	2.30190900
C	4.66925900	0.33296500	2.62727000
H	2.85568500	1.24888500	1.90873300
C	4.64643000	-2.07735700	2.77024300
H	2.80535100	-3.03719100	2.21319800
C	5.32151400	-0.86633100	2.92738800
H	5.18347600	1.28039400	2.75789300
H	5.13778200	-3.01192900	3.02339200
H	6.34326000	-0.85523400	3.29431000
H	1.34835300	-2.85411400	0.59975100
C	-1.58502000	-3.01946000	0.83023700
O	-1.28073800	-3.76978800	1.74165900
O	-2.75970900	-3.07547200	0.16844700
C	-3.73629000	-3.99182600	0.70664800
C	-4.98635000	-3.87417500	-0.14169100
H	-3.92408500	-3.72634700	1.75162500
H	-3.31751700	-5.00295400	0.69233600
H	-5.74859300	-4.56905300	0.22448000
H	-5.38720500	-2.85903000	-0.10013600
H	-4.77098600	-4.11946500	-1.18612500

**TS-2**

N	-0.52845900	-0.74294100	1.20760500
C	-1.63801200	1.35058000	1.24913700
C	-1.18897000	2.18269500	0.27536800
C	-1.04155000	-1.82911800	-2.56946200
C	-2.06727900	-2.29776000	-1.62910300
C	-2.96851400	-1.25059100	-1.41699000
C	-2.51997500	-0.09978300	-2.22631300
C	-1.38363100	-0.49602200	-2.99953600
Rh	-0.88747900	-0.48987800	-0.89594900
C	-0.65931300	0.39916500	1.93001800
O	-0.12897600	0.69405900	2.99841100
C	-0.67483300	0.30345000	-4.04738000
H	-1.04920800	0.05222800	-5.04722300
H	-0.82551500	1.37357400	-3.88896500
H	0.39767000	0.10499200	-4.01009500
C	0.01903200	-2.70197400	-3.15109700
H	-0.43655500	-3.36959100	-3.89445800
H	0.79427000	-2.11131400	-3.63704300
H	0.48419700	-3.31778700	-2.37979800
C	-2.03625500	-3.64105300	-0.97502200
H	-2.28926500	-4.42966400	-1.69352800



H	-1.03468600	-3.84705800	-0.58841100
H	-2.74183100	-3.69795400	-0.14451600
C	-4.15185100	-1.22780600	-0.50547000
H	-5.07990300	-1.31688800	-1.08346800
H	-4.11748100	-2.04950500	0.21154600
H	-4.20190900	-0.29586400	0.06132000
C	-3.25416200	1.19669200	-2.32998500
H	-4.01990500	1.12969400	-3.11370800
H	-3.75507500	1.44216200	-1.39238000
H	-2.57750800	2.01385500	-2.58662200
O	0.48529500	-1.56401600	1.81727200
C	1.21111400	-2.31545000	1.00577200
O	1.06464100	-2.36402400	-0.21488400
C	2.22326500	-3.18272500	1.75425700
C	2.43880100	-2.70938900	3.19888500
H	1.51527300	-2.75114100	3.77989200
H	3.18272600	-3.35249900	3.68005200
H	2.80399200	-1.68059300	3.22065100
C	1.65434200	-4.61913400	1.73931700
H	1.49695200	-4.96491800	0.71357200
H	2.35887400	-5.29868600	2.22879600
H	0.70211900	-4.67198500	2.27740600
C	3.54944100	-3.13543800	0.97364600
H	3.40538700	-3.45635000	-0.06043000
H	3.96583800	-2.12592500	0.96602100
H	4.27456300	-3.80332300	1.44915500
C	0.16287100	2.11167900	-0.33088600
C	0.57854400	0.93688800	-0.87003100
C	1.96721100	0.64200400	-1.39259200
O	2.00391900	-0.53437400	-2.20542900
H	1.79340300	-1.27668100	-1.61188200
H	2.26556200	1.45277900	-2.06355000
C	3.04065400	0.54258700	-0.30115400
C	4.34350600	0.23582200	-0.71776800
C	2.80097100	0.74963000	1.05928800
C	5.38922800	0.16269700	0.19979900
H	4.52765600	0.05436800	-1.77186400
C	3.84721200	0.66853200	1.98243000
H	1.80902300	0.98561900	1.41908800
C	5.14476900	0.38225400	1.55861300
H	6.39426100	-0.06526300	-0.14368100
H	3.63592500	0.83551000	3.03437900
H	5.95701900	0.32591500	2.27729100
C	-3.01821900	1.36529400	1.77437500

C	-3.38232900	0.49032400	2.81413000
C	-4.02187400	2.18891400	1.22822100
C	-4.69619300	0.42802800	3.27326900
H	-2.62443600	-0.13582700	3.27043300
C	-5.33381200	2.12679600	1.68940000
H	-3.77817300	2.88917800	0.43710800
C	-5.68168900	1.23959200	2.71057700
H	-4.94888700	-0.25746600	4.07671800
H	-6.08710400	2.77339800	1.24886100
H	-6.70612300	1.18763900	3.06615100
H	-1.82571500	2.99317100	-0.06957600
C	0.89791400	3.39811800	-0.26510700
O	0.40842600	4.42573400	0.17259000
O	2.16430300	3.32268000	-0.73091300
C	3.00809600	4.47312700	-0.52539700
C	4.44441100	3.98679000	-0.57119400
H	2.75359600	4.92729900	0.43539900
H	2.79571000	5.20986700	-1.30829700
H	5.12774000	4.82997300	-0.42854600
H	4.62523200	3.24838800	0.21396900
H	4.66969200	3.51880500	-1.53374300

**INT-3**

N	-0.74749500	-0.62504100	1.21425600
C	-1.97240800	1.40978000	0.94508300
C	-1.49609700	2.08570300	-0.12279200
C	-1.41795700	-2.92715900	-1.60075100
C	-2.42853600	-2.00041300	-1.28811500
C	-2.18667100	-0.78148000	-2.05545900
C	-1.04879900	-1.01683800	-2.91404200
C	-0.53164500	-2.30056000	-2.58439100
Rh	-0.43189900	-1.00762100	-0.79170900
C	-1.00907200	0.59078500	1.77582500
O	-0.57783000	1.00817500	2.84759200
C	0.65743100	-2.97006800	-3.19794500
H	0.34173100	-3.64337800	-4.00444800
H	1.35217800	-2.23634100	-3.60713200
H	1.19319400	-3.57296700	-2.45869200
C	-1.21262000	-4.29505600	-1.02746000
H	-1.45892900	-5.07388400	-1.75921200
H	-0.16973900	-4.44397900	-0.73013000
H	-1.83708500	-4.45391200	-0.14585700
C	-3.53417200	-2.14669100	-0.29188800
H	-4.50118600	-2.23162300	-0.80111800

H	-3.39919700	-3.03222600	0.33175800
H	-3.57928700	-1.27547000	0.36738600
C	-3.15377400	0.34948600	-2.18968500
H	-3.85025300	0.14556100	-3.01375300
H	-3.73993800	0.48465500	-1.28078900
H	-2.64212200	1.28805300	-2.40787300
C	-0.52906500	-0.07506600	-3.95363700
H	-1.04213800	-0.23770400	-4.90943000
H	-0.69539300	0.96116200	-3.65140200
H	0.54314900	-0.21123900	-4.10198900
O	0.27917800	-1.28552400	2.05318500
C	1.23127100	-1.88085200	1.39423200
O	1.28843900	-1.90265100	0.14547300
C	2.22872900	-2.64105500	2.25554400
C	2.37773400	-1.98167800	3.63641500
H	1.42453000	-1.93635700	4.16615500
H	3.08498200	-2.56387300	4.23494200
H	2.76243800	-0.96452000	3.53815800
C	1.65765100	-4.07151500	2.40569400
H	1.53228400	-4.55042200	1.42974000
H	2.35105500	-4.67635900	2.99759000
H	0.69065800	-4.05796400	2.91711700
C	3.58325200	-2.68142500	1.52979300
H	3.49615500	-3.16487900	0.55402900
H	3.98123200	-1.67542700	1.38121500
H	4.29601700	-3.24981000	2.13477400
C	-0.13577500	1.96950300	-0.67195900
C	0.51823500	0.79740200	-0.90322600
C	1.98003400	0.74138600	-1.32631500
O	2.28931200	-0.41743000	-2.11281100
H	2.22643700	-1.17310700	-1.51007800
H	2.19868300	1.57583600	-1.99692200
C	2.95429400	0.83834000	-0.14616700
C	2.56204300	1.17875100	1.15151900
C	4.31107700	0.59328900	-0.39796100
C	3.50829800	1.27857400	2.17415800
H	1.52340500	1.37994000	1.37712400
C	5.25782100	0.69992700	0.62031600
H	4.61535400	0.31393300	-1.40139900
C	4.85894500	1.04347700	1.91448300
H	3.17945600	1.54757600	3.17364400
H	6.30601700	0.51366200	0.40400300
H	5.59336600	1.12683900	2.71018500
C	-3.35713500	1.51778100	1.44599500

C	-3.71859600	0.93784800	2.67678200
C	-4.36751900	2.15586200	0.69987900
C	-5.03220900	0.99292300	3.13762900
H	-2.95592700	0.46682300	3.28557500
C	-5.67747400	2.21466300	1.16567200
H	-4.12870500	2.60885900	-0.25578800
C	-6.02041500	1.62944100	2.38649100
H	-5.28154400	0.54009900	4.09282800
H	-6.43487400	2.71508900	0.56927700
H	-7.04403100	1.67049700	2.74616900
H	-2.10578600	2.86099100	-0.57688600
C	0.40823000	3.31874300	-1.03616200
O	-0.27177200	4.22813300	-1.47753200
O	1.73083100	3.43857400	-0.80804300
C	2.34176300	4.70636400	-1.12167600
C	3.79522100	4.59946300	-0.70145900
H	1.80833600	5.49649600	-0.58504000
H	2.22953600	4.90096800	-2.19337700
H	4.31660400	5.53956100	-0.90609500
H	3.87060000	4.38070000	0.36706600
H	4.29883800	3.79435200	-1.24362200

**TS-3**

N	1.21605800	-0.42299300	-1.06812700
C	2.08123900	1.35647200	-1.02987600
C	1.50948600	2.17119500	-0.09660500
C	1.32471400	-2.86789800	1.59755300
C	2.39289500	-1.97049200	1.39619700
C	2.11721800	-0.75668700	2.15560300
C	0.90121500	-0.97035200	2.90626600
C	0.38011900	-2.23710200	2.51930500
Rh	0.48275600	-0.92118900	0.71368500
C	1.05647800	0.51563800	-1.93508100
O	0.59832700	0.85025700	-3.00231600
C	-0.87108600	-2.89088600	3.00963900
H	-0.62830500	-3.69553400	3.71422300
H	-1.52469900	-2.17306100	3.50398700
H	-1.42332400	-3.33321700	2.17497000
C	1.12849800	-4.22070300	0.98929800
H	1.30986400	-5.01362100	1.72503600
H	0.10410100	-4.33453400	0.62429800
H	1.80137800	-4.38002300	0.14504300
C	3.57388300	-2.15041700	0.49626200
H	4.48056900	-2.33229800	1.08497900

H	3.43183700	-2.99234600	-0.18309500
H	3.73963600	-1.25875400	-0.11344700
C	3.04469000	0.40657400	2.30769100
H	3.58809300	0.34856100	3.25894800
H	3.77939400	0.43077300	1.50165100
H	2.49945200	1.35459500	2.29384900
C	0.31258800	-0.02450700	3.90490800
H	0.67520900	-0.25870700	4.91319300
H	0.59738900	1.00559500	3.67791200
H	-0.77647300	-0.08567900	3.89669800
O	-0.29698500	-1.97231800	-2.12146500
C	-1.24410100	-2.13831400	-1.34796500
O	-1.25194000	-1.78069300	-0.09498400
C	-2.51238000	-2.88202200	-1.82680900
C	-2.80692200	-2.47082700	-3.27814600
H	-1.93685700	-2.64424300	-3.91359500
H	-3.65401800	-3.04836900	-3.66393800
H	-3.06383100	-1.40949000	-3.33220800
C	-2.17499200	-4.38678300	-1.76716400
H	-1.96273300	-4.70183300	-0.73934500
H	-3.02409800	-4.97558500	-2.13038900
H	-1.30382000	-4.61426000	-2.38772400
C	-3.72539100	-2.57871600	-0.93717500
H	-3.55418900	-2.89563000	0.09482700
H	-3.95791800	-1.51172600	-0.93226000
H	-4.60102600	-3.11670700	-1.31692700
C	0.18848700	2.05222600	0.47989300
C	-0.47208600	0.87573700	0.75119400
C	-1.93055900	0.85212600	1.18378700
O	-2.27934400	-0.31314000	1.92601200
H	-2.21207000	-1.04854800	1.28862300
H	-2.10706600	1.67966500	1.87680900
C	-2.90027600	1.01946900	0.01060100
C	-2.49951300	1.09684300	-1.32396200
C	-4.26793600	1.05393500	0.31082000
C	-3.44877000	1.21514000	-2.34168200
H	-1.45178000	1.06561500	-1.59025400
C	-5.21662900	1.17769600	-0.70216600
H	-4.58237400	0.96881900	1.34661500
C	-4.80895700	1.25845800	-2.03629100
H	-3.11457300	1.26957500	-3.37327400
H	-6.27325600	1.20682000	-0.45182200
H	-5.54574800	1.35017300	-2.82873400
C	3.48608100	1.36163800	-1.45402700

C	3.88231000	0.73680900	-2.65033600
C	4.47184300	1.97426300	-0.65774900
C	5.22088100	0.72504300	-3.03190100
H	3.13644400	0.27463600	-3.28688900
C	5.80720600	1.97252500	-1.05163200
H	4.18906400	2.44966500	0.27511900
C	6.18888300	1.34285400	-2.23756900
H	5.50742400	0.23750200	-3.95858600
H	6.55167500	2.45405600	-0.42483300
H	7.23161600	1.33268500	-2.53939300
H	2.04611600	3.07743400	0.17589700
C	-0.32793600	3.41087400	0.87529900
O	0.38607300	4.29733400	1.30927700
O	-1.64638300	3.55523300	0.67837300
C	-2.22485100	4.83466900	1.02291400
C	-3.69217500	4.76376700	0.64971300
H	-1.69067100	5.61650900	0.47542600
H	-2.07204100	5.01411400	2.09186000
H	-4.17912500	5.71838800	0.87094400
H	-3.80882000	4.54734200	-0.41534300
H	-4.19978900	3.97325100	1.20819000

#### INT-4

N	1.11495000	0.01592400	-0.98193000
C	1.82107200	1.26216000	-0.88969500
C	1.26070300	2.26199900	-0.17416800
C	1.62196600	-2.50777600	1.88218200
C	2.60076200	-1.56078800	1.54308600
C	2.24756100	-0.29642900	2.18803800
C	1.09567500	-0.53701000	3.03018500
C	0.66146900	-1.86759500	2.78669100
Rh	0.57046300	-0.70491800	0.88302300
C	0.45969300	-0.18354900	-2.11507700
O	0.39981400	0.43157900	-3.15271300
C	-0.48098800	-2.57894900	3.44206400
H	-0.12202500	-3.19369600	4.27698300
H	-1.21888900	-1.87273600	3.82278200
H	-0.98399000	-3.25047900	2.73875100
C	1.51601400	-3.92662900	1.41658700
H	1.80108100	-4.62617100	2.21183700
H	0.48843400	-4.16733400	1.12600900
H	2.16147400	-4.11517900	0.55610400
C	3.78230500	-1.74962800	0.64563600
H	4.70290500	-1.82211400	1.23741400

H	3.69331900	-2.66107800	0.05073500
H	3.89608900	-0.91161200	-0.04477300
C	3.10248300	0.93127800	2.21185700
H	3.77610700	0.91084300	3.07820300
H	3.71235800	1.01054800	1.31062000
H	2.49171400	1.83400700	2.27780900
C	0.48365900	0.45106400	3.97189700
H	0.97345500	0.39742700	4.95197000
H	0.59791200	1.46901800	3.59274700
H	-0.58254900	0.25927100	4.09957600
O	-0.28839800	-1.48226500	-2.18655700
C	-1.03457500	-2.04574500	-1.27182800
O	-1.01148700	-1.77590800	-0.05954900
C	-1.93317700	-3.15719200	-1.80299400
C	-2.62103800	-2.70475000	-3.10377200
H	-1.88715700	-2.42528700	-3.86165100
H	-3.23234800	-3.52589200	-3.49090900
H	-3.27116300	-1.84597400	-2.92129000
C	-1.01104300	-4.36663600	-2.08609000
H	-0.49987100	-4.69766800	-1.17595500
H	-1.61294100	-5.20055400	-2.45957000
H	-0.25864100	-4.11814100	-2.83887500
C	-2.98178800	-3.52173100	-0.74236100
H	-2.51291000	-3.87482200	0.17982700
H	-3.60856400	-2.65947500	-0.50001600
H	-3.62398300	-4.31915800	-1.12800500
C	-0.05649900	2.15971400	0.45625000
C	-0.59463400	0.97598500	0.86988300
C	-2.04567500	0.79082500	1.26842100
O	-2.24249200	-0.30785500	2.16573200
H	-2.04217100	-1.10763000	1.65757400
H	-2.38666100	1.66090200	1.83352500
C	-2.97245600	0.63581500	0.05118200
C	-2.60951600	1.01434500	-1.24507900
C	-4.24982000	0.09870900	0.26024700
C	-3.49968900	0.85776300	-2.30860200
H	-1.63162500	1.43714300	-1.43349700
C	-5.14458400	-0.05094500	-0.79956200
H	-4.53198400	-0.20539500	1.26239800
C	-4.77285800	0.32857100	-2.09115000
H	-3.18704500	1.14538400	-3.30776700
H	-6.13285100	-0.46301600	-0.61559500
H	-5.46660500	0.21049400	-2.91836400
C	3.15620700	1.33629400	-1.51450100

C	3.58838900	0.34542000	-2.41410000
C	4.05376400	2.37657900	-1.20295500
C	4.85673800	0.40074200	-2.98822200
H	2.92353800	-0.46947400	-2.66819800
C	5.31904600	2.43034900	-1.77840100
H	3.76472800	3.14237300	-0.49199200
C	5.73017400	1.44234600	-2.67625900
H	5.16092300	-0.37460400	-3.68535500
H	5.99044100	3.24328300	-1.51771300
H	6.71929600	1.48304500	-3.12204100
H	1.74309300	3.22901400	-0.11520300
C	-0.71038200	3.49984200	0.59083200
O	-0.09785700	4.54989600	0.67217600
O	-2.05961600	3.44612800	0.58760200
C	-2.76689800	4.70082400	0.63188600
C	-4.22797400	4.38080900	0.37955800
H	-2.34853300	5.36695300	-0.12797200
H	-2.60428000	5.16966700	1.60820500
H	-4.82086900	5.30053800	0.38098800
H	-4.34838900	3.88493500	-0.58743000
H	-4.62055400	3.71338500	1.15207000

**TS-4**

N	1.29743300	0.07751300	-0.95992800
C	2.00109100	1.32723300	-0.71634800
C	1.39341600	2.22760200	0.08089800
C	1.36474400	-2.71969000	1.73478200
C	2.41921300	-1.80628900	1.57679800
C	2.08666600	-0.57959800	2.30096900
C	0.84154000	-0.80601000	2.98803100
C	0.35358200	-2.08955600	2.58317700
Rh	0.49254700	-0.79797700	0.81455300
C	1.07551900	-0.24043700	-2.15427200
O	1.00316300	-0.26903300	-3.31781500
C	-0.88379900	-2.77895900	3.06088400
H	-0.62768100	-3.52880900	3.81969600
H	-1.59242300	-2.07032300	3.48682600
H	-1.37965100	-3.29836500	2.23567800
C	1.24260400	-4.08808900	1.14232900
H	1.45969600	-4.86155300	1.88952400
H	0.22925800	-4.26286000	0.77181500
H	1.92800400	-4.22256000	0.30366800
C	3.67205100	-2.02363900	0.78999800
H	4.43202700	-2.50727300	1.41596000



H	3.49356100	-2.66628000	-0.07547300
H	4.09031000	-1.08208700	0.43236600
C	2.99771000	0.59081500	2.50037200
H	3.64038100	0.43758700	3.37657200
H	3.64168900	0.74947300	1.63368700
H	2.42797700	1.50939400	2.65532300
C	0.17288500	0.13145900	3.94298600
H	0.47992700	-0.08903100	4.97261300
H	0.44061800	1.16730700	3.72418400
H	-0.91186200	0.03942400	3.86942700
O	0.14768600	-2.28571000	-1.87152600
C	-0.94436700	-2.30070400	-1.26866600
O	-1.15544700	-1.69569800	-0.15092600
C	-2.12681900	-3.08028000	-1.87009600
C	-2.38804500	-2.50439200	-3.27591400
H	-1.48052500	-2.54551500	-3.88216500
H	-3.17516500	-3.08003900	-3.77466500
H	-2.71748900	-1.46293200	-3.21224100
C	-1.69387800	-4.55496000	-1.98350000
H	-1.50812300	-4.98881200	-0.99403300
H	-2.48366400	-5.14251100	-2.46328800
H	-0.77971900	-4.64292000	-2.57489500
C	-3.39042500	-2.95881100	-1.00985200
H	-3.22847500	-3.36009100	-0.00461200
H	-3.70803400	-1.91830400	-0.91261600
H	-4.20615400	-3.52549300	-1.47205900
C	0.02742000	2.11941800	0.59694900
C	-0.59233200	0.92956500	0.85916800
C	-2.07367400	0.80552100	1.17289100
O	-2.40027700	-0.38345400	1.89128600
H	-2.23451100	-1.11071000	1.26530100
H	-2.37096600	1.61848900	1.83920300
C	-2.95123500	0.89722100	-0.08273100
C	-2.45518100	1.14076700	-1.36509300
C	-4.32929300	0.70795700	0.07937400
C	-3.31602300	1.20034900	-2.46253100
H	-1.39202700	1.28879800	-1.50966500
C	-5.19312000	0.77176100	-1.01292800
H	-4.71605000	0.49710000	1.07123700
C	-4.68884600	1.01851000	-2.29179400
H	-2.90937200	1.38635200	-3.45248500
H	-6.25963300	0.62630900	-0.86648100
H	-5.35819800	1.06506900	-3.14558600
C	3.34260200	1.47319500	-1.30904000

C	4.03145400	0.36789200	-1.84044400
C	3.97612100	2.73074000	-1.35835000
C	5.30848900	0.51016400	-2.38177800
H	3.57325700	-0.61303900	-1.82273700
C	5.25169600	2.86703100	-1.89284400
H	3.45718800	3.61042400	-0.99482300
C	5.92883700	1.75736700	-2.40710800
H	5.81630900	-0.36133100	-2.78378000
H	5.71567700	3.84835400	-1.92087500
H	6.92223700	1.86890200	-2.83006000
H	1.90439800	3.15670400	0.29875000
C	-0.57150100	3.47945300	0.78529500
O	0.08733800	4.49682900	0.92483100
O	-1.91823300	3.48773100	0.75388200
C	-2.57225300	4.77057700	0.82208800
C	-4.02716000	4.53532300	0.46333200
H	-2.07646700	5.45438000	0.12752200
H	-2.45172700	5.17901700	1.83117000
H	-4.57447200	5.48285100	0.47905300
H	-4.10938500	4.09569300	-0.53423900
H	-4.49937800	3.84922300	1.17174600

**INT-5**

N	1.27060800	0.12375100	-1.06961700
C	2.00842200	1.35060200	-0.82062500
C	1.39565300	2.27921400	-0.06100900
C	1.41238500	-2.63343200	1.73346700
C	2.46507200	-1.74296500	1.46964200
C	2.19854900	-0.48163600	2.16348500
C	0.98857800	-0.64978900	2.91791300
C	0.45669600	-1.94521500	2.59868900
Rh	0.51497000	-0.73545800	0.77886700
C	0.81428300	-0.17690800	-2.18029500
O	0.38037000	-0.43340700	-3.22976200
C	-0.75458700	-2.58585700	3.19478400
H	-0.46171800	-3.22566400	4.03685200
H	-1.46490200	-1.83824400	3.54429400
H	-1.26144500	-3.21835300	2.46128500
C	1.25295400	-4.02878900	1.21804300
H	1.65781200	-4.75662300	1.93247800
H	0.19958100	-4.26911800	1.05895700
H	1.75820600	-4.15708200	0.26037800
C	3.64962000	-2.00564500	0.59653700
H	4.48733800	-2.38480200	1.19492600

H	3.41621800	-2.74935200	-0.16832700
H	3.98727100	-1.09723100	0.09478000
C	3.14833200	0.66981900	2.27465400
H	3.79347600	0.55057700	3.15434200
H	3.79132500	0.74732300	1.39630100
H	2.61197300	1.61584700	2.37588400
C	0.38822700	0.33678600	3.86834900
H	0.74786400	0.15009100	4.88768300
H	0.65941800	1.35842700	3.59454400
H	-0.70031200	0.26021500	3.86142300
O	0.18728700	-2.73401800	-1.53313500
C	-0.93310400	-2.50410000	-1.06161200
O	-1.16151500	-1.62668400	-0.12681000
C	-2.17794500	-3.23060700	-1.60765200
C	-2.42870800	-2.66580600	-3.02168700
H	-1.54583500	-2.79937600	-3.65174800
H	-3.27502400	-3.18337900	-3.48665900
H	-2.66638600	-1.59871000	-2.97535400
C	-1.85338700	-4.73177200	-1.69444100
H	-1.69344300	-5.15853800	-0.69721500
H	-2.68405800	-5.27257600	-2.16032600
H	-0.94816000	-4.89322900	-2.28286200
C	-3.41561400	-2.99925100	-0.73144400
H	-3.24945500	-3.35076300	0.29248800
H	-3.68259100	-1.94152700	-0.68821700
H	-4.26814300	-3.55216300	-1.14160000
C	0.03460900	2.18195200	0.47034200
C	-0.56943900	0.99638900	0.79616500
C	-2.03915800	0.87756900	1.16473600
O	-2.32897700	-0.29354800	1.92448500
H	-2.17532400	-1.03452500	1.30873600
H	-2.31539900	1.70717000	1.81969800
C	-2.96498300	0.92841700	-0.05913900
C	-2.52446900	1.15375000	-1.36442300
C	-4.33082500	0.71087400	0.15929700
C	-3.42495000	1.16016000	-2.43070300
H	-1.47258500	1.32806200	-1.55194600
C	-5.23559300	0.72481300	-0.90132600
H	-4.67486700	0.51378900	1.16940500
C	-4.78513500	0.94756500	-2.20428400
H	-3.05884600	1.32694800	-3.43967200
H	-6.29180300	0.55654000	-0.71126500
H	-5.48599500	0.95158000	-3.03369300
C	3.37221900	1.41734000	-1.36728500

C	3.90045300	0.37014400	-2.14415500
C	4.19842700	2.53169100	-1.11526400
C	5.19499800	0.43981900	-2.65852600
H	3.30822000	-0.51595500	-2.33717100
C	5.48721300	2.59623800	-1.62982100
H	3.83056200	3.35355100	-0.51217200
C	5.99595400	1.55126300	-2.40714400
H	5.57451000	-0.38409600	-3.25509700
H	6.10023100	3.46795000	-1.42172600
H	7.00381100	1.60495500	-2.80626800
H	1.89699600	3.22292000	0.11294700
C	-0.57088000	3.54508700	0.61159900
O	0.08263100	4.57506300	0.65065200
O	-1.91622500	3.53971800	0.66025900
C	-2.58403700	4.81742700	0.67218900
C	-4.04680200	4.54481600	0.37728700
H	-2.11971200	5.46256100	-0.07864600
H	-2.43561200	5.28750000	1.65028400
H	-4.60600300	5.48530000	0.35713600
H	-4.15607100	4.04701000	-0.58983800
H	-4.48578300	3.89555400	1.13971000

**TS-5**

N	-1.32609200	-0.02540500	-1.11727700
C	-2.25281400	-1.09381500	-0.80935200
C	-1.79660800	-2.05987400	0.01171300
C	-0.87568000	2.86348400	1.65926900
C	-2.08681400	2.24196000	1.33456500
C	-2.12428800	0.93883300	2.01095300
C	-0.94082900	0.82559600	2.82519100
C	-0.13308800	1.97748100	2.56482700
Rh	-0.39562400	0.82894000	0.71974900
C	-0.81252600	0.09965200	-2.23810000
O	-0.37116200	0.19563300	-3.31098400
C	1.12656900	2.36389400	3.26690000
H	0.89056400	3.07282700	4.07142300
H	1.62095700	1.49487000	3.69905200
H	1.82139300	2.84451200	2.57658100
C	-0.35602700	4.17207100	1.16123300
H	-0.47474900	4.95051700	1.92492900
H	0.70742000	4.09123600	0.92681200
H	-0.87882300	4.49250300	0.25888000
C	-3.15362600	2.76434700	0.42617200
H	-3.89192400	3.34345100	0.99436000

H	-2.73335000	3.41669700	-0.34267500
H	-3.68567600	1.95250900	-0.07304900
C	-3.31241900	0.03481200	2.07806100
H	-3.95634900	0.33750400	2.91397700
H	-3.90742600	0.07344600	1.16494600
H	-3.01405800	-1.00217100	2.24004600
C	-0.62702100	-0.27417100	3.78807200
H	-0.98391300	-0.01332500	4.79189600
H	-1.10726700	-1.20697200	3.48647900
H	0.45002800	-0.44388200	3.82670500
O	0.54892800	1.97689500	-1.31799700
C	1.69165100	2.14660200	-0.81095400
O	1.95845800	1.78204600	0.37200400
C	2.76860000	2.85873600	-1.64978300
C	2.90801000	2.10713600	-2.98654300
H	1.94862100	2.06524800	-3.50687200
H	3.63613900	2.61658400	-3.62784500
H	3.25407000	1.08304900	-2.82391000
C	2.27716600	4.29545300	-1.91474900
H	2.16735000	4.85673700	-0.97965700
H	2.99811000	4.83072500	-2.54219300
H	1.31054500	4.28296300	-2.42435900
C	4.11220300	2.88277600	-0.91133900
H	4.02776700	3.40907100	0.04343500
H	4.46052800	1.86823600	-0.70402000
H	4.86616600	3.39228000	-1.52204200
C	-0.43156800	-2.14704700	0.52777500
C	0.37458200	-1.07024200	0.78598300
C	1.83459900	-1.22966000	1.18422400
O	2.27175700	-0.24388300	2.10690600
H	2.29591100	0.58929500	1.59401400
H	1.96121800	-2.17649600	1.71464500
C	2.75570500	-1.27287400	-0.04572200
C	2.31045200	-1.61649300	-1.32521800
C	4.11459200	-0.98875300	0.13658600
C	3.19988300	-1.67446300	-2.39924700
H	1.26576100	-1.85196400	-1.48485400
C	5.00682600	-1.05133800	-0.93313400
H	4.45988200	-0.70647800	1.12484000
C	4.55292600	-1.39409100	-2.20836900
H	2.82959700	-1.93227800	-3.38723000
H	6.05756100	-0.82818900	-0.77077100
H	5.24506200	-1.43697100	-3.04408200
C	-3.61195200	-0.96598500	-1.35478500

C	-3.98920500	0.16585300	-2.10053900
C	-4.58356400	-1.96286000	-1.13304800
C	-5.28355100	0.29647300	-2.60350000
H	-3.27100200	0.95687700	-2.27928000
C	-5.87192400	-1.82760800	-1.63517800
H	-4.32841700	-2.85301000	-0.56945800
C	-6.23302600	-0.69659200	-2.37402200
H	-5.54552500	1.18161900	-3.17524800
H	-6.59985300	-2.61207600	-1.45142000
H	-7.24058700	-0.59557000	-2.76464900
H	-2.44865800	-2.88650400	0.26629100
C	-0.06370100	-3.57775400	0.78917600
O	-0.85466200	-4.42168700	1.17488700
O	1.22370700	-3.85618300	0.51236300
C	1.67090800	-5.21029400	0.72918900
C	3.11075900	-5.26575000	0.25643600
H	1.01944200	-5.88989300	0.17177000
H	1.56980000	-5.45211100	1.79222600
H	3.51344600	-6.27414000	0.39154700
H	3.17786200	-4.99866000	-0.80160600
H	3.73067700	-4.56206200	0.81872500

**INT-6**

N	-1.55355100	-0.14706100	0.96904600
C	-2.37530800	0.99084400	0.69774800
C	-1.85982600	1.95010600	-0.09761700
C	-0.55362900	-2.98875000	-1.64351200
C	-1.83962400	-2.46813600	-1.43219700
C	-1.93920800	-1.19143400	-2.15065300
C	-0.71677400	-0.99569400	-2.86557300
C	0.17232800	-2.06933400	-2.51584100
Rh	-0.33670400	-0.90835100	-0.69214000
C	-1.44622900	-0.82519000	1.99354400
O	-1.32505900	-1.55409700	2.89795400
C	1.47315800	-2.39192100	-3.17546300
H	1.29196700	-3.11054500	-3.98623000
H	1.93583300	-1.49972200	-3.59353800
H	2.17161000	-2.83389700	-2.46530800
C	0.02980300	-4.24418400	-1.07700900
H	-0.02093300	-5.05948400	-1.80914000
H	1.07922900	-4.09018500	-0.81854400
H	-0.50160600	-4.56518600	-0.17838300
C	-2.93158100	-3.07362800	-0.60722400
H	-3.54274900	-3.75256100	-1.21428800

H	-2.53124500	-3.64875800	0.23182000
H	-3.59902900	-2.30630000	-0.21065000
C	-3.17735600	-0.36127700	-2.27961200
H	-3.79784400	-0.72962500	-3.10632000
H	-3.78223100	-0.38667500	-1.37112900
H	-2.93036000	0.68275200	-2.47955500
C	-0.41114800	0.10998200	-3.82487600
H	-0.66751600	-0.19478500	-4.84687300
H	-0.98132600	1.00974700	-3.58521200
H	0.65077800	0.35712700	-3.78749800
O	0.94989700	-1.36462500	0.89582300
C	2.11745400	-1.89421200	0.74855000
O	2.70719600	-2.01584600	-0.34089600
C	2.74365200	-2.44525000	2.04472300
C	2.44534900	-1.51301000	3.22986600
H	1.37087800	-1.42300300	3.39908700
H	2.90735800	-1.91386500	4.13922000
H	2.84922900	-0.51365900	3.05256800
C	2.09646800	-3.82454400	2.29519000
H	2.29519300	-4.51084700	1.46498800
H	2.50696700	-4.27089800	3.20742400
H	1.01348800	-3.72845000	2.41819000
C	4.25913100	-2.59985200	1.86062900
H	4.48647800	-3.24763000	1.01159200
H	4.72474500	-1.62819100	1.67607300
H	4.70297900	-3.03073100	2.76487600
C	-0.48645000	2.05565500	-0.58663300
C	0.37631900	1.00461800	-0.75963600
C	1.84858600	1.18689400	-1.09526800
O	2.36160100	0.16849800	-1.93011700
H	2.44791400	-0.65680000	-1.39418100
H	1.96173900	2.10236900	-1.68085300
C	2.70727500	1.36886300	0.16868900
C	2.21612200	1.93438600	1.34986300
C	4.05755600	1.00558200	0.11156900
C	3.05798200	2.14936600	2.44135200
H	1.17167300	2.21060000	1.41913300
C	4.90033600	1.21557600	1.20349700
H	4.43798400	0.55116000	-0.79529500
C	4.40575100	1.79323800	2.37340500
H	2.65549000	2.58750200	3.35039400
H	5.94574200	0.92763400	1.13718900
H	5.06021300	1.95684600	3.22449900
C	-3.73404300	1.00316200	1.26848400

C	-4.37785700	-0.18294300	1.66278400
C	-4.42878600	2.21722900	1.43181600
C	-5.67075900	-0.15969800	2.18471300
H	-3.87830300	-1.13805900	1.55272100
C	-5.72052100	2.23607700	1.94486500
H	-3.94118500	3.15151100	1.17701900
C	-6.35158800	1.04781600	2.32412300
H	-6.14435900	-1.09153500	2.47836200
H	-6.23262100	3.18592100	2.06488400
H	-7.35727000	1.06720200	2.73176900
H	-2.49544400	2.79314400	-0.33809400
C	-0.18244800	3.48807100	-0.92581900
O	-1.02579200	4.28449000	-1.30421200
O	1.10523400	3.83202000	-0.74392800
C	1.47035800	5.19775900	-1.03082200
C	2.92372200	5.34732400	-0.62484900
H	0.80783300	5.86336800	-0.46977700
H	1.31043200	5.39259300	-2.09621000
H	3.25852200	6.37467100	-0.79739600
H	3.05191300	5.10677700	0.43388300
H	3.56043200	4.67122000	-1.20209400

**TS-6**

N	1.51179800	0.40319600	-1.72488900
C	2.30226200	1.26473500	-0.93901500
C	1.77160400	2.02059400	0.04621600
C	1.12919300	-3.02769300	1.30041400
C	2.16740800	-2.07609100	1.02947500
C	2.12060200	-1.01990200	2.04437400
C	0.98856900	-1.26934400	2.86106000
C	0.35914600	-2.50641300	2.38197000
Rh	0.30155500	-0.98832100	0.83691600
C	0.57208500	0.46285700	-2.48222000
O	-0.30317100	0.41322200	-3.26941100
C	-0.86682700	-3.12256100	2.96676500
H	-0.57890900	-3.91127000	3.67342500
H	-1.45944700	-2.37679800	3.49615100
H	-1.49477300	-3.55453000	2.18615100
C	0.81058700	-4.24792100	0.49474900
H	1.34326800	-5.12720800	0.87592500
H	-0.26004400	-4.46144700	0.52214600
H	1.09316700	-4.11006000	-0.55159400
C	3.18905400	-2.19590800	-0.05103100
H	3.98061000	-2.88766800	0.26402200



H	2.74358000	-2.58786000	-0.96783300
H	3.64921600	-1.23652100	-0.28359300
C	3.14176700	0.04977900	2.25315000
H	3.84113200	-0.25986400	3.04017700
H	3.71669100	0.24384900	1.34912400
H	2.67427900	0.98565300	2.56461700
C	0.52436100	-0.46861700	4.03386000
H	0.80928900	-0.95856300	4.97290200
H	0.96582600	0.52968200	4.02096300
H	-0.56151600	-0.36005100	4.00740600
O	-0.73957800	-1.45383400	-0.91564700
C	-1.84146300	-2.11754000	-0.81186700
O	-2.45594200	-2.28872100	0.26301700
C	-2.41331100	-2.67787400	-2.12527800
C	-3.27199500	-1.55496900	-2.74602600
H	-2.65771400	-0.68632300	-2.98829200
H	-3.74425000	-1.91707600	-3.66619100
H	-4.05759300	-1.23554300	-2.05616100
C	-1.28390200	-3.06401800	-3.09296900
H	-0.63231900	-3.82889800	-2.65501900
H	-1.70909000	-3.47420900	-4.01541400
H	-0.67387000	-2.19684900	-3.34824600
C	-3.29182700	-3.89960500	-1.81888700
H	-2.70204000	-4.71112600	-1.37811600
H	-4.08445400	-3.64193800	-1.11460400
H	-3.74434600	-4.27398900	-2.74330700
C	0.37596900	2.06695700	0.50619200
C	-0.36200400	0.95624800	0.79105100
C	-1.80573800	0.94484200	1.26596700
O	-2.08061400	-0.26649700	1.99034300
H	-2.29512000	-0.99575300	1.35088700
H	-1.94074800	1.74165500	2.00261400
C	-2.84709300	1.16300000	0.16557300
C	-2.53837300	1.70558300	-1.08309600
C	-4.18259700	0.85191100	0.45104500
C	-3.53972300	1.94834900	-2.02332900
H	-1.51200900	1.94427100	-1.32485800
C	-5.18671300	1.09639200	-0.48472900
H	-4.42679000	0.41592300	1.41362900
C	-4.86964900	1.65064200	-1.72664200
H	-3.27365900	2.36064100	-2.99203800
H	-6.21753200	0.85335100	-0.24317400
H	-5.65006600	1.83885300	-2.45802600
C	3.74336900	1.23835000	-1.27700400

C	4.19347300	0.52098400	-2.39900500
C	4.70581900	1.90057500	-0.49010900
C	5.54737700	0.47231500	-2.72599000
H	3.46978200	-0.00223500	-3.01249600
C	6.05597400	1.85482600	-0.82175200
H	4.40107500	2.45448600	0.39026400
C	6.48737700	1.13909300	-1.94121400
H	5.86586200	-0.08890800	-3.59944100
H	6.77576600	2.37728500	-0.19879200
H	7.54221500	1.10077600	-2.19462100
H	2.42480400	2.75460300	0.50293000
C	-0.06502200	3.48308600	0.70399600
O	0.68658800	4.44107500	0.62211400
O	-1.38026400	3.61491600	0.96903900
C	-1.91292700	4.95272500	1.02252400
C	-3.42288400	4.82433700	0.94922400
H	-1.50220600	5.52747000	0.18783400
H	-1.57922500	5.43169900	1.94936800
H	-3.88511300	5.81563100	0.98848900
H	-3.72134000	4.33056100	0.02089500
H	-3.80480000	4.23074200	1.78460200

**INT-7**

N	-1.63121700	0.57674100	1.83696500
C	-2.34320100	1.39058700	0.94123000
C	-1.73427800	2.06551400	-0.05552000
C	-1.20644500	-3.01858400	-1.27442800
C	-2.12094500	-1.91308100	-0.97964800
C	-2.05693200	-0.98628300	-2.07170700
C	-1.00455200	-1.42009500	-2.94526100
C	-0.52974500	-2.72242300	-2.46871800
Rh	-0.10024900	-1.04319100	-1.02284400
C	-0.59785500	0.60387200	2.45825700
O	0.35193800	0.54186100	3.15533100
C	0.56385200	-3.50147900	-3.12800800
H	0.22017600	-3.92339700	-4.07971900
H	1.42097600	-2.85460600	-3.33820900
H	0.91093200	-4.32118600	-2.49671200
C	-1.00552600	-4.18744900	-0.36399300
H	-1.90202500	-4.81778200	-0.33807300
H	-0.16397200	-4.80665800	-0.68039500
H	-0.80851700	-3.84357600	0.65545600
C	-3.07737100	-1.91450100	0.16950500
H	-3.76595600	-2.76479000	0.09167300

H	-2.54210100	-1.99550300	1.11879100
H	-3.66949900	-1.00153700	0.20365700
C	-2.95707100	0.17817800	-2.33323000
H	-3.61408000	-0.05635500	-3.18005400
H	-3.58292400	0.40746600	-1.47270400
H	-2.38807500	1.07471800	-2.58831800
C	-0.59676800	-0.77218200	-4.23103200
H	-1.14435700	-1.20243800	-5.07928600
H	-0.79987000	0.30075300	-4.20779300
H	0.47129800	-0.90948400	-4.41648200
O	0.55579900	-1.55284000	0.94322600
C	1.72428600	-2.04495700	1.13498100
O	2.65288500	-2.04335900	0.28428200
C	2.02180900	-2.66648000	2.51065900
C	2.98681800	-1.70313800	3.23520600
H	2.50836800	-0.73750800	3.41251900
H	3.27879500	-2.12874900	4.20158700
H	3.88586700	-1.53777400	2.63676900
C	0.74966700	-2.86566600	3.34334700
H	0.03939300	-3.52446700	2.83338600
H	1.00838200	-3.32846900	4.30198700
H	0.25286300	-1.91646500	3.54355400
C	2.71682700	-4.02173700	2.28198700
H	2.05089000	-4.72451400	1.76802200
H	3.61510300	-3.89709400	1.67515000
H	2.99470600	-4.46449900	3.24435200
C	-0.31560800	2.03762500	-0.44491400
C	0.37758700	0.91023700	-0.75195300
C	1.81337700	0.80411100	-1.20473800
O	1.90874200	-0.61598900	-1.59584000
H	2.34932400	-1.18646100	-0.83478400
H	1.96823000	1.36862900	-2.12935500
C	2.93722300	1.12807600	-0.24129200
C	2.71765500	1.51350800	1.08005500
C	4.25164600	1.00056400	-0.70579100
C	3.79469000	1.76876600	1.92894800
H	1.70766600	1.61771700	1.44883700
C	5.32950200	1.25251600	0.13977700
H	4.42662300	0.69867800	-1.73477100
C	5.10330800	1.63948500	1.46304300
H	3.60581000	2.06270300	2.95693800
H	6.34441200	1.15130300	-0.23315500
H	5.94144200	1.83769000	2.12445800
C	-3.79984300	1.43971700	1.20406300

C	-4.33023000	0.82096900	2.34863100
C	-4.69566400	2.07564200	0.32399500
C	-5.69919800	0.84057200	2.60722100
H	-3.65594000	0.32042800	3.03335100
C	-6.06180100	2.09873000	0.58688400
H	-4.32819200	2.55556900	-0.57570800
C	-6.57395900	1.47965200	1.72923400
H	-6.08133200	0.35405800	3.49972800
H	-6.73008800	2.59858100	-0.10790000
H	-7.64090000	1.49399700	1.92898300
H	-2.33980700	2.78804500	-0.59052800
C	0.22770200	3.42013100	-0.58086600
O	-0.41232200	4.42231800	-0.30967700
O	1.49461200	3.46902500	-1.04878900
C	2.12217300	4.76810700	-1.06878300
C	3.61977200	4.55218400	-1.16867400
H	1.84229400	5.30652100	-0.15973300
H	1.72812500	5.33330600	-1.92052300
H	4.12864400	5.52059700	-1.20829500
H	3.99041000	3.99524200	-0.30504700
H	3.87801700	3.99146200	-2.07150400

**TS-7**

N	1.36429300	0.37778200	-1.97784700
C	2.02525700	1.39046300	-1.32194100
C	1.41379200	2.24564100	-0.44146900
C	1.34711600	-2.05693400	2.50129600
C	2.14958200	-0.98660600	1.92265300
C	1.65986600	0.26001700	2.45012900
C	0.46419600	-0.01105200	3.18504400
C	0.29854000	-1.46164900	3.24985300
Rh	0.12162300	-0.76651500	1.16899700
C	0.14996900	0.03108600	-1.83645100
O	-0.73484600	-0.62129000	-2.29790400
C	-0.83185900	-2.14782700	3.94798000
H	-0.73379400	-2.04634500	5.03505100
H	-1.78642600	-1.70437000	3.65020800
H	-0.86717300	-3.21099400	3.70484300
C	1.57085800	-3.50906000	2.23208300
H	2.53415000	-3.82930200	2.64465400
H	0.78666400	-4.12632000	2.67358200
H	1.57993900	-3.69236700	1.15376900
C	3.36002300	-1.18649700	1.06651600
H	4.23878900	-1.43198800	1.67622800

H	3.19435000	-2.00439900	0.36164800
H	3.58724900	-0.29210000	0.48420500
C	2.34170700	1.58364600	2.36468700
H	2.90581000	1.73053500	3.29555500
H	3.04686000	1.62014300	1.53573900
H	1.64289700	2.41536300	2.26240000
C	-0.38991300	0.99832700	3.88628800
H	-0.08886400	1.10833700	4.93564400
H	-0.30791000	1.97659900	3.40747800
H	-1.44014700	0.69651200	3.86958900
O	0.17933800	-2.28379700	-0.28205400
C	-0.85744500	-2.87825600	-0.74635000
O	-2.03883100	-2.65961900	-0.37659700
C	-0.60451700	-3.96918000	-1.79796000
C	-1.66345800	-3.83269300	-2.90609600
H	-1.56976500	-2.86542100	-3.40587800
H	-1.52942300	-4.62667200	-3.64894500
H	-2.66963700	-3.90298100	-2.48899800
C	0.80326000	-3.84553400	-2.39598400
H	1.57505900	-3.96112700	-1.63080000
H	0.95139000	-4.62040900	-3.15606300
H	0.93970400	-2.86762500	-2.86455500
C	-0.76463800	-5.32677600	-1.08198400
H	-0.02549900	-5.44027100	-0.28067700
H	-1.76344800	-5.41911200	-0.64679500
H	-0.61820600	-6.14607000	-1.79387300
C	0.04765700	2.10323500	-0.04267600
C	-0.58371600	0.87981000	-0.03504600
C	-2.03109200	0.65425000	0.34506700
O	-2.01567800	-0.63799500	1.02906900
H	-2.13877000	-1.46078800	0.37684700
H	-2.31680200	1.36445400	1.13126000
C	-3.10102500	0.70977000	-0.72990600
C	-2.94067300	1.47629200	-1.88641200
C	-4.30987100	0.03727200	-0.52160100
C	-3.97027300	1.56826400	-2.82099100
H	-2.00961200	2.00249900	-2.05457600
C	-5.33894000	0.12458200	-1.45888000
H	-4.44025300	-0.56468800	0.37175300
C	-5.17340400	0.89254000	-2.61165800
H	-3.82730400	2.16164600	-3.71940600
H	-6.26891200	-0.40966200	-1.28762900
H	-5.97335700	0.96060100	-3.34301200
C	3.44598900	1.54104600	-1.71076500

C	3.99716100	0.67686700	-2.67296600
C	4.29085300	2.49504100	-1.11301100
C	5.33818800	0.77358500	-3.03541800
H	3.35247400	-0.06864900	-3.12250800
C	5.63139000	2.58690900	-1.47406600
H	3.90532000	3.17150400	-0.35848900
C	6.16327100	1.72773900	-2.43878900
H	5.74125500	0.09676100	-3.78302100
H	6.26381200	3.33133900	-0.99949700
H	7.21054500	1.79904600	-2.71650900
H	1.92901900	3.13895000	-0.11851900
C	-0.59256900	3.33354400	0.51525500
O	-0.02310700	4.08659400	1.28980600
O	-1.86894400	3.48247800	0.13378800
C	-2.62563200	4.56211900	0.72678000
C	-4.05915000	4.38999000	0.26405900
H	-2.19145400	5.51268300	0.40183900
H	-2.52556700	4.50568100	1.81498100
H	-4.68355900	5.18858300	0.67578500
H	-4.12034800	4.42223800	-0.82661400
H	-4.45857800	3.42612600	0.59089200

**INT-8**

N	-1.24339900	-0.20501400	-1.92273100
C	-1.79092200	-1.35045900	-1.60913200
C	-1.06957000	-2.37843800	-0.90189200
C	-1.32313800	1.57875700	2.83509600
C	-2.13925900	0.61477800	2.10983800
C	-1.62830500	-0.69654200	2.39303300
C	-0.42488400	-0.55130000	3.16699700
C	-0.26456600	0.86339800	3.46508100
Rh	-0.13873200	0.55606000	1.29418000
C	0.09929200	0.04146400	-1.59425000
O	0.73661400	0.88191300	-2.22070100
C	0.86025300	1.43671900	4.26541000
H	0.71212800	1.23578800	5.33311000
H	1.81238600	0.99041500	3.96663100
H	0.93960600	2.51631500	4.12826800
C	-1.55952400	3.05358000	2.83610200
H	-2.44214500	3.29788400	3.43880600
H	-0.70592400	3.59792500	3.24374200
H	-1.73117700	3.40792600	1.81664000
C	-3.33995000	0.95533300	1.28496600
H	-4.20934300	1.16099000	1.92145900

H	-3.13861300	1.84019500	0.67661100
H	-3.59722800	0.14203300	0.60418600
C	-2.28095100	-1.97694600	2.00290300
H	-3.02588600	-2.23373100	2.76730400
H	-2.80642300	-1.88196100	1.05176900
H	-1.56862100	-2.79811400	1.92320300
C	0.41300800	-1.64945900	3.74364200
H	0.10165100	-1.87031000	4.77268500
H	0.32802200	-2.56655100	3.15979400
H	1.46648900	-1.35810500	3.77464600
O	-0.47841200	2.17652500	0.00046200
C	0.42525600	2.97287100	-0.43796200
O	1.63266400	2.94549600	-0.08039900
C	-0.03341500	4.05108100	-1.42760900
C	1.01880500	4.15971500	-2.54576100
H	1.09571700	3.21134700	-3.08166000
H	0.72795200	4.94704600	-3.24987300
H	2.00010700	4.39943600	-2.13147600
C	-1.40078600	3.69439100	-2.02655300
H	-2.17650800	3.65839300	-1.25665900
H	-1.68611000	4.44930500	-2.76765500
H	-1.35996500	2.71557600	-2.50984700
C	-0.11284600	5.37844300	-0.64528600
H	-0.85618200	5.32066200	0.15841400
H	0.85606400	5.62789700	-0.20372600
H	-0.40721800	6.19134700	-1.31750300
C	0.12545600	-2.05296800	-0.32211000
C	0.65472000	-0.70796600	-0.43634300
C	2.07264200	-0.38569000	0.05628400
O	1.95584900	0.74718400	0.95327600
H	1.92220000	1.69316200	0.46074100
H	2.37994800	-1.19793200	0.71698700
C	3.15916400	-0.21359900	-0.98388300
C	3.22801900	-1.09488900	-2.06882000
C	4.15340700	0.75496900	-0.83075800
C	4.26921000	-1.00329200	-2.98842200
H	2.45930600	-1.84849600	-2.19667900
C	5.19333000	0.85090300	-1.75700500
H	4.11106300	1.44473400	0.00409400
C	5.25713500	-0.02757900	-2.83714300
H	4.30343300	-1.68749300	-3.83144200
H	5.95255100	1.61749500	-1.63192200
H	6.06528400	0.04886800	-3.55858800
C	-3.22068300	-1.54375600	-1.97189500

C	-3.85298500	-0.59380500	-2.79169400
C	-3.97490200	-2.62392200	-1.48670100
C	-5.19869200	-0.72395500	-3.11698000
H	-3.26047700	0.23715100	-3.15599900
C	-5.32475400	-2.75187500	-1.81276100
H	-3.51812000	-3.36508600	-0.84034000
C	-5.94078400	-1.80379200	-2.62940000
H	-5.67232100	0.01696400	-3.75417300
H	-5.89407600	-3.59172100	-1.42597100
H	-6.99159800	-1.90412300	-2.88432600
H	-1.46058900	-3.38198700	-0.80720500
C	0.83536100	-3.16972900	0.38020400
O	0.32232600	-3.91333700	1.19936600
O	2.10123500	-3.29836400	-0.04135300
C	2.90959400	-4.33045700	0.57264300
C	4.32154100	-4.13938200	0.05655200
H	2.49119800	-5.30516300	0.30407000
H	2.84188600	-4.22585100	1.65955800
H	4.98132400	-4.89804200	0.48788300
H	4.35219500	-4.22700700	-1.03241900
H	4.70089800	-3.14972300	0.32429900

**INT-9**

N	-1.01125500	-0.38873400	-1.72654700
C	-1.18357100	-1.69685300	-1.62363700
C	-0.13626400	-2.53236000	-1.15336200
C	-1.59141900	0.85905300	2.80932200
C	-2.11840100	-0.28517800	2.08535000
C	-1.20009200	-1.36050500	2.26573600
C	-0.06900100	-0.88063400	3.03747200
C	-0.34743600	0.48807300	3.41433200
Rh	-0.13331100	0.32068300	1.25923400
C	0.27520400	0.18439400	-1.53447200
O	0.54905100	1.22800000	-2.11185500
C	0.57200900	1.35770200	4.21013800
H	0.72274600	0.94705300	5.21462500
H	1.54479500	1.41988900	3.71017400
H	0.17602600	2.36987400	4.31109500
C	-2.24711400	2.19834900	2.91213800
H	-2.79806500	2.27637300	3.85722600
H	-1.50920500	3.00217700	2.87780800
H	-2.95622400	2.35462500	2.09772900
C	-3.42264200	-0.33872700	1.35038800
H	-4.25682100	-0.52695800	2.03792100



H	-3.62046700	0.59727600	0.82363000
H	-3.41782400	-1.13308800	0.60176100
C	-1.39711500	-2.76630700	1.81342300
H	-1.86311900	-3.33418000	2.62943700
H	-2.06356800	-2.81756700	0.95293800
H	-0.45437000	-3.25180600	1.55803600
C	1.09319700	-1.68560700	3.52565500
H	0.90302600	-2.05168300	4.54291300
H	1.28250100	-2.54631300	2.88354400
H	1.99636200	-1.07072700	3.55298300
O	-0.65598800	2.19174500	0.21779200
C	-1.51957300	2.56087600	-0.59097200
O	-2.33753700	1.76652200	-1.24041900
C	-1.68770500	4.04236300	-0.91026800
C	-3.16152200	4.44091900	-0.70395000
H	-3.46098700	4.32373400	0.34384900
H	-3.29893100	5.49241400	-0.97508900
H	-3.82394700	3.83233400	-1.32307000
C	-0.77022000	4.88279300	-0.01470600
H	0.27491000	4.59594600	-0.14835200
H	-0.88160000	5.94215700	-0.26664900
H	-1.01918200	4.75394200	1.04276800
C	-1.28980200	4.21983900	-2.39322700
H	-0.27303400	3.85817800	-2.56684200
H	-1.96380300	3.65971000	-3.04505600
H	-1.34112400	5.28046100	-2.65997100
C	0.96615800	-1.93140600	-0.57195800
C	1.11288300	-0.51046300	-0.54662500
C	2.30053800	0.20657600	0.12285300
O	1.75045700	1.01597400	1.13422100
H	-1.92559200	0.82260800	-1.40735500
H	2.91948400	-0.57784000	0.58641700
C	3.19884100	0.98511200	-0.82420100
C	3.93025800	0.31896300	-1.81348400
C	3.32932500	2.36779400	-0.68958100
C	4.77905400	1.02986100	-2.66079500
H	3.82194700	-0.75508700	-1.92538300
C	4.18242300	3.07816100	-1.53441600
H	2.74481600	2.86508400	0.07577400
C	4.91027900	2.41343300	-2.52247000
H	5.33740500	0.50450800	-3.43112600
H	4.27607200	4.15541300	-1.42453400
H	5.57255000	2.96781400	-3.18148100
C	-2.52824500	-2.23398600	-1.94905500

C	-3.44026800	-1.43955100	-2.66449400
C	-2.93343500	-3.51380800	-1.53498000
C	-4.72126200	-1.90610600	-2.94323300
H	-3.12396100	-0.46108200	-3.00611800
C	-4.21561400	-3.98054900	-1.81807700
H	-2.25262500	-4.14451800	-0.97446700
C	-5.11535700	-3.17788600	-2.52046700
H	-5.41195300	-1.27906600	-3.49883600
H	-4.51257200	-4.97041900	-1.48510500
H	-6.11459400	-3.54155700	-2.73995200
H	-0.22040100	-3.60996800	-1.17471100
C	1.98179900	-2.85261800	0.03279200
O	1.72587300	-3.69932000	0.87214100
O	3.20231800	-2.67373400	-0.48844800
C	4.27780500	-3.46033900	0.08129700
C	5.55374600	-3.03404500	-0.61547000
H	4.05116900	-4.52046400	-0.06429500
H	4.30901900	-3.26894300	1.15820800
H	6.40519300	-3.57688800	-0.19429600
H	5.50263800	-3.24904900	-1.68644200
H	5.72293400	-1.96148800	-0.48882100

**TS-8**

N	-0.96301400	-0.36746600	-1.71162900
C	-1.11309200	-1.68709600	-1.64164900
C	-0.03891900	-2.49459300	-1.20927800
C	-1.60557500	0.75527300	2.81140100
C	-2.09230800	-0.40622900	2.09234400
C	-1.11841500	-1.43833100	2.24855900
C	-0.00171300	-0.91717500	3.01091500
C	-0.33277400	0.43608100	3.39605300
Rh	-0.15471100	0.31090500	1.24546100
C	0.31309500	0.24295900	-1.54212100
O	0.53995200	1.30308100	-2.10396000
C	0.55880700	1.34247100	4.18175300
H	0.74318800	0.93401700	5.18148900
H	1.51927900	1.44884300	3.66540800
H	0.12008500	2.33563000	4.29334800
C	-2.32073700	2.06151200	2.93184600
H	-2.87162700	2.10267800	3.87932800
H	-1.62103400	2.89873300	2.90297900
H	-3.03673100	2.19276700	2.11935100
C	-3.40782700	-0.51180800	1.38289100
H	-4.22847200	-0.65857100	2.09620600

H	-3.61612800	0.38716500	0.79875900
H	-3.41311600	-1.35302600	0.68745400
C	-1.25194000	-2.84553900	1.77721700
H	-1.68593800	-3.44567300	2.58776100
H	-1.92003300	-2.91687300	0.91948700
H	-0.28925500	-3.28315800	1.51017500
C	1.20790600	-1.66941200	3.46637300
H	1.05717300	-2.06027900	4.48088500
H	1.42705800	-2.51014800	2.80734000
H	2.07937600	-1.00997000	3.48581800
O	-0.76970500	2.13888300	0.23958900
C	-1.67783700	2.42285800	-0.57257400
O	-2.41337400	1.56764700	-1.20867000
C	-1.95835600	3.89520600	-0.87852600
C	-3.45391700	4.17605800	-0.63753700
H	-3.71843900	4.03919000	0.41756800
H	-3.68488400	5.21177600	-0.90674800
H	-4.07790400	3.51105700	-1.23845600
C	-1.09135400	4.80534300	-0.00125500
H	-0.02999300	4.59947200	-0.15499400
H	-1.28815500	5.85337600	-0.24987000
H	-1.30887500	4.65924400	1.06087800
C	-1.61244800	4.10904400	-2.36834800
H	-0.56906200	3.84783500	-2.56348200
H	-2.24265900	3.48313300	-3.00404100
H	-1.77206200	5.15880700	-2.63644500
C	1.06162100	-1.87214600	-0.63048500
C	1.18146000	-0.45664400	-0.59054100
C	2.31737400	0.29585900	0.12244000
O	1.71079700	1.07477700	1.12437700
H	-1.84313600	0.59621300	-1.46729000
H	2.95416500	-0.47033200	0.59328200
C	3.20841000	1.11709500	-0.79638200
C	3.97643300	0.48978500	-1.78344900
C	3.29281500	2.50072900	-0.63831800
C	4.81773300	1.23977400	-2.60411600
H	3.90239700	-0.58479700	-1.91527100
C	4.13850700	3.25020700	-1.45661100
H	2.67797400	2.96775800	0.12217600
C	4.90397900	2.62419600	-2.44142000
H	5.40474300	0.74430300	-3.37293200
H	4.19592500	4.32797400	-1.32896200
H	5.55992200	3.20931900	-3.07984300
C	-2.45190300	-2.23945400	-1.95271200

C	-3.40160500	-1.44488700	-2.61768200
C	-2.81681600	-3.54075700	-1.56743900
C	-4.67983100	-1.93276800	-2.87273200
H	-3.12585500	-0.44806800	-2.94020800
C	-4.09507100	-4.02857000	-1.82905400
H	-2.10612200	-4.17206600	-1.04623900
C	-5.03311900	-3.22529000	-2.47922600
H	-5.40021800	-1.30411400	-3.38701000
H	-4.35954500	-5.03496200	-1.51923200
H	-6.03031200	-3.60456700	-2.68052500
H	-0.09517100	-3.57338100	-1.24128200
C	2.09918200	-2.77867400	-0.03963900
O	1.85746200	-3.66459800	0.76269600
O	3.32190100	-2.53604700	-0.52715600
C	4.41460100	-3.30410700	0.03581300
C	5.68748500	-2.80495800	-0.61671200
H	4.23051200	-4.36538100	-0.15448000
H	4.41657300	-3.15310900	1.11953300
H	6.54993800	-3.33057000	-0.19612700
H	5.66738200	-2.98259200	-1.69552100
H	5.81277200	-1.73212600	-0.44842600

**INT-10**

N	-1.04292100	-0.34183200	-1.86181400
C	-1.68023200	-1.51783000	-1.61549300
C	-0.93959500	-2.54633400	-1.07444600
C	-1.47474800	1.54615500	2.68696000
C	-2.16331500	0.44398000	2.12706300
C	-1.44763600	-0.77732700	2.50189100
C	-0.32767700	-0.42621200	3.30192700
C	-0.28985600	1.02571600	3.37218000
Rh	-0.07743700	0.53099400	1.35616400
C	0.34196900	-0.10043700	-1.70589700
O	0.84135200	0.86765700	-2.26271100
C	0.73184200	1.82542000	4.10945300
H	0.45176000	1.92149500	5.16625800
H	1.70851900	1.33983400	4.05483500
H	0.82527800	2.82800500	3.68796000
C	-1.84345600	2.98774900	2.55831700
H	-2.47203000	3.29890000	3.40135600
H	-0.95270000	3.61897900	2.54630900
H	-2.38757400	3.16168600	1.62950700
C	-3.41219000	0.50340100	1.30829100
H	-4.29654800	0.48218400	1.95757100

H	-3.42588100	1.40876400	0.70192100
H	-3.47942900	-0.34538200	0.62595600
C	-1.89393900	-2.16004400	2.16284400
H	-2.51526900	-2.55031700	2.97929800
H	-2.50079200	-2.16035000	1.25741300
H	-1.05491500	-2.83948900	2.00631000
C	0.72167600	-1.33811600	3.84872200
H	0.80529000	-1.23557200	4.93587600
H	0.49897200	-2.37936100	3.61044900
H	1.68563700	-1.08912100	3.38941900
O	0.39430200	2.21139900	0.24038900
C	-0.50790600	2.65990100	-0.57252800
O	-1.63318400	2.14439000	-0.72983300
C	-0.13973200	3.94666200	-1.33470800
C	-0.83991500	5.10907500	-0.59955300
H	-0.46815000	5.20667300	0.42650300
H	-0.64546500	6.05410200	-1.11828400
H	-1.92227600	4.95169600	-0.56421000
C	1.37603900	4.17508700	-1.36461000
H	1.88269900	3.33432700	-1.84079000
H	1.60240300	5.08993100	-1.92464400
H	1.78047400	4.27957400	-0.35472600
C	-0.68379600	3.83502700	-2.76899200
H	-0.21557800	2.99100000	-3.28163300
H	-1.76521400	3.67953400	-2.75985000
H	-0.46437900	4.75212600	-3.32663100
C	0.38576600	-2.28661700	-0.64148800
C	1.00381100	-1.05874100	-0.82124000
C	2.25280600	-0.65707500	-0.03178200
O	1.84892200	-0.06351400	1.17916600
H	-1.56563500	0.51370700	-2.04086500
H	2.76887700	-1.58990200	0.22943100
C	3.26254700	0.15651100	-0.82380200
C	3.96101400	-0.45763300	-1.86846600
C	3.54492900	1.47969500	-0.49153700
C	4.91903000	0.25173100	-2.58989600
H	3.74292700	-1.49397300	-2.11890700
C	4.50731300	2.18967300	-1.21073600
H	2.97979600	1.94094400	0.30825800
C	5.19517700	1.58137300	-2.26171400
H	5.45183800	-0.23039700	-3.40510600
H	4.71348600	3.22553800	-0.95519500
H	5.94240300	2.13716100	-2.82115400
C	-3.12022500	-1.59903700	-1.92300800

C	-3.71042100	-0.72909500	-2.85451700
C	-3.93748800	-2.53543600	-1.26613400
C	-5.07828300	-0.78628000	-3.11062200
H	-3.09685000	-0.02080500	-3.40105200
C	-5.30276100	-2.59468000	-1.52900500
H	-3.50402500	-3.20683800	-0.53317900
C	-5.88011300	-1.71682300	-2.44885800
H	-5.51590200	-0.10653800	-3.83489300
H	-5.91872000	-3.32065300	-1.00737100
H	-6.94617200	-1.75917000	-2.64884700
H	-1.37181200	-3.52596000	-0.92918500
C	1.07262200	-3.40854100	0.07987500
O	0.60180200	-4.00628300	1.03068200
O	2.25243600	-3.71227800	-0.48029100
C	3.04326900	-4.72800900	0.18433600
C	4.38256500	-4.77482700	-0.52233700
H	2.50623800	-5.67978900	0.12978800
H	3.13883900	-4.45697600	1.23980300
H	5.02513900	-5.52525200	-0.05223700
H	4.25771200	-5.03763700	-1.57638900
H	4.88254000	-3.80395400	-0.46588600

**TS-9**

N	-3.68869900	1.66837600	-0.69828800
C	-3.96112000	0.32650100	-0.81227000
C	-2.94982600	-0.50874100	-1.21631800
C	1.90177400	-0.50862800	2.68322700
C	1.50135300	0.82503000	2.38642400
C	0.05178600	0.82576100	2.22777300
C	-0.42941000	-0.49737200	2.40539900
C	0.72342700	-1.35322100	2.64016500
Rh	0.96579200	-0.56416800	0.71113600
C	-2.47091100	2.33177400	-0.96150600
O	-2.44970400	3.56208500	-0.88783900
C	0.66291900	-2.81944800	2.92372200
H	0.48565100	-2.99763500	3.99176400
H	-0.14828100	-3.28767200	2.36198400
H	1.59664400	-3.31390300	2.64856800
C	3.28728800	-0.96830900	2.99819600
H	3.45979300	-0.89458400	4.07944100
H	3.43124200	-2.00991500	2.70363000
H	4.02161700	-0.36552500	2.46639600
C	2.39779700	2.01837700	2.36669300
H	2.66260600	2.31118600	3.39082200

H	3.31030400	1.78558500	1.81626400
H	1.91992800	2.86910700	1.88161500
C	-0.78476100	2.04448400	2.02060200
H	-0.89876700	2.56937000	2.97751800
H	-0.32519800	2.73785000	1.31750200
H	-1.77933600	1.79287400	1.65321400
C	-1.83795100	-0.98609400	2.29735100
H	-2.16972100	-1.42388400	3.24537700
H	-2.52358500	-0.17943100	2.03329700
H	-1.90265800	-1.74779000	1.51429700
O	2.48627600	-1.47521200	-0.31258500
C	3.65972300	-0.92343500	-0.44298500
O	4.07168300	0.05636300	0.18554700
C	4.50022200	-1.58659600	-1.55637100
C	5.95772400	-1.12253500	-1.45577800
H	6.40656300	-1.43555400	-0.50790500
H	6.54669000	-1.55229800	-2.27353200
H	6.02360200	-0.03377500	-1.50828100
C	4.41594800	-3.11839900	-1.44708200
H	3.38200700	-3.45749900	-1.53278900
H	5.00642500	-3.58520400	-2.24332800
H	4.81286600	-3.46731600	-0.48695900
C	3.88703000	-1.12885100	-2.89805300
H	2.82979900	-1.39867600	-2.95925200
H	3.96901200	-0.04232300	-3.01252600
H	4.42133100	-1.59460400	-3.73369900
C	-1.68639900	0.07387000	-1.43636600
C	-1.40523500	1.40881800	-1.27716600
C	0.05997900	1.62633400	-1.66184200
O	0.61765800	0.28856000	-1.47595300
H	-4.44774900	2.30870000	-0.50001800
H	0.08091900	1.80097000	-2.74964000
C	0.98665800	2.65303700	-1.05054000
C	0.55584200	3.92650100	-0.65713600
C	2.35634300	2.36060600	-1.03728600
C	1.48776400	4.87552800	-0.22998300
H	-0.49929200	4.17075700	-0.69772300
C	3.28104200	3.31258600	-0.61418500
H	2.70251300	1.38416400	-1.33904800
C	2.85098000	4.57560700	-0.20778100
H	1.14096500	5.85785300	0.07782700
H	4.33342200	3.04870600	-0.59183600
H	3.56969800	5.31978600	0.12296800
C	-5.31470600	-0.12783200	-0.44676200

C	-6.03600200	0.50507600	0.57866100
C	-5.89673000	-1.21732600	-1.11379200
C	-7.30892700	0.05847200	0.92706200
H	-5.58795000	1.32616600	1.13081400
C	-7.16752700	-1.66249800	-0.76098600
H	-5.35721500	-1.69569000	-1.92432200
C	-7.87870700	-1.02572800	0.25863400
H	-7.85128500	0.55223800	1.72731600
H	-7.60833900	-2.50147100	-1.29019100
H	-8.87083800	-1.37259500	0.52978500
H	-3.08601200	-1.57845800	-1.27966200
C	-0.45264200	-0.63195400	-1.91243900
O	-0.31198200	-1.31947700	-2.89502100
O	-0.28030500	-1.82925900	-0.33019700
C	0.17785100	-3.09488900	-0.76950400
C	-1.02204500	-4.00675500	-1.00063300
H	0.85370600	-3.51896300	-0.01680300
H	0.74961400	-2.98635400	-1.69878000
H	-0.69560600	-5.00385000	-1.31729600
H	-1.61772200	-4.11093500	-0.08654600
H	-1.65944700	-3.59346100	-1.78784300

**INT-4i**

N	1.81117000	0.64656300	0.73186000
C	2.35577400	-1.54416300	0.88938500
C	1.35337500	-2.22317800	0.28048700
C	0.13591800	2.65715800	-2.16790700
C	1.55345500	2.63641400	-1.94354500
C	1.99605000	1.29931200	-2.13890000
C	0.85541000	0.48558200	-2.52014500
C	-0.30062800	1.34998500	-2.56574600
Rh	0.44085400	1.06918200	-0.44317100
C	2.00189400	-0.29471000	1.67106200
O	2.05112700	-0.16990100	2.88850800
C	-1.65748800	1.02030300	-3.10363300
H	-1.70906700	1.25653100	-4.17390300
H	-1.90708200	-0.03352300	-2.98236800
H	-2.43504900	1.60242200	-2.60288700
C	-0.74181200	3.86200000	-2.06581900
H	-0.90559200	4.29354000	-3.06109500
H	-1.71934400	3.59759800	-1.65471200
H	-0.29492400	4.61704700	-1.42018200
C	2.39432400	3.80137100	-1.53422500
H	2.35928200	4.59262700	-2.29185500



H	2.02443500	4.20838200	-0.58989800
H	3.43601400	3.50397900	-1.40081700
C	3.39905500	0.81314100	-1.96510100
H	4.06703200	1.31756600	-2.67121400
H	3.74975600	1.01833500	-0.94931700
H	3.47489400	-0.26260800	-2.12880600
C	0.93750400	-0.93321200	-2.98497400
H	1.50719400	-0.98996800	-3.91997900
H	1.43631700	-1.56662200	-2.24635700
H	-0.05351400	-1.34890500	-3.16610000
O	0.39056200	3.84148000	0.92242200
C	-0.62169800	3.22040600	1.22461900
O	-0.93685100	2.02864800	0.75663900
C	-1.66524600	3.76455100	2.22302200
C	-1.47974900	2.99573800	3.54939700
H	-0.46337100	3.12010100	3.93462900
H	-2.18007300	3.37765000	4.29972600
H	-1.66498600	1.92487600	3.42984600
C	-1.41052200	5.26040400	2.44932100
H	-1.53168000	5.82531600	1.52000400
H	-2.12220200	5.65131000	3.18400800
H	-0.39617100	5.43413100	2.81337400
C	-3.09054900	3.54646600	1.68119000
H	-3.22632100	4.05168200	0.71828400
H	-3.31648200	2.48698600	1.54481700
H	-3.82019900	3.96496600	2.38232700
C	-0.06176600	-1.85675800	0.24285900
C	-0.61970100	-0.64580700	0.00196600
C	-2.12194300	-0.34459300	0.05700100
O	-2.50127600	-0.07526000	1.40109600
H	-2.02084800	0.74570000	1.60577900
H	-2.27552800	0.57363700	-0.52379700
C	-3.08349500	-1.35063200	-0.55694500
C	-2.74791700	-2.12856900	-1.66976100
C	-4.39012000	-1.41925900	-0.05806500
C	-3.69124600	-2.96862100	-2.26457300
H	-1.73324800	-2.11818400	-2.04950000
C	-5.33307000	-2.25670000	-0.65198600
H	-4.64652400	-0.81752800	0.80549300
C	-4.98873500	-3.03594900	-1.75924600
H	-3.40316400	-3.57827800	-3.11564700
H	-6.33993600	-2.30278200	-0.24686800
H	-5.72230200	-3.69143300	-2.21870700
C	3.77128900	-1.94391600	0.83283400

C	4.64844900	-1.63200400	1.88630900
C	4.27552500	-2.62887000	-0.28751900
C	5.98756700	-2.00978000	1.82133000
H	4.26208400	-1.11030100	2.75456000
C	5.61326100	-3.00872600	-0.34498400
H	3.61418600	-2.85151500	-1.11932600
C	6.47512000	-2.69963600	0.70981900
H	6.65211800	-1.76789200	2.64523400
H	5.98654400	-3.53667100	-1.21747100
H	7.51999400	-2.99104300	0.66288000
H	1.56707000	-3.21295400	-0.11679900
C	-0.89380900	-3.11191800	0.39884100
O	-0.69879200	-4.11439800	-0.26279400
O	-1.80600800	-3.00474500	1.36416000
C	-2.73793600	-4.10691100	1.48332500
C	-3.64715700	-3.78896400	2.65140900
H	-2.17199600	-5.03143900	1.62818300
H	-3.28856600	-4.18556600	0.54174800
H	-4.39217500	-4.58213700	2.76884500
H	-3.07514000	-3.70808900	3.57977700
H	-4.16445200	-2.84238700	2.48088100

**TS-4i**

N	1.94160900	0.07787100	0.42408700
C	1.81684400	-1.96602000	0.86569900
C	0.61011600	-2.42167400	0.42642900
C	0.73227600	2.55656800	-2.26203900
C	2.03420900	1.96513700	-2.22769800
C	1.87794300	0.57798400	-2.55442800
C	0.48454400	0.33014700	-2.85570300
C	-0.23066600	1.56568400	-2.67965900
Rh	0.63419000	0.85941200	-0.71492200
C	1.87819200	-0.58368200	1.56313900
O	1.98824300	-0.36676800	2.75619100
C	-1.66308000	1.82860600	-3.02810900
H	-1.75222000	2.14892700	-4.07355000
H	-2.28707400	0.94211900	-2.89702200
H	-2.08273100	2.62304700	-2.40612000
C	0.42490600	3.98204800	-1.93125400
H	0.45429500	4.59796300	-2.83846900
H	-0.57088500	4.07701900	-1.49240600
H	1.14890600	4.37446400	-1.21626300
C	3.30718500	2.66000100	-1.86273500
H	3.56231400	3.42326300	-2.60709300

H	3.20338800	3.13771000	-0.88535400
H	4.13560500	1.95110600	-1.80805300
C	2.97712400	-0.43632300	-2.60742800
H	3.59555000	-0.28591800	-3.49973500
H	3.61705700	-0.36152700	-1.72547600
H	2.57597300	-1.45080900	-2.63960000
C	-0.05712700	-0.95983900	-3.38872100
H	0.32800000	-1.14401700	-4.39847900
H	0.22967900	-1.80636300	-2.75892200
H	-1.14528900	-0.93756600	-3.44507700
O	1.88746800	3.12581500	0.98103600
C	0.74768300	2.90905100	1.38085700
O	-0.10350900	2.08738100	0.80450200
C	0.17969700	3.57122600	2.65394200
C	0.04779900	2.46831900	3.72785600
H	0.99719600	1.94660300	3.87491300
H	-0.25922800	2.91609100	4.67924200
H	-0.69859100	1.71977000	3.45071600
C	1.15308000	4.65374600	3.13683800
H	1.28585200	5.43214600	2.37987800
H	0.76556600	5.12032700	4.04876900
H	2.13556100	4.22776900	3.34985900
C	-1.19816300	4.19348400	2.35942400
H	-1.12687400	4.95712900	1.57665400
H	-1.92317500	3.44246200	2.03728900
H	-1.58719500	4.67592000	3.26239300
C	-0.64059700	-1.69233000	0.33855700
C	-0.84714900	-0.40486300	-0.05237800
C	-2.18384300	0.33437900	0.06137200
O	-2.35907900	0.74755900	1.41002400
H	-1.60329400	1.34878400	1.55401200
H	-2.09072900	1.23744700	-0.55373800
C	-3.43688100	-0.35893600	-0.44333800
C	-3.41144200	-1.25904500	-1.51310400
C	-4.67135700	-0.00615400	0.11479300
C	-4.59579300	-1.80861400	-2.00903200
H	-2.46279000	-1.56895500	-1.93440600
C	-5.85364600	-0.55335100	-0.38074000
H	-4.68411900	0.68873500	0.94617800
C	-5.82184200	-1.45753000	-1.44572300
H	-4.55414500	-2.52013400	-2.82825600
H	-6.80315600	-0.27569600	0.06799700
H	-6.74301100	-1.88676900	-1.82799500
C	3.07346400	-2.72119600	0.76610600

C	4.08874500	-2.56031600	1.72504600
C	3.28430200	-3.60930900	-0.30414700
C	5.27679100	-3.27886100	1.61671200
H	3.92871100	-1.88270800	2.55626600
C	4.47015300	-4.33090400	-0.40308300
H	2.51560800	-3.71952400	-1.06297100
C	5.47155500	-4.16658500	0.55682400
H	6.05138000	-3.14893200	2.36625500
H	4.61815300	-5.01344300	-1.23455200
H	6.39937100	-4.72469400	0.47624600
H	0.52548600	-3.48496200	0.21010200
C	-1.78962400	-2.64541700	0.59949000
O	-1.90132500	-3.70785600	0.01732500
O	-2.60901300	-2.21031500	1.55438600
C	-3.81238800	-2.98879200	1.76620800
C	-4.54464300	-2.35652700	2.93070400
H	-3.52919600	-4.02733300	1.95881000
H	-4.39977500	-2.95812700	0.84422600
H	-5.48195300	-2.89100200	3.11416500
H	-3.93814700	-2.39478000	3.83973900
H	-4.77235600	-1.31137600	2.71092800

**TS-3ii**

N	0.03673800	-0.20213300	0.91648600
C	-2.08188500	0.90223600	1.17749600
C	-1.73474700	1.75885000	0.14241100
C	-1.06152700	-3.14386500	-1.60738800
C	-2.11968300	-2.31488000	-1.20577000
C	-2.05746800	-1.08355200	-1.99815000
C	-0.99148100	-1.21478800	-2.95727600
C	-0.31803600	-2.43265800	-2.65774500
Rh	-0.15869600	-1.12868900	-0.91734100
C	-1.09882100	-0.00004100	1.75980300
O	-1.14996000	-0.57326600	2.84823100
C	0.89721900	-2.97212600	-3.34544100
H	0.61587300	-3.71112300	-4.10578800
H	1.45903200	-2.17463500	-3.83532500
H	1.56294200	-3.46707000	-2.63314800
C	-0.67695300	-4.48335400	-1.06040200
H	-0.92793300	-5.28842500	-1.76208700
H	0.40013100	-4.53616400	-0.87404700
H	-1.18765000	-4.68915500	-0.11716200
C	-3.12427600	-2.55127900	-0.12393300
H	-4.11919400	-2.72715300	-0.55005400

H	-2.86073700	-3.41386700	0.49107800
H	-3.20115500	-1.67977500	0.53280100
C	-3.11254100	-0.02726800	-2.03401000
H	-3.80056700	-0.22372700	-2.86643400
H	-3.69463600	-0.01428900	-1.11328700
H	-2.68387500	0.96663400	-2.17998300
C	-0.65028600	-0.21341700	-4.01612300
H	-1.24619200	-0.38272200	-4.92172500
H	-0.85514100	0.80147400	-3.66581800
H	0.40620400	-0.26534500	-4.28688400
O	1.08292000	-0.80828300	1.73731200
C	1.86988400	-1.63958800	1.10602200
O	1.73305400	-1.90285400	-0.10667300
C	2.89195100	-2.33106800	1.98977500
C	3.19942300	-1.49975700	3.24533300
H	2.30009200	-1.33363300	3.84149500
H	3.92810600	-2.04030500	3.85708100
H	3.62164300	-0.52819300	2.98153400
C	2.23220300	-3.67522500	2.39033600
H	2.00767300	-4.28272200	1.50881100
H	2.92257100	-4.23401600	3.02907500
H	1.30634700	-3.50546200	2.94737400
C	4.17008100	-2.58961300	1.17582100
H	3.95619400	-3.16738000	0.27372000
H	4.64101200	-1.64791400	0.88404200
H	4.87870200	-3.15283900	1.78977900
C	-0.51912800	1.85884000	-0.57174500
C	0.44248500	0.81681700	-0.62311400
C	1.91125200	1.09968100	-0.93329600
O	2.52343300	0.14630100	-1.79341100
H	2.48075200	-0.71851000	-1.35791000
H	1.89862200	2.01174900	-1.52951900
C	2.75692300	1.40982600	0.30121500
C	2.23151300	2.12170900	1.38637900
C	4.10762300	1.04733400	0.31826500
C	3.04057800	2.45085800	2.47216200
H	1.18724300	2.41239600	1.38291500
C	4.91908400	1.37981500	1.40558600
H	4.51625000	0.51714600	-0.53442700
C	4.38800400	2.08204200	2.48755000
H	2.61574500	2.99481200	3.31046500
H	5.96673000	1.09243700	1.40256700
H	5.01615500	2.34044200	3.33475000
C	-3.45059600	0.97053400	1.75101700

C	-3.75976400	0.52812800	3.05391800
C	-4.51301500	1.48734900	0.97784400
C	-5.06009400	0.60780600	3.54903200
H	-2.96831200	0.12146400	3.66601200
C	-5.80860900	1.57129300	1.48016800
H	-4.33182800	1.82150300	-0.03716400
C	-6.09430800	1.12924300	2.77203000
H	-5.26209600	0.26100900	4.55880000
H	-6.59822900	1.97464600	0.85239500
H	-7.10566900	1.18656600	3.16344900
H	-2.44583100	2.54198400	-0.09337800
C	-0.39559600	3.15506100	-1.28765000
O	-1.33302200	3.71665900	-1.83262400
O	0.84692200	3.70218100	-1.26273300
C	1.00696300	4.95433200	-1.96238000
C	2.45503100	5.36942800	-1.79160500
H	0.31260800	5.68454600	-1.53673500
H	0.73421100	4.81429100	-3.01308500
H	2.62926200	6.33325000	-2.27952200
H	2.70543200	5.46519100	-0.73146900
H	3.12847900	4.63065900	-2.23588500

**INT-4ii**

N	0.15044200	-0.71898900	-0.32690300
C	-2.09554100	-1.46054700	0.25920400
C	-1.87517200	-0.76534300	1.45911200
C	-0.63897900	2.64689000	-2.42324600
C	-1.75578300	2.09291000	-1.78136700
C	-1.69044100	2.46461800	-0.36579300
C	-0.57610900	3.35482600	-0.17598900
C	0.13644400	3.38080700	-1.41026400
Rh	0.15417700	1.31729200	-0.72744400
C	-1.05437700	-1.53441900	-0.70589400
O	-0.99173400	-2.07732200	-1.80102300
C	1.39228900	4.14110800	-1.70653900
H	1.16429200	5.08417900	-2.21892400
H	1.93867500	4.37804000	-0.79096100
H	2.05505900	3.56208300	-2.35493000
C	-0.22873900	2.49639700	-3.85502600
H	-0.37678300	3.43027200	-4.41116700
H	0.82993300	2.23062100	-3.93391000
H	-0.80506000	1.71282200	-4.35113100
C	-2.81241200	1.20434000	-2.35474100
H	-3.78640800	1.70806400	-2.35224100

H	-2.58262300	0.91269600	-3.38092800
H	-2.91898200	0.28963500	-1.76272100
C	-2.79403500	2.21666900	0.61139200
H	-3.55817600	2.99782600	0.50608100
H	-3.27553300	1.25535000	0.42769400
H	-2.44612300	2.22555700	1.64445400
C	-0.26106800	4.11839600	1.07190800
H	-0.82286700	5.06121400	1.10035600
H	-0.51820200	3.54136700	1.96020400
H	0.80234900	4.36186800	1.13322900
O	1.29974900	-1.37237400	-0.91394800
C	2.08672900	-0.59945800	-1.65613300
O	1.91563700	0.61724300	-1.76226400
C	3.18797000	-1.35889100	-2.37195600
C	3.17013100	-2.85634400	-2.02564700
H	2.21768900	-3.31515700	-2.30072000
H	3.96913600	-3.35382000	-2.58364100
H	3.33672800	-3.02429600	-0.95987000
C	2.93603200	-1.15765600	-3.88382900
H	2.94552600	-0.09677900	-4.14589400
H	3.72492600	-1.66427700	-4.44738100
H	1.97343600	-1.58470100	-4.18085700
C	4.53078900	-0.71950600	-1.96373500
H	4.55548000	0.34027600	-2.22876100
H	4.69039700	-0.80870600	-0.88743300
H	5.34349000	-1.23205500	-2.48666600
C	-0.72418700	-0.08679000	1.82581000
C	0.43024500	-0.04800700	0.92618600
C	1.81464300	-0.26414600	1.56012300
O	2.85741400	0.43483800	0.88294900
H	2.46075400	1.27268700	0.59422600
H	1.71703300	0.14720500	2.56621600
C	2.21988200	-1.72505800	1.69464800
C	1.26972400	-2.73192900	1.90115000
C	3.57598900	-2.06941400	1.66159900
C	1.66808000	-4.06047700	2.04276800
H	0.21456700	-2.48560200	1.93975800
C	3.97335000	-3.39919300	1.81029600
H	4.31460500	-1.29026100	1.51660400
C	3.02052100	-4.40140400	1.99486200
H	0.91611900	-4.83037500	2.18752500
H	5.02982000	-3.65038400	1.77956000
H	3.32823900	-5.43699000	2.10401600
C	-3.41701300	-2.05645700	-0.04031600

C	-3.56550400	-3.14699900	-0.91904600
C	-4.58313500	-1.53514700	0.55487600
C	-4.82156900	-3.69210300	-1.17593700
H	-2.68900100	-3.55644000	-1.40271700
C	-5.83604900	-2.08607500	0.29886300
H	-4.51448400	-0.67921200	1.21849600
C	-5.96509600	-3.17054700	-0.56956800
H	-4.90455600	-4.53617400	-1.85503000
H	-6.71478800	-1.65831500	0.77337200
H	-6.94189500	-3.59859900	-0.77400100
H	-2.67861000	-0.72971300	2.18596200
C	-0.80128300	0.68866000	3.06291200
O	-1.73058000	0.66280100	3.85782600
O	0.25900300	1.53790100	3.24216400
C	0.23272600	2.32112800	4.45013900
C	1.53176900	3.10143700	4.50624500
H	0.11390600	1.65330600	5.30817500
H	-0.64100900	2.98122500	4.42869300
H	1.56150400	3.71503900	5.41181700
H	2.39127800	2.42506200	4.51903500
H	1.62824800	3.76189800	3.63964900

**TS-5i**

N	-1.16704500	-0.12481600	-1.43905600
C	-1.75921900	-1.38833300	-1.21522700
C	-1.09623000	-2.37361200	-0.55068700
C	-1.86420500	1.96550800	1.99290600
C	-2.69133800	0.88340200	1.58022000
C	-2.10552600	-0.35736600	2.05231600
C	-0.90908300	-0.02084000	2.77361700
C	-0.73497900	1.40396400	2.71537500
Rh	-0.66384900	0.64481600	0.67718500
C	0.13688100	-0.00209500	-1.50938100
O	1.01226500	0.49653200	-2.12709100
C	0.35798800	2.19549200	3.35443400
H	0.02018500	2.59942000	4.31674600
H	1.24170400	1.57909700	3.51832700
H	0.64802400	3.03263500	2.71602700
C	-2.11706600	3.42045100	1.76289900
H	-2.75856800	3.82309300	2.55725500
H	-1.18256500	3.98378900	1.76892300
H	-2.59643500	3.59207200	0.79891900
C	-3.94937400	1.01201600	0.78567100
H	-4.79115000	1.23620600	1.45276500



H	-3.86736100	1.82316700	0.05905700
H	-4.18106100	0.09543300	0.24279400
C	-2.74281000	-1.70800600	2.00640800
H	-3.33216700	-1.86725800	2.91855200
H	-3.41566000	-1.80511400	1.15388300
H	-2.00054500	-2.50575200	1.94248800
C	-0.00675000	-0.98090300	3.47852100
H	-0.27023700	-1.02419800	4.54267800
H	-0.09874800	-1.98783700	3.06797800
H	1.03212200	-0.65894300	3.39086100
O	-0.86049300	3.10992900	-1.14858800
C	0.27938900	3.06914300	-0.69187200
O	0.69889700	2.13881400	0.13439500
C	1.35678000	4.11710400	-1.03561800
C	2.48594900	3.41808800	-1.81860800
H	2.10592000	2.97697400	-2.74384300
H	3.26277800	4.14661000	-2.07666000
H	2.93975100	2.61590100	-1.23366200
C	0.73329600	5.23019200	-1.88637100
H	-0.07186500	5.73707600	-1.34673800
H	1.49583700	5.97175200	-2.14853800
H	0.30762400	4.82389300	-2.80641400
C	1.92216100	4.70416900	0.27172500
H	1.13312600	5.17872200	0.86721300
H	2.39290900	3.92807700	0.87976500
H	2.67333500	5.46871700	0.04612800
C	0.21774600	-2.17404800	0.02123200
C	0.79500800	-0.93086900	0.17255500
C	2.21908500	-0.69360400	0.66969400
O	2.29413500	0.44348700	1.51929300
H	1.94935500	1.20715900	1.01227100
H	2.49987100	-1.53260600	1.31485300
C	3.27085800	-0.62881900	-0.44743800
C	3.24257600	-1.48641700	-1.55248000
C	4.32516000	0.28197400	-0.33182600
C	4.24113600	-1.42868200	-2.52207100
H	2.43198600	-2.19526500	-1.66369800
C	5.32340500	0.34518700	-1.30592700
H	4.35484400	0.94244600	0.52651500
C	5.28618600	-0.51013200	-2.40554500
H	4.19553400	-2.09568400	-3.37836000
H	6.12930800	1.06620600	-1.20204200
H	6.05990000	-0.46123100	-3.16611000
C	-3.12703900	-1.50830900	-1.74735300

C	-3.67447600	-0.45965900	-2.50871100
C	-3.93065500	-2.63353900	-1.48066500
C	-4.97726900	-0.54055800	-2.99450300
H	-3.06265200	0.41434600	-2.69818200
C	-5.23192900	-2.70818000	-1.96635400
H	-3.54275300	-3.45134600	-0.88338800
C	-5.76280200	-1.66237900	-2.72656700
H	-5.38072500	0.27914000	-3.58138700
H	-5.83598100	-3.58359900	-1.74761400
H	-6.78026300	-1.72160500	-3.10076900
H	-1.53006300	-3.35848200	-0.45190600
C	0.80587300	-3.42671600	0.60160100
O	0.14069000	-4.21022200	1.25830400
O	2.11366000	-3.57946800	0.36182400
C	2.76990400	-4.72039000	0.96486900
C	4.23613500	-4.62037800	0.59536000
H	2.30099500	-5.63264500	0.58435600
H	2.60564300	-4.68667600	2.04604100
H	4.78614600	-5.46633800	1.01814500
H	4.36274800	-4.62701700	-0.49028000
H	4.66987300	-3.69303700	0.97883300

**INT-6i**

N	-0.29193400	-0.69718100	0.34689100
C	-0.16967800	-1.93473900	-0.21610200
C	1.04001800	-2.59656700	-0.21310800
C	-4.12165900	0.60526200	0.46086200
C	-3.55049800	-0.38989500	1.33522500
C	-2.68701600	0.29604300	2.27226600
C	-2.72750100	1.69811200	1.96807200
C	-3.61753300	1.89647900	0.83834400
Rh	-1.95457000	0.62844600	0.26347200
C	0.75623000	-0.14381200	1.06228900
O	0.55165600	0.87732500	1.77530900
C	-3.95435300	3.21115100	0.20831900
H	-4.75362600	3.71799100	0.76221200
H	-3.08270000	3.86909700	0.19137400
H	-4.29014500	3.07813900	-0.82217300
C	-5.04837500	0.31544700	-0.67487200
H	-6.08577500	0.29763600	-0.31949000
H	-4.96780100	1.07372600	-1.45572900
H	-4.82350800	-0.65589800	-1.11936400
C	-3.90256400	-1.84086700	1.36339000
H	-4.76740800	-2.00037500	2.01998800

H	-4.15235100	-2.21646800	0.37096800
H	-3.07637700	-2.44196000	1.74200700
C	-1.90396700	-0.33228800	3.37924100
H	-2.45575700	-0.25643100	4.32402200
H	-1.71936900	-1.38912200	3.17775600
H	-0.93802100	0.16244800	3.48312500
C	-1.92542000	2.74725600	2.66489300
H	-2.30253300	2.89834100	3.68308800
H	-0.88144700	2.42817700	2.71247300
H	-1.97099300	3.69928100	2.13451700
O	-1.64564700	0.78419500	-1.90500200
C	-0.69246100	1.61944800	-1.71958900
O	-0.53263800	2.06283600	-0.54195600
C	0.28024300	1.95460600	-2.83598100
C	1.05215400	3.23815300	-2.49993900
H	1.58306500	3.14383000	-1.55205400
H	1.78522200	3.44258900	-3.28685600
H	0.37614900	4.09672300	-2.43179900
C	1.25299900	0.75181200	-2.90385700
H	0.71710700	-0.17117500	-3.14237600
H	2.00348400	0.93132600	-3.68054500
H	1.77411400	0.61979900	-1.95304500
C	-0.47749600	2.09552900	-4.16599000
H	-1.04699200	1.19104100	-4.39157900
H	-1.17434800	2.93998100	-4.13600800
H	0.23310600	2.27330700	-4.97946900
C	2.18688800	-1.98029100	0.34207200
C	2.07412200	-0.75764400	0.97826400
C	3.19472400	0.02598700	1.66153400
O	2.82709900	0.39032100	2.97848300
H	1.93638800	0.78519300	2.86070400
H	4.07011300	-0.61459300	1.75795700
C	3.58910500	1.22970500	0.79558100
C	4.05330800	1.04480000	-0.51368700
C	3.50875200	2.52736200	1.30368000
C	4.43314900	2.13573900	-1.29439800
H	4.12237700	0.04096100	-0.91683900
C	3.87992700	3.62166600	0.51997700
H	3.16323500	2.66635200	2.32087800
C	4.34584100	3.43137400	-0.78113000
H	4.79149900	1.97385800	-2.30739000
H	3.80650300	4.62539600	0.92942600
H	4.63474900	4.28280900	-1.39046400
C	-1.36388300	-2.65082900	-0.74730200

C	-2.19188200	-2.14217300	-1.75716800
C	-1.64428100	-3.92389900	-0.22389600
C	-3.28330500	-2.88371800	-2.21285400
H	-1.97218400	-1.17635400	-2.19051000
C	-2.73735100	-4.66094700	-0.67804900
H	-1.00231000	-4.32606800	0.55364900
C	-3.56643200	-4.14014500	-1.67271300
H	-3.90637400	-2.48020100	-3.00637300
H	-2.94102500	-5.63938000	-0.25331200
H	-4.41708500	-4.71213200	-2.03127300
H	1.12712100	-3.58006600	-0.65314800
C	3.44288200	-2.78815300	0.20129100
O	3.45143300	-3.99732200	0.08056800
O	4.56672500	-2.04361400	0.17206400
C	5.81093200	-2.76399500	0.02516800
C	6.92383900	-1.73625600	0.07474700
H	5.78783200	-3.30946600	-0.92327600
H	5.88716300	-3.50221600	0.82876800
H	7.89194300	-2.22932400	-0.05537100
H	6.80260700	-0.99191700	-0.71696200
H	6.92775800	-1.21286000	1.03478800

**INT-10i**

N	1.61385600	-1.12971800	-0.97941400
C	2.16635800	-0.13116300	-0.22003500
C	1.34322900	0.86955600	0.22449400
C	0.26651100	-1.24534400	-1.34060300
O	-0.09891200	-2.18621700	-2.04589700
C	-0.04416500	0.84408300	-0.10518600
C	-0.59008000	-0.17636400	-0.84239600
C	-2.06418000	-0.32245500	-1.17214200
O	-2.75644200	0.91838200	-1.09189900
H	-2.29186300	1.55501200	-1.65184600
H	-2.12944800	-0.74480200	-2.18287200
C	-2.71870600	-1.29650300	-0.20604400
C	-3.11193100	-0.86689400	1.06661600
C	-2.89047900	-2.63493300	-0.56865500
C	-3.68819500	-1.76928700	1.95880400
H	-2.96045800	0.16688700	1.35473200
C	-3.46204100	-3.53692000	0.32974100
H	-2.55285700	-2.96698600	-1.54437800
C	-3.86578000	-3.10580100	1.59356600
H	-3.99571000	-1.42881100	2.94336400
H	-3.59339700	-4.57538000	0.03976400

H	-4.31395100	-3.80693100	2.29176000
C	3.60633300	-0.21662700	0.08321700
C	4.22662000	-1.46048900	0.28322800
C	4.37967200	0.95078100	0.18063700
C	5.58735000	-1.53297300	0.57327300
H	3.63708900	-2.37205000	0.25071700
C	5.73825300	0.87480200	0.47485600
H	3.91493400	1.91398400	-0.00183500
C	6.34735300	-0.36660100	0.66994500
H	6.05111300	-2.50104600	0.73471900
H	6.32539400	1.78553200	0.54029000
H	7.40751500	-0.42415400	0.89568100
H	1.73679100	1.64957500	0.86225300
H	2.20855000	-1.84693400	-1.37570600
C	-0.85840600	1.97959900	0.45920800
O	-1.27633000	2.01381600	1.59458800
O	-0.94294500	3.00081900	-0.42263800
C	-1.67201700	4.17206100	0.03460700
C	-3.16499300	4.01533900	-0.20098400
H	-1.25123500	4.99468200	-0.54745200
H	-1.45252900	4.32321000	1.09342800
H	-3.68687800	4.91312800	0.14556000
H	-3.38470800	3.88367300	-1.26459000
H	-3.55256400	3.15184200	0.34218700

**TS-9i**

N	1.59462800	-1.11660600	-0.96854100
C	2.16517100	-0.16480000	-0.15713400
C	1.36104500	0.81079500	0.37688700
C	0.23798400	-1.22280000	-1.32552800
O	-0.13180300	-2.09927800	-2.10394300
C	-0.02026300	0.77511100	0.05591600
C	-0.58180800	-0.19930400	-0.71357500
C	-2.08658800	-0.11217100	-0.86017300
O	-2.45387500	1.13975800	-0.29900900
H	-2.00522100	2.14082000	-0.88750000
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C	-2.77771000	-1.25579500	-0.12942700
C	-3.23399900	-1.07493900	1.17917100
C	-2.92687100	-2.50012500	-0.74960200
C	-3.83869500	-2.13112000	1.86075000
H	-3.12537100	-0.10401900	1.64940700
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H	-2.54470500	-2.64417400	-1.75417700

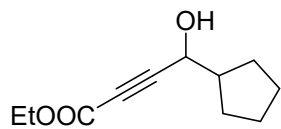
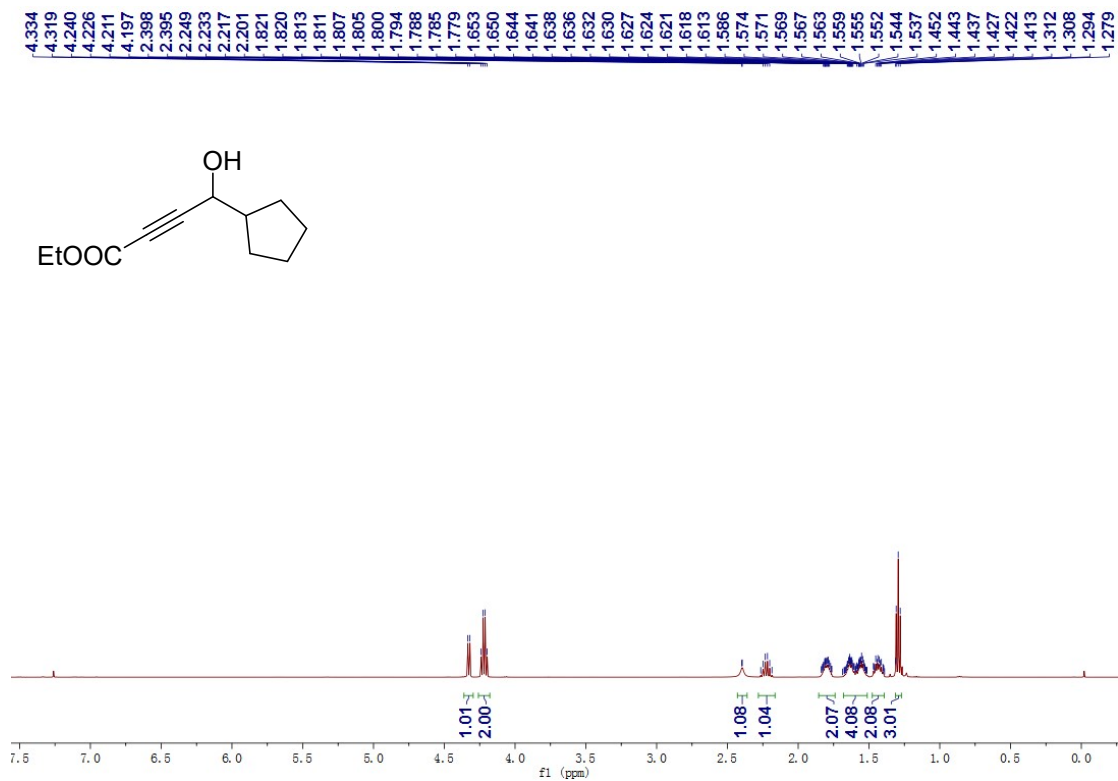
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H	-4.46118000	-4.19414600	1.77304500
C	3.61342000	-0.27113000	0.09942900
C	4.23539500	-1.52533900	0.20885000
C	4.39158500	0.88812100	0.24361200
C	5.60344400	-1.61575000	0.45622600
H	3.64277400	-2.43281600	0.13911100
C	5.75772000	0.79379800	0.49453000
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C	6.36860000	-0.45754000	0.59947500
H	6.06927200	-2.59190300	0.54780200
H	6.34874700	1.69855700	0.59664300
H	7.43451600	-0.52922200	0.79151800
H	1.75920700	1.55722500	1.04993600
H	2.19103800	-1.79342100	-1.42874500
C	-0.97091600	1.79080600	0.57946200
O	-1.10850900	2.27199600	1.65879400
O	-1.13950800	2.91704600	-0.76208700
C	-1.54779200	4.22234800	-0.32600700
C	-3.06201900	4.36358500	-0.25471300
H	-1.10812600	4.93763900	-1.02905800
H	-1.10589700	4.38916500	0.66313900
H	-3.33164200	5.37621800	0.06181300
H	-3.51999600	4.17946800	-1.23202000
H	-3.48073500	3.65379700	0.46338700

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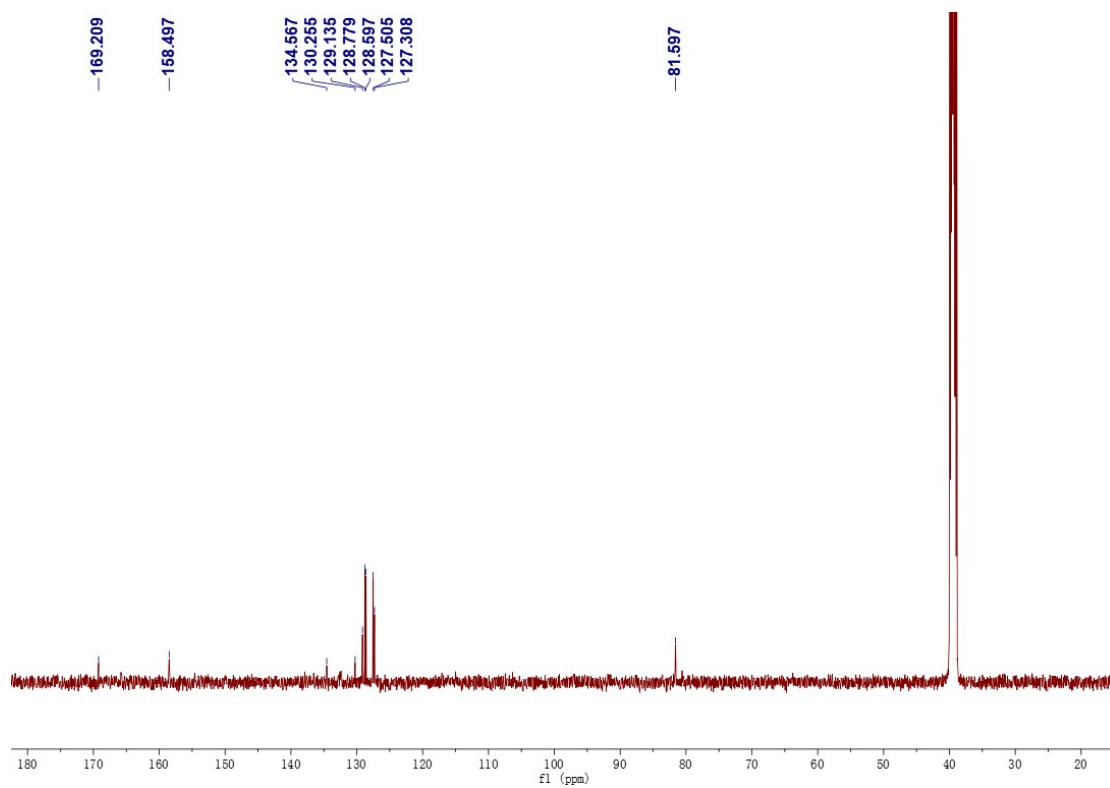
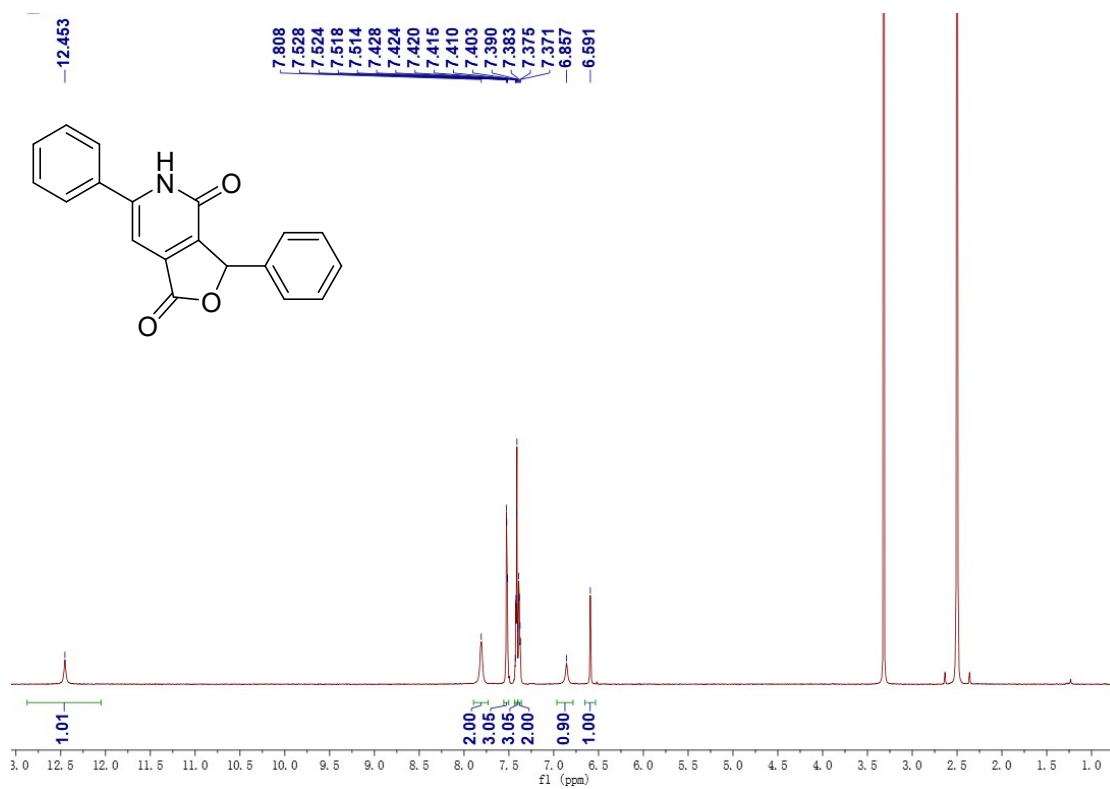
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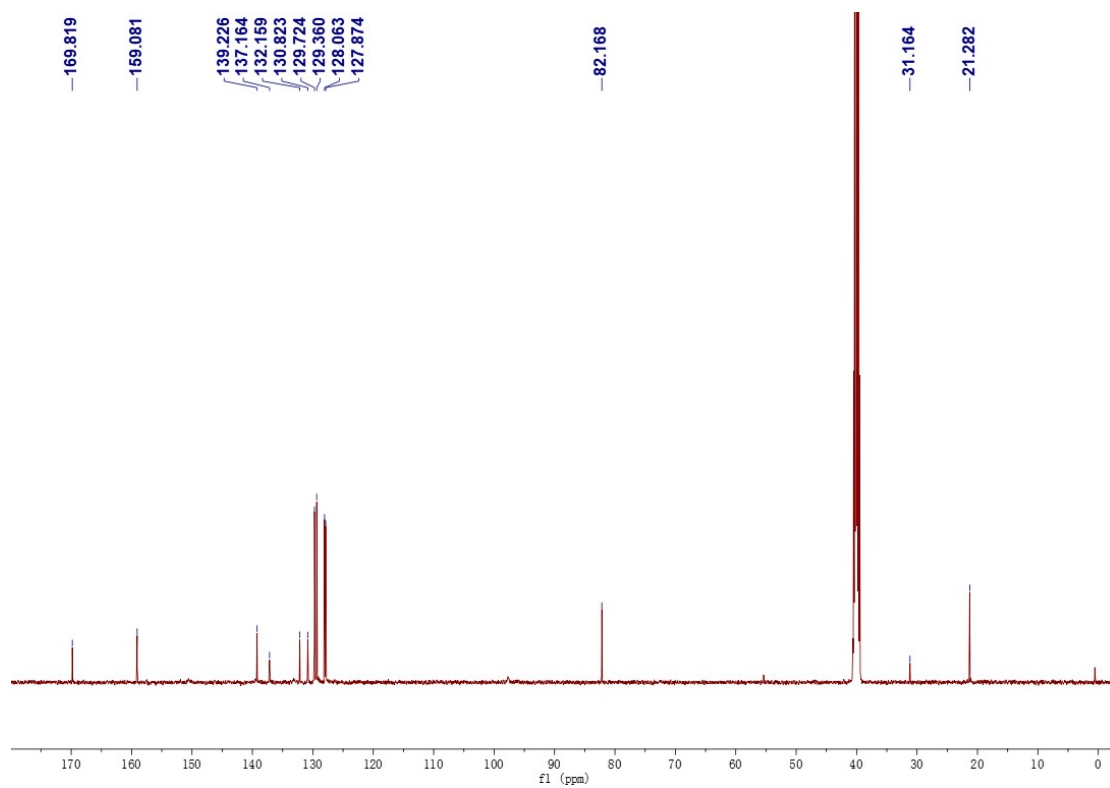
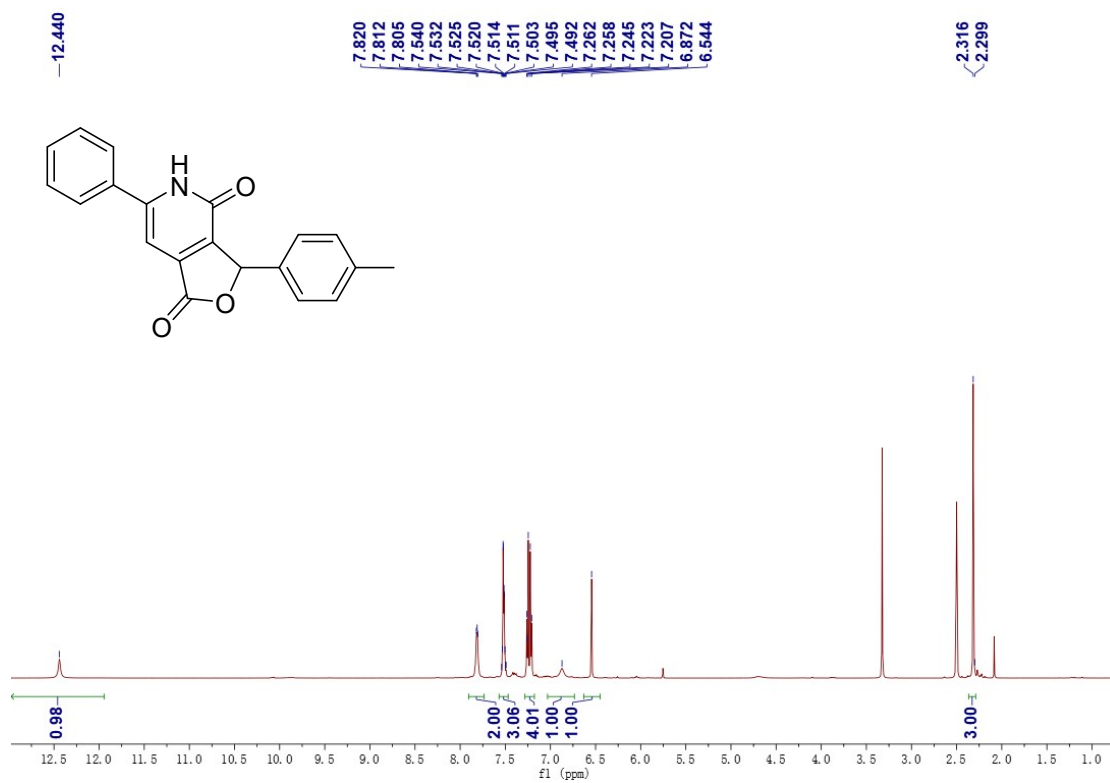




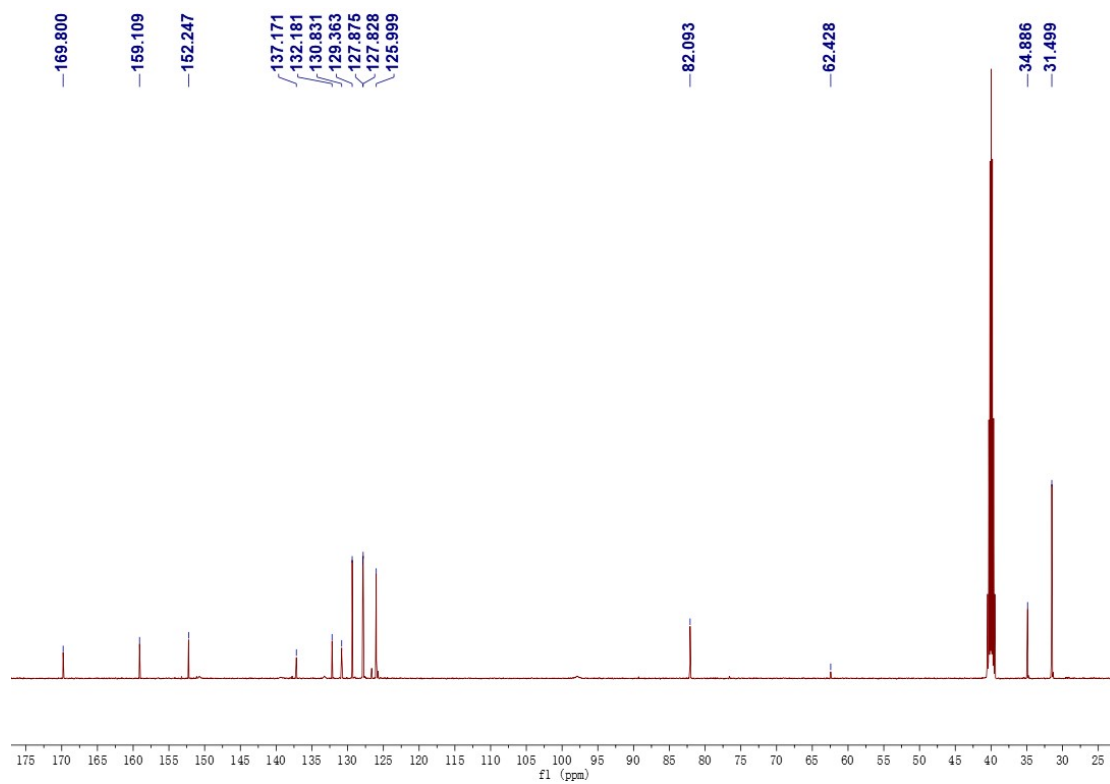
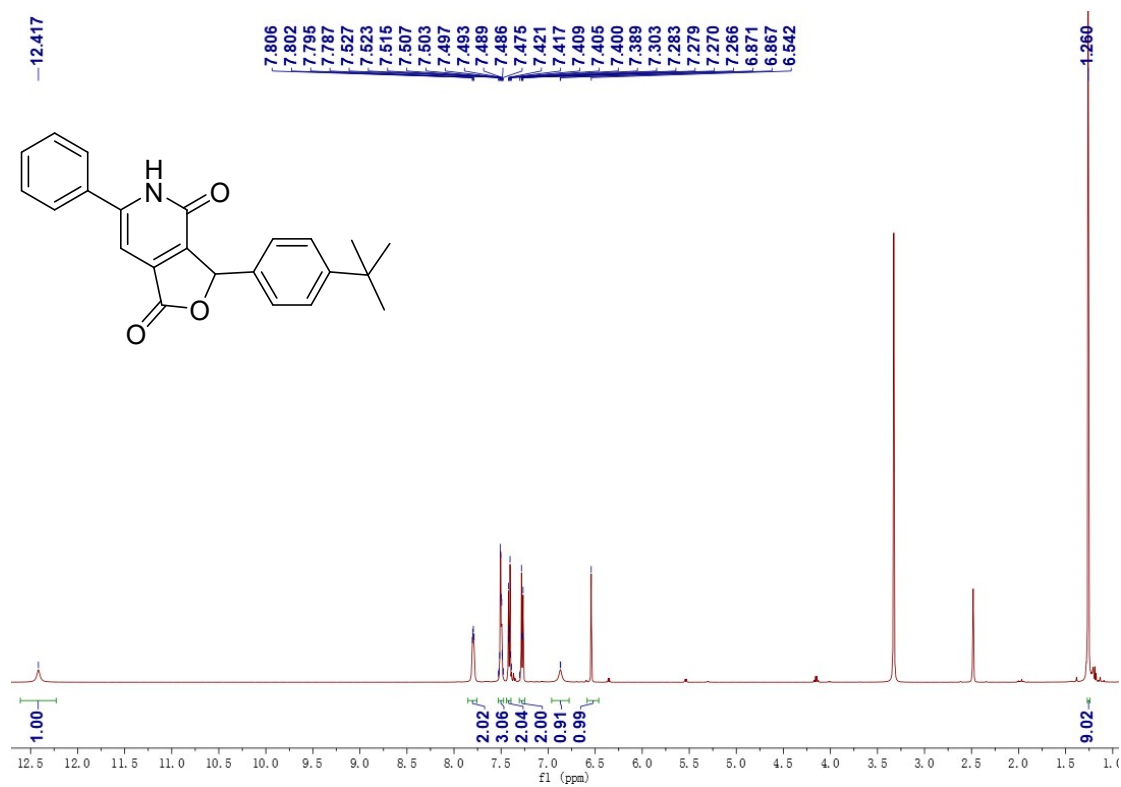
3,6-diphenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3a)



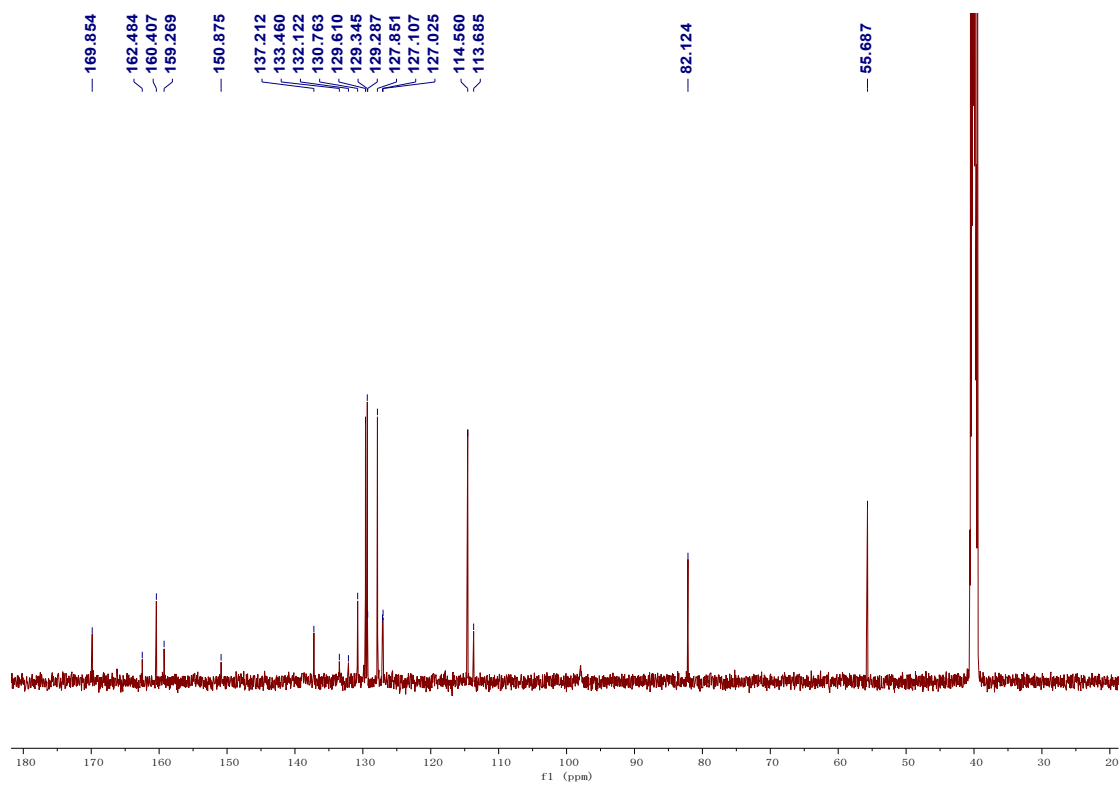
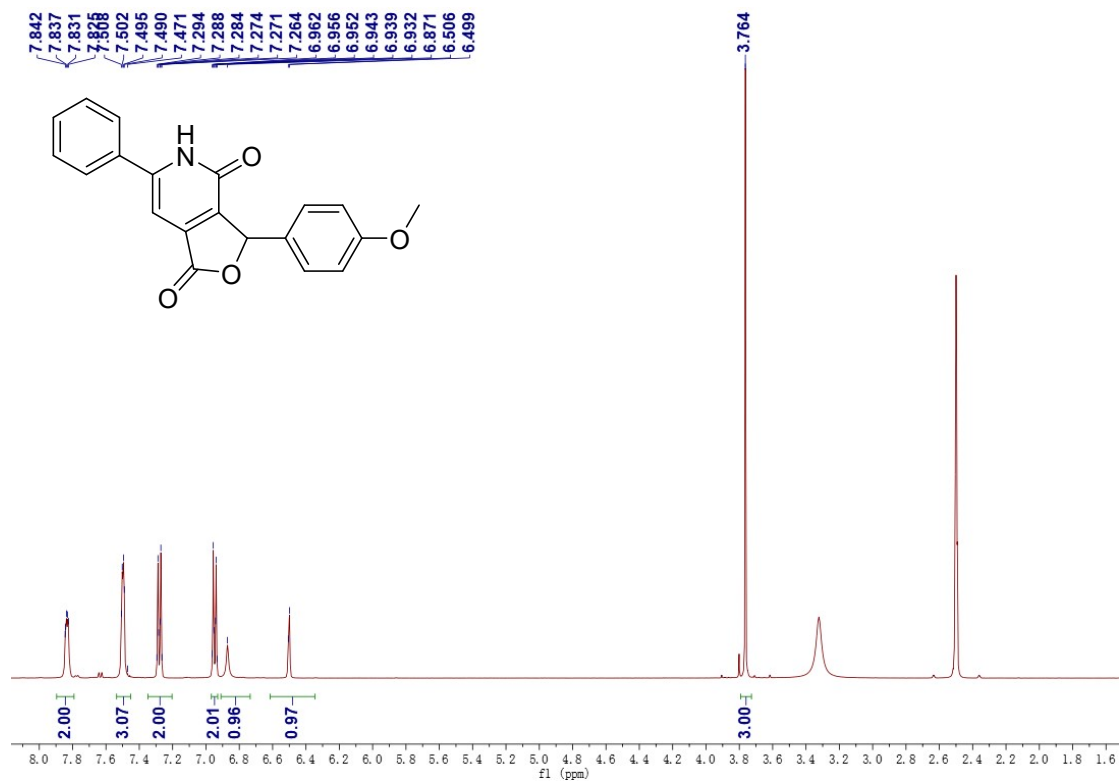
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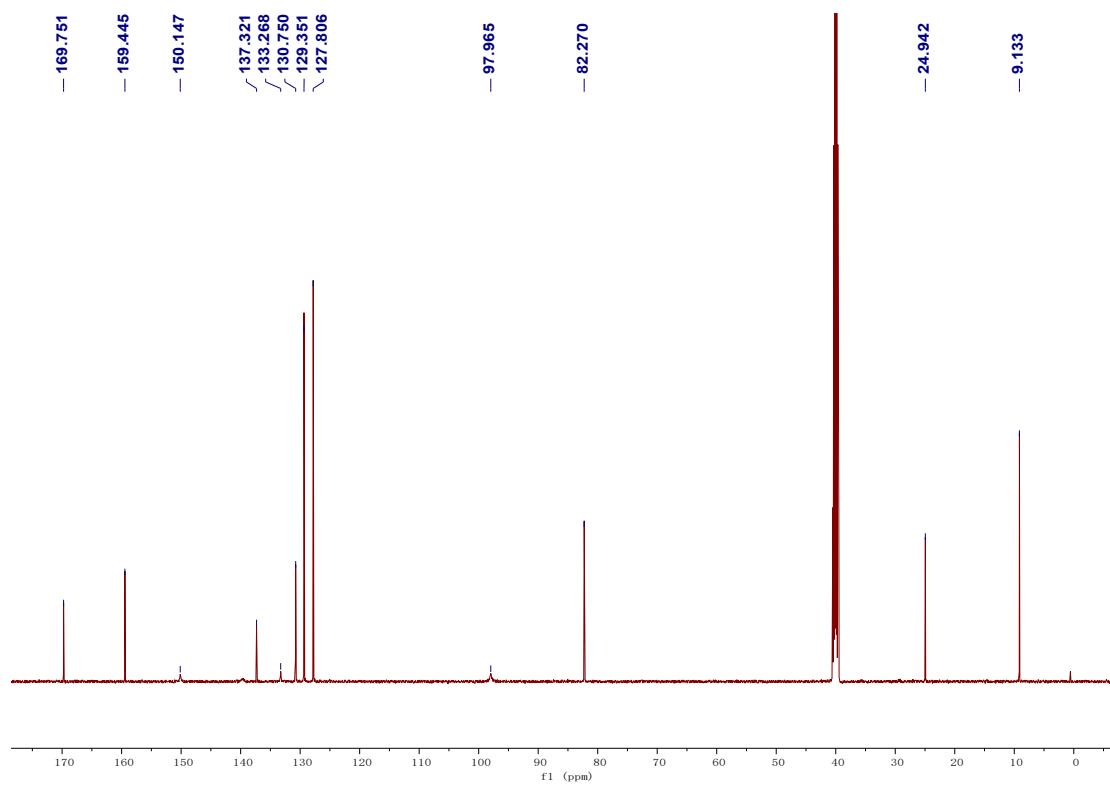
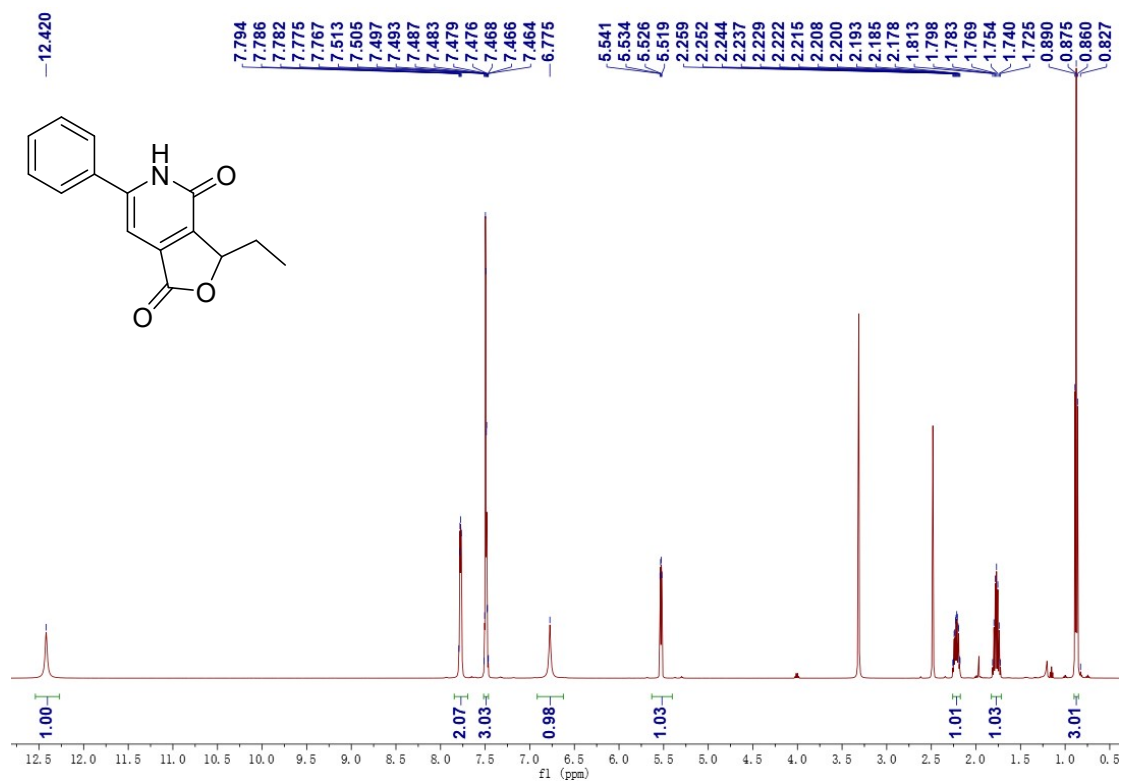
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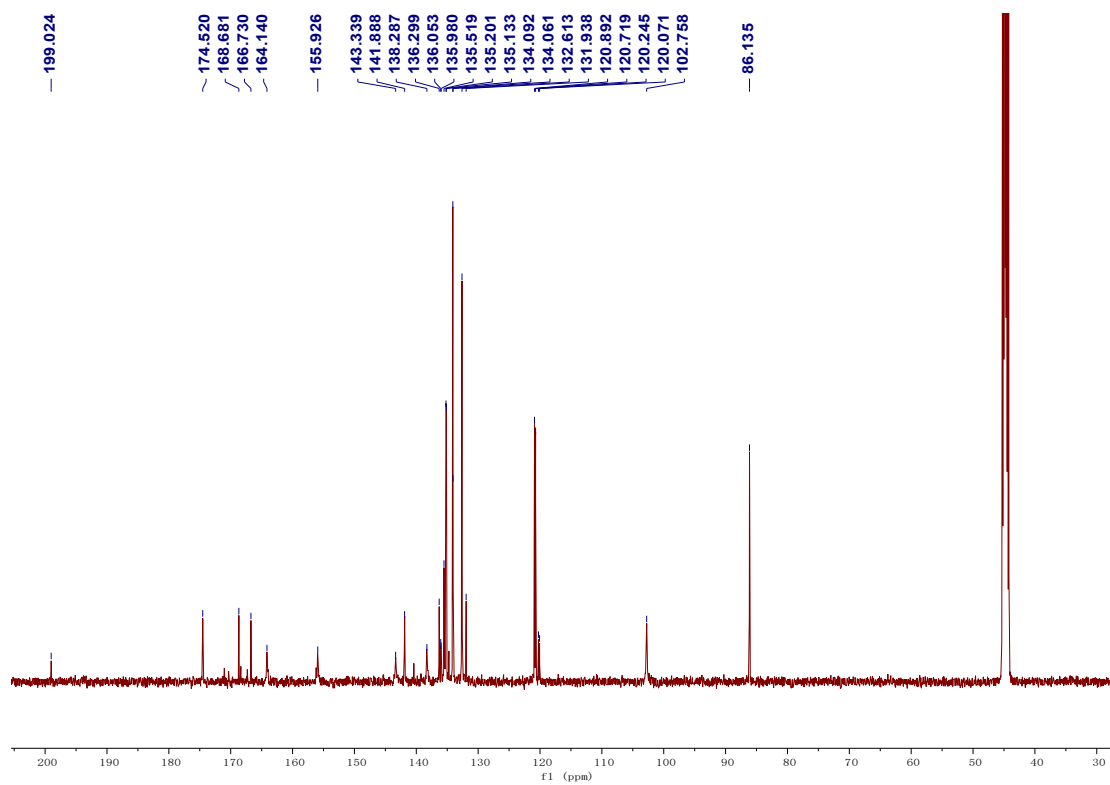
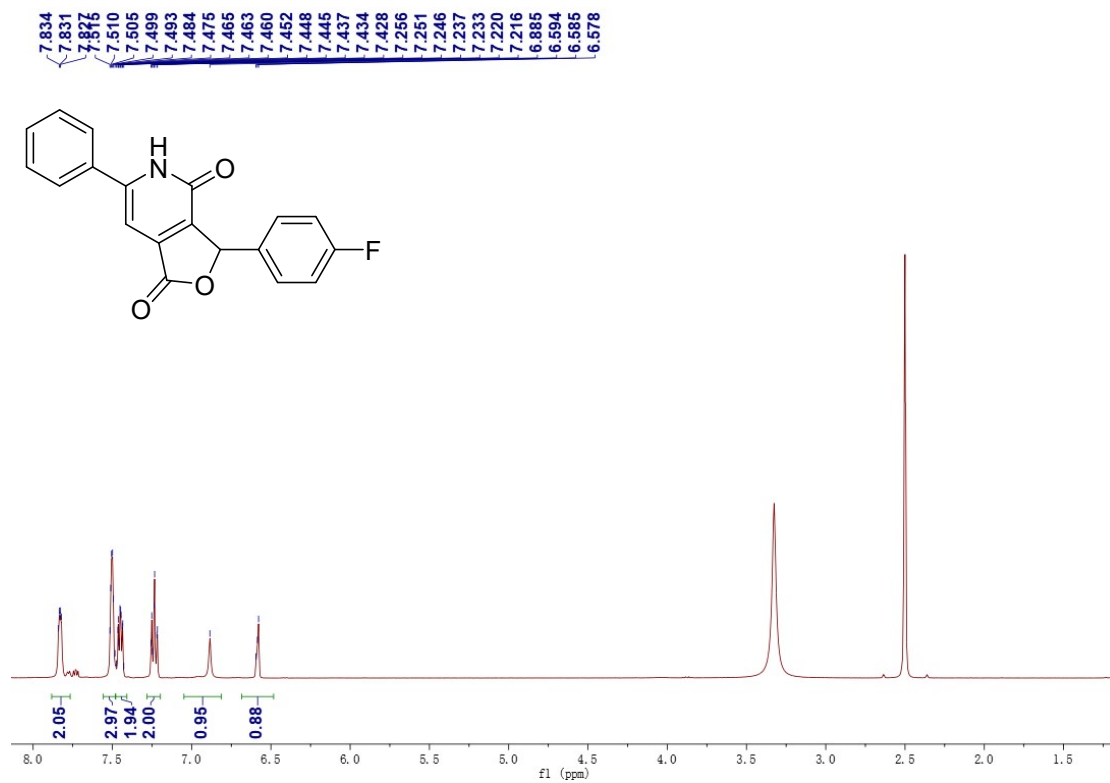
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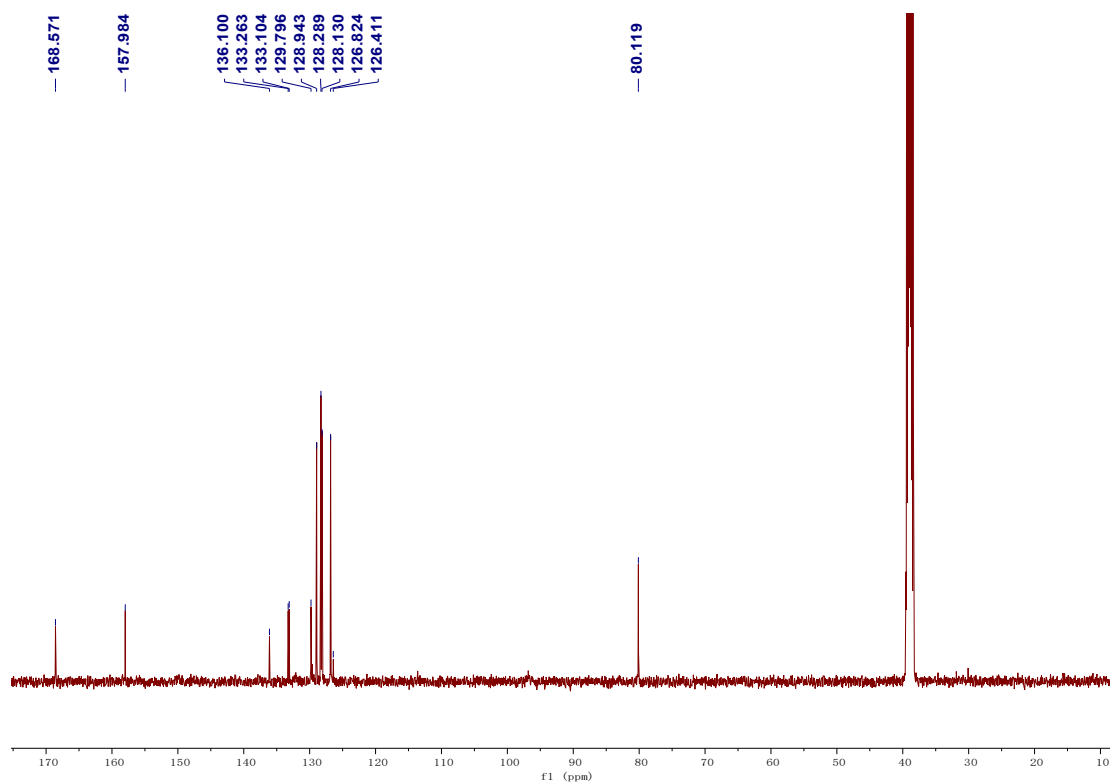
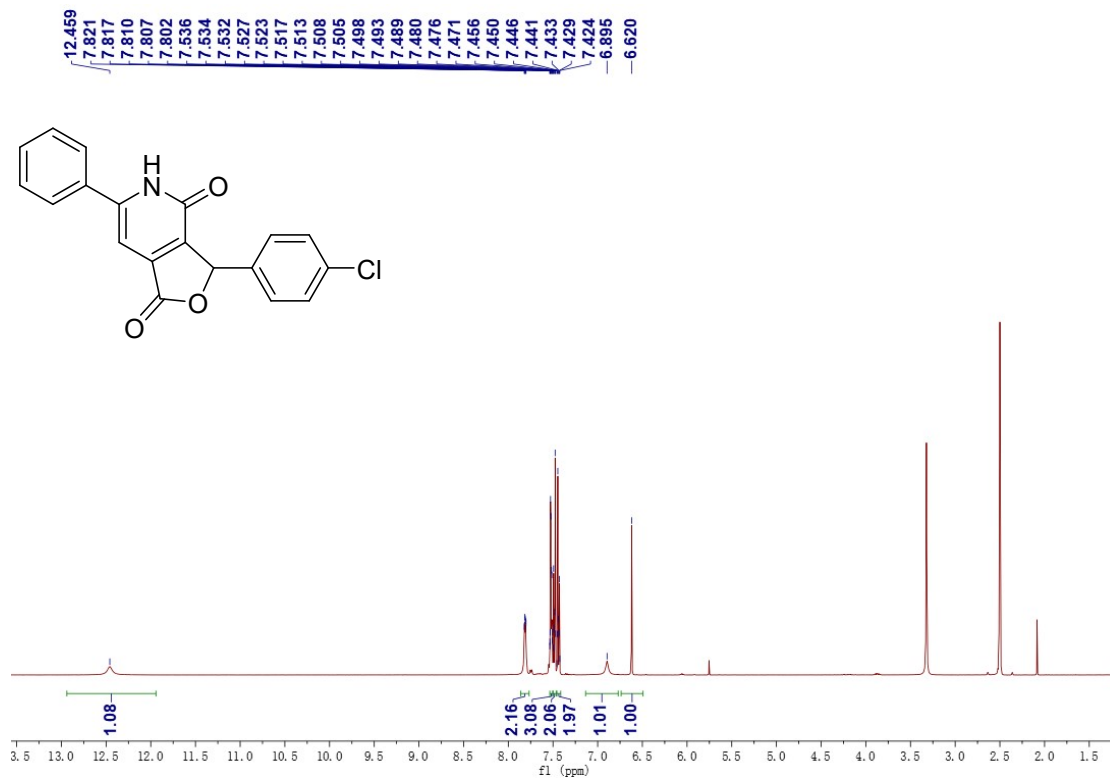
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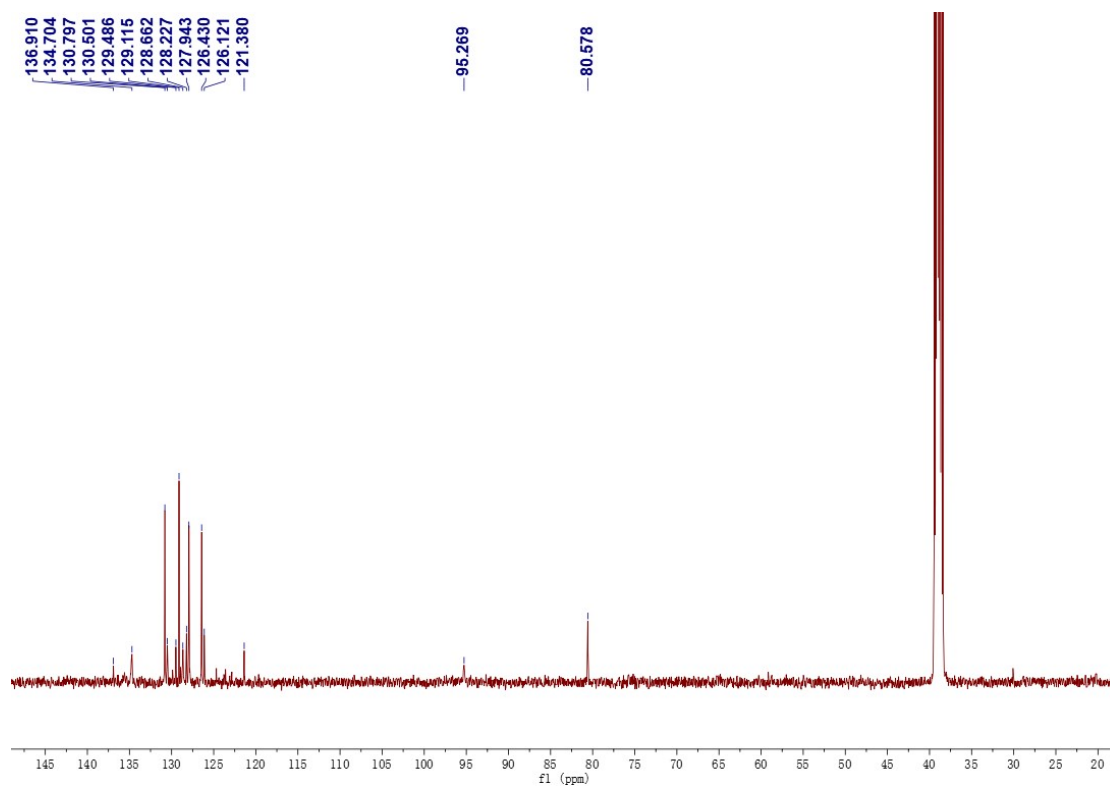
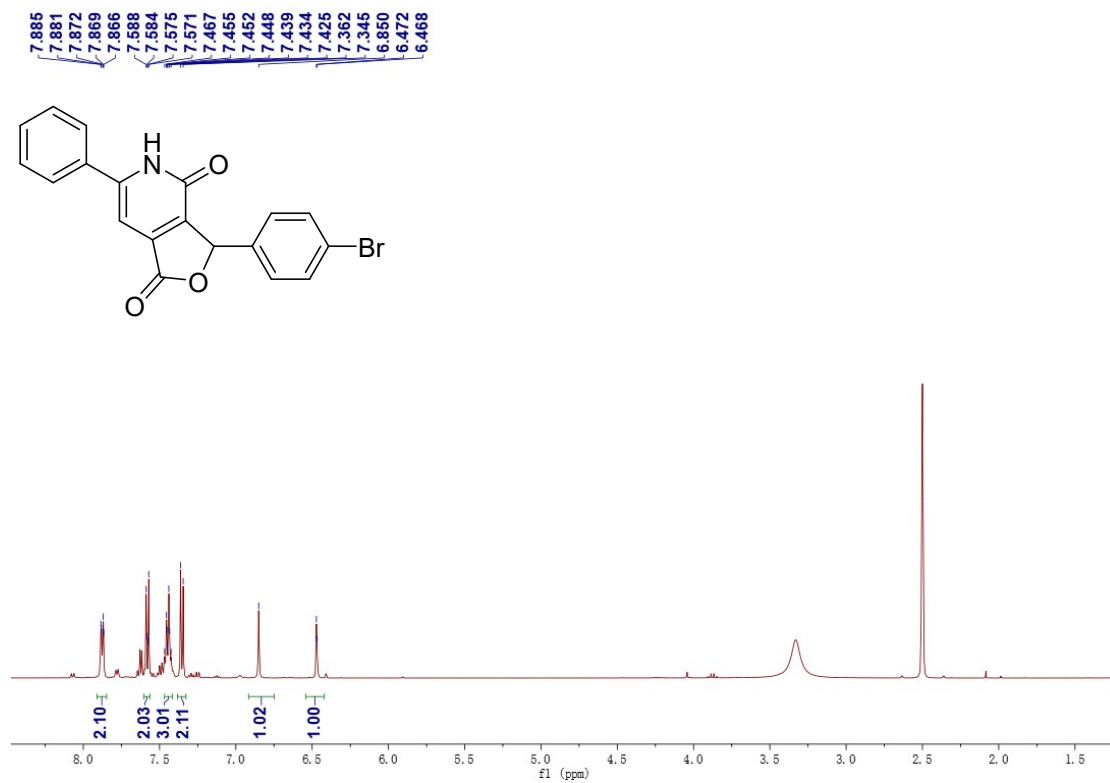
3-(4-fluorophenyl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3f)



3-(4-chlorophenyl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3g)

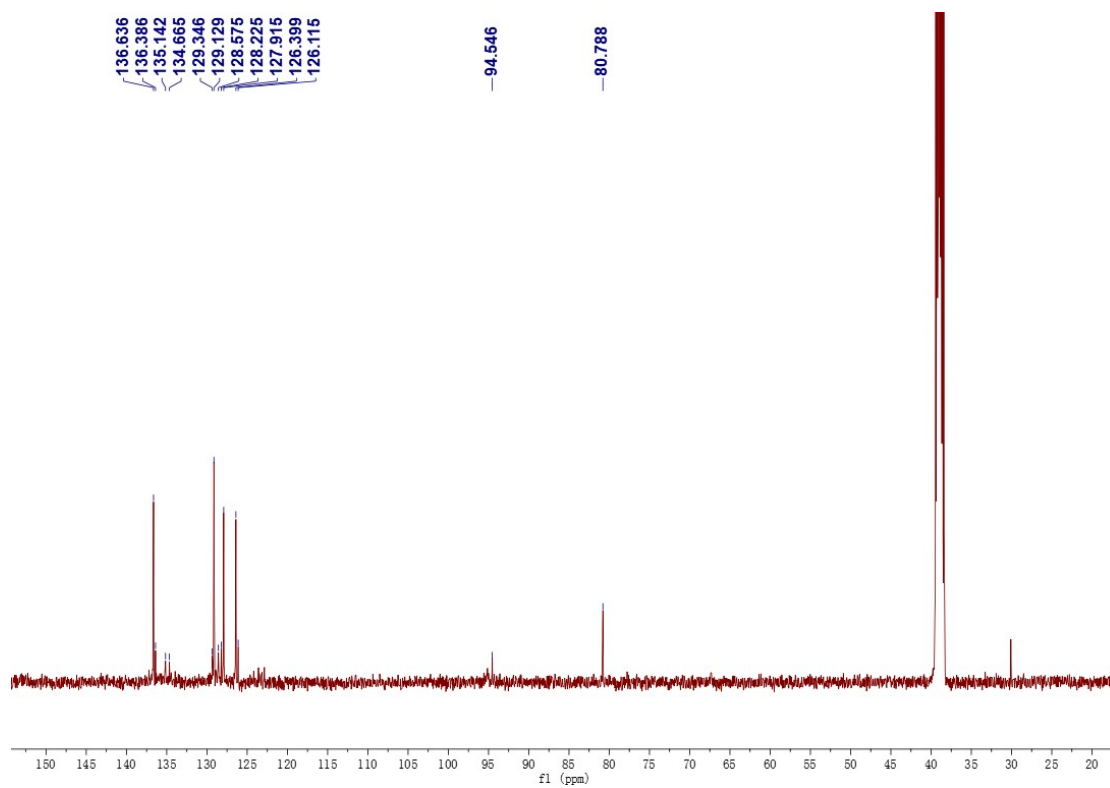
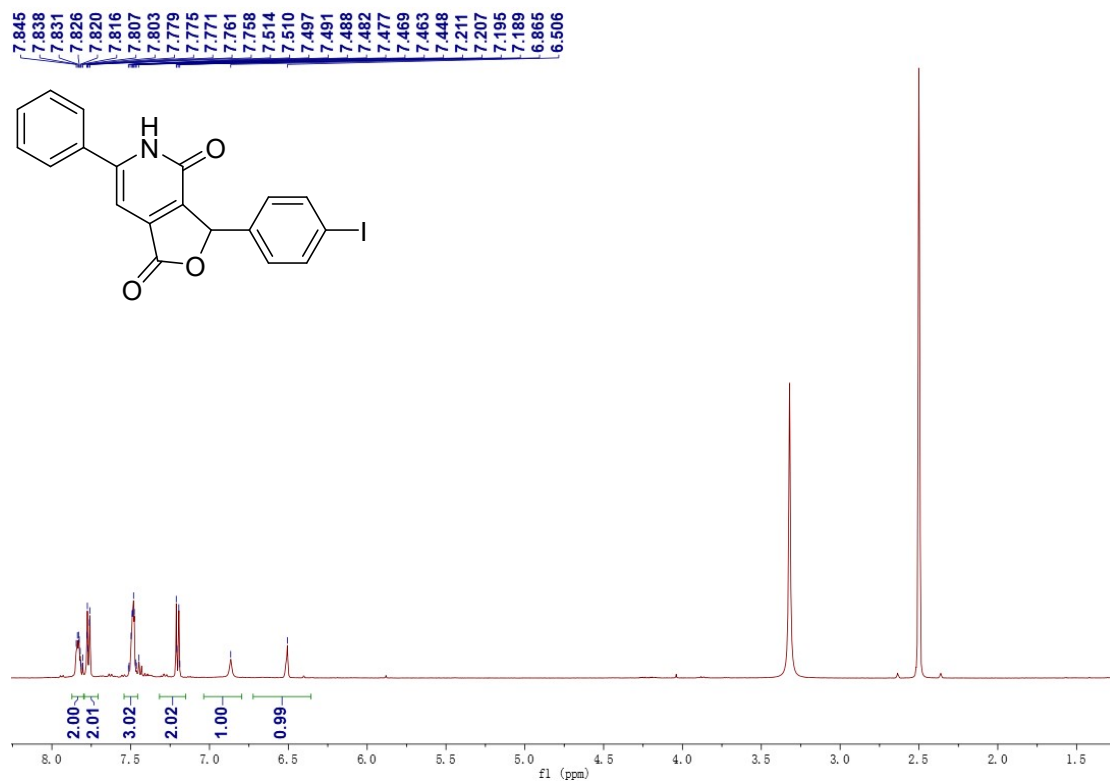


3-(4-bromophenyl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3h)

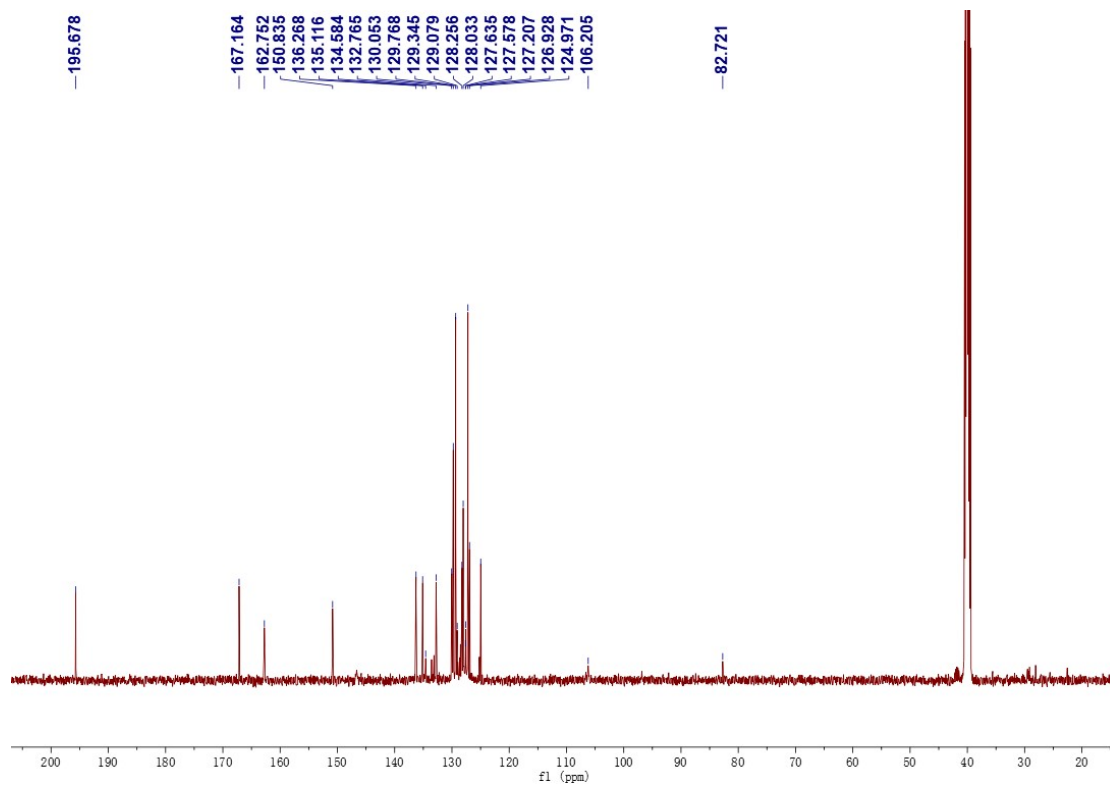
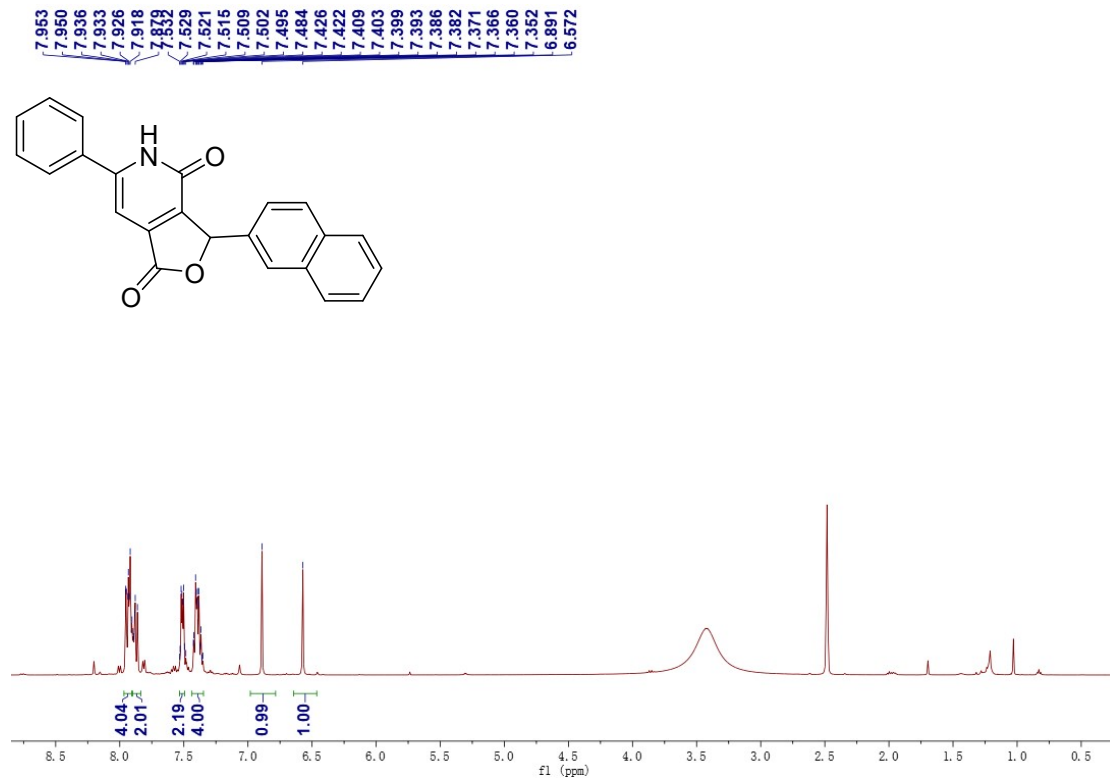




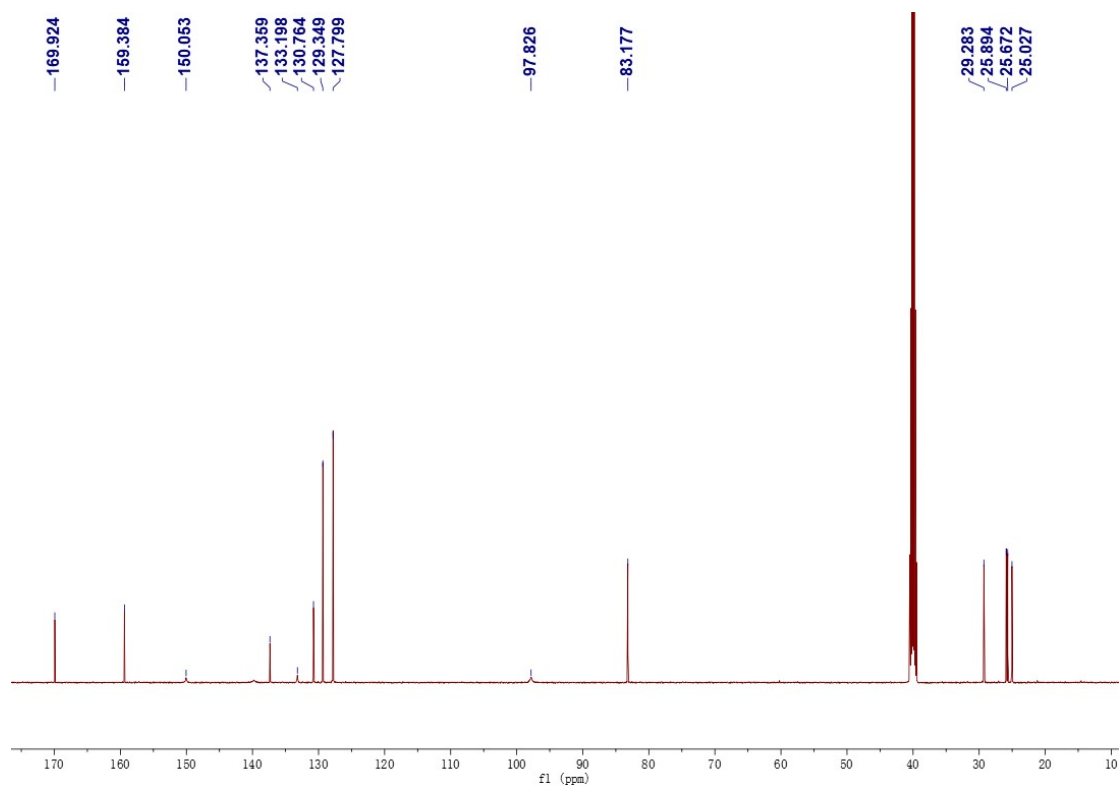
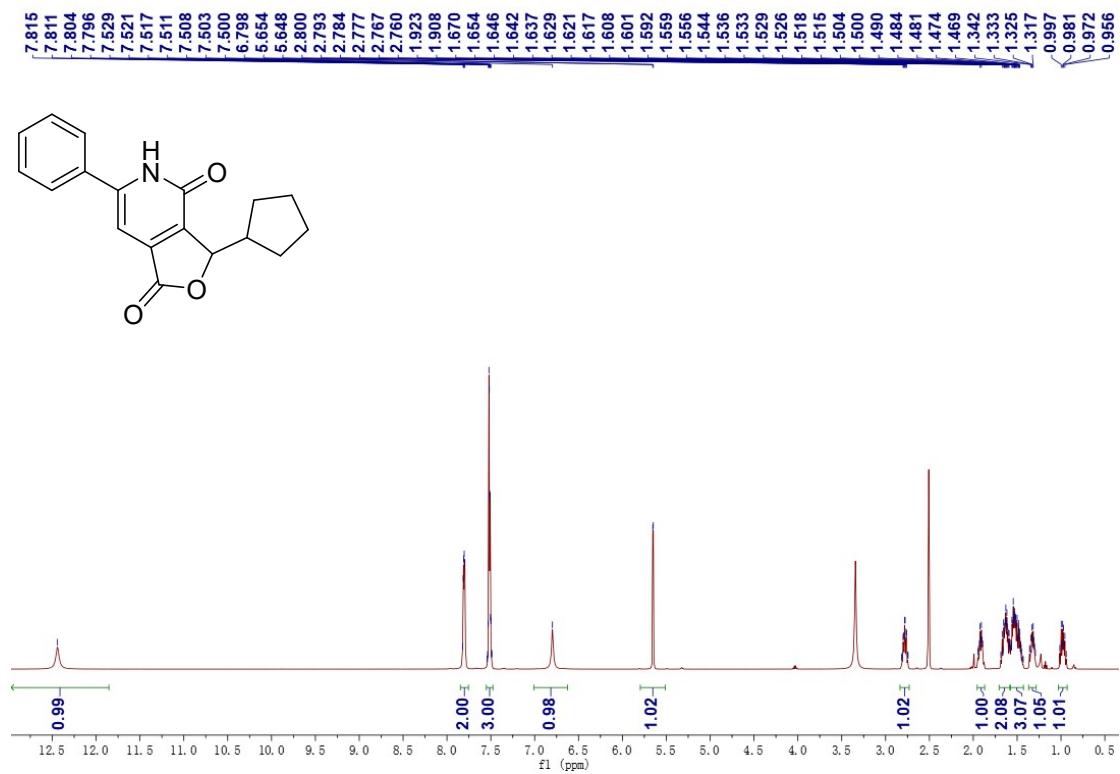
**3-(4-iodophenyl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3i)**



3-(naphthalen-2-yl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3j)

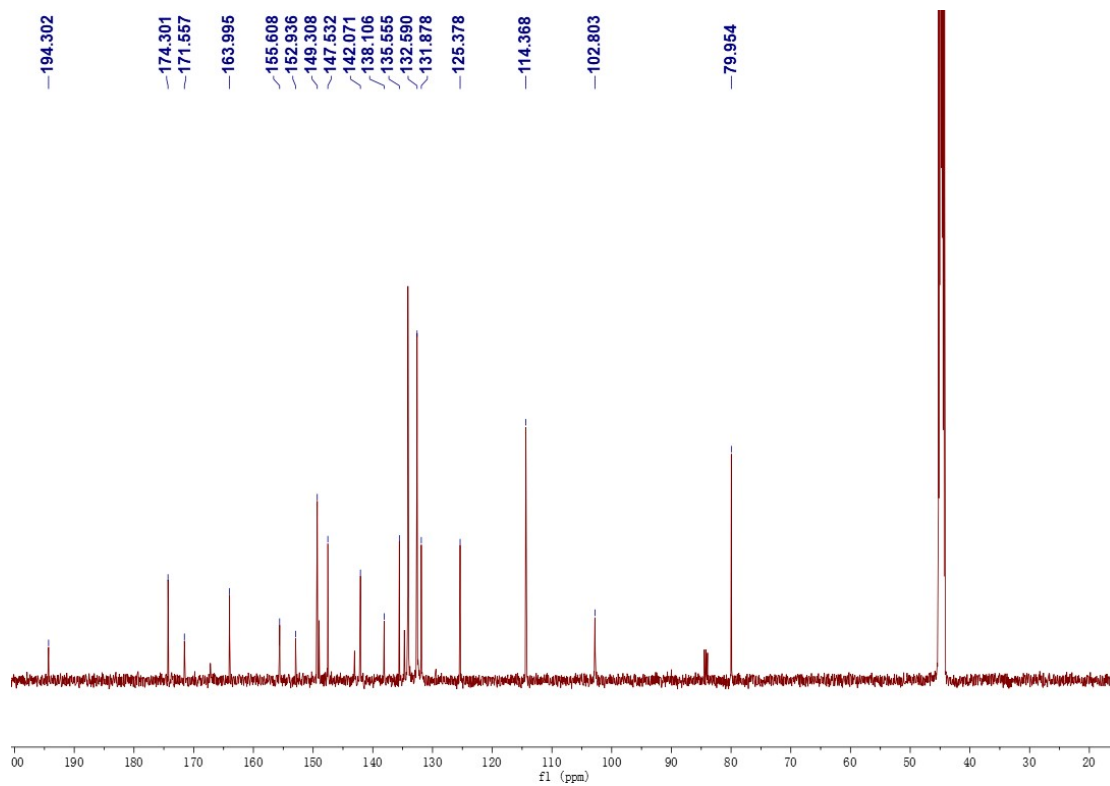
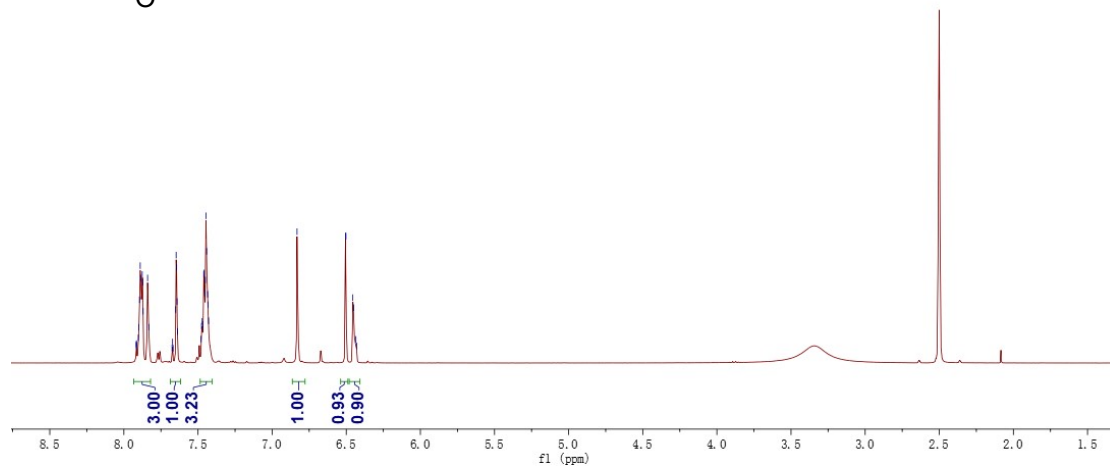
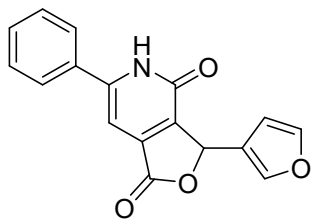


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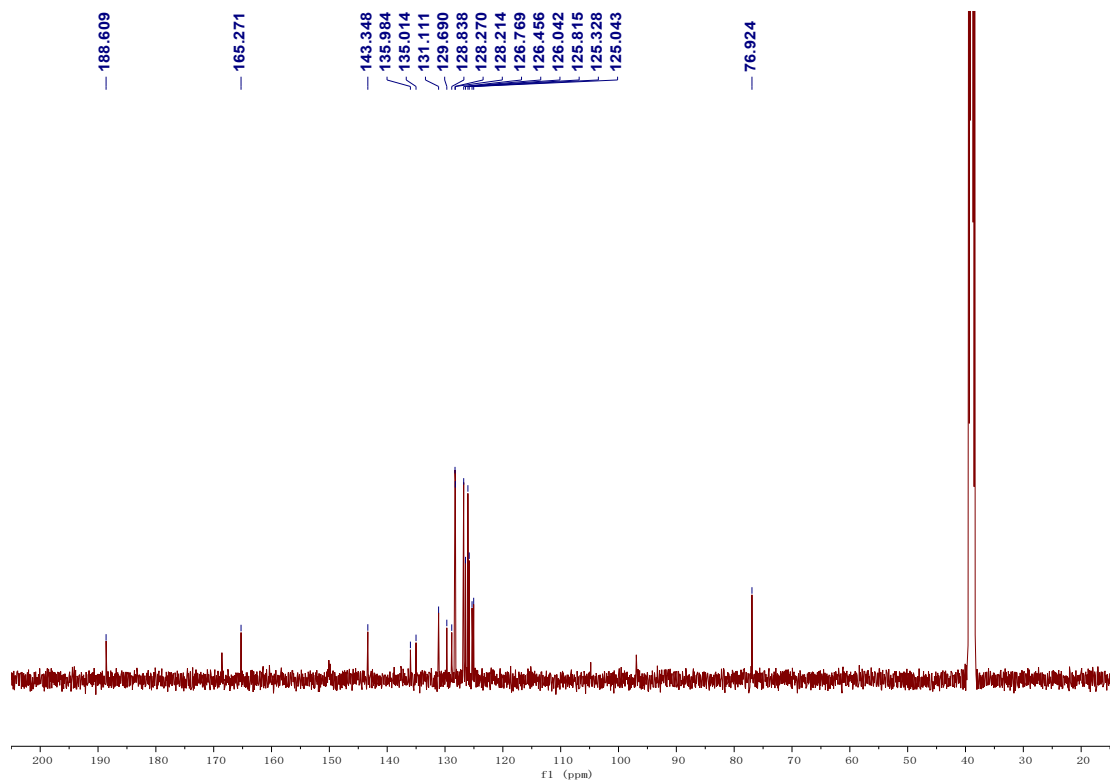
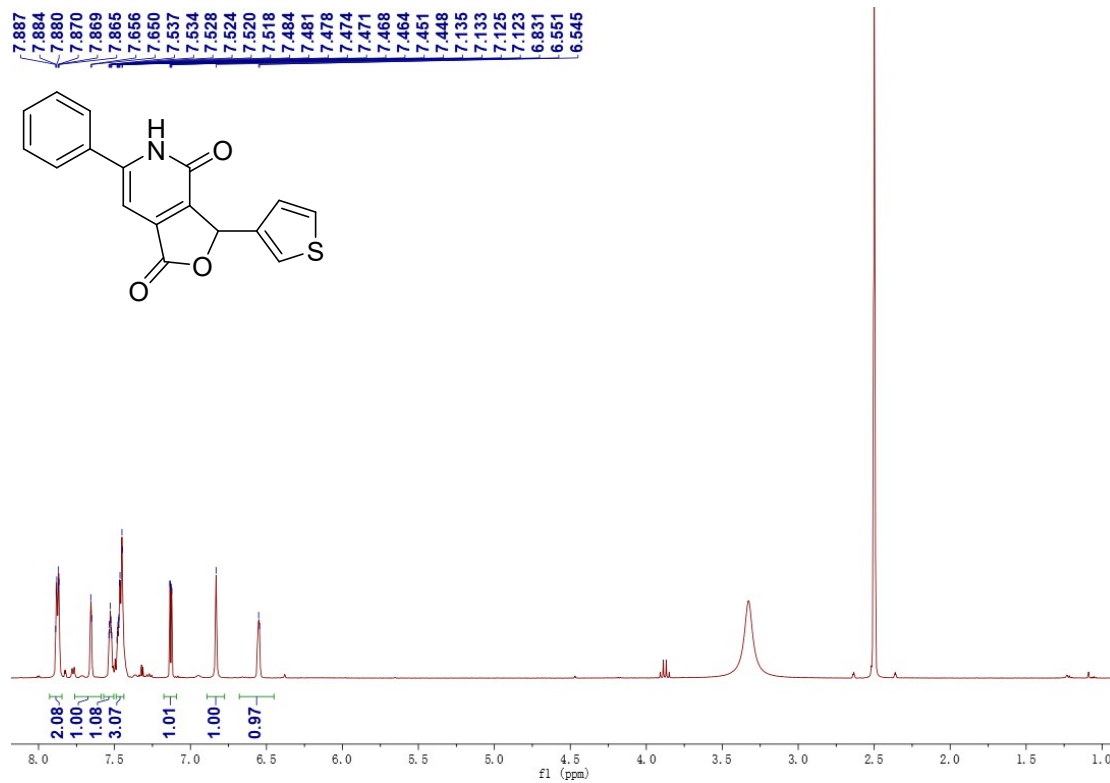


**3-(furan-3-yl)-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3l)**

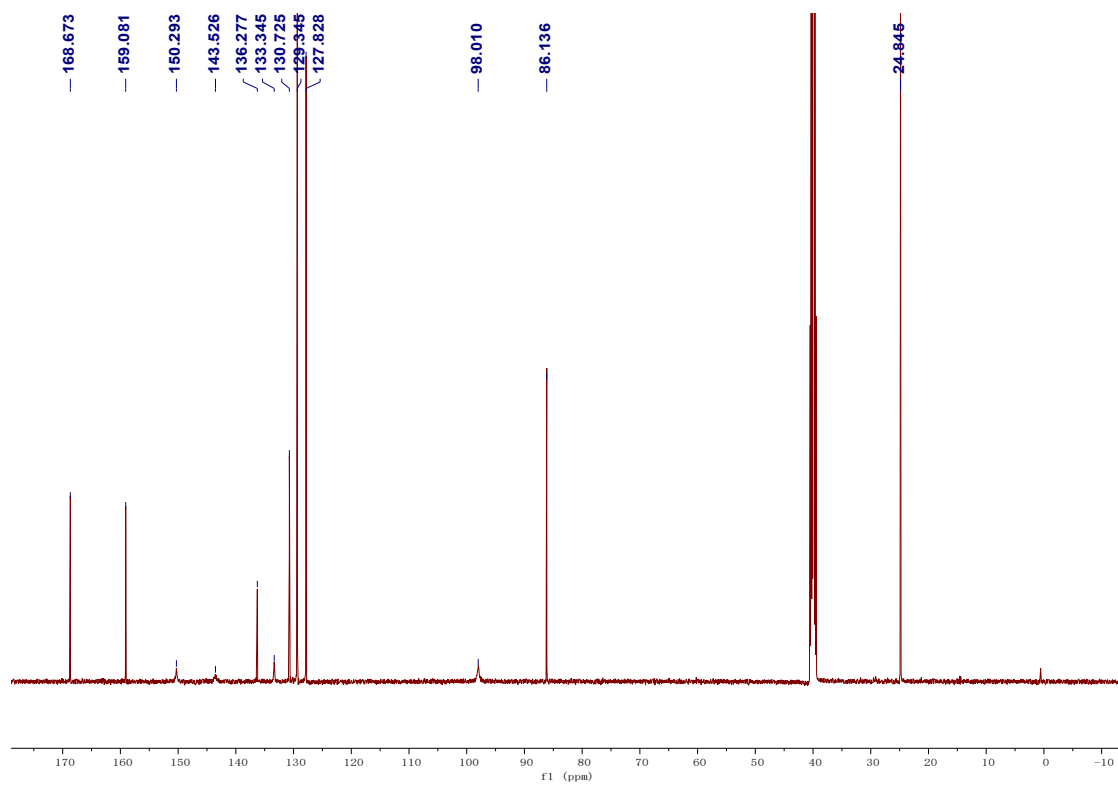
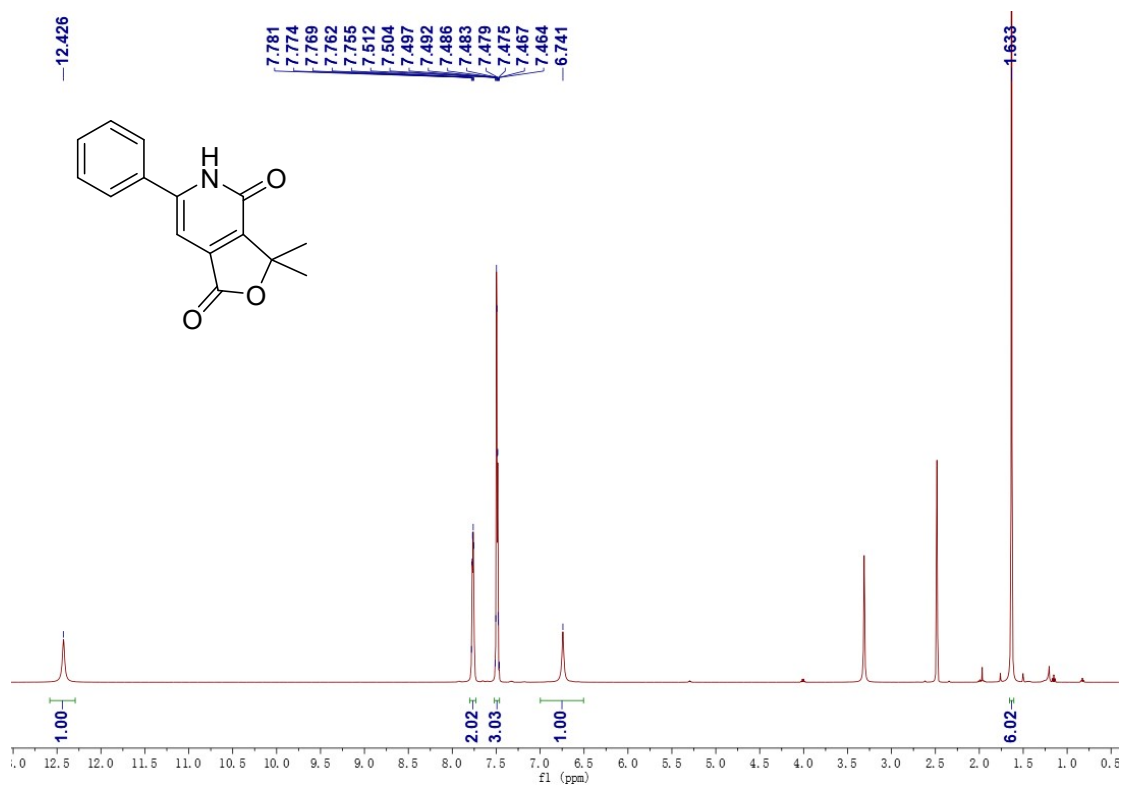
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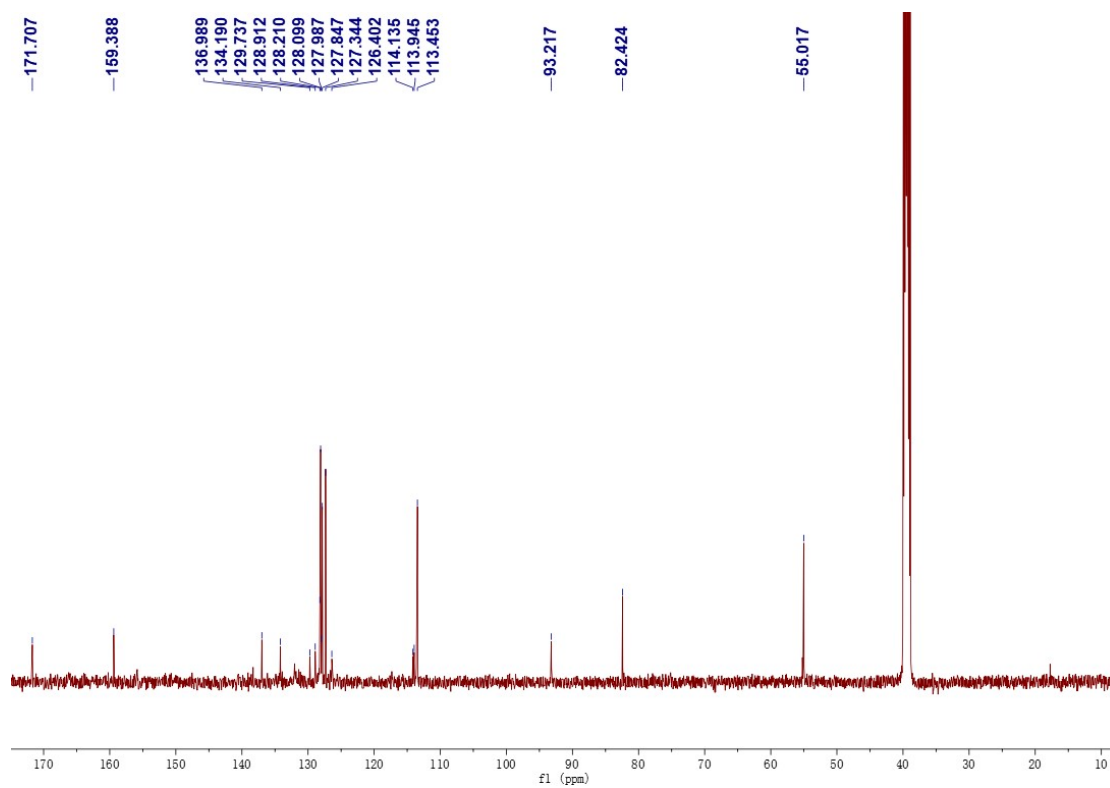
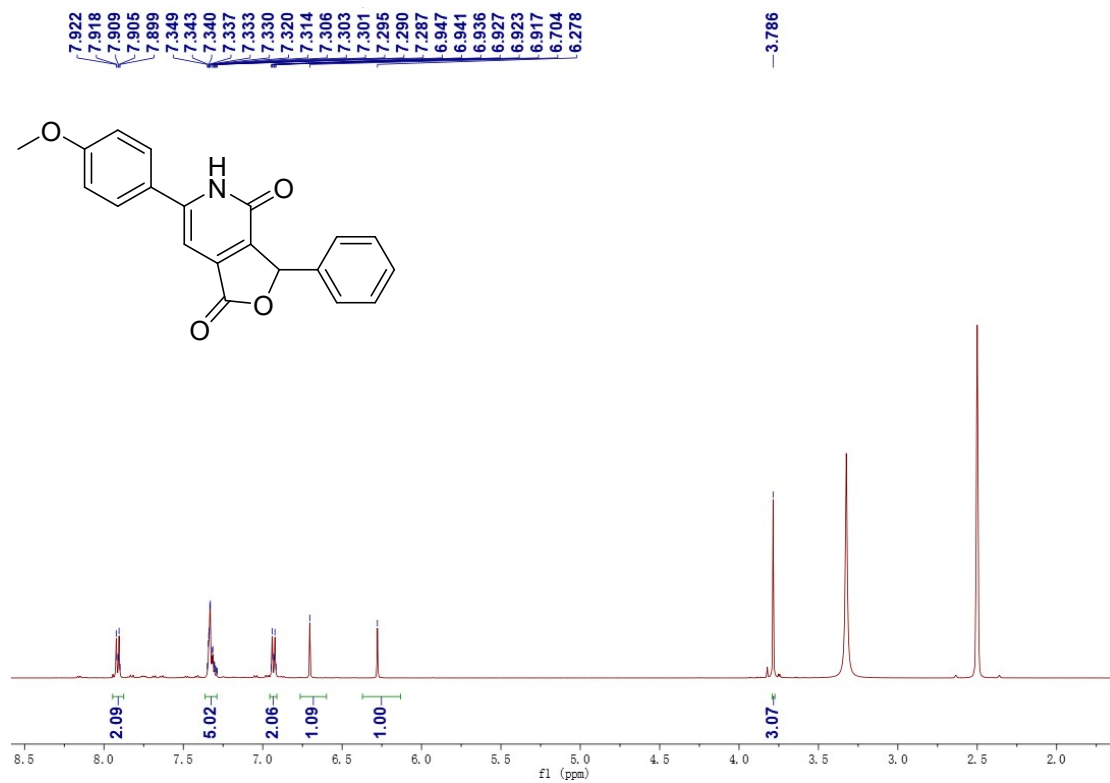
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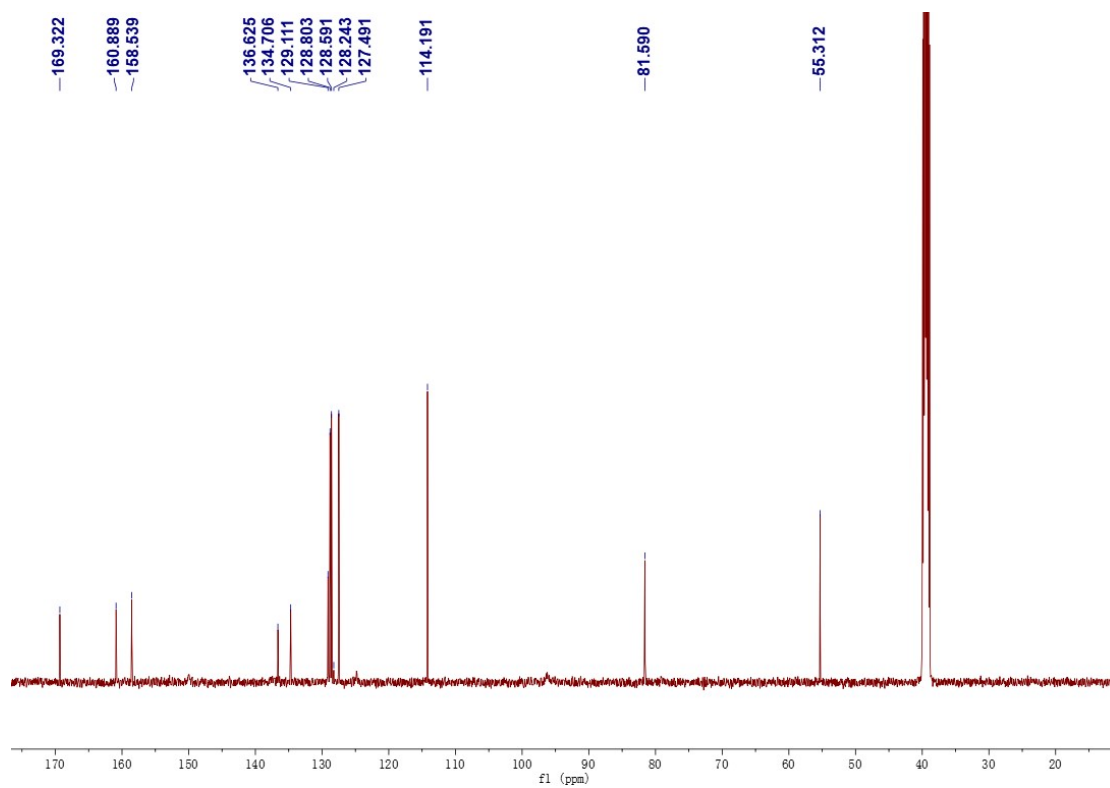
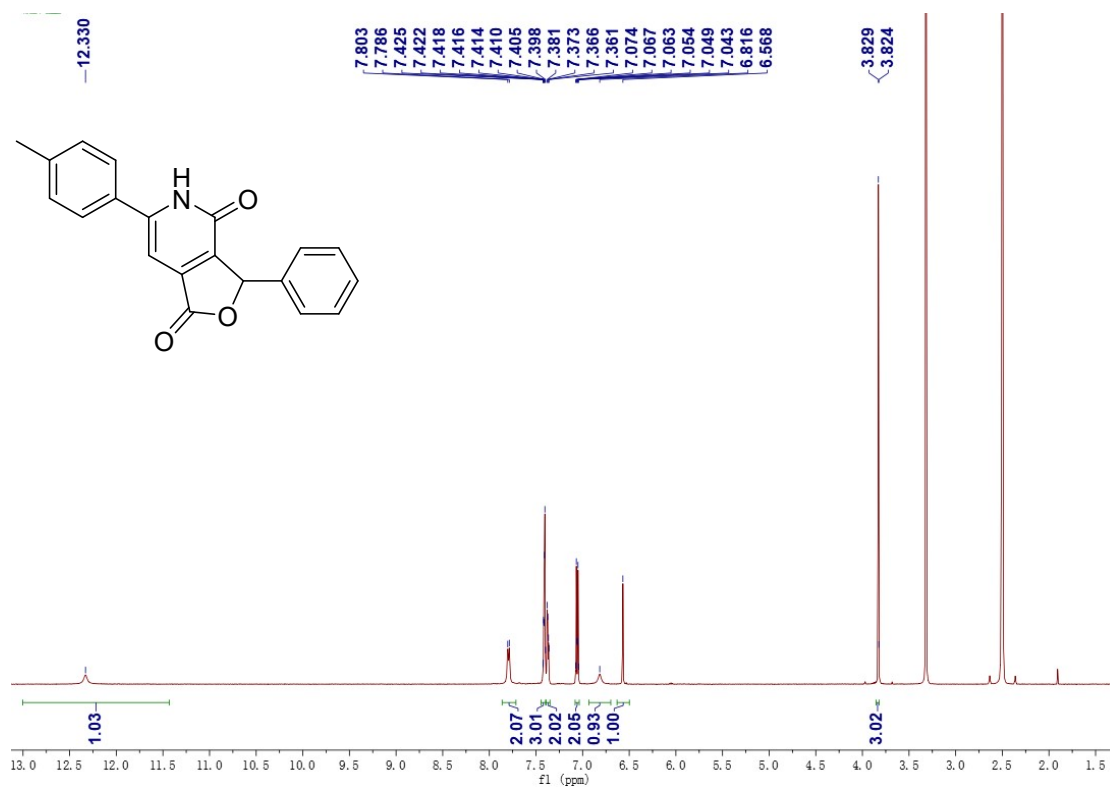
3,3-dimethyl-6-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3n)



6-(4-methoxyphenyl)-3-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (30)

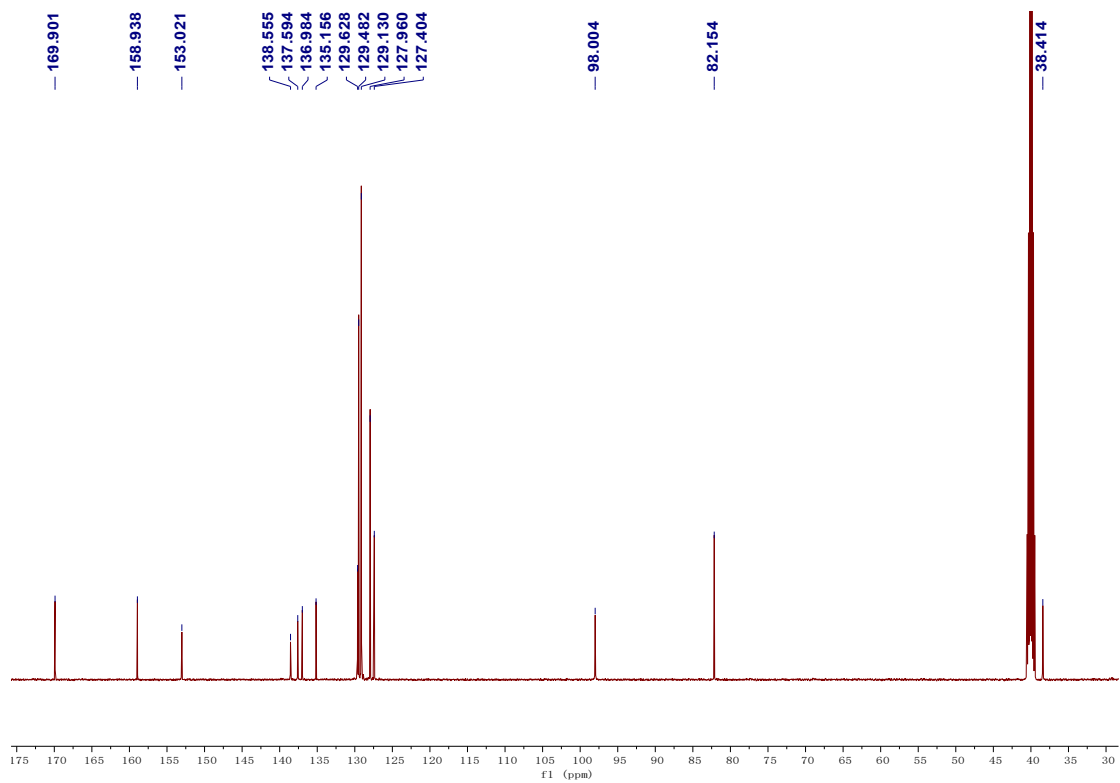
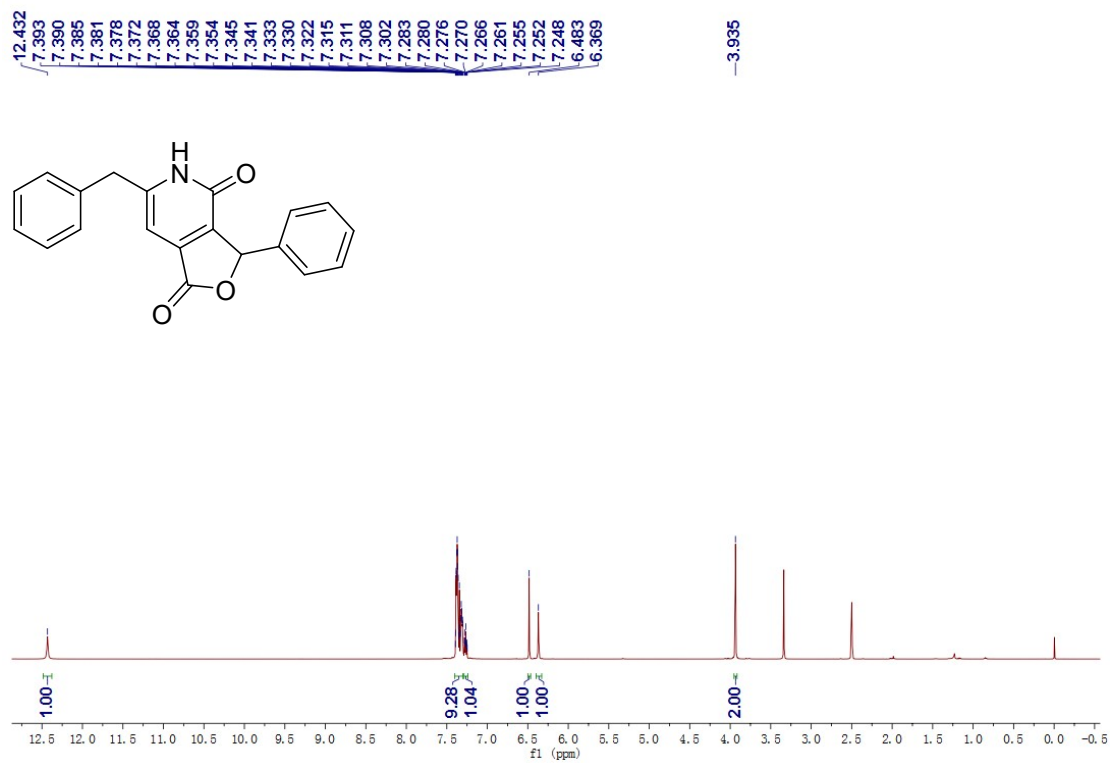


3-phenyl-6-(p-tolyl)-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3p)

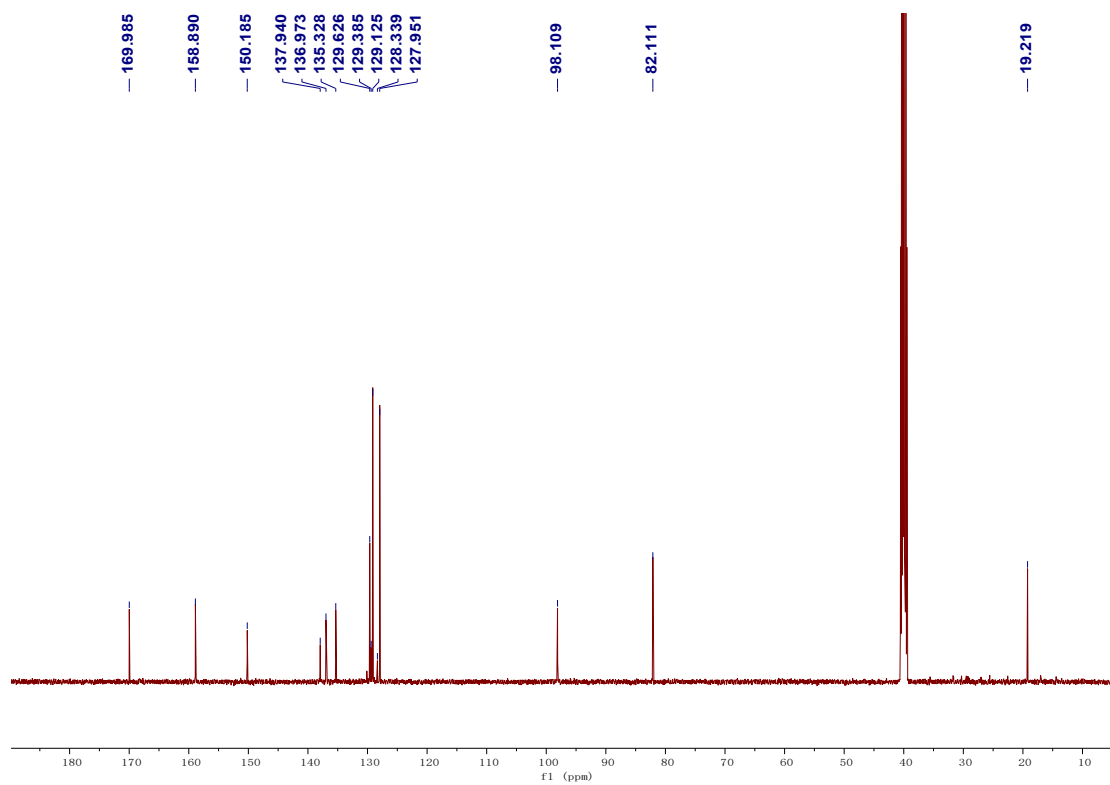
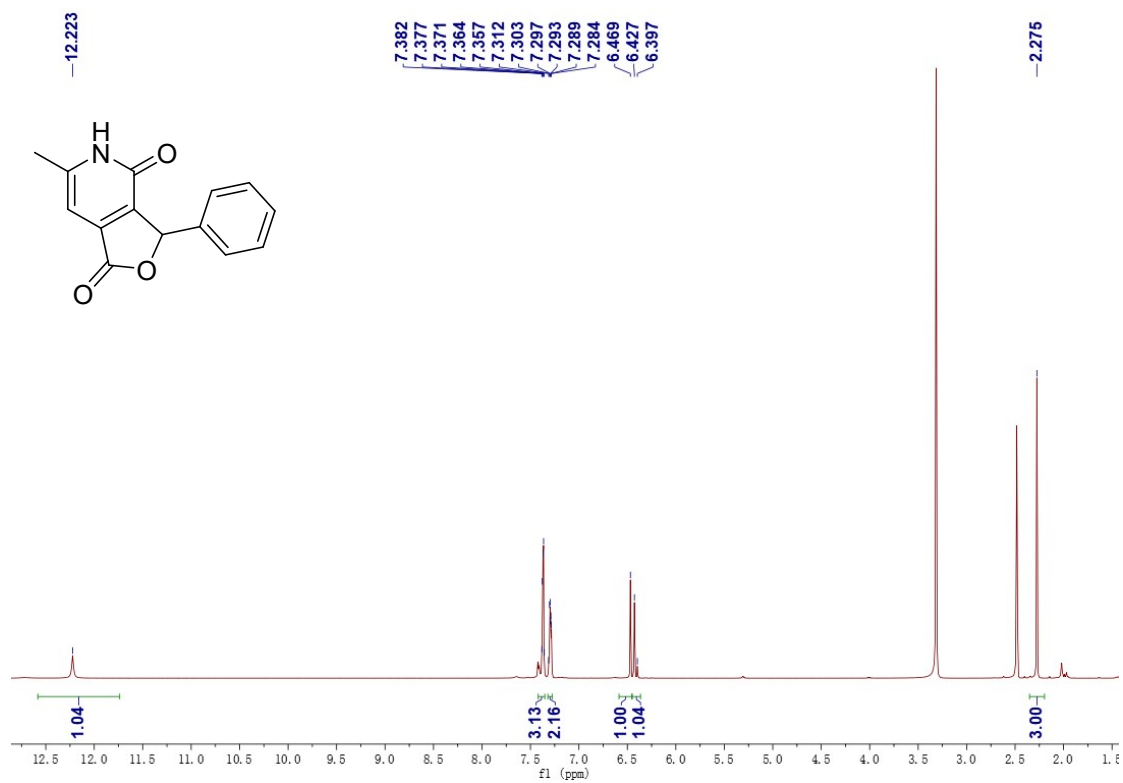




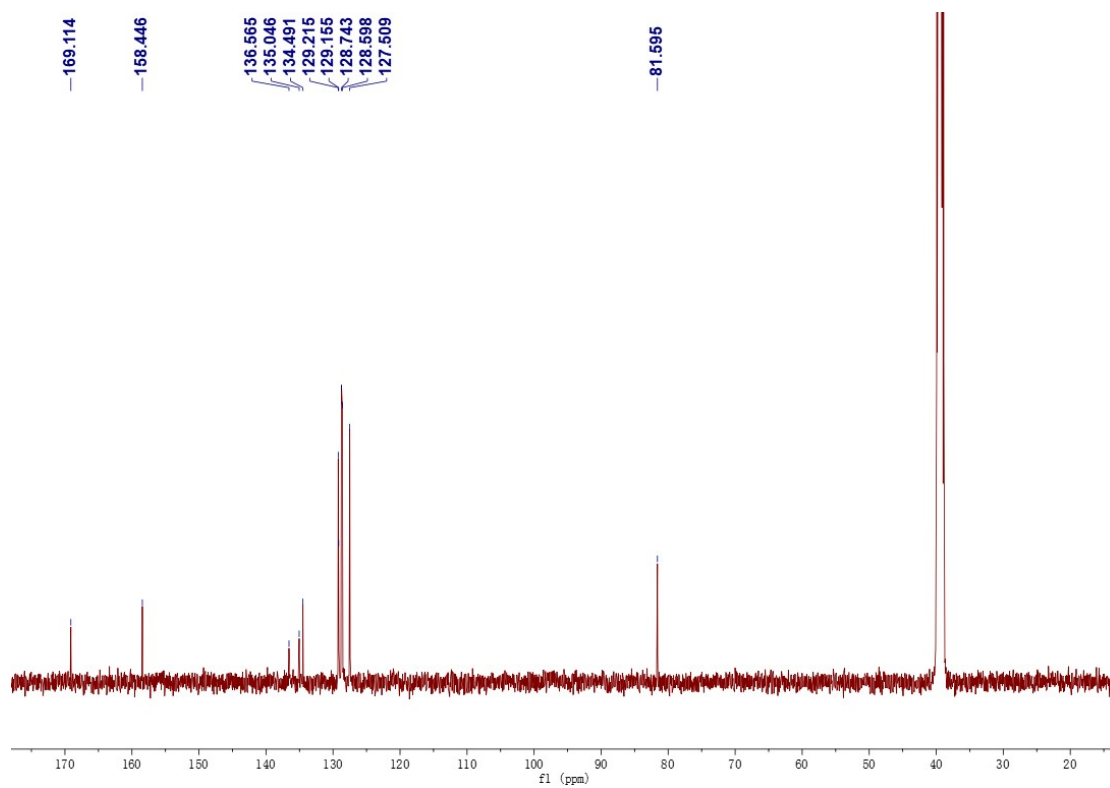
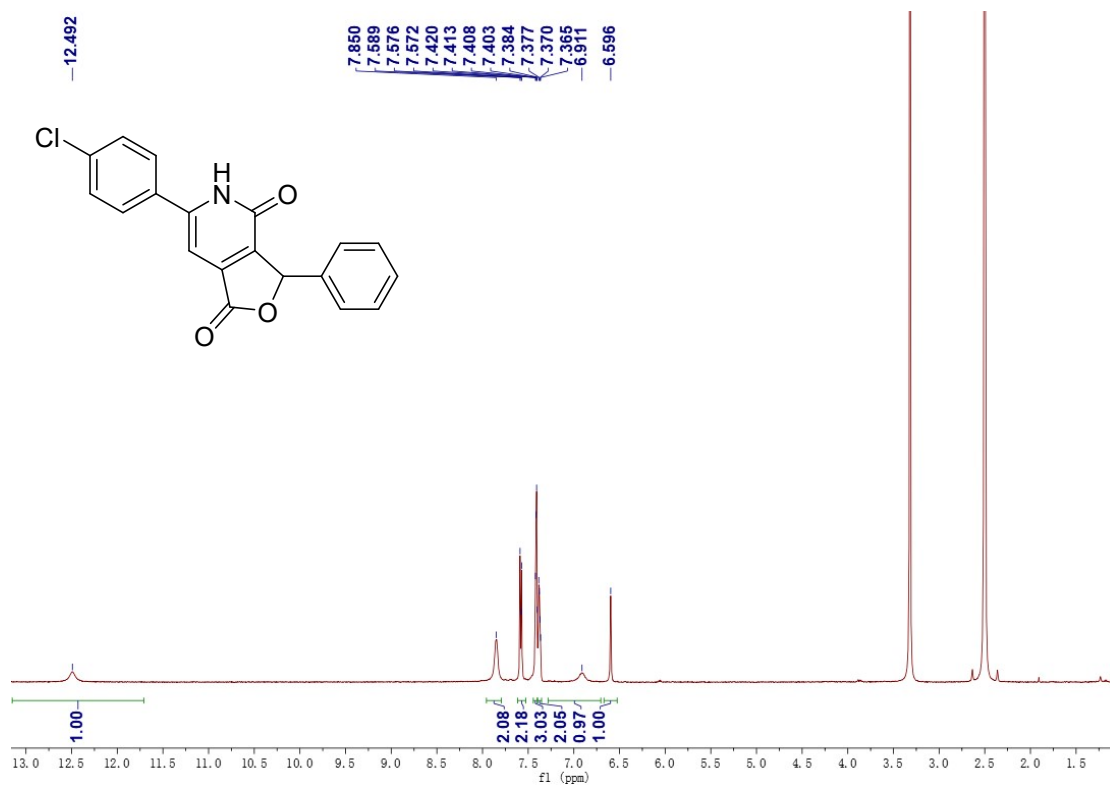
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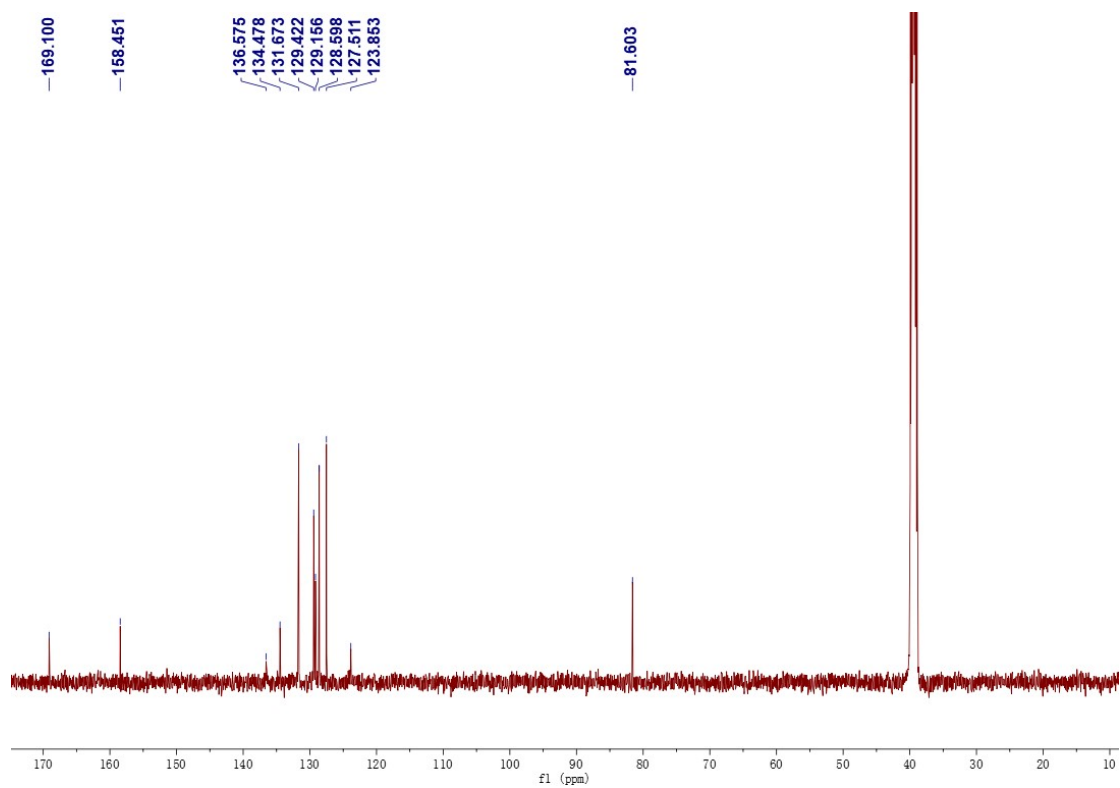
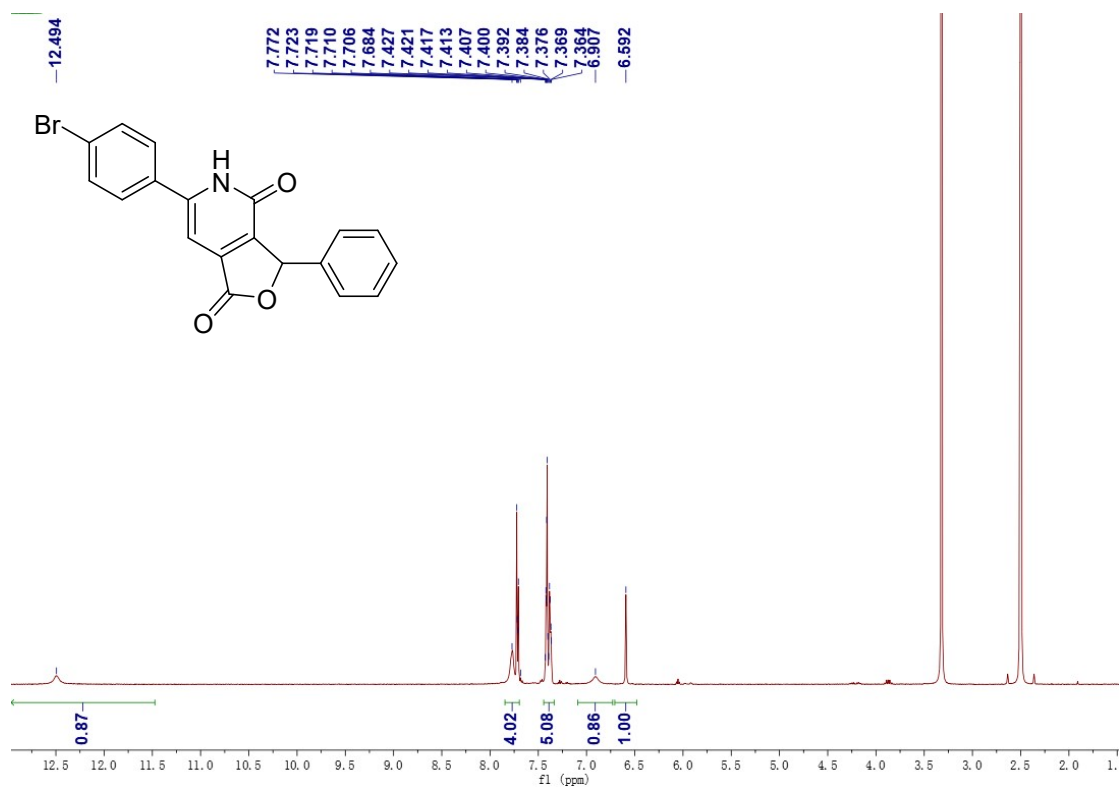
6-methyl-3-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3r)



6-(4-chlorophenyl)-3-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3s)



6-(4-bromophenyl)-3-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3t)



6-(4-iodophenyl)-3-phenyl-3,5-dihydrofuro[3,4-c]pyridine-1,4-dione (3u)

