

Supporting Information

Rhodium-catalyzed Regioselective C-H Activation/Lossen Rearrangement/Annulation for the Green Synthesis of Trisubstituted 2-Pyridones

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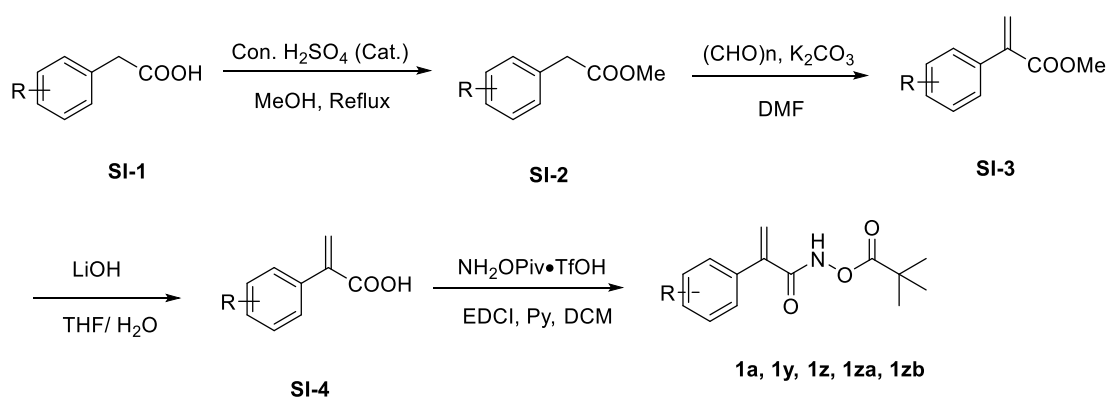
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General Information

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. ^1H , ^{13}C , and ^{19}F NMR spectra were collected on a Bruker 500 MHz instrument in chloroform-*d* or DMSO-*d*₆. Chemical shifts (δ) 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**, **1y**, **1z**, **1za**, **1zb**.¹



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 H₂O (30 mL) and brine (30 mL), dried with Na₂SO₄, filtered, and concentrated under reduced pressure. The crude product was used for the next step without further purification.

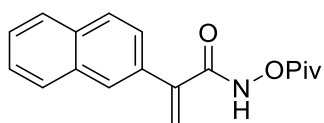
Step 2: A mixture of ester **SI-2** (7.0 mmol), paraformaldehyde (1.5 eq) and K₂CO₃ (1 eq) in DMF (10 mL) was heated at 80°C for 1-3 h. The mixture was cooled to room temperature, water (30 mL) and Et₂O (30 mL) were added, and the organic layer was separated. The collected organic layers were washed with brine (10 mL), dried with Na₂SO₄ 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/H₂O (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 Et₂O. 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.

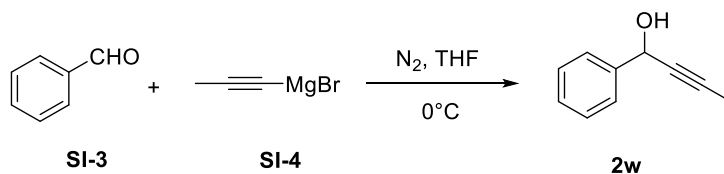
Step 4: To a solution of acrylic acid **SI-4** (2.0 mmol) in DCM (20 mL) was added pyridine (7.1 eq), EDCI (2eq) and NH₂OPiv.TfOH (1.2 eq), and stirred at room temperature overnight. The mixture was washed with 2N HCl (20 mL), saturated aq. NaHCO₃ (20 mL) and brine (20 mL), dried over Na₂SO₄ and concentrated under reduced pressure to give the crude products, which was purified by column chromatography eluting with PE/EtOAc from 20:1 to 5:1.

Characterization Data of **1zb**



2-(naphthalen-2-yl)-N-(pivaloyloxy)acrylamide: white solid (867 mg, yield 40%); ¹H NMR (500 MHz, Chloroform-*d*) δ 8.48 (s, 1H), 7.97 – 7.81 (m, 3H), 7.60 – 7.40 (m, 4H), 6.81 (d, *J* = 1.7 Hz, 1H), 5.77 (d, *J* = 1.7 Hz, 1H), 1.27 (s, 9H).

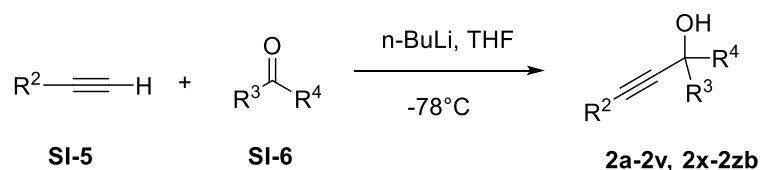
General procedure B for the preparation of **2w**²



To a solution of benzaldehyde (1.06g, 0.01 mol) in 20 mL THF, propynylmagnesium bromide (22 mL, 0.011 mol, 0.5M in THF) was added dropwise while stirring at 0°C. It was allowed to warm up to room temperature and then stirred overnight. Reaction mixture was quenched with 10 mL water at 0°C and then treated with saturated brine followed by extraction with ether. The ether extract was dried with anhydrous sodium sulfate, evaporated and then purified by column chromatography (10%

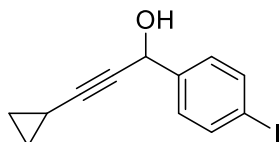
ethyl acetate/hexane).

General procedure C for the preparation of **2a-2v** and **2x-2zb**³

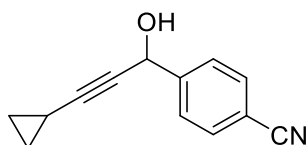


To a solution of alkyne (3.9 mmol) in anhydrous THF (5 mL) at -78 °C under N₂ atmosphere was added *n*-BuLi (1.6 M solution in hexanes, 2.06 mL, 3.3 mmol). The reaction was stirred at this temperature for 20 min then at room temperature for 1h. After cooling to -78 °C, aldehyde (3 mmol) was added to the mixture and was allowed to warm up to room temperature gradually and stirred for an additional hour before quenched with aqueous NH₄Cl. The mixture was extracted with EtOAc (30 x 2 mL), and the combined organic phases were washed with water and brine, dried with anhydrous MgSO₄, and filtered. The filtrate was concentrated under reduced pressure and the residue was purified by flash chromatography on silica gel (hexanes/ethyl acetate, v/v, 15:1) to produce the desired product.

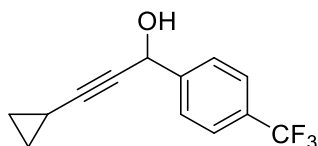
Characterization Data of **2h**, **2i**, **2j**, **2k**, **2l**, **2n**



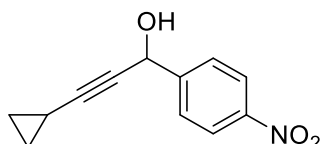
3-cyclopropyl-1-(4-iodophenyl)prop-2-yn-1-ol (2h): yellow liquid (626 mg, yield 70%); ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.78 – 7.59 (m, 2H), 7.31 – 7.06 (m, 2H), 5.92 (d, *J* = 5.5 Hz, 1H), 5.40 – 4.99 (m, 1H), 1.34 (m, 1H), 0.85 – 0.72 (m, 2H), 0.58 (m, 2H).



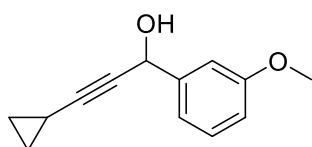
4-(3-cyclopropyl-1-hydroxyprop-2-yn-1-yl)benzonitrile (2i): yellow liquid (372 mg, yield 63%); ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.91 – 7.74 (m, 2H), 7.67 – 7.44 (m, 2H), 6.12 (d, *J* = 5.6 Hz, 1H), 5.39 (dd, *J* = 5.8, 1.9 Hz, 1H), 1.35 (m, 1H), 0.81 – 0.72 (m, 2H), 0.64 – 0.52 (m, 2H).



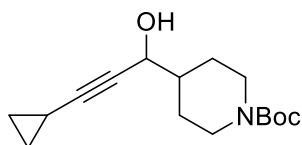
3-cyclopropyl-1-(4-(trifluoromethyl)phenyl)prop-2-yn-1-ol (2j): yellow liquid (439 mg, yield 61%); $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.72 (d, $J = 8.2$ Hz, 2H), 7.64 (d, $J = 8.1$ Hz, 2H), 6.08 (d, $J = 5.9$ Hz, 1H), 5.53 – 5.17 (m, 1H), 1.40 – 1.27 (m, 1H), 0.83 – 0.69 (m, 2H), 0.67 – 0.41 (m, 2H).



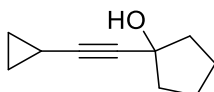
3-cyclopropyl-1-(4-nitrophenyl)prop-2-yn-1-ol (2k): yellow liquid (456 mg, yield 70%); $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 8.26 – 8.15 (m, 2H), 7.76 – 7.42 (m, 2H), 6.20 (d, $J = 5.9$ Hz, 1H), 5.46 (dd, $J = 5.9, 1.8$ Hz, 1H), 1.41 – 1.25 (m, 1H), 0.83 – 0.69 (m, 2H), 0.65 – 0.53 (m, 2H).



3-cyclopropyl-1-(3-methoxyphenyl)prop-2-yn-1-ol (2l): yellow liquid (545 mg, yield 90%); $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.26 (t, $J = 7.9$ Hz, 1H), 7.09 – 6.95 (m, 2H), 6.90 – 6.73 (m, 1H), 5.84 (d, $J = 6.0$ Hz, 1H), 5.27 (dd, $J = 6.1, 1.8$ Hz, 1H), 3.75 (s, 3H), 1.34 (m, 1H), 0.84 – 0.72 (m, 2H), 0.65 – 0.50 (m, 2H).

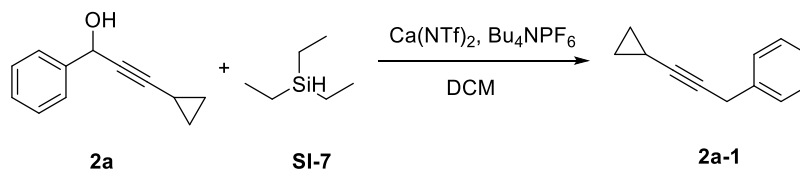


tert-butyl 4-(3-cyclopropyl-1-hydroxyprop-2-yn-1-yl)piperidine-1-carboxylate (2n): yellow liquid (670 mg, yield 80%); $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 5.18 (s, 1H), 3.95 (m, 3H), 1.69 – 1.61 (m, 2H), 1.50 (m, 1H), 1.38 (d, $J = 2.2$ Hz, 9H), 1.30 – 0.98 (m, 5H), 0.77 – 0.71 (m, 2H), 0.57 – 0.50 (m, 2H).



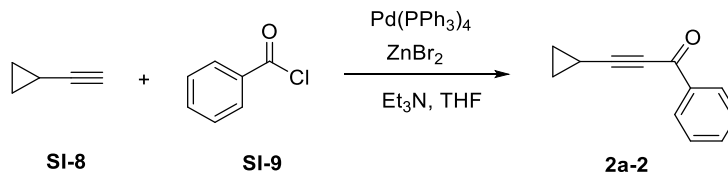
1-(cyclopropylethynyl)cyclopentan-1-ol (2t): yellow liquid (337 mg, yield 75%); $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 4.96 (s, 1H), 1.82 – 1.50 (m, 8H), 1.34 – 1.14 (m, 1H), 0.79 – 0.63 (m, 2H), 0.52 (m, 2H).

General procedure D for the preparation of **2a-1**⁴



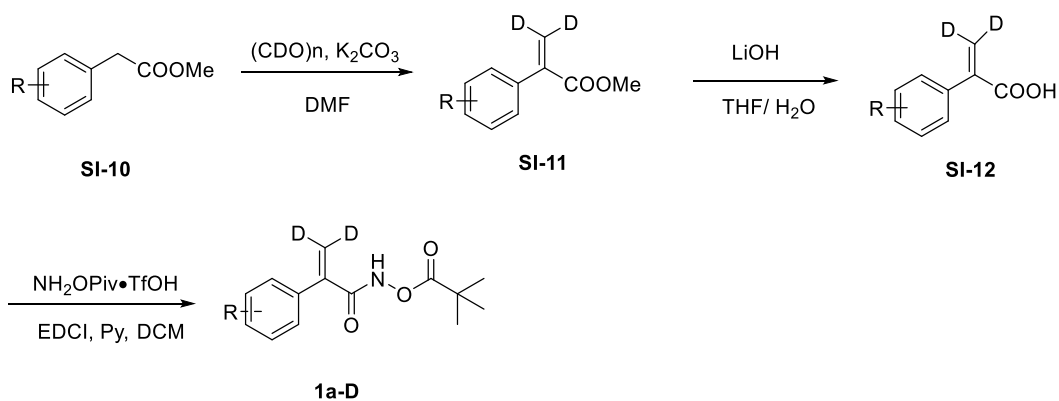
3-Cyclopropyl-1-phenylprop-2-yn-1-ol **2a** (0.5 mmol) and triethylsilane (1.5 mmol) are dissolved in 1 ml of DCM. Additive (5 mol%) and $\text{Ca}(\text{NTf}_2)_2$ (5 mol%) are added at room temperature and stirred until complete conversion of the alcohol (monitored by TLC). Next, 5 mL sat. NaHCO_3 -solution is added to the reaction mixture, the aqueous phase extracted with dichloromethane, the combined organic phases dried over Na_2SO_4 and concentrated under vacuum. The crude product is purified by column chromatography.

General procedure E for the preparation of **2a-2**⁵



A mixture of ZnBr_2 (1.2 mmol) in Et_3N (202 mg, 2 mmol) was stirred for 10 mins at room temperature. The reaction mixture was then successively treated with alkyne (1 mmol), $\text{Pd}(\text{PPh}_3)_4$ (6 mg, 0.5 mmol %) and acyl chloride (1 mmol), stirred for 30 mins at room temperature, diluted with Et_2O , washed with aqueous NH_4Cl and then with aqueous NaHCO_3 , dried over MgSO_4 , filtered, and concentrated under vacuum to give the product which was further purified by column chromatography using hexane/ EtOAc (20:1) as eluents.

Preparation of **1a-D**¹

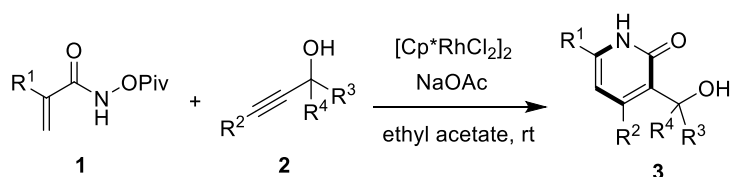


Step 1: A mixture of ester **SI-10** (7.0 mmol), D-paraformaldehyde (1.5 eq) and K_2CO_3 (1 eq) in DMF (10 mL) was heated at 80°C for 1-3 h. The mixture was cooled at room temperature, water (30 mL) and Et_2O (30 mL) were added, and the organic layer was separated. The collected organic layers were washed with brine (10 mL), dried with Na_2SO_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-11** (7.0 mmol), LiOH (5 eq) and THF/ H_2O (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_2O . 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.

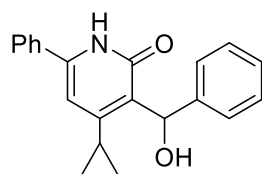
Step 3: To a solution of acrylic acid **SI-12** (2.0 mmol) in DCM (20 mL) was added pyridine (7.1 eq), EDCI (2eq) and $\text{NH}_2\text{OPiv}\cdot\text{TfOH}$ (1.2 eq), and stirred at room temperature overnight. The mixture was washed with 2N HCl (20 mL), saturated aq. NaHCO_3 (20 mL) and brine (20 mL), dried over Na_2SO_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 Products 3

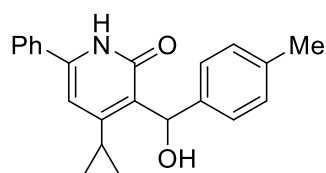


In an 8 mL reaction tube, the mixture of **1** (0.25 mmol), **2** (0.3 mmol), [Cp*RhCl₂]₂ (4.0 mol%) and NaOAc (1.0 eq.) was added EA (1.0 mL). Then the resulting mixture was stirred for 6 ~ 12 h. When the reaction was finished, the desired product precipitated out as a solid, and the product was simply collected by filtration. For some cases, if the precipitation did not occur, the reaction mixture was subjected directly to flash chromatography on silica gel (dichloromethane/methanol) to provide the desired products **3**.

Characterization Data of Products 3

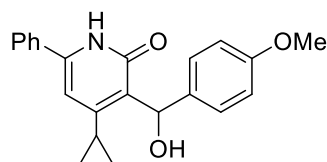


4-cyclopropyl-3-(hydroxy(phenyl)methyl)-6-phenylpyridin-2(1H)-one (3a): white solid (58mg, yield 73%), ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.75 (dd, *J* = 7.5, 2.1 Hz, 2H), 7.49 – 7.38 (m, 5H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.18 (t, *J* = 7.3 Hz, 1H), 6.23 (s, 1H), 5.98 (s, 1H), 2.23 (m, 1H), 0.90 (m, 2H), 0.80 (m, 1H), 0.72 (m, 1H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 175.04, 146.04, 130.12, 129.63, 129.03, 128.29, 127.28, 126.68, 126.18, 100.95, 69.11, 25.52, 12.55, 9.61, 9.08; HRMS (ESI) *m/z* calculated for C₂₁H₂₀NO₂⁺ [M+H]⁺ 318.1489, found: 318.1489.

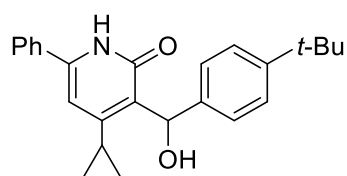


4-cyclopropyl-3-(hydroxy(p-tolyl)methyl)-6-phenylpyridin-2(1H)-one (3b): white solid (32 mg, yield 39%), ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.85 (s, 1H), 7.72 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.45 (dd, *J* = 5.0, 2.0 Hz, 3H), 7.30 (d, *J* = 7.9 Hz, 2H), 7.10 (d, *J* = 7.9 Hz, 2H), 6.40 (d, *J* = 7.4 Hz, 1H),

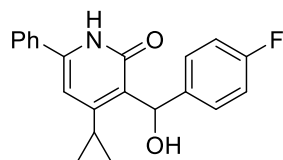
6.25 (d, $J = 6.8$ Hz, 1H), 5.93 (s, 1H), 3.33 (s, 3H), 2.33 – 2.27 (m, 1H), 1.00 – 0.87 (m, 2H), 0.85 – 0.67 (m, 2H). ^{13}C NMR (126 MHz, DMSO- d_6) δ 162.50, 153.36, 141.47, 134.60, 128.96, 128.08, 127.85, 126.33, 124.94, 67.43, 20.05, 11.53, 8.75, 8.29. HRMS (ESI) m/z calculated for $\text{C}_{22}\text{H}_{22}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 332.1645, found: 332.1643.



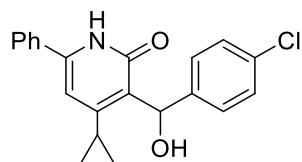
4-cyclopropyl-3-(hydroxy(4-methoxyphenyl)methyl)-6-phenylpyridin-2(1H)-one (3c): white solid (66 mg, yield 71%), ^1H NMR (500 MHz, DMSO- d_6) δ 11.86 (s, 1H), 7.72 (dd, $J = 6.7, 3.0$ Hz, 2H), 7.46 (dd, $J = 5.0, 2.0$ Hz, 3H), 7.37 – 7.25 (m, 2H), 6.93 – 6.77 (m, 2H), 6.44 (d, $J = 7.5$ Hz, 1H), 6.22 (d, $J = 7.3$ Hz, 1H), 5.94 (s, 1H), 3.72 (s, 3H), 2.29 (m, 1H), 0.93 (m, 2H), 0.85 – 0.68 (m, 2H). ^{13}C NMR (126 MHz, DMSO- d_6) δ 162.51, 157.23, 153.22, 136.44, 132.76, 128.97, 128.08, 126.34, 126.19, 112.70, 100.09, 67.39, 54.38, 11.50, 8.74, 8.25. HRMS (ESI) m/z calculated for $\text{C}_{22}\text{H}_{21}\text{NNaO}_3^+$ $[\text{M}+\text{Na}]^+$ 370.1414, found: 370.1413.



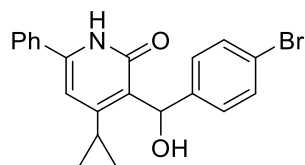
3-((4-(tert-butyl)phenyl)(hydroxy)methyl)-4-cyclopropyl-6-phenylpyridin-2(1H)-one (3d): white solid (60 mg, yield 64%), ^1H NMR (500 MHz, DMSO- d_6) δ 7.87 – 7.64 (m, 2H), 7.50 – 7.05 (m, 7H), 6.15 (s, 1H), 5.99 (s, 1H), 2.21 (m, 1H), 1.04 – 0.80 (m, 3H), 0.77 (m, 1H). ^{13}C NMR (126 MHz, DMSO- d_6) δ 163.58, 154.24, 149.10, 142.43, 130.06, 129.16, 127.43, 125.83, 125.11, 70.25, 68.79, 55.38, 34.57, 31.67, 12.61, 9.86, 9.39. HRMS (ESI) m/z calculated for $\text{C}_{25}\text{H}_{28}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 374.2115, found: 374.2111.



3-cyclopropyl-3-((4-fluorophenyl)(hydroxy)methyl)-6-phenylpyridin-2(1H)-one (3e): white solid (31 mg, yield 37%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.83 (s, 1H), 7.78 – 7.64 (m, 2H), 7.50 – 7.38 (m, 5H), 7.18 – 7.02 (m, 2H), 6.55 – 6.34 (m, 1H), 6.30 (s, 1H), 5.93 (s, 1H), 2.30 (m, 1H), 0.98 – 0.90 (m, 2H), 0.81 – 0.67 (m, 2H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 162.91, 161.70, 159.78, 154.17, 141.16, 129.51, 128.58, 127.33, 127.26, 126.87, 114.54, 114.38, 100.51, 67.31, 12.01, 9.29, 8.75. $^{19}\text{F NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ -117.04. HRMS (ESI) m/z calculated for $\text{C}_{21}\text{H}_{19}\text{FNO}_2^+$ $[\text{M}+\text{H}]^+$ 336.1394, found: 336.1393.

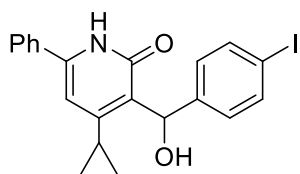


3-((4-chlorophenyl)(hydroxy)methyl)-4-cyclopropyl-6-phenylpyridin-2(1H)-one (3f): white solid (61 mg, yield 69%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.87 (s, 1H), 7.77 – 7.64 (m, 2H), 7.46 (m, 3H), 7.43 – 7.39 (m, 2H), 7.38 – 7.30 (m, 2H), 6.41 (d, $J = 6.9$ Hz, 1H), 6.32 (d, $J = 6.9$ Hz, 1H), 5.92 (s, 1H), 2.29 (m, 1H), 0.99 – 0.89 (m, 2H), 0.74 (m, 2H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 162.35, 153.84, 143.58, 132.74, 130.12, 129.02, 128.08, 127.23, 126.76, 126.36, 99.95, 66.59, 11.54, 8.82, 8.29. HRMS (ESI) m/z calculated for $\text{C}_{21}\text{H}_{19}\text{ClNO}_2^+$ $[\text{M}+\text{H}]^+$ 352.1099, found: 352.1099.

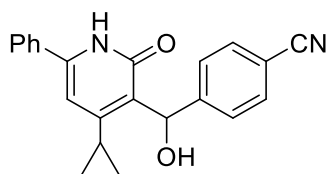


3-((4-bromophenyl)(hydroxy)methyl)-4-cyclopropyl-6-phenylpyridin-2(1H)-one (3g): white solid (64 mg, yield 65%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.86 (s, 1H), 7.77 – 7.64 (m, 2H), 7.53 – 7.43 (m, 5H), 7.38 – 7.31 (m, 2H), 6.40 (d, $J = 6.9$ Hz, 1H), 6.30 (d, $J = 6.5$ Hz, 1H), 5.92 (s, 1H), 2.29 (m, 1H), 1.02 – 0.87 (m, 2H), 0.74 (m, 2H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 162.34, 153.84, 144.03, 130.14, 129.01, 128.08, 127.15, 126.36, 118.63, 66.60, 54.31, 11.53, 8.82, 8.30. HRMS (ESI) m/z

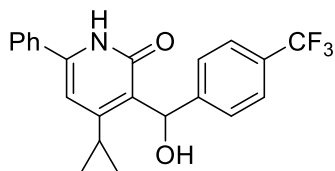
calculated for $C_{21}H_{19}BrNO_2^+$ $[M+H]^+$ 396.0594, found: 396.0593.



3-cyclopropyl-3-(hydroxy(4-iodophenyl)methyl)-6-phenylpyridin-2(1H)-one (3h): white solid (68 mg, yield 61%), 1H NMR (500 MHz, $DMSO-d_6$) δ 11.85 (s, 1H), 7.71 (dd, $J = 6.7, 2.9$ Hz, 2H), 7.69 – 7.62 (m, 2H), 7.52 – 7.39 (m, 3H), 7.27 – 7.15 (m, 2H), 6.38 (d, $J = 7.0$ Hz, 1H), 6.28 (d, $J = 6.9$ Hz, 1H), 5.91 (s, 1H), 2.29 (m, 1H), 0.93 (m, 2H), 0.75 (m, 2H). ^{13}C NMR (126 MHz, $DMSO-d_6$) δ 163.42, 154.90, 145.55, 137.08, 133.81, 130.10, 129.16, 128.44, 127.44, 92.44, 67.79, 55.38, 12.62, 9.91, 9.41. HRMS (ESI) m/z calculated for $C_{21}H_{19}INO_2^+$ $[M+H]^+$ 444.0455, found: 444.0456.

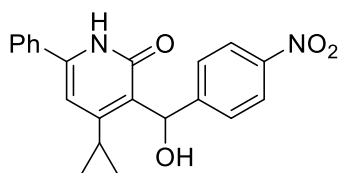


4-((4-cyclopropyl-2-oxo-6-phenyl-1,2-dihydropyridin-3-yl)(hydroxy)methyl)benzonitrile (3i): white solid (50 mg, yield 59%), 1H NMR (500 MHz, $DMSO-d_6$) δ 11.86 (s, 1H), 7.81 – 7.75 (m, 2H), 7.74 – 7.67 (m, 2H), 7.61 – 7.54 (m, 2H), 7.49 – 7.41 (m, 3H), 6.43 (s, 2H), 5.91 (s, 1H), 2.28 (m, 1H), 1.01 – 0.90 (m, 2H), 0.68 (m, 2H). ^{13}C NMR (126 MHz, $DMSO-d_6$) δ 162.24, 154.23, 150.53, 132.72, 131.34, 129.06, 128.08, 127.20, 126.39, 125.72, 118.48, 108.29, 99.86, 66.45, 11.60, 8.88, 8.28. HRMS (ESI) m/z calculated for $C_{22}H_{19}N_2O_2^+$ $[M+H]^+$ 343.1441, found: 343.1441.

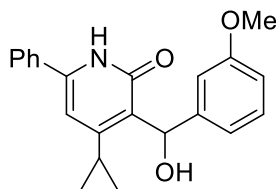


4-cyclopropyl-3-(hydroxy(4-(trifluoromethyl)phenyl)methyl)-6-phenylpyridin-2(1H)-one (3j): white solid (35 mg, yield 36%), 1H NMR (500 MHz, $DMSO-d_6$) δ 11.88 (s, 1H), 7.72 (dd, $J = 6.6, 2.9$ Hz, 2H), 7.67 (d, $J = 8.3$ Hz, 2H), 7.61 (d, $J = 8.2$ Hz, 2H), 7.46 (m, 3H), 6.43 (s, 2H), 5.92 (s, 1H), 2.37

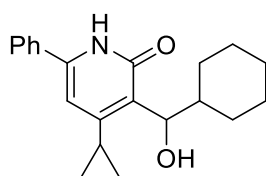
- 2.22 (m, 1H), 0.94 (dd, $J = 8.6, 6.3$ Hz, 2H), 0.70 (m, 2H). ^{13}C NMR (126 MHz, DMSO- d_6) δ 162.29, 154.07, 149.44, 129.04, 128.08, 126.38, 126.14, 125.52, 124.95, 124.23, 124.20, 66.56, 11.58, 8.83, 8.30. ^{19}F NMR (500 MHz, DMSO- d_6) δ -60.62. HRMS (ESI) m/z calculated for $\text{C}_{22}\text{H}_{19}\text{F}_3\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 386.1362, found: 386.1362.



4-cyclopropyl-3-(hydroxy(4-nitrophenyl)methyl)-6-phenylpyridin-2(1H)-one (3k): white solid (68 mg, yield 75%), ^1H NMR (500 MHz, DMSO- d_6) δ 11.89 (s, 1H), 8.24 – 8.15 (m, 2H), 7.76 – 7.69 (m, 2H), 7.68 – 7.61 (m, 2H), 7.47 – 7.40 (m, 3H), 6.54 – 6.36 (m, 2H), 5.92 (s, 1H), 2.33 – 2.24 (m, 1H), 0.95 (m, 2H), 0.66 (m, 2H). ^{13}C NMR (126 MHz, DMSO- d_6) δ 163.27, 155.46, 153.88, 146.46, 133.78, 130.16, 129.17, 127.46, 126.98, 123.69, 100.95, 67.38, 12.73, 9.99, 9.37. HRMS (ESI) m/z calculated for $\text{C}_{21}\text{H}_{19}\text{N}_2\text{O}_4^+$ $[\text{M}+\text{H}]^+$ 363.1339, found: 363.1334.

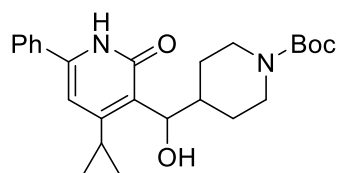


4-cyclopropyl-3-(hydroxy(3-methoxyphenyl)methyl)-6-phenylpyridin-2(1H)-one (3l): white solid (63 mg, yield 73%), ^1H NMR (500 MHz, DMSO- d_6) δ 7.83 – 7.60 (m, 2H), 7.50 – 7.29 (m, 3H), 7.19 (t, $J = 7.9$ Hz, 1H), 7.03 (t, $J = 2.0$ Hz, 1H), 6.97 (d, $J = 7.6$ Hz, 1H), 6.75 (dd, $J = 8.2, 2.6$ Hz, 1H), 6.19 (s, 1H), 5.97 (s, 1H), 3.71 (s, 3H), 2.24 (m, 1H), 0.99 – 0.63 (m, 4H). HRMS (ESI) m/z calculated for $\text{C}_{22}\text{H}_{22}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$ 348.1594, found: 348.1594

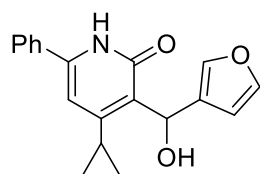


3-(cyclohexyl(hydroxy)methyl)-4-cyclopropyl-6-phenylpyridin-2(1H)-one (3m): white solid

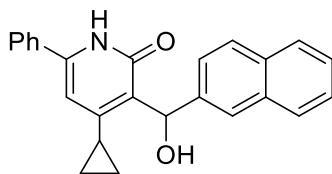
(53 mg, yield 62%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.75 (s, 1H), 7.78 – 7.64 (m, 2H), 7.49 – 7.38 (m, 3H), 5.93 (s, 1H), 5.66 (s, 1H), 4.71 (t, $J = 8.1$ Hz, 1H), 2.09 (d, $J = 12.9$ Hz, 1H), 1.91 – 1.53 (m, 4H), 1.37 (d, $J = 11.2$ Hz, 1H), 1.26 – 0.71 (m, 10H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 163.18, 153.26, 129.38, 128.55, 126.76, 72.42, 43.10, 29.26, 26.04, 25.81, 25.61, 11.88, 9.36, 8.83. HRMS (ESI) m/z calculated for $\text{C}_{21}\text{H}_{26}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 324.1958, found: 324.1958.



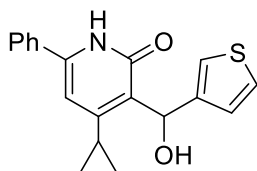
tert-butyl 4-((4-cyclopropyl-2-oxo-6-phenyl-1,2-dihydropyridin-3-yl)(hydroxy)methyl)piperidine-1-carboxylate (3n): white solid (29 mg, yield 27%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.80 (s, 1H), 7.71 (dd, $J = 6.6, 3.0$ Hz, 2H), 7.45 (dd, $J = 5.0, 2.0$ Hz, 3H), 5.93 (s, 1H), 5.75 (s, 1H), 4.76 (s, 1H), 4.00 (m, 2H), 1.39 (s, 9H), 1.34 – 1.08 (m, 7H), 1.03 – 0.76 (m, 5H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 163.18, 153.70, 129.45, 128.57, 126.80, 78.26, 41.35, 28.02, 26.90, 11.84, 9.47, 8.98. HRMS (ESI) m/z calculated for $\text{C}_{25}\text{H}_{33}\text{N}_2\text{O}_4^+$ $[\text{M}+\text{H}]^+$ 425.2435, found: 425.2434.



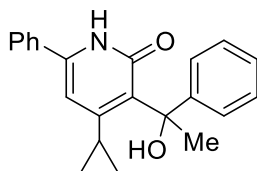
3-cyclopropyl-3-(furan-3-yl(hydroxy)methyl)-6-phenylpyridin-2(1H)-one (3o): white solid (36 mg, yield 47%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.85 (s, 1H), 7.71 (dd, $J = 6.7, 3.0$ Hz, 2H), 7.55 (t, $J = 1.7$ Hz, 1H), 7.46 (dd, $J = 5.1, 1.9$ Hz, 4H), 6.49 – 6.32 (m, 2H), 6.16 (d, $J = 7.4$ Hz, 1H), 5.94 (s, 1H), 2.36 (m, 1H), 0.94 (m, 3H), 0.87 – 0.76 (m, 1H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 163.35, 154.21, 143.56, 139.21, 130.07, 129.86, 129.16, 127.42, 110.20, 101.07, 63.07, 46.16, 12.39, 9.80, 9.35. HRMS (ESI) m/z calculated for $\text{C}_{19}\text{H}_{18}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$ 308.1281, found: 308.1.



3-cyclopropyl-3-(hydroxy(naphthalen-2-yl)methyl)-6-phenylpyridin-2(1H)-one (3p): white solid (76 mg, yield 83%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.87 (s, 1H), 7.95 – 7.91 (m, 1H), 7.90 – 7.82 (m, 3H), 7.77 – 7.70 (m, 2H), 7.55 (dd, $J = 8.5, 1.8$ Hz, 1H), 7.50 – 7.43 (m, 5H), 6.51 (d, $J = 3.4$ Hz, 2H), 5.94 (s, 1H), 2.41 (m, 1H), 1.02 – 0.86 (m, 2H), 0.77 – 0.58 (m, 2H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 163.01, 154.37, 142.64, 132.69, 131.80, 129.49, 128.58, 127.68, 127.33, 127.30, 126.84, 125.84, 125.29, 124.55, 123.27, 100.51, 67.84, 12.09, 9.28, 8.81. HRMS (ESI) m/z calculated for $\text{C}_{25}\text{H}_{22}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 368.1645, found: 368.1645.

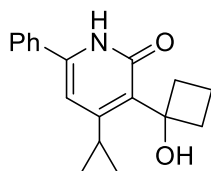


4-cyclopropyl-3-(hydroxy(thiophen-3-yl)methyl)-6-phenylpyridin-2(1H)-one (3q): white solid (42 mg, yield 52%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.85 (s, 1H), 7.71 (dd, $J = 6.6, 2.9$ Hz, 2H), 7.48 – 7.40 (m, 4H), 7.25 (dd, $J = 3.0, 1.4$ Hz, 1H), 7.07 (dd, $J = 5.0, 1.3$ Hz, 1H), 6.59 – 6.44 (m, 1H), 6.27 (d, $J = 5.5$ Hz, 1H), 5.94 (s, 1H), 2.36 (m, 1H), 0.99 – 0.91 (m, 2H), 0.86 (m, 1H), 0.82 – 0.75 (m, 1H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 162.80, 153.79, 146.27, 129.50, 128.59, 126.84, 126.42, 125.69, 119.91, 65.90, 11.88, 9.26, 8.76. HRMS (ESI) m/z calculated for $\text{C}_{19}\text{H}_{18}\text{NO}_2\text{S}^+$ $[\text{M}+\text{H}]^+$ 324.1053, found: 324.1052.

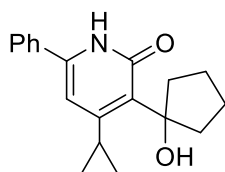


4-cyclopropyl-3-(1-hydroxy-1-phenylethyl)-6-phenylpyridin-2(1H)-one (3r): white solid (41 mg, yield 49%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 10.32 (s, 1H), 7.74 (d, $J = 7.6$ Hz, 2H), 7.46 – 7.34 (m, 6H), 7.32 – 7.26 (m, 2H), 7.13 (s, 1H), 6.80 (s, 1H), 2.00 (s, 3H), 1.23 – 1.13 (m, 1H), 0.64 (s, 1H),

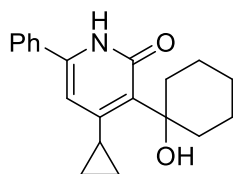
0.49 (s, 2H), 0.30 (s, 1H). ^{13}C NMR (126 MHz, DMSO- d_6) δ 158.86, 148.99, 144.45, 137.69, 136.28, 128.10, 128.07, 127.78, 113.97, 72.57, 26.90, 25.82, 10.33, 7.95, 6.14. HRMS (ESI) m/z calculated for $\text{C}_{22}\text{H}_{22}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 332.1645, found: 332.1642.



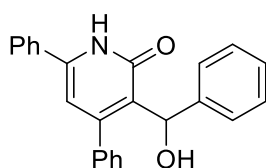
4-cyclopropyl-3-(1-hydroxycyclobutyl)-6-phenylpyridin-2(1H)-one (3s): white solid (52 mg, yield 74%), ^1H NMR (500 MHz, DMSO- d_6) δ 11.37 (s, 1H), 7.80 – 7.61 (m, 2H), 7.51 – 7.40 (m, 3H), 5.88 (s, 1H), 2.66 (m, 2H), 2.36 (m, 2H), 2.15 – 2.03 (m, 2H), 1.70 – 1.56 (m, 1H), 1.44 – 1.17 (m, 3H), 1.00 – 0.93 (m, 2H). ^{13}C NMR (126 MHz, DMSO- d_6) δ 160.94, 152.74, 130.99, 128.67, 128.01, 126.09, 75.61, 66.80, 37.40, 29.19, 27.75, 22.64, 21.79, 15.72, 13.29, 12.30, 10.20, 8.57. HRMS (ESI) m/z calculated for $\text{C}_{18}\text{H}_{20}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 282.1489, found: 282.1489.



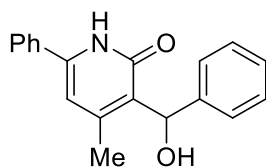
4-cyclopropyl-3-(1-hydroxycyclopentyl)-6-phenylpyridin-2(1H)-one (3t): white solid (53 mg, yield 72%), ^1H NMR (500 MHz, DMSO- d_6) δ 11.74 (s, 1H), 7.80 – 7.63 (m, 2H), 7.45 (m, 3H), 5.93 (d, $J = 27.6$ Hz, 1H), 2.67 – 2.54 (m, 1H), 2.48 – 2.42 (m, 1H), 2.32 – 2.17 (m, 2H), 2.06 – 1.91 (m, 3H), 1.81 (m, 1H), 1.68 (m, 1H), 1.05 – 1.00 (m, 1H), 0.95 (m, 2H), 0.89 – 0.82 (m, 1H). ^{13}C NMR (126 MHz, DMSO- d_6) δ 164.15, 161.28, 152.69, 138.96, 129.43, 128.58, 128.51, 126.76, 126.65, 101.78, 82.72, 35.10, 32.59, 23.92, 22.99, 14.10, 12.97, 10.04, 9.08. HRMS (ESI) m/z calculated for $\text{C}_{19}\text{H}_{22}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 296.1645, found: 296.1644.



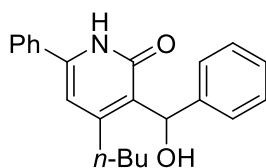
4-cyclopropyl-3-(1-hydroxycyclohexyl)-6-phenylpyridin-2(1H)-one (3u): white solid (58 mg, yield 75%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.93 (s, 1H), 7.70 (dd, $J = 6.6, 3.0$ Hz, 2H), 7.48 – 7.42 (m, 3H), 6.05 (s, 1H), 2.44 (m, 1H), 2.27 (m, 2H), 1.87 – 1.73 (m, 4H), 1.62 (d, $J = 13.1$ Hz, 1H), 1.50 – 1.38 (m, 2H), 1.28 – 1.24 (m, 1H), 1.09 – 1.00 (m, 2H), 0.96 – 0.88 (m, 2H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 164.50, 152.02, 129.49, 128.60, 126.78, 103.41, 74.12, 35.84, 25.02, 21.35, 15.50, 9.86. HRMS (ESI) m/z calculated for $\text{C}_{20}\text{H}_{24}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 310.1802, found: 310.1800.



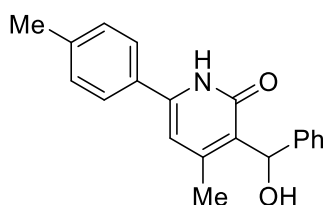
3-(hydroxy(phenyl)methyl)-4,6-diphenylpyridin-2(1H)-one (3v): white solid (37 mg, yield 42%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 12.25 (s, 1H), 7.81 (dd, $J = 6.6, 3.0$ Hz, 2H), 7.52 – 7.42 (m, 6H), 7.40 – 7.35 (m, 2H), 7.28 – 7.23 (m, 2H), 7.22 – 7.13 (m, 3H), 6.55 (s, 1H), 6.05 (d, $J = 9.7$ Hz, 1H), 5.55 (d, $J = 9.4$ Hz, 1H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 151.00, 144.22, 138.17, 129.79, 128.70, 128.40, 128.30, 127.91, 127.73, 126.97, 126.40, 125.53, 70.19. HRMS (ESI) m/z calculated for $\text{C}_{24}\text{H}_{20}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 354.1489, found: 354.1488.



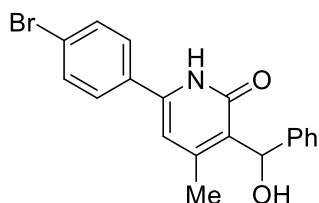
3-(hydroxy(phenyl)methyl)-4-methyl-6-phenylpyridin-2(1H)-one (3w): white solid (57 mg, yield 78%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 7.83 – 7.64 (m, 2H), 7.47 (d, $J = 6.5$ Hz, 3H), 7.39 (d, $J = 7.7$ Hz, 2H), 7.30 (t, $J = 7.5$ Hz, 2H), 7.19 (t, $J = 7.3$ Hz, 1H), 6.45 (s, 1H), 6.13 (s, 1H), 3.32 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 164.04, 149.07, 145.20, 133.79, 130.02, 129.23, 128.38, 127.19, 126.80, 125.95, 109.11, 68.44, 19.62. HRMS (ESI) m/z calculated for $\text{C}_{19}\text{H}_{18}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 292.1332, found: 292.1330.



4-butyl-3-(hydroxy(phenyl)methyl)-6-phenylpyridin-2(1H)-one (3x): white solid (26 mg, yield 31%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.89 (s, 1H), 7.81 – 7.68 (m, 2H), 7.51 – 7.44 (m, 3H), 7.40 – 7.34 (m, 2H), 7.32 – 7.26 (m, 2H), 7.22 – 7.14 (m, 1H), 6.45 (s, 1H), 6.24 – 6.04 (m, 2H), 2.56 (m, 1H), 2.48 – 2.43 (m, 1H), 1.44 – 1.32 (m, 1H), 1.27 – 1.21 (m, 1H), 1.16 – 1.06 (m, 1H), 0.77 (t, $J = 7.3$ Hz, 3H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 163.59, 153.17, 145.21, 133.09, 129.45, 128.64, 127.73, 126.63, 126.09, 125.28, 107.23, 67.38, 31.60, 31.28, 22.18, 13.60. HRMS (ESI) m/z calculated for $\text{C}_{22}\text{H}_{24}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 334.1802, found: 334.1801.

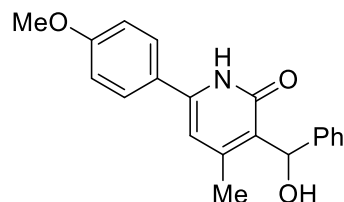


3-(hydroxy(phenyl)methyl)-4-methyl-6-(p-tolyl)pyridin-2(1H)-one (3y): white solid (22 mg, yield 29%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 10.88 (s, 1H), 7.70 – 7.60 (m, 2H), 7.46 (s, 1H), 7.44 – 7.39 (m, 2H), 7.36 (dd, $J = 8.4, 6.8$ Hz, 2H), 7.31 – 7.25 (m, 1H), 7.17 (d, $J = 8.0$ Hz, 2H), 6.48 – 6.19 (m, 1H), 5.77 (d, $J = 3.2$ Hz, 1H), 2.31 (s, 3H), 1.99 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 160.75, 142.87, 141.85, 136.81, 134.02, 128.91, 128.83, 128.38, 127.97, 126.85, 69.90, 21.26, 15.70. HRMS (ESI) m/z calculated for $\text{C}_{20}\text{H}_{20}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 306.1489, found: 306.1486.

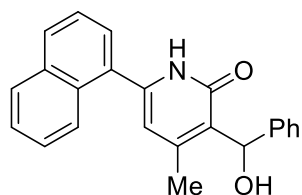


6-(4-bromophenyl)-3-(hydroxy(phenyl)methyl)-4-methylpyridin-2(1H)-one (3z): white solid (42 mg, yield 45%), $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 11.82 (s, 1H), 7.70 (d, $J = 8.7$ Hz, 2H), 7.44 – 7.35 (m, 2H), 7.29 (t, $J = 7.7$ Hz, 2H), 7.22 – 7.15 (m, 1H), 7.08 – 6.92 (m, 2H), 6.39 (s, 1H), 6.34 – 6.21 (m, 1H), 6.16 – 6.06 (m, 1H), 2.14 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, $\text{DMSO-}d_6$) δ 163.93, 160.89, 149.27, 145.25,

144.05, 128.61, 128.37, 126.78, 125.95, 125.79, 114.66, 108.08, 68.48, 55.81, 19.64. HRMS (ESI) m/z calculated for $C_{19}H_{17}BrNO_2^+$ $[M+H]^+$ 370.0437, found: 370.0437.

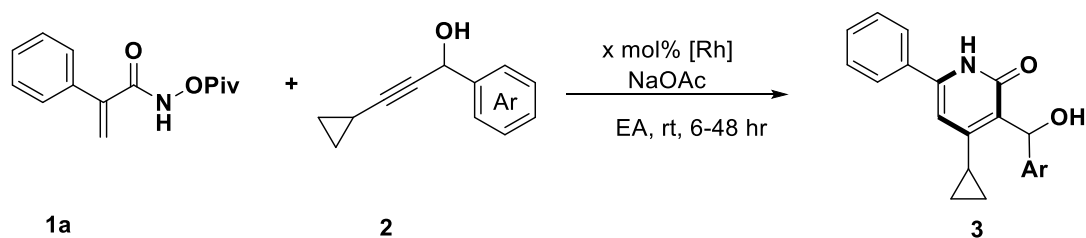


3-(hydroxy(phenyl)methyl)-6-(4-methoxyphenyl)-4-methylpyridin-2(1H)-one (3za): white solid (30 mg, yield 38%), 1H NMR (500 MHz, $DMSO-d_6$) δ 11.05 (s, 1H), 7.82 – 7.69 (m, 2H), 7.59 – 7.50 (m, 3H), 7.42 (d, $J = 8.3$ Hz, 2H), 7.39 – 7.32 (m, 2H), 7.30 – 7.22 (m, 1H), 6.41 (s, 1H), 5.76 (dd, $J = 12.3, 1.4$ Hz, 1H), 3.34 (s, 3H), 1.99 (s, 3H). ^{13}C NMR (126 MHz, $DMSO-d_6$) δ 160.54, 146.47, 143.55, 141.69, 136.09, 131.24, 130.54, 128.84, 128.02, 126.88, 126.34, 120.75, 69.97, 15.69. HRMS (ESI) m/z calculated for $C_{20}H_{19}KNO_3^+$ $[M+K]^+$ 360.0997, found: 360.0994.



3-(hydroxy(phenyl)methyl)-4-methyl-6-(naphthalen-1-yl)pyridin-2(1H)-one (3zb): white solid (42 mg, yield 61%), 1H NMR (500 MHz, $DMSO-d_6$) δ 11.02 (s, 1H), 8.05 – 7.80 (m, 2H), 7.62 (dd, $J = 8.4, 2.9$ Hz, 1H), 7.55 – 7.47 (m, 4H), 7.45 (m, 1H), 7.42 – 7.36 (m, 3H), 7.35 (s, 1H), 7.33 – 7.27 (m, 1H), 6.43 (s, 1H), 5.84 (d, $J = 3.5$ Hz, 1H), 2.02 (s, 3H). ^{13}C NMR (126 MHz, $DMSO-d_6$) δ 160.96, 145.62, 141.89, 135.93, 133.54, 131.84, 128.89, 128.52, 128.21, 128.03, 127.81, 126.97, 126.52, 126.23, 126.17, 125.91, 70.11, 15.71. HRMS (ESI) m/z calculated for $C_{23}H_{20}NO_2^+$ $[M+H]^+$ 342.1489, found: 342.1489.

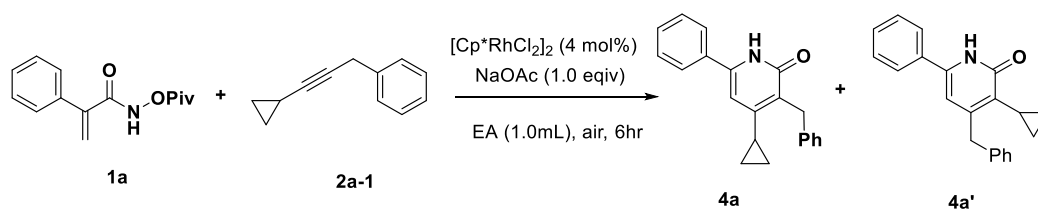
Scale-up Experiments



In a 50 mL reaction tube, the mixture of **1a** (494.6 mg, 2.0 mmol, 1.0 eq.), **2** (3.0 mmol, 1.5 eq.), [Cp**RhCl*₂]₂ (2.5 or 1.0 mol%) and NaOAc (2.0 mmol, 1.0 eq.) was added EA (10.0 mL). Then the resulting mixture was stirred at room temperature for 6.0~48 hours. When the reaction was finished, the product precipitated out was simply collected by filtration. The product **3a** or **3p** was obtained as a white solid. The rest reaction mixture was subjected to flash chromatography on silica gel (dichloromethane/methanol) to provide the rest products **3a** or **3p**, the total yields were reported.

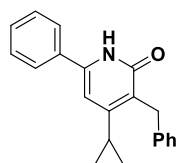
Control Experiments

a) Procedure for the Synthesis of **4a** and **4a'**



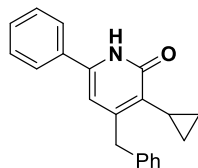
In a 10 mL reaction tube, the mixture of **1a** (0.2 mmol), **2a-1** (0.3 mmol), [Cp**RhCl*₂]₂ (4.0 mol%) and NaOAc (1.0 eq.) was added EA (1.0 mL). Then the resulting mixture was stirred for 12 h. When the reaction was finished, the solvent was removed under vacuum. The reaction mixture was subjected directly to flash chromatography on silica gel (dichloromethane/methanol) to provide the products **4a** in 32% yield and **4a'** in 42% yield.

Characterization Data of **4a**, **4a'**



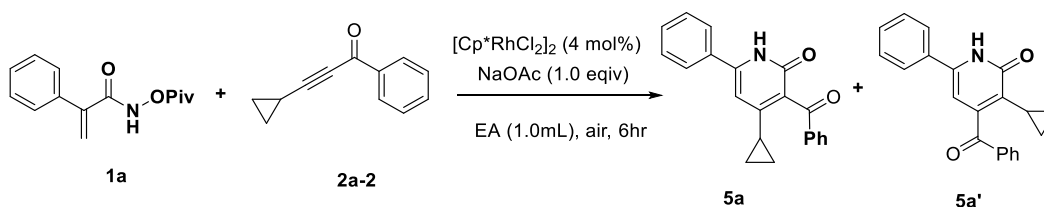
3-benzyl-4-cyclopropyl-6-phenylpyridin-2(1H)-one (4a): white solid (39 mg, yield 32%); ¹H

NMR (500 MHz, DMSO-*d*₆) δ 11.61 (s, 1H), 7.71 (dd, *J* = 7.3, 2.2 Hz, 2H), 7.46 – 7.38 (m, 3H), 7.29 – 7.19 (m, 4H), 7.17 – 7.05 (m, 1H), 5.94 (s, 1H), 4.02 (s, 2H), 2.04 – 1.90 (m, 1H), 0.92 (m, 2H), 0.86 – 0.77 (m, 2H). **¹³C NMR** (126 MHz, DMSO-*d*₆) δ 163.39, 153.45, 141.28, 134.32, 129.79, 129.12, 128.64, 127.22, 126.08, 100.76, 31.15, 13.19, 9.07. LCMS (ESI) *m/z* calculated for C₂₁H₂₀NO⁺ [M+H]⁺ 302.2, found: 302.2.



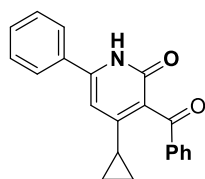
4-benzyl-3-cyclopropyl-6-phenylpyridin-2(1H)-one (4a'): white solid (51 mg, yield 42%); **¹H NMR** (500 MHz, DMSO-*d*₆) δ 11.42 (s, 1H), 7.72 – 7.58 (m, 2H), 7.40 (q, *J* = 7.3, 6.8 Hz, 3H), 7.27 (m, 3H), 7.18 (t, *J* = 7.1 Hz, 1H), 6.41 (s, 1H), 4.05 (s, 2H), 1.70 – 1.51 (m, 1H), 1.02 (m, 2H), 0.75 (m, 2H). **¹³C NMR** (126 MHz, DMSO-*d*₆) δ 163.46, 151.84, 143.67, 139.93, 134.14, 129.69, 129.19, 129.11, 128.97, 126.86, 126.63, 107.77, 38.51, 10.33, 6.62. LCMS (ESI) *m/z* calculated for C₂₁H₂₀NO⁺ [M+H]⁺ 302.2, found: 302.2.

b) Procedure for the Synthesis of **5a** and **5a'**

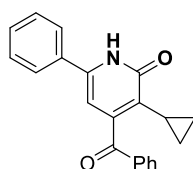


In a 10 mL reaction tube, the mixture of **1a** (0.2 mmol), **2a-2** (0.3 mmol), [Cp*RhCl₂]₂ (4.0 mol%) and NaOAc (1.0 eq.) was added EA (1.0 mL). Then the resulting mixture was stirred for 12 h. When the reaction was finished, the solvent was removed under vacuum. The reaction mixture was subjected directly to flash chromatography on silica gel (dichloromethane/ methanol) to provide the products **5a** in 8% yield and **5a'** in 24% yield.

Characterization Data of **5a**, **5a'**



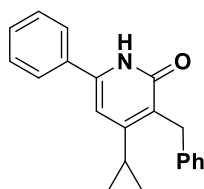
3-benzoyl-4-cyclopropyl-6-phenylpyridin-2(1H)-one (5a): yellow liquid (10 mg, yield 8%); ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 11.92 (s, 1H), 7.87 – 7.82 (m, 2H), 7.78 (dd, $J = 6.6, 3.0$ Hz, 2H), 7.68 – 7.62 (m, 1H), 7.54 (t, $J = 7.7$ Hz, 2H), 7.50 – 7.45 (m, 3H), 6.07 (s, 1H), 1.51 (m, 1H), 0.99 – 0.93 (m, 2H), 0.90 (m, 2H). ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 196.68, 174.75, 161.16, 155.65, 137.48, 134.16, 130.43, 130.11, 129.40, 129.37, 129.20, 127.65, 13.50, 9.97. LCMS (ESI) m/z calculated for $\text{C}_{21}\text{H}_{18}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 316.1, found: 316.2.



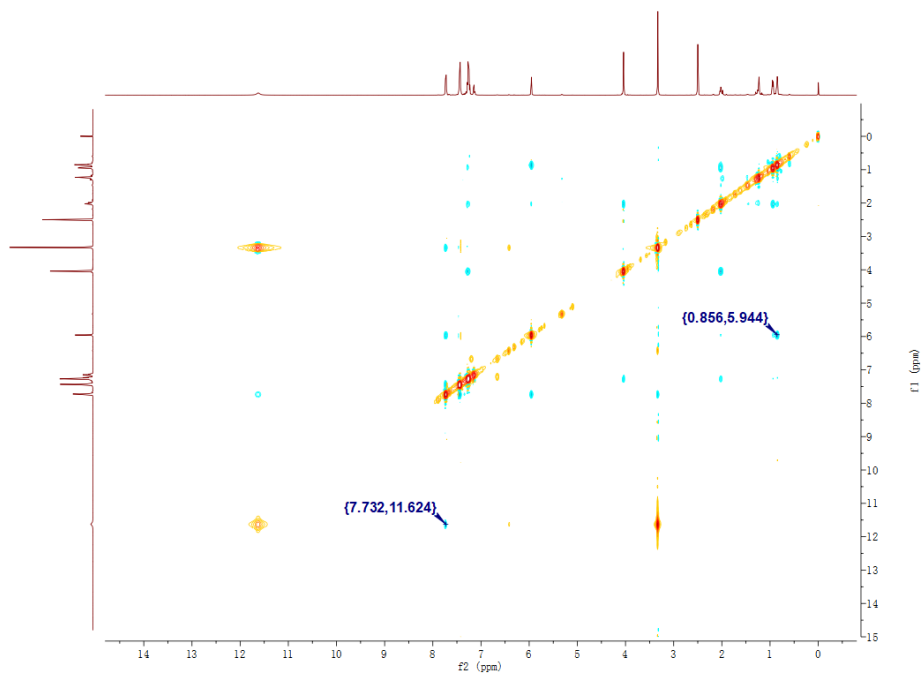
4-benzoyl-3-cyclopropyl-6-phenylpyridin-2(1H)-one (5a'): yellow liquid (29 mg, yield 24%); ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 11.90 (s, 1H), 7.93 – 7.86 (m, 2H), 7.80 – 7.75 (m, 2H), 7.74 – 7.69 (m, 1H), 7.59 (t, $J = 7.7$ Hz, 2H), 7.45 (dd, $J = 5.2, 1.9$ Hz, 3H), 6.50 (s, 1H), 1.39 (m, 1H), 0.93 – 0.83 (m, 2H), 0.61 – 0.49 (m, 2H). ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 196.87, 163.26, 149.14, 145.16, 135.98, 134.79, 133.68, 130.11, 129.92, 129.64, 129.23, 127.17, 102.93, 12.09, 6.33. LCMS (ESI) m/z calculated for $\text{C}_{21}\text{H}_{18}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 316.1, found: 316.2.

NOESY Experiments for Product 4a, 4a', 5a, 5a'

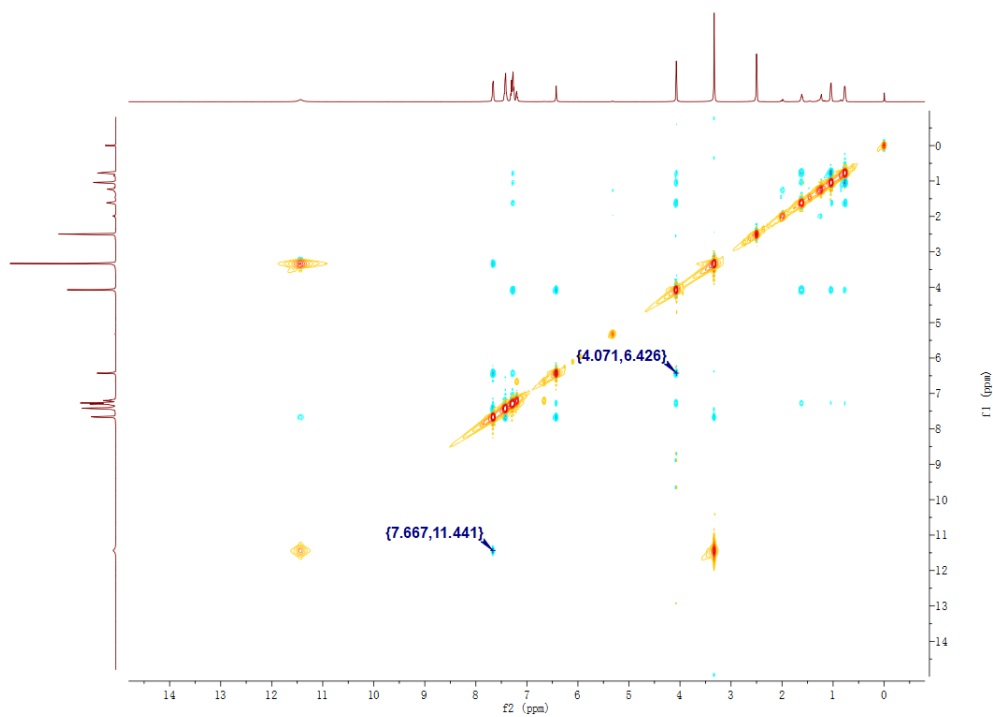
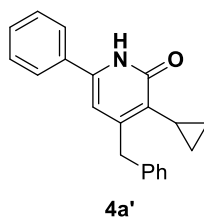
1) NOESY spectra of product 4a



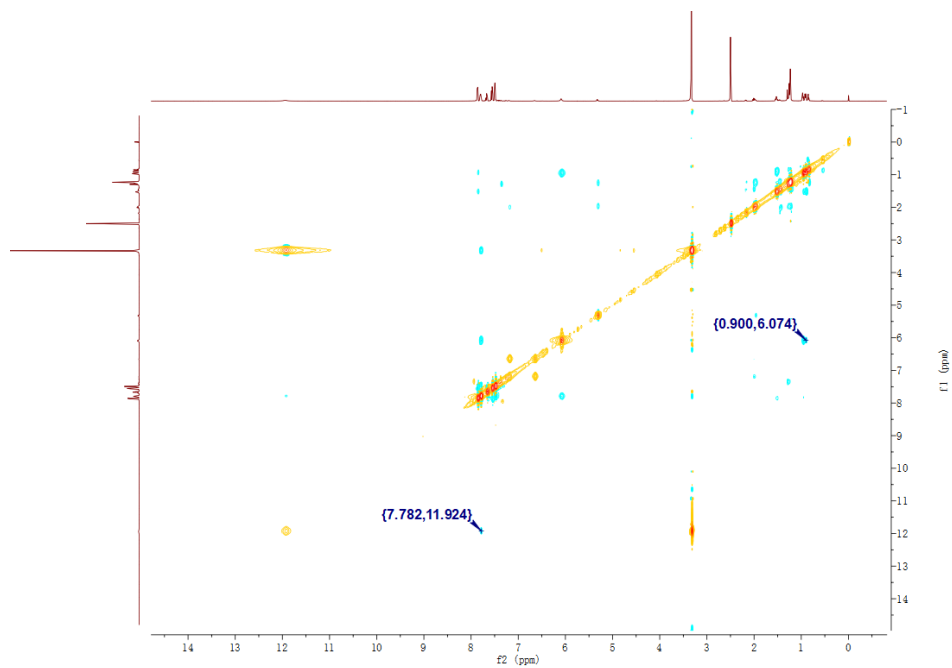
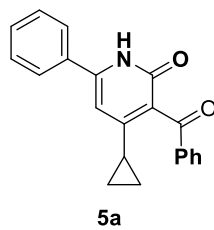
4a



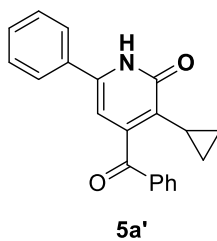
2) NOESY spectra of product 4a'

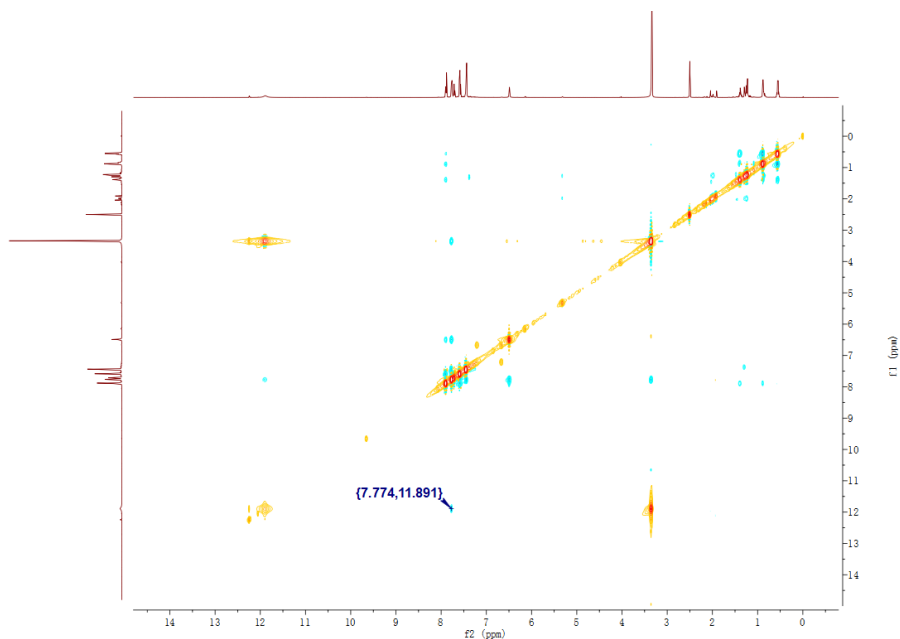


3) NOESY spectra of product **5a**



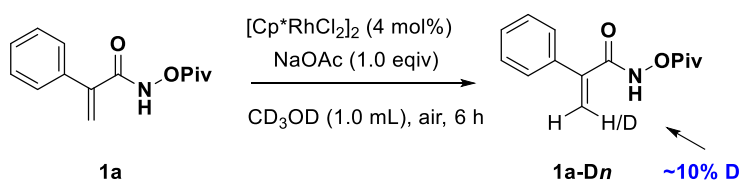
4) NOESY spectra of product **5a'**



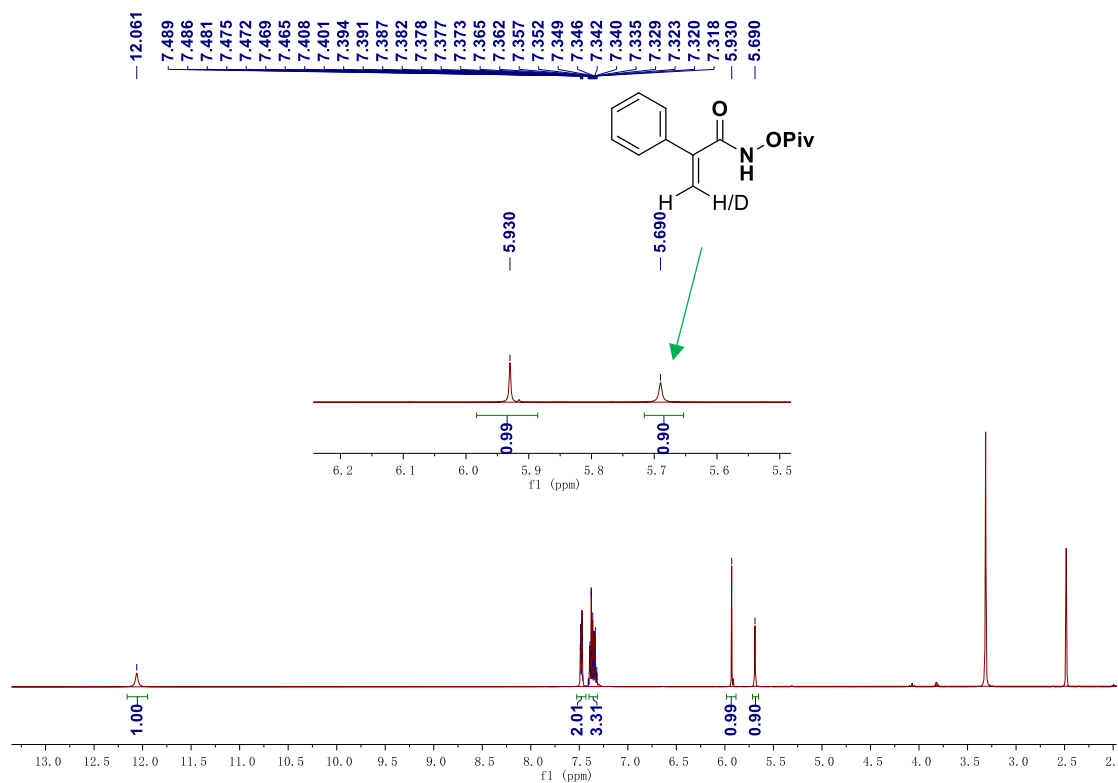


Mechanistic Experiments

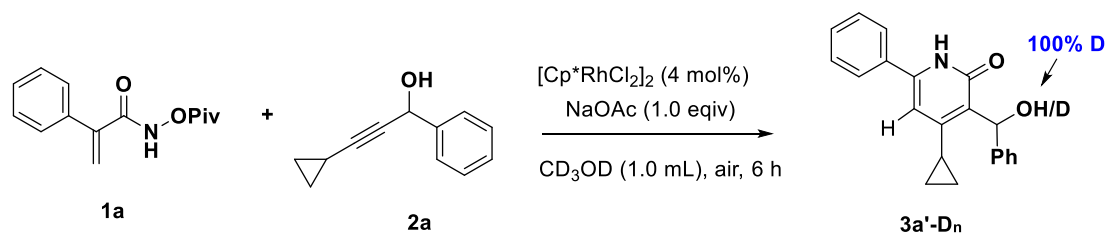
Deuterium Incorporation Experiment A



To a mixture of **1a** (49.5 mg, 0.2 mmol, 1.0 eq.), $[\text{Cp}^*\text{RhCl}_2]_2$ (4.9 mg, 0.008 mmol, 4 mol%) and NaOAc (16.4 mg, 0.2 mmol, 1.0 eq.) in a 10 mL reaction tube was added CD_3OD (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 ^1H NMR analysis. The reaction of **1a** (49.5 mg, 0.2 mmol, 1.0 eq.) without **2a** provided the product **1a-D_n**. Found ~10% H/D exchange occurred at the olefinic bond of **1a**.

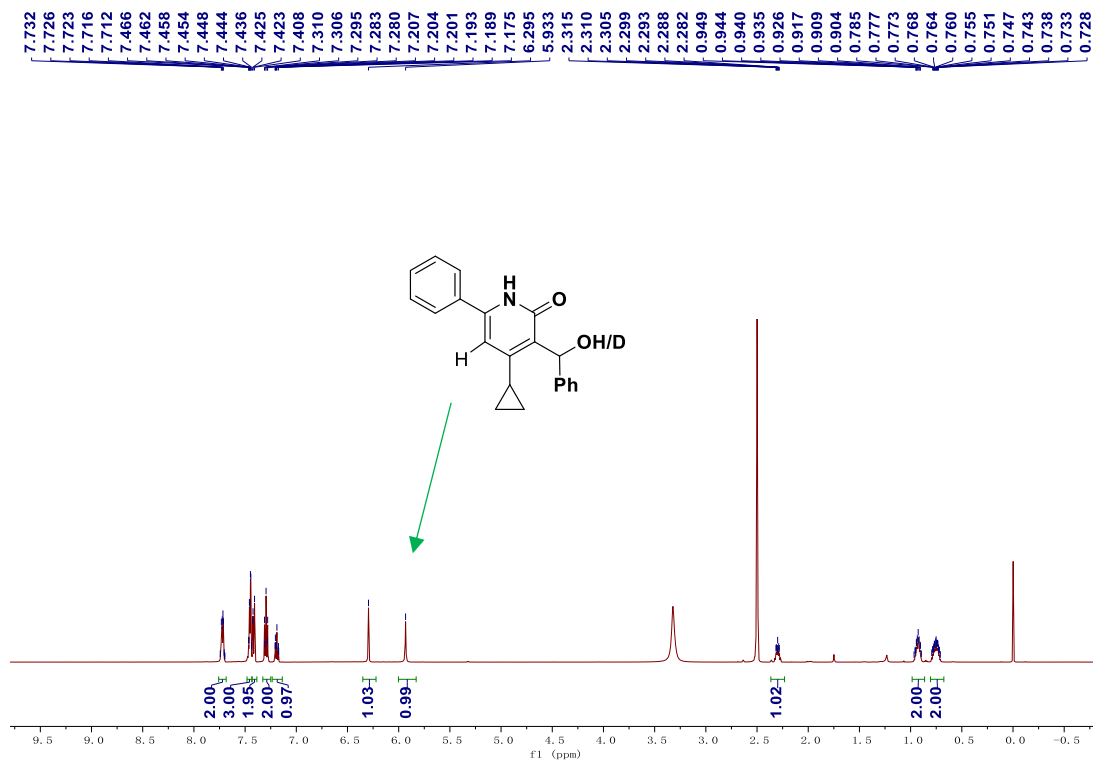


Deuterium Incorporation Experiment B



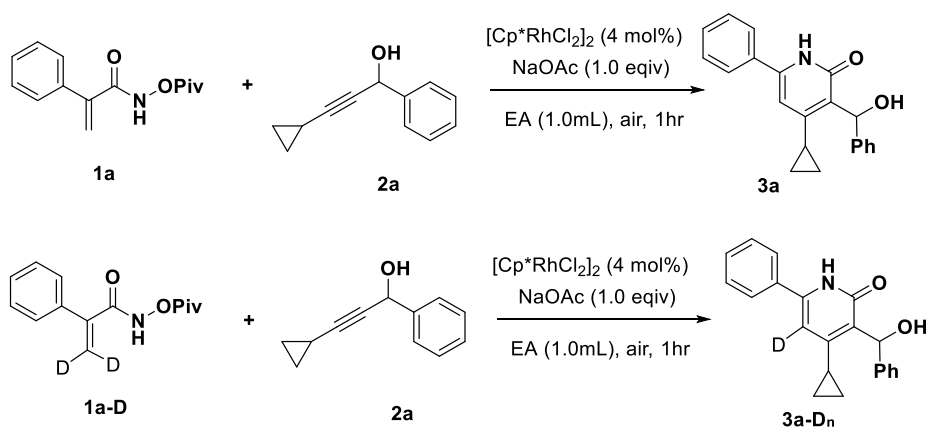
To a mixture of **1a** (49.5 mg, 0.2 mmol, 1.0 eq.), **2a** (51.7 mg, 0.3 mmol, 1.5 eq.), $[\text{Cp}^*\text{RhCl}_2]_2$ (4.9 mg, 0.008 mmol, 4 mol%) and NaOAc (16.4 mg, 0.2 mmol, 1.0 eq.) in a 10 mL reaction tube was added CD_3OD (1.0 mL). Then the resulting mixture was stirred at the temperature for 6.0 h. After removal of the solvents under vacuum, the residue obtained was directly used for ^1H 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_n**, found almost 100% deuterium incorporation at the hydrogen of hydroxyl group.



Determination of the KIE

Two parallel reactions for KIE value measurement

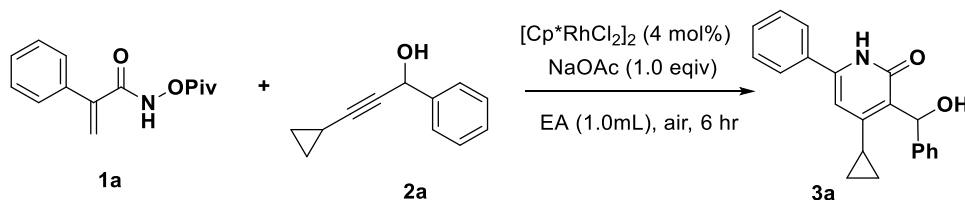


To a mixture of **1a** (49.5 mg, 0.2 mmol, 1.0 eq.), **2a** (51.7 mg, 0.3 mmol, 1.5 eq.), $[\text{Cp}^*\text{RhCl}_2]_2$ (4.9 mg, 0.008 mmol, 4 mol%) and NaOAc (16.4 mg, 0.2 mmol, 1.0 eq.) in a 10 mL reaction tube was added EA (1.0 mL). Then the resulting mixture was stirred at the temperature for 1.0 h. The reaction was finished to provide the product **3a** (19.0 mg, 30% yield).

To a mixture of **1a-D** (49.8 mg, 0.2 mmol, 1.0 eq.), **2a** (51.7 mg, 0.3 mmol, 1.5 eq.), $[\text{Cp}^*\text{RhCl}_2]_2$ (4.9 mg, 0.008 mmol, 4 mol%) and NaOAc (16.4 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_n** (17.0 mg, 27% yield). The ratio of **3aa/3aa-D_n** was 1.12 (0.30/0.27)

Catalyst Recycling Experiments



In a 10 mL reaction tube, the mixture of **1a** (0.3 mmol), **2a** (0.45 mmol), $[\text{Cp}^*\text{RhCl}_2]_2$ (4.0 mol%) and NaOAc (1.0 eq.) was added EA (1.0 mL). Then the resulting mixture was stirred for 6.0 ~ 24 h. When the reaction was finished, the desired product precipitated out as a solid, and the product **3a** was simply collected by filtration. The precipitation was washed with H₂O and EA. The filtrate (concentrated to ~1 mL) was reused in the next cycle without adding additional rhodium catalyst. **1aa** (0.3 mmol), **2aa** (0.45 mmol), and NaOAc (1.0 eq.) were added to the filtrate in each cycle. Repeating the above-mentioned procedure for 4 times, the results were shown as below.

Number of runs	Isolated yield (%)
1	63
2	53
3	42
4	45

X-ray data of compound 3c (Deposition Data: CCDC 2213771)

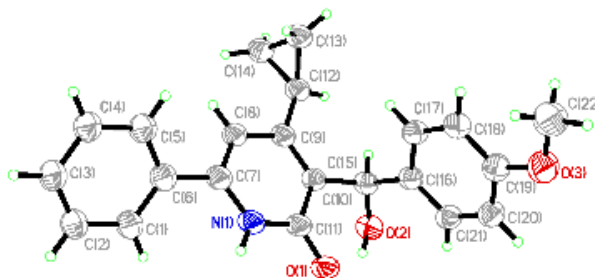
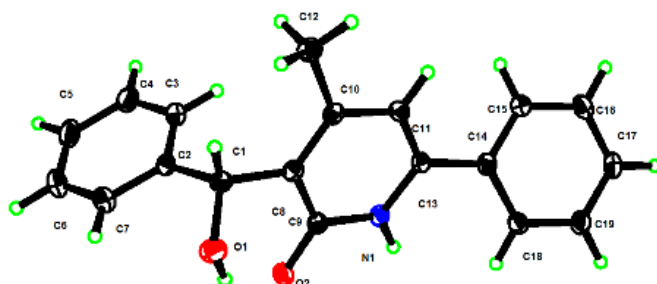


Table S1. Crystal data and structure refinement for compound **3c**.

Identification code	fast
Empirical formula	C ₂₂ H ₁₁ NO ₃
Formula weight	347.4
Temperature/K	293.15
Crystal system	monoclinic
Space group	P 2 ₁ /c
a/Å	13.3096(4)
b/Å	10.8544(4)
c/Å	12.5557(4)
α/°	90
β/°	91.697(2)
γ/°	90
Volume/Å ³	1813.10(10)
Z	4
ρ _{calc} /cm ³	1.273
μ/mm ⁻¹	0.679
F(000)	736
Crystal size/mm ³	0.22 × 0.18 × 0.16
Radiation	Cu Kα (λ = 1.54178)
2θ range for data collection/°	6.64 to 153.08
Index ranges	-16 ≤ h ≤ 16, -13 ≤ k ≤ 13, -15 ≤ l ≤ 14
Reflections collected	16770
Independent reflections	3689 [R _{int} = 0.0896, R _{sigma} = 0.1247]
Data/restraints/parameters	3689/411/281
Goodness-of-fit on F ²	1.144
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.1063, wR ₂ = 0.2709
Final R indexes [all data]	R ₁ = 0.1208, wR ₂ = 0.2778
Largest diff. peak/hole / e Å ⁻³	0.55/-0.32

X-ray data of compound 3w (Deposition Data: CCDC 2234440)**Table S2.** Crystal data and structure refinement for compound **3w**.

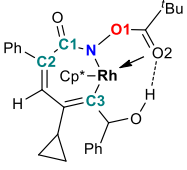
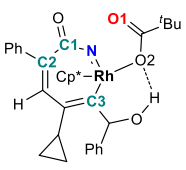
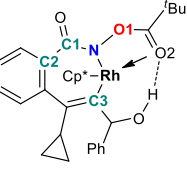
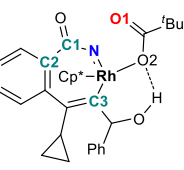
Identification code	A
Empirical formula	C ₁₉ H ₁₇ NO ₂
Formula weight	291.33
Temperature/K	150
Crystal system	monoclinic
Space group	P 21/c
a/Å	14.0628(8)
b/Å	9.8424(7)
c/Å	11.6643(7)
α/°	90
β/°	114.207(2)
γ/°	90
Volume/Å ³	1472.52(16)
Z	4
ρ _{calc} /cm ³	1.314
μ/mm ⁻¹	0.085
F(000)	616.0
Crystal size/mm ³	0.12 × 0.08 × 0.05
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	5.216 to 52.784
Index ranges	-17 ≤ h ≤ 17, -12 ≤ k ≤ 12, -14 ≤ l ≤ 12
Reflections collected	10699
Independent reflections	2991 [R _{int} = 0.0829, R _{sigma} = 0.0766]
Data/restraints/parameters	2991/0/201
Goodness-of-fit on F ²	1.075
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0619, wR ₂ = 0.1580
Final R indexes [all data]	R ₁ = 0.0921, wR ₂ = 0.1846
Largest diff. peak/hole / e Å ⁻³	0.27/-0.31

Computational Mechanistic Studies

Computational details:

Density functional theory (DFT)⁶ calculations were performed by using Gaussian 09 quantum chemical package.⁷ Unless otherwise specified, geometry optimizations were performed using B3LYP⁸ functional with Grimme D3 correction (EmpiricalDispersion=GD3BJ).⁹ Herein, the Stuttgart/Dresden effective core potential (SDD)¹⁰ was used for Rh in conjunction with a standard 6-31G(d,p) basis set¹¹ 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) calculations¹² were carried out to confirm that all transition state structures connect the corresponding reactants and products. Solvent effects in ethyl acetate (EA) were estimated by using the SMD¹³ solvation method (solvent=EthylEthanoate) at the M06¹⁴ 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. 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 ΔG for clarity). The 3D diagrams of optimized structures are illustrated using CYLView.¹⁵ Multiwfn¹⁶ was utilized to analyze interactions with the independent gradient model based on Hirshfeld partition of molecular density (IGMH)¹⁷ and the graphics are displayed using VMD program.¹⁸ The Mulliken atomic charge was analyzed by Multiwfn.

Table S3. Comparison of intermediates INT-3 and INT-4i with their analogues.

		 INT-3	 INT-4i	 INT-3 _{Ph}	 INT-4i _{Ph}
Bond	C1-C2	1.51	1.51	1.51	1.51
	N-O1	1.48	-	1.48	-
	N-C2	2.38	2.27	2.38	2.27
	N-C3	2.85	2.84	2.88	2.86
Mulliken atomic charge	Rh	0.0920	0.2572	0.0879	0.2531
	N	-0.2947	-0.3958	-0.2965	-0.3828
	O1	-0.3229	-0.4573	-0.3246	-0.4558
	C2	0.0346	-0.0153	0.0216	-0.0038
	C3	-0.0506	-0.0089	-0.0395	-0.0075

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

Table S4. 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 of the transition states.

Structures	corr. to ZPE	corr. to <i>E</i>	corr. to <i>H</i>	corr. to <i>G</i>	SP _{SMD}	Imaginary frequency
2a	0.205697	0.218059	0.219004	0.163764	-539.379153	—
PC1	0.352129	0.372144	0.373088	0.301751	-1016.419180	—
PC2	0.351575	0.371776	0.372721	0.301292	-1016.413484	—
HOAc	0.062006	0.066586	0.067531	0.034715	-229.0377862	—
Cp*Rh(OAc)(OPiv)	0.411727	0.439702	0.440646	0.353085	-1075.257734	—
INT-0	0.488166	0.520121	0.521066	0.424395	-1323.079708	—
INT-1	0.698184	0.742556	0.743500	0.619754	-1862.502940	—
TS-1	0.697186	0.740865	0.741809	0.620156	-1862.485075	-358.95
INT-2	0.700549	0.743721	0.744665	0.627050	-1862.531136	—
TS-2	0.700024	0.742785	0.743729	0.626430	-1862.520257	-158.68
INT-3	0.701510	0.744409	0.745353	0.627583	-1862.535260	—
TS-3	0.696825	0.740395	0.741339	0.621582	-1862.518086	-337.63
INT-4	0.699479	0.743648	0.744592	0.622505	-1862.590483	—
TS-4	0.697777	0.741324	0.742268	0.622042	-1862.555455	-420.71
INT-5	0.702989	0.745772	0.746717	0.628405	-1862.655912	—
TS-5	0.762009	0.810191	0.811135	0.680714	-2091.686754	-814.92
INT-1i	0.697183	0.741956	0.742900	0.618325	-1862.493430	—
TS-1i	0.696121	0.740413	0.741357	0.615375	-1862.478477	-418.85

INT-2i	0.699082	0.743086	0.744031	0.622471	-1862.518971	—
INT-4i	0.697727	0.741979	0.742923	0.620559	-1862.499250	—
TS-4i	0.696831	0.740521	0.741465	0.620365	-1862.499285	-117.19
TS-3ii	0.699916	0.742212	0.743156	0.626679	-1862.497687	-346.82
INT-4ii	0.701289	0.744034	0.744978	0.626925	-1862.526865	—
TS-4ii	0.698362	0.741452	0.742396	0.623915	-1862.492084	-206.45
INT-5ii	0.699254	0.742782	0.743726	0.624153	-1862.499161	—
TS-5ii	0.698997	0.741767	0.742711	0.625238	-1862.499647	-43.72
INT-6ii	0.702888	0.745818	0.746763	0.627027	-1862.654825	—

Cartesian coordinates of the optimized structures

2a

C	-2.02220200	0.15719600	0.10039900
C	-0.99847200	-0.43573200	0.36197800
C	0.22324800	-1.17598900	0.70323700
O	0.30127400	-1.44493700	2.10497400
H	-0.60312600	-1.57499500	2.41683800
H	0.21086800	-2.12618000	0.14355200
C	1.46415800	-0.40087800	0.28141900
C	2.11139100	0.44751100	1.18190800
C	1.93896400	-0.50958700	-1.02798000
C	3.22588800	1.18015300	0.77312600
H	1.74179000	0.51199300	2.19859600
C	3.04981400	0.22651500	-1.43794000
H	1.43553600	-1.17124100	-1.72841000
C	3.69667000	1.07403600	-0.53661400
H	3.72864300	1.83429100	1.47963900
H	3.41350200	0.13408900	-2.45708500
H	4.56528300	1.64429800	-0.85235200
C	-3.22524300	0.87440900	-0.21963100
C	-4.10860800	0.39582200	-1.36369400
C	-4.58324100	0.23999800	0.04919300
H	-3.16952200	1.95180500	-0.08212200
H	-3.78287200	-0.49152100	-1.89525700
H	-4.56604100	1.15829300	-1.98573500
H	-5.37108900	0.89388500	0.40894500
H	-4.58367600	-0.75454900	0.48195600

PC1

C	-0.21465000	-0.44290600	0.29859000
C	-0.60680300	0.85145900	0.02590000
C	2.12320800	0.13895800	-0.07727500
C	1.16847400	-0.79571900	0.22453900

H	1.46838400	-1.80894600	0.45597900
N	1.71454200	1.43301800	-0.27175600
H	2.39139300	2.15348800	-0.48860400
C	0.39880600	1.88582100	-0.17223800
O	0.16097200	3.09811400	-0.24645000
C	3.56658100	-0.14738800	-0.16932600
C	4.52107800	0.79632200	0.24364100
C	4.00919300	-1.38066400	-0.67363400
C	5.88228000	0.51324200	0.15249200
H	4.20110200	1.74087800	0.67406500
C	5.36974200	-1.66240300	-0.75921000
H	3.27983400	-2.10484000	-1.02088800
C	6.31137200	-0.71612800	-0.34913200
H	6.60733600	1.25017500	0.48365700
H	5.69636600	-2.61776700	-1.15815700
H	7.37204400	-0.93553800	-0.42047500
C	-1.16882600	-1.52417900	0.70771300
C	-0.88156000	-2.31743900	1.96404800
C	-2.03813200	-1.35067600	1.92310300
H	-1.61126500	-2.07304700	-0.11977000
H	-0.01035000	-2.03980700	2.55042800
H	-1.09382600	-3.38204700	1.95606100
H	-3.04742600	-1.74288600	1.87344000
H	-1.94783800	-0.41054600	2.45678800
C	-2.01527700	1.42467300	0.02206100
H	-1.98608100	2.22845600	-0.72698300
O	-2.30942900	2.01304000	1.29256900
H	-1.72565000	2.78347000	1.34830000
C	-3.12842500	0.48875900	-0.39096400
C	-4.30227400	0.38511400	0.35790400
C	-3.01756000	-0.23222100	-1.58626700
C	-5.33582900	-0.45311400	-0.06479900
H	-4.38981200	0.95952000	1.27204300
C	-4.04770600	-1.06979000	-2.00819500
H	-2.11152400	-0.14322200	-2.17996100
C	-5.21126100	-1.18799500	-1.24371100
H	-6.24140300	-0.53078400	0.53027100
H	-3.94479800	-1.62818200	-2.93426600
H	-6.01522000	-1.84107700	-1.57003200

PC2

C	-0.32606800	0.55823600	-0.19576700
C	-0.73376200	-0.68086100	-0.63272000
C	2.02019200	-0.25582300	-0.09099500

C	1.06340000	0.72042600	0.07500500
H	1.37400800	1.68893300	0.45382200
C	3.45026200	0.01167700	0.16817000
C	4.31855000	-0.99268200	0.63251400
C	3.97238600	1.30292200	-0.03032600
C	5.65216300	-0.70089400	0.91181700
H	3.93989800	-1.99778100	0.75870700
C	5.30548000	1.58995300	0.24855400
H	3.33338700	2.08286700	-0.43267000
C	6.15246600	0.58828800	0.72617900
H	6.30477500	-1.48926800	1.27545800
H	5.68605100	2.59326400	0.08087800
H	7.19407500	0.80852600	0.94023100
C	-1.26896500	1.69064000	0.06100800
C	-0.90682500	3.09087400	-0.38272600
C	-2.03400500	2.35540100	-1.05636000
H	-1.80337000	1.62240300	1.00617700
H	0.01366400	3.22182800	-0.94418000
H	-1.14358200	3.91457500	0.28308900
H	-3.05561200	2.65545800	-0.84885200
H	-1.87586000	1.97351100	-2.05753200
C	-2.14459700	-1.08574500	-1.02980700
H	-2.14977500	-2.18873400	-1.09579600
O	-2.50511000	-0.54293300	-2.29662900
H	-1.80748800	-0.76967300	-2.92440100
C	-3.19476700	-0.69746100	-0.00681100
C	-4.37824800	-0.06555800	-0.39163500
C	-2.98723600	-1.00832500	1.34161900
C	-5.33622800	0.26867000	0.56723700
H	-4.53531400	0.17042700	-1.43671700
C	-3.94449400	-0.67531200	2.29754100
H	-2.06557000	-1.49690400	1.64632000
C	-5.12263900	-0.03128300	1.91240700
H	-6.25124200	0.76645400	0.25996400
H	-3.76943700	-0.91510400	3.34195900
H	-5.86809100	0.23235800	2.65648600
N	0.21155900	-1.66249800	-0.78495500
C	1.58990400	-1.58177500	-0.53164400
O	2.27902200	-2.58888200	-0.69695100
H	-0.07453400	-2.58933300	-1.07918600

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

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	-0.21836000	-0.12677100	1.02944200
C	2.06749300	-0.53452900	0.81990800
C	2.00724900	0.64607200	0.17837000
C	0.00572000	3.09562300	1.28386800
C	0.94630000	3.53164200	0.28573300
C	0.26235500	3.58047400	-0.97190500
C	-1.13698300	3.27260400	-0.73335100
C	-1.29599300	2.97681900	0.64286900
Rh	0.19089800	1.47326800	-0.19783200
C	0.73227300	-1.09849100	1.20548700
O	0.50815600	-2.23797600	1.62335000
C	-2.57872500	2.63743600	1.33579200

H	-3.11457400	3.55320900	1.61489900
H	-3.23078000	2.04999800	0.68491500
H	-2.39097000	2.06802100	2.24675100
C	0.26558500	2.89764500	2.74462100
H	-0.12222500	3.74321700	3.32588000
H	-0.21336600	1.98079000	3.09687600
H	1.33565400	2.81339800	2.94379000
C	2.38315300	3.87441200	0.52228000
H	2.48825100	4.94053100	0.75527400
H	2.79509300	3.30459700	1.35751200
H	2.99549800	3.66611700	-0.35878800
C	0.83806400	3.99609400	-2.29034100
H	0.60216400	5.04421100	-2.51106800
H	1.92523500	3.89033600	-2.29895600
H	0.43579900	3.38579600	-3.10336900
C	-2.21758200	3.28809900	-1.76869500
H	-2.68011300	4.28105300	-1.82809700
H	-1.81585400	3.05128000	-2.75713700
H	-2.98864300	2.55311700	-1.53295300
O	-1.53211600	-0.66442500	1.19612600
C	-1.98558300	-0.65082100	2.49435300
O	-1.47861400	0.00691000	3.37070400
C	-3.15185400	-1.61906100	2.68333800
C	-3.96979200	-1.83625500	1.39998400
H	-3.37477600	-2.29449700	0.60798800
H	-4.80662800	-2.50577100	1.62300500
H	-4.38744900	-0.90017800	1.01687200
C	-2.49231600	-2.95393500	3.11024600
H	-1.97991100	-2.84048600	4.06945300
H	-3.26440900	-3.72333900	3.21396700
H	-1.75403100	-3.27270500	2.37122600
C	-4.05130500	-1.08292700	3.80693300
H	-3.46915800	-0.88303100	4.70834600
H	-4.54508200	-0.15247400	3.50708600
H	-4.82675900	-1.81850900	4.04136500
C	0.61843500	0.47219500	-2.13404000
C	-0.59040000	0.32293800	-1.84641600
C	-1.95688200	-0.21537800	-2.11798300
O	-2.89979200	0.10214100	-1.10949900
H	-2.52640800	-0.20105700	-0.26286700
H	-2.33142400	0.27424400	-3.02414200
C	-1.83321600	-1.70756100	-2.40438300
C	-1.29757700	-2.58320100	-1.44830200
C	-2.22444600	-2.21019800	-3.64767800

C	-1.16925100	-3.93974200	-1.73699900
H	-0.97488900	-2.21840000	-0.48100900
C	-2.08905700	-3.56990100	-3.93875600
H	-2.63758600	-1.53459400	-4.39261900
C	-1.56157200	-4.43723800	-2.98300200
H	-0.75152500	-4.60418100	-0.98679400
H	-2.39623100	-3.94774800	-4.90952100
H	-1.45368500	-5.49433200	-3.20687100
C	3.31549700	-1.26597500	1.12463400
C	3.39861600	-2.15133500	2.21314900
C	4.46196900	-1.07651400	0.33241400
C	4.59371300	-2.80785500	2.50235500
H	2.51623600	-2.32865300	2.81408600
C	5.65547400	-1.72988200	0.62666700
H	4.40757800	-0.42103700	-0.53071700
C	5.72782100	-2.60012700	1.71621600
H	4.63779600	-3.48672300	3.34928800
H	6.52709000	-1.56890100	-0.00178200
H	6.65585700	-3.11624700	1.94405500
H	2.89994600	1.16907900	-0.15960500
C	1.85395200	0.19838200	-2.83635900
C	2.46101900	-1.18984300	-2.70839800
C	1.79209500	-0.79508500	-3.98956600
H	2.54783800	1.02857700	-2.93164900
H	1.94488000	-1.88314200	-2.05409200
H	3.54318800	-1.25827900	-2.68080900
H	2.40722700	-0.58257900	-4.85827500
H	0.82267800	-1.23108000	-4.20887800

TS-1

N	-0.05820500	0.18206400	1.06900600
C	2.03204500	-0.71822300	0.56023000
C	1.96069200	0.08027600	-0.54296600
C	0.54245800	3.37106200	0.50461000
C	1.46179900	3.36894800	-0.57454800
C	0.71109200	3.20834600	-1.80667000
C	-0.69094000	3.19811600	-1.47652900
C	-0.80402100	3.24385600	-0.05564600
Rh	0.32300100	1.41396100	-0.55895300
C	0.72192500	-0.92221400	1.26461000
O	0.40493600	-1.93545200	1.89763700
C	-2.07503700	3.28968700	0.73411000
H	-2.43299500	4.32316100	0.82614500
H	-2.85699000	2.70289300	0.24732400

H	-1.92153900	2.89983100	1.74161400
C	0.84650300	3.48402000	1.96518000
H	0.55360600	4.47107500	2.34390500
H	0.30724000	2.72155800	2.53320600
H	1.91371500	3.35460400	2.15700500
C	2.95216700	3.47989500	-0.48231300
H	3.27778000	4.51361000	-0.64991800
H	3.31368600	3.16687800	0.49905300
H	3.44525300	2.85504400	-1.23203200
C	1.29050500	3.20489800	-3.18769500
H	1.37138200	4.22406800	-3.58628300
H	2.29265900	2.76848900	-3.19550400
H	0.66922300	2.62645300	-3.87564900
C	-1.83147100	3.14491000	-2.44561400
H	-2.20854900	4.15472000	-2.64935800
H	-1.51987200	2.71091000	-3.39893700
H	-2.64644100	2.53817600	-2.04751900
O	-1.41374000	-0.10875700	1.44571300
C	-1.75282200	0.29362900	2.70785600
O	-1.08569700	1.04843400	3.37583200
C	-3.03784700	-0.39350500	3.16883300
C	-4.01437400	-0.65717000	2.01002500
H	-3.59864200	-1.34574500	1.27246100
H	-4.92964700	-1.10485900	2.41012200
H	-4.29520900	0.26858400	1.49741600
C	-2.57702600	-1.74033600	3.77833200
H	-1.95316300	-1.57066000	4.66048000
H	-3.45366000	-2.32355200	4.07887500
H	-1.98916400	-2.31133400	3.05602700
C	-3.70394900	0.48074400	4.24028000
H	-3.00237800	0.71485400	5.04302000
H	-4.05789600	1.42540800	3.81423000
H	-4.56520700	-0.04497000	4.66394200
C	0.66452300	-0.54578300	-1.83303500
C	-0.53259000	-0.12230800	-1.62398400
C	-1.97342200	-0.40106900	-1.91461300
O	-2.83699900	0.32971400	-1.04437100
H	-2.49637300	0.19893800	-0.14323500
H	-2.21168900	-0.03687400	-2.92107700
C	-2.25058900	-1.89590800	-1.86189500
C	-1.86787600	-2.65591700	-0.74635000
C	-2.89027100	-2.52676600	-2.93153900
C	-2.12078100	-4.02561600	-0.71425900
H	-1.35890600	-2.19205500	0.09107800

C	-3.13906100	-3.90075300	-2.90033100
H	-3.18739400	-1.94083100	-3.79761500
C	-2.75272800	-4.65314600	-1.79136400
H	-1.81195800	-4.60323600	0.15170700
H	-3.63055200	-4.38040700	-3.74169100
H	-2.94033300	-5.72244400	-1.76622700
C	3.25050000	-1.37624200	1.04632900
C	3.34819500	-1.81741800	2.37987100
C	4.35642700	-1.57226200	0.19653800
C	4.51891800	-2.41019500	2.84566600
H	2.49445900	-1.70405600	3.03566300
C	5.52312100	-2.16650100	0.66572000
H	4.28796200	-1.27690900	-0.84514200
C	5.61200300	-2.58564800	1.99556200
H	4.57593000	-2.74024000	3.87874800
H	6.36188100	-2.31267800	-0.00883300
H	6.52134300	-3.05290400	2.36157700
H	2.85436400	0.31782200	-1.11406400
C	1.50279400	-1.43003000	-2.66026900
C	1.89618600	-2.78727000	-2.12357200
C	0.89497700	-2.69188400	-3.24318400
H	2.24083500	-0.91519300	-3.27204400
H	1.51887200	-3.03958400	-1.13731600
H	2.89612700	-3.15238400	-2.33470000
H	1.20545800	-2.96662000	-4.24668700
H	-0.14096800	-2.90707000	-3.01266100

INT-2

N	0.06626100	-0.22355700	1.28119600
C	-1.56233200	1.27794200	0.75606700
C	-1.38115700	1.78811000	-0.52900700
C	-0.79628300	-2.41973000	-1.69571400
C	-1.66678700	-2.62633200	-0.54778200
C	-2.80554000	-1.80721600	-0.68586600
C	-2.62414400	-1.01923500	-1.89635300
C	-1.41599500	-1.44314900	-2.54390300
Rh	-0.91306700	-0.44565800	-0.62722000
C	-0.31007300	1.03689000	1.60060500
O	0.18795700	1.87749000	2.34005700
C	-0.91284200	-0.99795800	-3.88152600
H	-1.28973200	-1.65670300	-4.67400600
H	-1.23862800	0.02007400	-4.10767900
H	0.17778300	-1.01787200	-3.89544700
C	0.33238500	-3.32757500	-2.06797700

H	-0.07947300	-4.26494000	-2.46583400
H	0.96762200	-2.87865600	-2.83033200
H	0.95220800	-3.56785100	-1.20468300
C	-1.35859100	-3.57028100	0.56952500
H	-1.56438400	-4.60513000	0.26953600
H	-0.30169400	-3.50014500	0.83691200
H	-1.95607900	-3.34859300	1.45614800
C	-4.00677900	-1.77182800	0.20321800
H	-4.77591800	-2.46179100	-0.16694500
H	-3.75751000	-2.06606500	1.22389400
H	-4.45019600	-0.77583200	0.24997500
C	-3.63514000	-0.06372600	-2.44850600
H	-4.39302400	-0.60686200	-3.02687200
H	-4.15478500	0.47062200	-1.64932800
H	-3.17190900	0.66890100	-3.11306800
O	1.34984800	-0.50315800	1.86231900
C	2.09221000	-1.46101400	1.31696900
O	1.80063000	-2.08095500	0.30279200
C	3.35250800	-1.75298000	2.13418300
C	3.61182800	-0.70647300	3.22608400
H	2.78871900	-0.65869800	3.94252600
H	4.52694200	-0.97040300	3.76647300
H	3.74141100	0.28676200	2.79235900
C	3.13210900	-3.14408600	2.76967400
H	2.93168500	-3.89449000	2.00034000
H	4.02853400	-3.44180400	3.32264600
H	2.29071500	-3.12904300	3.47068200
C	4.53825100	-1.80937400	1.15325900
H	4.34768400	-2.53116200	0.35592600
H	4.71813000	-0.83340600	0.69779900
H	5.44294800	-2.11089700	1.69089900
C	-0.03994100	2.05348000	-1.13444600
C	0.51885800	0.85622600	-1.33975700
C	1.86781200	0.54819800	-1.93834800
O	2.03229100	-0.82884800	-2.25849900
H	1.95167600	-1.31633800	-1.41742400
H	1.92239200	1.05846900	-2.91105400
C	3.05894000	1.04581900	-1.10984800
C	4.34134100	0.81695700	-1.63123900
C	2.93780000	1.70771400	0.11398400
C	5.47643700	1.25334500	-0.95321000
H	4.43719500	0.27990900	-2.56994000
C	4.07731100	2.14547000	0.79611900
H	1.96479700	1.88878400	0.54727900

C	5.34736400	1.92422500	0.26707300
H	6.46138400	1.06901000	-1.37275300
H	3.95977300	2.65975800	1.74538300
H	6.23043900	2.26652800	0.79866500
C	-2.87783800	1.16830000	1.42141000
C	-2.99822000	0.40601100	2.59575500
C	-4.02153800	1.81899300	0.92884700
C	-4.22459800	0.28199700	3.24269300
H	-2.12317700	-0.10248200	2.98590500
C	-5.25006200	1.68908600	1.57417100
H	-3.95016600	2.44903100	0.04886800
C	-5.35840200	0.91722500	2.73234900
H	-4.29549500	-0.31271600	4.14841900
H	-6.12074800	2.20349900	1.17860800
H	-6.31420900	0.82189500	3.23806400
H	-2.26117000	2.07879400	-1.09864100
C	0.48136300	3.42133700	-1.36518200
C	-0.42419400	4.62776700	-1.22705400
C	0.61829100	4.36309000	-0.17848800
H	1.27080500	3.48488800	-2.10931900
H	-1.46288800	4.45546200	-0.95910000
H	-0.27614600	5.45269400	-1.91684500
H	1.49863700	4.99705900	-0.14748100
H	0.29810600	3.97969200	0.78590900

TS-2

N	-0.15153500	0.05994200	1.29524800
C	-1.70647000	1.63810600	0.48862600
C	-1.48757700	1.92732600	-0.81910900
C	-0.52657000	-2.85251200	-1.37372300
C	-1.38683100	-2.98297400	-0.18952900
C	-2.50838700	-2.17225300	-0.38026900
C	-2.36848300	-1.51410800	-1.69383200
C	-1.19150500	-2.01187700	-2.33791200
Rh	-0.65472900	-0.85754000	-0.59761200
C	-0.49904200	1.36631400	1.37960700
O	0.00884900	2.26479100	2.05161300
C	-0.72508500	-1.72461400	-3.73025700
H	-1.04885700	-2.51370800	-4.42004800
H	-1.12868900	-0.77463900	-4.08747100
H	0.36380800	-1.65518700	-3.75198700
C	0.69516500	-3.67501300	-1.61186600
H	0.39220100	-4.69310500	-1.89075000
H	1.30068500	-3.25811700	-2.41556000

H	1.30736700	-3.73565800	-0.71078400
C	-1.01823000	-3.78566400	1.01613800
H	-1.10940000	-4.85928500	0.81252600
H	0.01846600	-3.58530600	1.29973900
H	-1.65766900	-3.54505700	1.86726300
C	-3.64127600	-1.93030200	0.56403500
H	-4.53572600	-2.47361200	0.23492700
H	-3.39595200	-2.26145100	1.57445500
H	-3.89849100	-0.87006600	0.61656300
C	-3.40005400	-0.62070000	-2.30231300
H	-4.15920900	-1.22413300	-2.81692100
H	-3.90771300	-0.02707100	-1.54002200
H	-2.95408100	0.05640800	-3.03328800
O	1.04264600	-0.16178600	2.07001800
C	1.89306100	-1.06223200	1.59999500
O	1.72512400	-1.70473800	0.56586600
C	3.09185700	-1.28096400	2.52285800
C	3.26214500	-0.14043400	3.53634000
H	2.39212600	-0.04862100	4.18972200
H	4.14323600	-0.33857800	4.15520300
H	3.40352800	0.81475500	3.02690800
C	2.83018400	-2.61461600	3.25824800
H	2.70363800	-3.43425600	2.54496600
H	3.67969600	-2.84970700	3.90700700
H	1.93283500	-2.55138500	3.88256800
C	4.34687700	-1.40640100	1.64016400
H	4.23211000	-2.21141500	0.91104200
H	4.54147900	-0.47849600	1.09814100
H	5.21426600	-1.62613000	2.27066500
C	-0.16097200	1.84003700	-1.48050100
C	0.44926400	0.63790700	-1.47744200
C	1.84960900	0.40799200	-2.00483900
O	2.14306800	-0.98124000	-2.19400500
H	2.12974500	-1.36775300	-1.30105900
H	1.91782100	0.83258000	-3.01626000
C	2.96361000	1.04671000	-1.16567900
C	4.28699700	0.84576000	-1.58613600
C	2.73355600	1.79911100	-0.01165400
C	5.35364400	1.39484900	-0.87846300
H	4.47081200	0.24180300	-2.46940800
C	3.80280100	2.34878800	0.70147500
H	1.72813600	1.96779900	0.34306500
C	5.11422700	2.15294800	0.27199400
H	6.37142700	1.23087800	-1.22124800

H	3.59601800	2.93219800	1.59377600
H	5.94356800	2.58290500	0.82614700
C	-3.03387700	1.62238500	1.13380700
C	-3.14446200	1.29260100	2.49685000
C	-4.22205900	1.87372700	0.42065500
C	-4.38974400	1.20099800	3.11491400
H	-2.24465600	1.11034500	3.07298300
C	-5.46562800	1.78215300	1.03936500
H	-4.17800400	2.14563100	-0.62833500
C	-5.55805200	1.43842100	2.39023300
H	-4.44554400	0.94285400	4.16824700
H	-6.36580700	1.97966100	0.46461600
H	-6.52838600	1.36293200	2.87120200
H	-2.32322800	2.25531100	-1.43569400
C	0.43045100	3.09998500	-2.02154400
C	-0.37668900	4.37613300	-2.15020400
C	0.66353600	4.26340500	-1.07155600
H	1.20451700	2.95543900	-2.77005900
H	-1.41869700	4.36422600	-1.84691700
H	-0.17266900	5.01149400	-3.00665500
H	1.59110100	4.81719200	-1.17349300
H	0.32427000	4.12584400	-0.04877700

INT-3

N	-0.44370100	0.06397500	1.25322600
C	-2.09989200	1.44722700	0.24687300
C	-1.80862500	1.61875700	-1.05936700
C	-0.65687900	-3.39792500	-0.07518600
C	-1.84400500	-2.64532500	-0.10945900
C	-1.89390900	-1.92157100	-1.37759500
C	-0.74460900	-2.31493900	-2.15799100
C	0.05284300	-3.15749600	-1.33311300
Rh	-0.11434700	-1.17139100	-0.38067300
C	-0.94323300	1.33154600	1.21427600
O	-0.56988900	2.29476400	1.88169500
C	1.35615100	-3.79141500	-1.70471300
H	1.19280100	-4.81115200	-2.07479500
H	1.86359800	-3.21657200	-2.48007600
H	2.02089200	-3.85895000	-0.83863400
C	-0.14485800	-4.26497900	1.03330200
H	-0.21439600	-5.32777300	0.77126300
H	0.90684600	-4.05028100	1.24820300
H	-0.71120400	-4.11086700	1.95431100
C	-2.87535700	-2.50759400	0.96477000

H	-3.79692600	-3.03038900	0.68277900
H	-2.52649300	-2.92096300	1.91285100
H	-3.12585700	-1.45632000	1.13009600
C	-3.08793800	-1.18871700	-1.89685800
H	-3.75028700	-1.88129100	-2.43297800
H	-3.66057200	-0.73479900	-1.08796500
H	-2.79393100	-0.39950000	-2.59029900
C	-0.45325700	-1.90664400	-3.56761800
H	-0.85925200	-2.64037300	-4.27494400
H	-0.90277200	-0.93598100	-3.78596200
H	0.62236000	-1.81565000	-3.72786600
O	0.73300200	0.08264500	2.15347300
C	1.77534200	-0.56069800	1.71062100
O	1.79706200	-1.15493300	0.61154300
C	2.94875900	-0.62843000	2.67681700
C	2.95787200	0.58215200	3.62376400
H	2.03917300	0.64170500	4.21029900
H	3.80599100	0.49276300	4.30952900
H	3.06432800	1.51169700	3.06106900
C	2.75913100	-1.93539300	3.48364400
H	2.74339800	-2.80708200	2.82245900
H	3.59165100	-2.05116700	4.18412800
H	1.82812100	-1.91302500	4.05787600
C	4.25415300	-0.68917600	1.86684700
H	4.26504800	-1.55348700	1.19904100
H	4.38703200	0.21205900	1.26505800
H	5.09955000	-0.77300800	2.55634900
C	-0.46104900	1.55027500	-1.65066200
C	0.38860700	0.51460600	-1.43425100
C	1.81389600	0.56169000	-1.96359000
O	2.38315500	-0.73876900	-2.18403200
H	2.50381600	-1.12341700	-1.30324100
H	1.80947400	1.00128700	-2.96799500
C	2.76772500	1.39975700	-1.10349900
C	2.33775800	2.19459900	-0.03721000
C	4.13608900	1.36648100	-1.40887800
C	3.25427100	2.94548100	0.70360100
H	1.29052600	2.23623000	0.22576700
C	5.05150700	2.11618300	-0.67215600
H	4.47552600	0.73640400	-2.22469500
C	4.61278900	2.91166300	0.39028600
H	2.89321400	3.55774000	1.52473100
H	6.10735800	2.07915000	-0.92533500
H	5.32380300	3.49726200	0.96573600

C	-3.45756500	1.47389200	0.82374400
C	-3.63528500	1.45670900	2.22002500
C	-4.61198300	1.47907800	0.01661400
C	-4.91010500	1.44073400	2.78183700
H	-2.76485500	1.48059900	2.86538600
C	-5.88435600	1.46762900	0.58009200
H	-4.51687000	1.48716300	-1.06364300
C	-6.04276600	1.44422600	1.96748700
H	-5.01660800	1.43036700	3.86261900
H	-6.75623200	1.47172200	-0.06776000
H	-7.03589800	1.42995200	2.40593300
H	-2.61096700	1.89760300	-1.73843300
C	-0.05936500	2.75756300	-2.45427700
C	-0.98627800	3.92608200	-2.72076700
C	0.14533000	4.08550700	-1.74485200
H	0.65127900	2.56428800	-3.25230000
H	-1.99279500	3.90692100	-2.31810300
H	-0.90728500	4.40684200	-3.69119400
H	1.00727500	4.68533300	-2.01857400
H	-0.11042700	4.11086300	-0.68977100

TS-3

N	1.00123100	0.09496600	1.08981000
C	2.22814000	-1.36981400	0.57875500
C	1.84564200	-1.94756700	-0.60629600
C	0.56107300	3.27618000	-0.63932300
C	1.80846000	2.62445200	-0.61674400
C	1.84597300	1.67967900	-1.72820200
C	0.63019300	1.84153000	-2.49142500
C	-0.18738500	2.77143500	-1.79226100
Rh	0.18987600	1.00226200	-0.47278500
C	1.05424500	-1.08661300	1.60849900
O	0.66027800	-1.81894900	2.48894600
C	-1.54527400	3.25814500	-2.18277500
H	-1.48356400	4.28166900	-2.57242800
H	-1.99260200	2.61828500	-2.94287800
H	-2.21122700	3.27132400	-1.31499300
C	0.02770400	4.28996700	0.32320100
H	-0.05596600	5.27540900	-0.15066700
H	-0.96840500	4.00356400	0.67170200
H	0.67108200	4.38848300	1.19919800
C	2.89455800	2.76355500	0.40249100
H	3.78376800	3.22588700	-0.04118400
H	2.57340900	3.37851000	1.24467100

H	3.18302000	1.78584100	0.79874300
C	3.03191400	0.86296400	-2.13014700
H	3.58163500	1.34741700	-2.94680300
H	3.71718200	0.73195100	-1.29191400
H	2.73033600	-0.13047400	-2.47364000
C	0.30153800	1.14614700	-3.77496000
H	0.60799000	1.75545800	-4.63383800
H	0.82337300	0.18832700	-3.83832300
H	-0.77009800	0.95224000	-3.83999500
O	-0.94424000	0.82213100	2.44926400
C	-1.85643400	1.08738400	1.66520200
O	-1.71980600	1.19730300	0.37118700
C	-3.27907500	1.39823600	2.18813100
C	-3.51677200	0.62055500	3.49077500
H	-2.73755800	0.83966800	4.22257700
H	-4.49132900	0.88955200	3.91239300
H	-3.51092900	-0.45634200	3.30245300
C	-3.31136200	2.91547400	2.46978800
H	-3.15680000	3.48783400	1.54886100
H	-4.28506600	3.19950700	2.88331900
H	-2.53652300	3.19610000	3.18955800
C	-4.35624200	1.03790400	1.15420800
H	-4.24034400	1.62043600	0.23705200
H	-4.31849000	-0.02177200	0.89251200
H	-5.34753300	1.25175400	1.56899900
C	0.55357100	-1.90644800	-1.23380600
C	-0.31331600	-0.83805000	-1.16523500
C	-1.72735000	-1.01012900	-1.69286600
O	-2.35964300	0.21142100	-2.06619500
H	-2.45862900	0.70829900	-1.23162400
H	-1.68748800	-1.58925500	-2.62311300
C	-2.62076800	-1.77771200	-0.71467200
C	-2.27152000	-2.01215100	0.61806400
C	-3.87264100	-2.20757300	-1.17109300
C	-3.15189200	-2.67384200	1.47627800
H	-1.31821100	-1.68131000	1.00489700
C	-4.75594300	-2.86335600	-0.31540500
H	-4.15590000	-2.01193100	-2.20137800
C	-4.39686200	-3.10048900	1.01401000
H	-2.85601900	-2.84736300	2.50624200
H	-5.72335700	-3.19077700	-0.68527500
H	-5.08323700	-3.61204100	1.68218600
C	3.60277600	-1.22398900	1.07086700
C	3.85660500	-0.96711000	2.43085200

C	4.69809800	-1.32021700	0.19175500
C	5.16096900	-0.80902300	2.89003700
H	3.02810000	-0.90886500	3.12769100
C	6.00198400	-1.17715500	0.65900400
H	4.52497200	-1.49899400	-0.86403100
C	6.23944900	-0.91480100	2.00922700
H	5.33591700	-0.61077200	3.94299800
H	6.83272300	-1.25796400	-0.03566200
H	7.25551200	-0.79276300	2.37149500
H	2.58246300	-2.59526400	-1.07849400
C	0.19463000	-3.11585900	-2.06804300
C	0.80856800	-4.47916600	-1.83686500
C	-0.63500700	-4.24439800	-1.49005800
H	-0.02094500	-2.88858200	-3.11111700
H	1.50096300	-4.60472900	-1.01054300
H	1.04781100	-5.07811100	-2.71013100
H	-1.41087100	-4.67596000	-2.11427600
H	-0.89439400	-4.17490400	-0.44000000

INT-4

N	1.12790100	0.24117100	-1.05226100
C	2.01741900	1.31630100	-0.66257500
C	1.50744100	2.24113400	0.18024300
C	0.87877900	-2.84714900	1.44708100
C	2.03355400	-2.06538000	1.29777300
C	1.89199900	-0.85731500	2.11426300
C	0.64712500	-0.95711700	2.82239400
C	-0.02490500	-2.13599300	2.34991200
Rh	0.24394800	-0.74094500	0.69019000
C	0.53167500	0.16657400	-2.12999700
O	-0.05183200	0.06894400	-3.13449900
C	-1.33284500	-2.66566900	2.84273100
H	-1.16823200	-3.35026200	3.68473800
H	-1.98644200	-1.85417200	3.16116200
H	-1.85096100	-3.22225800	2.05848900
C	0.59482700	-4.16871500	0.80647400
H	0.99061100	-4.98769100	1.42038000
H	-0.47943300	-4.32835800	0.69692300
H	1.03242200	-4.22949000	-0.19031600
C	3.20454100	-2.37095900	0.42051800
H	4.00488000	-2.84601700	1.00150400
H	2.92129700	-3.04897100	-0.38690800
H	3.61569500	-1.46428500	-0.02821000
C	2.96196200	0.15947400	2.36112100

H	3.56986000	-0.12343300	3.22996300
H	3.62863200	0.25675100	1.50254900
H	2.52729500	1.14208500	2.55720500
C	0.14472900	-0.01867100	3.87296500
H	0.48692600	-0.34033700	4.86437200
H	0.51008800	0.99546400	3.69881000
H	-0.94586100	0.00749900	3.87429100
O	-0.19088800	-2.55258000	-1.75106200
C	-1.29805800	-2.19553300	-1.33988900
O	-1.47399400	-1.27281800	-0.42839600
C	-2.60691900	-2.79987000	-1.88546900
C	-3.43606500	-1.67183000	-2.52952700
H	-2.87393800	-1.18496500	-3.33364200
H	-4.35620900	-2.08169000	-2.96014100
H	-3.70568500	-0.91117600	-1.79462500
C	-2.28282000	-3.87833500	-2.92601000
H	-1.68055900	-4.67916500	-2.48869600
H	-3.20993800	-4.31238100	-3.31624200
H	-1.71486400	-3.45853000	-3.75961600
C	-3.39474200	-3.41449600	-0.71279300
H	-2.82103400	-4.21293100	-0.22771100
H	-3.63685900	-2.65879100	0.03802100
H	-4.33084300	-3.85264100	-1.07526000
C	0.15667500	2.25882300	0.72579300
C	-0.57047700	1.12128500	0.93342200
C	-2.02077700	1.21784400	1.39751500
O	-2.58760600	-0.04172600	1.75197400
H	-2.45168600	-0.62380700	0.97914000
H	-2.05894200	1.80558800	2.32470800
C	-2.90520600	1.92135700	0.37363600
C	-3.85866400	2.85308400	0.79217900
C	-2.80772500	1.62166000	-0.99003800
C	-4.69142700	3.48712700	-0.13081200
H	-3.94064300	3.09138900	1.84979700
C	-3.64099000	2.24853700	-1.91517600
H	-2.08453900	0.88704700	-1.32010900
C	-4.58231400	3.18834100	-1.48978800
H	-5.42319600	4.21398800	0.21036200
H	-3.55320200	2.00189900	-2.96941400
H	-5.22725100	3.68166500	-2.21102800
C	3.39416600	1.22805600	-1.16197300
C	3.76200500	0.25713500	-2.11247100
C	4.39719000	2.10059800	-0.69079000
C	5.07075200	0.17599600	-2.58595800

H	3.02662600	-0.45235800	-2.47225200
C	5.69954900	2.01697600	-1.16789400
H	4.15887900	2.84261600	0.06280200
C	6.04701200	1.05508400	-2.12102900
H	5.32433600	-0.58353200	-3.31922600
H	6.45125400	2.70222400	-0.78768000
H	7.06638400	0.98949000	-2.48778800
H	2.15703600	3.06286300	0.45821500
C	-0.41291100	3.61271800	1.06287400
C	0.25773800	4.92065100	0.69339800
C	-0.99832400	4.50107100	-0.01610100
H	-0.96008400	3.64274000	2.00265000
H	1.18331700	4.90170400	0.12758200
H	0.20249700	5.73028500	1.41480800
H	-1.93203800	5.01045300	0.19447700
H	-0.90779100	4.14450300	-1.03699300

TS-4

N	-0.87997900	-0.62117400	-1.31977200
C	-1.04069900	-1.97169700	-0.92352100
C	-0.05566400	-2.60334500	-0.23075100
C	-1.86166300	1.70385600	2.07500800
C	-2.63115700	0.58370100	1.68468200
C	-1.91875600	-0.61765600	2.10927800
C	-0.71761300	-0.21328400	2.76330500
C	-0.63349400	1.22609800	2.69562000
Rh	-0.61286200	0.48363500	0.66544800
C	0.32326800	-0.16439400	-1.53718000
O	0.99937300	0.46274100	-2.27508600
C	0.42414300	2.08212800	3.31602600
H	0.23102900	2.21947600	4.38783700
H	1.41467000	1.64539500	3.18426200
H	0.44970200	3.06650000	2.84614200
C	-2.21653300	3.14064700	1.87605500
H	-2.71217500	3.52934700	2.77433600
H	-1.32270800	3.74190500	1.70101200
H	-2.87966100	3.26782500	1.02112600
C	-3.93322300	0.62048700	0.95055200
H	-4.76797400	0.78665700	1.64278000
H	-3.92288400	1.42205200	0.20899800
H	-4.11543700	-0.31818500	0.42321000
C	-2.45231300	-2.01114700	2.05367200
H	-2.99978500	-2.23470300	2.97792700
H	-3.13577900	-2.15118500	1.21625200

H	-1.64718200	-2.74087900	1.95207600
C	0.25972900	-1.11819500	3.44249500
H	-0.07005900	-1.32216900	4.46866500
H	0.35067000	-2.07157700	2.91938300
H	1.24945300	-0.66123700	3.49528800
O	-2.02112400	2.47455800	-1.23458500
C	-0.85235600	2.83073400	-1.09121900
O	0.02487600	2.19977500	-0.34723000
C	-0.28456500	4.10305000	-1.75518300
C	0.95574800	3.73304200	-2.58998700
H	0.70424500	3.00328100	-3.36484900
H	1.35502700	4.62908200	-3.07790100
H	1.73882100	3.29960900	-1.96464000
C	-1.35705300	4.73476300	-2.65035000
H	-2.25102300	4.98737200	-2.07466200
H	-0.96763200	5.64857500	-3.11228300
H	-1.65987500	4.04604600	-3.44313700
C	0.12088700	5.08748900	-0.63971100
H	-0.74437600	5.37022000	-0.02958400
H	0.87771100	4.64662700	0.01413600
H	0.53275900	6.00309400	-1.07756500
C	1.16836000	-1.93562900	0.18036100
C	1.23662400	-0.55316300	0.28311400
C	2.50719500	0.16096900	0.74859200
O	2.38601800	1.57525600	0.78067200
H	1.65873900	1.86862900	0.19912500
H	2.63865500	-0.14838000	1.80048700
C	3.80635500	-0.21917000	0.04151500
C	4.89611700	-0.65213600	0.80328700
C	3.95902700	-0.10586800	-1.34454700
C	6.10544700	-0.99877800	0.19971400
H	4.79317600	-0.72556500	1.88375100
C	5.16633400	-0.44922200	-1.95182500
H	3.13177800	0.24647300	-1.94657500
C	6.24193900	-0.90348800	-1.18562000
H	6.93856500	-1.33639800	0.80972100
H	5.26702000	-0.36250700	-3.03004000
H	7.17941400	-1.17317200	-1.66304300
C	-2.33207700	-2.55430600	-1.31253800
C	-3.32526400	-1.72423900	-1.86495400
C	-2.62789400	-3.91610000	-1.11500200
C	-4.57629600	-2.24089200	-2.19729200
H	-3.09842700	-0.67547800	-2.01788600
C	-3.87737700	-4.42587900	-1.44864700

H	-1.87709100	-4.58313100	-0.70528300
C	-4.86032900	-3.59056400	-1.98899100
H	-5.33058200	-1.58353400	-2.61919400
H	-4.08587000	-5.47991600	-1.29161200
H	-5.83547800	-3.99212600	-2.24690500
H	-0.16995500	-3.64860700	0.01889100
C	2.34778400	-2.79176200	0.50430400
C	2.39580400	-4.29180400	0.29744300
C	3.17993500	-3.39656700	-0.61451600
H	2.94059500	-2.42922800	1.33722200
H	1.53207200	-4.80008500	-0.11745200
H	2.93129200	-4.86901200	1.04494600
H	4.25787000	-3.32762600	-0.51880100
H	2.80398600	-3.25355500	-1.62219700

INT-5

N	-0.13346200	-0.70744900	0.48152000
C	-0.11708100	-1.95889500	-0.05915200
C	0.99906900	-2.76330000	0.03839000
C	-3.09868400	2.32298300	0.58367100
C	-3.73945000	1.10112500	0.18891800
C	-3.39868400	0.06948700	1.14098500
C	-2.53836900	0.66438500	2.13977200
C	-2.35084800	2.04465100	1.79754100
Rh	-1.58582600	0.81371300	0.20046000
C	0.92906600	-0.27390900	1.25716900
O	0.81115700	0.80350900	1.91313800
C	-1.47299200	2.99764900	2.53992500
H	-1.90339100	3.22434000	3.52226300
H	-0.48827500	2.54327800	2.67601400
H	-1.35005500	3.93278200	1.99189400
C	-3.17940100	3.64876500	-0.10561200
H	-3.89716400	4.30827300	0.39658400
H	-2.20566200	4.14368600	-0.10738900
H	-3.49691000	3.53444600	-1.14404600
C	-4.57571900	0.89470000	-1.03214800
H	-5.63492300	1.05873000	-0.80034000
H	-4.28738300	1.58422300	-1.82767200
H	-4.46106200	-0.12334100	-1.40939200
C	-3.95487000	-1.31621900	1.17248800
H	-4.89304600	-1.32740300	1.74203200
H	-4.15880600	-1.69538800	0.17079800
H	-3.26241500	-2.00966000	1.64910400
C	-1.94601000	-0.02313700	3.32689300

H	-2.54475200	0.18038000	4.22291600
H	-1.91493900	-1.10348800	3.17586800
H	-0.92441300	0.32371700	3.48737600
O	-1.07948500	0.79753300	-1.93151900
C	-0.05137200	1.52776700	-1.70960500
O	0.05984400	2.03451400	-0.55134400
C	1.05648100	1.66349600	-2.73864800
C	2.07100500	0.54622200	-2.38996600
H	1.60482600	-0.44186300	-2.45548700
H	2.91045200	0.58215600	-3.09081400
H	2.46564600	0.67645100	-1.38155700
C	0.50400200	1.45675100	-4.15596800
H	-0.23351400	2.22466700	-4.41165200
H	1.32128600	1.51580200	-4.88188900
H	0.02349500	0.48059100	-4.25327500
C	1.72926900	3.03805000	-2.60372400
H	1.02955800	3.84569400	-2.84480000
H	2.09918000	3.18711500	-1.58882700
H	2.57695700	3.10333400	-3.29325900
C	2.17328200	-2.30613300	0.68751800
C	2.14299300	-1.06343900	1.29720800
C	3.34825400	-0.40459200	1.97178600
O	3.00933400	0.22647000	3.18765000
H	2.15121900	0.66300700	2.98861900
H	4.08357200	-1.17226300	2.22813800
C	4.01110300	0.53995100	0.96381800
C	4.85450000	0.02746300	-0.02975000
C	3.75779000	1.91401200	0.99155500
C	5.43293600	0.86922900	-0.97894600
H	5.05245800	-1.03992800	-0.06637600
C	4.33326800	2.75764100	0.04014300
H	3.10820100	2.31204200	1.76068200
C	5.17121800	2.24020700	-0.94895900
H	6.08780400	0.45543400	-1.74086000
H	4.12714900	3.82388900	0.07322400
H	5.61873200	2.89921900	-1.68730400
C	-1.35011700	-2.54518300	-0.66049900
C	-2.00849800	-2.00647200	-1.77421600
C	-1.84644900	-3.73213800	-0.09618900
C	-3.14586900	-2.62991100	-2.29061500
H	-1.62360100	-1.10890000	-2.23762300
C	-2.98415500	-4.35238400	-0.61209200
H	-1.33606600	-4.15753500	0.76249800
C	-3.64331000	-3.79898800	-1.71064700

H	-3.63642800	-2.20434800	-3.16181800
H	-3.35573500	-5.26418000	-0.15378200
H	-4.52853500	-4.27935400	-2.11690300
H	0.95715800	-3.74678400	-0.41081600
C	3.39202600	-3.16452300	0.67436000
C	3.31988000	-4.66304900	0.46699700
C	3.85894900	-3.79336200	-0.62987900
H	4.18857500	-2.84352500	1.33330900
H	2.34476300	-5.12016400	0.33633300
H	4.01897800	-5.26949400	1.03417500
H	4.92478600	-3.80794600	-0.83607700
H	3.23259800	-3.62223400	-1.49974100

TS-5

N	0.18037300	0.54316100	1.04284400
C	0.38006300	1.91436900	0.96899200
C	1.51935000	2.42606600	0.40375000
C	-2.85472800	-0.03450000	-2.22286400
C	-2.41751000	1.34750400	-2.05937200
C	-1.03525600	1.40838500	-2.36999700
C	-0.57201300	0.06110500	-2.67328000
C	-1.71503400	-0.80510600	-2.65155700
Rh	-1.41034900	-0.03255400	-0.65383900
C	1.28089300	-0.29596300	0.78184500
O	1.32556900	-1.42704400	1.29187800
C	-1.70886300	-2.26126200	-2.97834300
H	-1.87333900	-2.39573400	-4.05464800
H	-0.74978000	-2.71213300	-2.71812500
H	-2.49617600	-2.78370900	-2.43438800
C	-4.25322300	-0.53255400	-2.06666200
H	-4.74291000	-0.59724300	-3.04633400
H	-4.24917300	-1.51281800	-1.58794800
H	-4.83393100	0.14246900	-1.43574700
C	-3.31105300	2.46651700	-1.63078700
H	-4.01865000	2.72246900	-2.42783600
H	-3.88322700	2.17059300	-0.74756200
H	-2.74103200	3.35753600	-1.36714700
C	-0.18419900	2.62672100	-2.46940000
H	0.24347400	2.69108400	-3.47601000
H	-0.76215000	3.53314200	-2.28599200
H	0.64485600	2.59417000	-1.75925200
C	0.80368900	-0.31995200	-3.11916600
H	0.80619000	-0.53302200	-4.19546700
H	1.50992900	0.49018300	-2.93166100

H	1.16746700	-1.20386300	-2.58742600
O	-3.18712200	-2.65089700	0.03737000
C	-1.98131200	-2.80859000	0.25453600
O	-1.05056200	-1.91989500	0.04980700
C	-1.42119000	-4.13174300	0.82282900
C	-0.84600000	-3.84518400	2.22425500
H	-1.62411800	-3.46515700	2.89466100
H	-0.44915900	-4.77079100	2.65717600
H	-0.05069500	-3.10103700	2.17001100
C	-2.54589800	-5.17013600	0.90968300
H	-2.97595900	-5.37446700	-0.07510100
H	-2.15456100	-6.10809600	1.31881400
H	-3.35479800	-4.81909400	1.55491900
C	-0.30045300	-4.64012800	-0.10266300
H	-0.68439700	-4.85543100	-1.10677500
H	0.49566800	-3.89993000	-0.19162800
H	0.12576000	-5.56700000	0.29635800
C	2.49213400	1.56764700	-0.20429400
C	2.33216200	0.20617400	-0.09107100
C	3.26799700	-0.82081200	-0.72344500
O	2.60521000	-2.05893800	-0.95281400
H	2.13988100	-2.25697100	-0.11419100
H	3.53377200	-0.45858500	-1.72257300
C	4.56599500	-0.99454700	0.05566600
C	5.79458400	-0.85390900	-0.59587400
C	4.55387100	-1.30429300	1.42232000
C	6.99543500	-1.01032000	0.09882200
H	5.81123300	-0.62617700	-1.65953100
C	5.75122700	-1.46641700	2.11606300
H	3.60211800	-1.42559600	1.92893500
C	6.97549700	-1.31620600	1.45896500
H	7.94187100	-0.89710900	-0.42222000
H	5.73027400	-1.70867400	3.17473600
H	7.90663700	-1.43921800	2.00431800
C	-0.65867100	2.81679300	1.52189600
C	-1.26166900	2.56982700	2.76412400
C	-1.02016600	3.97925800	0.82283700
C	-2.22317000	3.44136700	3.27106800
H	-0.97516000	1.69674200	3.33600300
C	-1.98038200	4.85178000	1.33082000
H	-0.54995900	4.19092100	-0.13043800
C	-2.59315700	4.58101300	2.55482300
H	-2.67780900	3.23307200	4.23493200
H	-2.25159400	5.74109300	0.76933000

H	-3.34460700	5.25679100	2.95156400
H	1.66865600	3.49839700	0.42183500
C	3.65536200	2.15878400	-0.91608500
C	3.55024600	3.48477600	-1.65189600
C	4.33864000	3.40451200	-0.38058400
H	4.33184000	1.43853100	-1.35633700
H	2.59560000	4.00054200	-1.62969000
H	4.08406600	3.57550600	-2.59259700
H	5.42190900	3.43257900	-0.43364800
H	3.92256900	3.85719300	0.51365200
O	-1.53771700	-0.45139800	2.57954100
C	-2.67941100	-0.24141900	2.04396300
O	-2.83778600	0.26154700	0.89523000
C	-3.90479900	-0.65170300	2.80977400
H	-4.22353800	-1.61381700	2.39438300
H	-3.68732500	-0.76383100	3.87212300
H	-4.70910800	0.06826900	2.64739700
H	-0.69217700	-0.01311100	1.88573000

INT-ii

N	-0.50707300	-0.94984400	1.21180700
C	-2.31356300	0.36284300	0.50913800
C	-1.82257100	0.02698500	-0.69612800
C	-0.01387800	-3.44451700	-0.75459000
C	-1.30432400	-2.99661000	-1.23977800
C	-1.08979000	-2.31519300	-2.49681100
C	0.31708900	-2.25274000	-2.71820300
C	0.98054000	-2.98949700	-1.65496900
Rh	-0.17980600	-1.15885900	-0.79483300
C	-1.49898600	-0.11551000	1.67571100
O	-1.67081900	0.18178800	2.85654500
C	2.44982200	-3.27115300	-1.59434000
H	2.70034900	-4.14353900	-2.21062000
H	3.03448500	-2.42541400	-1.96135800
H	2.77702600	-3.48212500	-0.57371500
C	0.18498500	-4.21544500	0.51299600
H	-0.20815500	-5.23396000	0.41292600
H	1.24162600	-4.28506600	0.77836800
H	-0.33617200	-3.72631200	1.33990300
C	-2.61525200	-3.32125300	-0.59401700
H	-2.89481600	-4.36717100	-0.76922200
H	-2.55552600	-3.15848600	0.48512400
H	-3.41503700	-2.68567000	-0.97748800
C	-2.14937200	-1.76882900	-3.40055200

H	-2.40035700	-2.49308000	-4.18428200
H	-3.06447500	-1.54617100	-2.84763000
H	-1.81880400	-0.84569600	-3.88347300
C	1.01189200	-1.62510500	-3.88564000
H	1.27895400	-2.37533500	-4.63958700
H	0.37773700	-0.87464000	-4.36162500
H	1.93573600	-1.13472100	-3.56463900
O	0.48426600	-1.23577500	2.18080100
C	1.12979100	-0.14390800	2.70869200
O	1.08189200	0.96831300	2.24319400
C	1.88857300	-0.55154300	3.97083400
C	2.72192300	0.64463600	4.44759400
H	2.08394700	1.50828800	4.64672400
H	3.25584000	0.38148500	5.36616800
H	3.45553700	0.94238600	3.69314500
C	0.83561900	-0.92766900	5.03662600
H	0.26015900	-1.80094300	4.72312800
H	1.33632200	-1.15249300	5.98447900
H	0.13175100	-0.10667700	5.19313900
C	2.80113600	-1.75907400	3.68236300
H	2.22354500	-2.61781400	3.33347400
H	3.55310300	-1.51488400	2.92405300
H	3.33067600	-2.04711200	4.59632600
C	1.61768000	0.04138900	-0.58135400
C	0.78631800	0.74290800	-1.20038200
C	0.27274800	1.96946900	-1.84844200
O	0.09235700	1.77351300	-3.25378800
H	0.92998200	1.42921200	-3.59416400
H	-0.73180800	2.17575600	-1.46736100
C	1.17839100	3.14882600	-1.50551600
C	1.66487100	3.99561500	-2.50177200
C	1.50023900	3.39699700	-0.16327300
C	2.48564500	5.07560400	-2.16612400
H	1.38596600	3.81537900	-3.53419600
C	2.31251500	4.48054100	0.16683000
H	1.12874200	2.73656700	0.61502000
C	2.81287600	5.31944200	-0.83321500
H	2.86296500	5.72804400	-2.94831100
H	2.55624000	4.66735100	1.20853600
H	3.44881400	6.16017300	-0.57230500
C	-3.53572300	1.16747600	0.72216000
C	-4.33177700	0.99142800	1.86679500
C	-3.94182800	2.11433400	-0.23392900
C	-5.50525800	1.72501900	2.03214800

H	-4.00921200	0.29238400	2.62746400
C	-5.11637300	2.84324800	-0.06761400
H	-3.32101800	2.28988500	-1.10758200
C	-5.90675800	2.64960600	1.06702500
H	-6.10818200	1.57406900	2.92316500
H	-5.40806200	3.57259800	-0.81805900
H	-6.81985200	3.22202700	1.20195200
H	-2.29639700	0.32549700	-1.62937400
C	2.87254500	-0.34998700	0.02671900
C	4.17254600	-0.05942700	-0.71377200
C	3.82793800	0.72204200	0.51697000
H	2.84031500	-1.26660200	0.60439900
H	4.08776600	0.44487400	-1.67110600
H	4.95274700	-0.81265100	-0.66023900
H	4.36552100	0.50874200	1.43503300
H	3.50985400	1.75100500	0.40156900

TS-1i

N	0.85799000	-0.79082100	1.15197100
C	-1.24083900	-1.70142600	0.72695100
C	-0.98312800	-1.28333500	-0.54469000
C	3.10293300	-1.19693500	-1.14377900
C	2.27906000	-2.37135300	-1.39563800
C	1.47939500	-2.09504500	-2.54038000
C	1.78014200	-0.75409400	-2.99187000
C	2.82467800	-0.22554600	-2.15165300
Rh	0.96964200	-0.62993500	-0.90981000
C	-0.28861300	-1.21106700	1.77403800
O	-0.49114800	-1.19882600	2.98923700
C	3.49800500	1.10148900	-2.31924700
H	4.31855500	1.03393800	-3.04400300
H	2.79963300	1.86254500	-2.67505400
H	3.91893700	1.45443200	-1.37496800
C	4.11771100	-1.09351100	-0.04835100
H	5.03118800	-1.63703200	-0.31974900
H	4.38789600	-0.05462400	0.14963100
H	3.72973600	-1.51490800	0.88057100
C	2.30099600	-3.62312600	-0.57535400
H	3.19967900	-4.21774600	-0.77969600
H	2.28652500	-3.38245200	0.49110000
H	1.42976400	-4.24736500	-0.78414000
C	0.47547000	-3.00825000	-3.17242400
H	0.93066300	-3.58307200	-3.98769300
H	0.06952700	-3.71657000	-2.44693000

H	-0.36033100	-2.44300400	-3.59301800
C	1.20404300	-0.08920600	-4.20434800
H	1.71913300	-0.41565200	-5.11633100
H	0.14111100	-0.31509900	-4.31563700
H	1.31128900	0.99730600	-4.14085200
O	1.74610400	-0.09655200	2.00563800
C	1.25350900	1.04565900	2.58396000
O	0.19278900	1.54940000	2.30870000
C	2.24904000	1.56885100	3.61967300
C	1.73053400	2.90860500	4.15697700
H	0.74237800	2.79205600	4.60724300
H	2.41957200	3.29651700	4.91403100
H	1.64343900	3.64742600	3.35509600
C	2.33669700	0.53087100	4.75823600
H	2.73357300	-0.41777200	4.39069200
H	2.99230200	0.90562000	5.55161700
H	1.34782200	0.33700100	5.18233700
C	3.63105200	1.75710500	2.96363000
H	4.02266800	0.80976100	2.58764300
H	3.57673600	2.46467100	2.12823200
H	4.33809700	2.15848700	3.69708500
C	0.17805200	1.24971200	-0.61944000
C	-0.89922800	0.60479400	-0.92442300
C	-2.15559500	0.87802600	-1.70497600
O	-1.88400000	0.97377100	-3.10491500
H	-1.10011000	1.53344400	-3.19490500
H	-2.85580800	0.04305800	-1.62207900
C	-2.82102700	2.12073500	-1.12300400
C	-3.19404300	3.18834700	-1.94022600
C	-3.06966800	2.18231800	0.25519700
C	-3.79491800	4.32053900	-1.38415400
H	-3.02006800	3.12197600	-3.00859400
C	-3.68014900	3.30725300	0.80503500
H	-2.75793700	1.36349100	0.89636000
C	-4.03804500	4.38310000	-0.01275500
H	-4.07558400	5.15065900	-2.02579500
H	-3.86265100	3.34905600	1.87435200
H	-4.50503200	5.26334000	0.41869900
C	-2.36373500	-2.58070100	1.08263600
C	-2.31568800	-3.38450800	2.23822200
C	-3.51090700	-2.65701500	0.26922900
C	-3.36505400	-4.24684000	2.54584600
H	-1.45849800	-3.30652800	2.89397500
C	-4.55632600	-3.52086100	0.57965500

H	-3.59220900	-2.01821900	-0.60476300
C	-4.48736500	-4.32494200	1.71959000
H	-3.30626900	-4.86008000	3.44050400
H	-5.43233700	-3.55723900	-0.06163700
H	-5.30507300	-4.99562200	1.96632500
H	-1.56246700	-1.67012800	-1.37810500
C	0.85945200	2.52253100	-0.46155900
C	0.51463300	3.70845900	-1.36674400
C	0.14554900	3.74061600	0.08355000
H	1.90715400	2.43700200	-0.19096600
H	-0.29355800	3.57322900	-2.07845300
H	1.34008800	4.31907400	-1.72100400
H	0.71742200	4.37269700	0.75469100
H	-0.89649300	3.61932400	0.34813400

INT-2i

N	0.33259200	1.18378400	0.84170600
C	1.10756000	-0.85422800	1.40003700
C	0.59373200	-1.78386300	0.49603300
C	2.64310800	1.57127800	-1.52284400
C	3.36382600	0.39202400	-1.25832100
C	2.74948200	-0.67987100	-2.03225000
C	1.71966800	-0.12311900	-2.85197600
C	1.58831900	1.26573000	-2.48534200
Rh	1.09802600	0.06991700	-0.72312100
C	0.24721700	0.33050400	1.88215100
O	-0.27594300	0.41509200	2.98301900
C	0.71825400	2.30062800	-3.12999500
H	1.30114000	2.92998900	-3.81450900
H	-0.08617900	1.84547000	-3.71121200
H	0.26459700	2.95265800	-2.37913000
C	2.84906100	2.92385200	-0.91575300
H	3.21733100	3.63420200	-1.66565100
H	1.90937700	3.31340000	-0.51369500
H	3.57259100	2.88859800	-0.09927200
C	4.54775000	0.22850300	-0.35966500
H	5.47835500	0.22999000	-0.94109300
H	4.60739900	1.03303500	0.37457900
H	4.50541000	-0.71147800	0.19492400
C	3.23353200	-2.09740400	-2.04484800
H	4.11067200	-2.20457100	-2.69515500
H	3.52716000	-2.41660000	-1.04126200
H	2.46250100	-2.78080700	-2.40743400
C	0.94027400	-0.85257500	-3.90231800

H	1.47794100	-0.84659700	-4.85824600
H	0.77473000	-1.89387900	-3.61576400
H	-0.03866400	-0.39877300	-4.06385300
O	-0.40958700	2.38737000	0.84285900
C	-1.77132000	2.27589100	0.95861400
O	-2.35679000	1.23342700	1.09669100
C	-2.41904900	3.65862300	0.85546000
C	-3.93119500	3.49466000	1.05628700
H	-4.15101400	3.06943300	2.03867300
H	-4.42336300	4.46936700	0.97888600
H	-4.35763400	2.82508400	0.30542800
C	-1.83168900	4.58995500	1.93349200
H	-0.75625100	4.72362600	1.79789000
H	-2.31546600	5.57083000	1.87742800
H	-2.00070800	4.18308700	2.93507200
C	-2.12807700	4.22382000	-0.55088900
H	-1.05577400	4.37104600	-0.70209100
H	-2.49714100	3.54665400	-1.32856800
H	-2.63021900	5.18881700	-0.67503800
C	-0.80675300	-0.68311100	-0.93286800
C	-0.76548500	-1.75046100	-0.11643400
C	-1.68754700	-2.93582800	0.08643400
O	-1.64439100	-3.81323700	-1.05245300
H	-1.63746100	-3.24381800	-1.83283600
H	-1.26175600	-3.53374300	0.90304400
C	-3.10552600	-2.56050600	0.49287100
C	-4.21266500	-3.15323900	-0.11774400
C	-3.30149800	-1.62779700	1.51947100
C	-5.50589200	-2.79236000	0.26612500
H	-4.04866800	-3.89236900	-0.89399100
C	-4.59252200	-1.27415300	1.90556200
H	-2.45089400	-1.14171400	1.98491100
C	-5.69924300	-1.84989100	1.27609700
H	-6.36081400	-3.24957100	-0.22420700
H	-4.73005200	-0.53218700	2.68593100
H	-6.70500300	-1.56527800	1.57173000
C	2.42871700	-1.01493400	2.05221300
C	2.99331000	0.07117600	2.74298400
C	3.15357200	-2.21802800	2.00247900
C	4.24503000	-0.03602000	3.34325300
H	2.44323500	1.00333900	2.80263800
C	4.40720000	-2.32368900	2.60205700
H	2.73267900	-3.08764900	1.50992600
C	4.96195400	-1.23158300	3.27181100

H	4.66040100	0.81699800	3.87142400
H	4.94598200	-3.26534400	2.55456000
H	5.93654900	-1.31584500	3.74252600
H	1.19974300	-2.66246300	0.27700200
C	-1.78073100	-0.10333200	-1.87561000
C	-2.89867500	-0.88329300	-2.56502600
C	-3.24264100	0.15716000	-1.54744600
H	-1.34908600	0.66797900	-2.50153100
H	-3.06314000	-1.91389000	-2.27208900
H	-3.06922700	-0.68047300	-3.61873100
H	-3.65313600	1.10382400	-1.88688900
H	-3.59810100	-0.17147000	-0.58137800

INT-4i

N	-1.39205600	1.07071100	-0.65905800
C	-2.70464100	-0.76666500	-0.88178900
C	-1.97010000	-1.79187400	-0.39125700
C	0.96832400	2.14007900	2.27464500
C	-0.36881000	2.63649700	2.13042400
C	-1.24977300	1.52758100	2.25600700
C	-0.46086700	0.33656700	2.51887800
C	0.92567900	0.73293200	2.55589700
Rh	0.06947000	0.89467800	0.46134400
C	-1.96207400	0.32683900	-1.62135500
O	-2.01995200	0.54402800	-2.82672900
C	2.09498400	-0.09159900	2.99503400
H	2.26955700	0.03963000	4.07045900
H	1.94729700	-1.15521800	2.80902200
H	3.00929400	0.20906200	2.47724500
C	2.21380300	2.96298600	2.20771100
H	2.56211300	3.20160000	3.22034000
H	3.01533400	2.41746100	1.70272100
H	2.04044700	3.89022300	1.66322300
C	-0.75506800	4.05183200	1.84702600
H	-0.48332000	4.70625100	2.68364600
H	-0.24253000	4.40362300	0.94835400
H	-1.83136600	4.13775700	1.68618200
C	-2.73867000	1.57895200	2.13266300
H	-3.16661100	2.19105500	2.93387600
H	-3.02874000	2.01456600	1.17225000
H	-3.18028200	0.58332500	2.18738600
C	-1.02926600	-0.99214900	2.90300300
H	-1.56173300	-0.91199600	3.85805600
H	-1.73578200	-1.35440600	2.15106900

H	-0.24463300	-1.74040500	3.01418300
O	1.08389000	3.55969300	-0.69647600
C	1.80290100	2.65030400	-1.09340800
O	1.67891800	1.38746800	-0.73173000
C	2.95349500	2.87739200	-2.09602900
C	2.48740300	2.33773700	-3.46583300
H	1.56832700	2.83516000	-3.78948700
H	3.26084900	2.52233000	-4.21876400
H	2.29634800	1.26160800	-3.43659400
C	3.23731300	4.38158000	-2.19995000
H	3.55469100	4.78981200	-1.23568900
H	4.03547400	4.55960600	-2.92816800
H	2.34545100	4.92744600	-2.51361300
C	4.21931700	2.12898800	-1.63781300
H	4.54611700	2.47579800	-0.65088800
H	4.05604000	1.05079900	-1.58380500
H	5.03542200	2.31757600	-2.34324300
C	-0.51448500	-1.96860100	-0.47626600
C	0.42961000	-1.05469800	-0.15424500
C	1.93467300	-1.30070600	-0.27684500
O	2.37200400	-1.04591100	-1.61118900
H	2.19964000	-0.09340700	-1.71537400
H	2.42869800	-0.56911600	0.37490100
C	2.45868000	-2.64945600	0.18875000
C	1.91311100	-3.30635200	1.29740900
C	3.58417000	-3.20149100	-0.43137400
C	2.47254000	-4.49078100	1.77495900
H	1.01812200	-2.90883600	1.76305700
C	4.14263500	-4.38931900	0.04215200
H	4.00385500	-2.69523400	-1.29217600
C	3.59200000	-5.03905100	1.14760600
H	2.02722200	-4.98983400	2.63106500
H	5.01202700	-4.80839400	-0.45651600
H	4.02763600	-5.96368000	1.51415200
C	-4.16602200	-0.64806500	-0.74755300
C	-4.92380100	0.02463200	-1.72191400
C	-4.82882400	-1.18943200	0.36842100
C	-6.30546900	0.13757500	-1.58492500
H	-4.41729800	0.43827200	-2.58667900
C	-6.21043200	-1.07897300	0.49806700
H	-4.25193200	-1.68586800	1.14294600
C	-6.95470400	-0.41370000	-0.47871200
H	-6.87802100	0.65539300	-2.34854100
H	-6.70579500	-1.50153100	1.36730400

H	-8.03161800	-0.32205200	-0.37511600
H	-2.51098900	-2.66780300	-0.03248900
C	-0.20768800	-3.37121300	-0.96095600
C	-0.78781600	-3.81333900	-2.29161900
C	0.69868600	-3.64876400	-2.12887000
H	-0.21337400	-4.12444900	-0.17473500
H	-1.31501000	-3.06406700	-2.87521300
H	-1.20389400	-4.81393600	-2.36100800
H	1.31948900	-4.53669400	-2.06500900
H	1.17797500	-2.79657100	-2.59405700

TS-4i

N	-1.72761100	0.43022200	-0.21998600
C	-2.19865700	-1.53227200	-0.71085300
C	-1.13213400	-2.31560600	-0.40435200
C	0.43003200	2.45583800	2.22567400
C	-0.97300900	2.22890200	2.38186800
C	-1.13986200	0.85134800	2.74190600
C	0.16843500	0.24918000	2.87981900
C	1.14902900	1.24909900	2.56209800
Rh	-0.12842400	0.79092400	0.74663800
C	-1.91710500	-0.16033200	-1.38727100
O	-2.01767200	0.11613200	-2.56387800
C	2.63344000	1.12736600	2.71846500
H	2.93885300	1.41574300	3.73201200
H	2.98129600	0.10688800	2.54410900
H	3.16187400	1.78084500	2.01976700
C	1.04675500	3.74878600	1.79763700
H	1.26116700	4.37638200	2.67135000
H	1.98520400	3.58227900	1.26461000
H	0.37133500	4.29232600	1.13577400
C	-2.05732300	3.23389700	2.15351900
H	-2.01632500	4.03052100	2.90559200
H	-1.95498200	3.67699100	1.15987400
H	-3.04134200	2.76480700	2.21407700
C	-2.44454300	0.16131800	2.99113700
H	-2.83786900	0.42979600	3.97863700
H	-3.18547100	0.43993100	2.23934400
H	-2.32998100	-0.92375100	2.95594600
C	0.42132600	-1.12781200	3.41027400
H	0.13536300	-1.18548700	4.46720800
H	-0.15492400	-1.87974500	2.86475900
H	1.47628400	-1.39106400	3.33629300
O	-1.00650700	3.26316900	-0.89148400

C	0.01847300	2.80205400	-1.38611700
O	0.69428000	1.78745000	-0.89381500
C	0.63307200	3.36513400	-2.68529500
C	0.42308100	2.31304600	-3.79648100
H	-0.63178200	2.04095000	-3.88419200
H	0.76483000	2.71776300	-4.75529000
H	0.98442800	1.39653100	-3.59823400
C	-0.08721400	4.66663100	-3.05981500
H	0.02908800	5.42173500	-2.27689300
H	0.32885800	5.06691900	-3.99055500
H	-1.15647600	4.49454900	-3.19790400
C	2.13664700	3.63211700	-2.48428900
H	2.30456500	4.34700500	-1.67083800
H	2.68292400	2.71559700	-2.25054000
H	2.56287600	4.05926700	-3.39819700
C	0.28567400	-1.98366800	-0.49129900
C	0.86408100	-0.82323000	-0.08313700
C	2.32773500	-0.47041200	-0.36018000
O	2.46198000	-0.05004400	-1.71612300
H	1.86046400	0.71823400	-1.76610700
H	2.57340300	0.38903400	0.27458400
C	3.37181700	-1.52096800	-0.03201700
C	3.25252600	-2.32991400	1.10313100
C	4.52533800	-1.62185700	-0.81553700
C	4.26109900	-3.22953200	1.44748500
H	2.34512900	-2.28144200	1.69439600
C	5.53366200	-2.52366200	-0.47397400
H	4.61160600	-0.99739800	-1.69660500
C	5.40780200	-3.33029600	0.65822000
H	4.14656100	-3.85742800	2.32664600
H	6.42087900	-2.59724000	-1.09653400
H	6.19318900	-4.03253300	0.92119200
C	-3.61709900	-1.90863000	-0.54449300
C	-4.58506800	-0.93789600	-0.24052900
C	-4.02458500	-3.24377800	-0.70019800
C	-5.91942200	-1.29986500	-0.06936400
H	-4.27973200	0.09659700	-0.12786100
C	-5.35980500	-3.60037200	-0.52823000
H	-3.29815600	-4.00009600	-0.97978800
C	-6.31268800	-2.63146600	-0.20809900
H	-6.65393600	-0.53697700	0.17059500
H	-5.65795900	-4.63679300	-0.65529400
H	-7.35364500	-2.91121200	-0.07892500
H	-1.34139900	-3.35780500	-0.16355800

C	1.06828000	-3.16359600	-1.03923300
C	0.59511300	-3.84114200	-2.31145400
C	1.88252500	-3.06389700	-2.30125600
H	1.46793400	-3.82601600	-0.27396200
H	-0.25169500	-3.40009800	-2.82975300
H	0.63607600	-4.92528100	-2.35903500
H	2.82201000	-3.60648400	-2.32052600
H	1.91066000	-2.09770600	-2.78917000

TS-3ii

N	0.08024200	-0.43700600	-0.64130400
C	-2.18426300	-1.20501400	-0.45680000
C	-1.98583300	-1.42187200	0.91126200
C	-0.25533500	3.55255200	-0.25033100
C	-1.46741800	2.86068200	-0.37734600
C	-1.77756700	2.25766600	0.92220500
C	-0.78183400	2.68878800	1.87247600
C	0.20654700	3.39764200	1.13846600
Rh	0.11934300	1.35016600	0.36107900
C	-1.09013400	-0.86257000	-1.34241800
O	-1.07263400	-0.89793800	-2.57741100
C	1.46615600	3.99819100	1.68270200
H	1.31962600	5.05824000	1.92525300
H	1.78846500	3.48281300	2.58972700
H	2.27885400	3.93663800	0.95352200
C	0.51057900	4.28169300	-1.31029900
H	0.52277300	5.36155400	-1.11857000
H	1.55196600	3.94497300	-1.34510700
H	0.07501900	4.12075900	-2.29863300
C	-2.29729000	2.65518800	-1.60531200
H	-3.27691300	3.13575900	-1.49899200
H	-1.81155800	3.06754000	-2.49179000
H	-2.47172000	1.59008400	-1.78774400
C	-3.07251300	1.60079600	1.27074300
H	-3.75746500	2.33635000	1.71218200
H	-3.55405500	1.17346400	0.39179800
H	-2.92509500	0.79613600	1.99410300
C	-0.79078800	2.38325300	3.33740600
H	-1.38776100	3.12097400	3.88833700
H	-1.22479500	1.39709700	3.52175800
H	0.21992200	2.38550900	3.75121400
O	1.21266100	-0.55089500	-1.57973200
C	2.18599400	0.29148200	-1.36349700
O	2.13973300	1.15744100	-0.46421400

C	3.32827700	0.21029600	-2.36112300
C	3.42968200	-1.19016300	-2.98517700
H	2.50483500	-1.46605100	-3.49546600
H	4.24504600	-1.19398900	-3.71511700
H	3.64159800	-1.94546200	-2.22602400
C	2.98430500	1.25506900	-3.45294100
H	2.90725600	2.25969800	-3.02696000
H	3.77863900	1.25838900	-4.20517600
H	2.04015600	1.00870900	-3.94690600
C	4.64067400	0.59159800	-1.65771800
H	4.57302600	1.58164500	-1.20127000
H	4.88802300	-0.13504700	-0.88013200
H	5.45179500	0.60081400	-2.39155900
C	-0.83318600	-1.25292900	1.68812200
C	0.28197000	-0.50068700	1.24674800
C	1.65570500	-0.85527100	1.81357200
O	2.45970200	0.26610600	2.15830600
H	2.60005100	0.77947200	1.34792200
H	1.44680600	-1.32379000	2.77861700
C	2.42335500	-1.89802100	0.99731800
C	1.76602000	-2.91003200	0.28628300
C	3.82222700	-1.89502900	1.03015600
C	2.49390300	-3.89883400	-0.37373800
H	0.68343500	-2.91374200	0.23587600
C	4.55159900	-2.88336200	0.36581500
H	4.32825700	-1.11680100	1.59003800
C	3.88995900	-3.89183300	-0.33583200
H	1.96751200	-4.67118600	-0.92638500
H	5.63713700	-2.86683300	0.40307800
H	4.45528800	-4.66240100	-0.85127300
C	-3.54266400	-1.39602900	-1.02039100
C	-3.77121400	-1.74886400	-2.36726700
C	-4.67847200	-1.22971800	-0.19816600
C	-5.06449900	-1.93412600	-2.85088500
H	-2.92116300	-1.86915600	-3.02301900
C	-5.96896100	-1.42159100	-0.68493100
H	-4.55424200	-0.92729100	0.83559200
C	-6.17327900	-1.77542000	-2.01857700
H	-5.20419100	-2.21067800	-3.89247100
H	-6.81689500	-1.28064100	-0.02019900
H	-7.17872500	-1.91832100	-2.40344900
H	-2.82515900	-1.87512300	1.42698600
C	-0.76876500	-1.90852700	3.04667000
C	-1.67026500	-3.05250800	3.44450100

C	-0.19811100	-3.30134600	3.26071800
H	-0.54782500	-1.21919800	3.86167800
H	-2.33975000	-3.47148700	2.70158100
H	-2.07440500	-3.04744400	4.45191400
H	0.42086100	-3.47284800	4.13654800
H	0.11020300	-3.85214300	2.37901700

INT-4ii

N	0.20487000	-0.46769000	-0.33516900
C	-2.01529400	-1.44519800	-0.32986700
C	-1.88089100	-1.42418000	1.08760500
C	-0.56613600	3.49450700	-0.76285400
C	-1.69768900	2.67123400	-0.68786900
C	-1.88457700	2.29821100	0.71852300
C	-0.92166600	3.01440700	1.51637400
C	-0.04026400	3.65777800	0.60333700
Rh	0.08980800	1.51792100	0.21579500
C	-0.93952900	-1.03013300	-1.13957500
O	-0.78728300	-0.96381800	-2.36048300
C	1.15343700	4.49124900	0.95509500
H	0.88628300	5.55460300	1.00231900
H	1.56514100	4.20267200	1.92482500
H	1.94366900	4.38228600	0.20755000
C	0.07406500	4.07459700	-1.98541200
H	-0.06249200	5.16220800	-2.02902500
H	1.15113200	3.87889600	-1.99351200
H	-0.34845300	3.64388500	-2.89546500
C	-2.55153500	2.15470500	-1.80146900
H	-3.57091300	2.55192600	-1.72517300
H	-2.14998900	2.43229300	-2.77760800
H	-2.62216800	1.06298300	-1.77094600
C	-3.07349500	1.55910300	1.24147400
H	-3.87645100	2.26923400	1.47813800
H	-3.45514900	0.85049300	0.50605700
H	-2.83392500	1.00180100	2.14837700
C	-0.86466400	3.05198800	3.01201900
H	-1.42889700	3.90844900	3.40426700
H	-1.29770100	2.14648100	3.44289500
H	0.16360900	3.13477700	3.37169500
O	1.41209300	-0.75598900	-1.11047600
C	2.22353700	0.26489300	-1.30175700
O	2.07961200	1.34539100	-0.70709500
C	3.30079400	0.01724200	-2.33850000
C	3.37080600	-1.46337900	-2.74341400

H	2.42006700	-1.80338100	-3.15931500
H	4.14758700	-1.58217500	-3.50477400
H	3.62114700	-2.09914400	-1.89185300
C	2.88650300	0.88157300	-3.55597900
H	2.84349300	1.94085800	-3.28961800
H	3.62539400	0.74991500	-4.35187700
H	1.90827300	0.57326000	-3.93633200
C	4.64804100	0.49810900	-1.76984500
H	4.59443300	1.54260700	-1.45373700
H	4.94712300	-0.11219900	-0.91361500
H	5.41674700	0.40666200	-2.54242200
C	-0.80352200	-0.97767300	1.80552800
C	0.35554000	-0.42279900	1.11435200
C	1.71991600	-0.70877600	1.77803100
O	2.58369400	0.41057000	1.93583500
H	2.50364300	0.97728800	1.15602100
H	1.45709800	-0.98011800	2.80015100
C	2.43898200	-1.92145700	1.18963800
C	1.72307600	-3.06220200	0.80364200
C	3.83198700	-1.92446400	1.08265300
C	2.39119300	-4.17676600	0.30057000
H	0.63950000	-3.06990500	0.87467500
C	4.50139700	-3.04364100	0.58163300
H	4.37877000	-1.04458000	1.40143400
C	3.78352200	-4.17214000	0.18492200
H	1.82222900	-5.04874900	-0.00797300
H	5.58498100	-3.03214300	0.50356500
H	4.30210700	-5.04109300	-0.20877300
C	-3.29609800	-1.83431200	-0.95313200
C	-3.37584200	-2.28555100	-2.28781500
C	-4.50357000	-1.75794700	-0.22615900
C	-4.59591100	-2.65145600	-2.85046100
H	-2.46942400	-2.33675800	-2.87524400
C	-5.72060900	-2.12890200	-0.79260800
H	-4.49898700	-1.38472700	0.79261900
C	-5.77800900	-2.58111600	-2.11096400
H	-4.62066500	-2.99950800	-3.87970400
H	-6.62920200	-2.05340800	-0.20116900
H	-6.72656500	-2.86735800	-2.55542500
H	-2.72207000	-1.80442900	1.65415400
C	-0.77975000	-0.99676700	3.30037600
C	-1.74820400	-1.81629100	4.11424700
C	-0.29524400	-2.20877500	4.08474300
H	-0.50153700	-0.04273300	3.74718200

H	-2.44953700	-2.46149500	3.59649300
H	-2.14422600	-1.37228300	5.02209400
H	0.31004200	-2.04485300	4.97155600
H	-0.02629100	-3.08843100	3.50815900

TS-4ii

N	0.91144300	-1.02278200	-1.04782600
C	2.77702800	0.33795000	-1.00770000
C	2.09466200	1.45625900	-0.65973200
C	-1.00870200	-2.06251500	2.28576500
C	0.23454200	-2.67262500	1.95339600
C	1.24181200	-1.64108800	1.96110200
C	0.62523600	-0.40794800	2.37704400
C	-0.78676700	-0.66110100	2.55090600
Rh	-0.22757400	-0.93388500	0.41363400
C	2.08773600	-0.87887200	-1.61666600
O	2.57886600	-1.59063100	-2.50428700
C	-1.80975100	0.28197000	3.10033900
H	-1.85916600	0.19601700	4.19302800
H	-1.58608500	1.32058100	2.85509500
H	-2.80368600	0.05557500	2.70715400
C	-2.33176200	-2.75217700	2.37635900
H	-2.58337300	-2.94848000	3.42574200
H	-3.12431700	-2.12841100	1.95517400
H	-2.32015600	-3.69326100	1.82827500
C	0.44341100	-4.10830000	1.60238600
H	0.24231900	-4.75101900	2.46746500
H	-0.23511800	-4.38877800	0.79265100
H	1.46849300	-4.28812300	1.27436000
C	2.70011500	-1.85447800	1.70670900
H	3.14674000	-2.41488000	2.53620200
H	2.86658500	-2.42234700	0.78836500
H	3.23187600	-0.90910100	1.60983000
C	1.35701100	0.85555900	2.69633500
H	2.03530300	0.69016500	3.54110900
H	1.95145500	1.19305500	1.84407100
H	0.66687200	1.65461000	2.96797300
O	-1.69992900	-3.41677000	-0.64230900
C	-2.33746600	-2.41672500	-0.95708800
O	-2.02569000	-1.18832600	-0.59924700
C	-3.60054500	-2.48580200	-1.84216300
C	-3.20002400	-2.00687600	-3.25474200
H	-2.38992000	-2.62079300	-3.65977100
H	-4.05859800	-2.08439300	-3.93011300

H	-2.86753400	-0.96513600	-3.25248900
C	-4.08934400	-3.93859400	-1.90656300
H	-4.36901800	-4.30388200	-0.91375900
H	-4.96753700	-4.00671900	-2.55721000
H	-3.30998500	-4.59684400	-2.29493600
C	-4.70768300	-1.57880100	-1.27323700
H	-4.98010700	-1.88232900	-0.25609000
H	-4.40068700	-0.53138200	-1.24539700
H	-5.60549600	-1.65669100	-1.89538600
C	0.66609400	1.80399900	-0.67916300
C	-0.37030800	1.06945000	-0.21295600
C	-1.83093200	1.51879500	-0.19524500
O	-2.44111600	1.30303800	-1.46499600
H	-2.42168500	0.33220000	-1.54642900
H	-2.34957800	0.88034000	0.53036600
C	-2.09240400	2.94084500	0.27529600
C	-1.35544300	3.51324200	1.31843600
C	-3.16075700	3.66057000	-0.26827000
C	-1.67274200	4.78054700	1.80580200
H	-0.50178300	2.97942800	1.72107700
C	-3.47664700	4.93057900	0.21563400
H	-3.72648400	3.21759800	-1.07878400
C	-2.73645400	5.49635600	1.25452900
H	-1.08239400	5.21215500	2.60919100
H	-4.30460100	5.48034000	-0.22289600
H	-2.98289700	6.48544800	1.62868200
C	4.23801100	0.24230500	-0.78034500
C	5.08917200	-0.43798100	-1.67110000
C	4.80931400	0.84868300	0.35596600
C	6.46058900	-0.49482500	-1.43004700
H	4.65404800	-0.91614000	-2.53818300
C	6.18090900	0.79514900	0.58749100
H	4.16802300	1.35613500	1.07011700
C	7.01430000	0.12022400	-0.30631200
H	7.10173100	-1.02082600	-2.13126500
H	6.59688700	1.27010600	1.47128000
H	8.08389900	0.07115800	-0.12537400
H	2.71655100	2.31313400	-0.39895900
C	0.49827600	3.22164100	-1.18983000
C	1.00610600	3.54647700	-2.58106500
C	-0.46872900	3.58232500	-2.28324700
H	0.67363100	3.98815200	-0.43682100
H	1.38095000	2.72035500	-3.17822100
H	1.53833100	4.48194600	-2.72462000

H	-0.96261800	4.54531800	-2.20375400
H	-1.09439700	2.78624100	-2.66692100

INT-5ii

N	0.67183300	-0.96579700	-1.24133600
C	2.71526200	0.34002300	-0.89485900
C	2.03986500	1.49779700	-0.67042600
C	-0.90579600	-1.97714800	2.33819000
C	0.36251700	-2.53370300	1.97254900
C	1.34266400	-1.47138100	2.00028700
C	0.66731600	-0.26942300	2.39323700
C	-0.73251200	-0.58062200	2.59525800
Rh	-0.17564800	-0.94442800	0.41847900
C	2.03816500	-0.94922400	-1.22227600
O	2.63854000	-2.00138300	-1.48134800
C	-1.78542900	0.34086300	3.12500400
H	-1.81095000	0.30379900	4.22116200
H	-1.61477800	1.37711000	2.83209800
H	-2.77623100	0.05579500	2.76365600
C	-2.18953200	-2.73571200	2.44680900
H	-2.32483600	-3.10182100	3.47192800
H	-3.04370500	-2.10002100	2.20320800
H	-2.19415600	-3.58266000	1.76164100
C	0.63172300	-3.96058900	1.62699100
H	0.59427500	-4.58281900	2.53007100
H	-0.11698500	-4.31818000	0.91735800
H	1.61714100	-4.07297400	1.17194800
C	2.81664300	-1.65493400	1.82509500
H	3.21786600	-2.23738400	2.66267100
H	3.05444900	-2.18635800	0.89978300
H	3.33944600	-0.69899000	1.79803900
C	1.33800100	1.02859800	2.70436200
H	1.83701500	0.95938100	3.67863200
H	2.09125700	1.27344000	1.95444500
H	0.62280000	1.84910800	2.75079700
O	-1.59331200	-3.51263600	-0.57653800
C	-2.22509800	-2.53333600	-0.96744000
O	-1.93573500	-1.29103600	-0.66354500
C	-3.45924500	-2.66500500	-1.88621000
C	-3.04420200	-2.19472700	-3.29640900
H	-2.20320800	-2.78552500	-3.67218800
H	-3.88297600	-2.31330000	-3.99076600
H	-2.74710600	-1.14265600	-3.30116800
C	-3.89805500	-4.13394900	-1.93659900

H	-4.18744200	-4.49198300	-0.94411200
H	-4.75799400	-4.24326800	-2.60607500
H	-3.08796600	-4.77209800	-2.29486100
C	-4.60965800	-1.78779900	-1.35674500
H	-4.89295300	-2.08488700	-0.34065100
H	-4.33715800	-0.73050300	-1.33853900
H	-5.49115300	-1.90428100	-1.99631600
C	0.61562700	1.84767100	-0.64454500
C	-0.40229700	1.08253400	-0.19344700
C	-1.88728800	1.44207300	-0.21490600
O	-2.42998500	1.17282200	-1.50184000
H	-2.35645900	0.19958100	-1.56603600
H	-2.38518400	0.77991700	0.50398900
C	-2.24767100	2.85590200	0.21618400
C	-1.56715800	3.50963000	1.24889600
C	-3.35253100	3.48559700	-0.36527100
C	-1.97424500	4.76818200	1.68980600
H	-0.68632200	3.04839900	1.68117000
C	-3.75929400	4.74647700	0.07205800
H	-3.87486300	2.98094700	-1.16879600
C	-3.07417400	5.39369700	1.10117500
H	-1.42556200	5.26338600	2.48592100
H	-4.61503100	5.22504000	-0.39558900
H	-3.39090600	6.37587800	1.43874800
C	4.19764100	0.32832200	-0.81717700
C	4.98477900	-0.38239200	-1.73954300
C	4.84927300	1.05646200	0.19328900
C	6.37503300	-0.34921900	-1.65503800
H	4.50127100	-0.95987000	-2.51597500
C	6.23955500	1.08895700	0.27537400
H	4.25677400	1.59283500	0.92890200
C	7.00922600	0.38391300	-0.65048000
H	6.96632800	-0.89997600	-2.38045900
H	6.71982100	1.65649200	1.06705500
H	8.09301800	0.40134900	-0.58674600
H	2.67295100	2.37712900	-0.56265300
C	0.41522500	3.26563000	-1.13738400
C	0.91849300	3.61681000	-2.52507700
C	-0.55755100	3.60831000	-2.23095300
H	0.56775900	4.03004200	-0.37746200
H	1.31600900	2.80732300	-3.13039600
H	1.42554800	4.56762900	-2.65817900
H	-1.07901400	4.55593400	-2.14540500
H	-1.15714300	2.79703300	-2.62557800

TS-5ii

N	0.62973300	-0.85133900	-1.25700800
C	2.71717800	0.39942600	-0.90352100
C	2.05878200	1.55780700	-0.64204600
C	-0.87481100	-2.02939400	2.31953700
C	0.38992000	-2.57285500	1.92698000
C	1.36662900	-1.50699100	1.96589800
C	0.69340900	-0.31610000	2.39448600
C	-0.70412700	-0.63593300	2.60335800
Rh	-0.17801600	-0.94643300	0.43316600
C	1.99723400	-0.84886800	-1.27957800
O	2.55834400	-1.90102000	-1.61776400
C	-1.76080500	0.26915700	3.15390800
H	-1.80944500	0.18434800	4.24662300
H	-1.57761700	1.31554700	2.90966500
H	-2.74581700	0.00799800	2.75957800
C	-2.15582000	-2.79247600	2.42785500
H	-2.28558100	-3.16618100	3.45094400
H	-3.01222500	-2.15668800	2.19254300
H	-2.16165500	-3.63381000	1.73601200
C	0.66086800	-3.99082200	1.54785900
H	0.64283600	-4.63186000	2.43829600
H	-0.09765400	-4.33753200	0.84351600
H	1.63911200	-4.08845800	1.07411100
C	2.83672900	-1.68290000	1.75298300
H	3.25660800	-2.29600100	2.55887700
H	3.05326500	-2.18082400	0.80390500
H	3.35975300	-0.72695400	1.74936500
C	1.36100800	0.98078700	2.71844300
H	1.85692300	0.90545600	3.69382000
H	2.11570800	1.23339000	1.97255800
H	0.64407800	1.79994000	2.76856400
O	-1.59265400	-3.50684200	-0.61073000
C	-2.23358000	-2.52129000	-0.97067700
O	-1.94943300	-1.28525800	-0.64015900
C	-3.47297200	-2.64107100	-1.88493500
C	-3.04918500	-2.19349900	-3.30019100
H	-2.21907800	-2.80360300	-3.66907400
H	-3.88993500	-2.30352200	-3.99360200
H	-2.73283800	-1.14696300	-3.31680800
C	-3.93521500	-4.10341600	-1.92097100
H	-4.23296500	-4.44587400	-0.92526700
H	-4.79557000	-4.20656200	-2.59094500

H	-3.13429900	-4.75780800	-2.27006500
C	-4.60962900	-1.74020000	-1.36697500
H	-4.89860600	-2.02108300	-0.34792500
H	-4.32031600	-0.68736800	-1.35976000
H	-5.49231100	-1.84974800	-2.00623900
C	0.63429100	1.89257200	-0.61773000
C	-0.37766700	1.09298700	-0.20954300
C	-1.86915800	1.43163900	-0.25001800
O	-2.38592000	1.18015600	-1.54980300
H	-2.32276900	0.20707900	-1.61757100
H	-2.36962600	0.74964600	0.44712700
C	-2.25451200	2.82950900	0.20940400
C	-1.61383100	3.45337000	1.28530400
C	-3.34731200	3.46755800	-0.38489700
C	-2.04707800	4.69245800	1.75487500
H	-0.74376700	2.98412300	1.73111800
C	-3.78078300	4.70900900	0.08193800
H	-3.84009500	2.98468500	-1.21985700
C	-3.13469800	5.32733800	1.15307100
H	-1.52935200	5.16501100	2.58478000
H	-4.62701700	5.19475300	-0.39547500
H	-3.47236400	6.29417700	1.51383400
C	4.19660600	0.34855800	-0.81877400
C	4.97095700	-0.36939700	-1.74689500
C	4.86135000	1.04700700	0.20476300
C	6.36124000	-0.37370700	-1.65329000
H	4.47688600	-0.92230900	-2.53420100
C	6.25111300	1.04258800	0.29493300
H	4.27879100	1.58829500	0.94464700
C	7.00798900	0.32951100	-0.63577200
H	6.94245000	-0.92974300	-2.38280800
H	6.74122800	1.58730100	1.09652400
H	8.09148100	0.31831800	-0.56570300
H	2.69253800	2.43177100	-0.50281400
C	0.41633800	3.32358700	-1.06191400
C	0.95357500	3.73931900	-2.41857700
C	-0.53036800	3.68122000	-2.17353700
H	0.52243700	4.06208500	-0.26943100
H	1.39199600	2.96438300	-3.04064500
H	1.43752600	4.70782600	-2.50036300
H	-1.08019600	4.61085400	-2.07121900
H	-1.09460100	2.86957400	-2.61691100

N	-0.24973400	0.26147500	0.88189700
C	1.01688800	2.30094000	1.04171500
C	-0.17233700	2.95354600	0.72916800
C	0.71025400	-3.63613100	-0.34711500
C	1.78317900	-3.45317600	0.58191300
C	1.19650500	-3.12776700	1.87485200
C	-0.22566000	-3.10394100	1.72315000
C	-0.53689900	-3.39708400	0.33457500
Rh	0.67080400	-1.59541500	0.43256500
C	0.94494100	0.88013700	1.05564100
O	1.91971400	0.02532300	1.12568200
C	-1.89823500	-3.54556200	-0.27591800
H	-2.05320900	-4.57504400	-0.61825500
H	-2.68368200	-3.31444600	0.44593200
H	-2.02829100	-2.87514900	-1.12996800
C	0.84611100	-3.97059300	-1.79742400
H	0.85985400	-5.05951400	-1.92921100
H	0.00460600	-3.57040300	-2.36693900
H	1.76498200	-3.54944700	-2.20597700
C	3.24134700	-3.58425700	0.27876500
H	3.53629400	-4.64019300	0.24425900
H	3.46531200	-3.11289700	-0.67976400
H	3.84324900	-3.08910600	1.04325300
C	1.97283200	-2.86041000	3.12451900
H	2.34136900	-3.79845800	3.55625700
H	2.83202700	-2.21859800	2.91589700
H	1.35865300	-2.35848400	3.87411800
C	-1.22762200	-2.82526900	2.79855500
H	-1.54574900	-3.76045600	3.27474800
H	-0.80933000	-2.17625900	3.57001300
H	-2.11649700	-2.33462900	2.39649200
O	2.68644500	-1.26356300	-1.99368200
C	1.67140700	-0.59480100	-2.17776700
O	0.59186200	-0.65961700	-1.43403600
C	1.55386700	0.43922600	-3.31697100
C	1.30749800	1.82341500	-2.68166100
H	2.11834300	2.09633900	-1.99845300
H	1.25144100	2.58960400	-3.46281700
H	0.37269800	1.83437200	-2.11698400
C	2.85040600	0.45315300	-4.13478000
H	3.04705300	-0.52740800	-4.57629100
H	2.77633800	1.19075900	-4.94119600
H	3.70642900	0.70802800	-3.50547500
C	0.36206000	0.06716300	-4.22056600

H	0.48279300	-0.93814900	-4.63930200
H	-0.58230600	0.10048900	-3.67224400
H	0.29279500	0.77152100	-5.05670200
C	-1.37155300	2.29054700	0.39317600
C	-1.36502900	0.89746500	0.47114600
C	-2.41678300	-0.06610800	-0.05043400
O	-2.17703500	-0.31309500	-1.43336400
H	-1.20662900	-0.40337400	-1.55277900
H	-2.23918400	-0.99383600	0.51207800
C	-3.86094400	0.30871000	0.18427300
C	-4.27147400	0.68507600	1.46861600
C	-4.80861500	0.21655200	-0.83627100
C	-5.60731800	0.98761500	1.72429400
H	-3.53480000	0.75976200	2.26509000
C	-6.14780600	0.51679300	-0.57969900
H	-4.48219900	-0.07812300	-1.82619800
C	-6.55137200	0.90641200	0.69756000
H	-5.91168900	1.28865800	2.72253100
H	-6.87688000	0.44795400	-1.38201500
H	-7.59276700	1.14316500	0.89416800
C	2.28625700	3.03174000	1.23300600
C	3.50999200	2.49095800	0.79872700
C	2.28784000	4.30837800	1.82013700
C	4.69004800	3.22010700	0.93336200
H	3.52395400	1.50162300	0.35853400
C	3.47040300	5.03135000	1.95591700
H	1.35686900	4.72792800	2.18962900
C	4.67778800	4.49127900	1.50945500
H	5.62451200	2.79076900	0.58377100
H	3.44997100	6.01444700	2.41731700
H	5.60053100	5.05401400	1.61521700
H	-0.15946800	4.03566000	0.64552000
C	-2.55162100	3.07866800	-0.08135800
C	-2.34635300	4.19785700	-1.07932600
C	-3.04609700	2.93327100	-1.49982100
H	-3.32807700	3.24417500	0.66227300
H	-1.34058000	4.36512200	-1.45294900
H	-2.93476100	5.10225200	-0.96013600
H	-4.11891900	2.95493800	-1.65644200
H	-2.51441700	2.23179400	-2.13300800

INT-3_{Ph}

N	0.22084800	-0.22981500	-1.64212300
C	1.15871300	-3.26571800	0.36077000

C	2.18300400	-2.58460100	-0.31058500
C	2.68584100	-1.53003300	0.56941600
C	1.99705300	-1.64084000	1.83302900
C	1.00675200	-2.65275100	1.68504800
Rh	0.59496300	-1.02331400	0.25009700
C	0.51024500	1.05033800	-2.02401400
O	-0.20658900	1.81323200	-2.66736300
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H	-0.75832400	-4.17256700	0.01790300
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C	0.24942400	0.85164500	1.02351200
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INT-4i_{ph}

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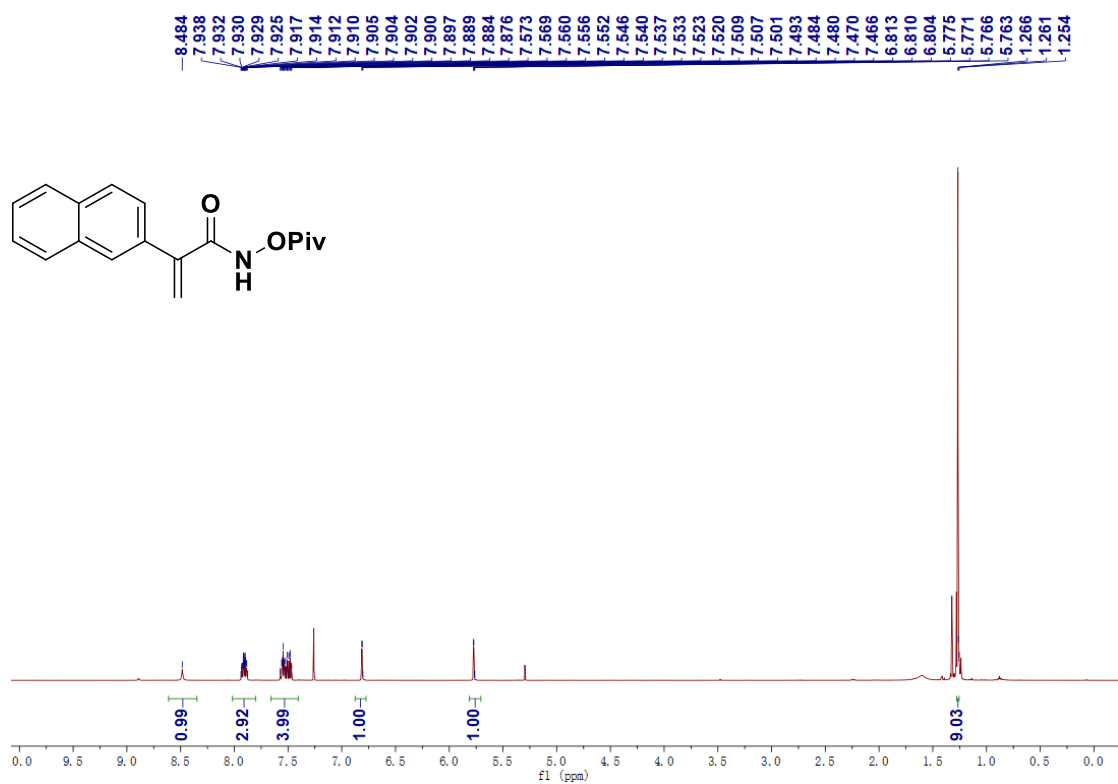
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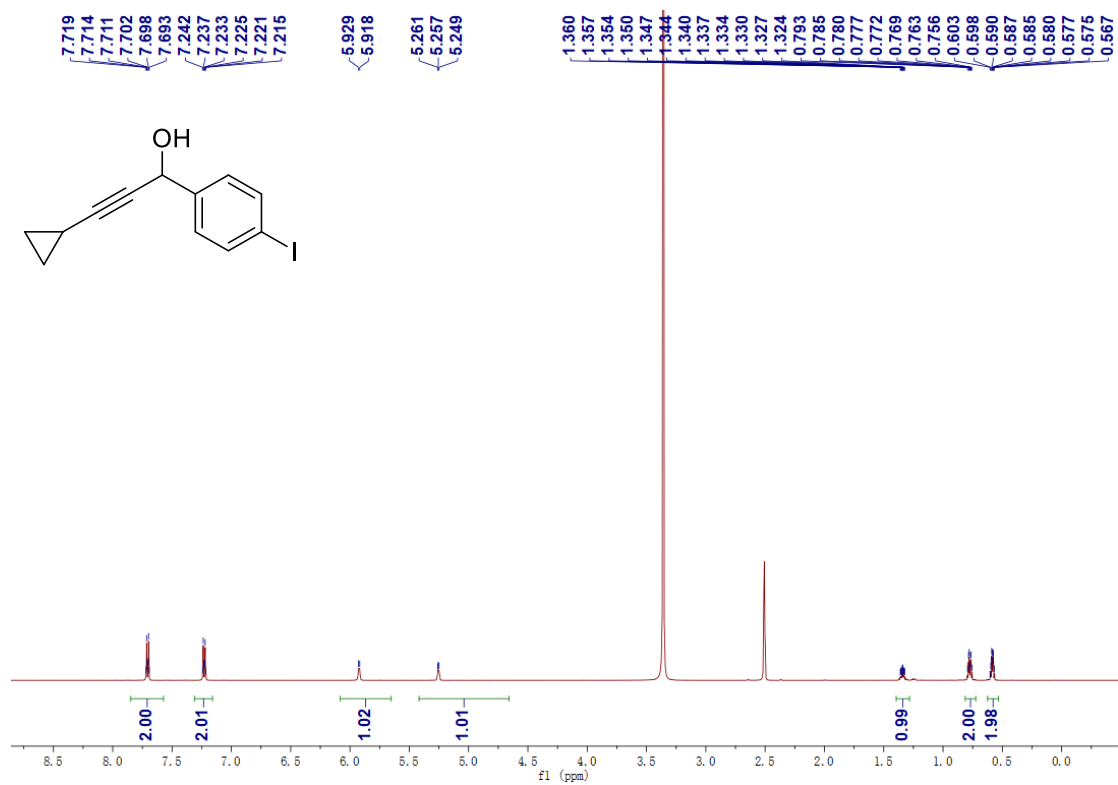
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Copies of ^1H , ^{13}C NMR and ^{19}F NMR spectra

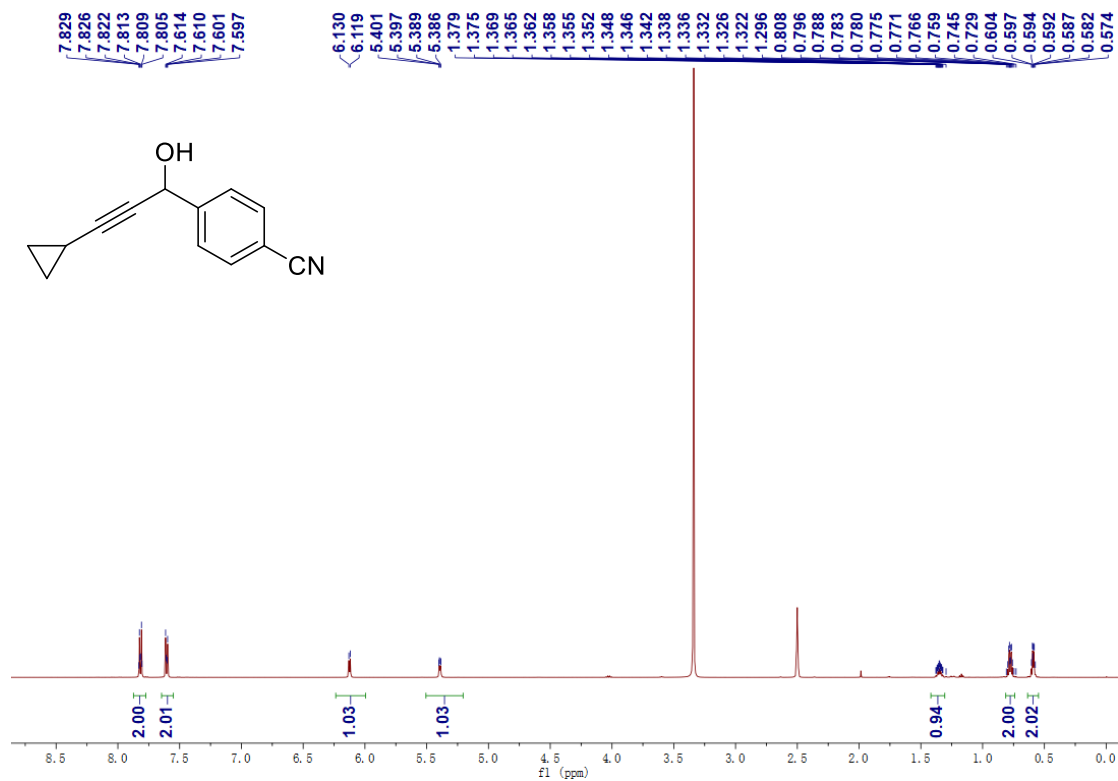
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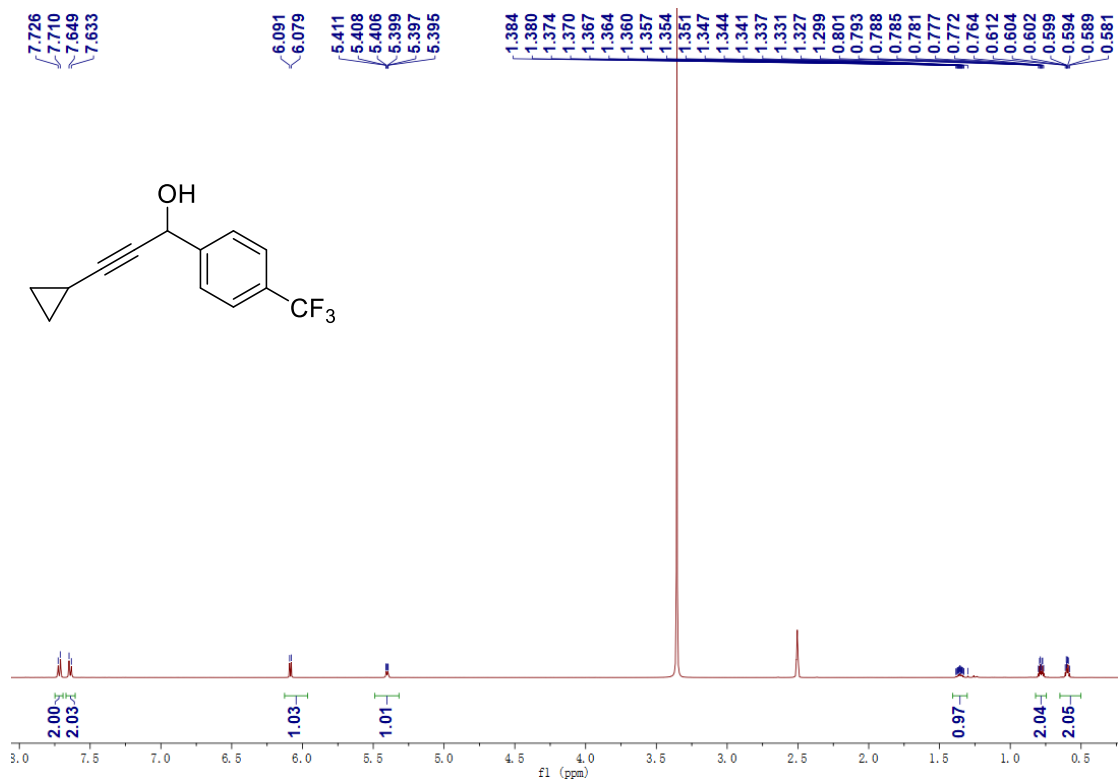
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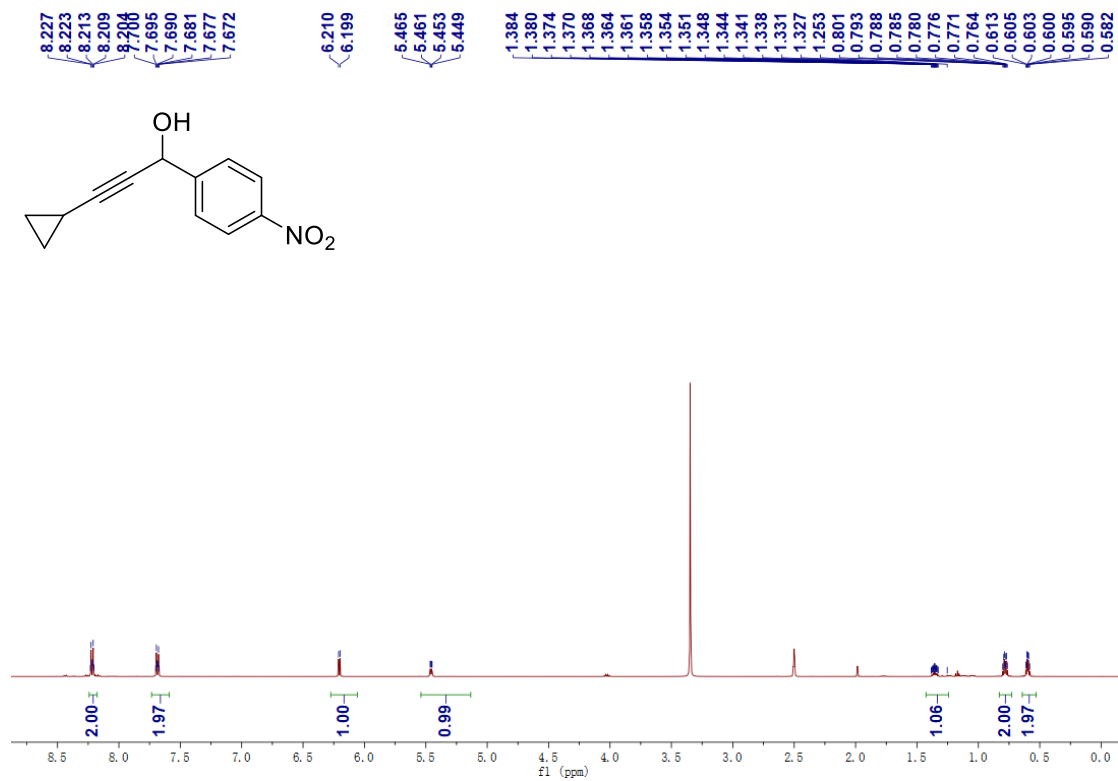
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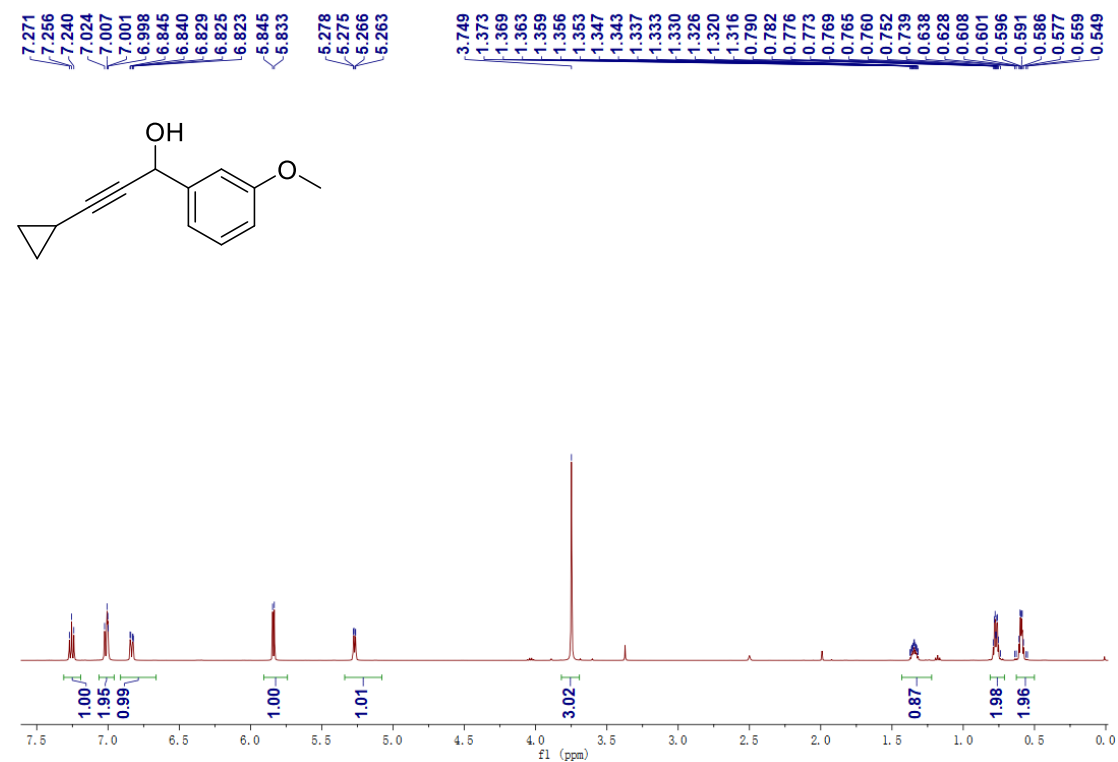
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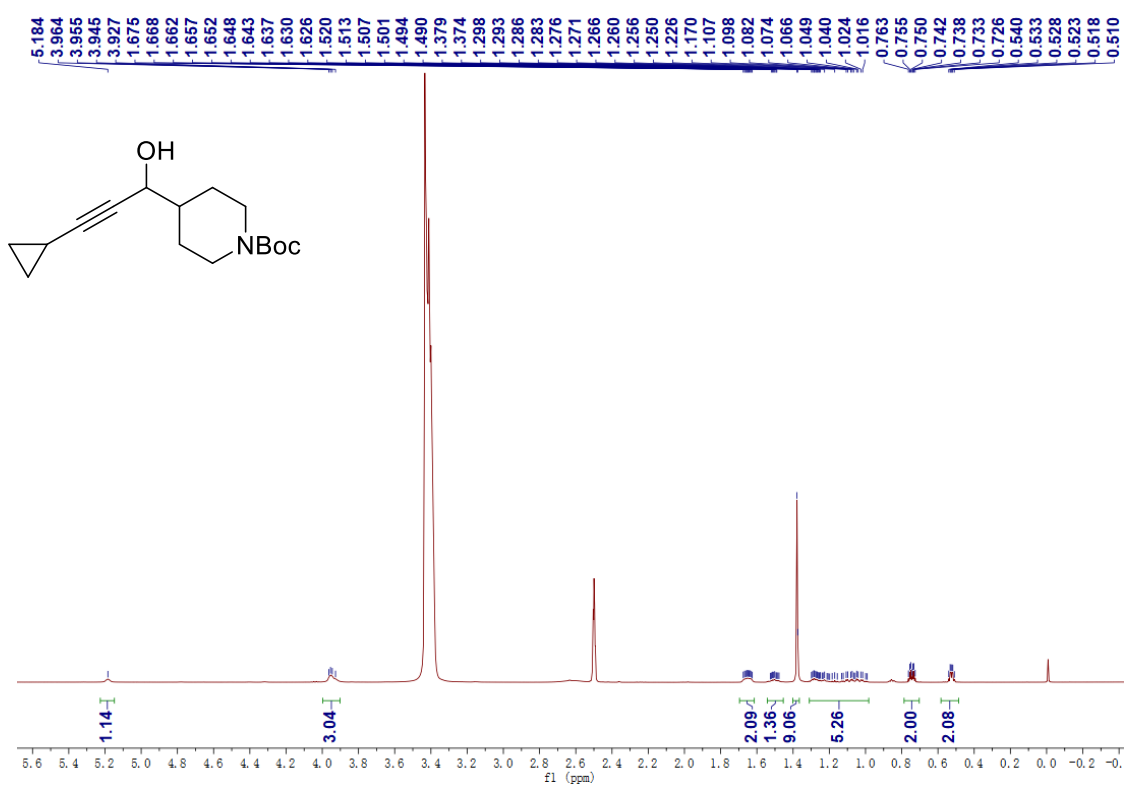
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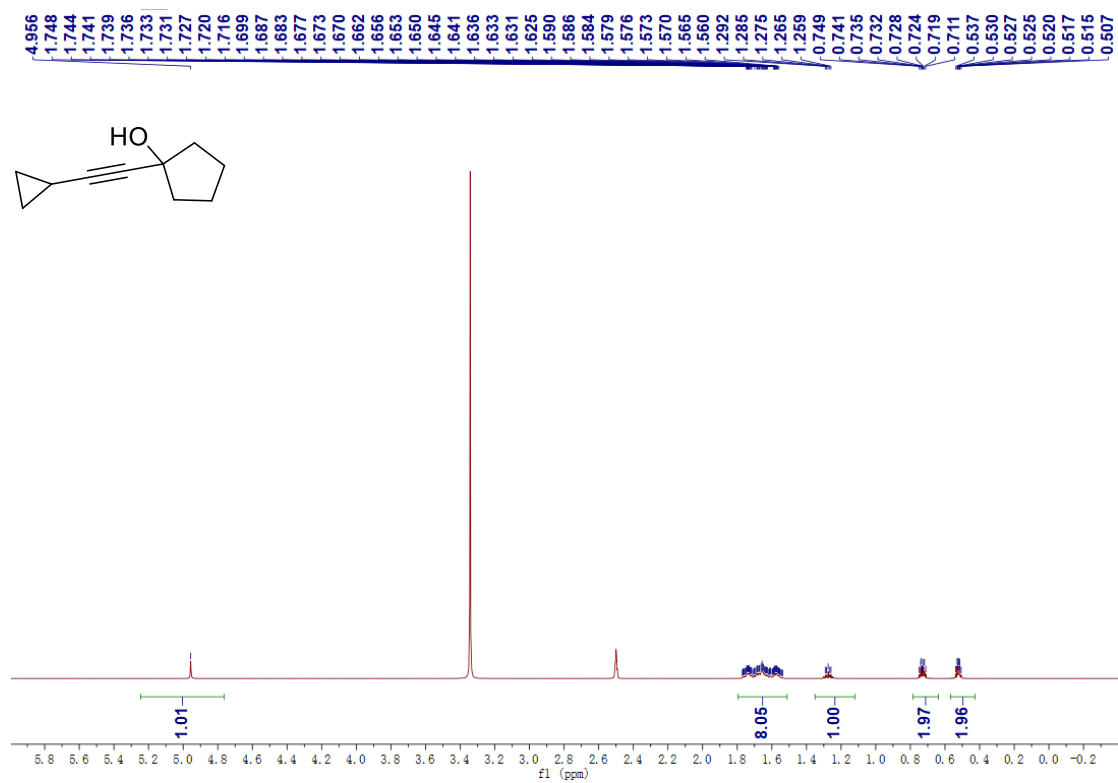
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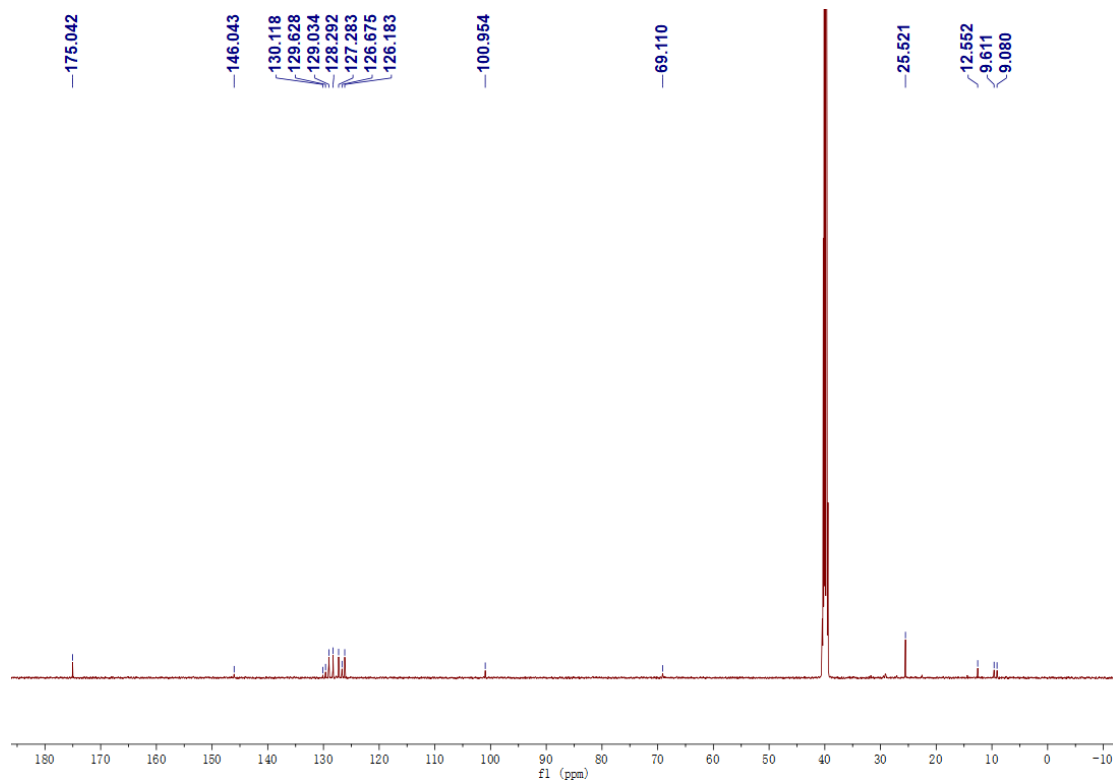
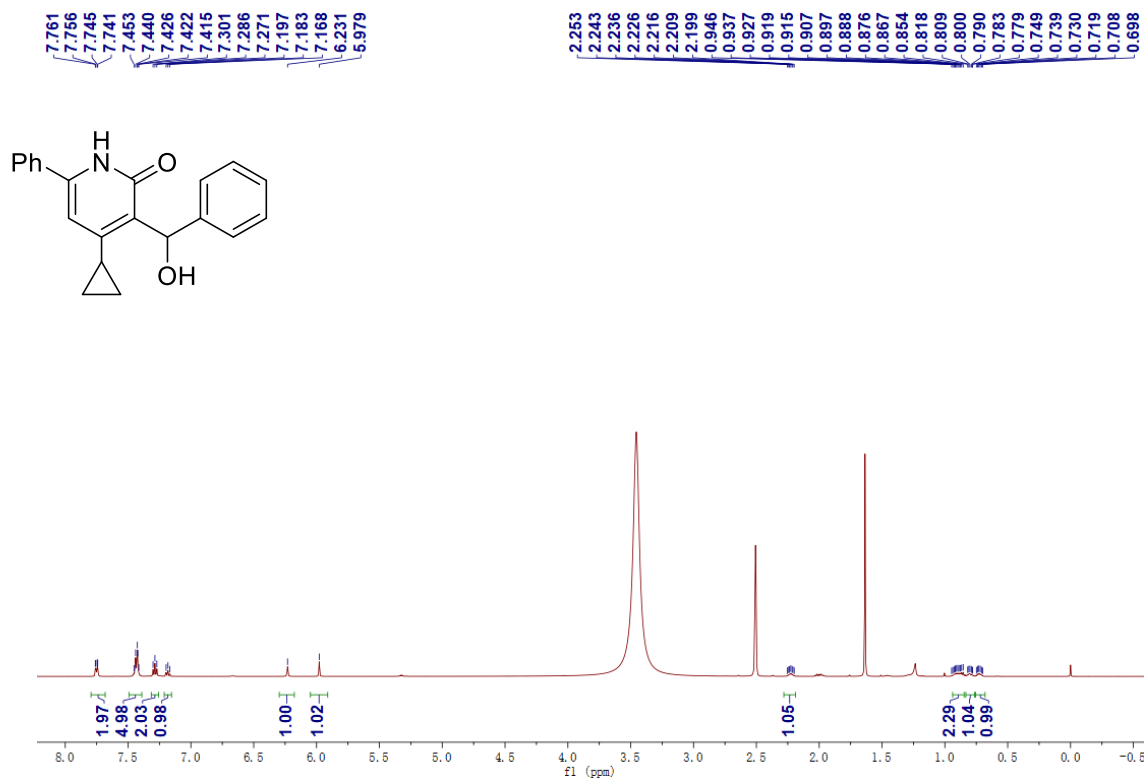
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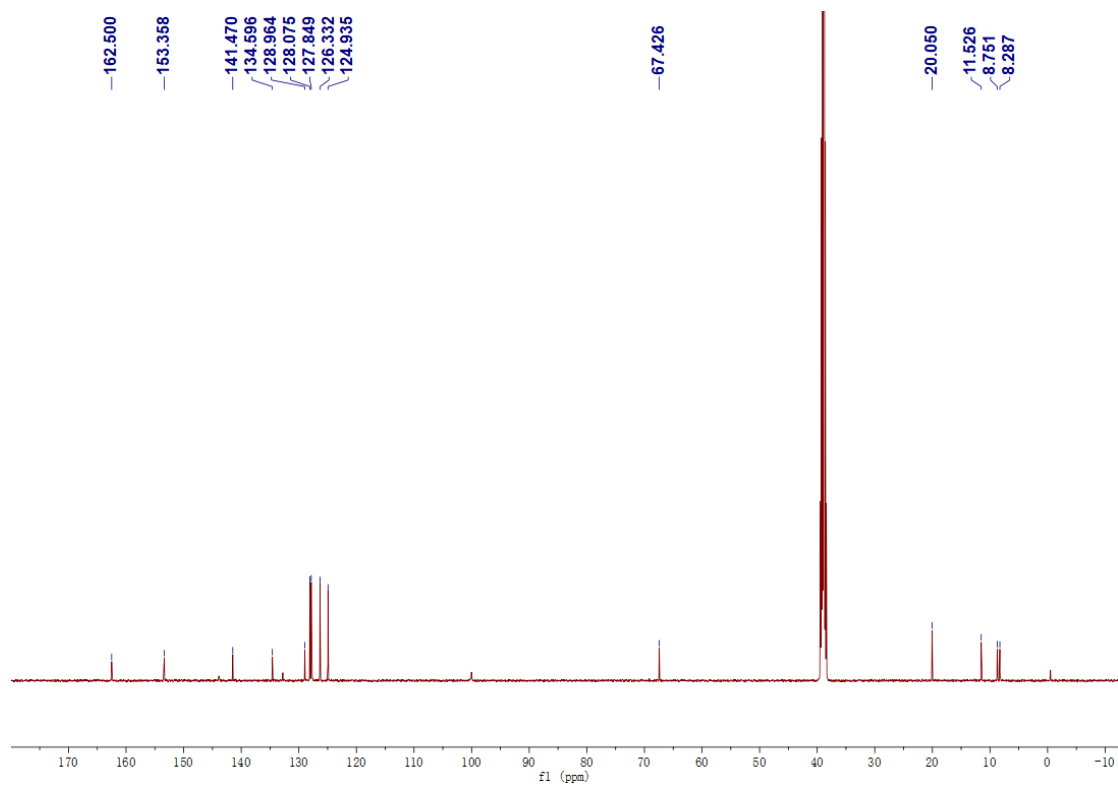
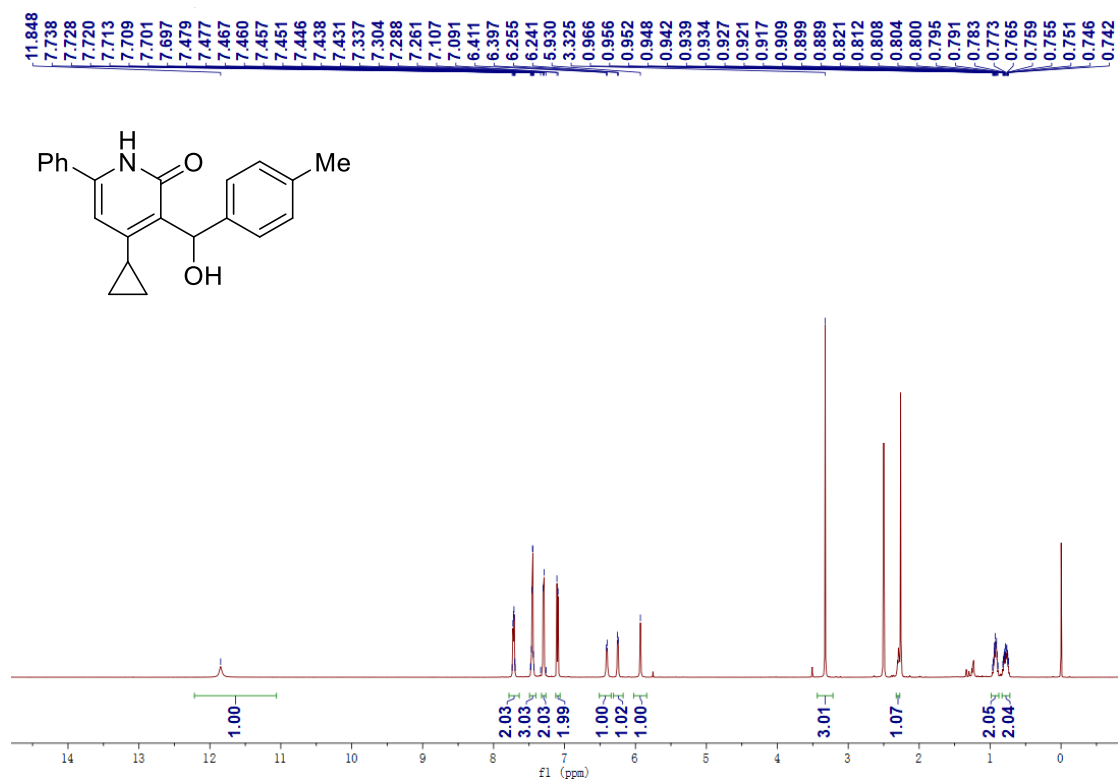
1-(cyclopropylethynyl)cyclopentan-1-ol (2t)



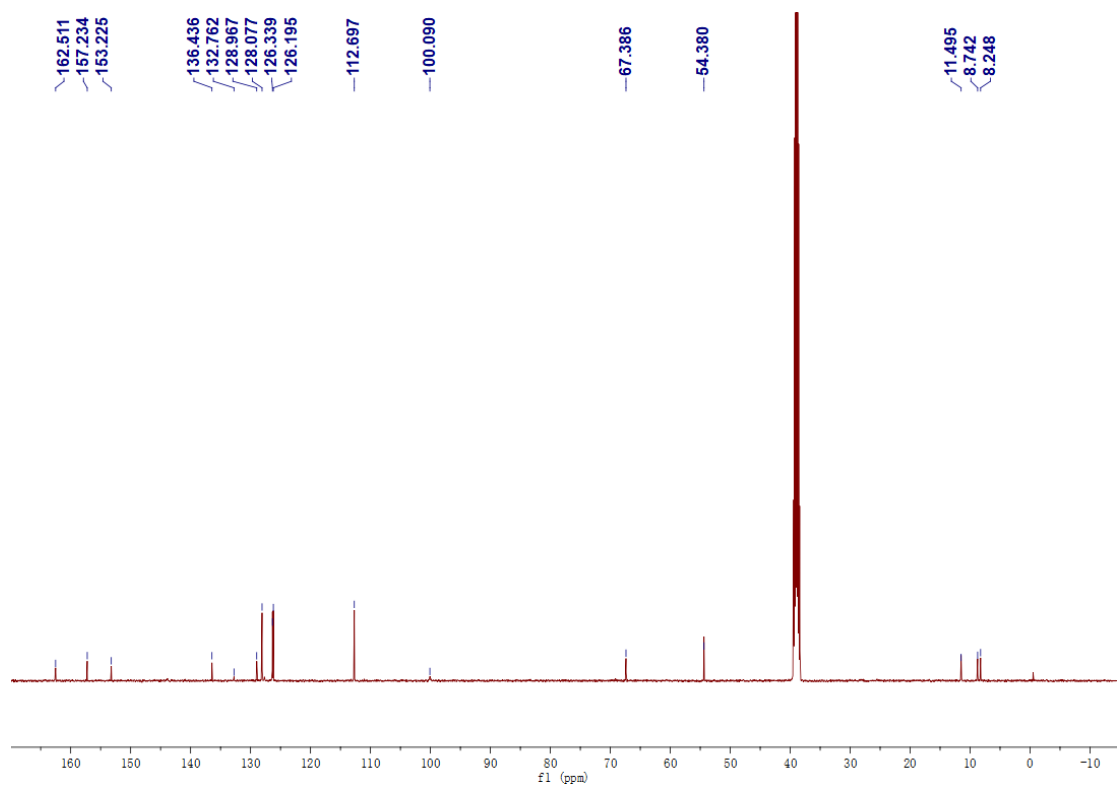
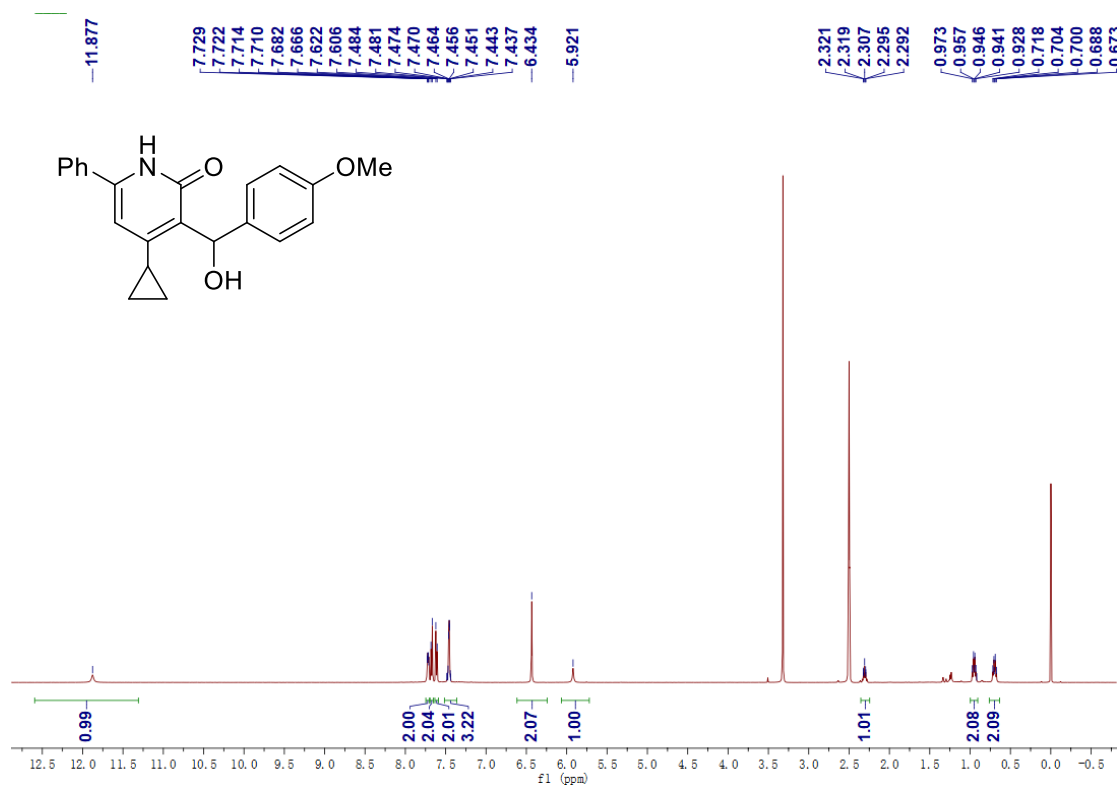
4-cyclopropyl-3-(hydroxy(phenyl)methyl)-6-phenylpyridin-2(1H)-one (3a)



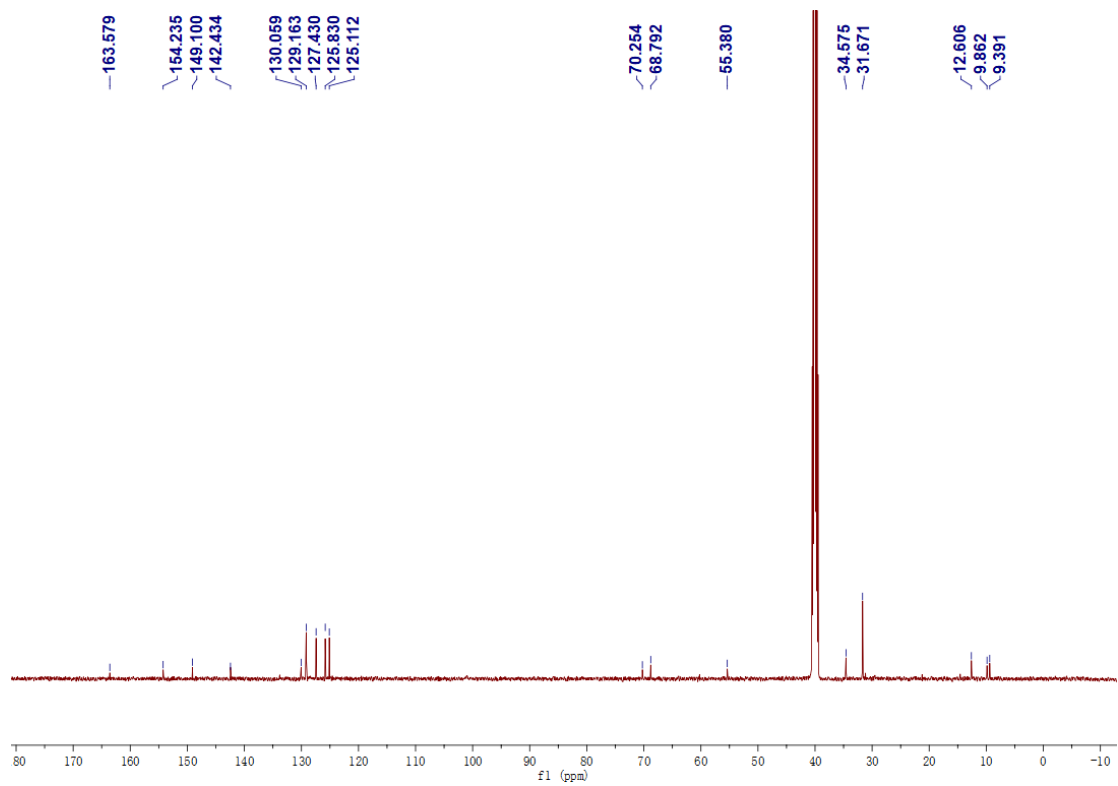
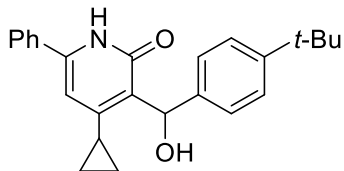
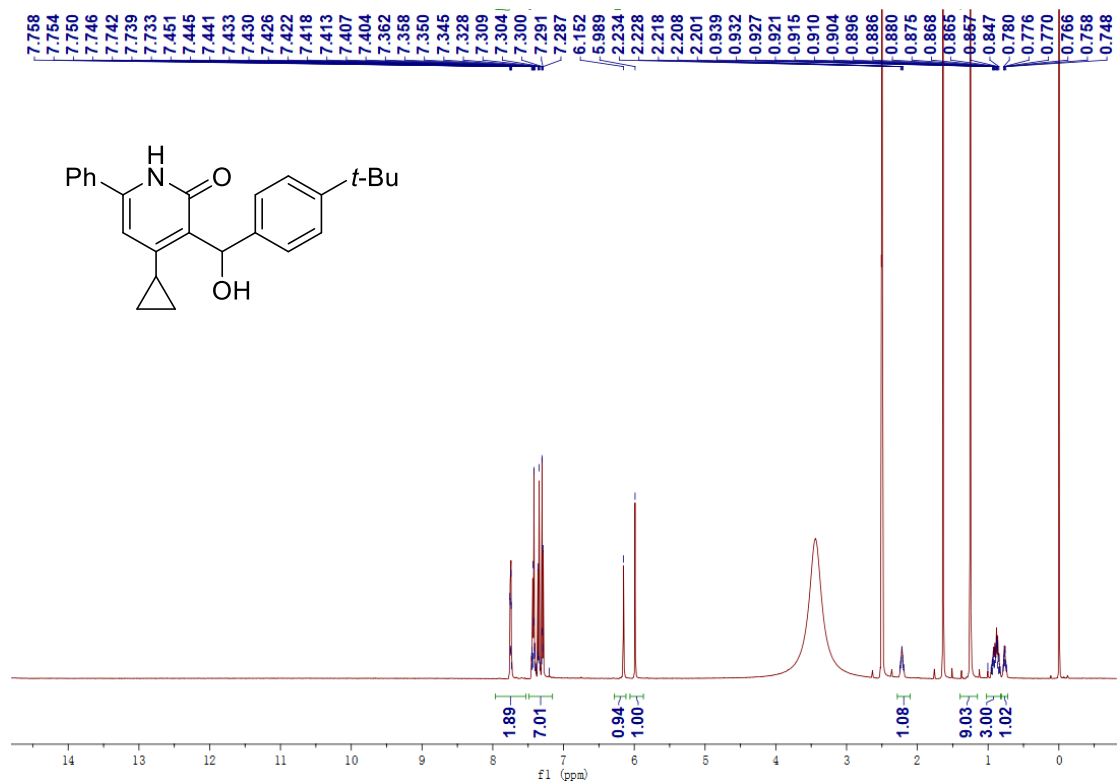
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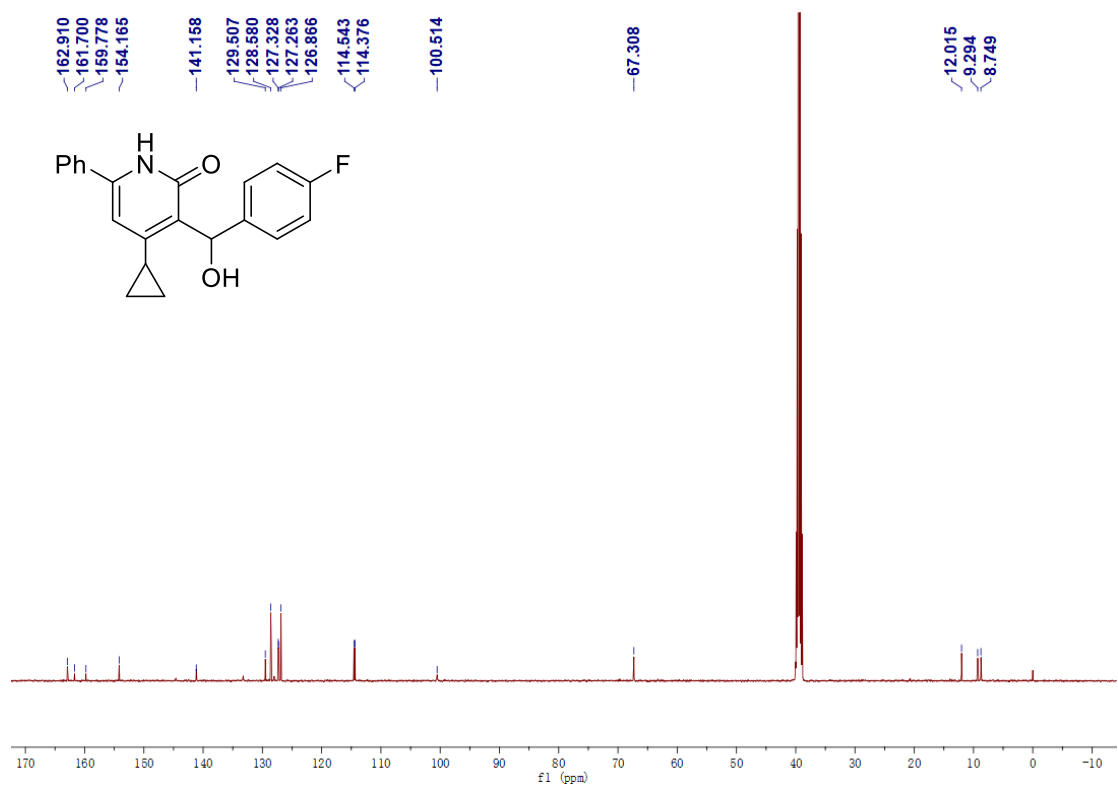
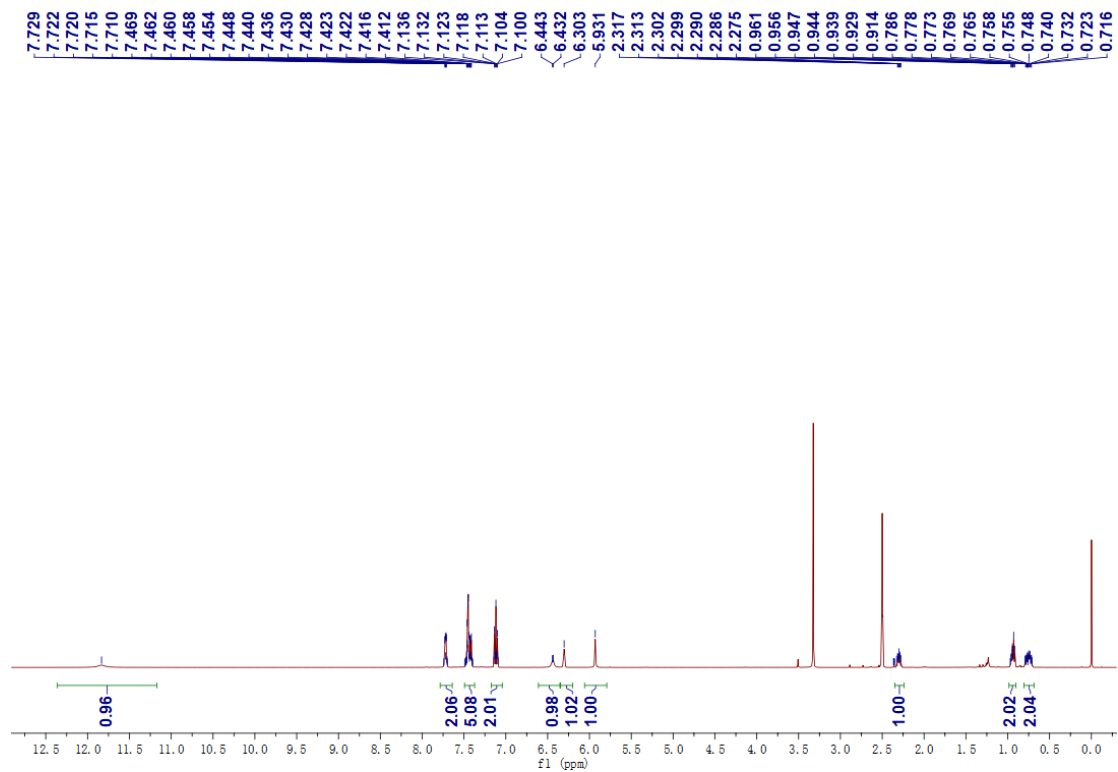
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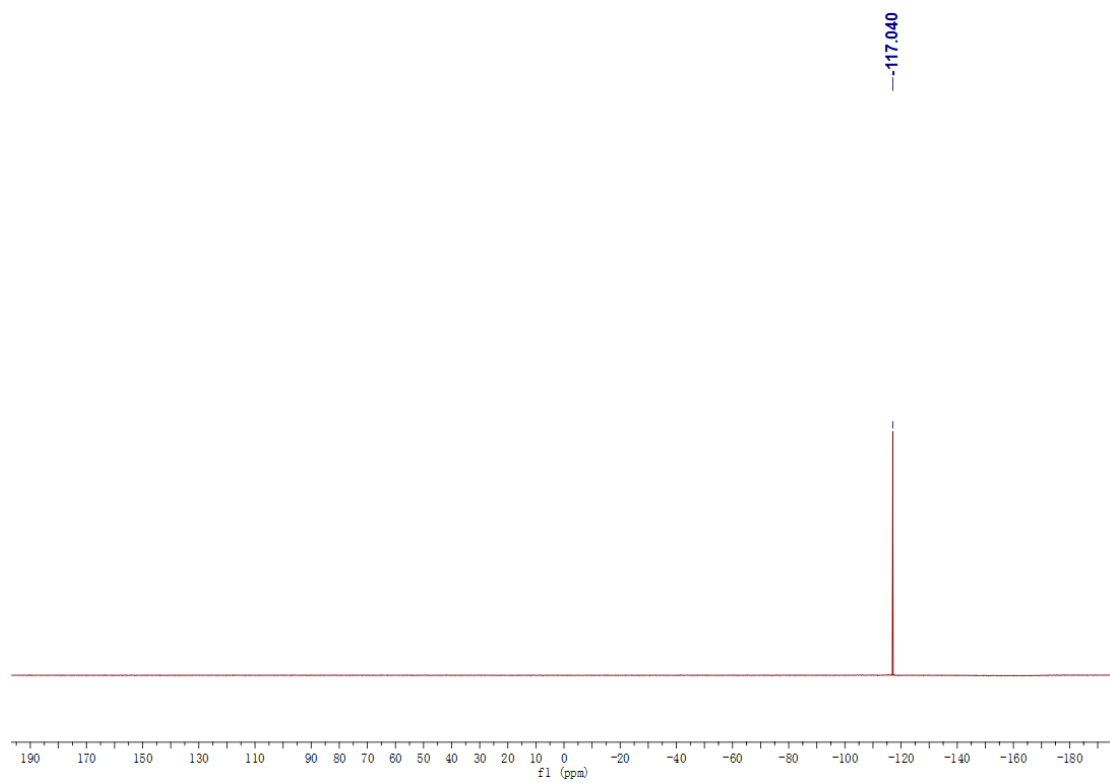


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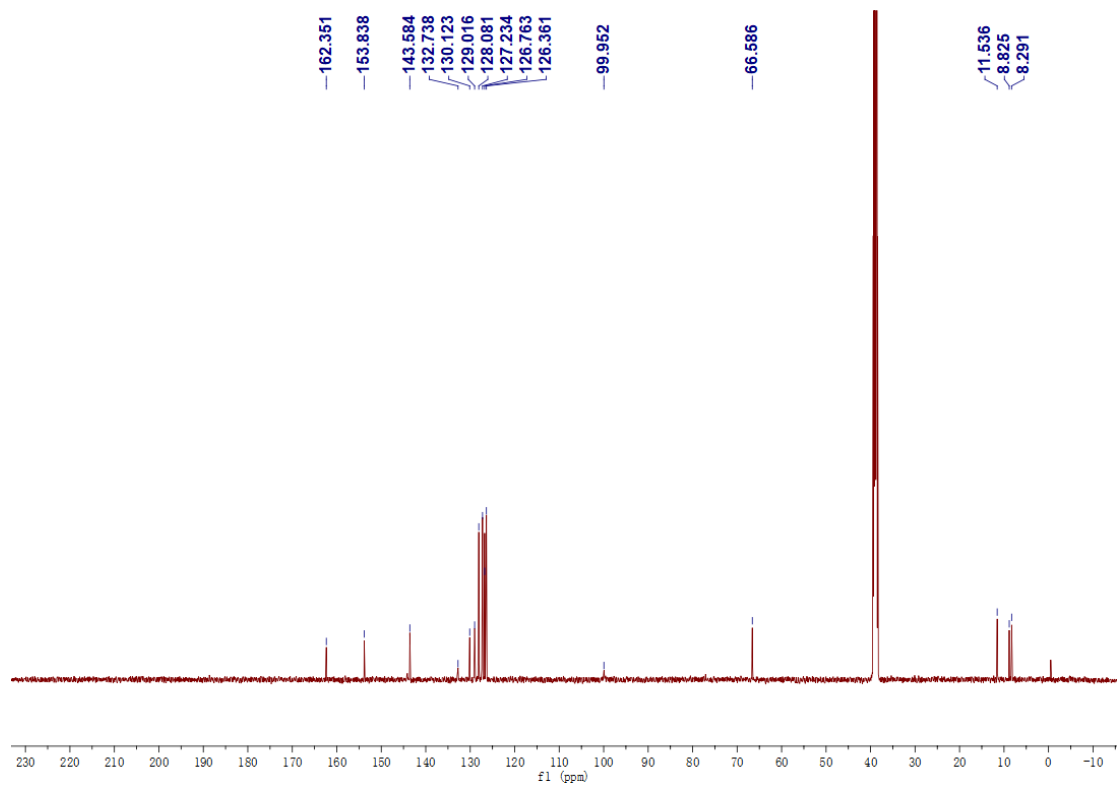
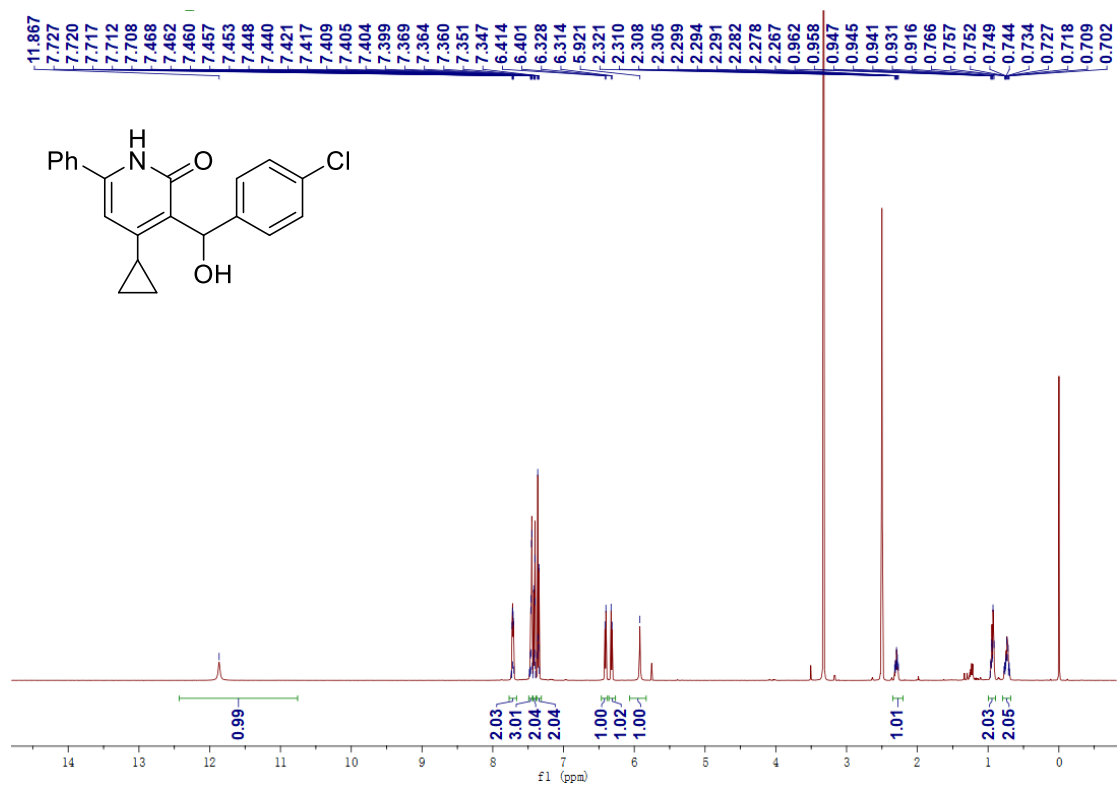


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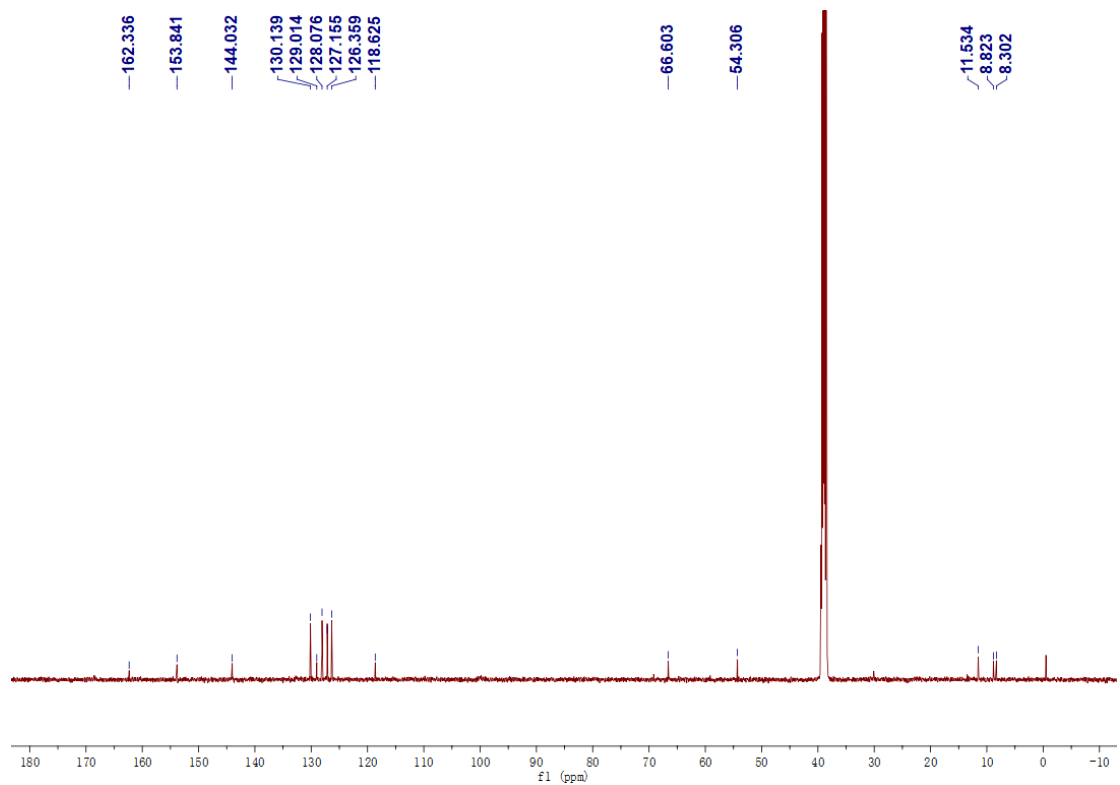
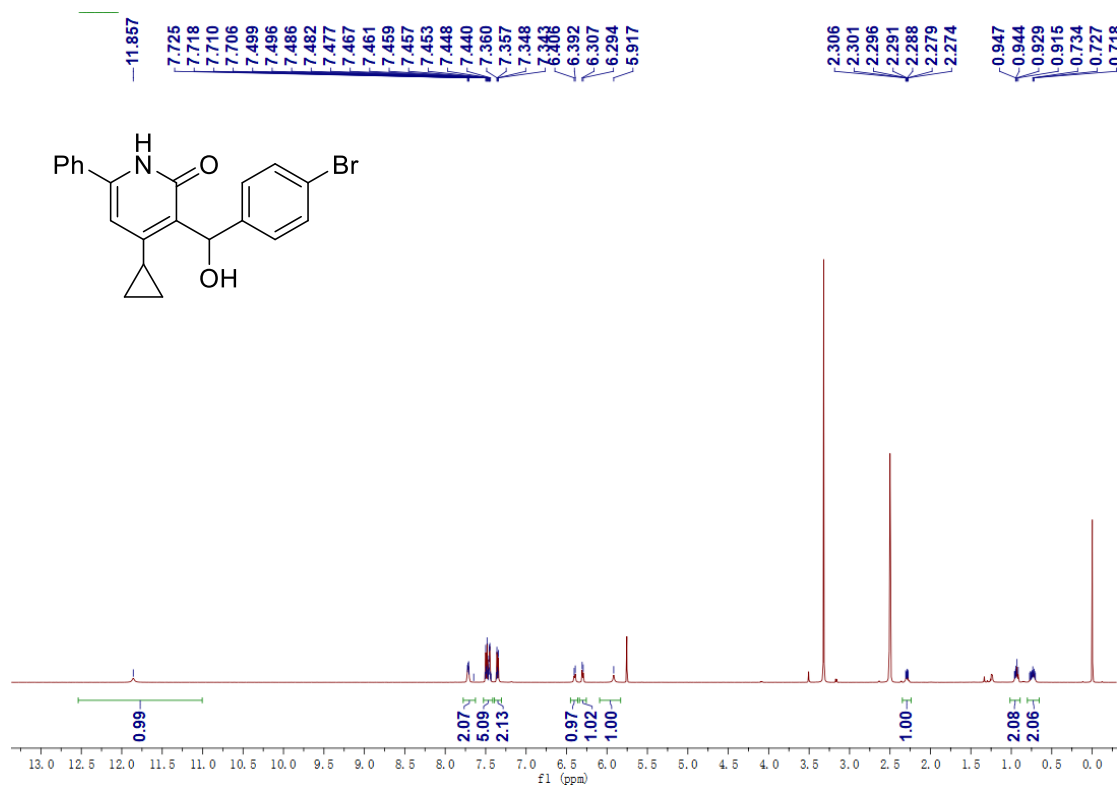




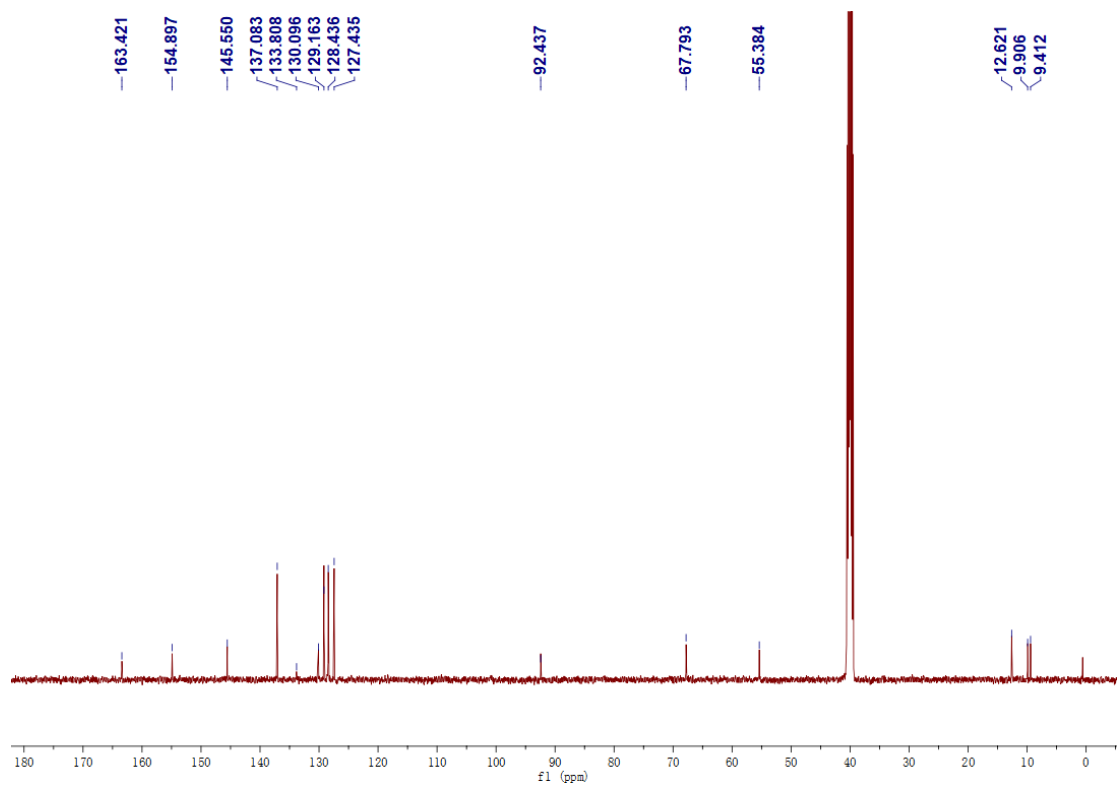
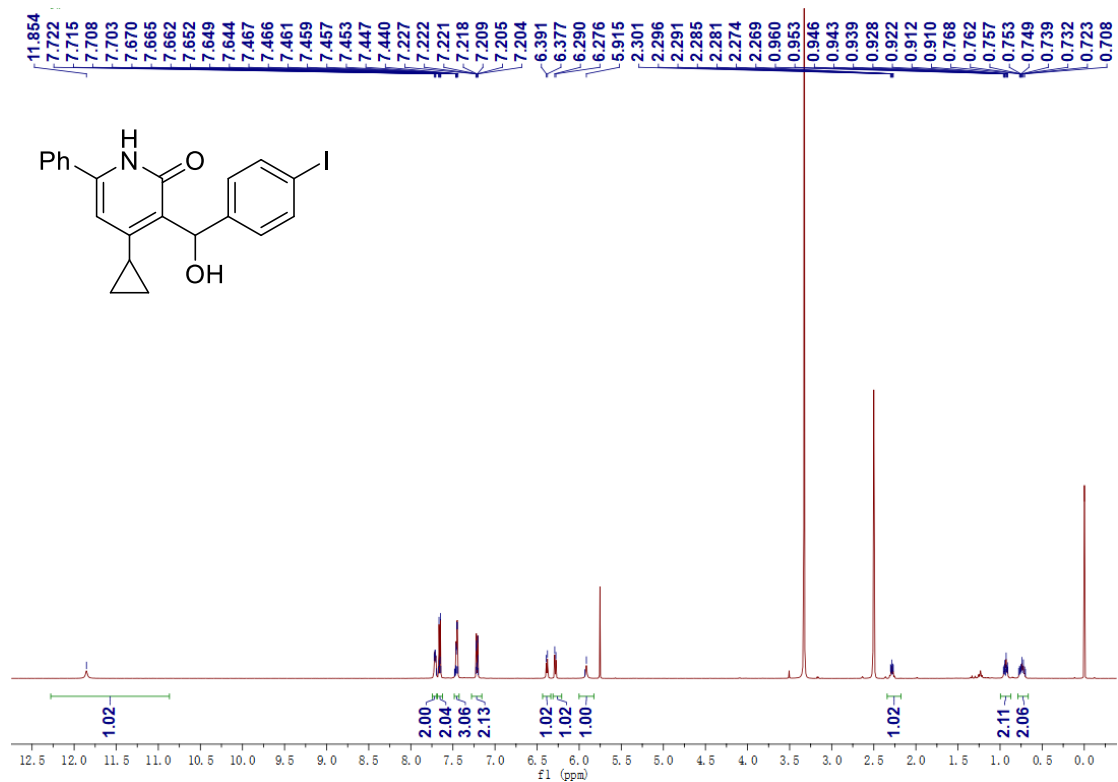
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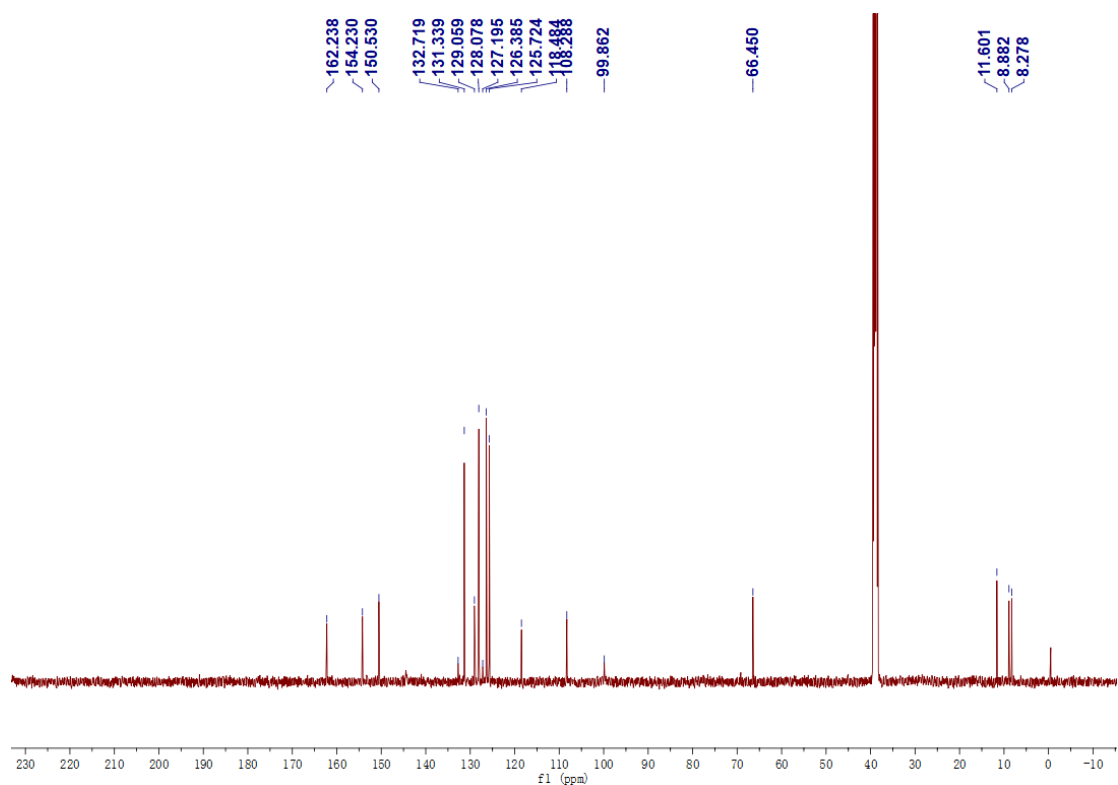
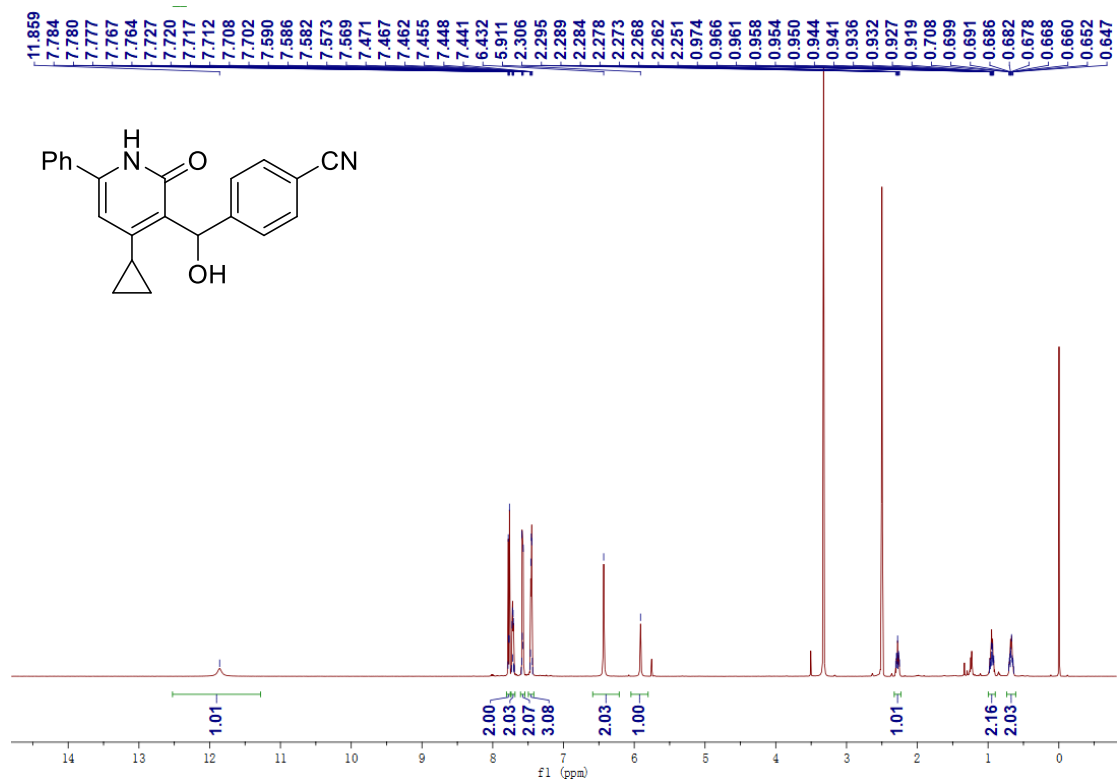
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3-cyclopropyl-3-(hydroxy(4-iodophenyl)methyl)-6-phenylpyridin-2(1H)-one (3h)

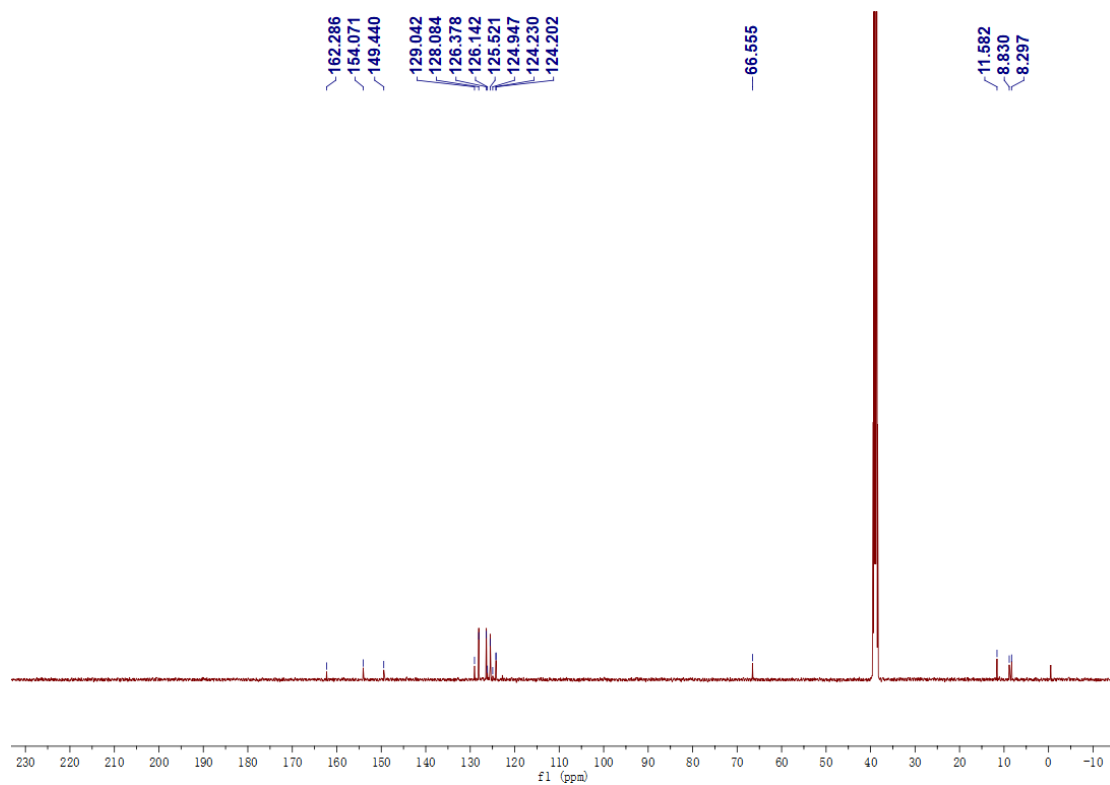
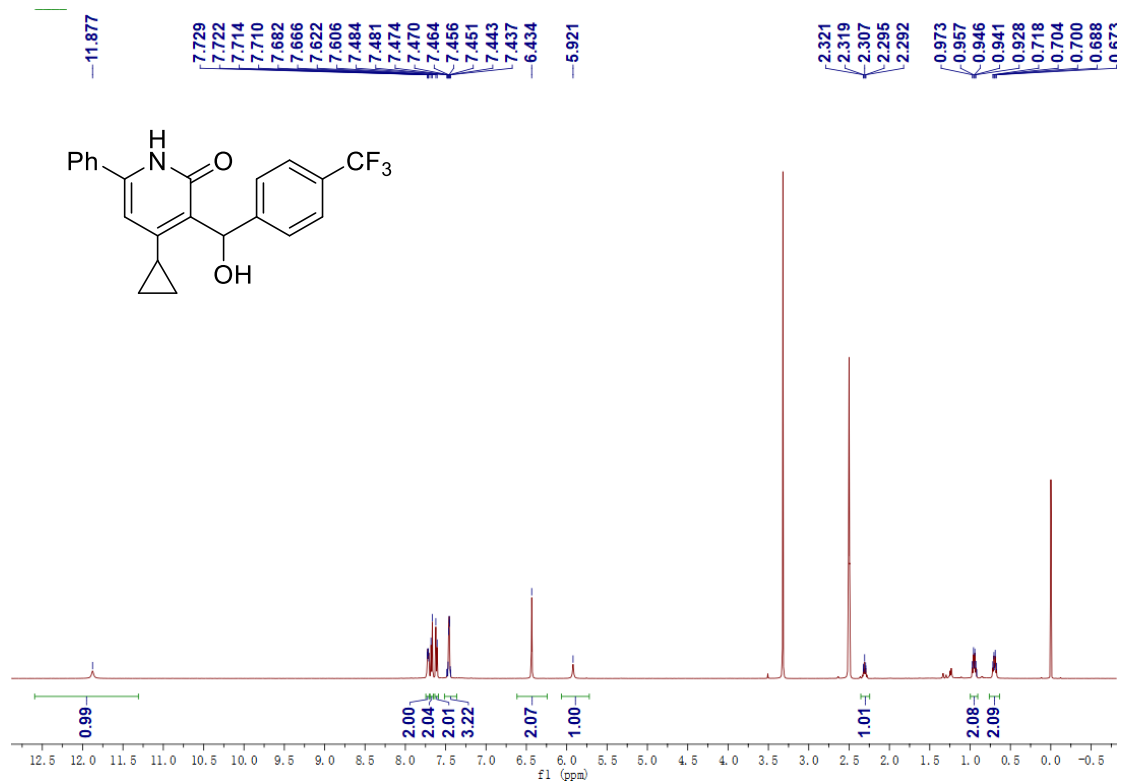


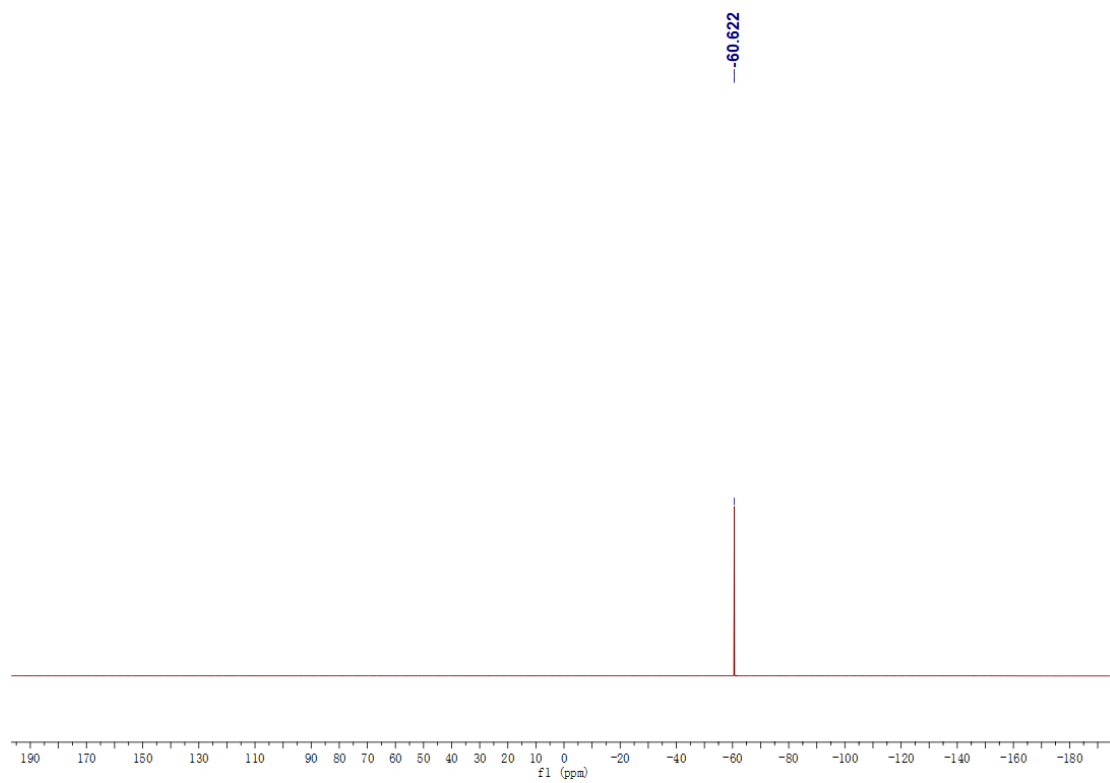
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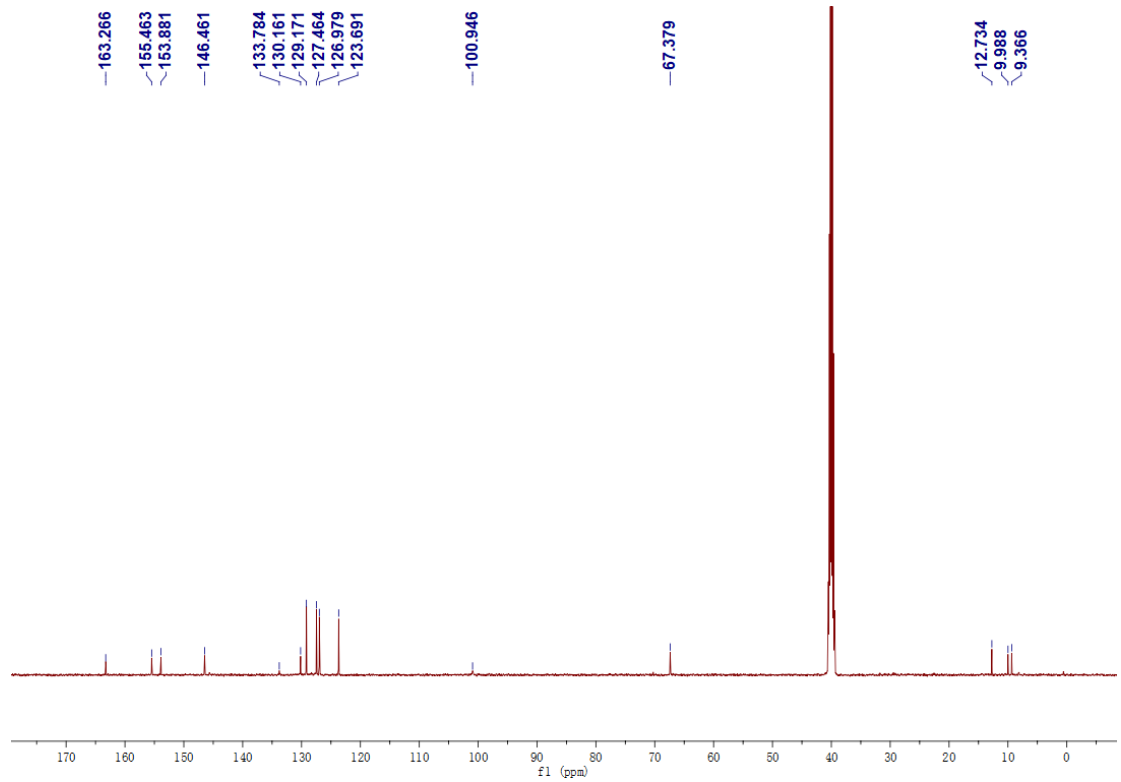
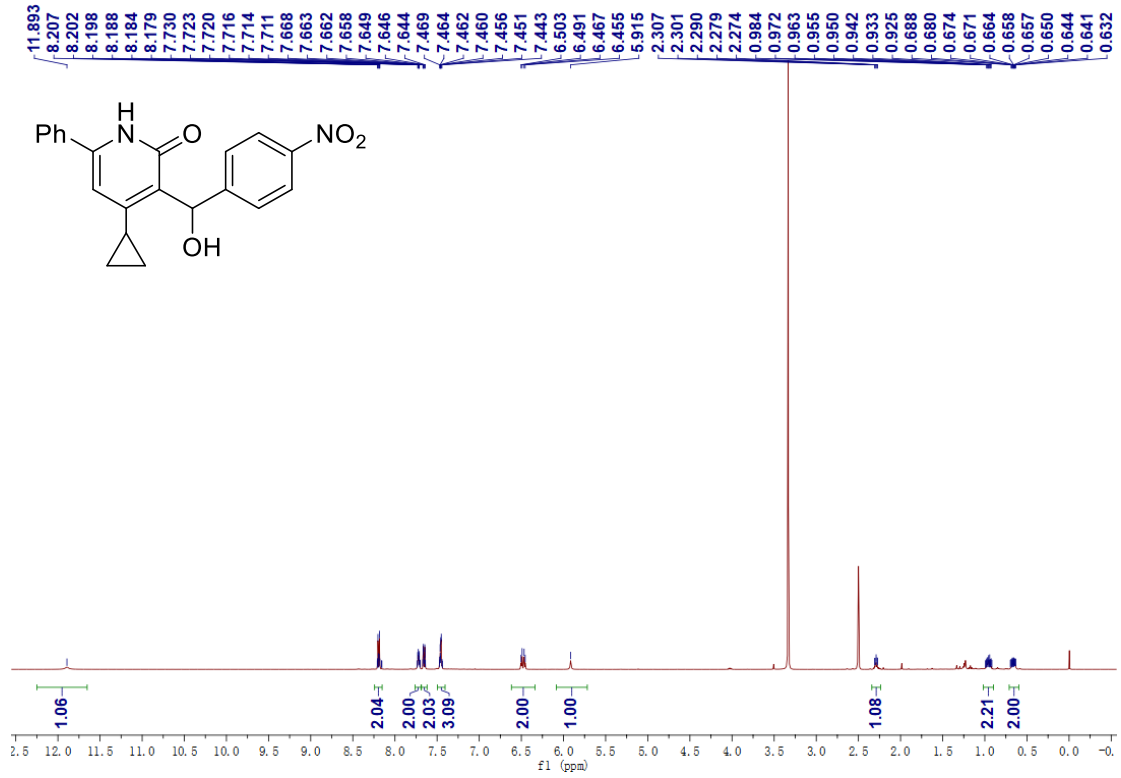
4-cyclopropyl-3-(hydroxy(4-(trifluoromethyl)phenyl)methyl)-6-phenylpyridin-2(1H)-one

(3j)

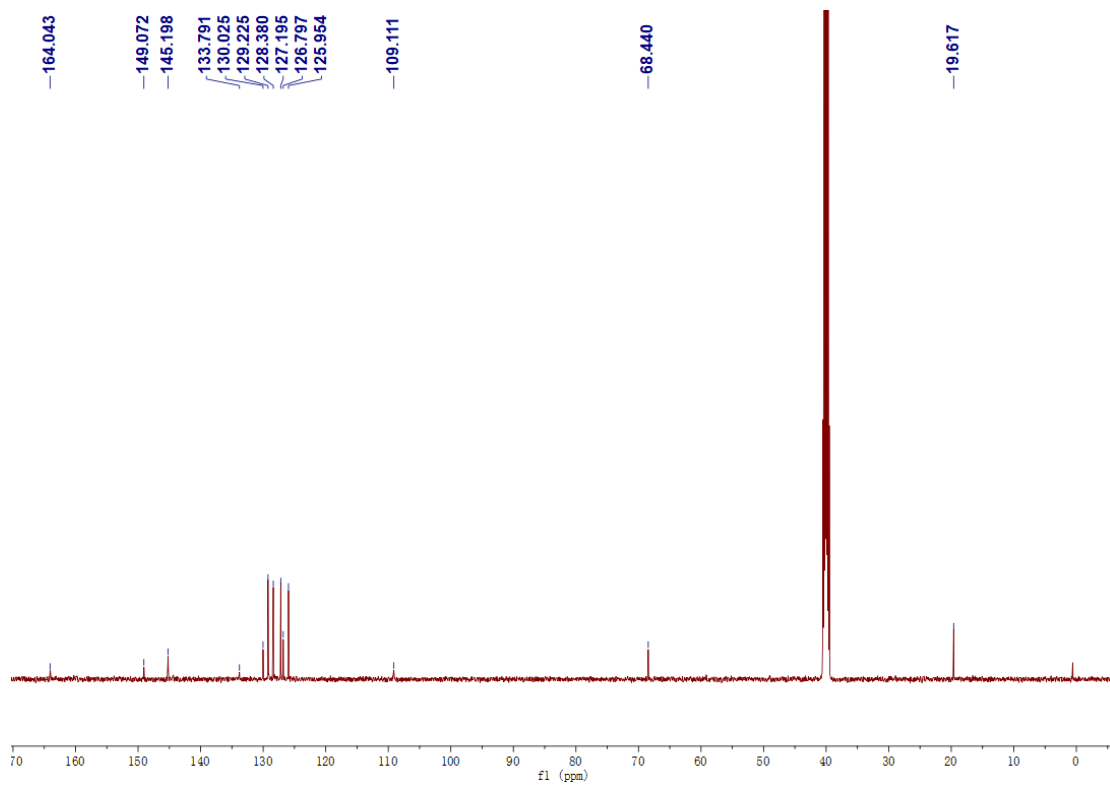
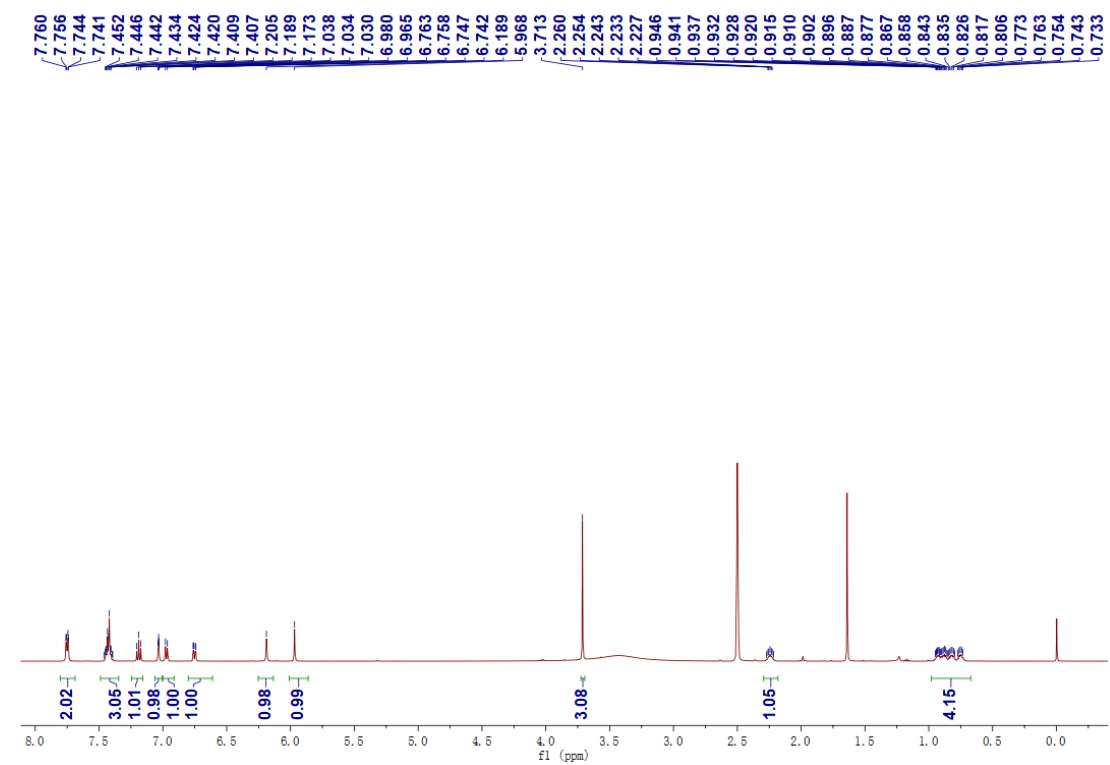




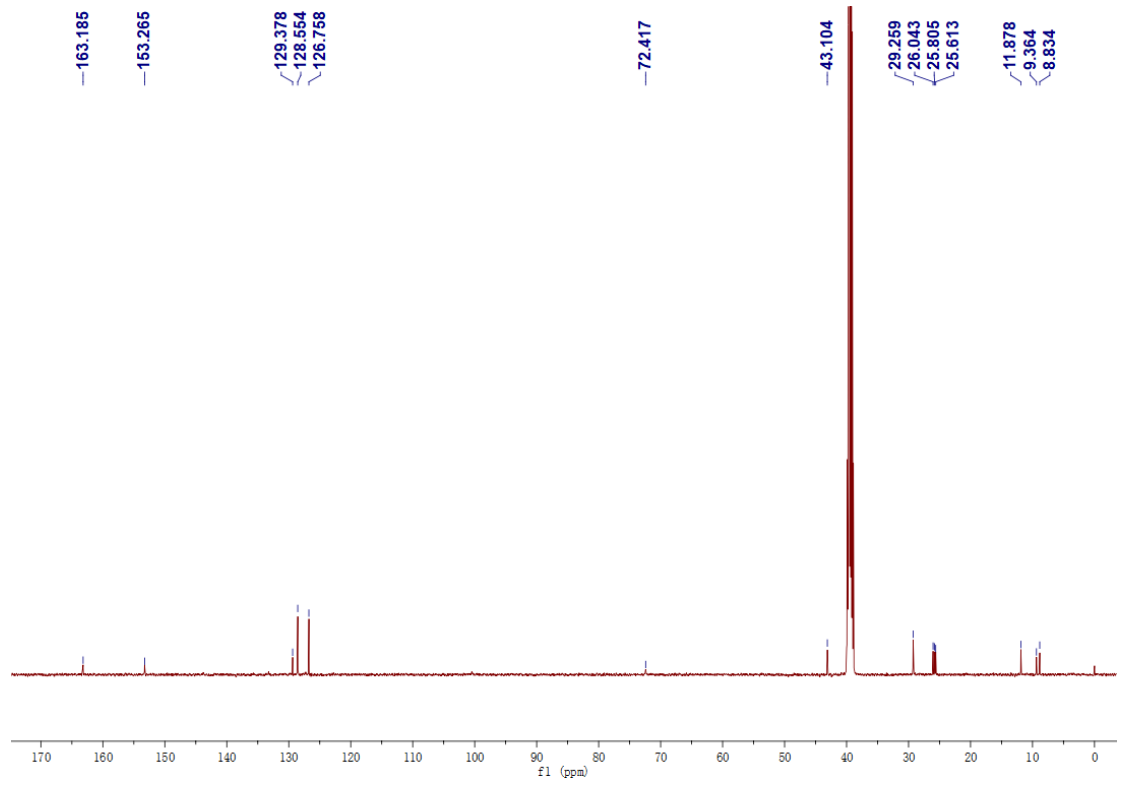
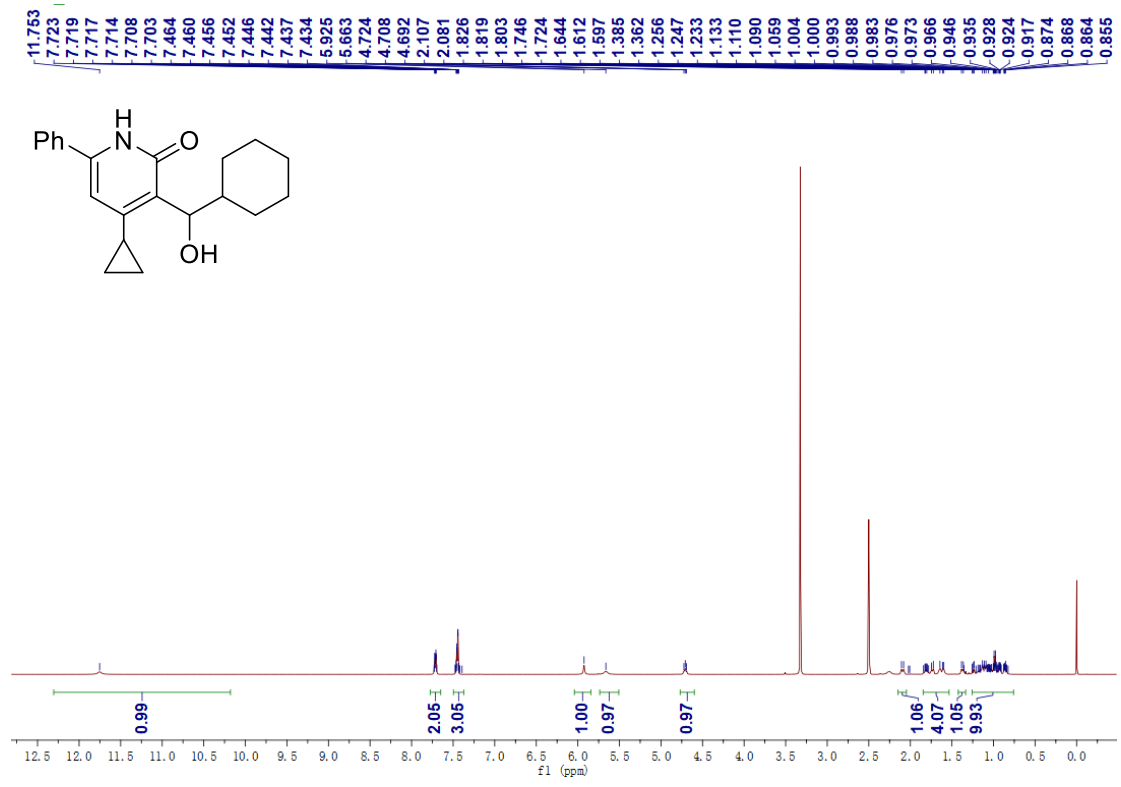
4-cyclopropyl-3-(hydroxy(4-nitrophenyl)methyl)-6-phenylpyridin-2(1H)-one (3k)



4-cyclopropyl-3-(hydroxy(3-methoxyphenyl)methyl)-6-phenylpyridin-2(1H)-one (3l)



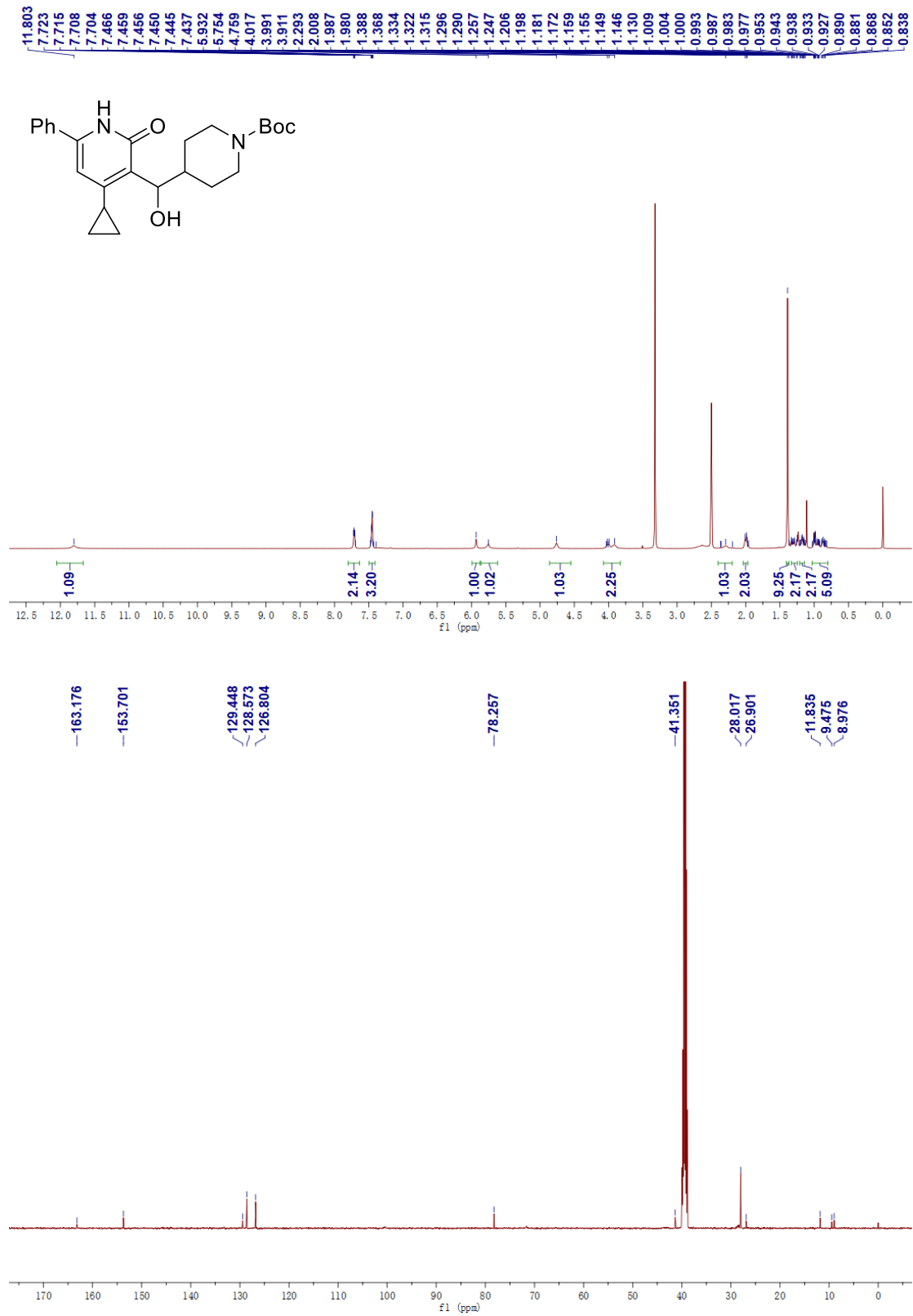
3-(cyclohexyl(hydroxy)methyl)-4-cyclopropyl-6-phenylpyridin-2(1H)-one (3m)



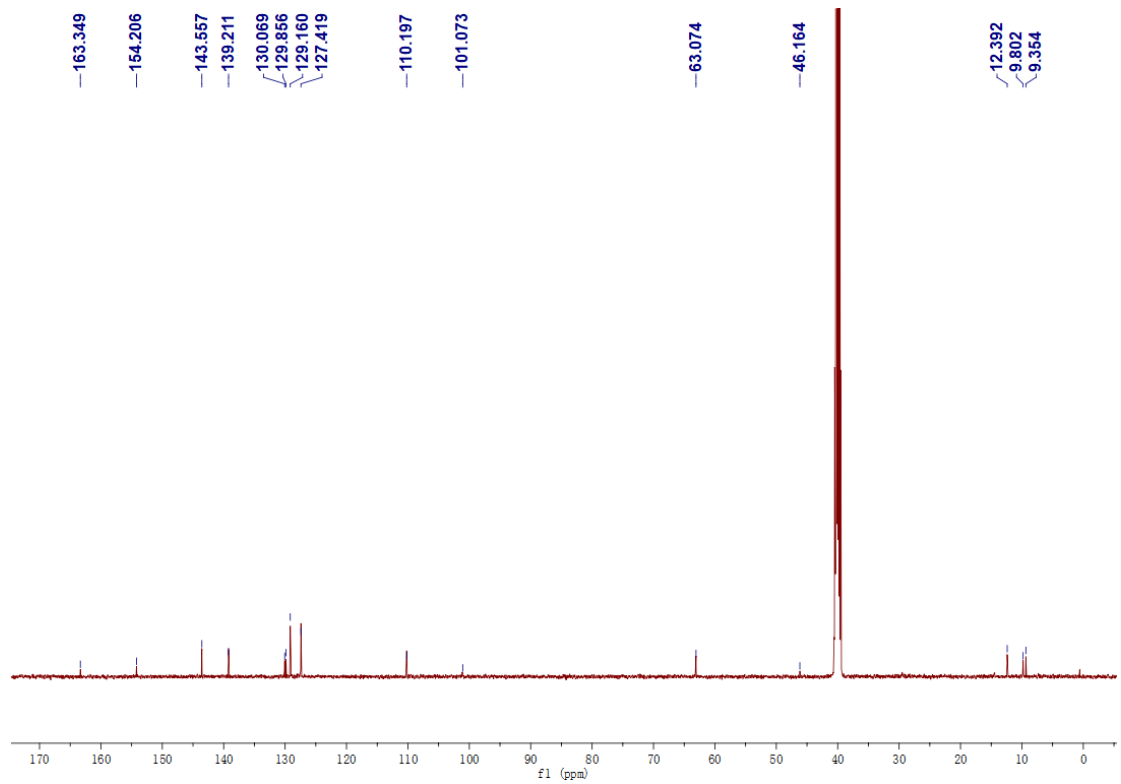
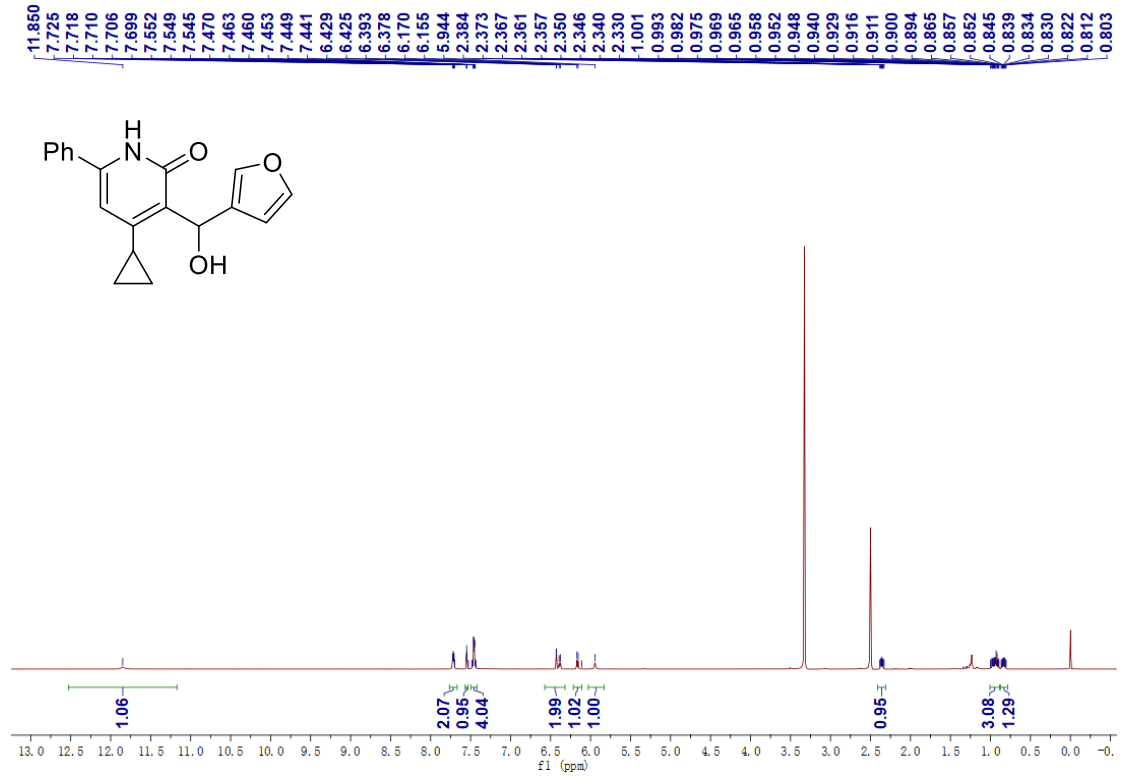
tert-butyl

4-((4-cyclopropyl-2-oxo-6-phenyl-1,2-dihydropyridin-3-

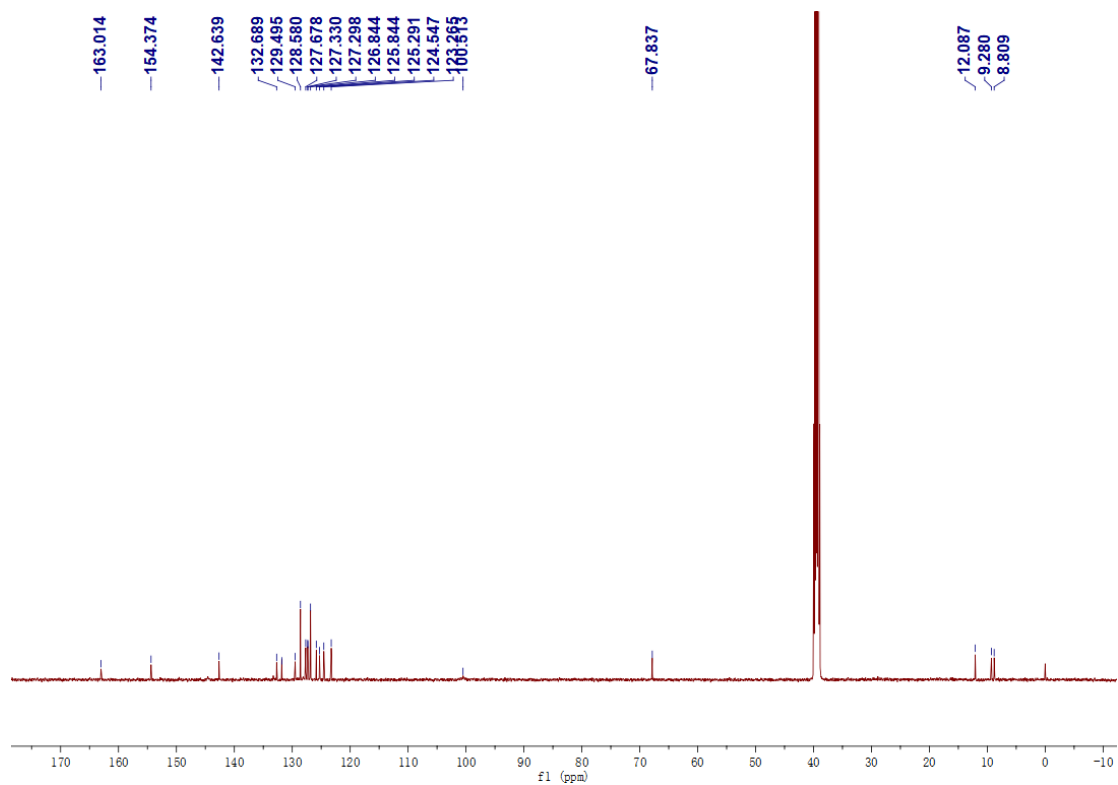
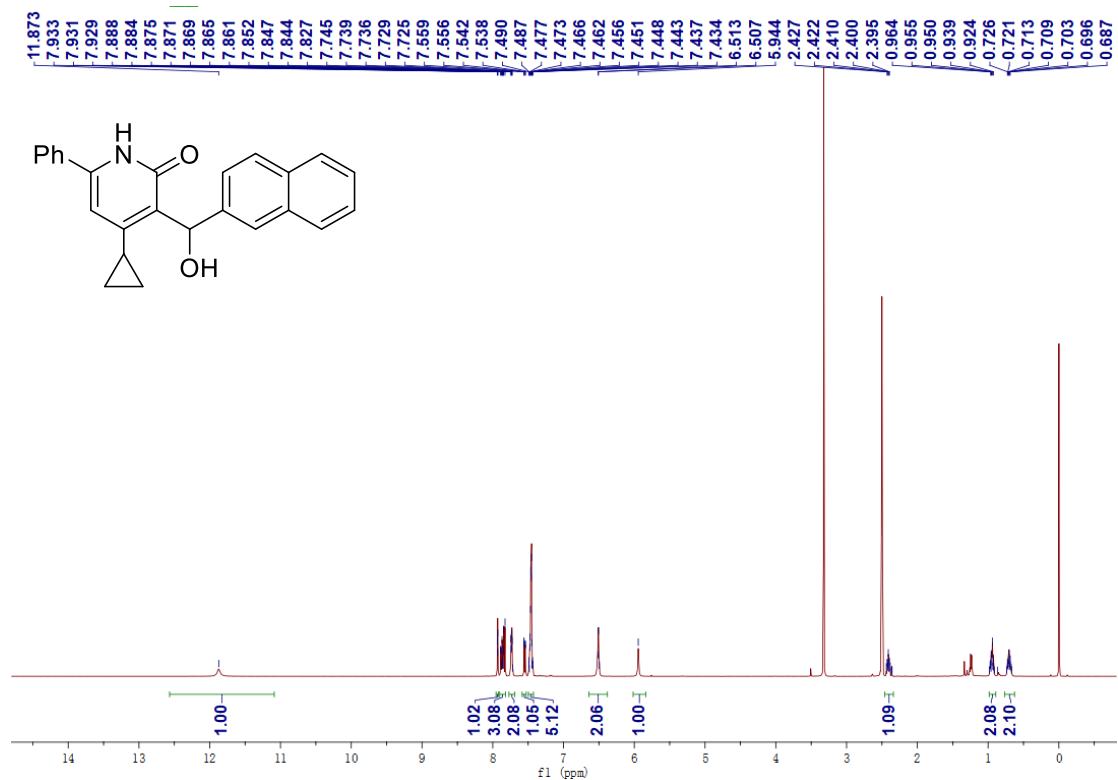
yl)(hydroxy)methyl)piperidine-1-carboxylate (3n)



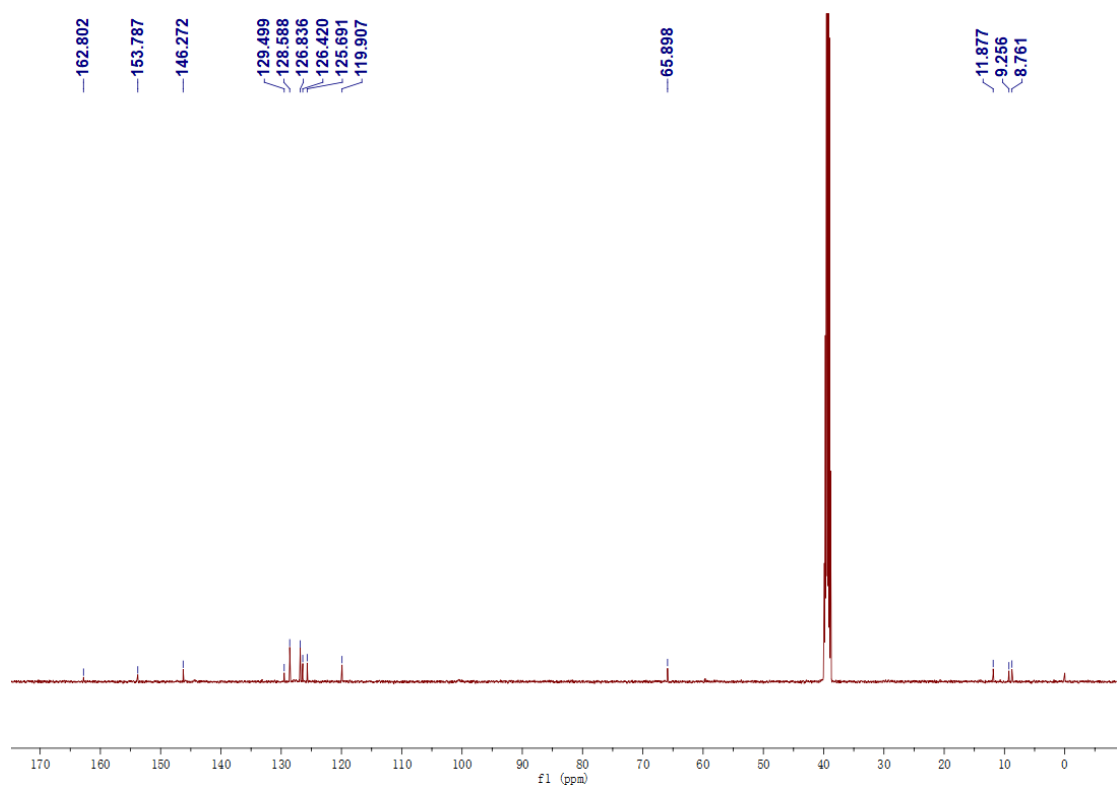
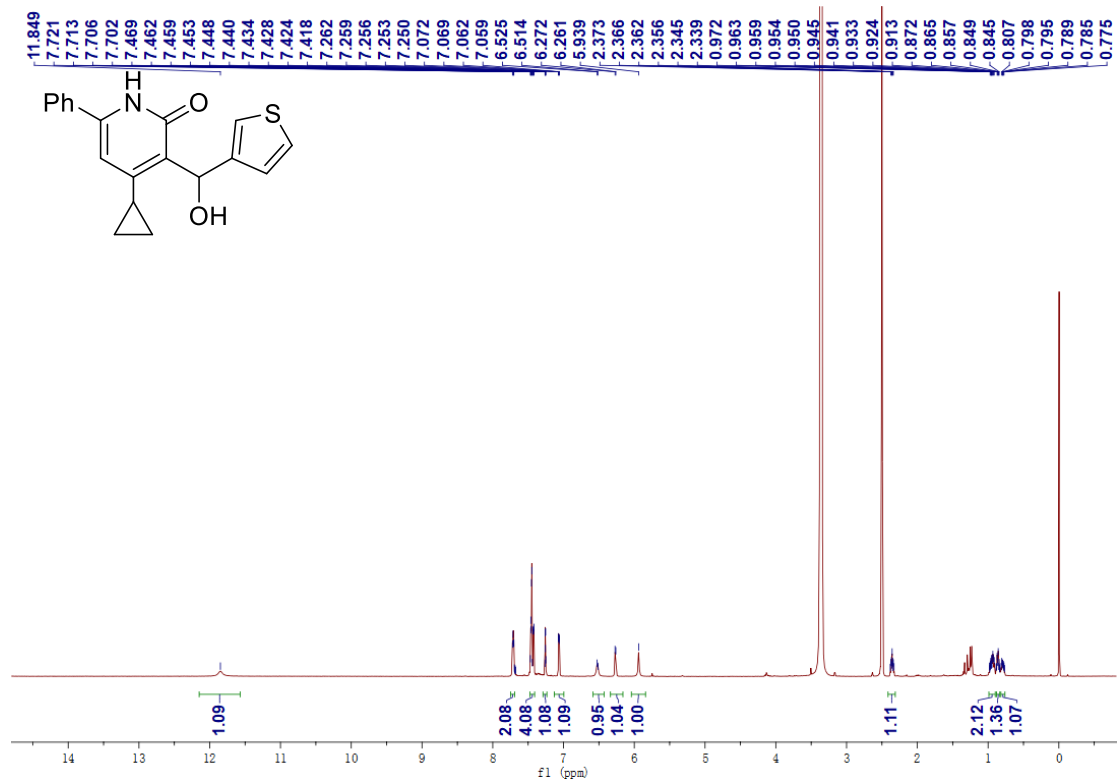
3-cyclopropyl-3-(furan-3-yl(hydroxy)methyl)-6-phenylpyridin-2(1H)-one (3o)



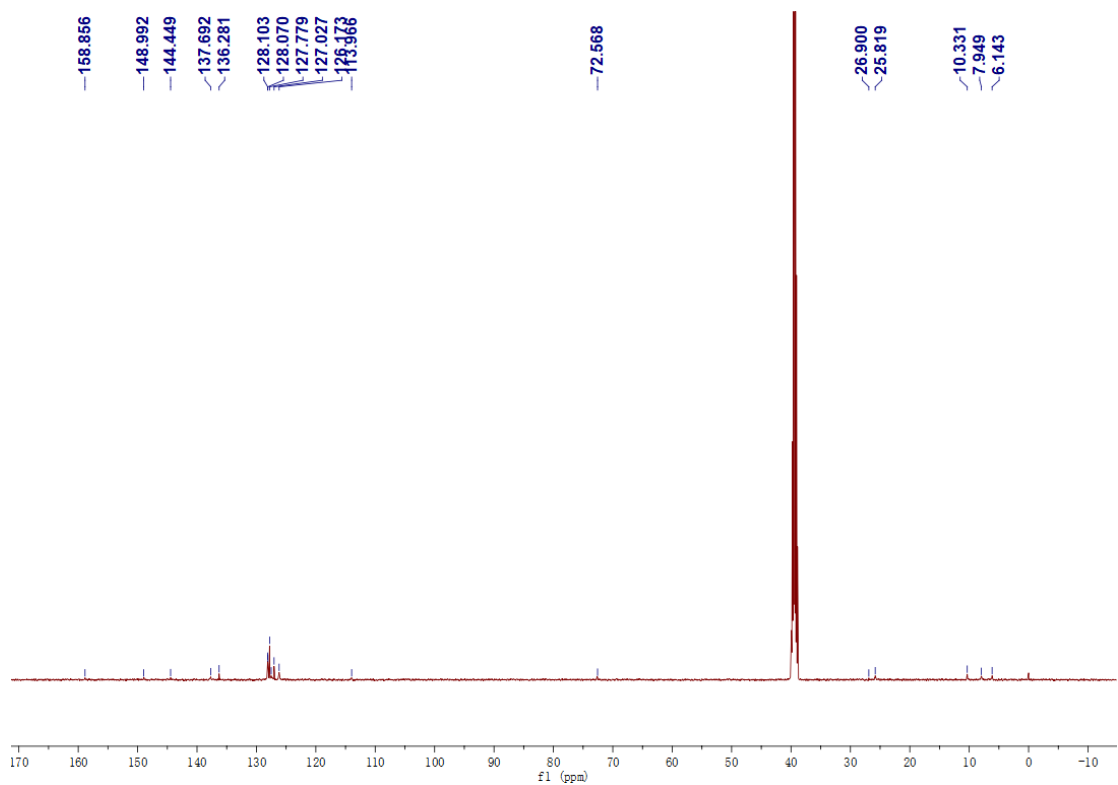
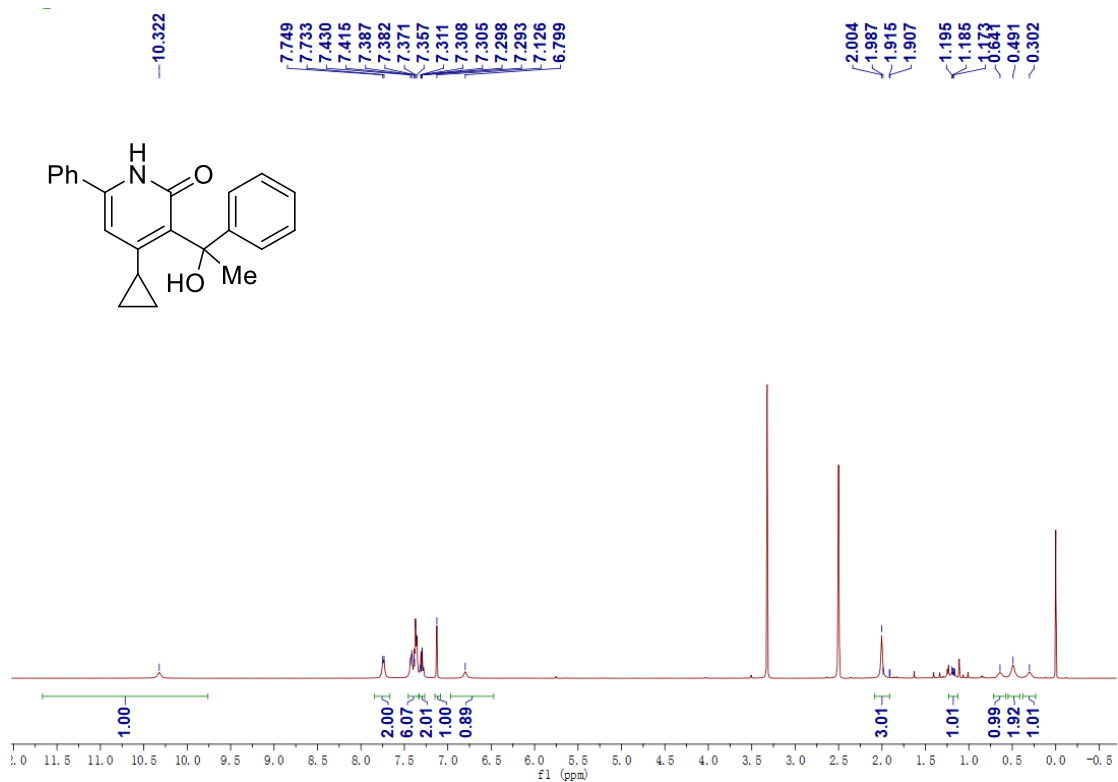
3-cyclopropyl-3-(hydroxy(naphthalen-2-yl)methyl)-6-phenylpyridin-2(1H)-one (3p)



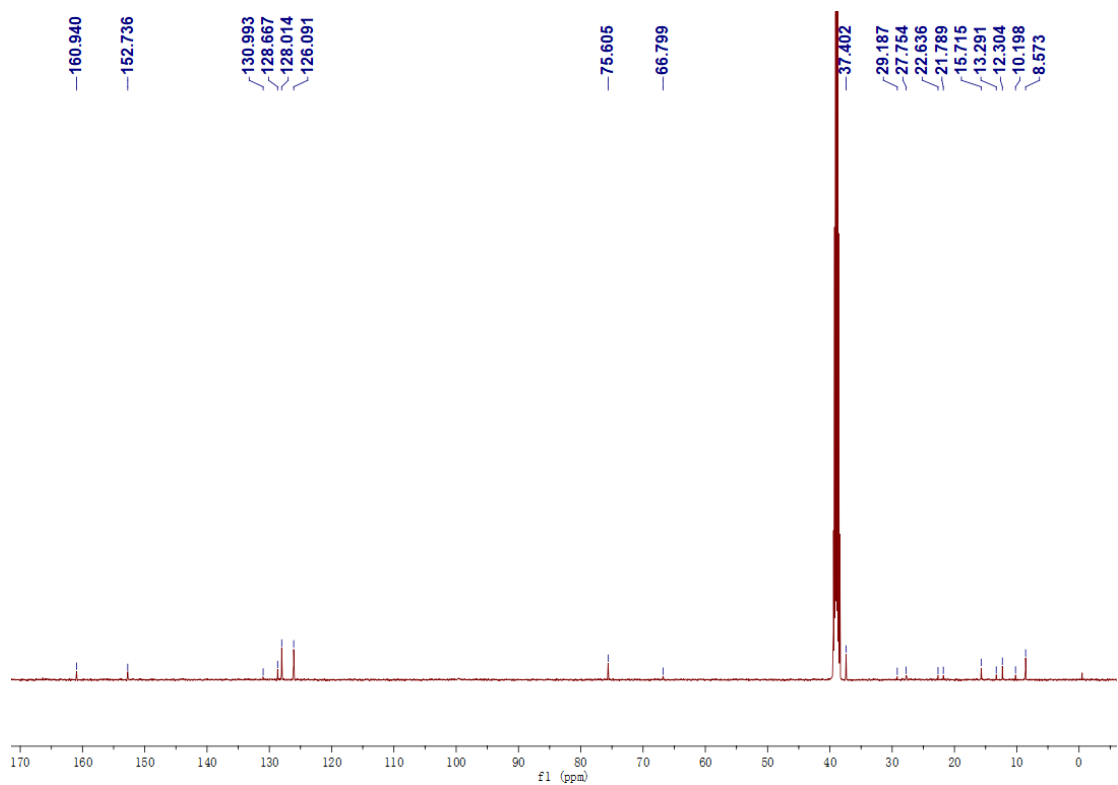
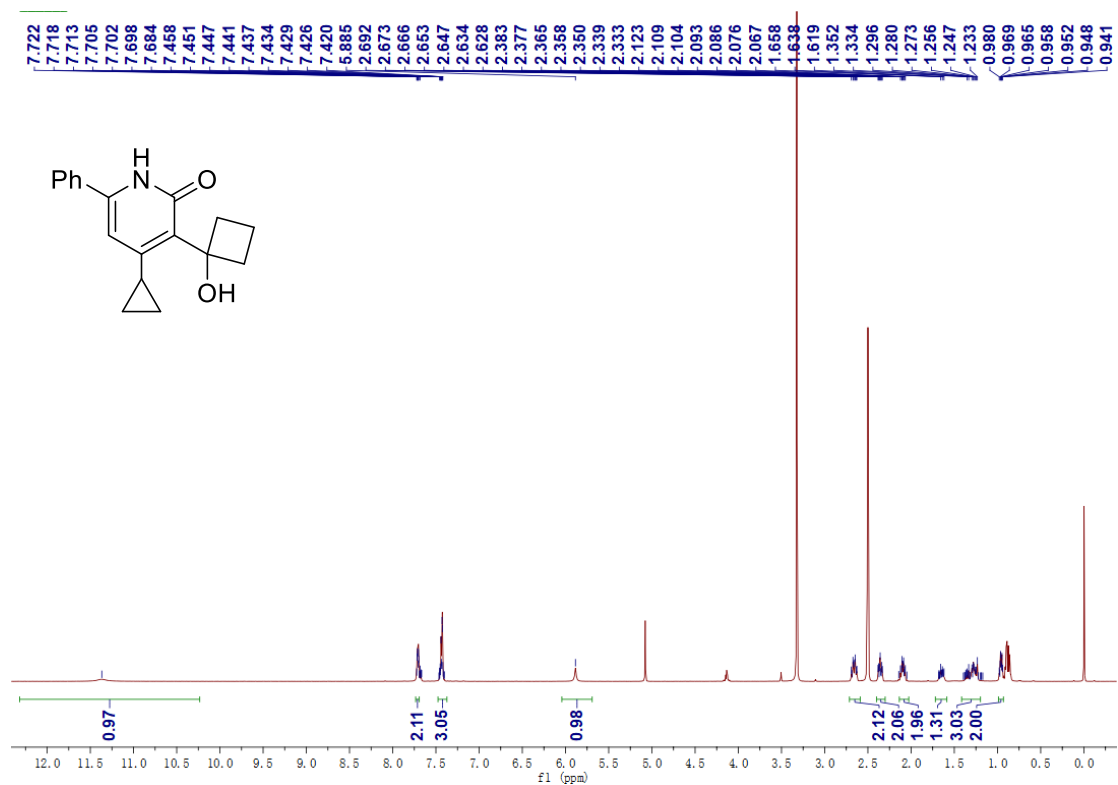
4-cyclopropyl-3-(hydroxy(thiophen-3-yl)methyl)-6-phenylpyridin-2(1H)-one (3q)



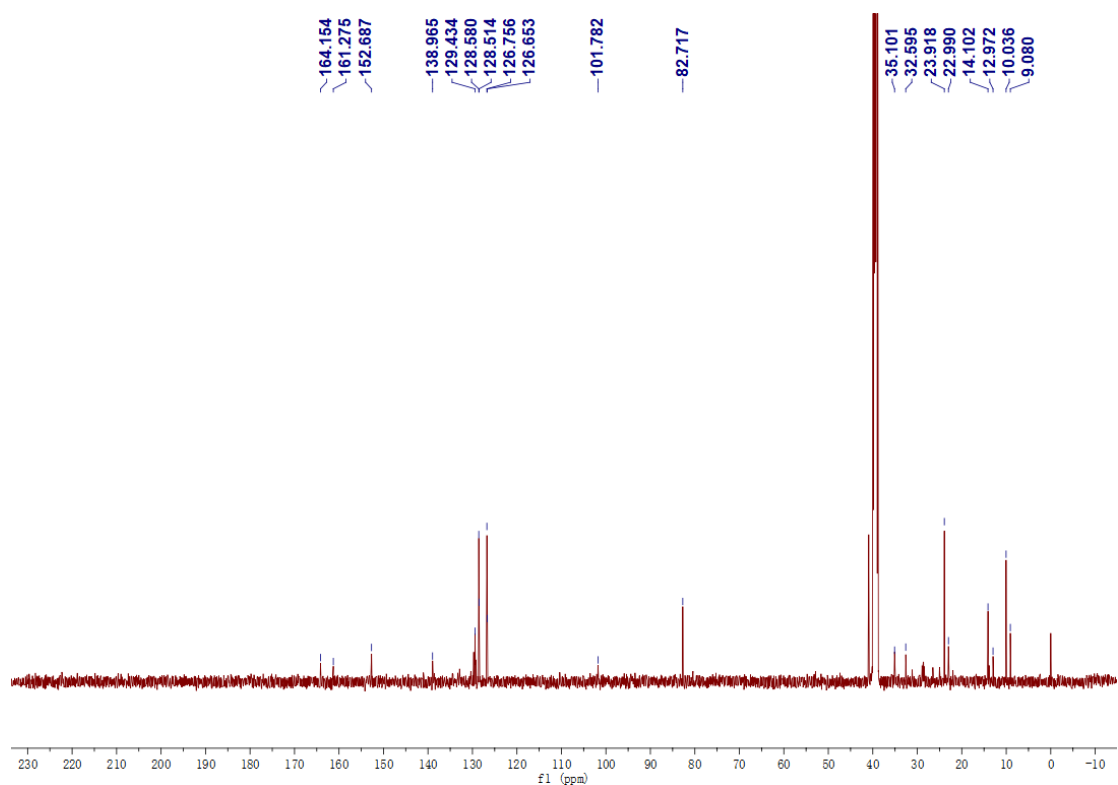
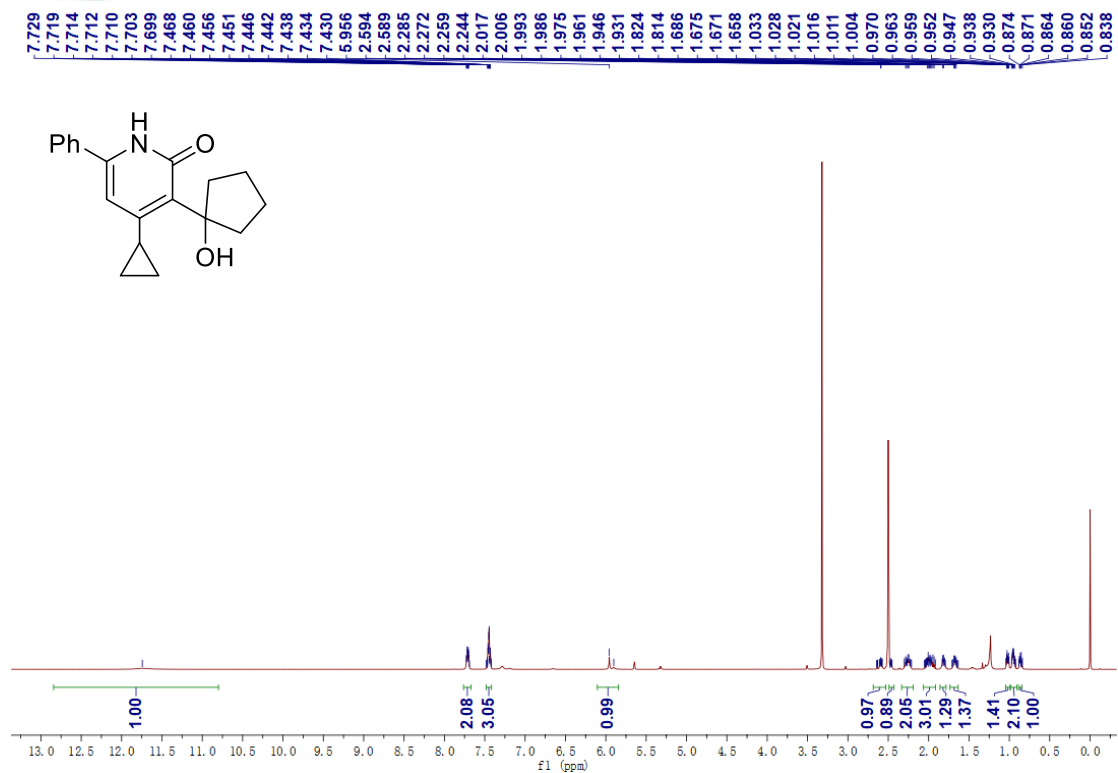
4-cyclopropyl-3-(1-hydroxy-1-phenylethyl)-6-phenylpyridin-2(1H)-one (3r)



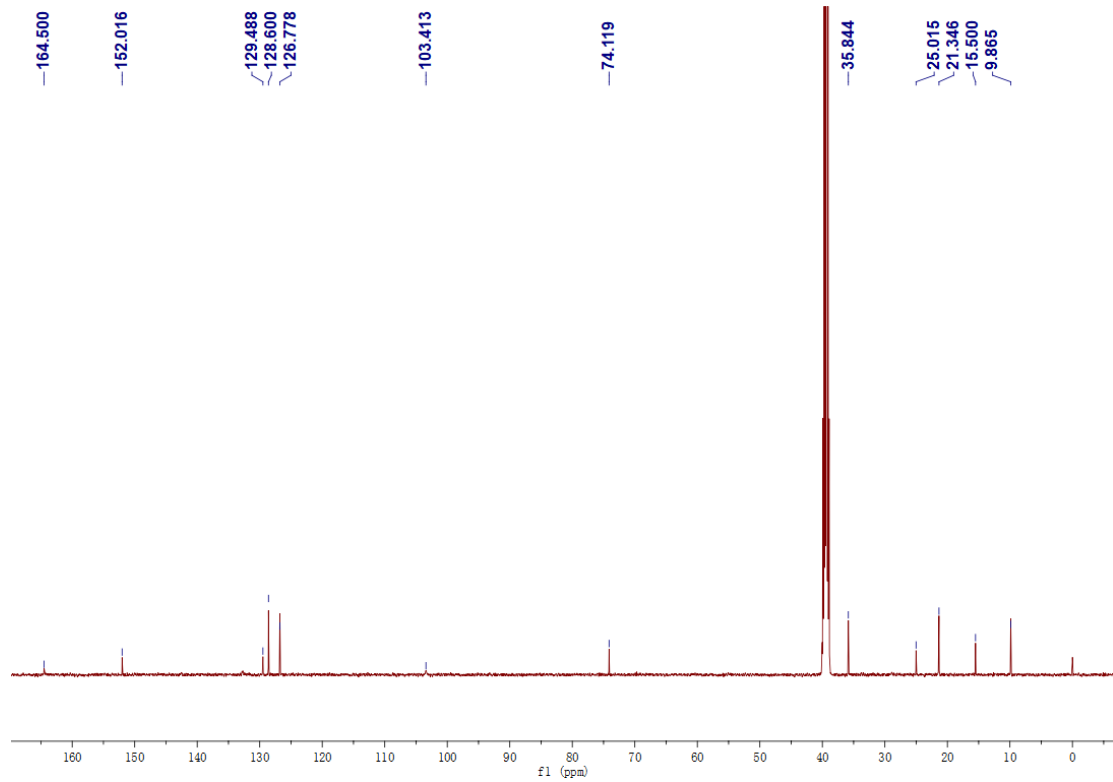
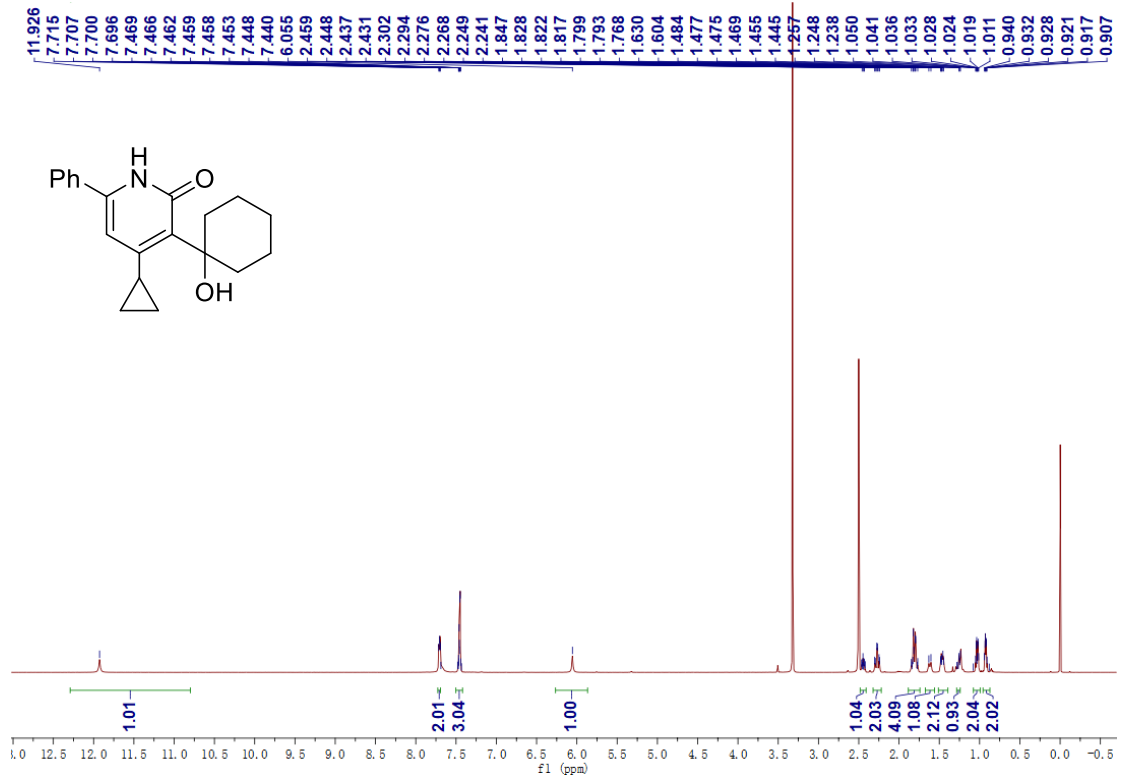
4-cyclopropyl-3-(1-hydroxycyclobutyl)-6-phenylpyridin-2(1H)-one (3s)



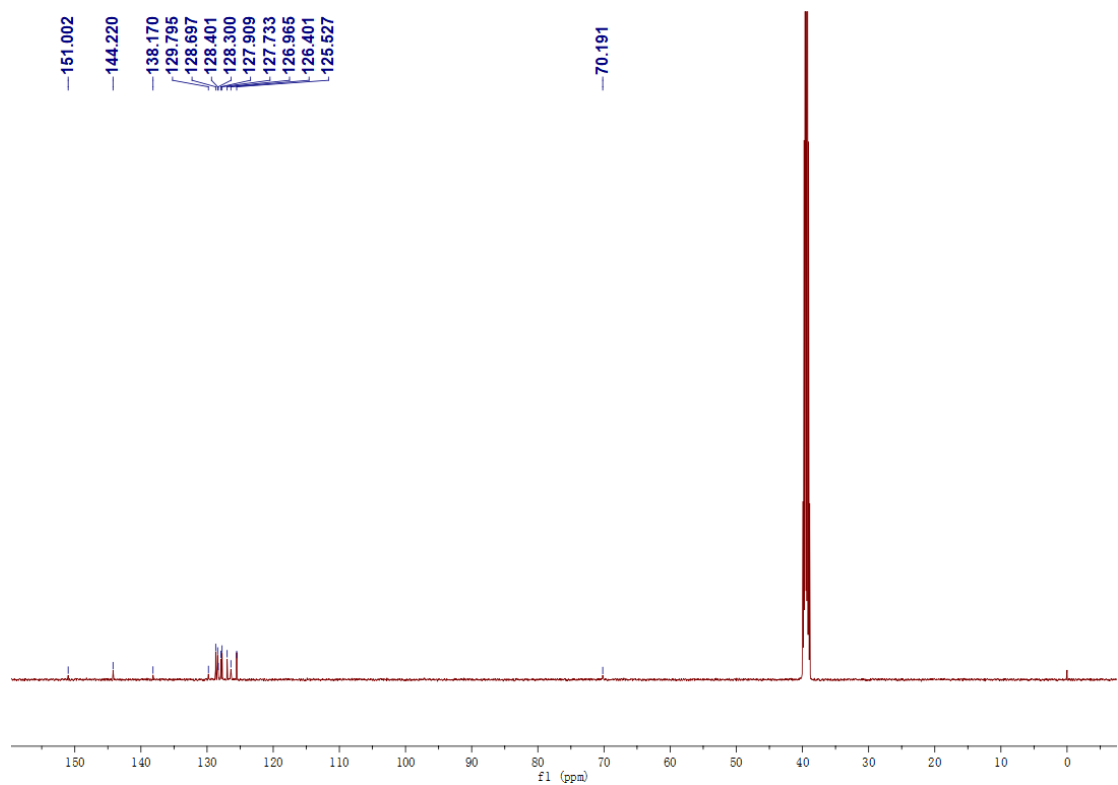
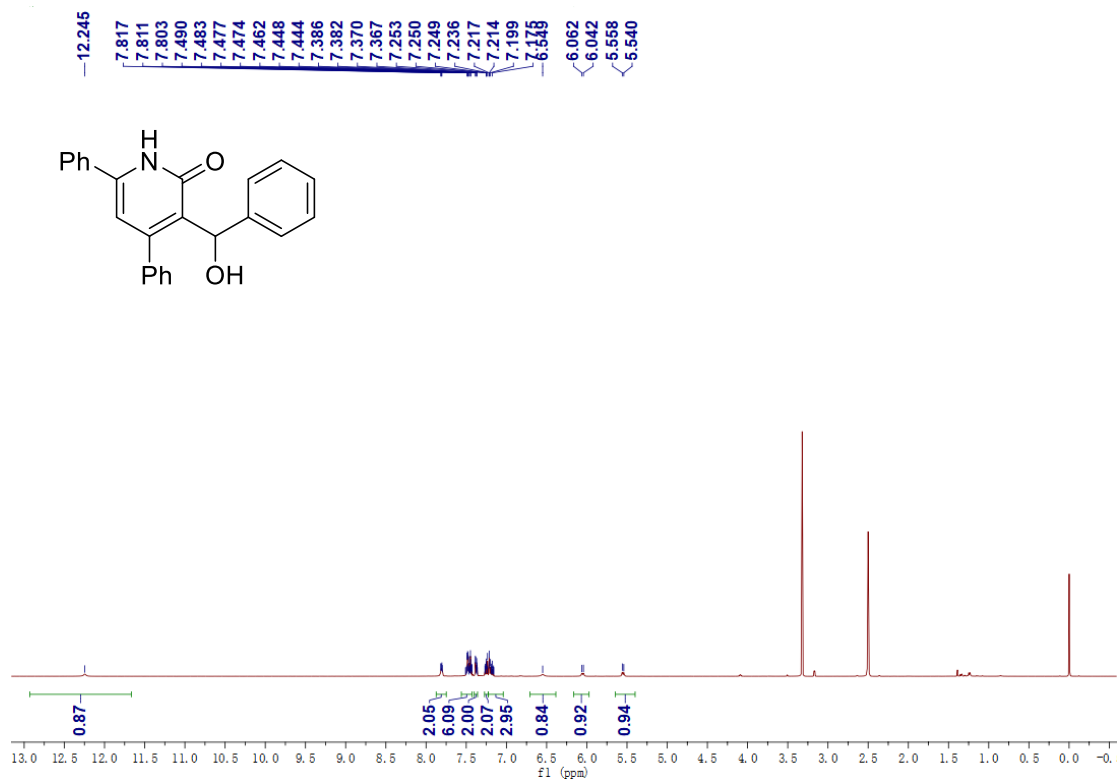
4-cyclopropyl-3-(1-hydroxycyclopentyl)-6-phenylpyridin-2(1H)-one (3t)



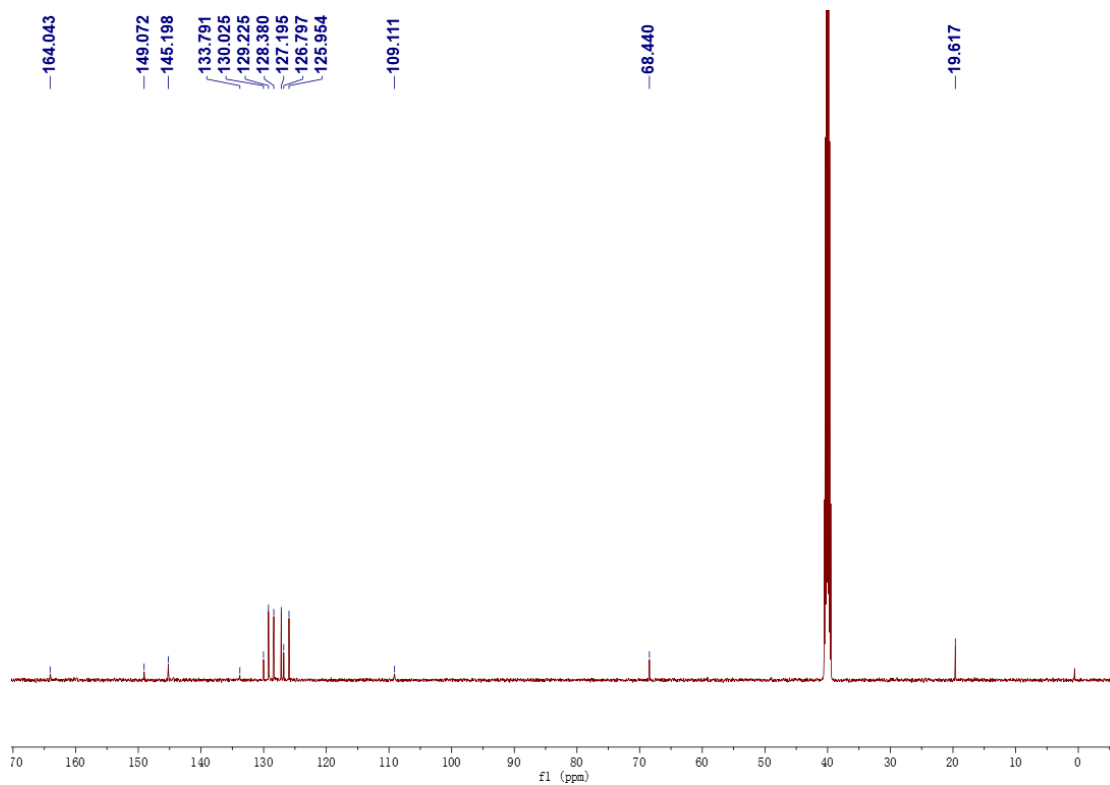
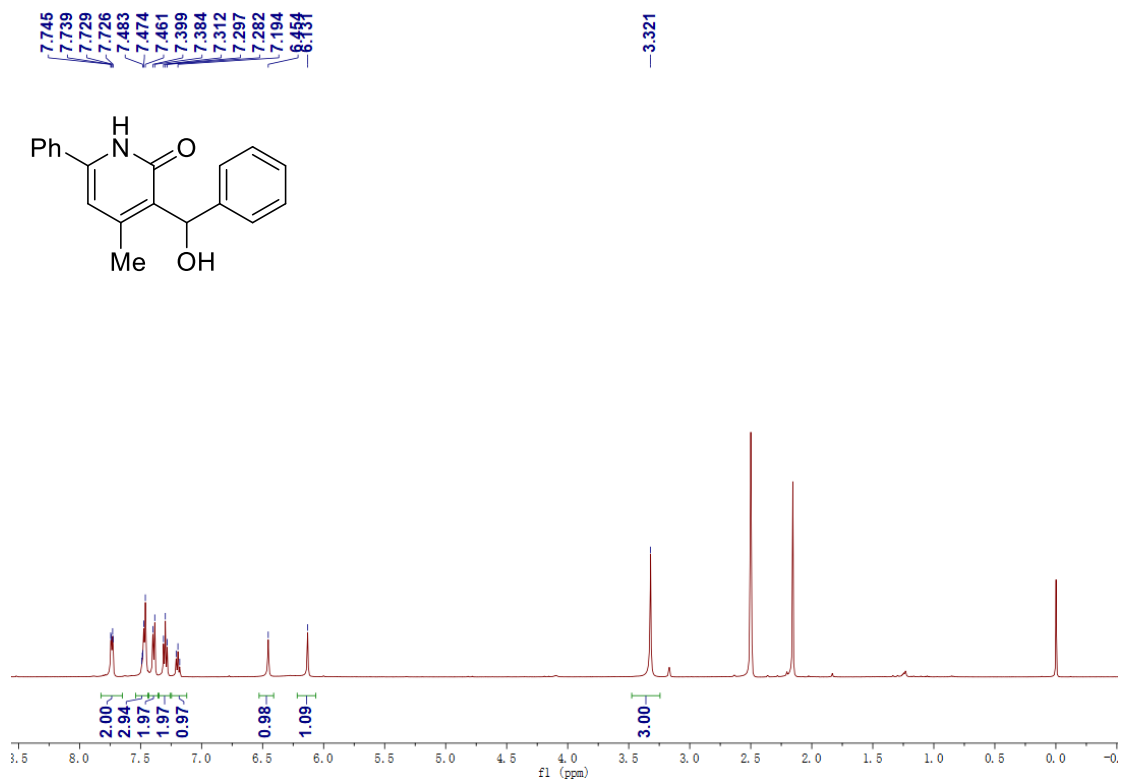
4-cyclopropyl-3-(1-hydroxycyclohexyl)-6-phenylpyridin-2(1H)-one (3u)



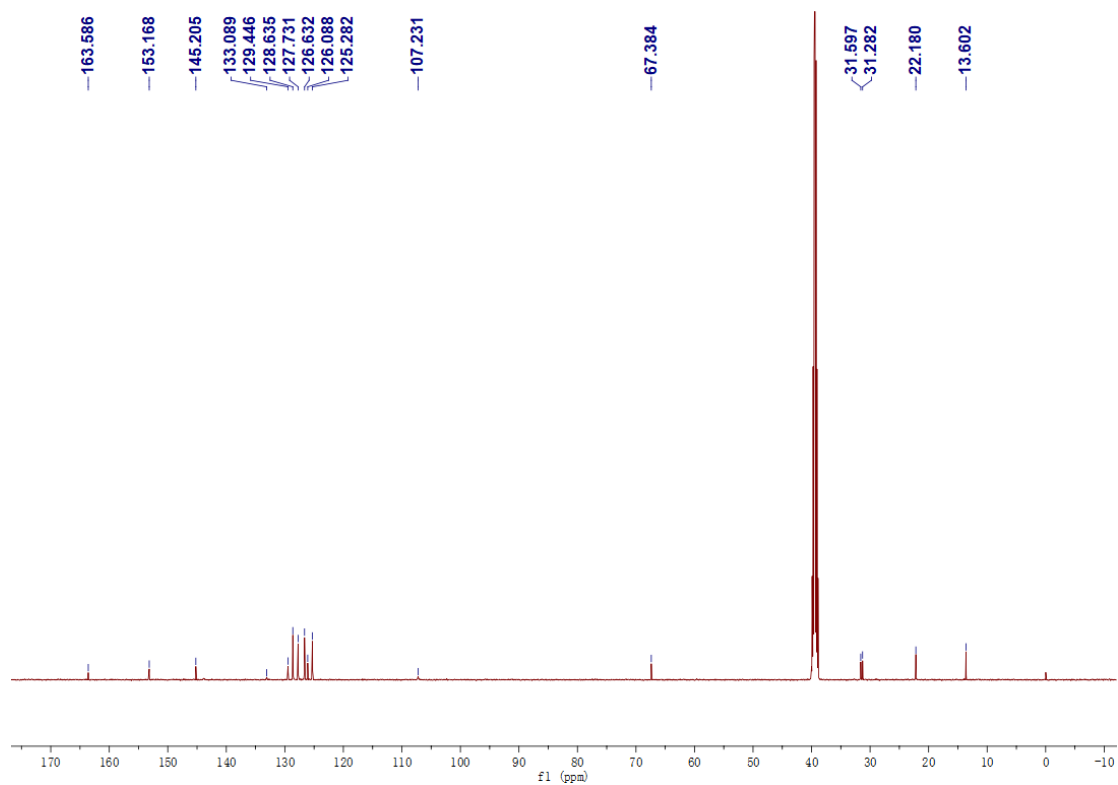
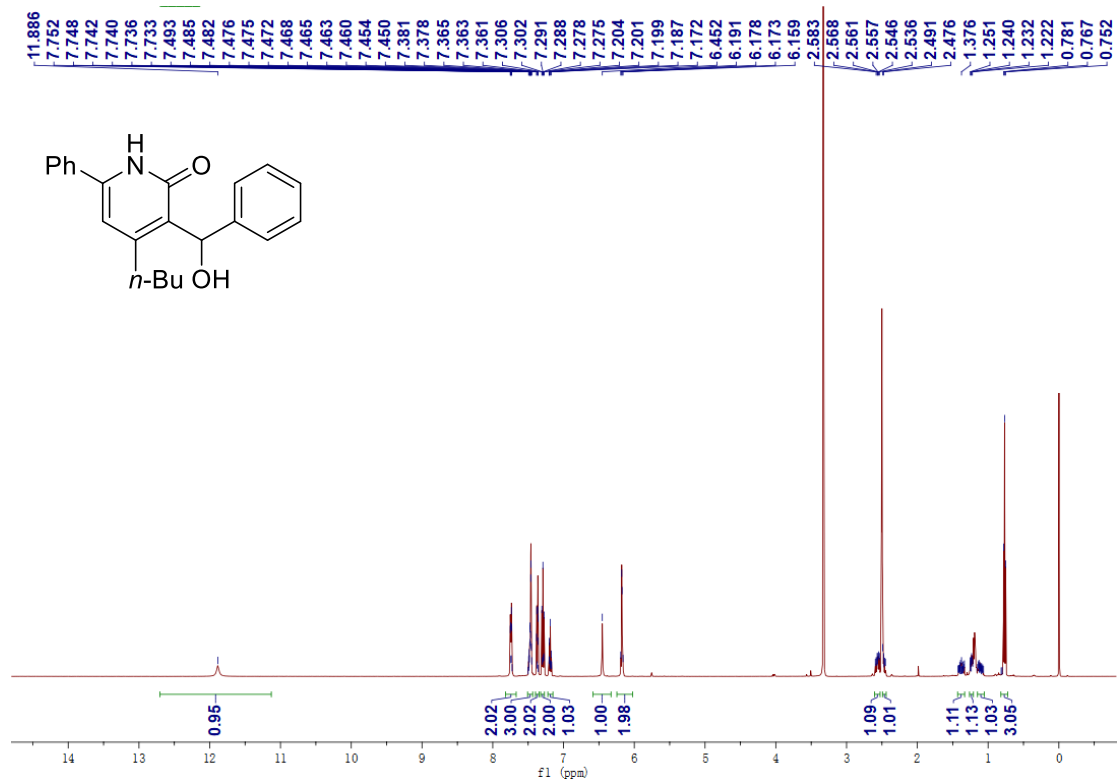
3-(hydroxy(phenyl)methyl)-4,6-diphenylpyridin-2(1H)-one (3v)



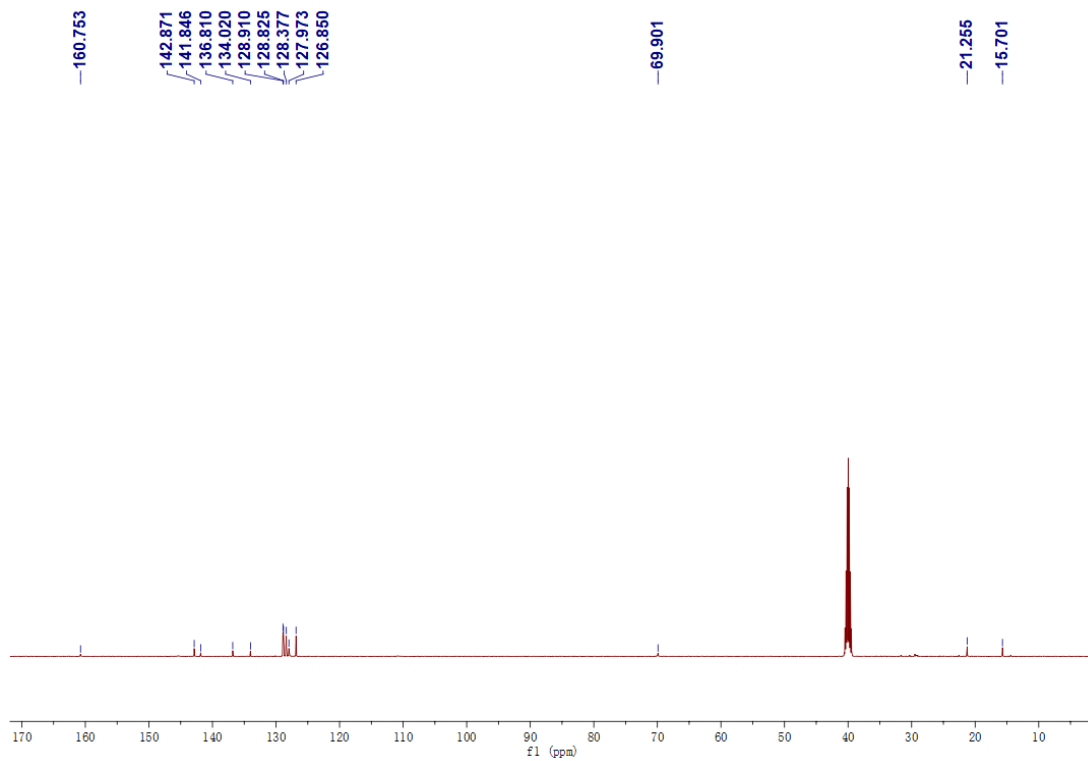
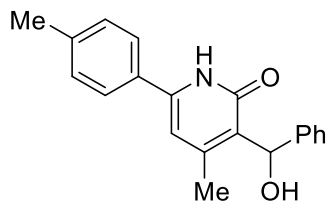
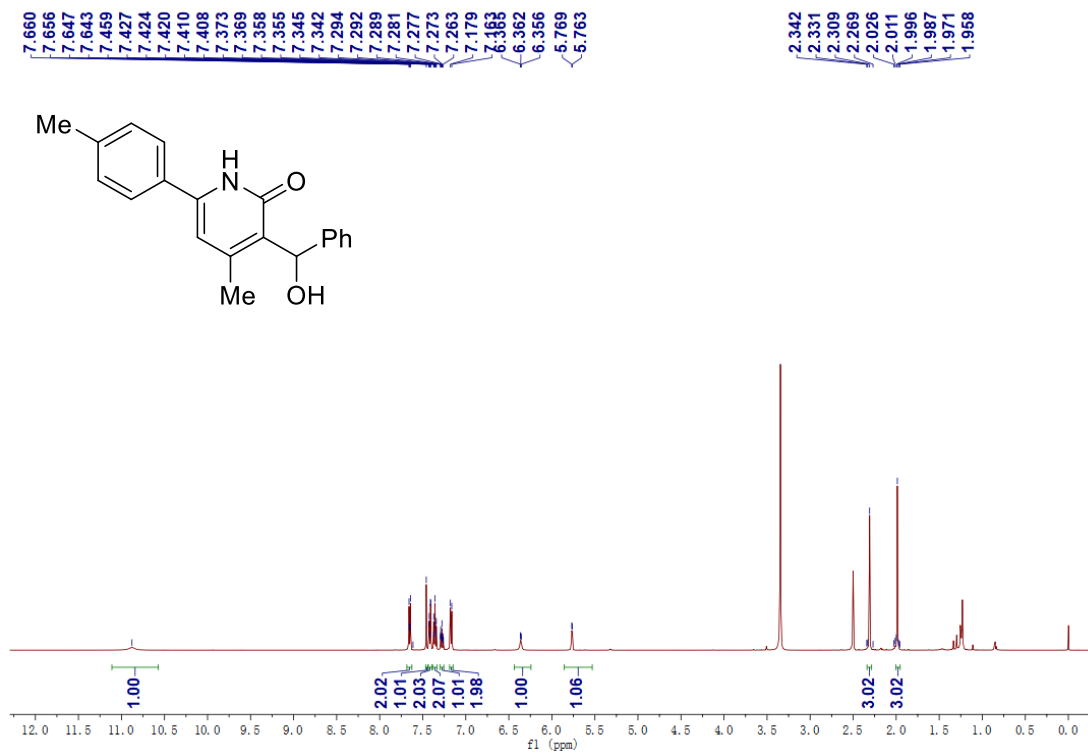
3-(hydroxy(phenyl)methyl)-4-methyl-6-phenylpyridin-2(1H)-one (3w)



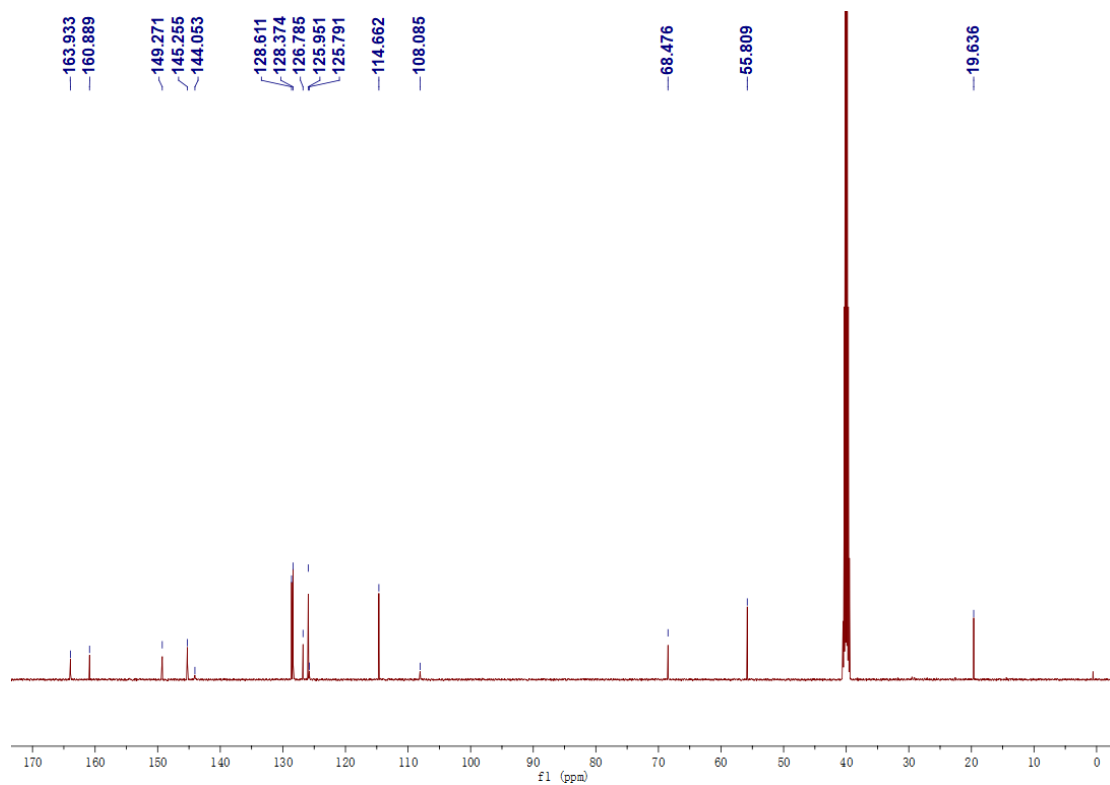
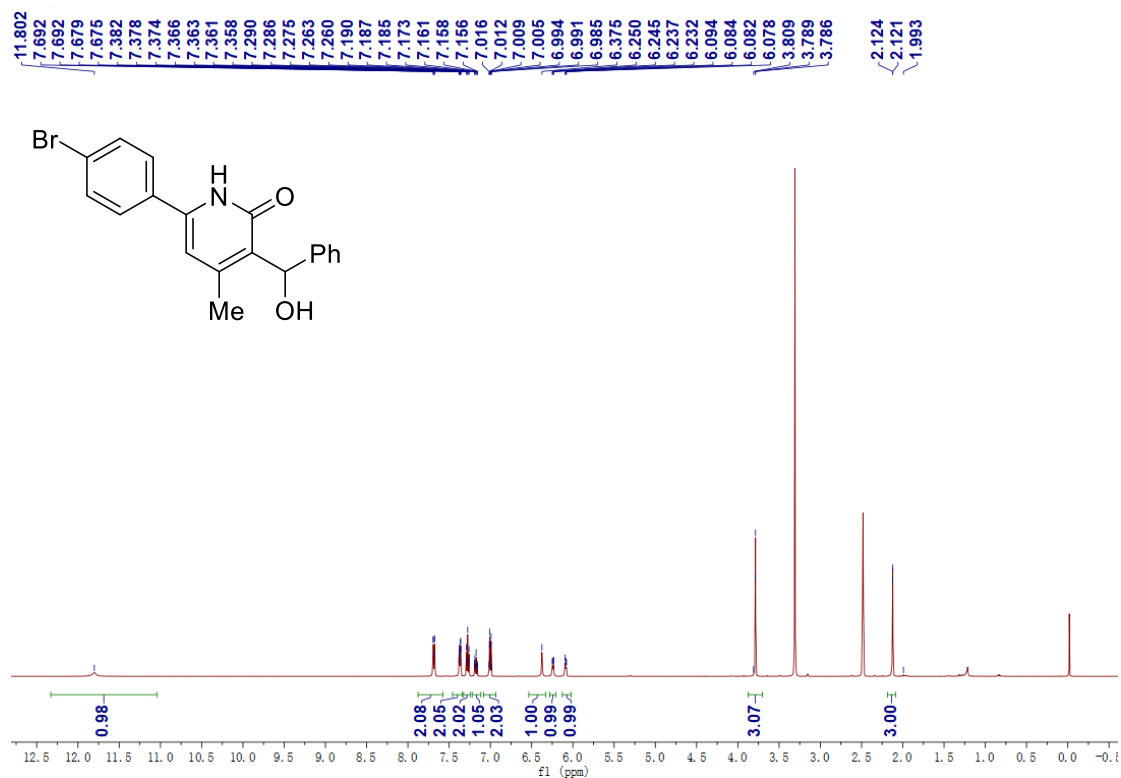
4-butyl-3-(hydroxy(phenyl)methyl)-6-phenylpyridin-2(1H)-one (3x)



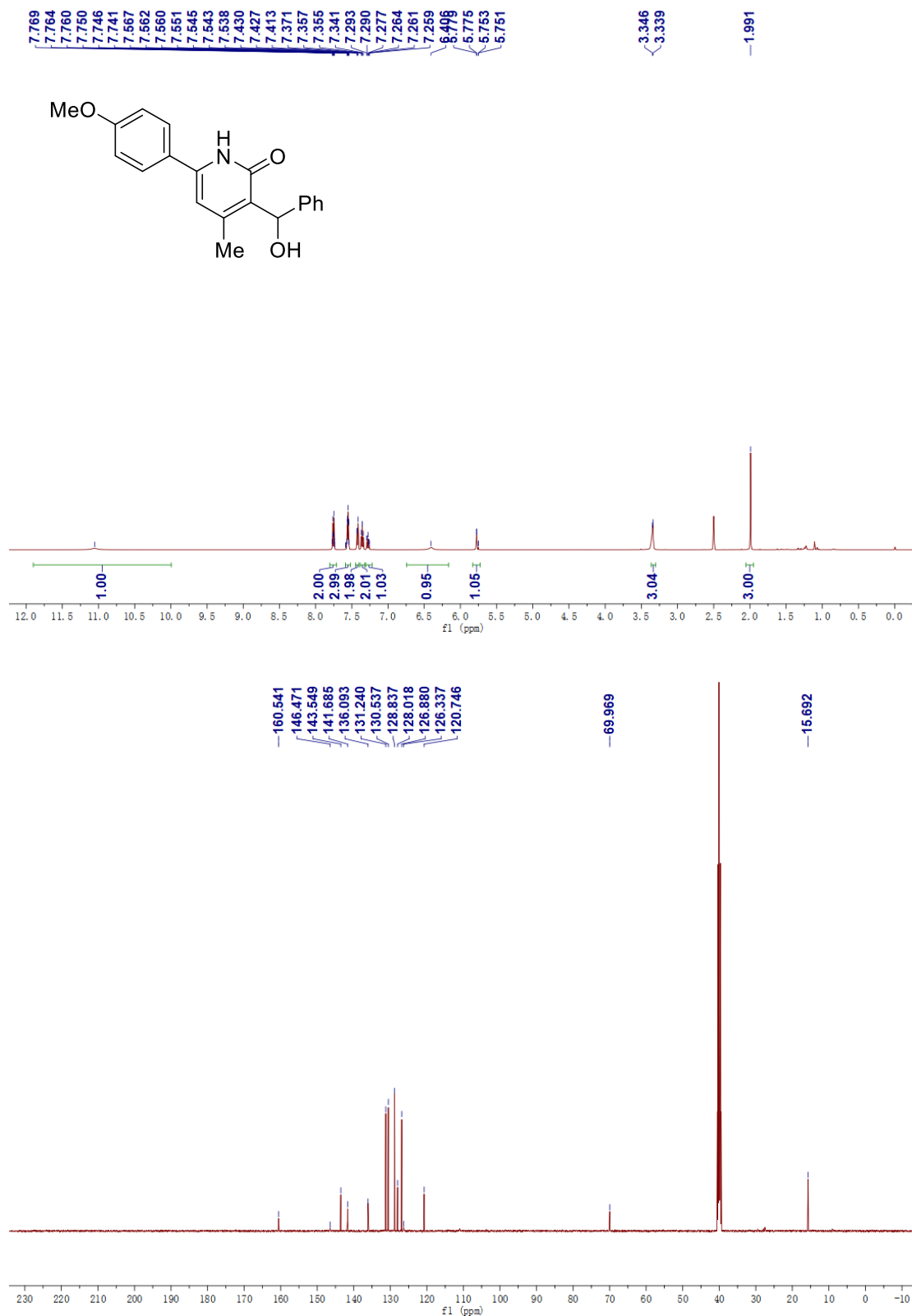
3-(hydroxy(phenyl)methyl)-4-methyl-6-(p-tolyl)pyridin-2(1H)-one (3y)



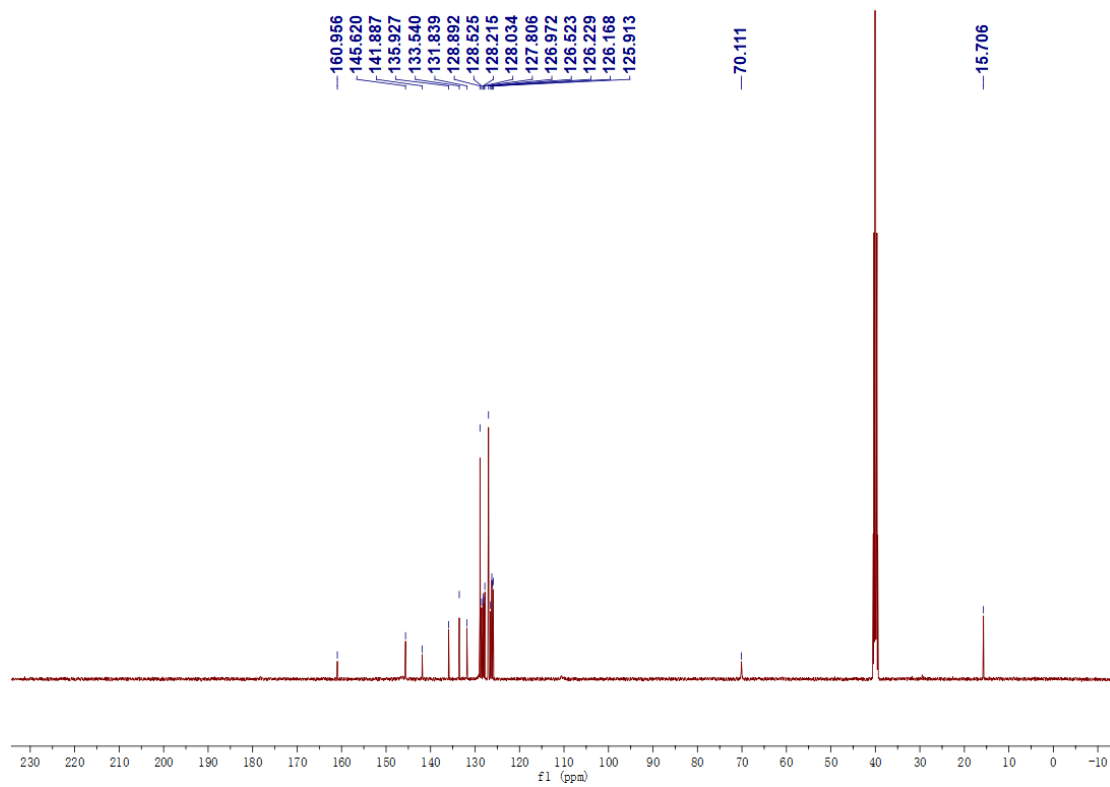
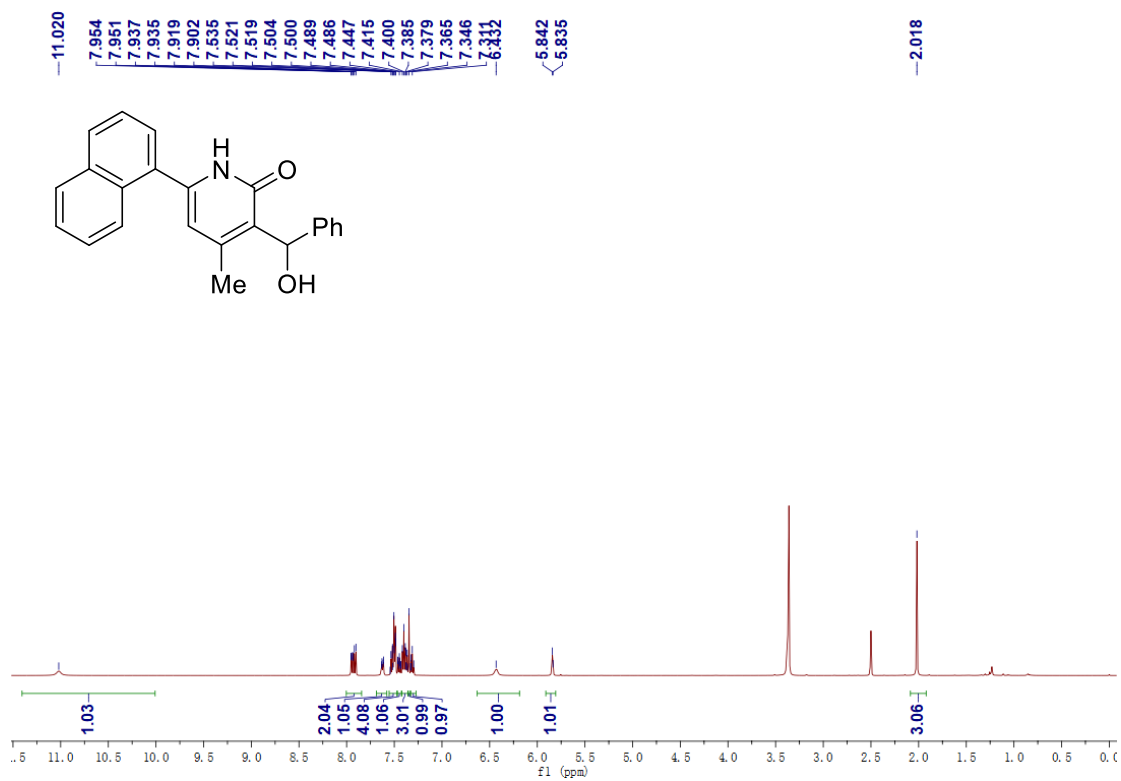
6-(4-bromophenyl)-3-(hydroxy(phenyl)methyl)-4-methylpyridin-2(1H)-one (3z)



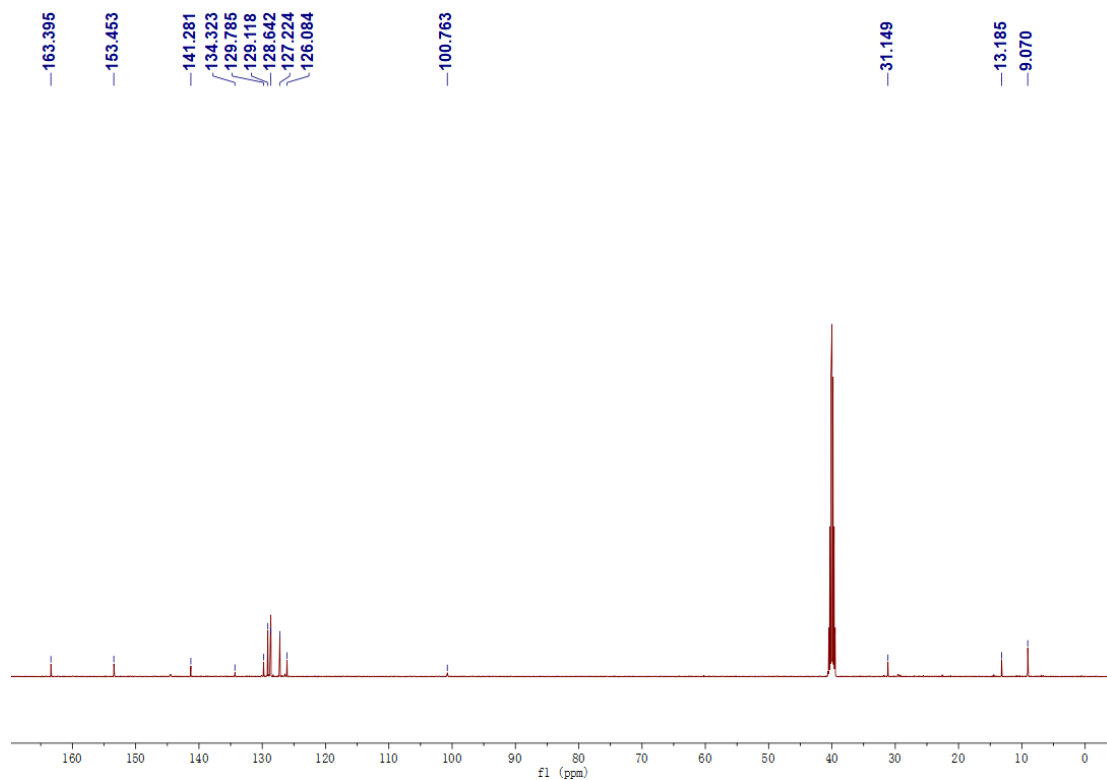
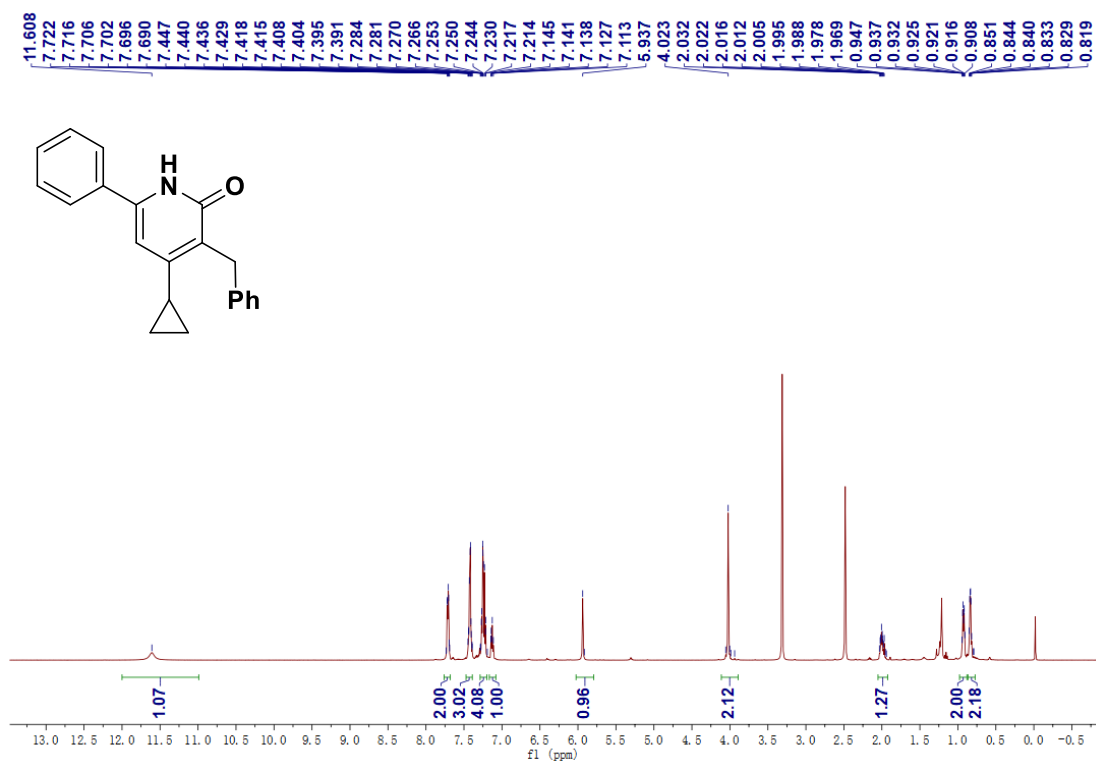
3-(hydroxy(phenyl)methyl)-6-(4-methoxyphenyl)-4-methylpyridin-2(1H)-one (3za)



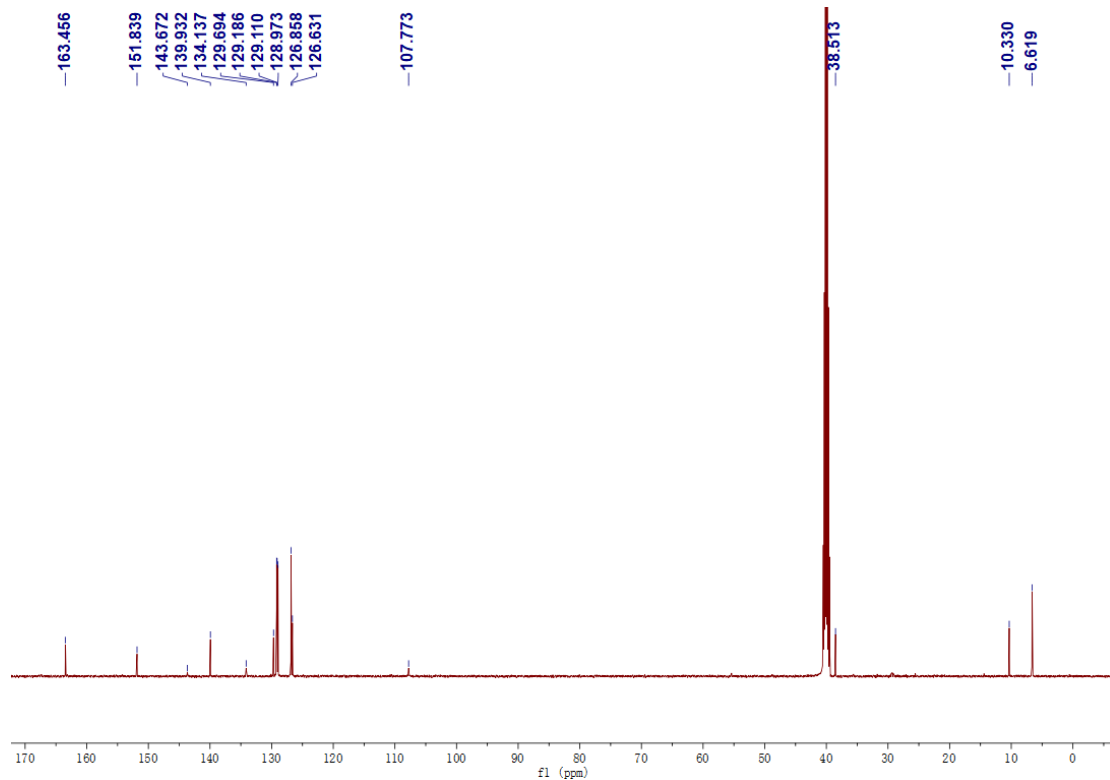
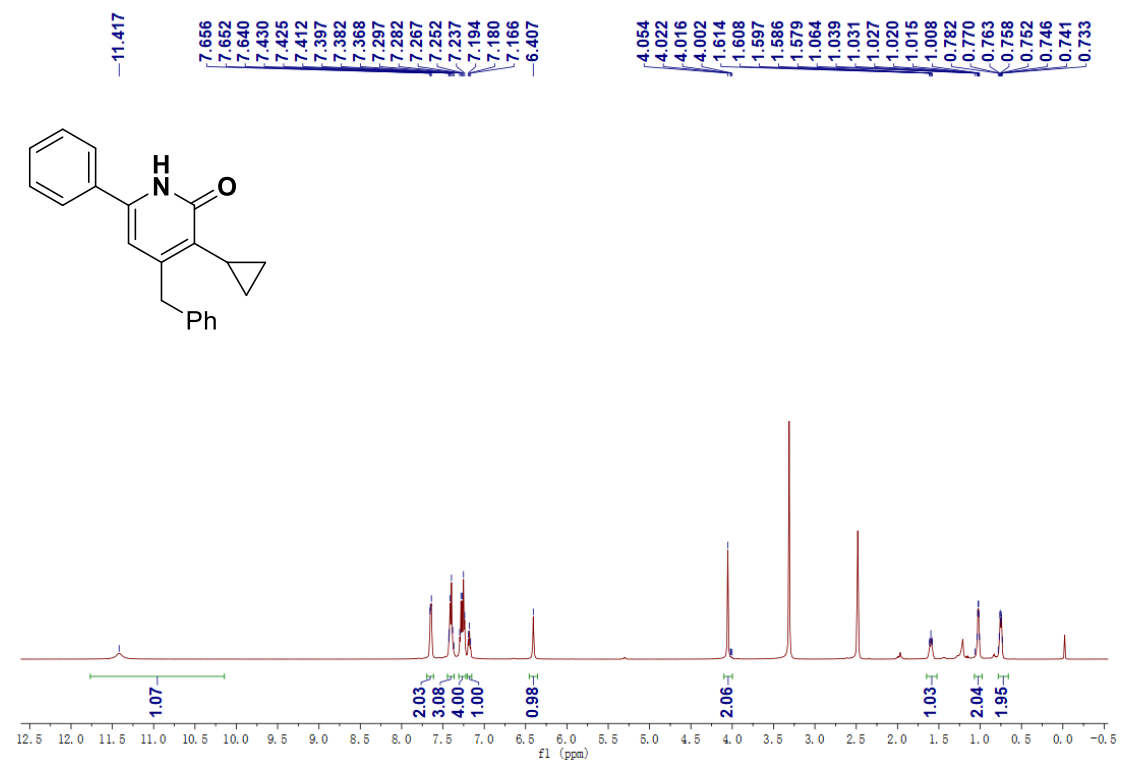
3-(hydroxy(phenyl)methyl)-4-methyl-6-(naphthalen-1-yl)pyridin-2(1H)-one (3zb)



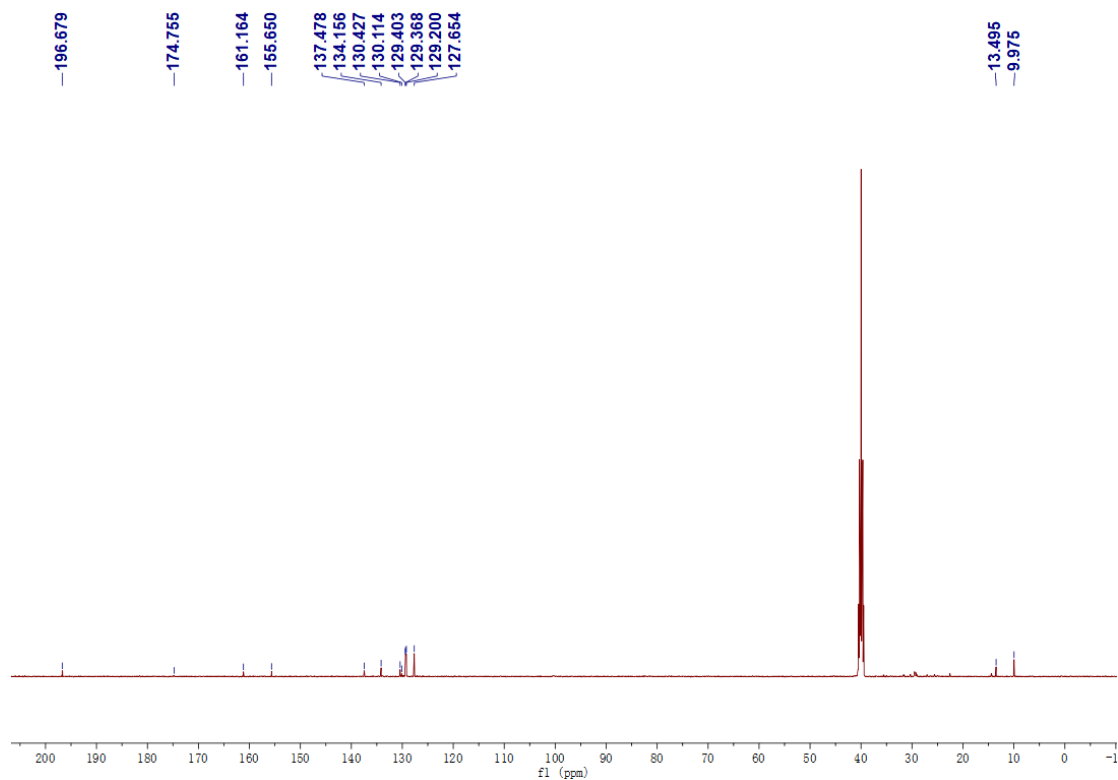
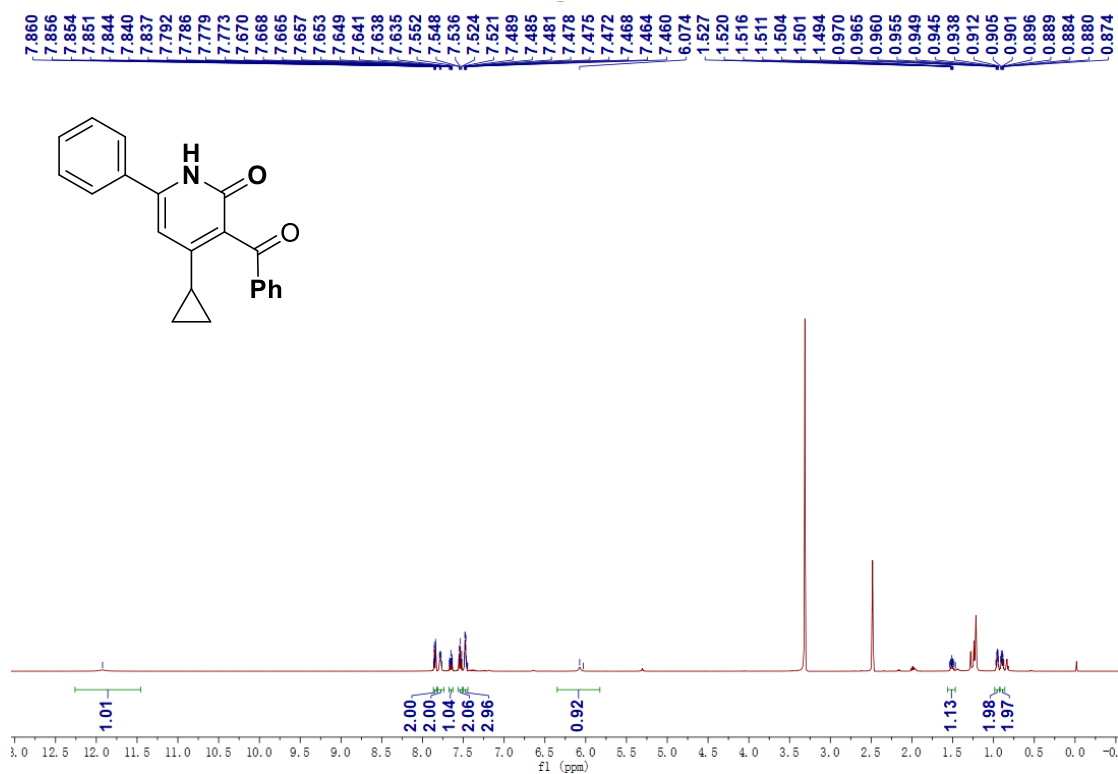
3-benzyl-4-cyclopropyl-6-phenylpyridin-2(1H)-one (4a)



4-benzyl-3-cyclopropyl-6-phenylpyridin-2(1H)-one (4a')

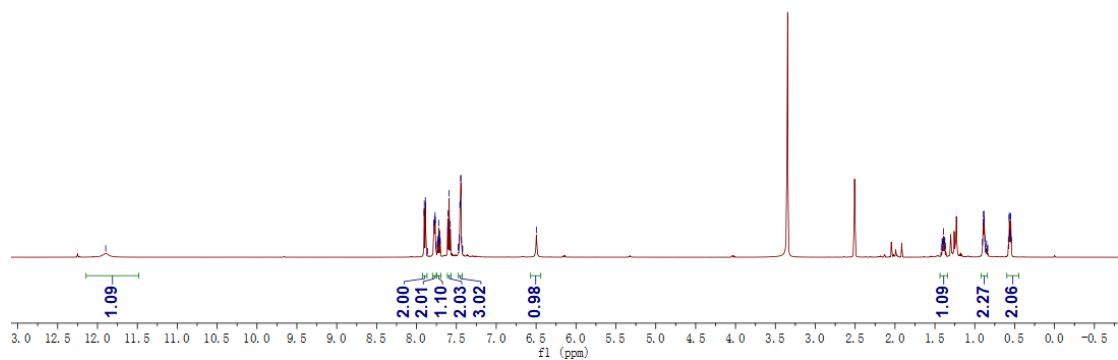
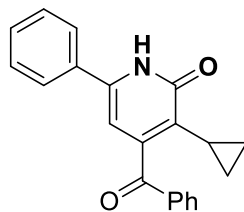


3-benzoyl-4-cyclopropyl-6-phenylpyridin-2(1H)-one (5a)



4-benzoyl-3-cyclopropyl-6-phenylpyridin-2(1H)-one (5a')

7.905
7.902
7.889
7.886
7.782
7.777
7.774
7.767
7.763
7.756
7.738
7.735
7.732
7.720
7.717
7.708
7.705
7.703
7.607
7.604
7.591
7.576
7.475
7.472
7.465
7.457
7.453
7.447
7.443
7.435
7.435
6.497
1.421
1.410
1.404
1.399
1.393
1.387
1.382
1.376
1.365
0.904
0.896
0.892
0.885
0.880
0.873
0.864
0.851
0.837
0.578
0.571
0.566
0.561
0.558
0.554
0.549
0.541



—196.867
—163.258
—149.138
—145.162
—135.976
—134.789
—133.681
—130.111
—129.925
—129.641
—129.230
—127.169
—102.930
—12.085
—6.327

