Supporting Information

Recyclable rhodium-catalyzed C-H activation/[4+2] annulation with unconventional regioselectivity at ambient temperature: experimental development and mechanistic insight

Haifang Meng,[a] Huiying Xu,[c] Zhi Zhou,[c] Zhenhao Tang,[a] Yidi Li,[b,d] Yu Zhou,*[,b,d] Wei Yi*[,c] and Xiaowei Wu*[,a,b,d]

[a]Zhongshan Institute for Drug Discovery, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Zhongshan 528400, China

[b]Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai 201203, China

[c]Guangzhou Municipal and Guangdong Provincial Key Laboratory of Protein Modification and Degradation & Molecular Target and Clinical Pharmacology, State Key Laboratory of Respiratory Disease, School of Pharmaceutical Sciences & the Fifth Affiliated Hospital, Guangzhou Medical University, Guangzhou, Guangdong 511436, China.

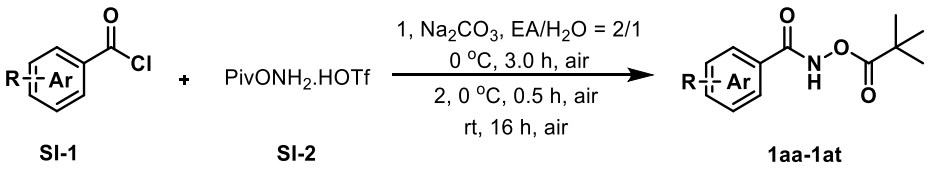
[d]University of Chinese Academy of Sciences, No.19A Yuquan Road, Beijing 100049, China

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 HSFG 254 (0.4-0.5 mm thickness). Yields refer to isolated compounds. ^{1}H, ^{13}C, and ^{19}F NMR spectra were collected on a Brucker 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.

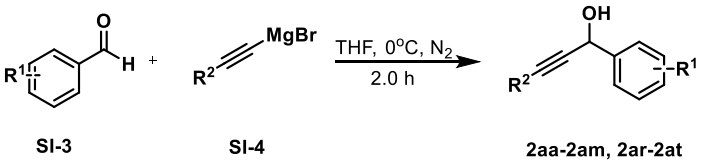
Preparation of Starting Materials

General procedure A for the preparation of **1aa-1at**.[1-5]



In a 100 mL round-bottom flask, O-pivaloylhydroxamine triflic acid (**SI-2**, 801 mg, 3.0 mmol, 1.0 eq.) and Na_2CO_3 (635 mg, 6.0 mmol, 2.0 eq.) were combined in a 2:1 mixed solvent of EtOAc (20 mL) and H_2O (10 mL). The mixture was cooled under an ice bath and stirred at 0°C for 1.0 h. Then acid chloride (**SI-1**, 3.0 mmol, 1.0 eq.) was added dropwise under an ice bath and stirred at 0 °C for 1.0 h. Then, the mixture was stirred for 16.0 h and slowly warmed up to room temperature. The reaction mixture was then diluted with EtOAc (20 mL) and washed twice with sat. $NaHCO_3$ and brine. The organic layer was dried over Na_2SO_4, filtered, and concentrated. The purification was made by flash column chromatography using an appropriate solvent mixture (petroleum ether/ethyl acetate) to afford the pure products **1aa-1at**. Compounds were prepared similarly according to the literature procedure, and their characterization data were in accordance with that previously reported.

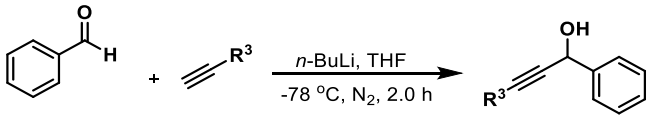
General procedure B for the preparation of propargyl alcohols **2aa-2am, 2ar-2at**.[6-11]



SI-3 **SI-4** **2aa-2am, 2ar-2at**

In a 100 mL round-bottom flask, the solution of the aldehyde (**SI-3**, 5.0 mmol, 1.0 eq.) in dry THF (10 mL) was added dropwise to the Grignard reagent (**SI-4**, 1.2 eq., 6.0 mmol, 0.5 M in THF) at 0°C under nitrogen atmosphere. The reaction mixture was stirred at 0°C for one hour and then another hour at room temperature. The completion of the reactions was confirmed by TLC, the mixture was quenched with a saturated solution of NH_4Cl (added slowly under cooling) and extracted with ethyl acetate (3 × 100 mL), dried with anhydrous Na_2SO_4. The combined organic solvent was removed under vacuum. The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to obtain the pure products. Compounds were prepared similarly according to the literature procedure, and their characterization data were in accordance with that previously reported.

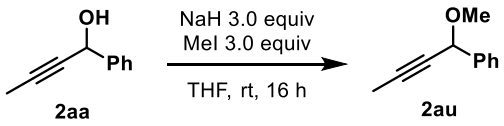
General procedure C for the preparation of **2ap** and **2aq**.



SI-3 **SI-5** **2ap, 2aq**

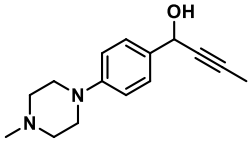
In a 100 mL round-bottom flask, a mixture solution of the benzaldehyde (**SI-3**, 5.0 mmol, 1.0 eq.) and alkyne (**SI-5**, 5.0 mmol, 1.0 eq.) in dry THF (15 mL) were added the *n*-BuLi (1.2 eq., 6.0 mmol, 1.6 M in THF) dropwise at -78°C under nitrogen atmosphere. The reaction mixture was stirred at 0°C for 2.0 h until the completion of the reaction. The mixture was quenched with a saturated solution of NH_4Cl (added slowly under cooling) and extracted with ethyl acetate (3 × 100 mL), dried with anhydrous Na_2SO_4. The combined organic solvent was removed under vacuum. The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to give the pure products. Compounds were prepared similarly according to the literature procedure, and their characterization data were in accordance with that previously reported.

General procedure D for the preparation of **2au**.[12]

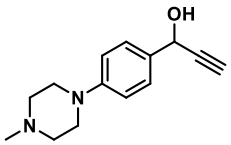


In a 50 mL round-bottom flask, 108 mg NaH were suspended in dry THF (10 mL) at room temperature under nitrogen atmosphere. **2aa** (1.5 mmol, 1.0 eq.) were added and the suspension was stirred for 30 min, followed by the addition of 0.28 mL (4.5 mmol, 3.0 eq.). The reaction mixture solution was stirred at room temperature for 16.0 h until the completion of the reaction. The mixture was quenched with water and extracted with DCM (3 × 20 mL), dried with anhydrous Na_2SO_4. No further purification was necessary. Compound was prepared similarly according to the literature procedure, and their characterization data were in accordance with that previously reported.

Characterization Data of **2am** and **2an**

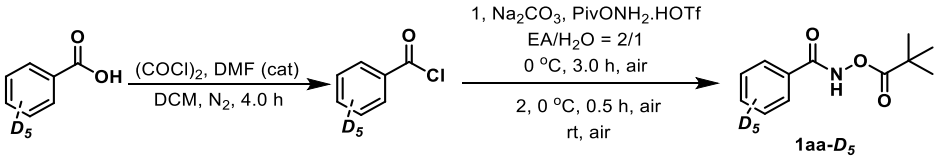


1-(4-(4-methylpiperazin-1-yl)phenyl)but-2-yn-1-ol (2am): yellow solid (696 mg, yield 57%); ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.26 (d, J = 8.5 Hz, 2H), 6.88 (d, J = 9.0 Hz, 2H), 5.61 (d, J = 5.0 Hz, 1H), 5.18 (s, 1H), 3.10 (t, 4H), 2.44 (t, 4H), 2.21 (s, 3H), 1.82 (d, J = 2.5 Hz, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 150.39, 133.15, 127.15, 114.92, 81.63, 80.46, 62.33, 54.55, 48.19, 45.76, 3.19.



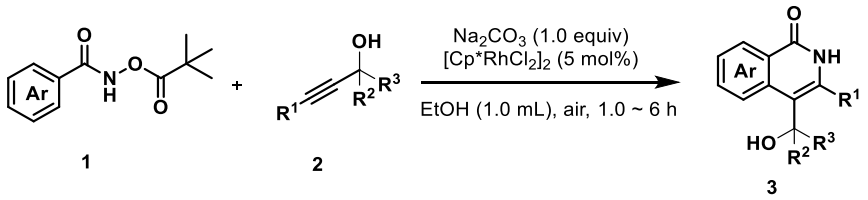
1-(4-(4-methylpiperazin-1-yl)phenyl)prop-2-yn-1-ol (2an)： yellow solid (921 mg, yield 80%); ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.28 (d, J = 8.5 Hz, 2H), 6.90 (d, J = 9.0 Hz, 2H), 5.80 (d, J = 6.0 Hz, 1H), 5.22 (dd, J = 5.5, 2.0 Hz, 1H), 3.42 (d, J = 2.5 Hz, 1H), 3.11 (t, 4H), 2.44 (t, 4H), 2.21 (s, 3H).^{13}C NMR (126 MHz, DMSO-d_6) δ 150.54, 132.15, 127.24, 114.92, 85.90, 75.34, 62.03, 54.53, 48.09, 45.74.

Preparation of 1aa-D_5



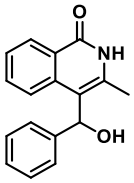
To a solution of the deuterium benzoic acid (99% Deuteration, 254.3 mg, 2.0 mmol, 1.0 eq.) in CH_2Cl_2 (10 mL) at 0°C under nitrogen atmosphere was added dropwise oxalyl chloride (1.2 eq., 2.4 mmol, 2.0 M in CH_2Cl_2), then followed by a catalytic amount of DMF (2 drops). The reaction was allowed to stir at 0°C for 4.0 h until completion. The solvent was then removed under reduce pressure to afford the corresponding crude acid chloride. O-pivaloylhydroxamine triflic acid (**SI-2**, 534 mg, 2.0 mmol, 1.0 eq.) and Na_2CO_3 (424 mg, 4.0 mmol, 2.0 eq.) was stirred at 0°C under air for 3.0 h in a 2:1 mixture of EtOAc (20 mL) and H_2O (10 mL). The resulting solution was followed by addition of a solution unpurified acid chloride in a minimum amount of EtOAc dropwise at 0°C under air. The reaction was stirred until the acid chloride disappeared. The two layers were separated and extracted with EtOAc (40 mL x 2). The combined organic phase was dried over anhydrous Na_2SO_4, filtered, and evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate) to obtain the product **1aa-D_5**. The NMR spectral data was in accordance with that previously reported.

General Procedure for the Synthesis of Isoquinolinones 3

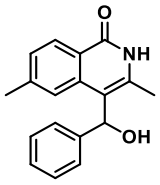


In an 8 mL reaction tube, the mixture of **1** (0.25 mmol), **2** (0.3 mmol), $[Cp^*RhCl_2]_2$ (5.0 mol%) and Na_2CO_3 (1.0 eq.) was added EtOH (1.0 mL). Then the resulting mixture was stirred for 1 ~ 6 h. When the reaction was finished, the desired product precipitated out as a solid, and the product 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 (petroleum ether/ethyl acetate) to provide the desired products **3**.

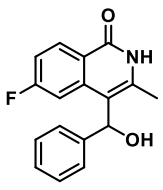
Characterization Data of Products 3 and 4



4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3aa): white solid (54 mg, yield 81%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.22 (br, 1H), 8.14 (dd, J = 8.0, 1.5 Hz, 1H), 7.76 (d, J = 8.0 Hz, 1H), 7.43 – 7.38 (m, 1H), 7.36 (s, 1H), 7.34 (s, 1H), 7.32 – 7.26 (m, 3H), 7.16 (t, J = 7.5 Hz, 1H), 6.14 (d, J = 3.5 Hz, 1H), 5.95 (d, J = 3.5 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.90, 144.58, 136.82, 136.37, 131.13, 128.03, 126.55, 126.15, 125.80, 125.49, 125.28, 124.88, 114.00, 68.01, 16.78; HRMS (ESI) *m/z* calculated for $C_{17}H_{14}NO_2^-$ [M-H]$^-$ 264.1030, found: 264.1024.

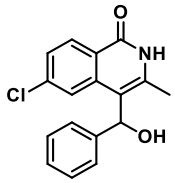


4-(hydroxy(phenyl)methyl)-3,6-dimethylisoquinolin-1(2H)-one (3ab): white solid (58 mg, yield 83%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.12 (br, 1H), 8.04 (d, J = 8.0 Hz, 1H), 7.60 (s, 1H), 7.37 – 7.33 (m, 2H), 7.30 – 7.25 (m, 2H), 7.18 – 7.12 (m, 2H), 6.14 (s, 1H), 5.93 (br, 1H), 2.34 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.81, 144.67, 140.84, 137.01, 136.47, 127.97, 126.62, 126.36, 126.11, 125.34, 125.27, 123.24, 113.88, 67.93, 21.68, 16.84; HRMS (ESI) *m/z* calculated for $C_{18}H_{16}NO_2^-$ [M-H]$^-$ 278.1187, found: 278.1184.

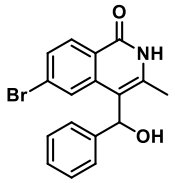


6-fluoro-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3ac): white solid (51 mg, yield 55%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.33 (br, 1H), 8.23 – 8.15 (m, 1H), 7.46 – 7.42 (m, 1H), 7.38 – 7.34 (m, 2H), 7.32 – 7.27 (m, 2H), 7.20 – 7.12 (m, 2H), 6.16 – 6.0 (m, 2H), 2.39 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 163.47 (d, J = 246.8 Hz), 161.19, 144.12, 139.21 (d, J =

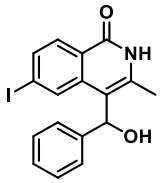
10.7 Hz), 138.15, 129.95 (d, J = 10.2 Hz), 128.15, 126.35, 125.25, 122.41, 113.60, 113.58, 113.42 (d, J = 23.7 Hz), 110.76 (d, J = 23.5 Hz), 67.92, 16.75; ^{19}F NMR (471 MHz, DMSO-d_6) δ -107.49 (s); HRMS (ESI) *m/z* calculated for $C_{17}H_{13}FNO_2^-$ $[M-H]^-$ 282.0936, found: 282.0931.



6-chloro-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3ad): white solid (53 mg, yield 71%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.37 (s, 1H), 8.12 (d, J = 8.5 Hz, 1H), 7.78 (d, J = 2.0 Hz, 1H), 7.36 – 7.29 (m, 5H), 7.19 (t, J = 7.0 Hz, 1H), 6.11 – 6.05 (m, 2H), 2.39 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.25, 144.08, 138.20, 138.16, 136.22, 128.86, 128.15, 126.38, 125.22, 125.10, 124.14, 113.19, 67.87, 16.77; HRMS (ESI) *m/z* calculated for $C_{17}H_{14}ClNO_2^+$ $[M+H]^+$ 300.0791, found: 300.0787.

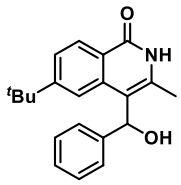


6-bromo-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3ae): white solid (68 mg, yield 79%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.38 (br, 1H), 8.04 (d, J = 8.5 Hz, 1H), 7.95 (d, J = 2.0 Hz, 1H), 7.44 (dd, J = 8.5, 2.0 Hz, 1H), 7.35 (d, J = 7.5 Hz, 2H), 7.30 (t, J = 7.5 Hz, 2H), 7.22 – 7.16 (m, 1H), 6.15 – 6.02 (m, 2H), 2.40 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.37, 144.08, 138.33, 138.14, 128.88, 128.22, 128.13, 127.82, 126.35, 125.47, 125.20, 124.39, 113.08, 67.84, 16.78; HRMS (ESI) *m/z* calculated for $C_{17}H_{13}BrNO_2^-$ $[M-H]^-$ 342.0135, found: 342.1024.

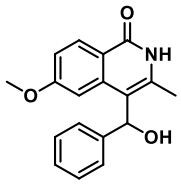


4-(hydroxy(phenyl)methyl)-6-iodo-3-methylisoquinolin-1(2H)-one (3af): white solid (65 mg, yield 66%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.35 (br, 1H), 8.18 (s, 1H), 7.85 (d, J = 8.0 Hz,

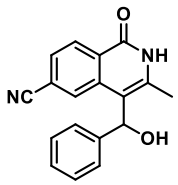
1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.35 – 7.28 (m, 4H), 7.21 – 7.17 (m, 1H), 6.25 – 5.9 (m, 1H), 2.39 (s, 3H); ^{13}C NMR (126 MHz, DMSO-*d*$_6$) δ 161.65, 144.19, 138.19, 137.83, 134.60, 133.43, 128.48, 128.12, 126.35, 125.20, 124.65, 112.93, 99.93, 67.85, 16.83; HRMS (ESI) *m/z* calculated for $C_{17}H_{13}INO_2^-$ [M-H]$^-$ 389.9996, found: 389.9988.



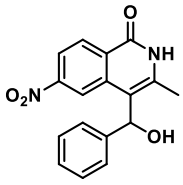
6-(tert-butyl)-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3ag): white solid (56 mg, yield 70%), ^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 11.09 (br, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.72 (s, 1H), 7.40 – 7.31 (m, 3H), 7.27 (t, *J* = 7.0 Hz, 2H), 7.15 (t, *J* = 7.0 Hz, 1H), 6.12 (s, 1H), 5.91 (br, 1H), 2.41 (s, 3H), 1.08 (s, 9H); ^{13}C NMR (126 MHz, DMSO-*d*$_6$) δ 161.74, 153.33, 144.94, 136.41, 136.14, 127.83, 126.18, 125.92, 125.13, 123.29, 122.58, 122.56, 114.39, 67.98, 34.76, 30.73, 16.71; HRMS (ESI) *m/z* calculated for $C_{21}H_{22}NO_2^-$ [M-H]$^-$ 320.1656, found: 320.1656.



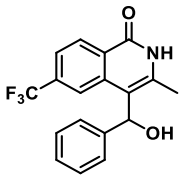
4-(hydroxy(phenyl)methyl)-6-methoxy-3-methylisoquinolin-1(2H)-one (3ah): white solid (42 mg, yield 59%), ^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 11.05 (s, 1H), 8.03 (d, *J* = 9.0 Hz, 1H), 7.39 – 7.35 (m, 2H), 7.30 – 7.26 (m, 2H), 7.19 – 7.15 (m, 2H), 6.88 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.11 (s, 1H), 5.93 (br, 1H), 3.56 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (126 MHz, DMSO-*d*$_6$) δ 161.51, 161.02, 144.68, 138.64, 137.08, 128.48, 127.97, 126.09, 125.18, 119.29, 113.79, 107.82, 68.00, 54.96, 16.76; HRMS (ESI) *m/z* calculated for $C_{18}H_{16}NO_3^-$ [M-H]$^-$ 294.1136, found: 294.1134.



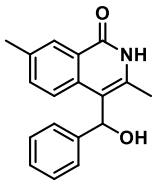
4-(hydroxy(phenyl)methyl)-3-methyl-1-oxo-1,2-dihydroisoquinoline-6-carbonitrile (3ai): white solid (52 mg, yield 72%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.49 (br, 1H), δ 8.26 (d, J = 7.5 Hz, 1H), 8.14 (s, 1H), 7.65 (d, J = 7.5 Hz, 1H), 7.38 – 7.29 (m, 4H), 7.20 (t, J = 7.5 Hz, 1H), 6.50 – 5.8 (m, 2H), 2.41 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.03, 143.97, 139.02, 136.81, 130.60, 128.25, 128.06, 128.05, 126.61, 126.52, 125.26, 118.57, 113.45, 113.32, 67.80, 16.89; HRMS (ESI) *m/z* calculated for $C_{18}H_{13}N_2O_2^-$ [M-H]$^-$ 289.0983, found: 289.0980.



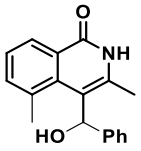
4-(hydroxy(phenyl)methyl)-3-methyl-6-nitroisoquinolin-1(2H)-one (3aj): pale green solid (77 mg, yield 99%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.70 (d, J = 2.0 Hz, 1H), 8.33 (d, J = 8.5 Hz, 1H), 8.01 (dd, J = 8.5, 2.0 Hz, 1H), 7.43 – 7.38 (m, 2H), 7.32 – 7.28 (m, 2H), 7.18 (t, J = 7.0 Hz, 1H), 6.45 – 6.0 (m, 2H), 2.46 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.95, 148.72, 143.97, 139.33, 137.32, 129.27, 128.87, 128.20, 126.49, 125.25, 121.37, 118.43, 114.16, 67.94, 16.91; HRMS (ESI) *m/z* calculated for $C_{17}H_{13}N_2O_4^-$ [M-H]$^-$ 309.0881, found: 309.0875.



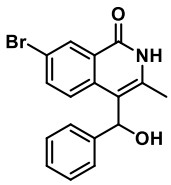
4-(hydroxy(phenyl)methyl)-3-methyl-6-(trifluoromethyl)isoquinolin-1(2H)-one (3ak): pale yellow solid (65 mg, yield 78%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.55 (br, 1H), 8.30 (d, J = 8.3 Hz, 1H), 8.14 (s, 1H), 7.57 (d, J = 8.4 Hz, 1H), 7.39 – 7.34 (m, 2H), 7.29 (t, J = 7.7 Hz, 2H), 7.17 (t, J = 7.3 Hz, 1H), 6.30 – 5.90 (m, 2H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.09, 144.11, 138.34, 136.81, 128.07, 127.97, 126.34, 125.15, 124.95, 123.57, 123.24, 122.78, 120.57, 113.97, 67.87, 16.77; ^{19}F NMR (471 MHz, DMSO-d_6) δ -60.98 (s); HRMS (ESI) *m/z* calculated for $C_{18}H_{13}F_3NO_2^-$ [M-H]$^-$ 332.0904, found: 332.0899.



4-(hydroxy(phenyl)methyl)-3,7-dimethylisoquinolin-1(2H)-one (3al): The major regioisomer was isolated from a ~8:1 mixture of regioisomers (the ratio was determined by ^{1}H-NMR of crude products), yellow solid (54 mg, 77% yield), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.12 (s, 1H), 7.93 (s, 1H), 7.65 (d, *J* = 8.5 Hz, 1H), 7.35 – 7.32 (m, 2H), 7.28 – 7.21 (m, 3H), 7.15 (t, *J* = 7.0 Hz, 1H), 6.11 (d, *J* = 3.5 Hz, 1H), 5.95 (d, *J* = 3.5 Hz, 1H), 2.35 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.84, 144.69, 135.25, 134.54, 134.25, 132.57, 128.01, 126.12, 126.05, 125.82, 125.47, 125.31, 113.99, 68.01, 20.72, 16.66; HRMS (ESI) *m/z* calculated for $C_{18}H_{14}NO_2^+$ $[M+H]^+$ 280.1337, found: 280.1331.

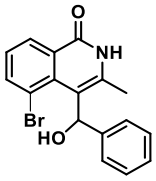


4-(hydroxy(phenyl)methyl)-3,5-dimethylisoquinolin-1(2H)-one (3al'): yellow solid (7.0 mg, 10% yield), ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.14 (s, 1H), 8.02 (s, 1H), 7.64 (d, *J* = 8.5 Hz, 1H), 7.57 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.44 – 7.40 (m, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.26 (d, *J* = 7.5 Hz, 1H), 6.34 (d, *J* = 4.5 Hz, 1H), 5.97 (d, *J* = 4.5 Hz, 1H), 2.43 (s, 3H), 2.19 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.04, 142.27, 137.91, 136.22, 135.56, 133.88, 128.31, 127.33, 126.48, 126.20, 125.05, 123.49, 106.11, 68.89, 20.81, 11.76； HRMS (ESI) *m/z* calculated for $C_{18}H_{14}NO_2^+$ $[M+H]^+$ 280.1337, found: 280.1329.

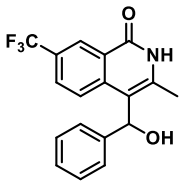


7-bromo-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3am): The major regioisomer was isolated from a ~11:1 mixture of regioisomers (the ratio was determined by ^{1}H-NMR of crude products), pale yellow solid (58 mg, isolated yield 67%), ^{1}H NMR (500 MHz,

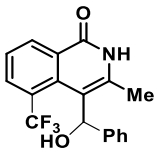
DMSO-d_6) δ 11.43 (s, 1H), 8.22 (d, *J* = 2.5 Hz, 1H), 7.70 (d, *J* = 9.0 Hz, 1H), 7.58 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.27 (t, *J* = 7.5 Hz, 2H), 7.17 (t, *J* = 7.5 Hz, 1H), 6.11 (d, *J* = 4.0 Hz, 1H), 6.05 (d, *J* = 4.0 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.71, 144.20, 137.22, 135.76, 133.94, 128.65, 128.34, 128.10, 127.20, 126.29, 125.29, 117.96, 113.79, 67.86, 16.77; HRMS (ESI) *m/z* calculated for $C_{17}H_{13}BrNO_2^-$ [M-H]$^-$ 342.0135, found: 342.0137.



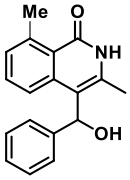
5-bromo-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3am'): The minor isomer contained some inseparable impurities. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.57 (br, 1H), 8.35 – 8.30 (m, 1H), 8.06 – 8.00 (m, 1H), 7.41 – 7.32 (m, 6H), 6.51 (d, *J* = 4.6 Hz, 1H), 5.96 (d, *J* = 4.6 Hz, 1H), 2.44 (s, 3H).



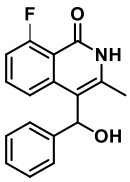
4-(hydroxy(phenyl)methyl)-3-methyl-7-(trifluoromethyl)isoquinolin-1(2H)-one (3an): The major regioisomer was isolated from a ~12:1 mixture of regioisomers (the ratio was determined by ^{1}H-NMR of crude products), yellow solid (53 mg, yield 64%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.60 (br, 1H), 8.39 (s, 1H), 7.95 (d, *J* = 9.0 Hz, 1H), 7.73 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.38 – 7.33 (m, 2H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.18 (t, *J* = 7.0 Hz, 1H), 6.16 (d, *J* = 4.0 Hz, 1H), 6.11 (d, *J* = 4.0 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.26, 144.07, 139.76, 139.60, 128.15, 127.25, 126.97 (m), 126.36, 125.32, 125.19, 124.92, 123.66 (m), 123.02, 113.88, 67.84, 16.96; ^{19}F NMR (471 MHz, DMSO-d_6) δ -61.02; HRMS (ESI) *m/z* calculated for $C_{18}H_{13}F_3NO_2^-$ [M-H]$^-$ 332.0909, found: 332.0907.



4-(hydroxy(phenyl)methyl)-3-methyl-5-(trifluoromethyl)isoquinolin-1(2H)-one (3an'): yellow solid (4 mg, yield 5%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.78 (s, 1H), 8.46 (s, 1H), 8.03 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.95 (d, *J* = 8.5 Hz, 1H), 7.44 (d, *J* = 7.5 Hz, 2H), 7.34 (dd, *J* = 7.5, 2.0 Hz, 2H), 7.28 – 7.25 (m, 1H), 6.47 (d, *J* = 4.5 Hz, 1H), 6.01 (d, *J* = 4.5 Hz, 1H), 2.23 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.53, 142.17, 141.73, 141.40, 128.35, 127.47, 126.27, 125.92, 125.21, 125.16, 124.87, 123.91 (m), 106.02, 69.21, 11.72; ^{19}F NMR (471 MHz, DMSO-d_6) δ -60.86; HRMS (ESI) *m/z* calculated for $C_{18}H_{13}F_3NO_2^-$ $[M-H]^-$ 332.0909, found: 332.0907.

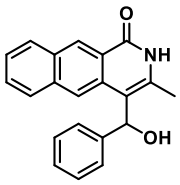


4-(hydroxy(phenyl)methyl)-3,8-dimethylisoquinolin-1(2H)-one (3ao): white solid (12 mg, yield 17%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.96 (s, 1H), 7.59 (d, *J* = 8.5 Hz, 1H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.26 (t, *J* = 7.5 Hz, 2H), 7.22 – 7.18 (m, 1H), 7.15 (t, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 7.0 Hz, 1H), 6.09 (s, 1H), 5.98 (br, 1H), 2.76 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.95, 144.68, 140.06, 138.43, 136.52, 130.19, 127.98, 127.75, 126.03, 125.20, 124.00, 123.80, 113.65, 68.12, 23.72, 16.54; HRMS (ESI) *m/z* calculated for $C_{18}H_{18}NO_2^+$ $[M+H]^+$ 280.1337, found: 280.1325.

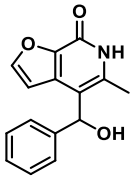


8-fluoro-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3ap): yellow solid (35 mg, yield 49%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.22 (s, 1H), 7.54 (d, J = 8.4 Hz, 1H), 7.41 – 7.31 (m, 3H), 7.29 – 7.24 (m, 2H), 7.19 – 7.15 (m, 1H), 7.03 – 6.97 (m, 1H), 6.10 (s, 1H), 6.00 (br, 1H), 2.36 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.64 (d, *J* = 260.3 Hz), 159.29 (d, *J* = 3.1

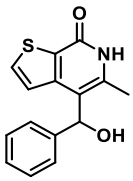
Hz), 144.31, 139.68, 138.12, 132.12 (d, *J* = 10.6 Hz), 128.06, 126.20, 125.22, 124.19, 121.84, 114.41 (d, *J* = 5.1 Hz), 113.23, 111.42 (d, *J* = 21.0 Hz), 67.94, 16.71; ^{19}F NMR (471 MHz, DMSO-d_6) δ -111.34; HRMS (ESI) *m/z* calculated for $C_{17}H_{15}FNO_2^+$ $[M+H]^+$ 284.1087, found: 284.1076.



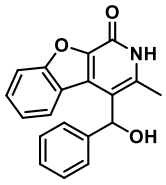
4-(hydroxy(phenyl)methyl)-3-methylbenzo[g]isoquinolin-1(2H)-one (3aq): yellow solid (35 mg, yield 44%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.04 (br, 1H), 8.83 (s, 1H), 8.32 (s, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.5 Hz, 1H), 7.53 – 7.43 (m, 4H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.15 (t, *J* = 7.5 Hz, 1H), 6.27 (s, 1H), 5.97 (br, 1H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.31, 144.67, 135.36, 134.22, 132.58, 129.89, 128.86, 127.98, 127.87, 127.73, 127.50, 126.13, 125.62, 125.34, 124.48, 123.90, 113.63, 68.20, 16.95; HRMS (ESI) *m/z* calculated for $C_{21}H_{16}NO_2^-$ $[M-H]^-$ 314.1187, found: 314.1182.



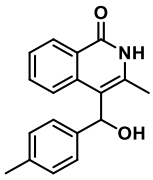
4-(hydroxy(phenyl)methyl)-5-methylfuro[2,3-c]pyridin-7(6H)-one (3ar): yellow solid (41 mg, yield 54%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.39 (br, 1H), 7.89 (d, *J* = 2.0 Hz, 1H), 7.37 – 7.32 (m, 2H), 7.29 (t, *J* = 7.5 Hz, 2H), 7.19 (t, *J* = 7.5 Hz, 1H), 6.63 (d, *J* = 2.0 Hz, 1H), 6.10 – 5.62 (m, 2H), 2.32 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 152.67, 147.98, 144.18, 141.73, 135.28, 133.53, 128.00, 126.50, 125.70, 113.31, 107.95, 68.46, 15.81; HRMS (ESI) *m/z* calculated for $C_{15}H_{14}NO_3^+$ $[M+H]^+$ 256.0973, found: 256.0969.



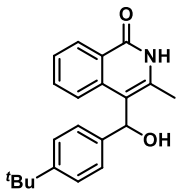
4-(hydroxy(phenyl)methyl)-5-methylthieno[2,3-c]pyridin-7(6H)-one (3as): white solid (64 mg, yield 94%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.40 (br, 1H), 7.79 (d, J = 5.5 Hz, 1H), 7.37 – 7.33 (m, 2H), 7.30 – 7.25 (m, 3H), 7.18 (t, J = 7.0 Hz, 1H), 6.20 – 5.65 (m, 2H), 2.37 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 158.23, 145.83, 144.29, 136.87, 132.42, 128.00, 127.79, 126.35, 125.53, 125.25, 115.49, 68.24, 16.09; HRMS (ESI) *m/z* calculated for $C_{15}H_{13}NO_2S^+$ $[M+H]^+$ 272.0745, found: 272.0740.



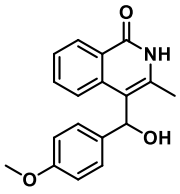
4-(hydroxy(phenyl)methyl)-3-methylbenzofuro[2,3-c]pyridin-1(2H)-one (3at): white solid (47 mg, yield 62%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.82 (br, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.66 (d, J = 8.5 Hz, 1H), 7.43 (t, J = 7.5 Hz, 1H), 7.38 – 7.35 (m, 2H), 7.27 (t, J = 7.5 Hz, 2H), 7.19 – 7.11 (m, 2H), 6.40 – 5.75 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 155.94, 153.61, 143.15, 142.98, 136.65, 129.11, 128.11, 126.86, 126.61, 125.96, 122.67, 122.60, 113.41, 111.83, 68.02, 16.42; HRMS (ESI) *m/z* calculated for $C_{19}H_{14}NO_3^-$ $[M-H]^-$ 304.0979, found: 304.0973.



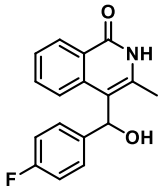
4-(hydroxy(p-tolyl)methyl)-3-methylisoquinolin-1(2H)-one (3au): white solid (57 mg, yield 82%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.20 (br, 1H), 8.13 (dd, J = 8.0, 1.2 Hz, 1H), 7.76 (d, J = 8.3 Hz, 1H), 7.46 – 7.37 (m, 1H), 7.33 – 7.26 (m, 1H), 7.24 – 7.20 (m, 2H), 7.10 – 7.06 (m, 2H), 6.08 (s, 1H), 5.94 (br, 1H), 2.36 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.86, 141.53, 136.83, 136.17, 135.02, 131.07, 128.60, 126.49, 125.87, 125.46, 125.21, 124.83, 114.04, 67.87, 20.56, 16.73; HRMS (ESI) *m/z* calculated for $C_{18}H_{18}NO_2^+$ $[M+H]^+$ 280.1337, found: 280.1328.



4-((4-(tert-butyl)phenyl)(hydroxy)methyl)-3-methylisoquinolin-1(2H)-one (3av): white solid (65 mg, yield 81%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.21 (br, 1H), 8.14 (d, J = 7.0 Hz, 1H), 7.81 (d, J = 8.5 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.32 – 7.24 (m, 5H), 6.09 (s, 1H), 5.93 (br, 1H), 2.36 (s, 3H), 1.23 (s, 9H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.85, 148.33, 141.46, 136.88, 136.11, 131.13, 126.50, 125.88, 125.45, 125.01, 124.84, 124.76, 113.98, 67.92, 34.04, 31.16, 16.74; HRMS (ESI) *m/z* calculated for $C_{21}H_{22}NO_2^-$ [M-H]$^-$ 320.1656, found: 320.1660.

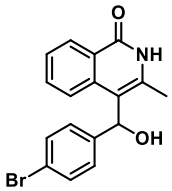


4-(hydroxy(4-methoxyphenyl)methyl)-3-methylisoquinolin-1(2H)-one (3aw): white solid (63 mg, yield 85%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.20 (br, 1H), 8.14 (dd, J = 7.5, 1.0 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.32 – 7.28 (m, 1H), 7.23 (d, J = 8.5 Hz, 2H), 6.85 – 6.81 (m, 2H), 6.07 (s, 1H), 5.87 (br, 1H), 3.69 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.86, 157.64, 136.86, 136.36, 136.11, 131.06, 126.49, 126.43, 125.89, 125.48, 124.82, 114.01, 113.40, 67.69, 54.91, 16.72; HRMS (ESI) *m/z* calculated for $C_{18}H_{16}NO_3^-$ [M-H]$^-$ 294.1136, found: 294.1135.

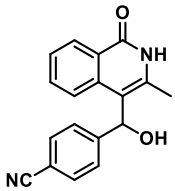


4-((4-fluorophenyl)(hydroxy)methyl)-3-methylisoquinolin-1(2H)-one (3ax): white solid (55 mg, yield 78%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.23 (br, 1H), 8.16 – 8.13 (m, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.44 – 7.40 (m, 1H), 7.37 – 7.34 (m, 2H), 7.30 (t, J = 7.5 Hz, 1H), 7.12 – 7.08 (m, 2H), 6.20 – 5.80 (m, 2H), 2.37 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.84, 160.75 (d, J = 242.0 Hz), 140.64, 136.67, 136.49, 131.16, 127.21 (d, J = 8.1 Hz), 126.58, 125.64, 125.50, 124.90,

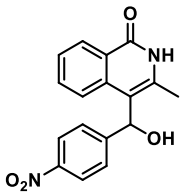
114.69 (d, *J* = 21.0 Hz), 113.63, 67.58, 16.71; ^{19}F NMR (471 MHz, DMSO-d_6) δ -117.32. HRMS (ESI) *m/z* calculated for $C_{17}H_{13}FNO_2^-$ [M-H]$^-$ 282.0936, found: 282.0935.



4-((4-bromophenyl)(hydroxy)methyl)-3-methylisoquinolin-1(2H)-one (3ay): white solid (74 mg, yield 82%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.25 (br, 1H), 8.14 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.69 (d, *J* = 8.5 Hz, 1H), 7.48 – 7.40 (m, 3H), 7.33 – 7.28 (m, 3H), 6.25 – 5.90 (m, 2H), 2.37 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.86, 144.14, 136.67, 136.59, 131.25, 130.88, 127.68, 126.61, 125.55, 125.49, 124.95, 119.24, 113.42, 67.62, 30.68, 16.73; HRMS (ESI) *m/z* calculated for $C_{17}H_{13}BrNO_2^-$ [M-H]$^-$ 342.0135, found: 342.0134.

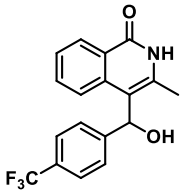


4-(hydroxy(3-methyl-1-oxo-1,2-dihydroisoquinolin-4-yl)methyl)benzonitrile (3az): pale red solid (68 mg, yield 97%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.28 (br, 1H), 8.14 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.74 (d, *J* = 8.5 Hz, 2H), 7.62 (d, *J* = 8.5 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.31 (t, *J* = 7.5 Hz, 1H), 6.40 – 6.10 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.83, 150.68, 137.10, 136.43, 132.05, 131.36, 126.69, 126.39, 125.46, 125.28, 125.03, 118.94, 113.06, 108.99, 67.87, 16.75; HRMS (ESI) *m/z* calculated for $C_{18}H_{13}N_2O_2^-$ [M-H]$^-$ 289.0983, found: 289.0980.

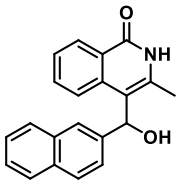


4-(hydroxy(3-methyl-1-oxo-1,2-dihydroisoquinolin-4-yl)methyl)benzonitrile (3ba): yellow solid (30 mg, yield 38%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.30 (br, 1H), 8.17 – 8.14 (m, 3H),

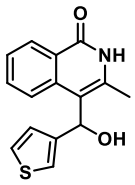
7.69 – 7.60 (m, 3H), 7.44 – 7.40 (m, 1H), 7.31 (t, *J* = 7.0 Hz, 1H), 6.41 – 6.05 (m, 2H), 2.40 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.85, 152.90, 146.07, 137.17, 136.41, 131.44, 127.67, 126.65, 125.48, 125.23, 125.09, 123.30, 113.07, 67.91, 16.77; HRMS (ESI) *m/z* calculated for $C_{17}H_{13}N_2O_4^-$ [M-H]$^-$ 309.0881, found: 309.0875.



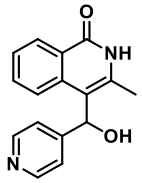
4-(hydroxy(phenyl)methyl)-3-methyl-6-(trifluoromethyl)isoquinolin-1(2H)-one (3bb): white solid (34 mg, yield 41%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.28 (br, 1H), 8.15 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.68 – 7.63 (m, 3H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.44 – 7.40 (m, 1H), 7.33 – 7.29 (m, 1H), 6.19 (br, 2H), 2.39 (s, 3H); ^{13}C NMR (126 MHz,DMSO-d_6) δ 161.88, 149.59, 136.93, 136.54, 131.36, 127.04, 126.68, 126.14, 125.50, 125.40, 125.03, 124.97 (m), 123.32, 113.33, 67.83, 16.76; ^{19}F NMR (471 MHz, DMSO-d_6) δ -60.69; HRMS (ESI) *m/z* calculated for $C_{18}H_{13}F_3NO_2^-$ [M-H]$^-$ 332.0904, found: 332.0898.



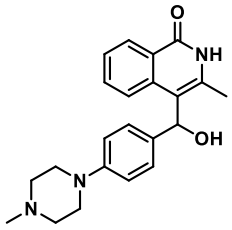
4-(hydroxy(naphthalen-2-yl)methyl)-3-methylisoquinolin-1(2H)-one (3bc): yellow solid (75 mg, yield 95%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.28 (br, 1H), 8.15 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.97 (s, 1H), 7.88 (d, *J* = 7.0 Hz, 1H), 7.84 – 7.78 (m, 3H), 7.46 – 7.44 (m, 3H), 7.38 – 7.34 (m, 1H), 7.27 (t, *J* = 7.0 Hz, 1H), 6.30 (s, 1H), 6.13 (br, 1H), 2.44 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.93, 142.32, 136.86, 136.62, 132.84, 131.79, 131.16, 127.84, 127.55, 127.39, 126.56, 125.97, 125.66, 125.50, 125.43, 124.87, 124.19, 123.39, 113.83, 68.19, 16.86; HRMS (ESI) *m/z* calculated for $C_{21}H_{16}NO_2^-$ [M-H]$^-$ 314.1187, found: 314.1186.



4-(hydroxy(thiophen-3-yl)methyl)-3-methylisoquinolin-1(2H)-one (3bd): white solid (55 mg, yield 81%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.19 (br, 1H), 8.14 (dd, J = 8.0, 1.5 Hz, 1H), 7.91 (d, J = 8.5 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.40 – 7.38 (m, 1H), 7.32 (t, J = 7.0 Hz, 1H), 7.23 – 7.22 (m, 1H), 6.88 (dd, J = 5.0, 1.0 Hz, 1H), 6.11 (s, 1H), 5.93 (br, 1H), 2.36 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.85, 146.43, 136.90, 135.80, 131.10, 126.48, 126.34, 125.93, 125.64, 125.38, 124.86, 119.92, 113.78, 66.57, 16.64; HRMS (ESI) *m/z* calculated for $C_{15}H_{12}NO_2S^-$ $[M-H]^-$ 270.0594, found: 270.0591.

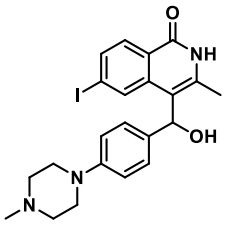


4-(hydroxy(pyridin-4-yl)methyl)-3-methylisoquinolin-1(2H)-one (3be): yellow solid (66 mg, yield 83%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.28 (s, 1H), 8.45 (d, J = 5.0 Hz, 2H), 8.15 (d, J = 7.1 Hz, 1H), 7.64 (d, J = 8.5 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.38 – 7.28 (m, 3H), 6.21 (br, 1H), 6.11 (s, 1H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.86, 153.75, 149.37, 137.13, 136.44, 131.36, 126.69, 125.45, 125.28, 125.05, 120.68, 112.89, 67.30, 16.76; HRMS (ESI) *m/z* calculated for $C_{16}H_{13}N_2O_2^-$ $[M-H]^-$ 265.0983, found: 265.0981.

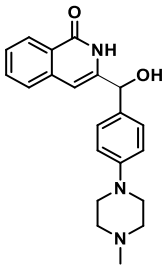


4-(hydroxy(4-(4-methylpiperazin-1-yl)phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3bf): white solid (43 mg, yield 47%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.18 (br, 1H), 8.15 – 8.12 (m, 1H), 7.80 (d, J = 8.5 Hz, 1H), 7.44 – 7.39 (m, 1H), 7.30 (t, J = 7.5 Hz, 1H), 7.15 (d, J = 8.5 Hz, 2H), 6.83 (d, J = 9.0 Hz, 2H), 6.05 (s, 1H), 5.81 (br, 1H), 3.06 – 3.03 (m, 4H), 2.51 – 2.39 (m, 4H),

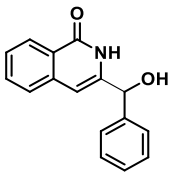
2.35 (s, 3H), 2.19 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.86, 149.37, 136.95, 135.93, 134.64, 131.03, 126.46, 125.99, 125.96, 125.45, 124.79, 115.02, 114.13, 67.75, 54.63, 48.16, 45.75, 16.72; HRMS (ESI) *m/z* calculated for $C_{22}H_{24}N_3O_2^-$ [M-H]$^-$ 362.1874, found: 362.1870.



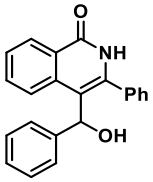
4-(hydroxy(4-(4-methylpiperazin-1-yl)phenyl)methyl)-6-iodo-3-methylisoquinolin-1(2H)-one (3bg): white solid (70 mg, yield 72%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.32 (br, 1H), 8.26 (d, *J* = 1.5 Hz, 1H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.62 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.14 (d, *J* = 8.5 Hz, 2H), 6.85 (d, *J* = 9.0 Hz, 2H), 6.00 (s, 1H), 5.87 (br, 1H), 3.08 – 3.05 (m, 4H), 2.42 – 2.39 (m, 4H), 2.35 (s, 3H), 2.19 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.61, 149.48, 138.37, 137.35, 134.77, 134.13, 133.37, 128.42, 125.90, 124.63, 115.01, 113.10, 99.93, 67.65, 54.61, 48.13, 45.77, 16.78; HRMS (ESI) *m/z* calculated for $C_{22}H_{23}IN_3O_2^-$ [M-H]$^-$ 488.0840, found: 488.0850.



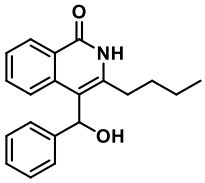
3-(hydroxy(4-(4-methylpiperazin-1-yl)phenyl)methyl)isoquinolin-1(2H)-one (3bh): yellow solid (39 mg, yield 45%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.97 (br, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.42 – 7.39 (m, 1H), 7.29 (d, *J* = 8.5 Hz, 2H), 6.88 (d, *J* = 8.5 Hz, 2H), 6.57 (s, 1H), 5.43 (s, 1H), 3.10 – 3.07 (m, 4H), 2.43 – 2.40 (m, 4H), 2.19 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.09, 150.47, 145.66, 137.87, 132.68, 132.40, 127.43, 126.55, 126.31, 125.82, 124.70, 114.91, 100.24, 70.83, 54.54, 48.07, 45.75; HRMS (ESI) *m/z* calculated for $C_{21}H_{22}N_3O_2^-$ [M-H]$^-$ 348.1718, found: 348.1717.



3-(hydroxy(phenyl)methyl)isoquinolin-1(2H)-one (3bi): yellow oil (42 mg, yield 63%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.06 (br, 1H), 8.11 (d, J = 8.0 Hz, 1H), 7.68 – 7.63 (m, 2H), 7.50 – 7.48 (m, 2H), 7.45 – 7.41 (m, 1H), 7.36 – 7.32 (m, 2H), 7.28 – 7.24 (m, 1H), 6.60 (s, 1H), 6.20 (br, 1H), 5.54 (s, 1H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.24, 145.20, 142.57, 137.86, 132.59, 128.25, 127.61, 126.72, 126.66, 126.47, 126.10, 124.84, 100.85, 71.21; HRMS (ESI) *m/z* calculated for $C_{16}H_{14}NO_2^+$ $[M+H]^+$ 252.1024, found: 252.1019.

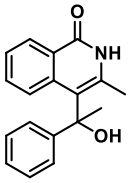


4-(hydroxy(phenyl)methyl)-3-phenylisoquinolin-1(2H)-one (3bj): yellow solid (51 mg, yield 95%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.40 (s, 1H), 8.24 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.69 – 7.60 (m, 2H), 7.52 – 7.46 (m, 3H), 7.46 – 7.41 (m, 1H), 7.40 – 7.34 (m, 3H), 7.25 (t, *J* = 7.5 Hz, 2H), 7.14 (t, *J* = 7.5 Hz, 1H), 6.08 (br, 1H), 5.71 (s, 1H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.65, 144.50, 140.07, 136.20, 134.51, 131.18, 129.35, 129.00, 128.41, 128.06, 127.17, 126.69, 126.52, 126.18, 125.79, 125.24, 114.00, 69.20; HRMS (ESI) *m/z* calculated for $C_{22}H_{16}NO_2^-$ $[M-H]^-$ 326.1187, found: 326.1191.

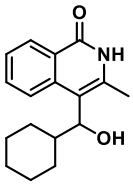


3-butyl-4-(hydroxy(phenyl)methyl)isoquinolin-1(2H)-one (3bk): yellow solid (51 mg, yield 70%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.21 (br, 1H), 8.14 (d, *J* = 7.8 Hz, 1H), 7.68 (d, *J* = 8.3 Hz, 1H), 7.40 – 7.32 (m, 3H), 7.30 – 7.23 (m, 3H), 7.16 (t, *J* = 7.1 Hz, 1H), 6.10 (s, 1H), 6.04 (br, 1H), 2.75 – 2.62 (m, 2H), 1.65 – 1.53 (m, 2H), 1.39 – 1.30 (m, 2H), 0.87 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.04, 144.84, 140.92, 136.84, 130.97, 128.02, 126.48, 126.15,

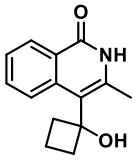
126.27, 125.65, 125.31, 124.92, 113.29, 67.74, 31.69, 27.03, 22.07, 13.70; HRMS (ESI) *m/z* calculated for $C_{20}H_{20}NO_2^-$ $[M-H]^-$ 306.1500, found: 306.1497.



4-(1-hydroxy-1-phenylethyl)-3-methylisoquinolin-1(2H)-one (3bl): yellow solid (51 mg, yield 70%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.99 (s, 1H), 8.27 (dd, *J* = 8.0, 0.5 Hz, 1H), 7.74 – 7.70 (m, 1H), 7.65 (d, *J* = 8.5 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.44 – 7.40 (m, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 6.66 (s, 1H), 1.92 (s, 3H), 1.75 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.23, 145.51, 142.04, 139.30, 132.54, 128.29, 127.44, 126.81, 126.12, 125.85, 124.91, 123.18, 105.06, 72.83, 26.67, 12.89; HRMS (ESI) *m/z* calculated for $C_{18}H_{18}NO_2^+$ $[M+H]^+$ 280.1337, found: 280.1329.

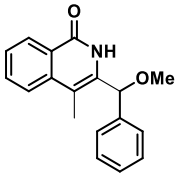


4-(cyclohexyl(hydroxy)methyl)-3-methylisoquinolin-1(2H)-one (3bm): white solid (55 mg, yield 81%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.06 (s, 1H), 8.39 – 8.15 (m, 2H), 7.68 – 7.58 (m, 1H), 7.42 – 7.35 (m, 1H), 5.17 (br, 1H), 4.54 (br, 1H), 2.26 (s, 3H), 1.99 – 1.83 (m, 1H), 1.76 – 1.72 (m, 1H), 1.62 – 1.49 (m, 2H), 1.30 – 0.9 (m, 6H), 0.88 – 0.75 (m, 1H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.66, 137.29, 131.24, 126.69, 125.40, 124.89, 113.40, 73.18, 42.69, 30.46, 29.16, 26.04, 25.74, 25.63, 17.15.; HRMS (ESI) *m/z* calculated for $C_{17}H_{22}NO_2^+$ $[M+H]^+$ 272.1651, found: 272.1645.

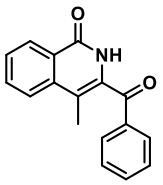


4-(1-hydroxycyclobutyl)-3-methylisoquinolin-1(2H)-one (3bn): white solid (30 mg, yield 53%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.98 (s, 1H), 8.16 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.81 (d, *J* = 8.0 Hz,

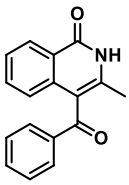
1H), 7.63 – 7.59 (m, 1H), 7.40 – 7.36 (m, 1H), 5.48 (br, 1H), 2.56 – 2.53 (m, 2H), 2.47 – 2.42 (m, 2H), 2.26 – 2.18 (m, 4H), 1.75 –1.67 (m, 1H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.59, 137.28, 135.46, 131.19, 126.58, 124.88, 124.78, 124.75, 117.57, 76.78, 38.90, 18.27, 16.46; HRMS (ESI) *m/z* calculated for $C_{14}H_{14}NO_2^-$ $[M-H]^-$ 228.1030, found: 228.1024.



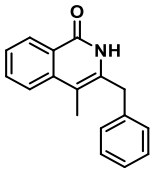
3-(methoxy(phenyl)methyl)-4-methylisoquinolin-1(2H)-one (4a): yellow solid (30 mg, yield 43%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.39 (br, 1H), 8.43 (d, *J* = 7.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.48 – 7.44 (m, 1H), 7.40 – 7.36 (m, 2H), 7.34 – 7.30 (m, 2H), 7.29 – 7.24 (m, 3H), 2.63 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.19, 139.14, 138.40, 136.77, 132.17, 128.57, 127.50, 125.65, 125.58, 125.29, 125.23, 110.99, 71.66, 21.09, 17.78; HRMS (ESI) *m/z* calculated for $C_{18}H_{18}NO_2^+$ $[M+H]^+$ 280.1338, found: 280.1329.



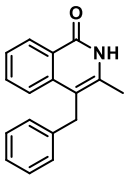
3-benzoyl-4-methylisoquinolin-1(2H)-one (4b): yellow solid (51 mg, yield 78%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.64 (s, 1H), 8.24 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.84 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.70 – 7.66 (m, 1H), 7.60 – 7.55 (m, 1H), 7.53 (t, *J* = 8.0 Hz, 2H), 7.48 – 7.44 (m, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 2.05 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 196.01, 161.76, 138.14, 137.75, 135.83, 134.05, 132.72, 129.31, 129.19, 126.97, 126.05, 124.06, 123.71, 113.41, 17.34; HRMS (ESI) *m/z* calculated for $C_{17}H_{14}NO_2^+$ $[M+H]^+$ 264.1025, found: 264.1019.



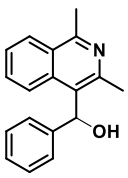
4-benzoyl-3-methylisoquinolin-1(2H)-one (4b'): yellow solid (9 mg, yield 14%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.47 (br, 1H), 8.49 (d, *J* = 7.5 Hz, 1H), 7.85 (d, *J* = 7.5 Hz, 2H), 7.82 – 7.77 (m, 2H), 7.68 – 7.60 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 2H), 2.21 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.00, 161.69, 137.70, 137.11, 133.98, 133.02, 132.50, 129.61, 128.98, 128.50, 128.01, 127.17, 124.57, 115.27, 14.80; HRMS (ESI) *m/z* calculated for $C_{17}H_{14}NO_2^+$ $[M+H]^+$ 264.1025, found: 264.1018.



3-benzyl-4-methylisoquinolin-1(2H)-one (4c): withe solid (yield 27%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.27 (s, 1H), 8.21 (d, J = 8.1 Hz, 1H), 7.76 – 7.68 (m, 2H), 7.49 – 7.42 (m, 1H), 7.33 – 7.27 (m, 2H), 7.26 – 7.23 (m, 2H), 7.20 (t, J = 7.1 Hz, 1H), 3.99 (s, 2H), 2.22 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.76, 138.51, 138.45, 136.83, 132.42, 128.51, 128.10, 126.80, 126.31, 125.59, 124.95, 123.29, 107.19, 35.70, 12.30; HRMS (ESI) *m/z* calculated for $C_{17}H_{16}NO^+$ $[M+H]^+$ 250.1232, found: 250.1221.



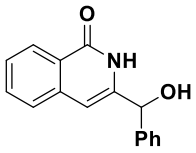
4-benzyl-3-methylisoquinolin-1(2H)-one (4c'): withe solid (yield 45%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.27 (s, 1H), 8.21 – 8.16 (m, 1H), 7.62 – 7.50 (m, 2H), 7.43 – 7.33 (m, 1H), 7.28 – 7.21 (m, 2H), 7.18 – 7.13 (m, 3H), 4.07 (s, 2H), 2.29 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.73, 140.19, 138.01, 136.37, 132.30, 128.45, 127.69, 126.90, 125.90, 125.11, 124.99, 123.29, 109.22, 31.38, 16.65; HRMS (ESI) *m/z* calculated for $C_{17}H_{16}NO^+$ $[M+H]^+$ 250.1232, found: 250.1223.



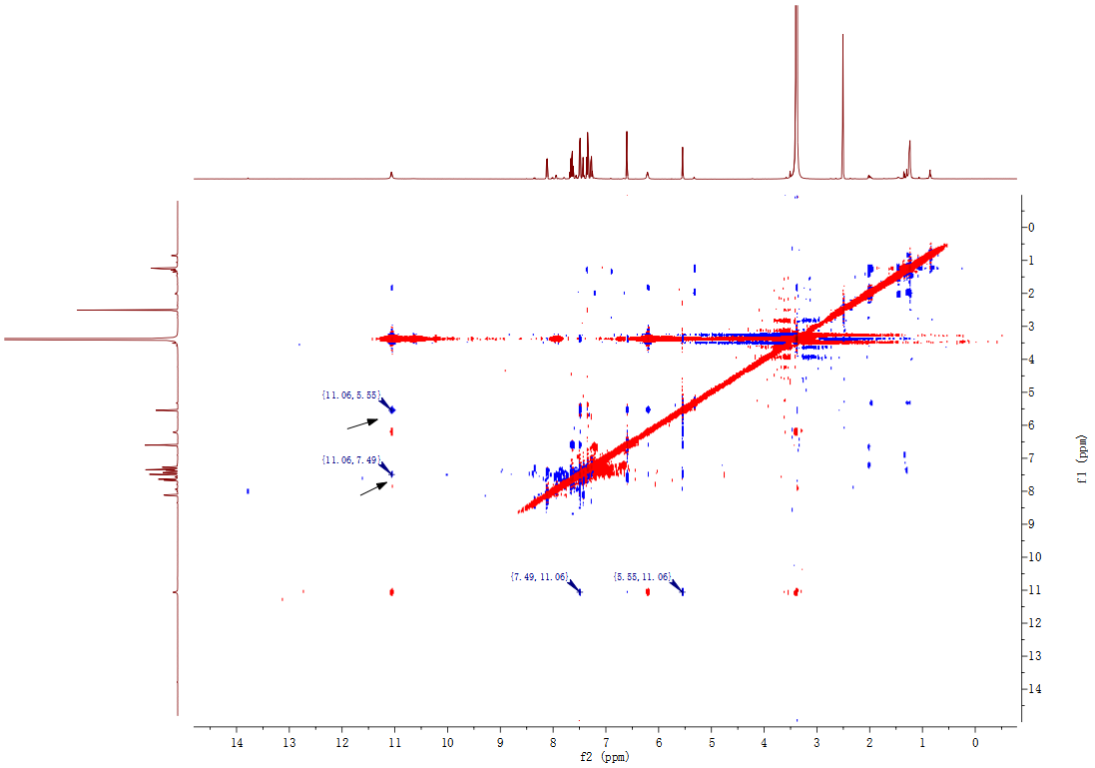
(1,3-dimethylisoquinolin-4-yl)(phenyl)methanol (4d): withe solid (yield 72%), ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.16 – 8.10 (m, 2H), 7.53 – 7.45 (m, 2H), 7.28 – 7.25 (m, 4H), 7.22 – 7.12 (m, 1H), 6.47 (d, J = 4.2 Hz, 1H), 6.20 (d, J = 4.2 Hz, 1H), 2.85 (s, 3H), 2.68 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 156.86, 147.64, 144.65, 134.16, 128.94, 128.23, 128.04, 126.25, 126.20, 125.92, 125.82, 125.55, 125.25, 68.98, 22.70, 22.15; HRMS (ESI) *m/z* calculated for $C_{18}H_{18}NO^{+}$ $[M+H]^{+}$ 264.1388, found: 264.1376.

NOESY Experiments for Product 3bi, 3bj, 3bk, 4a, 4b, 4c, and **4d**

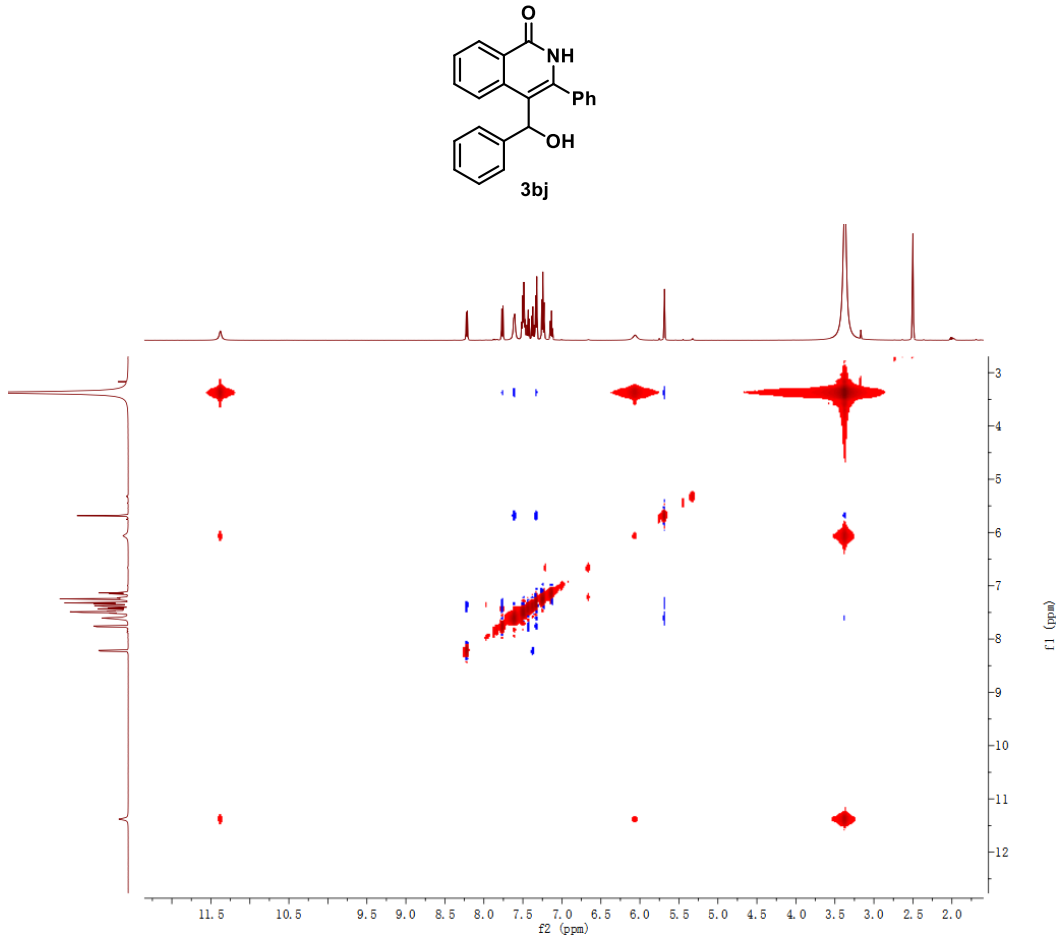
1) NOESY spectra of product **3bi**



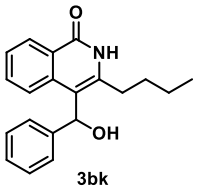
3bi

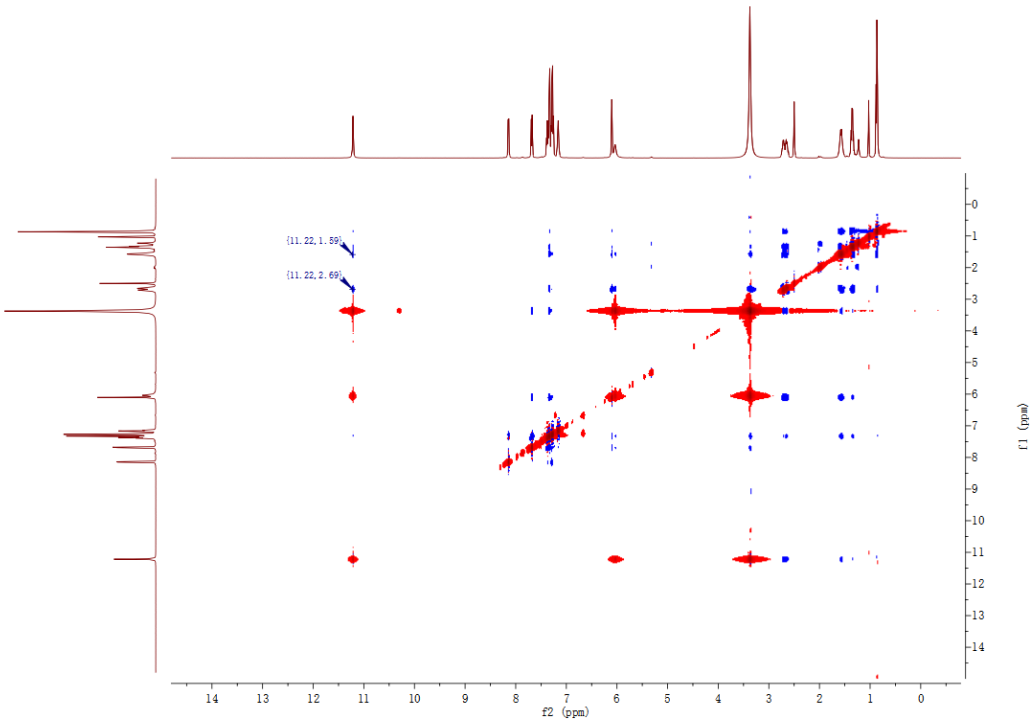


2) NOESY spectra of product **3bj**

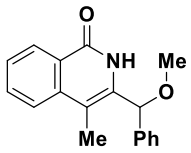


3) NOESY data of product **3bk**

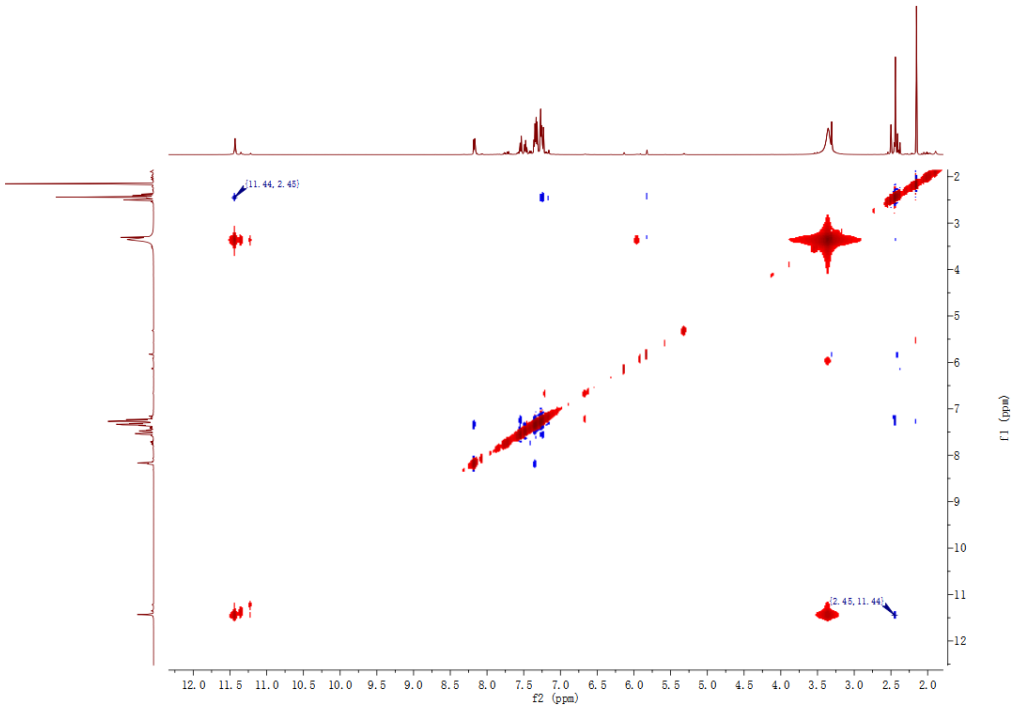




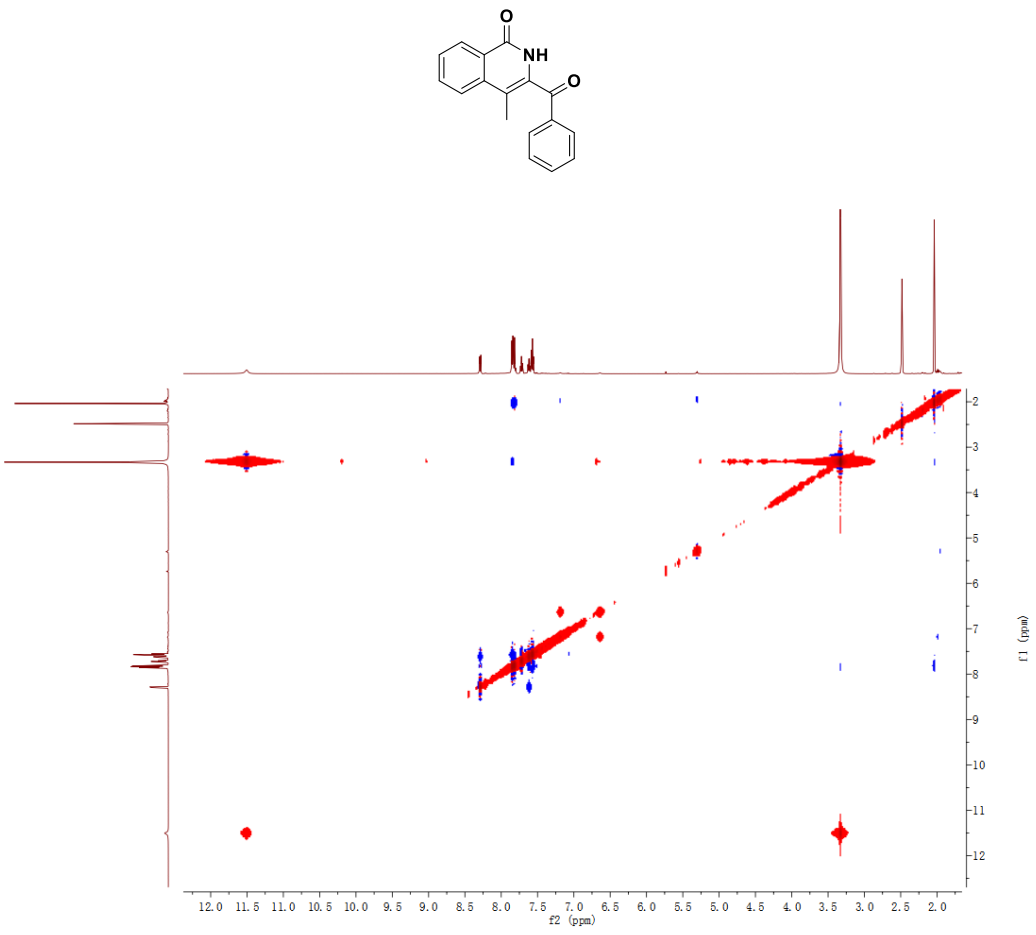
4) NOESY data of product **4a**



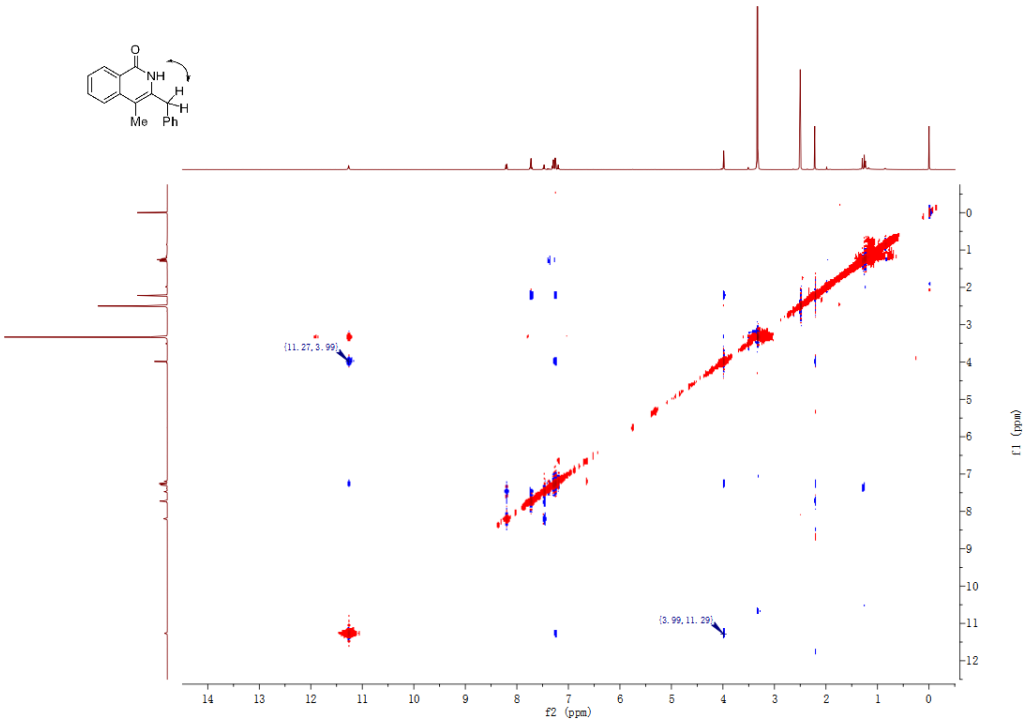
4a



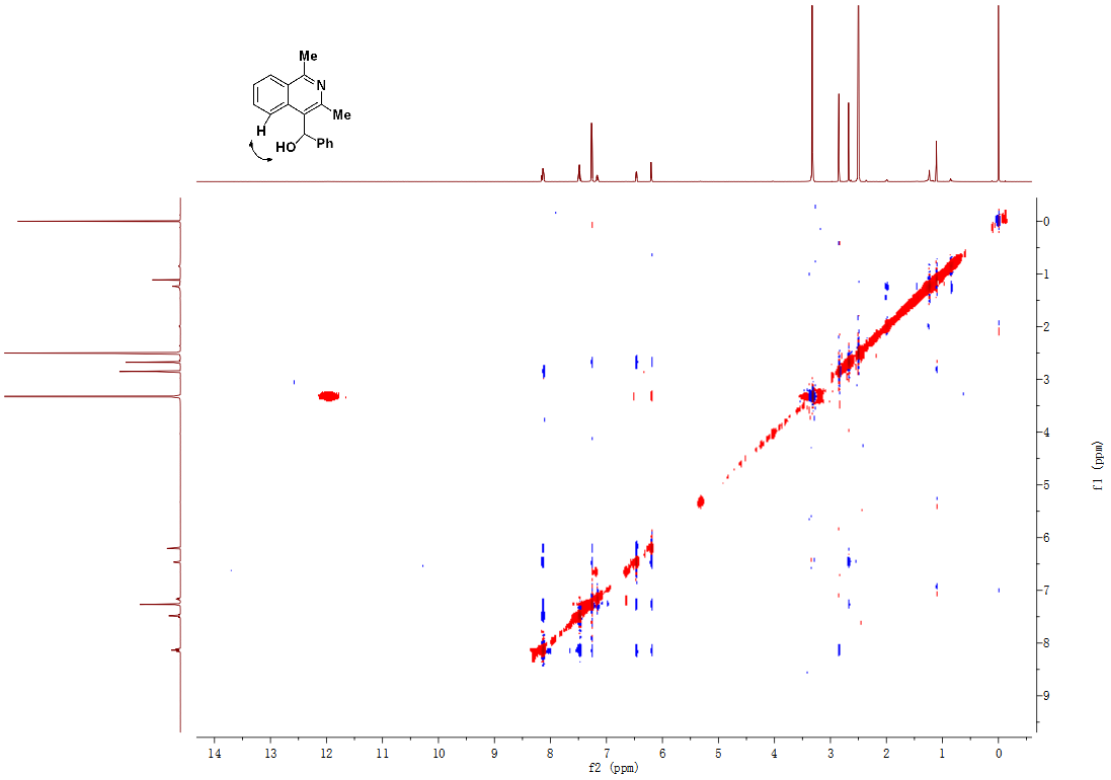
5) NOESY data of product **4b**



6) NOESY data of product **4c**

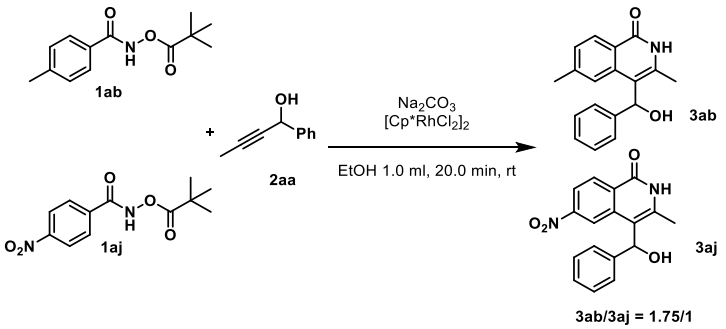


7) NOESY data of product **4d**



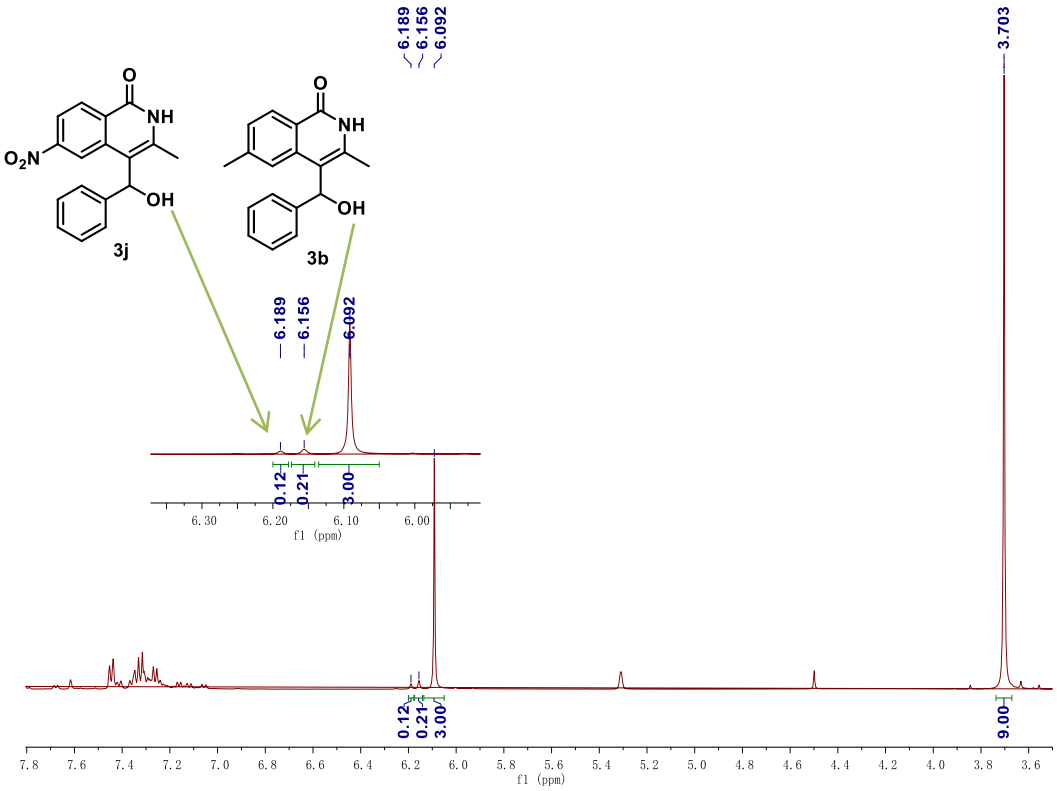
Intermolecular Competition Experiment

The competition experiment between **1ab** and **1aj**



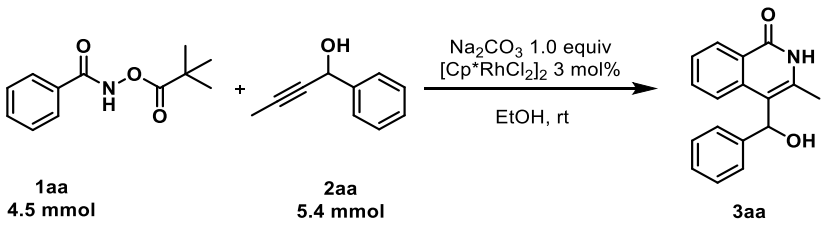
To a mixture of **1ab** (29.4 mg, 0.125 mmol, 1.0 eq.), **1aj** (33.3 mg, 0.125 mmol, 1.0 equiv), **2aa** (43.9 mg, 0.3 mmol, 1.2 eq.), $[Cp^*RhCl_2]_2$ (7.7 mg, 0.0125 mmol, 5 mol%) and Na_2CO_3 (26.5 mg, 0.25 mmol, 1.0 eq.) in a 10 mL reaction tube was added EtOH (1.0 mL). Then the resulting mixture was stirred at the temperature for 20.0 min. The solvent was removed in vacuum and ^1H NMR was taken using 0.25 mmol 1,3,5-trimethoxybenzene as the internal standard.

The reaction of **1ab** (29.4 mg, 0.125 mmol, 1.0 eq.), **1aj** (33.3 mg, 0.125 mmol, 1.0 equiv) with **2aa** (43.9 mg, 0.3 mmol, 1.2 eq.) provided the product **3ab** in 21% NMR yield，**3aj** in 12% NMR yield. The ratio of **3ab**/**3aj** was 1.75 (0.21/0.12)

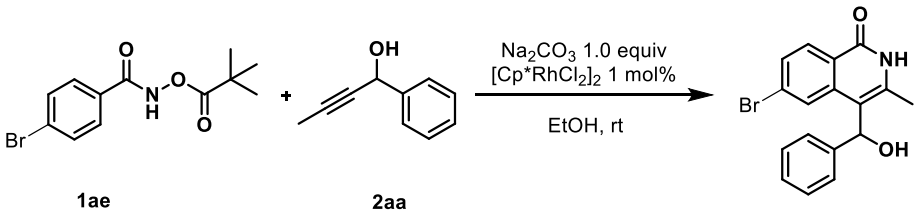


^{1}H NMR of the products **3ab**/**3aj**.

Gram-Scale Experiments



In a 100 mL reaction tube, the mixture of **1aa** (995.7 mg, 4.5 mmol, 1.0 eq.), **2aa** (789.4 mg, 6.0 mmol, 1.2 eq.), $[Cp^*RhCl_2]_2$ (83.0 mg, 0.135 mmol, 3 mol%) and Na_2CO_3 (477 mg, 4.5 mmol, 1.0 eq.) was added EtOH (8.0 mL). Then the resulting mixture was stirred at the temperature for 1.0 h. When the reaction was finished, the product precipitated out was simply collected by filtration, and the precipitation was washed with water. The product **3aa** was obtained as a white solid (1.10 g, 92% yield).

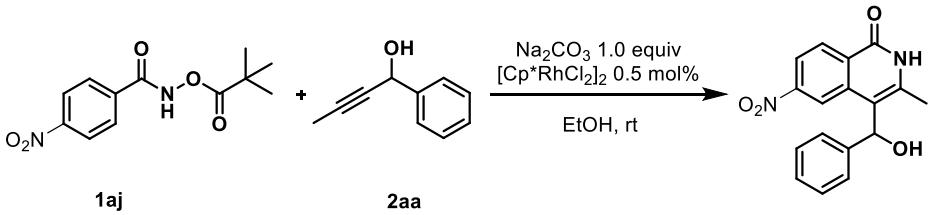


1ae
3 mmol

2aa
3.6 mmol

3ae

In a 100 mL reaction tube, the mixture of **1ae** (900.5 mg, 3 mmol, 1.0 eq.), **2aa** (526.3 mg, 3.6 mmol, 1.2 eq.), $[Cp^*RhCl_2]_2$ (18.5 mg, 1 mol%) and Na_2CO_3 (318.0 mg, 3 mmol, 1.0 eq.) was added EtOH (8.0 mL). Then the resulting mixture was stirred at the temperature for 2.0 h. When the reaction was finished, the product precipitated out was simply collected by filtration, and the precipitation was washed with water. The product **3ae** was obtained as a white solid (0.919 g, 89% yield).



1aj
8.0 mmol

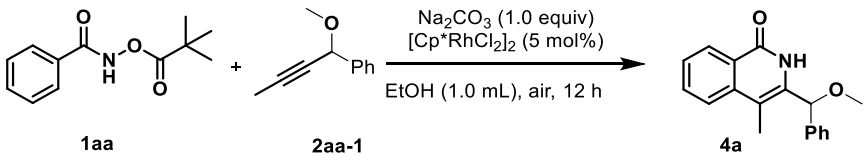
2aa
9.6 mmol

3aj

In a 100 mL reaction tube, the mixture of **1aj** (2130 mg, 8 mmol, 1.0 eq.), **2aa** (1403 mg, 9.6 mmol, 1.2 eq.), $[Cp^*RhCl_2]_2$ (24.7 mg, 0.5 mol%) and Na_2CO_3 (848.0 mg, 8 mmol, 1.0 eq.) was added EtOH (15.0 mL). Then the resulting mixture was stirred at the temperature for 3.5 h. When the reaction was finished, the product precipitated out was simply collected by filtration, and the precipitation was washed with water. The product **3aj** was obtained as a white solid (2.035 g, 82% yield).

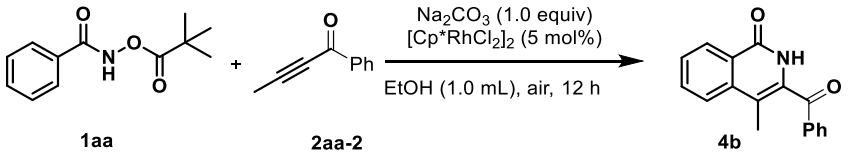
Control Experiments

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



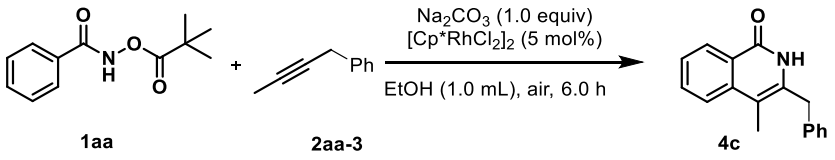
In a 10 mL reaction tube, the mixture of **1aa** (0.25 mmol), **2aa-1** (0.3 mmol), $[Cp^*RhCl_2]_2$ (5.0 mol%) and Na_2CO_3 (1.0 eq.) was added EtOH (1.0 mL). Then the resulting mixture was stirred for 12 h. When the reaction was finished, the solvent was removed under vacuum. The reaction mixture was subjected directly to flash chromatography on silica gel (petroleum ether/ethyl acetate) to provide the products **4a** in 43% yield.

b) Procedure for the Synthesis of **4b**



In a 10 mL reaction tube, the mixture of **1aa** (0.25 mmol), **2aa-2** (0.3 mmol), $[Cp^*RhCl_2]_2$ (5.0 mol%) and Na_2CO_3 (1.0 eq.) was added EtOH (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 (petroleum ether/ethyl acetate) to provide the products **4b** (78% yield) and **4b'** (14% yield).

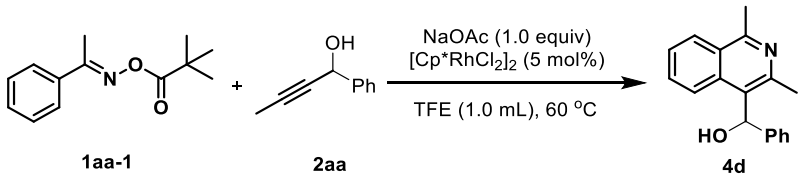
c) Procedure for the Synthesis of **4c**



In a 10 mL reaction tube, the mixture of **1aa** (0.25 mmol), **2aa-1** (0.3 mmol), $[Cp^*RhCl_2]_2$ (5.0 mol%) and Na_2CO_3 (1.0 eq.) was added EtOH (1.0 mL). Then the resulting mixture was stirred for 6.0 h. When the reaction was finished, the solvent was removed under vacuum. The reaction

mixture was subjected directly to flash chromatography on silica gel (petroleum ether/ethyl acetate) to provide the products **4c** (27% yield) and **4c'** (45% yield).

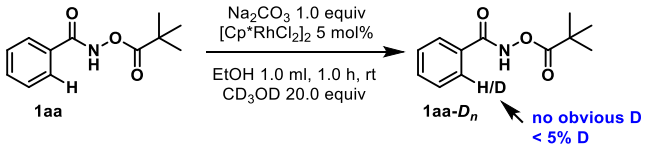
d) Procedure for the Synthesis of **4d**



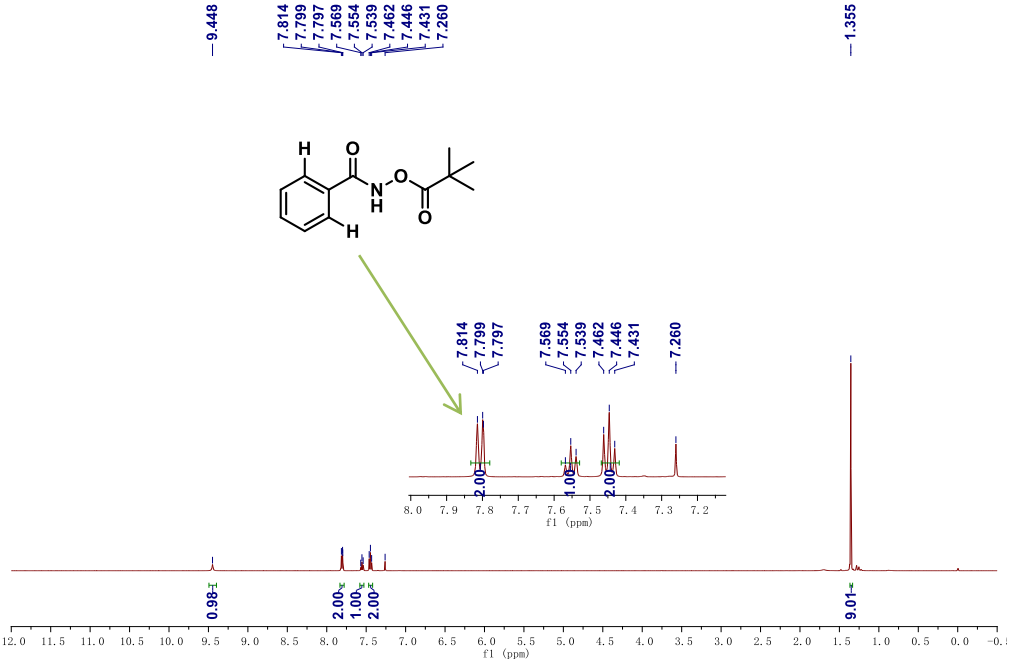
In a 10 mL reaction tube, the mixture of **1aa-1** (0.25 mmol), **2aa** (0.3 mmol), $[Cp^*RhCl_2]_2$ (5.0 mol%) and Na_2CO_3 (1.0 eq.) was added TFE (1.0 mL). Then the resulting mixture was stirred for 12 h at 60 ºC. When the reaction was finished, the solvent was removed under vacuum. The reaction mixture was subjected directly to flash chromatography on silica gel (petroleum ether/ethyl acetate) to provide the products **4d** (72% yield).

Mechanistic Experiments

Deuterium Incorporation Experiment A

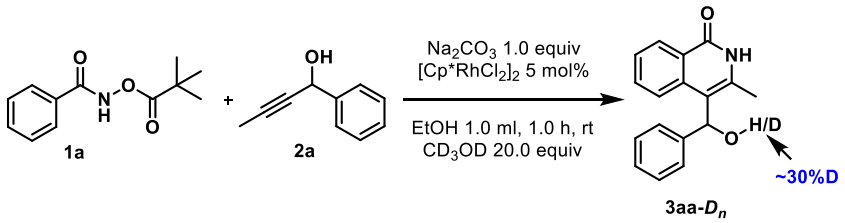


To a mixture of **1aa** (55.3 mg, 0.25 mmol, 1.0 eq.), $[Cp^*RhCl_2]_2$ (7.7 mg, 0.0125 mmol, 5 mol%) and Na_2CO_3 (26.5 mg, 0.25 mmol, 1.0 eq.) in a 10 mL reaction tube was added CD_3OD (180.4 mg, 5.0 mmol, 20.0 eq.). Then the resulting mixture was stirred at the temperature for 1.0 h. After removal of the solvents under vacuum, the residue obtained was directly used for ^{1}HNMR analysis. The reaction of **1aa** (55.3 mg, 0.25 mmol, 1.0 equiv) without **2aa** provided the product **1aa-*D*$_n$.** Found no obvious H/D exchange occurred at the C2-position of the **1aa** (< 5% D).



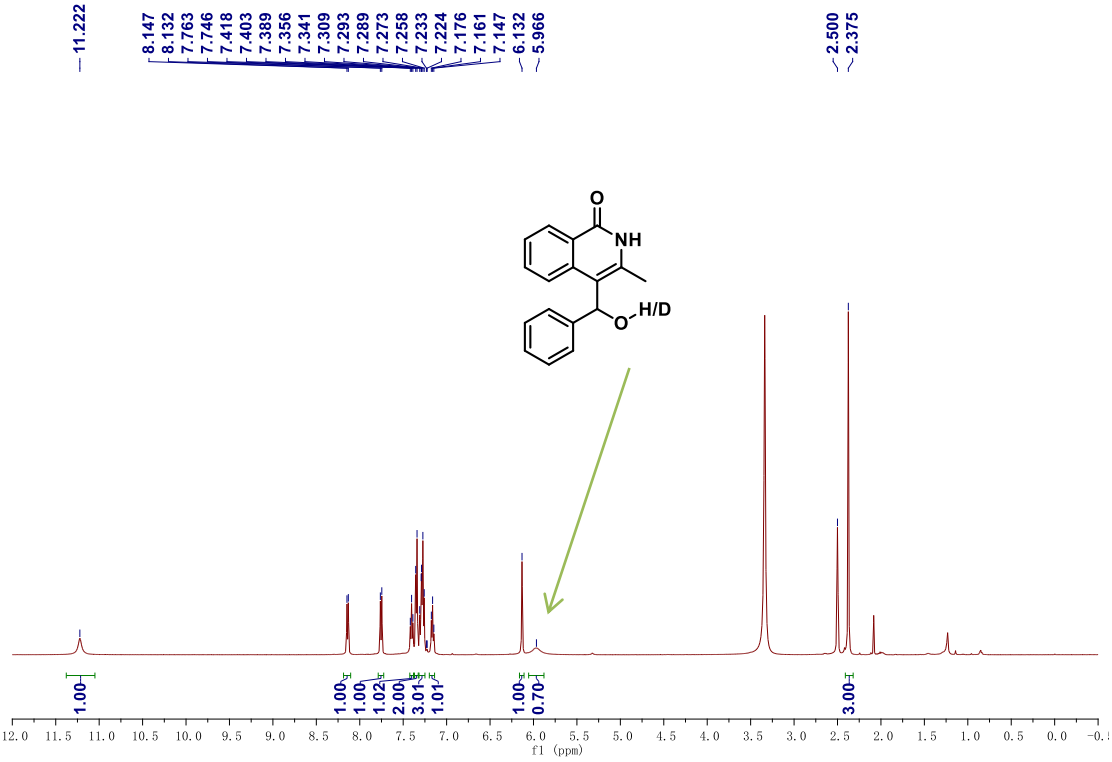
^{1}H NMR of the product **1aa-*D$_n$*** of this reaction.

Deuterium Incorporation Experiment B



To a mixture of **1aa** (55.3 mg, 0.25 mmol, 1.0 eq.), **2aa** (43.9 mg, 0.3 mmol, 1.2 eq.), $[Cp^*RhCl_2]_2$ (7.7 mg, 0.0125 mmol, 5 mol%) and Na_2CO_3 (26.5 mg, 0.25 mmol, 1.0 eq.), CD_3OD (180.4 mg, 5.0 mmol, 20.0 eq.) in a 10 mL reaction tube was added EtOH (1.0 mL). Then the resulting mixture was stirred at the temperature for 1.0 h. After removal of the solvents under vacuum, the residue obtained was directly used for ^{1}HNMR analysis.

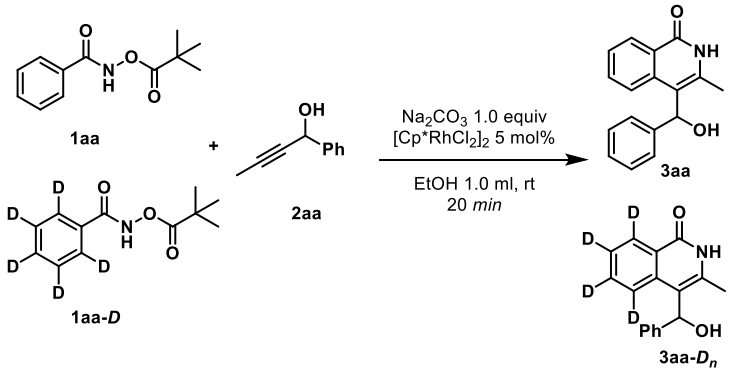
The reaction of **1aa** (55.3 mg, 0.25 mmol, 1.0 equiv) with **2aa** (43.9 mg, 0.3 mmol, 1.2 eq.) provided the product **3aa-*D*,** found 30% deuterium incorporation at the hydrogen of hydroxyl group.



^{1}H NMR of the product **3aa-*D*** of this reaction.

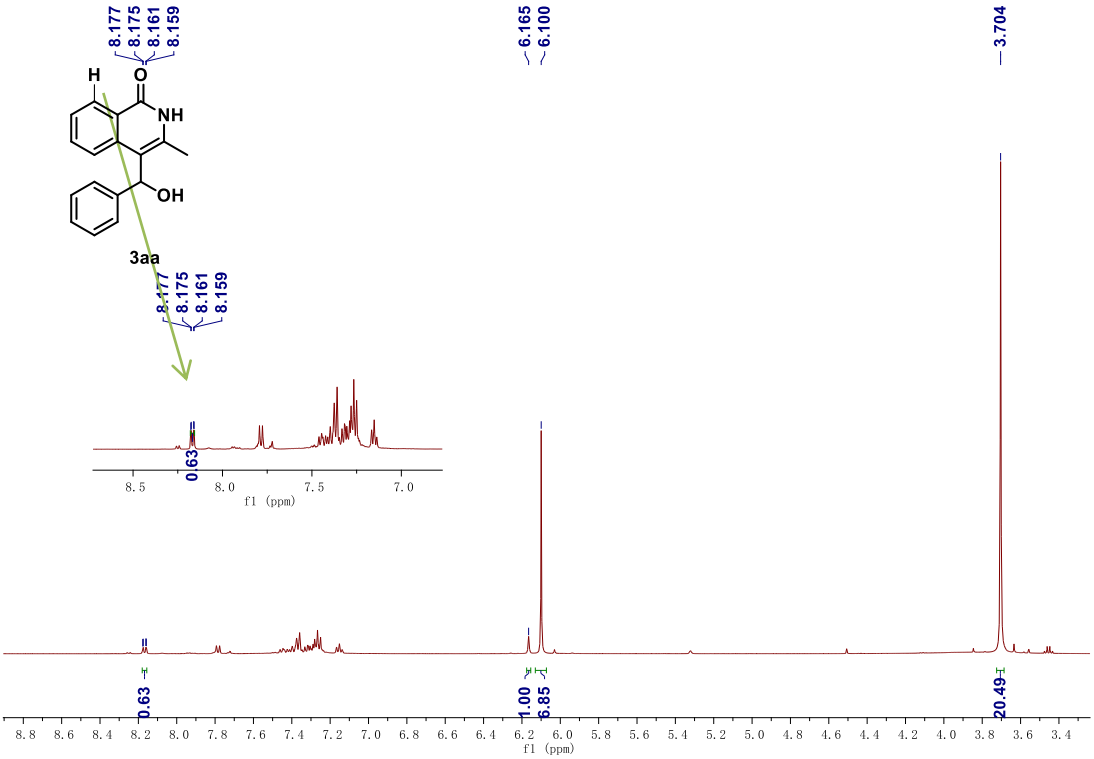
Determination of the KIE

(1) The intermolecular competition experiments



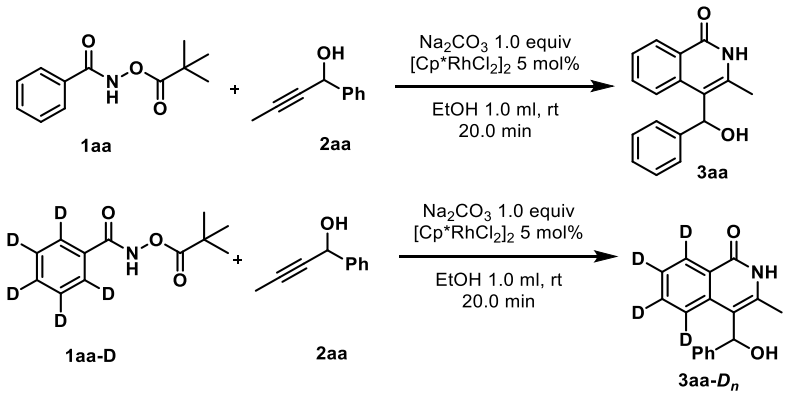
To a mixture of **1aa** (27.7 mg, 0.125 mmol, 1.0 eq.), **1aa-*D*** (28.3 mg, 0.125 mmol, 1.0 equiv.), **2aa** (43.9 mg, 0.3 mmol, 1.2 eq.), $[Cp^*RhCl_2]_2$ (7.7 mg, 0.0125 mmol, 5 mol%) and Na_2CO_3 (26.5 mg, 0.25 mmol, 1.0 eq.) in a 10 mL reaction tube was added EtOH (1.0 mL). Then the resulting mixture was stirred at the temperature for 20.0 min. The solvent was removed under vacuum and ^{1}H NMR was taken by using 0.25 mmol 1,3,5-trimethoxybenzene as the internal standard.

The ratio of **3aa**/**3aa-*D*$_n$** was 1.70 [0.63/(1.0 - 0.63)] based on ^{1}H NMR.



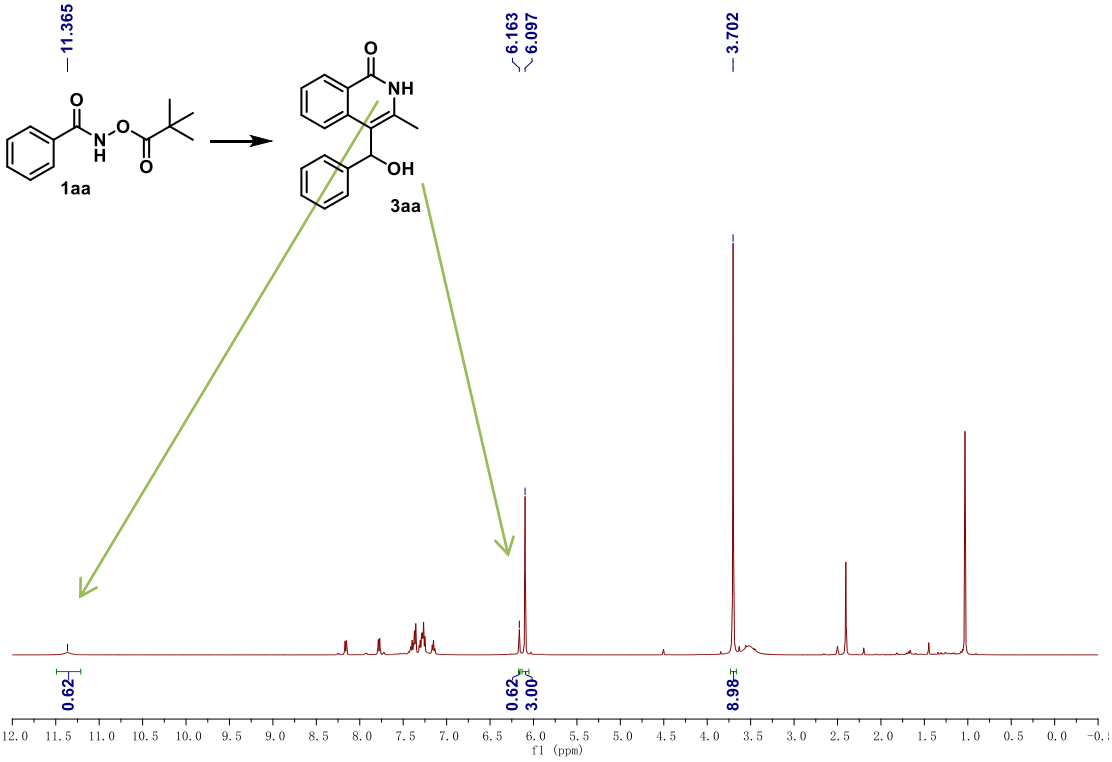
^{1}H NMR of the products **3aa**/**3aa-*D*$_n$** of this reaction.

(2) Two parallel reactions for KIE value measurement



To a mixture of **1aa** (55.3 mg, 0.25 mmol, 1.0 eq.), **2aa** (43.9 mg, 0.3 mmol, 1.2 eq.), $[Cp^*RhCl_2]_2$ (7.7 mg, 0.0125 mmol, 5 mol%) and Na_2CO_3 (26.5 mg, 0.25 mmol, 1.0 eq.), in a 10 mL reaction tube was added EtOH (1.0 mL). Then the resulting mixture was stirred at the temperature for 20.0 min. The solvent was removed under vacuum and ^{1}H NMR was taken using 0.25 mmol 1,3,5-trimethoxybenzene as the internal standard.

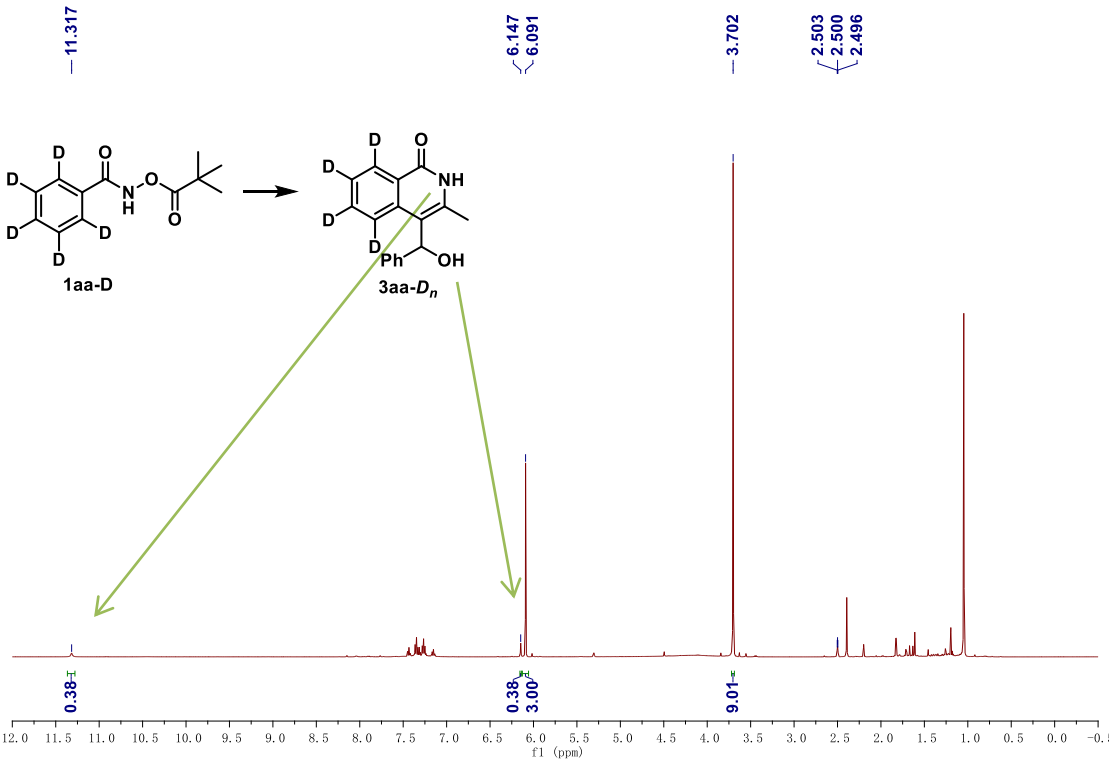
The reaction of **1aa** (55.3 mg, 0.25 mmol, 1.0 equiv) with **2aa** (43.9 mg, 0.3 mmol, 1.2 eq.) provided the product **3aa** in 62% NMR yield.



^{1}H NMR of the crude product **3aa**.

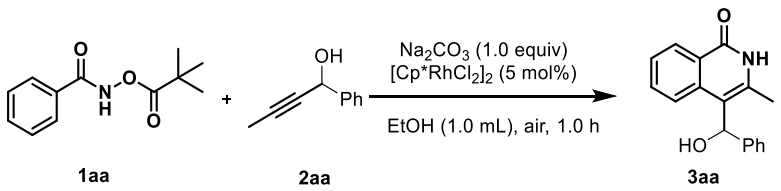
To a mixture of **1aa-D** (56.6 mg, 0.25 mmol, 1.0 equiv), **2aa** (43.9 mg, 0.3 mmol, 1.2 eq.), $[Cp^*RhCl_2]_2$ (7.7 mg, 0.0125 mmol, 5 mol%) and Na_2CO_3 (26.5 mg, 0.25 mmol, 1.0 eq.) in a 10 mL reaction tube was added EtOH (1.0 mL). Then the resulting mixture was stirred at the temperature for 20.0 min. The solvent was removed in vacuum and ^{1}H NMR was taken using 0.25 mmol 1,3,5-trimethoxybenzene as the internal standard.

The reaction of **1aa-D** (56.6 mg, 0.25 mmol, 1.0 equiv) with **2aa** (43.9 mg, 0.3 mmol, 1.2 eq.) provided the product **3aa-*D$_n$*** in 38% yield. The ratio of **3aa**/**3aa-*D$_n$*** was 1.63 (0.62/0.38)



^{1}H NMR of the crude product **3aa-*D*$_n$**

Catalyst Recycling Experiments



In a 10 mL reaction tube, the mixture of **1aa** (0.25 mmol), **2aa** (0.3 mmol), $[Cp^*RhCl_2]_2$ (5.0 mol%) and Na_2CO_3 (1.0 eq.) was added EtOH (1.0 mL). Then the resulting mixture was stirred for 1.0 h. When the reaction was finished, the desired product precipitated out as a solid, and the product **3aa** was simply collected by filtration. Due to Na_2CO_3 are coarse white granules in EtOH, it can be separated from the product easily by using Pasteur pipet during filtration. The precipitation was washed with ethanol (1.0 mL) and dried under vacuum. The filtrate (concentrated to ~1 mL) was reused in the next cycle without adding additional rhodium catalyst. **1aa** (0.25 mmol), **2aa** (0.3 mmol), and Na_2CO_3 (1.0 eq.) were added to the filtrate in each cycle. Repeating the above-mentioned procedure for 10 times in three days, the overall results showed that no obvious decrease in catalytic activity was observed.

X-ray data of compound 3aa (Deposition Data: CCDC 2156445)

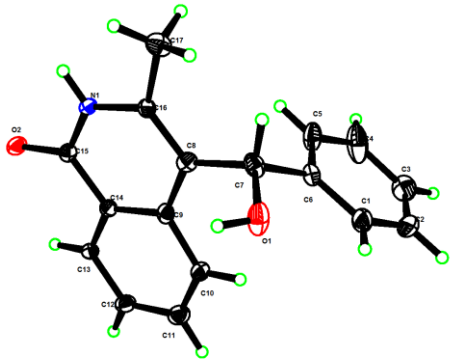


Table S1. Crystal data and structure refinement for compound 3aa.

Identification code	mo_2022197_0m
Empirical formula	$C_{17}H_{15}NO_2$
Formula weight	265.30
Temperature/K	150.0
Crystal system	monoclinic
Space group	Pc
a/Å	6.9187(10)
b/Å	12.6378(19)
c/Å	14.994(2)
α/°	90
β/°	96.541(5)
γ/°	90
Volume/Å^3	1302.5(3)
Z	4
ρ_{calc}g/cm^3	1.353
μ/mm^{-1}	0.089
F(000)	560.0
Crystal size/mm^3	0.12 × 0.08 × 0.05
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.226 to 52.848
Index ranges	-8 ≤ h ≤ 8, -15 ≤ k ≤ 15, -18 ≤ l ≤ 18
Reflections collected	11327
Independent reflections	4770 [R_{int} = 0.0896, R_{sigma} = 0.1247]
Data/restraints/parameters	4770/2/365
Goodness-of-fit on F^2	1.008
Final R indexes [I>=2σ (I)]	R_1 = 0.0692, wR_2 = 0.1402
Final R indexes [all data]	R_1 = 0.1481, wR_2 = 0.1807
Largest diff. peak/hole / e Å^{-3}	0.39/-0.32

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for mo_2022197_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O3	-8256(7)	-6753(4)	-4125(4)	26.6(12)
O2	-1599(7)	-5714(4)	-5871(4)	30.3(13)
C20	-4466(15)	-6492(9)	-3156(7)	25(2)
O4	-2157(8)	-3585(5)	-5470(4)	40.1(15)
N1	-2030(9)	-7165(5)	-5052(4)	24.6(15)
O1	-7663(9)	-8868(5)	-4477(5)	46.2(17)
N2	-7840(9)	-5286(5)	-4958(4)	25.0(15)
C12	-7135(13)	-6150(8)	-7278(7)	31(2)
C24	-4144(11)	-4939(6)	-4094(5)	22.7(17)
C26	-6796(12)	-4429(7)	-5214(6)	25(2)
C18	-7199(11)	-5992(6)	-4305(5)	24.5(18)
C31	-4157(18)	-1499(9)	-3082(8)	38(3)
C19	-5286(11)	-5807(6)	-3842(5)	22.8(17)
C25	-4984(13)	-4230(7)	-4802(6)	25(2)
C14	-4594(10)	-6676(6)	-6157(5)	22.0(17)
C10	-7606(11)	-7627(6)	-6320(5)	27.9(19)
C15	-2654(10)	-6484(6)	-5707(5)	22.3(17)
C7	-6008(15)	-9171(7)	-4900(7)	32(2)
C11	-8315(13)	-6945(8)	-7003(6)	35(2)
C6	-6660(12)	-9941(7)	-5661(6)	29(2)
C3	-7740(18)	-11327(9)	-7067(8)	47(3)
C27	-7839(11)	-3815(7)	-5980(5)	31(2)
C16	-3075(12)	-8030(7)	-4777(6)	24(2)
C8	-4883(12)	-8231(7)	-5188(6)	26(2)
C30	-4678(14)	-2208(7)	-3777(6)	40(2)
C28	-3858(15)	-3280(7)	-5091(7)	29(2)
C29	-3313(12)	-2501(7)	-4335(6)	29(2)
C9	-5680(11)	-7532(6)	-5883(5)	24.4(18)
C1	-8529(13)	-10346(7)	-5793(7)	40(2)
C23	-2249(11)	-4831(7)	-3670(5)	28.2(19)
C22	-1543(12)	-5530(8)	-3005(5)	32(2)
C17	-2005(12)	-8640(7)	-4019(6)	36(2)
C21	-2683(15)	-6348(8)	-2735(7)	32(3)
C33	-1005(14)	-1335(7)	-3502(7)	44(2)
C35	-1466(13)	-2046(6)	-4199(6)	37(2)
C5	-5333(14)	-10267(7)	-6227(7)	41(2)

C2	-9060(13)	-11029(7)	-6496(7)	44(2)
C32	-2360(20)	-1068(9)	-2933(8)	47(3)
C13	-5248(14)	-6007(8)	-6855(8)	25(2)
C4	-5830(20)	-10951(10)	-6931(10)	65(5)

Table S3. Anisotropic Displacement Parameters ($Å^2×10^3$) for mo_2022197_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O3	20(3)	25(3)	35(3)	2(3)	5(2)	-3(2)
O2	21(3)	31(3)	38(3)	5(3)	1(2)	-4(3)
C20	28(5)	28(6)	22(5)	4(4)	10(4)	3(4)
O4	39(4)	40(4)	45(4)	-10(3)	19(3)	-9(3)
N1	18(3)	23(4)	31(4)	3(3)	-3(3)	-2(3)
O1	50(4)	37(4)	59(4)	-16(3)	35(3)	-16(3)
N2	17(3)	32(4)	27(4)	1(3)	3(3)	-3(3)
C12	25(5)	35(6)	31(6)	0(4)	-2(4)	3(4)
C24	21(4)	24(4)	23(4)	-2(4)	6(3)	3(3)
C26	22(5)	26(5)	29(5)	6(4)	12(4)	4(4)
C18	24(4)	25(5)	26(4)	-3(4)	8(4)	5(4)
C31	54(7)	35(7)	27(6)	-4(5)	12(5)	-8(5)
C19	25(4)	22(4)	22(4)	-5(3)	3(3)	-1(4)
C25	32(5)	19(4)	26(5)	-5(4)	10(4)	-8(4)
C14	21(4)	22(4)	22(4)	-3(3)	4(3)	1(3)
C10	22(4)	28(5)	35(5)	-2(4)	5(4)	-2(4)
C15	20(4)	24(4)	24(4)	-2(3)	8(3)	-2(3)
C7	40(6)	24(5)	33(6)	-1(4)	14(6)	1(5)
C11	27(5)	40(6)	38(5)	-6(5)	5(4)	2(4)
C6	34(5)	20(5)	34(5)	0(4)	4(4)	-3(4)
C3	59(8)	44(7)	35(7)	-3(6)	-12(6)	-4(6)
C27	24(4)	34(5)	36(5)	7(4)	2(4)	4(4)
C16	22(5)	20(5)	30(5)	5(4)	4(4)	-2(4)
C8	24(5)	30(5)	24(5)	-3(4)	7(4)	1(4)
C30	49(6)	35(5)	38(5)	-7(4)	17(5)	-11(4)
C28	36(6)	24(5)	30(5)	3(4)	14(5)	-9(5)
C29	35(5)	27(5)	27(5)	9(4)	5(4)	-4(4)
C9	27(4)	23(4)	25(4)	-9(4)	6(3)	-2(3)
C1	34(5)	28(5)	59(6)	-11(5)	13(5)	-2(4)
C23	24(4)	33(5)	27(5)	-2(4)	1(4)	1(4)
C22	22(5)	47(6)	25(5)	-8(5)	-6(4)	-4(4)
C17	38(5)	36(5)	35(5)	12(4)	10(4)	3(4)
C21	38(6)	31(6)	28(5)	-1(4)	2(5)	4(5)

C33	48(6)	22(5)	57(7)	4(5)	-12(5)	-5(4)
C35	41(5)	29(5)	41(5)	1(4)	1(4)	1(4)
C5	46(6)	32(5)	50(6)	-9(5)	24(5)	-14(4)
C2	32(5)	36(6)	60(7)	-10(5)	-9(5)	-4(4)
C32	77(9)	28(6)	36(7)	-5(5)	3(6)	0(6)
C13	18(5)	23(5)	34(6)	-1(5)	4(4)	1(4)
C4	104(12)	41(7)	58(9)	-23(7)	45(9)	-24(8)

Table S4. Bond Lengths for mo_2022197_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O3	C18	1.256(9)	C14	C9	1.405(10)
O2	C15	1.258(9)	C14	C13	1.382(14)
C20	C19	1.413(14)	C10	C11	1.385(12)
C20	C21	1.332(16)	C10	C9	1.421(11)
O4	C28	1.418(11)	C7	C6	1.528(13)
N1	C15	1.340(10)	C7	C8	1.510(12)
N1	C16	1.398(10)	C6	C1	1.384(11)
O1	C7	1.423(11)	C6	C5	1.383(12)
N2	C26	1.380(11)	C3	C2	1.374(15)
N2	C18	1.361(10)	C3	C4	1.399(18)
C12	C11	1.386(12)	C16	C8	1.354(12)
C12	C13	1.397(14)	C16	C17	1.497(11)
C24	C19	1.427(10)	C8	C9	1.428(12)
C24	C25	1.459(12)	C30	C29	1.382(12)
C24	C23	1.397(11)	C28	C29	1.515(13)
C26	C25	1.356(12)	C29	C35	1.395(11)
C26	C27	1.501(11)	C1	C2	1.378(13)
C18	C19	1.442(11)	C23	C22	1.379(12)
C31	C30	1.391(15)	C22	C21	1.388(13)
C31	C32	1.350(17)	C33	C35	1.388(12)
C25	C28	1.521(12)	C33	C32	1.381(15)
C14	C15	1.453(10)	C5	C4	1.377(17)

Table S5. Bond Angles for mo_2022197_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C21	C20	C19	122.3(10)	C1	C6	C7	122.3(8)
C15	N1	C16	125.7(7)	C5	C6	C7	119.2(8)
C18	N2	C26	125.2(7)	C5	C6	C1	118.5(8)
C11	C12	C13	120.7(10)	C2	C3	C4	120.0(11)
C19	C24	C25	118.5(7)	N1	C16	C17	113.5(7)

C23	C24	C19	118.3(7)	C8	C16	N1	119.7(8)
C23	C24	C25	123.1(7)	C8	C16	C17	126.9(8)
N2	C26	C27	113.4(7)	C16	C8	C7	119.8(9)
C25	C26	N2	120.3(8)	C16	C8	C9	118.4(8)
C25	C26	C27	126.3(8)	C9	C8	C7	121.8(9)
O3	C18	N2	120.5(7)	C29	C30	C31	119.3(10)
O3	C18	C19	123.1(7)	O4	C28	C25	112.0(7)
N2	C18	C19	116.5(7)	O4	C28	C29	109.2(8)
C32	C31	C30	122.6(11)	C29	C28	C25	113.1(7)
C20	C19	C24	118.3(8)	C30	C29	C28	119.8(8)
C20	C19	C18	121.4(8)	C30	C29	C35	118.6(8)
C24	C19	C18	120.2(7)	C35	C29	C28	121.6(8)
C24	C25	C28	121.2(9)	C14	C9	C10	115.7(7)
C26	C25	C24	119.3(8)	C14	C9	C8	121.0(7)
C26	C25	C28	119.5(9)	C10	C9	C8	123.2(8)
C9	C14	C15	119.3(7)	C2	C1	C6	120.3(9)
C13	C14	C15	117.1(8)	C22	C23	C24	120.2(8)
C13	C14	C9	123.6(8)	C23	C22	C21	121.4(8)
C11	C10	C9	121.5(8)	C20	C21	C22	119.4(10)
O2	C15	N1	119.7(7)	C32	C33	C35	120.6(10)
O2	C15	C14	124.3(7)	C33	C35	C29	120.4(9)
N1	C15	C14	115.9(7)	C4	C5	C6	122.2(10)
O1	C7	C6	108.7(8)	C3	C2	C1	120.7(10)
O1	C7	C8	112.5(7)	C31	C32	C33	118.5(11)
C8	C7	C6	113.9(7)	C14	C13	C12	118.3(10)
C10	C11	C12	120.0(9)	C5	C4	C3	118.3(12)

Table S6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for mo_2022197_0m.

Atom	*x*	*y*	*z*	U(eq)
H20	-5212.79	-7074.58	-2987.76	30
H4	-2331.21	-4180.99	-5713.69	60
H1	-859.95	-7058.45	-4769.18	29
H1A	-7455.7	-8278.62	-4225.5	69
H2	-9013.05	-5383.2	-5239.17	30
H12	-7615.11	-5698.8	-7759.91	37
H31	-5100.97	-1309.25	-2696.98	46
H10	-8425.43	-8170.89	-6139.34	33
H7	-5120.87	-9569.65	-4444.92	38
H11	-9609.82	-7021.35	-7282.27	42

H3	-8126.51	-11789.07	-7554.86	57
H27A	-9054.35	-4177.2	-6197.6	47
H27B	-7012.37	-3764.94	-6467.27	47
H27C	-8131.8	-3102.61	-5775	47
H30	-5959.99	-2488.36	-3867.4	48
H28	-4720.59	-2899.64	-5566.8	35
H1B	-9450.86	-10153.17	-5398.64	48
H23	-1444.1	-4273.97	-3839.74	34
H22	-248.21	-5450.3	-2725.6	39
H17A	-1173.95	-9171.83	-4260.35	54
H17B	-2942.29	-8992.48	-3675.7	54
H17C	-1198.42	-8154.95	-3625.68	54
H21	-2196.7	-6800.83	-2255.96	39
H33	256.23	-1028.41	-3414.99	53
H35	-518.21	-2223.16	-4585.11	45
H5	-4036.35	-10009.36	-6127.84	49
H2A	-10350.59	-11296.46	-6585.51	53
H32	-2042.26	-593.42	-2447.09	57
H13	-4436.17	-5463.41	-7042.91	30
H4A	-4893.85	-11162.96	-7313.36	78

Crystal structure determination of compound 3aa

Crystal data for $C_{17}H_{15}NO_2$ (M =265.30 g/mol): monoclinic, space group Pc (no. 7), a = 6.9187(10) Å, b = 12.6378(19) Å, c = 14.994(2) Å, β = 96.541(5)°, V = 1302.5(3) Å^3, Z = 4, T = 150.0 K, μ (MoKα) = 0.089 mm-1, Dcalc = 1.353 g/cm^3, 11327 reflections measured (4.226° ≤ 2Θ ≤ 52.848°), 4770 unique (R_{int} = 0.0896, R_{sigma} = 0.1247) which were used in all calculations. The final R_1 was 0.0692 (I > 2σ(I)) and wR_2 was 0.1807 (all data).

DFT Calculations

Computational details:

Density functional theory (DFT)[13] calculations were performed by using Gaussian 09 quantum chemical package.[14] Unless otherwise specified, geometry optimizations were performed using B3LYP[15] functional with Grimme D3 correction[16] Herein, the Stuttgart/Dresden effective core potential (SDD)[17] for Rh in conjunction with a standard 6-31G(d,p) basis set[18] for all other atoms. This level of theory is denoted as B3LYP-D3(BJ)/6-31G(d,p) SDD. Frequency analysis was conducted at the same level of theory to verify the stationary points to be real minima or saddle points and to obtain the thermodynamic energy corrections. Intrinsic reaction coordinate (IRC) calculations[19] were carried out to confirm that all transition state structures connect the corresponding reactants and products. Solvent effects in dichloromethane were estimated by using the SMD[20] solvation method at the M06[21] level of theory with Grimme D3 correction. Herein, SDD was used for Rh and the 6-311++G(d,p) basis set was used for all other atoms (BS2). This level of theory is denoted as M06-D3 SMD/6-311++G(d,p) SDD. If not noted, the energies presented in this paper are the M06-D3 SMD -calculated single point energies with B3LYP-D3(BJ)-calculated thermodynamic corrections which were calculated under standard conditions (1 atm and 298.15 K) (denoted as ΔG_{sol} (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.[22] Multiwfn was utilized to analyze interactions with the independent gradient model based on Hirshfeld partition of molecular density (IGMH) and the graphics are displayed using VMD program.

Table S7. Gibbs free energy differences between **TS-a** and **TS-b** at several levels of theory.

Computational level	ΔG(**TS-b**)-ΔG(**TS-a**) (kcal/mol)
B3LYP-D3(BJ)/6-31G(d,p) SDD (gas)	-5.03
M06-D3 SMD/6-311++G(d,p) SDD//B3LYP-D3(BJ)/6-31G(d,p) SDD	0.57
M06-D3 SMD/def2-TZVPP//B3LYP-D3(BJ)/6-31G(d,p) SDD	0.94
M06-D3 SMD/def2-QZVP//B3LYP-D3(BJ)/6-31G(d,p) SDD	0.82
M062x-D3 SMD/def2-TZVPP//B3LYP-D3(BJ)/6-31G(d,p) SDD	1.08
M06-D3 SMD/6-31G(d,p) SDD*	-0.69
M06-D3 SMD/6-311++G(d,p) SDD//M06-D3 SMD/6-31G(d,p) SDD*	0.36

* Geometry optimizations were done with SMD solvation model (**TS-a$_{SMD}$** and **TS-b$_{SMD}$**).

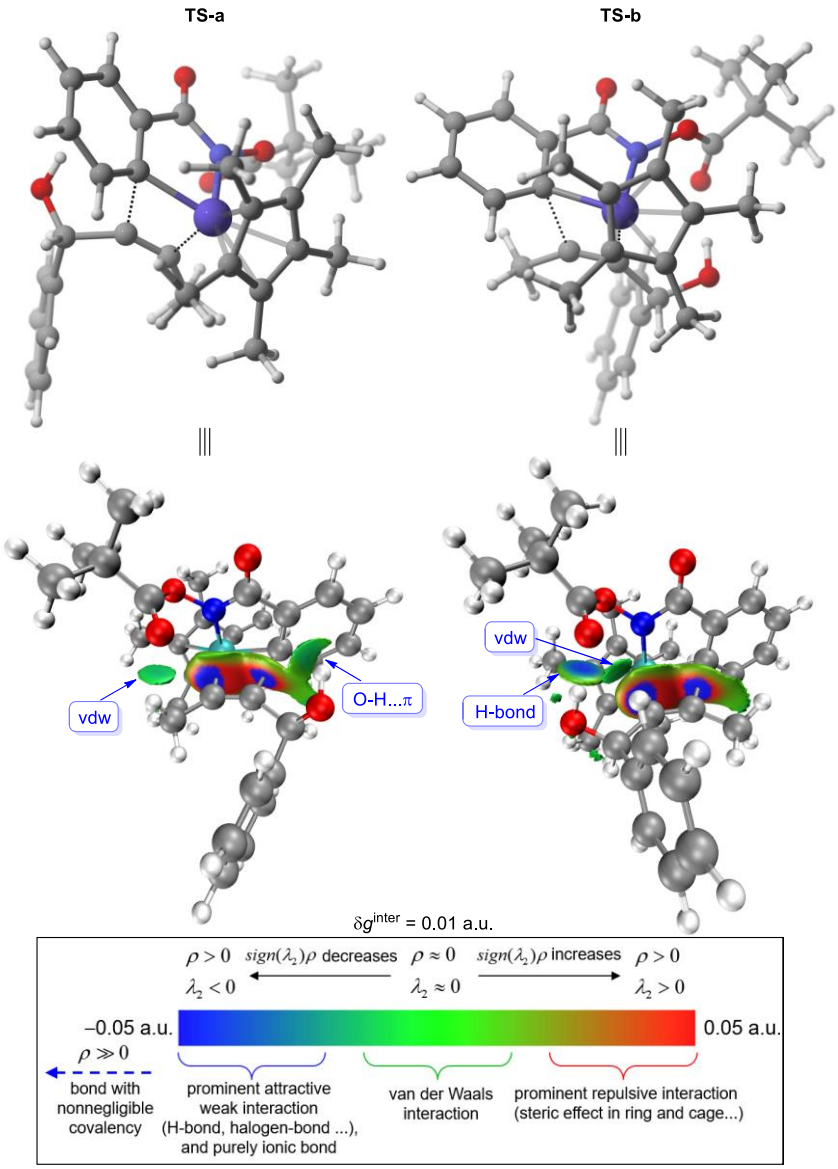


Figure S1. Interaction analysis using IGMH method (below shows IGMH colorbar).

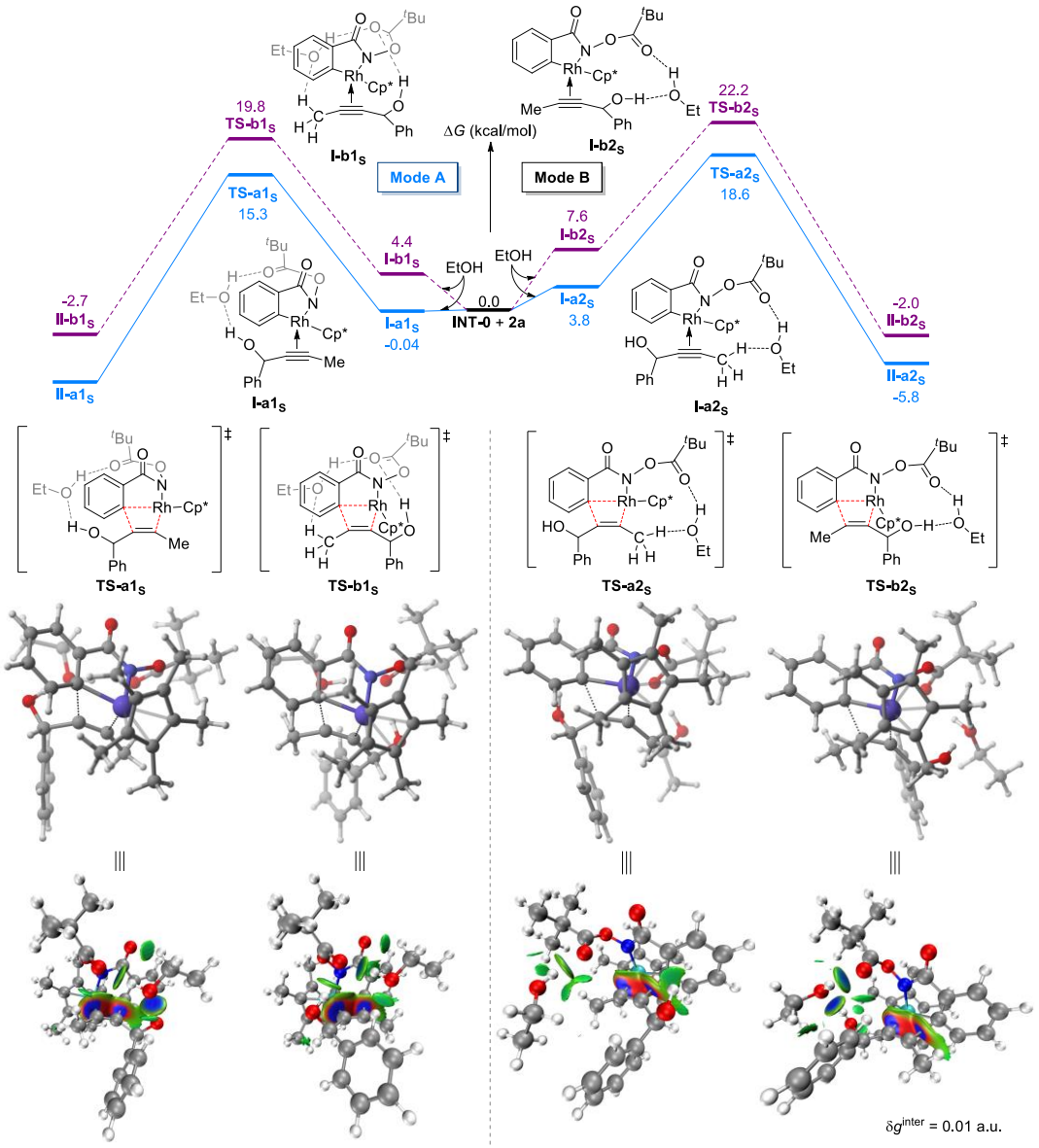


Figure S2. Computed Gibbs free energies for regioselective alkyne insertion involving one molecule of ethanol and interaction analysis of the four transition states using IGMH method.

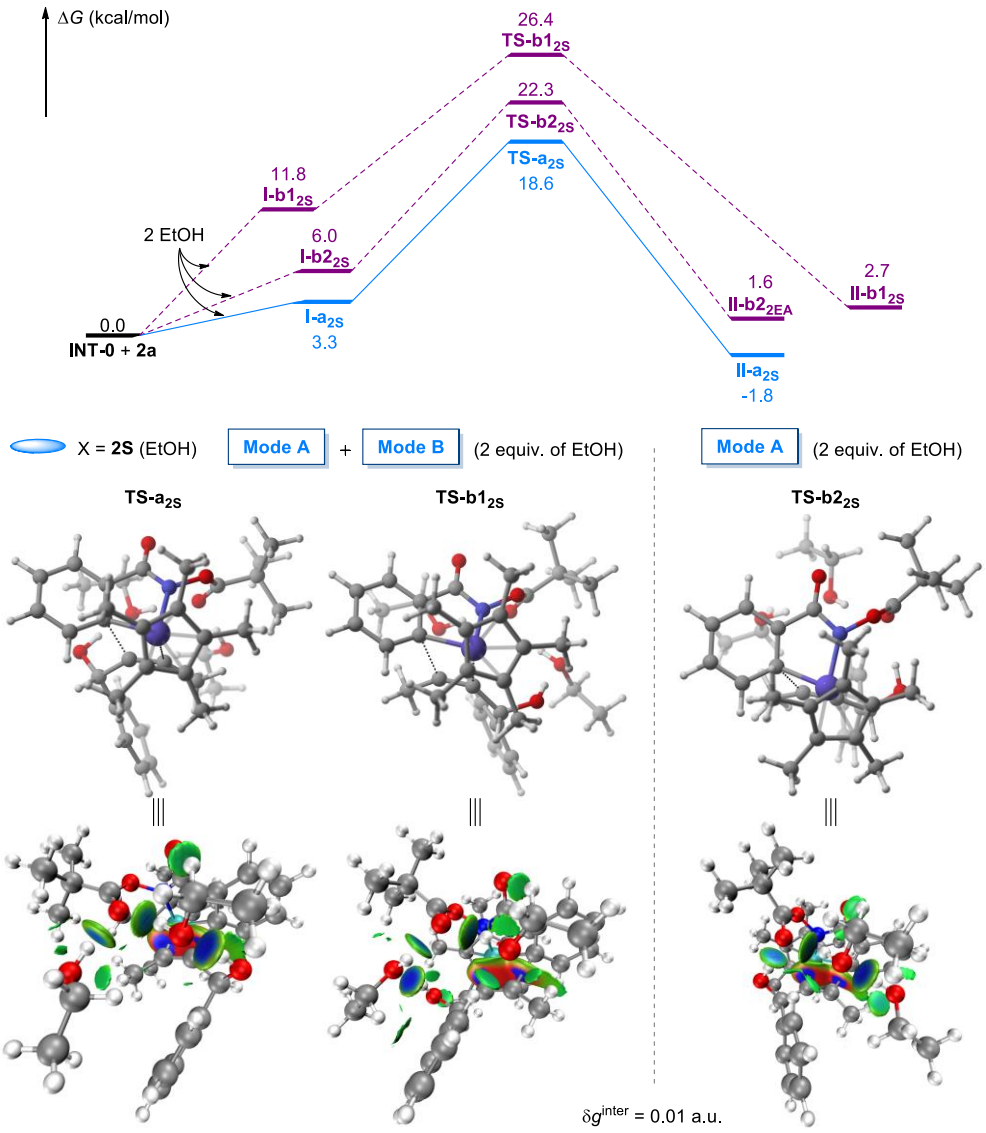


Figure S3. Computed Gibbs free energies for regioselective alkyne insertion involving two molecules of ethanol and interaction analysis of the three transition states using IGMH method.

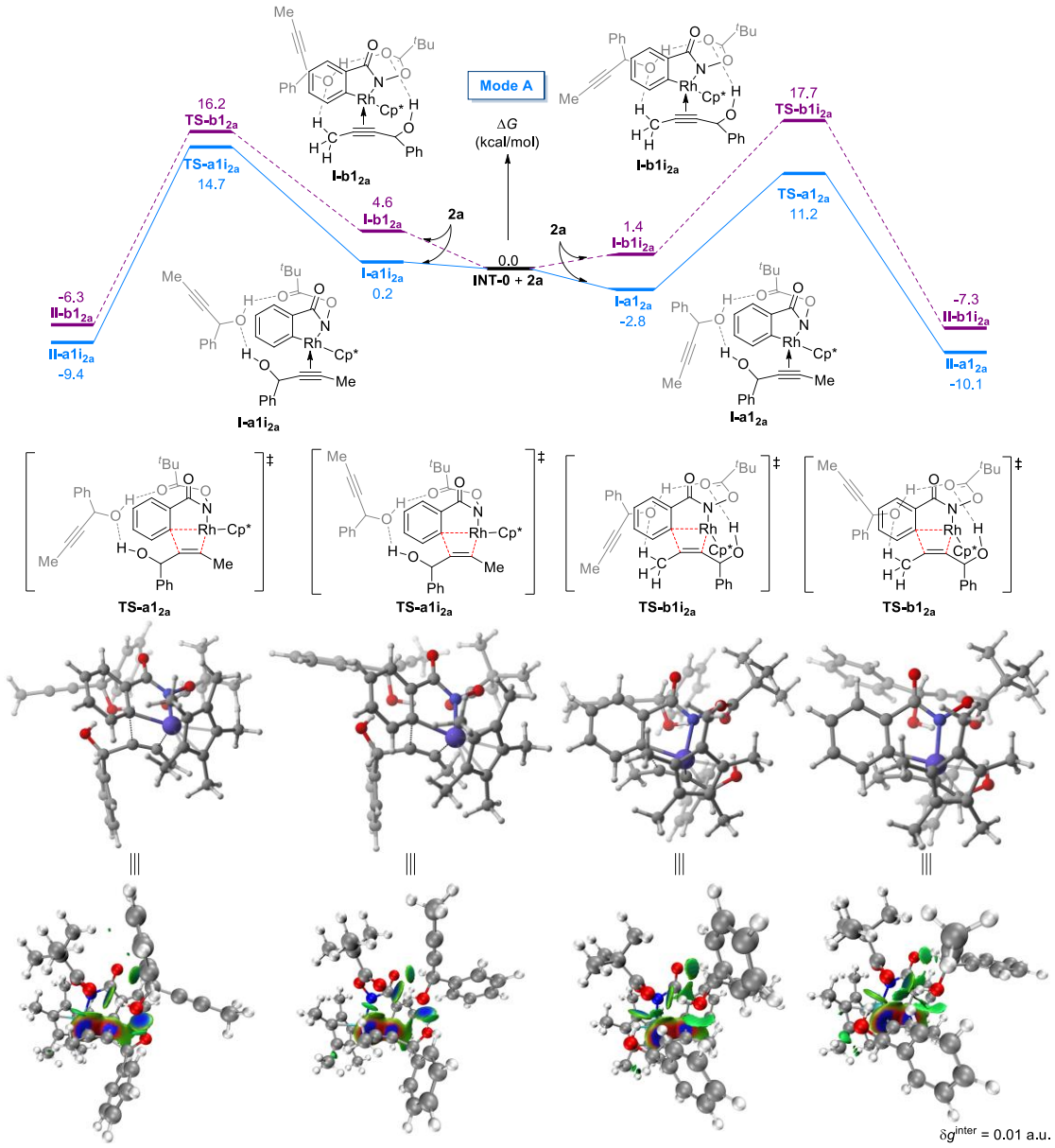


Figure S4. Computed Gibbs free energies for regioselective alkyne insertion involving another molecule of substrate **2a** and interaction analysis of the four transition states using IGMH method.

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

Table S8. 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 *E*	corr. to *H*	corr. to *G*	SP_{SMD}	Imaginary frequency
2a (*R*-type)	0.170816	0.181758	0.182702	0.130782	-462.036668	—
INT-0	0.455282	0.484919	0.485864	0.395527	-1245.745977	—
EtOH	0.080201	0.084484	0.085428	0.054820	-154.994401	—
I-a	0.628772	0.669945	0.670889	0.555135	-1707.811359	—
TS-a	0.627809	0.668287	0.669231	0.555103	-1707.788088	-290.31
II-a	0.630583	0.670928	0.671873	0.557532	-1707.832535	—
I-b	0.629918	0.670474	0.671418	0.557448	-1707.806073	—
TS-b	0.629268	0.669293	0.670237	0.557199	-1707.789281	-282.29
II-b	0.632192	0.671892	0.672837	0.561562	-1707.828576	—
I-a1$_S$	0.712736	0.758715	0.759660	0.633473	-1862.829452	—
TS-a1$_S$	0.712017	0.757229	0.758173	0.634290	-1862.805762	-277.75
II-a1$_S$	0.713443	0.759205	0.760149	0.633326	-1862.842257	—
I-b1$_S$	0.712466	0.758760	0.759705	0.632635	-1862.821587	—
TS-b1$_S$	0.711904	0.757364	0.758308	0.633362	-1862.797661	-304.44
II-b1$_S$	0.714484	0.759872	0.760816	0.636686	-1862.836927	—
I-a2$_S$	0.711585	0.758134	0.759078	0.631408	-1862.821344	—
TS-a2$_S$	0.710472	0.756533	0.757477	0.630485	-1862.796824	-281.75
II-a2$_S$	0.713513	0.759275	0.760219	0.634697	-1862.839780	—
I-b2$_S$	0.712669	0.758521	0.759465	0.634080	-1862.817934	—
TS-b2$_S$	0.712578	0.757545	0.758489	0.635801	-1862.796393	-284.60
II-b2$_S$	0.714751	0.759975	0.760919	0.637372	-1862.836459	—
I-a$_{2S}$	0.795332	0.846927	0.847871	0.709004	-2017.839291	—
TS-a$_{2S}$	0.795198	0.845666	0.846610	0.710849	-2017.816677	-302.74
II-a$_{2S}$	0.796709	0.847574	0.848518	0.710900	-2017.849252	—
I-b1$_{2S}$	0.796391	0.847401	0.848345	0.713042	-2017.829726	—
TS-b1$_{2S}$	0.795493	0.845856	0.846800	0.712395	-2017.805813	-297.03
II-b1$_{2S}$	0.797836	0.848317	0.849261	0.714523	-2017.845728	—
I-b2$_{2S}$	0.795174	0.846880	0.847824	0.707284	-2017.833160	—
TS-b2$_{2S}$	0.795166	0.845834	0.846778	0.709559	-2017.809567	-285.86
II-b2$_{2S}$	0.797465	0.848223	0.849167	0.712289	-2017.845205	—
I-a1$_{2a}$	0.802493	0.855706	0.856650	0.711907	-2169.878610	—
TS-a1$_{2a}$	0.801796	0.854177	0.855121	0.712957	-2169.857408	-273.28
II-a1$_{2a}$	0.804470	0.856891	0.857835	0.715605	-2169.893850	—
I-a1i$_{2a}$	0.802705	0.855755	0.856700	0.712635	-2169.874613	—
TS-a1i$_{2a}$	0.802617	0.854614	0.855558	0.715015	-2169.853807	-263.85
II-a1i$_{2a}$	0.804944	0.857090	0.858034	0.717323	-2169.894587	—
I-b1$_{2a}$	0.803946	0.856580	0.857524	0.715392	-2169.870360	—
TS-b1$_{2a}$	0.802897	0.854934	0.855879	0.715468	-2169.851816	-279.85
II-b1$_{2a}$	0.804720	0.857049	0.857994	0.717669	-2169.889877	—
I-b1i$_{2a}$	0.803038	0.856102	0.857046	0.712958	-2169.872913	—
TS-b1i$_{2a}$	0.802823	0.854808	0.855753	0.715207	-2169.849264	-298.96
II-b1i$_{2a}$	0.804667	0.857213	0.858157	0.714784	-2169.888623	—

Table S9. Energy, enthalpy and free energy corrections of the structures calculated at M06-D3 SMD/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 *E*	corr. to *H*	corr. to *G*	SP_{SMD}	Imaginary frequency
TS-a$_{SMD}$	0.626505	0.664995	0.665939	0.558767	-1707.797976	-260.42
TS-b$_{SMD}$	0.626826	0.665364	0.666308	0.559692	-1707.798330	-275.22

Cartesian coordinates of the optimized structures

2a (*R*-type)

C	-2.77382800	-0.58976000	-0.01820000
C	-1.86587900	0.17508400	-0.24274500
C	-0.74102300	1.06499300	-0.54115600
O	-0.90303000	2.25704200	0.23148800
H	-0.10052900	2.78058800	0.09809000
C	-3.87029800	-1.50812400	0.26618100
H	-3.49568000	-2.48719700	0.58504600
H	-4.50825700	-1.11846500	1.06714600
H	-4.50106600	-1.66160800	-0.61647300
H	-0.76960800	1.30508000	-1.61739300
C	0.58850100	0.37763700	-0.24850600
C	1.34791300	-0.17677500	-1.28068200
C	1.05136800	0.29420300	1.06931800
C	2.55780800	-0.81458400	-1.00190000
H	0.99112700	-0.10891900	-2.30537600
C	2.26107900	-0.33861400	1.34805600
H	0.45596600	0.73419200	1.86279500
C	3.01662800	-0.89596800	0.31313700
H	3.14329800	-1.24131400	-1.81090900
H	2.61575400	-0.39899100	2.37285100
H	3.95963100	-1.38826300	0.53130700

INT-0

Rh	-0.83303500	-0.34696100	0.24083100
N	0.64967000	0.86836800	0.65942000
C	-2.19901100	-2.05181400	0.51691900
C	-2.19719000	-1.68257900	-0.85318900
C	-0.83137900	-1.80078100	-1.32832200
C	-0.02708900	-2.40676300	-0.27752600

C	-0.84804200	-2.51386400	0.86217600
O	1.99676400	0.47185400	0.83236500
C	0.53256000	2.24298600	0.44458800
C	-0.90478000	2.56819400	0.21069400
C	-1.77693800	1.47086200	0.09038100
C	-1.34699100	3.88471500	0.12873300
C	-3.13518100	1.73992700	-0.09460800
C	-2.70817600	4.13335200	-0.06695900
H	-0.62421700	4.69050400	0.21747400
C	-3.59670800	3.06242700	-0.16947700
H	-3.85383700	0.93056000	-0.17791600
H	-3.07310000	5.15380900	-0.13503800
H	-4.65778100	3.25290800	-0.31060500
O	1.46400400	3.03365000	0.44764000
C	-0.44538900	-3.01081700	2.21333400
H	0.63903100	-2.99270400	2.33709900
H	-0.88712200	-2.40042000	3.00549700
H	-0.78783900	-4.04262100	2.36148100
C	1.41151500	-2.79913300	-0.40244200
H	1.94248700	-2.67197300	0.54395100
H	1.50211200	-3.85108000	-0.69958000
H	1.91582900	-2.19181500	-1.15468000
C	-0.35109700	-1.48823600	-2.70763200
H	0.62492500	-0.99931700	-2.67178400
H	-0.26236100	-2.41033600	-3.29677200
H	-1.04591400	-0.82157200	-3.22166100
C	-3.36878900	-1.28747500	-1.69618200
H	-3.15832100	-0.39333200	-2.28697500
H	-3.62447600	-2.09912700	-2.38762000
H	-4.24996900	-1.08535700	-1.08501600
C	-3.37358000	-2.07936700	1.44313300
H	-4.14375100	-1.37259500	1.12759000
H	-3.82330100	-3.07984300	1.47682200
H	-3.07746800	-1.81350800	2.46095100
C	2.70837200	0.33828700	-0.32587500
O	2.21118100	0.34977400	-1.42974600
C	4.20163000	0.21806800	-0.02608100
C	4.89626500	-0.43481600	-1.22861000
H	4.68069500	0.11224800	-2.14828700
H	5.97896600	-0.44593200	-1.06932300
H	4.56274200	-1.46892000	-1.36504900
C	4.70830000	1.66783100	0.16392500
H	4.15451000	2.17322800	0.95774100
H	5.77340000	1.65180900	0.41761300

H	4.57753900	2.24608600	-0.75473900
C	4.46238200	-0.59804300	1.25211500
H	3.99377300	-0.13727800	2.12317800
H	4.08147900	-1.62040200	1.15671400
H	5.54114900	-0.65834900	1.42894400

EtOH

C	-1.22175200	-0.22226100	0.00000300
C	0.08754100	0.54848800	-0.00005900
H	-1.28770400	-0.85931900	-0.88675400
H	-1.28573400	-0.86158700	0.88528300
H	-2.07407000	0.46438800	0.00189200
H	0.13623900	1.20150900	0.88663300
H	0.13638300	1.20137100	-0.88682500
O	1.14954000	-0.39872200	-0.00004100
H	1.98383400	0.08605200	0.00043800

I-a

N	1.61132500	-0.02953300	0.59969700
C	0.90904300	-1.81488300	1.90419800
C	0.98565500	-2.68340300	2.99313700
H	1.86808100	-2.63892200	3.62450600
C	-0.05503100	-3.57952600	3.23625700
H	-0.01043600	-4.25458900	4.08531200
C	-1.15608800	-3.60510700	2.37740800
H	-1.97175700	-4.30013600	2.55850100
C	-1.22342000	-2.73471700	1.27958700
H	-2.09296200	-2.77981300	0.62965500
C	-0.18929700	-1.82577200	1.03138100
C	0.66692600	-0.08343200	-2.68901000
C	1.13684300	-1.38765700	-2.25398800
C	-0.00151700	-2.23104300	-2.04741700
C	-1.17905600	-1.43457300	-2.25350400
C	-0.75169500	-0.11810100	-2.68543500
Rh	-0.02923800	-0.53539400	-0.55342500
C	2.02590600	-0.88035600	1.58348700
O	3.13240800	-0.88413500	2.12367800
C	-1.68904200	0.99088400	-3.04654600
H	-2.20516600	0.76671000	-3.98712400
H	-2.44908400	1.13225800	-2.27224500
H	-1.16170500	1.93840400	-3.17032000
C	1.55377500	1.04917500	-3.10195900
H	2.01507600	0.84868700	-4.07654500
H	0.99432900	1.98347900	-3.18705200

H	2.35196700	1.19869200	-2.37423800
C	2.57477500	-1.78903500	-2.14398700
H	2.97771600	-2.05417900	-3.12921300
H	3.17283900	-0.97404700	-1.73312400
H	2.69526000	-2.65183700	-1.48616700
C	0.03137700	-3.69086900	-1.72288100
H	0.04746600	-4.28159000	-2.64702500
H	0.91666400	-3.94963000	-1.13905400
H	-0.84188000	-3.99304500	-1.14274500
C	-2.59452800	-1.92239800	-2.24945800
H	-2.87040400	-2.33267200	-3.22912100
H	-2.74703500	-2.71145400	-1.50927900
H	-3.28954400	-1.11014300	-2.02621900
O	2.69743100	0.69932600	0.03677000
C	3.17128100	1.71362000	0.83033500
O	2.56136600	2.18937400	1.75744600
C	4.57962500	2.12777200	0.39868400
C	4.87100200	3.52195500	0.97115400
H	4.73909800	3.53140700	2.05443000
H	5.90042100	3.81084800	0.73645400
H	4.19848200	4.27362300	0.54567100
C	5.54881500	1.08822400	1.00688600
H	5.31558800	0.08281700	0.65214900
H	6.57704700	1.34390200	0.72841400
H	5.46992100	1.07599300	2.09634300
C	4.72989000	2.14315800	-1.13249300
H	4.58593500	1.14859300	-1.55957400
H	4.01576600	2.82964600	-1.59980600
H	5.73760300	2.48164300	-1.39412700
C	-0.83039800	1.37383900	0.19064200
C	-1.67361100	0.49594000	0.45926400
C	-2.95238100	-0.00508100	1.03705300
O	-2.82013400	-0.29855600	2.41639800
H	-2.10661800	-0.95041300	2.49777500
C	-0.16440500	2.67470000	0.10328900
H	-0.88777100	3.46560600	0.33227200
H	0.65711200	2.71693200	0.82360300
H	0.24306100	2.84870200	-0.89702400
H	-3.27139600	-0.89538000	0.47784700
C	-3.99620100	1.08072500	0.85629700
C	-4.88220000	1.03437700	-0.22223500
C	-4.03274100	2.16958100	1.73321300
C	-5.79270700	2.07079500	-0.43391900
H	-4.86842400	0.17867200	-0.89275300

C	-4.94578600	3.20194300	1.52530500
H	-3.35216100	2.18732200	2.57724400
C	-5.82424300	3.15830500	0.43943100
H	-6.48085800	2.02391800	-1.27277200
H	-4.97406700	4.04247400	2.21245100
H	-6.53370000	3.96467400	0.27972100

TS-a

N	1.39968800	0.22221000	0.73423900
C	0.06405400	-0.49495400	2.48276700
C	-0.10467300	-0.81601300	3.83034500
H	0.52042300	-0.30590000	4.55678000
C	-1.04082200	-1.78221800	4.20474700
H	-1.17718800	-2.03196200	5.25225500
C	-1.79692800	-2.43524600	3.22453000
H	-2.51779800	-3.19527600	3.51238600
C	-1.64907100	-2.09830000	1.87893100
H	-2.27896300	-2.57334200	1.13272300
C	-0.72569500	-1.11320900	1.48620500
C	1.56081300	-1.61696600	-2.11296500
C	1.94817500	-2.42652500	-0.95719500
C	0.85850600	-3.26413900	-0.61176900
C	-0.23360700	-2.95520500	-1.51353800
C	0.23096800	-1.99254100	-2.47296500
Rh	0.26299500	-1.06108600	-0.41800400
C	1.16897400	0.42197500	2.05549700
O	1.78067800	1.17536900	2.81582000
C	-0.55422200	-1.51127500	-3.65253900
H	-0.54581200	-2.26497900	-4.44931100
H	-1.59754700	-1.32024100	-3.38810900
H	-0.13681800	-0.59147300	-4.06619400
C	2.46642900	-0.66492200	-2.83085100
H	3.16283000	-1.19802000	-3.49045200
H	1.89726300	0.03928100	-3.44297800
H	3.05142000	-0.08391500	-2.11576100
C	3.28939800	-2.35696000	-0.29621200
H	4.04189700	-2.88014000	-0.89874200
H	3.60720600	-1.31904500	-0.17654200
H	3.27121500	-2.81424900	0.69476000
C	0.80598100	-4.27252400	0.49269400
H	0.87492500	-5.29282000	0.09658500
H	1.62676700	-4.12984400	1.19817300
H	-0.12673100	-4.19366000	1.05829200
C	-1.55639300	-3.65690400	-1.56137000

H	-1.53806900	-4.47504100	-2.29271900
H	-1.81049100	-4.09051400	-0.59191000
H	-2.36060000	-2.97477600	-1.85029400
O	2.49196900	0.96746700	0.23697700
C	2.28005900	2.31785500	0.13234200
O	1.19411500	2.84074200	0.20272100
C	3.61026100	3.05181600	-0.03465900
C	3.32631900	4.46439700	-0.56235100
H	2.63506900	4.99324000	0.09641900
H	4.26017100	5.03196800	-0.62500800
H	2.87807000	4.43113200	-1.56051600
C	4.24350500	3.12350600	1.37407000
H	4.40551200	2.12306100	1.77969000
H	5.20166200	3.65142200	1.31745800
H	3.58757400	3.65649500	2.06678400
C	4.55180300	2.30314600	-0.99498300
H	4.79284000	1.30600400	-0.62115100
H	4.10725300	2.20229300	-1.99102800
H	5.48593900	2.86425400	-1.10135900
C	-0.94609900	0.55754100	-0.74961200
C	-1.61276400	0.18926300	0.28410600
C	-2.91507900	0.47847100	0.99864300
O	-2.72194100	1.05455300	2.27221900
H	-1.97773800	0.60710700	2.70056300
C	-0.92412600	1.58895600	-1.80982900
H	-1.91206800	2.04341500	-1.93291800
H	-0.21605800	2.36608500	-1.50871300
H	-0.59650100	1.17467600	-2.76595500
H	-3.48133400	-0.46110600	1.08171000
C	-3.68781200	1.44873500	0.12589900
C	-4.49181200	0.96326700	-0.90926700
C	-3.53250400	2.82690500	0.29283500
C	-5.13363300	1.84642300	-1.77629200
H	-4.60975700	-0.11021000	-1.03693100
C	-4.17815900	3.71093800	-0.57232300
H	-2.90466500	3.18750200	1.09895800
C	-4.97573300	3.22454600	-1.60980000
H	-5.75874000	1.46197400	-2.57691500
H	-4.05363800	4.78140300	-0.43869500
H	-5.47538700	3.91452600	-2.28328900

II-a

N	0.54549300	1.37072000	0.75243800
C	0.85641800	-0.33637800	2.26263000

C	1.91434200	-0.52103300	3.16948700
H	2.28467400	0.34302900	3.71186500
C	2.46360500	-1.77881700	3.37201700
H	3.28171100	-1.90830200	4.07427800
C	1.95342000	-2.88729100	2.67552700
H	2.37854900	-3.87334800	2.83792300
C	0.89388700	-2.72443200	1.79676100
H	0.47817700	-3.58052600	1.27333700
C	0.31141100	-1.45531800	1.56517300
C	2.13183900	0.62194300	-2.15278500
C	3.19036900	0.86884000	-1.16082300
C	3.61533500	-0.36967700	-0.67365500
C	2.85708600	-1.42072500	-1.36947900
C	2.03559400	-0.81022300	-2.35427500
Rh	1.29930500	-0.18797300	-0.37230700
C	0.30914500	1.06675800	2.04770600
O	-0.18903700	1.75794400	2.92943200
C	1.24615100	-1.50494900	-3.41853100
H	1.87249300	-1.67830600	-4.30248000
H	0.87511900	-2.47323000	-3.07542000
H	0.38701800	-0.90970800	-3.73135600
C	1.47830800	1.68976100	-2.97115200
H	2.15160500	2.04739900	-3.76088000
H	0.56753200	1.32143500	-3.44787100
H	1.20715400	2.54117800	-2.34265400
C	3.60204600	2.23534500	-0.71247400
H	4.06640700	2.79311100	-1.53393100
H	2.73231500	2.80224600	-0.36674500
H	4.31662500	2.18806600	0.11143000
C	4.59913100	-0.64839200	0.41788100
H	5.44532000	-1.23493500	0.04145200
H	4.99093200	0.27466800	0.84903800
H	4.13315800	-1.22137600	1.22699500
C	3.06791500	-2.88737300	-1.15640400
H	3.97709100	-3.22989400	-1.66668200
H	3.17473100	-3.11515600	-0.09280300
H	2.22618300	-3.46788400	-1.54002000
O	-0.02109700	2.58461700	0.28769300
C	-1.38071900	2.66574300	0.32164800
O	-2.12188200	1.75318800	0.61183300
C	-1.83197600	4.08254500	-0.03202000
C	-3.35455500	4.07673100	-0.22013100
H	-3.85811400	3.72155900	0.68125600
H	-3.70276400	5.09030800	-0.44202400

H	-3.64796900	3.42131700	-1.04520200
C	-1.44132400	4.99328200	1.15309400
H	-0.35778200	5.01410700	1.28915300
H	-1.79350300	6.01269400	0.96420600
H	-1.89095600	4.63599700	2.08361900
C	-1.13546000	4.56181900	-1.32012100
H	-0.05131200	4.60081100	-1.19468900
H	-1.36267100	3.89972600	-2.16265200
H	-1.48882800	5.56559100	-1.57692800
C	-0.64527400	-0.73637800	-0.48935100
C	-0.90235700	-1.34644000	0.67311600
C	-2.23846000	-1.71174300	1.30281500
O	-2.65006200	-0.65801600	2.16263100
H	-2.46421300	0.18236900	1.70654200
C	-1.55091100	-0.36262600	-1.61831900
H	-2.58973800	-0.26839700	-1.29801000
H	-1.24202800	0.59295700	-2.05289400
H	-1.51736000	-1.11734100	-2.41249900
H	-2.07159900	-2.57180300	1.96725400
C	-3.30434900	-2.11756300	0.29519000
C	-3.05951900	-3.16431600	-0.60177200
C	-4.53874100	-1.46713600	0.25869500
C	-4.02419400	-3.54127600	-1.53331900
H	-2.09825000	-3.67170500	-0.57647200
C	-5.50554300	-1.83973600	-0.67797000
H	-4.72235100	-0.66829800	0.96805300
C	-5.25168300	-2.87423900	-1.57833800
H	-3.82024100	-4.35291800	-2.22633900
H	-6.45974400	-1.32079400	-0.70182600
H	-6.00356200	-3.16304900	-2.30694000

I-b

N	-0.40080500	0.67001100	0.72582700
C	0.83789900	-0.07207100	2.57578500
C	1.05999700	-0.28915700	3.93828300
H	0.32215600	0.07561800	4.64668700
C	2.22324400	-0.93454600	4.35039900
H	2.40901200	-1.11105400	5.40548700
C	3.15919300	-1.34207500	3.39432400
H	4.07430600	-1.83751800	3.70929500
C	2.92889600	-1.12228700	2.03228900
H	3.66351000	-1.46637500	1.31046600
C	1.75927800	-0.48737300	1.60468600
C	1.28708400	1.41055100	-2.07341400

C	2.13821400	1.83299300	-0.96937900
C	3.20637500	0.88117500	-0.84449800
C	2.95395800	-0.18427900	-1.76698900
C	1.78087200	0.17386800	-2.54756600
Rh	1.22322000	-0.07579000	-0.33622600
C	-0.30808100	0.74463100	2.10107200
O	-1.03802000	1.42417100	2.82209500
C	1.21581400	-0.62684200	-3.67784100
H	1.75153900	-0.40712300	-4.60958400
H	1.31085100	-1.69898900	-3.48739400
H	0.15876200	-0.39872000	-3.82309300
C	0.12484500	2.16462900	-2.64019300
H	0.41367000	2.66477800	-3.57274400
H	-0.70698700	1.48734900	-2.84702300
H	-0.22324500	2.92479600	-1.94176400
C	2.01888500	3.12660200	-0.22521700
H	2.45683300	3.94900000	-0.80467600
H	0.97291600	3.36439600	-0.02831100
H	2.53790600	3.07822300	0.73451600
C	4.39870300	1.03382100	0.04575300
H	5.11329000	1.72916400	-0.41141600
H	4.12246300	1.42583100	1.02617400
H	4.91341200	0.08464700	0.20104200
C	3.82291200	-1.37685700	-2.02170000
H	4.52339200	-1.18610800	-2.84414100
H	4.41200400	-1.63941300	-1.13966200
H	3.22151900	-2.24747400	-2.29547200
O	-1.00194200	1.89610300	0.26973100
C	-2.34432000	1.89072900	0.16074000
O	-3.01597100	0.88562200	0.01281900
C	-2.94876600	3.29140600	0.24460600
C	-3.88000500	3.48325100	-0.96547900
H	-4.60675300	2.67031800	-1.02314200
H	-4.41773900	4.43214200	-0.87393500
H	-3.31254000	3.50397200	-1.90236200
C	-3.76771700	3.29276300	1.55710300
H	-3.11709400	3.08282100	2.40970900
H	-4.23799900	4.27225200	1.69239800
H	-4.54713300	2.52802900	1.52126100
C	-1.89103900	4.40203100	0.30032100
H	-1.22481200	4.26563400	1.15448200
H	-1.28535500	4.43326100	-0.61072300
H	-2.39104400	5.37097800	0.39965200
C	-0.08279200	-1.74691200	-0.85738500

C	0.86674500	-2.29740200	-0.26877700
C	1.65666000	-3.38987600	0.31316000
C	-1.37867900	-1.77085500	-1.60573600
H	-1.18537600	-2.33340300	-2.52726000
H	2.70440300	-3.34562400	0.00124600
O	-1.82899300	-0.50095400	-2.02636700
H	-2.24463100	-0.06620900	-1.25165400
C	-2.41398800	-2.53468000	-0.79272700
C	-3.15048300	-3.56115900	-1.38834400
C	-2.65498800	-2.19885000	0.54577400
C	-4.12088600	-4.25003400	-0.65880900
H	-2.96542300	-3.82055300	-2.42778400
C	-3.62761300	-2.88254500	1.27129700
H	-2.08943900	-1.39380600	1.00194000
C	-4.36025100	-3.91101100	0.67291000
H	-4.68695900	-5.04848600	-1.12964000
H	-3.81369500	-2.61176500	2.30629300
H	-5.11447400	-4.44539900	1.24319000
H	1.63266000	-3.35692500	1.40441700
H	1.23643700	-4.34514300	-0.02001300

TS-b

N	0.16670500	1.11256400	0.81147500
C	0.96990500	-0.20844000	2.54221400
C	1.42717400	-0.36280400	3.84961700
H	1.09193400	0.35172100	4.59513400
C	2.31781300	-1.39286800	4.15885400
H	2.67750000	-1.51442900	5.17612900
C	2.75674800	-2.26092200	3.15332100
H	3.46032300	-3.05470500	3.38914400
C	2.27541900	-2.12609900	1.85041900
H	2.57293700	-2.84071400	1.08802200
C	1.37134600	-1.10260000	1.52773500
C	1.59869400	0.96303200	-2.21799800
C	2.65245200	1.20762000	-1.23096600
C	3.34096900	-0.01009500	-1.00573000
C	2.70158500	-1.03612500	-1.80850500
C	1.67787200	-0.40796200	-2.60216400
Rh	1.14302400	-0.23415000	-0.42747200
C	0.17667500	1.00480600	2.16518100
O	-0.31851000	1.79234400	2.97603200
C	0.85818600	-1.06420200	-3.66853100
H	1.35319400	-0.96128900	-4.64215700
H	0.73175500	-2.13260700	-3.47645500

H	-0.12960800	-0.60560300	-3.73770000
C	0.68553400	1.99895700	-2.79534500
H	1.13790900	2.48010300	-3.67188600
H	-0.26595600	1.55166200	-3.08985900
H	0.47389500	2.77299200	-2.05592100
C	2.93710700	2.53792700	-0.60670500
H	3.51637400	3.16919600	-1.29162200
H	2.00889900	3.05918000	-0.36561300
H	3.50707200	2.42977000	0.31821200
C	4.51046200	-0.22777100	-0.09819500
H	5.43887400	-0.31748000	-0.67506800
H	4.62781700	0.60172400	0.60156000
H	4.39285900	-1.13929600	0.49350000
C	3.15739300	-2.45772200	-1.93093900
H	3.87915700	-2.57069500	-2.74995400
H	3.64682900	-2.79623600	-1.01469900
H	2.31882800	-3.12909300	-2.13315600
O	-0.28700600	2.39421900	0.39680700
C	-1.62087200	2.53992200	0.27094000
O	-2.40821900	1.61298800	0.20612300
C	-2.03604100	4.00777900	0.27228300
C	-3.22988900	4.18433800	-0.67836500
H	-4.02991300	3.48459300	-0.42988600
H	-3.61656700	5.20523000	-0.60204800
H	-2.93569100	4.00926800	-1.71874400
C	-2.46249200	4.28773000	1.73525300
H	-1.65071000	4.04558700	2.42549500
H	-2.73181600	5.34379600	1.84055100
H	-3.32823300	3.67699000	2.00463400
C	-0.88719400	4.94859700	-0.12235100
H	-0.04602300	4.86289000	0.56789500
H	-0.52653800	4.73995900	-1.13489700
H	-1.24671700	5.98234100	-0.10262100
C	-0.60463500	-1.30122400	-0.46306900
C	-0.21532900	-1.92511100	0.58280400
C	-0.52873800	-3.07587300	1.46601600
C	-1.73444900	-1.33675600	-1.44937500
H	-1.40264700	-1.93915900	-2.30208400
H	0.21072100	-3.87617200	1.37117400
O	-2.03121800	-0.06051200	-1.98434800
H	-2.17871500	0.53934300	-1.22757400
C	-2.93132900	-2.03716700	-0.82410400
C	-3.31006600	-3.30460100	-1.27314700
C	-3.62443900	-1.45187300	0.24408900

C	-4.36824800	-3.98691800	-0.66832900
H	-2.77195600	-3.76138800	-2.10056000
C	-4.68338800	-2.13030800	0.84340700
H	-3.32934300	-0.47143700	0.60226200
C	-5.05695700	-3.39966700	0.39237700
H	-4.65315900	-4.97169600	-1.02715300
H	-5.21643700	-1.66969000	1.67000300
H	-5.88054200	-3.92609700	0.86564500
H	-0.56958200	-2.77410400	2.51580900
H	-1.50773400	-3.45955500	1.15936400

II-b

N	-0.28283500	0.74097500	0.97737800
C	1.23877300	-0.60374900	2.21074400
C	2.34903500	-0.25880800	3.01239500
H	2.27787200	0.64940300	3.60044900
C	3.47923000	-1.05745100	3.06604100
H	4.32052900	-0.76888700	3.68881800
C	3.52248700	-2.24938400	2.32518200
H	4.40076700	-2.88702200	2.36595300
C	2.43009600	-2.62095100	1.55934200
H	2.44974700	-3.55444700	1.00525900
C	1.26352900	-1.82338100	1.47359400
C	1.25926700	1.25438400	-2.12573100
C	2.19031500	1.87689600	-1.17883200
C	3.17330100	0.93081100	-0.86823600
C	2.90264300	-0.29160500	-1.64047700
C	1.78424900	-0.05159700	-2.48241600
Rh	1.10913500	0.00533000	-0.39637500
C	0.12306100	0.43846700	2.24121800
O	-0.20445300	0.99006400	3.28796200
C	1.25397400	-0.94088900	-3.56085400
H	1.70687900	-0.67303600	-4.52385000
H	1.49045800	-1.98826400	-3.35997300
H	0.17114300	-0.83908600	-3.63816300
C	0.14840100	1.97480200	-2.81844500
H	0.54295500	2.53022500	-3.67986300
H	-0.60977500	1.27374100	-3.16474500
H	-0.32943100	2.69516400	-2.15099000
C	2.02226900	3.25499900	-0.62070300
H	2.18130000	4.01251100	-1.39726300
H	1.01477300	3.38967500	-0.22139400
H	2.72862300	3.44801300	0.18919000
C	4.29649100	1.05268600	0.10993600

H	5.26253200	1.02544300	-0.40818600
H	4.23942500	1.98424500	0.67569400
H	4.28248600	0.22541700	0.82680100
C	3.77820600	-1.50537000	-1.62984400
H	4.66453500	-1.35012600	-2.25810300
H	4.12092200	-1.73536900	-0.61787000
H	3.24418300	-2.37865500	-2.00994900
O	-0.84565900	2.05492200	0.97873700
C	-1.96492700	2.23178700	0.25830300
O	-2.43606300	1.42039500	-0.51485000
C	-2.59300000	3.58789000	0.58585300
C	-3.70973300	3.87698900	-0.42425100
H	-4.45698700	3.08094700	-0.42145100
H	-4.20018900	4.82184000	-0.17061000
H	-3.31270300	3.95673400	-1.44064500
C	-3.16968300	3.46531100	2.01580600
H	-2.38885400	3.18869300	2.72843400
H	-3.61002900	4.42096900	2.31803600
H	-3.95382100	2.70252500	2.05269300
C	-1.53165000	4.70338000	0.54622800
H	-0.74088000	4.52694700	1.27801500
H	-1.07671400	4.78392100	-0.44726800
H	-2.00463800	5.66403100	0.77366100
C	-0.20205600	-1.56938500	-0.39357900
C	0.10557100	-2.33484500	0.66212400
C	-0.51876800	-3.63344500	1.12132300
C	-1.32405400	-1.78240600	-1.38839800
H	-1.00147700	-2.53806800	-2.11695100
H	0.25483200	-4.36625400	1.37832600
O	-1.58784400	-0.61802600	-2.16708800
H	-1.86185200	0.08236300	-1.54267000
C	-2.61202900	-2.27030300	-0.73966000
C	-3.33901100	-3.31486300	-1.31672600
C	-3.10538700	-1.65642700	0.41900200
C	-4.53574500	-3.75131500	-0.74558300
H	-2.96207400	-3.79252800	-2.21781900
C	-4.30231500	-2.08672600	0.98711000
H	-2.53810500	-0.85040200	0.87105000
C	-5.01988700	-3.13765100	0.40966700
H	-5.08696500	-4.56888000	-1.20148000
H	-4.67366800	-1.60555500	1.88752000
H	-5.94866700	-3.47651700	0.85935500
H	-1.12343800	-3.47329500	2.02310400
H	-1.16868500	-4.06903700	0.36322900

TS-a$_{SMD}$

N	1.50032100	-0.06066100	0.77571000
C	0.16173500	-0.81024600	2.48720000
C	-0.01592400	-1.24209200	3.79953400
H	0.70437700	-0.92683300	4.55305600
C	-1.07504600	-2.08140700	4.12391100
H	-1.21263200	-2.42344100	5.14691500
C	-1.95107000	-2.49803900	3.11908000
H	-2.77130500	-3.17283500	3.35681700
C	-1.79653900	-2.04394300	1.81190400
H	-2.51402500	-2.35329000	1.05187600
C	-0.74894300	-1.17229900	1.47105400
C	1.19288700	-1.57212000	-2.32930700
C	1.52570200	-2.54305900	-1.29392100
C	0.34800500	-3.25120400	-0.93783700
C	-0.73892300	-2.68564500	-1.69769800
C	-0.20100800	-1.69154000	-2.59206200
Rh	0.11858400	-1.05161500	-0.46882100
C	1.36579900	-0.02589400	2.11490700
O	2.12170800	0.53526400	2.92379600
C	-1.00048400	-0.95493000	-3.60833800
H	-1.22157100	-1.60745900	-4.46402500
H	-1.96351200	-0.62278800	-3.20068100
H	-0.47023900	-0.07665600	-3.98974300
C	2.17328400	-0.69399300	-3.02510200
H	2.71665700	-1.24819200	-3.80287900
H	1.68309800	0.15818200	-3.50920800
H	2.91871500	-0.29721000	-2.32566300
C	2.88559200	-2.77742100	-0.73972000
H	3.39171300	-3.57963300	-1.29378500
H	3.51222600	-1.88182100	-0.80929700
H	2.84180400	-3.07868100	0.31339100
C	0.26265100	-4.34699200	0.06624400
H	0.59222700	-5.30172900	-0.36485300
H	0.89927200	-4.14166500	0.93615700
H	-0.76063100	-4.48658000	0.43051600
C	-2.15722100	-3.13817300	-1.69846100
H	-2.34516000	-3.80663800	-2.55016700
H	-2.41500400	-3.68673300	-0.78662600
H	-2.84937800	-2.29259200	-1.79377100
O	2.57740500	0.69341700	0.28670100
C	2.48438800	2.03876100	0.45187400
O	1.51630300	2.59938700	0.91096400

C	3.78147500	2.71152200	0.04336300
C	3.52101600	4.20160500	-0.13655900
H	3.14175500	4.65571900	0.78539100
H	4.45356800	4.70862100	-0.41228500
H	2.78536400	4.38183500	-0.93126100
C	4.75872300	2.48096100	1.20325800
H	4.96643300	1.41338800	1.34275200
H	5.70566700	2.99518900	0.99562000
H	4.35077000	2.87430500	2.14344600
C	4.34045300	2.11933400	-1.24885400
H	4.61066500	1.06343700	-1.13618800
H	3.61858100	2.20727700	-2.07237100
H	5.24538300	2.66957200	-1.53560100
C	-0.71602800	0.83337900	-0.54013500
C	-1.46515100	0.32970200	0.37243300
C	-2.85730400	0.55794200	0.91094900
O	-2.89363800	0.79781800	2.29784400
H	-2.73557700	-0.04377900	2.74859800
C	-0.44668500	1.93093800	-1.47725000
H	-0.86659300	2.87642700	-1.10879200
H	0.62952200	2.06971200	-1.64183500
H	-0.90236500	1.71208900	-2.45277900
H	-3.48087400	-0.31472900	0.65109500
C	-3.39101400	1.76891100	0.18490100
C	-3.99980400	1.60794000	-1.05982300
C	-3.19169700	3.05177100	0.69275800
C	-4.40393700	2.71772300	-1.79434300
H	-4.15119700	0.60219800	-1.45428400
C	-3.60207600	4.16302700	-0.04025400
H	-2.71045600	3.17764800	1.66037400
C	-4.20393000	3.99953600	-1.28510900
H	-4.87914300	2.58230800	-2.76385200
H	-3.44581600	5.16175400	0.36257300
H	-4.51865300	4.86950900	-1.85771100

TS-b_{SMD}

N	0.19666200	1.14392600	0.90465500
C	1.04945400	-0.23923400	2.53689500
C	1.53061000	-0.45862200	3.82599900
H	1.20522500	0.20610800	4.62508700
C	2.44014700	-1.48241600	4.06633400
H	2.82067700	-1.65227600	5.07100800
C	2.88028700	-2.27498800	3.00518800
H	3.61449100	-3.05959600	3.17929200

C	2.37396900	-2.08268300	1.72409500
H	2.69081300	-2.74374600	0.91664500
C	1.43326000	-1.07581900	1.47046600
C	1.51951800	1.01135400	-2.26709200
C	2.55083100	1.30279100	-1.27793800
C	3.29260200	0.11807500	-1.03222400
C	2.69665400	-0.93512500	-1.81880100
C	1.64329700	-0.36333200	-2.61778500
Rh	1.13598500	-0.17312800	-0.45120800
C	0.25326700	0.97995600	2.23907700
O	-0.21910000	1.74070300	3.09868200
C	0.86397900	-1.11448700	-3.63758600
H	1.43862500	-1.19105700	-4.57080300
H	0.65438300	-2.13742200	-3.30232300
H	-0.08775700	-0.62589000	-3.87153000
C	0.59567800	2.02286700	-2.85393900
H	1.15552300	2.76951800	-3.43341400
H	-0.13796100	1.56122600	-3.52243700
H	0.04284100	2.56102200	-2.07293500
C	2.80385500	2.63785400	-0.67295900
H	3.60992700	3.15433600	-1.21156900
H	1.91443700	3.27484200	-0.71569200
H	3.10938800	2.55169400	0.37641100
C	4.45524100	-0.00616600	-0.11284000
H	5.38995700	0.24742700	-0.63049700
H	4.35856600	0.66901100	0.74604600
H	4.55915200	-1.02421700	0.27766000
C	3.15864500	-2.34697100	-1.92178400
H	3.65593200	-2.51919500	-2.88626600
H	3.87298700	-2.60026400	-1.13217000
H	2.31667300	-3.04851000	-1.86078800
O	-0.33675800	2.39084100	0.52864700
C	-1.67089800	2.50477600	0.56937300
O	-2.42226300	1.58141300	0.82723600
C	-2.14822500	3.91148900	0.26946400
C	-3.17787900	3.81105700	-0.85712300
H	-4.00473300	3.14547000	-0.58545200
H	-3.59085600	4.80504900	-1.06827800
H	-2.71767300	3.42992900	-1.77906400
C	-2.81292400	4.40231900	1.56104500
H	-2.09197700	4.41528000	2.38940400
H	-3.19249200	5.42124800	1.41632400
H	-3.65122200	3.75692500	1.84632100
C	-1.02744800	4.86432600	-0.12773700

H	-0.27268800	4.95916200	0.66141800
H	-0.52569700	4.54365200	-1.04951500
H	-1.45414700	5.85863000	-0.30908500
C	-0.67227000	-1.17612900	-0.44769100
C	-0.11922000	-1.87586400	0.47021300
C	-0.24872200	-3.18349700	1.15469600
C	-1.84846800	-1.13993900	-1.35886600
H	-1.52795100	-1.56839400	-2.32073100
H	0.53877500	-3.88208200	0.84770600
O	-2.27841100	0.17410700	-1.65685400
H	-2.45466500	0.62313100	-0.81261300
C	-2.94080900	-2.01944100	-0.79261300
C	-3.18304200	-3.27396400	-1.34981300
C	-3.65447500	-1.62367000	0.34205700
C	-4.12651800	-4.12803300	-0.78271300
H	-2.62156100	-3.58397600	-2.23139200
C	-4.59909200	-2.47344900	0.90523400
H	-3.46152900	-0.64943500	0.79137100
C	-4.83489800	-3.72920100	0.34662300
H	-4.30684000	-5.10567300	-1.22528100
H	-5.15063800	-2.15880700	1.78890800
H	-5.57092700	-4.39506700	0.79228900
H	-0.21296400	-3.08783200	2.24625000
H	-1.21623400	-3.61646100	0.86629000

I-a1$_S$

N	1.51459400	0.13777100	0.29175700
C	0.77847000	-0.09581500	2.47122100
C	0.78002200	0.16700700	3.84254300
H	1.58928900	0.76335300	4.25324800
C	-0.24812700	-0.33469000	4.63776600
H	-0.26330200	-0.13400000	5.70467600
C	-1.26830800	-1.08896300	4.05081400
H	-2.08328800	-1.46651800	4.66279200
C	-1.26277900	-1.34952400	2.67745600
H	-2.08539500	-1.90939900	2.24282600
C	-0.23176100	-0.86098200	1.87632600
C	0.93164800	-2.56682000	-1.75193100
C	1.39149400	-2.99016200	-0.44495100
C	0.26123100	-3.44855100	0.30486300
C	-0.91443100	-3.22990800	-0.49491400
C	-0.48418100	-2.72109600	-1.77783100
Rh	0.04232900	-1.23314800	-0.12857400
C	1.84768000	0.42903500	1.58241800

O	2.84623400	1.05873400	1.94457300
C	-1.41509200	-2.42307700	-2.91124200
H	-1.90856400	-3.33999400	-3.25200900
H	-2.19284600	-1.71796700	-2.60162300
H	-0.88789400	-1.99019500	-3.76285200
C	1.82486000	-2.11208500	-2.86485300
H	2.36838900	-2.95878100	-3.30138900
H	1.25578500	-1.63656500	-3.66666500
H	2.55968600	-1.39032500	-2.50330400
C	2.82146900	-3.00156400	-0.00127700
H	3.33549500	-3.89868500	-0.36749200
H	3.34944400	-2.12437700	-0.38087800
H	2.89809900	-2.98883700	1.08759400
C	0.31068200	-4.08919400	1.65502600
H	0.46980100	-5.16963500	1.55210700
H	1.12331500	-3.68033800	2.25851900
H	-0.61515900	-3.93112500	2.20902700
C	-2.31876900	-3.62767800	-0.15883900
H	-2.55040200	-4.62507600	-0.55359300
H	-2.47773800	-3.65636800	0.92086800
H	-3.03966100	-2.92615900	-0.58698200
O	2.57674700	0.41136500	-0.61521200
C	2.74146800	1.72721500	-0.89507400
O	1.91990600	2.58738900	-0.64148900
C	4.09981600	2.00594000	-1.53087500
C	5.04757600	2.32013200	-0.34797800
H	5.07550400	1.48887200	0.35931200
H	6.05559000	2.50934100	-0.73158300
H	4.70543100	3.20508900	0.19417500
C	4.63318400	0.79994900	-2.32132500
H	3.95419500	0.52192800	-3.13414800
H	5.59903200	1.05890100	-2.76630900
H	4.77643400	-0.07022800	-1.67768700
C	3.97153300	3.23116500	-2.44840500
H	3.31566600	3.02181400	-3.30021200
H	3.55699100	4.08144500	-1.90425600
H	4.95657900	3.50585700	-2.83791700
C	-0.86165600	0.36992600	-1.27920800
C	-1.63076100	0.13861400	-0.32034700
C	-2.83193100	0.51507500	0.48125900
O	-2.50306600	1.30007000	1.59568700
H	-1.68788900	1.81677000	1.39342800
C	-0.36937800	1.03620900	-2.49029600
H	-1.18067600	1.64348400	-2.90815100

H	0.46390100	1.69842000	-2.24674500
H	-0.03877400	0.32119100	-3.24831900
H	-3.32823500	-0.39086300	0.85205800
C	-3.76346000	1.22258500	-0.50047000
C	-4.79260000	0.52674200	-1.13708100
C	-3.53321700	2.56456700	-0.82408500
C	-5.58851300	1.16049600	-2.09331000
H	-4.97548000	-0.51424200	-0.87867100
C	-4.32657100	3.19701000	-1.77984000
H	-2.73260200	3.09938700	-0.32198300
C	-5.35453400	2.49712300	-2.41833000
H	-6.39226800	0.61394400	-2.57838800
H	-4.14566200	4.23935400	-2.02644000
H	-5.97298100	2.99350900	-3.16032100
C	-0.66896800	3.56156300	3.27904400
C	0.29528300	3.50920700	2.10643300
H	-1.60580800	4.04659100	2.98699900
H	-0.90009000	2.55286500	3.63188000
H	-0.22964100	4.12840500	4.10634300
H	1.21690800	2.98684500	2.38579800
H	0.56844700	4.52568400	1.78767700
O	-0.33881400	2.82338400	1.01889400
H	0.35706200	2.53962500	0.39625300

TS-a1$_S$

N	1.16127300	0.82332800	0.46743100
C	-0.03205500	0.17179700	2.34002000
C	-0.31864600	0.26143900	3.70017000
H	-0.08622500	1.19092200	4.21076200
C	-0.86276200	-0.83385400	4.37081500
H	-1.09279600	-0.76585600	5.42963300
C	-1.09949200	-2.02518800	3.67815300
H	-1.51225000	-2.88416600	4.19987800
C	-0.82938900	-2.11169700	2.31294300
H	-1.06370500	-3.02583300	1.77573400
C	-0.30792400	-1.01024700	1.61792700
C	2.69648900	-1.58158200	-1.40306100
C	3.11445100	-1.69693800	-0.00469300
C	2.40041600	-2.76633100	0.59001500
C	1.49064400	-3.29272400	-0.40952800
C	1.73357200	-2.60614200	-1.64861700
Rh	0.95253000	-1.14292000	-0.12167300
C	0.69622700	1.28021700	1.65367700
O	0.86376600	2.41558300	2.11926100

C	1.08013100	-2.93800300	-2.95428500
H	1.51322800	-3.85180300	-3.37876300
H	0.00618700	-3.10508100	-2.83304100
H	1.21597400	-2.13892000	-3.68558400
C	3.28088900	-0.62545300	-2.39594600
H	4.23480300	-0.99469200	-2.79347100
H	2.60330400	-0.46900100	-3.23880800
H	3.46002400	0.34614200	-1.93171400
C	4.14377400	-0.82165800	0.63988800
H	5.15366300	-1.12979900	0.34300200
H	4.00577400	0.22075900	0.34490600
H	4.08087300	-0.86835200	1.72858700
C	2.51293900	-3.26043200	1.99817500
H	3.02645700	-4.22870300	2.03465600
H	3.07345100	-2.55923400	2.61933100
H	1.52639500	-3.38284400	2.45417200
C	0.59490200	-4.48075600	-0.23769000
H	1.09616900	-5.39918200	-0.56933700
H	0.31756400	-4.61784600	0.80930600
H	-0.32307400	-4.37628500	-0.82217600
O	1.93886700	1.77694200	-0.23701100
C	1.24882500	2.81672400	-0.75880700
O	0.03555900	2.87685300	-0.82619700
C	2.17840300	3.94299900	-1.20145000
C	2.26311900	4.89048000	0.02023200
H	2.62883500	4.35753200	0.90086900
H	2.93877100	5.72144600	-0.20769500
H	1.27691900	5.29535300	0.26119400
C	3.58196700	3.43779400	-1.57116400
H	3.54315600	2.72142600	-2.39814900
H	4.19845000	4.28422600	-1.88991500
H	4.07174800	2.95717900	-0.72211400
C	1.53899600	4.66977600	-2.39403700
H	1.48719500	4.01771400	-3.27242300
H	0.52490000	4.99295800	-2.15279500
H	2.13744800	5.54730600	-2.65746900
C	-0.70599600	-0.46544800	-1.10788700
C	-1.37549600	-0.75291600	-0.05098600
C	-2.80694600	-0.90364800	0.42857100
O	-3.11843400	-0.06131900	1.49780700
H	-2.74771000	0.82994000	1.29869400
C	-0.85771200	0.09279000	-2.47048000
H	-1.89937500	0.03925800	-2.80167700
H	-0.55616300	1.14486600	-2.45161600

H	-0.22438400	-0.43027700	-3.19121700
H	-2.94791200	-1.93065500	0.78364800
C	-3.68356000	-0.69829300	-0.80465200
C	-3.99179300	-1.78845400	-1.62399700
C	-4.13008300	0.57769200	-1.16192800
C	-4.73649100	-1.61209600	-2.78979700
H	-3.64520400	-2.78107600	-1.34470700
C	-4.87473400	0.75420300	-2.32894100
H	-3.87622300	1.42725100	-0.53722600
C	-5.17910500	-0.33626500	-3.14612500
H	-4.97563000	-2.46725900	-3.41547000
H	-5.21604200	1.74859600	-2.60198100
H	-5.76046100	-0.19450100	-4.05242600
C	-3.08098200	3.01845200	2.92574100
C	-2.13130300	3.40427100	1.80396000
H	-4.09747300	2.87423400	2.54570500
H	-2.75753800	2.08481600	3.39521500
H	-3.10537400	3.80206500	3.68983700
H	-1.10932600	3.49990700	2.18159100
H	-2.43508000	4.36264800	1.35748700
O	-2.17145200	2.37859000	0.80257400
H	-1.37619000	2.44668400	0.24005600

II-a1$_S$

N	0.64867900	1.04459700	0.40889200
C	0.34835800	-0.41132000	2.20498800
C	1.11493800	-0.68272300	3.35499300
H	1.58299100	0.15737700	3.85650200
C	1.25714300	-1.97466500	3.83599200
H	1.85284700	-2.16147500	4.72440400
C	0.62145100	-3.03825900	3.17567200
H	0.72579400	-4.05295800	3.54833500
C	-0.16146900	-2.78472100	2.06219100
H	-0.68265500	-3.59926300	1.56843200
C	-0.33312800	-1.47787800	1.54373500
C	2.55633100	-0.59709700	-1.94440600
C	3.45955900	-0.44796600	-0.79027300
C	3.41963700	-1.63780300	-0.05909800
C	2.51355400	-2.56678800	-0.74932900
C	2.08450900	-1.96629200	-1.96336700
Rh	1.24006400	-0.81128900	-0.28547500
C	0.40203600	1.03754000	1.73529800
O	0.35303600	1.99632200	2.50688300
C	1.32722000	-2.64009200	-3.06407200

H	2.00177900	-3.27227200	-3.65447800
H	0.52751900	-3.27444400	-2.67391700
H	0.87870800	-1.91363700	-3.74312500
C	2.38612700	0.42192300	-3.02636600
H	3.21057500	0.37353200	-3.74949800
H	1.44935600	0.27089500	-3.56707000
H	2.36882900	1.42913300	-2.60346400
C	4.20138600	0.81125400	-0.46883200
H	5.00893900	0.98162400	-1.19100700
H	3.53236000	1.67404600	-0.50277900
H	4.64326800	0.77114000	0.52871000
C	4.08916300	-1.94964700	1.24152600
H	4.82100200	-2.75731600	1.12091100
H	4.60994200	-1.07836600	1.64302900
H	3.35917400	-2.27466100	1.99057700
C	2.25465600	-3.97392000	-0.31010100
H	3.09914400	-4.62402200	-0.57218600
H	2.11409700	-4.02645000	0.77224300
H	1.35819500	-4.37745100	-0.78590900
O	1.14414600	2.29412800	-0.05841400
C	0.23051500	3.09759200	-0.64219000
O	-0.92139600	2.78201000	-0.87004400
C	0.80737200	4.48779500	-0.90317400
C	0.57338900	5.27025800	0.41285800
H	1.03835400	4.75728500	1.25883300
H	1.00044800	6.27426500	0.32352000
H	-0.49630100	5.36641600	0.61901800
C	2.31068400	4.44391500	-1.22242600
H	2.51281500	3.83766200	-2.11178200
H	2.66757200	5.45905400	-1.42287400
H	2.88635600	4.03748400	-0.38883600
C	0.03159800	5.14013300	-2.05593800
H	0.20229900	4.60873100	-2.99776400
H	-1.04116800	5.13332000	-1.85566300
H	0.36198300	6.17548400	-2.18374700
C	-0.74427500	-0.89634100	-0.73010900
C	-1.31984000	-1.28242100	0.41382100
C	-2.77276300	-1.54214700	0.82470200
O	-3.12452400	-0.69230700	1.89505100
H	-2.92598000	0.23165300	1.62159800
C	-1.28649000	-0.44892200	-2.04482100
H	-2.37516000	-0.48744200	-2.09316100
H	-0.97717700	0.58863900	-2.21130600
H	-0.88829200	-1.05197900	-2.86646700

H	-2.80117200	-2.55788700	1.24605500
C	-3.75339000	-1.52016700	-0.33395100
C	-3.83951000	-2.63038700	-1.18142600
C	-4.55330700	-0.40367900	-0.59148100
C	-4.68883500	-2.61990700	-2.28618700
H	-3.22490200	-3.50431000	-0.97643100
C	-5.40440700	-0.39128600	-1.69803700
H	-4.48511800	0.46012400	0.05972400
C	-5.47259400	-1.49417100	-2.55076200
H	-4.74374500	-3.48786500	-2.93739000
H	-6.01555600	0.48500000	-1.89512000
H	-6.13609300	-1.48087500	-3.41057300
C	-2.94607200	2.45422500	3.32777700
C	-2.60937500	2.93853700	1.92821500
H	-3.92075600	1.95615500	3.34228000
H	-2.18416700	1.74838700	3.66745000
H	-2.97590500	3.29684200	4.02635200
H	-1.59464200	3.34761500	1.92019100
H	-3.30933100	3.72536200	1.60868500
O	-2.69304800	1.83315200	1.02309500
H	-2.07061500	1.97742300	0.28674900

I-a2s

N	1.80668400	0.44381200	0.58866600
C	1.28074400	-0.78449600	2.48021000
C	1.29134000	-1.06858000	3.84786900
H	1.81281400	-0.38328100	4.50941200
C	0.62887900	-2.19994500	4.32142400
H	0.62435100	-2.42800600	5.38282200
C	-0.04253400	-3.03281800	3.42212900
H	-0.57000500	-3.91075000	3.78569500
C	-0.05407600	-2.74050000	2.05309600
H	-0.59926300	-3.39647200	1.38053100
C	0.61313000	-1.61255600	1.56420700
C	2.00306700	-1.20763700	-2.33958500
C	2.65939100	-1.94097700	-1.27672900
C	1.80978100	-3.02720200	-0.88646100
C	0.58797000	-2.92387100	-1.63519400
C	0.73740800	-1.82110000	-2.56023100
Rh	0.80603800	-1.05376100	-0.40498800
C	1.94076300	0.44270500	1.94658700
O	2.49570500	1.30497900	2.62679000
C	-0.28467500	-1.45564300	-3.59001300
H	-0.36111400	-2.24823200	-4.34327300

H	-1.27312100	-1.33304800	-3.13839000
H	-0.02904000	-0.52745000	-4.10264900
C	2.60126700	-0.04530300	-3.07137400
H	3.40839800	-0.37368300	-3.73698500
H	1.85629100	0.46956900	-3.68129000
H	3.01628400	0.68258300	-2.36982400
C	4.02539800	-1.64393100	-0.74496800
H	4.79611800	-2.10319700	-1.37606500
H	4.20192100	-0.56709800	-0.71414700
H	4.14589500	-2.02588000	0.27050500
C	2.17893600	-4.10974300	0.07693500
H	2.74853200	-4.88986600	-0.44275300
H	2.79465800	-3.72545300	0.89219300
H	1.29867200	-4.57422400	0.52165200
C	-0.56575600	-3.87946500	-1.61825500
H	-0.47988600	-4.62149600	-2.42212200
H	-0.61671500	-4.42445300	-0.67330700
H	-1.51579100	-3.35506900	-1.75196700
O	2.25761600	1.63599300	-0.02349000
C	1.55495300	2.75415900	0.32934000
O	0.51169900	2.71549800	0.94373000
C	2.27883800	4.01743300	-0.12680400
C	1.35991000	5.22497600	0.10429800
H	1.09292400	5.31474200	1.15981400
H	1.87624700	6.14017500	-0.20124200
H	0.43210500	5.14363500	-0.46861900
C	3.55299400	4.13849200	0.73984700
H	4.22998600	3.30125300	0.55771700
H	4.06994800	5.07342300	0.49938600
H	3.30122400	4.13664700	1.80317700
C	2.66102500	3.91630600	-1.61593400
H	3.32467300	3.06892000	-1.80155000
H	1.77306300	3.81019700	-2.24773000
H	3.17976200	4.83049500	-1.92124800
C	-0.72500500	0.44400500	-0.91934600
C	-1.26851200	-0.35556500	-0.13293800
C	-2.32300600	-0.82024400	0.80498200
O	-2.18369600	-0.18364400	2.06567600
H	-1.27993600	-0.35140600	2.37232800
C	-0.54861700	1.56161200	-1.85578200
H	-1.00240300	1.31640600	-2.82177900
H	-1.04233100	2.45193500	-1.44485500
H	0.50630800	1.78362000	-2.02069600
H	-2.22470500	-1.90802100	0.92943000

C	-3.71904500	-0.53995100	0.26620400
C	-4.01490500	-0.72377200	-1.08832000
C	-4.73773200	-0.15489200	1.14193800
C	-5.30983500	-0.52276500	-1.56396700
H	-3.22380600	-1.01194900	-1.77397900
C	-6.03366300	0.04634300	0.66492800
H	-4.50154100	-0.00590100	2.18823100
C	-6.32467600	-0.13563700	-0.68745300
H	-5.52443200	-0.66159200	-2.61955600
H	-6.81659300	0.35128700	1.35312600
H	-7.33269800	0.02639700	-1.05699600
C	-4.02470900	3.02672300	-0.52501500
C	-2.96752800	3.20313500	0.55233000
H	-4.25841400	3.98997500	-0.98977600
H	-3.67299700	2.34404600	-1.30415500
H	-4.94109300	2.60642800	-0.10268900
H	-2.69840700	2.23054800	0.98349000
H	-3.36938600	3.82264700	1.37047500
O	-1.82549400	3.83467500	-0.02668100
H	-1.05075300	3.60836800	0.51555500

TS-a2$_S$

N	0.85478400	1.22817100	0.94523300
C	1.35254100	-0.48582300	2.41461100
C	1.83505600	-0.93400900	3.64501800
H	1.73958600	-0.27163500	4.49993200
C	2.43682600	-2.19023200	3.74189600
H	2.81038600	-2.54341000	4.69789000
C	2.56698800	-2.98936600	2.60024800
H	3.04570300	-3.96200000	2.67060900
C	2.06372200	-2.55447000	1.37414500
H	2.12380000	-3.20243700	0.50504300
C	1.43489800	-1.30211500	1.26358500
C	2.14163900	1.12047000	-2.20802100
C	3.20520700	1.04805500	-1.20641400
C	3.62632800	-0.30013400	-1.09711900
C	2.79957000	-1.09084800	-1.98795400
C	1.93935300	-0.19950600	-2.71524100
Rh	1.41700800	-0.10915600	-0.52349200
C	0.84209800	0.91616100	2.26639700
O	0.52659000	1.64449800	3.20664900
C	1.02633100	-0.60308300	-3.83053400
H	1.59650200	-0.74757900	-4.75632000
H	0.51134900	-1.54150900	-3.60886700

H	0.26964200	0.15905000	-4.02579100
C	1.51191700	2.38770300	-2.69689700
H	2.13611400	2.86995500	-3.46012500
H	0.52918600	2.20190300	-3.13675800
H	1.37919300	3.09461000	-1.87555300
C	3.74038000	2.22942700	-0.45969500
H	4.41761700	2.81174600	-1.09618300
H	2.92840600	2.88340500	-0.13505900
H	4.29128100	1.92165600	0.43082000
C	4.70510700	-0.84054200	-0.21181200
H	5.60000900	-1.09179000	-0.79366100
H	4.99305700	-0.11250600	0.54892900
H	4.37710400	-1.74428300	0.30941700
C	2.95092900	-2.55802000	-2.25120200
H	3.59642200	-2.73352600	-3.12123400
H	3.40387400	-3.06893100	-1.39901900
H	1.98614900	-3.02943700	-2.45640900
O	0.42589800	2.54659600	0.66147800
C	-0.90236300	2.76831300	0.80545400
O	-1.69370800	1.89661500	1.10767000
C	-1.27428900	4.21412100	0.47439400
C	-2.46146900	4.62383000	1.36507800
H	-2.20290400	4.54512600	2.42494600
H	-2.73031200	5.66307400	1.15155100
H	-3.33574000	3.99955900	1.17235300
C	-0.09122900	5.17006900	0.69903300
H	0.74339800	4.94465300	0.03123300
H	-0.41589700	6.19750000	0.50564500
H	0.27415100	5.11018100	1.72781700
C	-1.70867500	4.23664800	-1.01057200
H	-0.88555300	3.93775800	-1.66673500
H	-2.55943700	3.57234200	-1.18201400
H	-2.00564900	5.25473500	-1.28271400
C	-0.55939400	-0.64963700	-0.60566100
C	-0.29170200	-1.51690700	0.30346600
C	-0.89569200	-2.72138300	0.99180100
O	-1.14084500	-2.49893900	2.36320600
H	-0.39713500	-1.99772300	2.72800800
C	-1.67103200	-0.18991600	-1.46819600
H	-2.41620300	-0.98270700	-1.59153500
H	-2.17018200	0.66999200	-1.01430200
H	-1.31286400	0.11536600	-2.45373600
H	-0.21220400	-3.57301600	0.85810800
C	-2.20618100	-3.03220400	0.29323000

C	-2.19176700	-3.71041800	-0.92987900
C	-3.42044700	-2.59497200	0.82474100
C	-3.37855200	-3.93981600	-1.62338600
H	-1.24422300	-4.05046900	-1.34102000
C	-4.61030700	-2.83215900	0.13393700
H	-3.41653400	-2.07765800	1.77651200
C	-4.59302500	-3.49672500	-1.09262500
H	-3.35822100	-4.46606300	-2.57314700
H	-5.55178700	-2.49130400	0.55351800
H	-5.51948700	-3.67374500	-1.63035500
C	-5.67914800	0.40111700	-1.13243600
C	-4.94108400	0.86741400	0.11230600
H	-6.20758200	1.23948100	-1.59694500
H	-4.97653500	-0.01029700	-1.86340200
H	-6.41034000	-0.37492700	-0.88382800
H	-4.37316100	0.03060900	0.53964300
H	-5.66506200	1.19589900	0.87568500
O	-4.06988500	1.93410900	-0.24054300
H	-3.33433900	1.95389300	0.39971200

II-a2S

N	0.97804700	1.42944100	0.87497000
C	1.36949800	-0.33809200	2.30067700
C	2.49280600	-0.52101100	3.12666300
H	2.89789500	0.34278700	3.64409000
C	3.05994300	-1.77687000	3.28818500
H	3.92783300	-1.90396500	3.92820200
C	2.49766000	-2.88655200	2.63618800
H	2.93132400	-3.87311500	2.77056900
C	1.37835000	-2.72489200	1.83389500
H	0.92833000	-3.58357700	1.34404700
C	0.78273100	-1.45640500	1.63856100
C	2.33885600	0.77623200	-2.17040900
C	3.46656500	1.01168900	-1.25376500
C	3.93345200	-0.23331300	-0.82666100
C	3.13813500	-1.27654000	-1.49498800
C	2.24408200	-0.65222300	-2.40395000
Rh	1.64489500	-0.08351100	-0.36099300
C	0.79049600	1.06382000	2.16345300
O	0.31694800	1.70276300	3.09480500
C	1.38842300	-1.32541800	-3.42977500
H	1.94673800	-1.44554000	-4.36652200
H	1.07001100	-2.31649600	-3.09944800
H	0.49276700	-0.74229300	-3.64813800

C	1.61399500	1.85342600	-2.91233600
H	2.20177300	2.20466400	-3.77024600
H	0.65162400	1.49765800	-3.28601800
H	1.42616700	2.70692800	-2.25683000
C	3.89924100	2.37107900	-0.80402800
H	4.31579200	2.94464200	-1.64012600
H	3.05013600	2.93029300	-0.39952100
H	4.65904900	2.31116100	-0.02261600
C	4.99552700	-0.52860400	0.18425400
H	5.83674000	-1.05915000	-0.27714400
H	5.37960100	0.38558400	0.64027900
H	4.60591200	-1.16293900	0.98768800
C	3.37104900	-2.74513000	-1.32571200
H	4.25772800	-3.06700600	-1.88635200
H	3.53146800	-2.99487900	-0.27370000
H	2.51714500	-3.32492600	-1.68232600
O	0.38834200	2.66357300	0.48024400
C	-0.95903600	2.71602400	0.49592800
O	-1.66964700	1.78573600	0.83418600
C	-1.48743600	4.05068100	-0.02846400
C	-2.75280700	4.41569000	0.76879600
H	-2.53305100	4.51511900	1.83573200
H	-3.14480100	5.37109700	0.40688200
H	-3.52534500	3.65682100	0.63857000
C	-0.44068100	5.16965100	0.08774800
H	0.44481100	4.95964800	-0.51642600
H	-0.87927400	6.10944500	-0.26197300
H	-0.11873300	5.30546100	1.12389400
C	-1.86205400	3.81683400	-1.51228600
H	-0.98961400	3.50510000	-2.09587900
H	-2.64438800	3.05915200	-1.60309000
H	-2.23738100	4.75223300	-1.93948300
C	-0.28423900	-0.68333700	-0.35862600
C	-0.45885400	-1.34573200	0.79278600
C	-1.76765100	-1.86924400	1.35621900
O	-2.50361300	-0.80950700	1.97054200
H	-2.13001300	0.02930000	1.65552700
C	-1.28783600	-0.37146000	-1.42163800
H	-2.30858200	-0.32187100	-1.03430900
H	-1.06807500	0.59021000	-1.89526300
H	-1.27227500	-1.13980500	-2.20312900
H	-1.51837700	-2.57566000	2.16279800
C	-2.60972800	-2.63670500	0.34236400
C	-2.00908200	-3.53804000	-0.54495900

C	-3.99943000	-2.49998900	0.32435000
C	-2.77902800	-4.27351400	-1.44480100
H	-0.92774600	-3.64496000	-0.54274900
C	-4.77285800	-3.23335600	-0.57745000
H	-4.46206300	-1.81057400	1.01899900
C	-4.16693800	-4.11979900	-1.46779300
H	-2.29614100	-4.96316200	-2.13186500
H	-5.85212000	-3.11032400	-0.58198000
H	-4.76871100	-4.68661600	-2.17207200
C	-6.25328600	0.39224900	-0.40416700
C	-5.14656500	1.05507600	0.39838800
H	-6.60961700	1.06549000	-1.19027800
H	-5.87739000	-0.51807700	-0.87922000
H	-7.10040300	0.13268300	0.23966600
H	-4.78606100	0.38047400	1.18573200
H	-5.53389800	1.96018300	0.89508900
O	-4.08352600	1.38464100	-0.49034300
H	-3.28323100	1.52568300	0.04346800

I-b1$_S$

N	0.47466000	1.22324500	0.13208100
C	1.86095400	0.83453800	1.95151600
C	2.44767000	1.14269800	3.18009500
H	2.30130000	2.13911000	3.58606000
C	3.19627200	0.17381200	3.84606700
H	3.65436100	0.39793900	4.80459200
C	3.35141700	-1.09164900	3.27217900
H	3.93078400	-1.85329200	3.78798400
C	2.76394900	-1.39098700	2.03797100
H	2.88604400	-2.38646700	1.62105600
C	2.01435300	-0.42623700	1.36275700
C	1.35986400	-0.37713800	-2.74657000
C	2.52299800	0.15257700	-2.06441500
C	3.19109400	-0.93174300	-1.40350900
C	2.40834900	-2.12045500	-1.60138600
C	1.30582800	-1.77310000	-2.46660600
Rh	1.14244500	-0.62362300	-0.49476700
C	1.06374900	1.83922000	1.20149200
O	0.93240100	3.02690700	1.50941000
C	0.32728300	-2.75991800	-3.01991200
H	0.84060500	-3.46517200	-3.68399600
H	-0.14671400	-3.34267700	-2.22405600
H	-0.45322200	-2.26291500	-3.59810700
C	0.41755300	0.39233600	-3.62492500

H	0.47815800	0.04330300	-4.66251100
H	-0.61524600	0.30024200	-3.27921700
H	0.66826300	1.45356700	-3.61511100
C	2.98930500	1.57487300	-2.11484100
H	3.56332700	1.76086600	-3.03073600
H	2.14316300	2.26335500	-2.09149300
H	3.63021700	1.80997200	-1.26271600
C	4.51012800	-0.84496500	-0.70471500
H	5.32333600	-0.99037300	-1.42647600
H	4.64681200	0.12780700	-0.22924900
H	4.60565300	-1.60356500	0.07261000
C	2.75419300	-3.51095200	-1.16577500
H	3.27559200	-4.05815600	-1.96155900
H	3.40793900	-3.50232900	-0.29107800
H	1.85464300	-4.07609700	-0.90809100
O	-0.02261300	2.18473700	-0.79520700
C	-1.23655600	2.66716600	-0.48656300
O	-1.97220300	2.17463100	0.35776300
C	-1.59829800	3.91209700	-1.28517700
C	-3.07870100	3.80866500	-1.68989200
H	-3.70997900	3.66152700	-0.81156400
H	-3.38834000	4.72742200	-2.19733900
H	-3.24031500	2.96681700	-2.37097900
C	-1.38548800	5.09111700	-0.30534600
H	-0.35552800	5.10880300	0.05987400
H	-1.60538100	6.03408100	-0.81626700
H	-2.04839500	4.99545200	0.55811300
C	-0.71511100	4.09641600	-2.52786500
H	0.33812300	4.20129200	-2.25853000
H	-0.81512100	3.25167900	-3.21523000
H	-1.02485400	5.00258200	-3.05802800
C	-0.89483700	-1.36233200	-0.27484500
C	-0.28586700	-1.81554500	0.71659900
C	-0.19442100	-2.48824700	2.01718000
C	-2.10885600	-1.21411000	-1.12422300
H	-1.96075200	-1.77558400	-2.05040400
H	0.66156900	-3.16364200	2.08085000
O	-2.35103600	0.11807000	-1.55105400
H	-2.43993500	0.67458100	-0.75818700
C	-3.30273100	-1.81576900	-0.39331200
C	-4.14795800	-2.69984200	-1.06957100
C	-3.58764300	-1.46860000	0.93475000
C	-5.27032900	-3.23387100	-0.43559500
H	-3.92874100	-2.96706700	-2.10048500

C	-4.71210800	-2.00138700	1.56433500
H	-2.93265100	-0.79903600	1.48648300
C	-5.55474400	-2.88384100	0.88462600
H	-5.91949900	-3.92034100	-0.97126100
H	-4.92687500	-1.72801200	2.59327700
H	-6.42685500	-3.29796800	1.38209000
H	-0.11136800	-1.73215600	2.80059000
H	-1.11825200	-3.05562700	2.17520000
C	-0.87001500	0.62011900	4.88577300
C	-1.33539300	1.36505000	3.64528800
H	-1.53815700	-0.22078300	5.09993500
H	0.14102400	0.23000800	4.73428600
H	-0.85995700	1.28270300	5.75761200
H	-0.64363500	2.18442700	3.41300700
H	-2.32854900	1.80898700	3.82022200
O	-1.38301000	0.44115900	2.56299900
H	-1.40896200	0.95106400	1.73397500

TS-b1$_S$

N	-0.42785500	-1.22871800	0.37254500
C	-0.69872000	-0.25649300	2.45980100
C	-0.93234700	-0.35160400	3.83011900
H	-0.67720700	-1.28237200	4.32711600
C	-1.51058400	0.71837300	4.51537500
H	-1.69255000	0.64666800	5.58335900
C	-1.87176100	1.87691000	3.81939700
H	-2.33899900	2.70457700	4.34586100
C	-1.61539200	1.98219600	2.45206700
H	-1.85108700	2.90432200	1.92844500
C	-1.01083500	0.92535300	1.75308600
C	-2.39494900	-0.15858700	-2.16678200
C	-3.23716100	-0.52329200	-1.02415100
C	-3.64218800	0.66509500	-0.37123100
C	-3.02208100	1.78067800	-1.06305300
C	-2.32350600	1.26549400	-2.20900200
Rh	-1.36180300	0.48258800	-0.33224800
C	-0.26360800	-1.46491900	1.69622100
O	0.13870000	-2.51584700	2.21154600
C	-1.68297700	2.09044400	-3.28029500
H	-2.43720400	2.41372400	-4.00857100
H	-1.21520100	2.99059000	-2.87276900
H	-0.92358300	1.52207800	-3.82060000
C	-1.83280700	-1.11577000	-3.17146500
H	-2.54236700	-1.29034700	-3.99055300

H	-0.89668900	-0.74215200	-3.59165100
H	-1.61565900	-2.07574700	-2.70127500
C	-3.59562300	-1.92842900	-0.65341300
H	-4.39894900	-2.30484500	-1.29836200
H	-2.73373800	-2.58923200	-0.76300600
H	-3.93361500	-1.99307100	0.38254300
C	-4.52222400	0.78209300	0.83348700
H	-5.50871900	1.17498500	0.55954300
H	-4.66813400	-0.18756500	1.31316800
H	-4.08737000	1.45300100	1.57943700
C	-3.24435400	3.22929100	-0.75432900
H	-4.08762300	3.62815700	-1.33270800
H	-3.47369700	3.37619800	0.30313600
H	-2.36307300	3.82888900	-0.99668300
O	-0.23558700	-2.40220700	-0.40854000
C	1.04384700	-2.76978400	-0.58804700
O	2.00457000	-2.06283200	-0.31729900
C	1.16999900	-4.19229700	-1.11770000
C	2.40713200	-4.27216900	-2.02540200
H	3.29584700	-3.91544300	-1.50198200
H	2.57076700	-5.30902900	-2.33449300
H	2.27543100	-3.66343400	-2.92577700
C	1.37240100	-5.06540500	0.14591700
H	0.54246400	-4.93690600	0.84456000
H	1.44247500	-6.11775300	-0.14773100
H	2.29235400	-4.78312500	0.66423800
C	-0.08413400	-4.65143100	-1.87721800
H	-0.96949400	-4.63442400	-1.23862000
H	-0.27360700	-4.01958900	-2.75040300
H	0.06474000	-5.67657200	-2.23045400
C	0.52239900	1.24552200	-0.55471500
C	0.48031500	1.66960000	0.65390300
C	1.18618500	2.53169600	1.63461300
C	1.40270500	1.24800200	-1.76617600
H	0.88547000	1.81431900	-2.54573600
H	0.58630400	3.39893700	1.92170500
O	1.55008700	-0.06087400	-2.30455800
H	1.83792300	-0.64598300	-1.58187200
C	2.73755300	1.93132100	-1.51476200
C	3.10390400	3.03025400	-2.29706700
C	3.61609100	1.47718300	-0.52148900
C	4.32798200	3.67137600	-2.10005200
H	2.42631000	3.38400300	-3.07070600
C	4.83932900	2.11699500	-0.32633300

H	3.34068200	0.65521200	0.13140100
C	5.20066100	3.21329400	-1.11333900
H	4.59852900	4.52363200	-2.71672700
H	5.50873200	1.76028700	0.45103900
H	6.15423800	3.70865700	-0.95545900
H	1.44276300	1.95795900	2.52661300
H	2.10889300	2.87497200	1.15739900
C	2.93922800	-0.19655300	4.26211700
C	2.90932600	-1.13831900	3.06916000
H	3.61367200	0.64485200	4.07100200
H	1.93776500	0.20137900	4.45367500
H	3.28369100	-0.71747200	5.16163300
H	2.19783700	-1.95314200	3.24597800
H	3.90694300	-1.58161600	2.91556500
O	2.51219700	-0.38966400	1.92553600
H	2.24827000	-1.00831600	1.22315100

II-b1s

N	0.00968000	1.05785400	0.59449600
C	1.02717900	-0.18413100	2.32449200
C	2.07796000	0.02720300	3.24257700
H	2.19674000	1.02989900	3.63761900
C	2.91640300	-1.00269400	3.63279500
H	3.71836900	-0.81366500	4.33988600
C	2.71926600	-2.29238400	3.11330900
H	3.37145800	-3.10806600	3.41117100
C	1.67326600	-2.52557600	2.23764700
H	1.49584100	-3.52786100	1.85973700
C	0.78781100	-1.49865900	1.82068800
C	2.07361500	0.66878400	-2.11229500
C	2.99532600	1.19460700	-1.10034900
C	3.66608000	0.10277700	-0.53547100
C	3.20594500	-1.12463800	-1.19960000
C	2.30817600	-0.75541400	-2.24027300
Rh	1.38776300	-0.24976400	-0.31099800
C	0.29201000	1.08847600	1.92969100
O	0.11681400	2.01458800	2.71554100
C	1.76523900	-1.62585400	-3.32643400
H	2.41544600	-1.55991400	-4.20815400
H	1.72781700	-2.67420900	-3.02241800
H	0.76323400	-1.30680500	-3.61554500
C	1.22741000	1.50718300	-3.01318000
H	1.80919900	1.85457300	-3.87696300
H	0.36492400	0.94021300	-3.36398100

H	0.86596800	2.38723200	-2.47804400
C	3.10066000	2.64027900	-0.72571300
H	3.55848000	3.22092800	-1.53533600
H	2.11269600	3.06242500	-0.52750400
H	3.70683800	2.77695400	0.17192900
C	4.65066200	0.10818800	0.58843900
H	5.63299200	-0.23084000	0.23865700
H	4.76744400	1.10414900	1.01903000
H	4.33463000	-0.56662400	1.39011400
C	3.74332000	-2.49129000	-0.91026000
H	4.73193000	-2.63146100	-1.36566200
H	3.84512700	-2.64805600	0.16688300
H	3.07912200	-3.26569000	-1.29965200
O	-0.23481000	2.39225200	0.13007100
C	-1.39388300	2.55276400	-0.53386900
O	-2.12392800	1.63680500	-0.86764300
C	-1.69837200	4.03550500	-0.74882700
C	-2.85188900	4.16491900	-1.75110100
H	-3.73148200	3.61619700	-1.40887200
H	-3.11849700	5.21950200	-1.87021200
H	-2.57126800	3.76727200	-2.73092500
C	-2.11174000	4.60140600	0.63078400
H	-1.32503700	4.43913800	1.37156700
H	-2.30315600	5.67542900	0.54051300
H	-3.02549000	4.12077100	0.99100000
C	-0.45574100	4.78786400	-1.25999100
H	0.36888900	4.72824900	-0.54700000
H	-0.11637900	4.39247800	-2.22287900
H	-0.70760800	5.84309600	-1.40481100
C	-0.25584600	-1.47770100	-0.31245900
C	-0.36914800	-1.93163000	0.94249300
C	-1.38961400	-2.83410800	1.60287900
C	-1.07490100	-1.73716000	-1.55560400
H	-0.50480000	-2.44306600	-2.17074700
H	-0.90343100	-3.46420700	2.35529200
O	-1.18233000	-0.56170400	-2.35992700
H	-1.50763700	0.15777100	-1.78782900
C	-2.43462900	-2.36563300	-1.30984300
C	-2.65647000	-3.70036500	-1.66019400
C	-3.47095800	-1.63723400	-0.71471300
C	-3.88410700	-4.31253100	-1.40135400
H	-1.85637900	-4.26813000	-2.12984000
C	-4.69638100	-2.24598500	-0.45546500
H	-3.31370000	-0.60773000	-0.41864900

C	-4.90739300	-3.58505100	-0.79340500
H	-4.04056100	-5.35187700	-1.67585100
H	-5.48618300	-1.67464700	0.02326100
H	-5.86318700	-4.05695300	-0.58509200
H	-2.13471200	-2.21339700	2.11182300
H	-1.90636200	-3.47563200	0.89152700
C	-4.03302200	1.08613600	3.50381900
C	-3.17415700	1.34619700	2.27813500
H	-4.81679000	0.35750300	3.27368300
H	-3.41990600	0.68392900	4.31579800
H	-4.50671800	2.01064400	3.84989700
H	-2.37902100	2.06341100	2.52084000
H	-3.78926800	1.78006100	1.47331500
O	-2.61564800	0.10641400	1.86233100
H	-1.96991900	0.27909100	1.15879600

I-b2$_S$

N	0.28965500	0.88760700	0.75099200
C	1.92741700	0.48411100	2.36107600
C	2.48536300	0.59044500	3.63721800
H	2.05784900	1.31057400	4.32852800
C	3.57257400	-0.20978500	3.98042800
H	4.01458500	-0.14108700	4.96985600
C	4.09537900	-1.10030100	3.03776100
H	4.94564800	-1.72654300	3.29663600
C	3.53547700	-1.19472300	1.75914100
H	3.96202300	-1.89849700	1.05061100
C	2.44146600	-0.40049300	1.40450600
C	1.47916400	0.91521700	-2.38225700
C	2.56471900	1.33968000	-1.51275600
C	3.49876100	0.25278400	-1.40989400
C	2.93615700	-0.87595000	-2.08977700
C	1.70171900	-0.44100300	-2.72037400
Rh	1.53136200	-0.28674300	-0.43839600
C	0.81302500	1.36738700	1.92775800
O	0.42948800	2.37080700	2.52939500
C	0.83275600	-1.27944600	-3.60393400
H	1.19308600	-1.24578900	-4.63965100
H	0.84013800	-2.32506100	-3.28590100
H	-0.19854300	-0.92301200	-3.58357700
C	0.36041700	1.77136700	-2.88180300
H	0.53335400	2.04714500	-3.92961000
H	-0.59333700	1.24556100	-2.80667600
H	0.28770500	2.68709000	-2.29689900

C	2.73744000	2.70996800	-0.93360700
H	3.19563700	3.39274200	-1.65948500
H	1.77467700	3.12526400	-0.62919000
H	3.37494100	2.67815500	-0.04746000
C	4.84535100	0.32560600	-0.76446800
H	5.56602100	0.75899600	-1.46893500
H	4.82917900	0.94671000	0.13243500
H	5.21135800	-0.66055100	-0.47603600
C	3.57135400	-2.21993200	-2.26965600
H	4.13090200	-2.27169000	-3.21197600
H	4.26852300	-2.44156000	-1.45815700
H	2.81658300	-3.01039800	-2.28959300
O	-0.47345400	1.92017500	0.11617100
C	-1.68750300	2.14319200	0.66056500
O	-2.24616100	1.37384400	1.42180500
C	-2.27416100	3.47744200	0.18722000
C	-3.51846000	3.78012700	1.03564200
H	-3.27083100	3.82129700	2.09920400
H	-3.93614000	4.74606500	0.73499200
H	-4.28536900	3.01551900	0.89263900
C	-1.21900100	4.58525800	0.38122500
H	-0.37401900	4.44680100	-0.29705400
H	-1.67097800	5.56097500	0.17406100
H	-0.83007100	4.57835400	1.40228900
C	-2.67872200	3.37026000	-1.29811000
H	-1.81423800	3.17105000	-1.93269000
H	-3.40929500	2.57099100	-1.44352900
H	-3.12581500	4.31770800	-1.61759600
C	-0.06340100	-1.75496500	-0.45915700
C	0.87313500	-2.33635300	0.12548300
C	1.54118900	-3.43320900	0.83866100
C	-1.44744700	-1.74379200	-1.02244400
H	-1.43864200	-2.47471000	-1.84599300
H	2.49549600	-3.69884000	0.37303200
O	-1.81567500	-0.48980500	-1.56061600
H	-2.64867000	-0.17942100	-1.13927700
C	-2.39896800	-2.26998200	0.04200500
C	-3.28295500	-3.30826300	-0.26057800
C	-2.39230900	-1.71931800	1.33065000
C	-4.15870000	-3.79840200	0.71150400
H	-3.28478100	-3.73668000	-1.25971400
C	-3.27302000	-2.20188900	2.29623000
H	-1.71294300	-0.90504800	1.55944800
C	-4.15391800	-3.24542500	1.99209600

H	-4.83942400	-4.60876200	0.46801500
H	-3.26845500	-1.76467800	3.29015400
H	-4.83229600	-3.62438300	2.75085600
H	1.74328400	-3.16401800	1.87762400
H	0.89162100	-4.31528100	0.82240200
C	-5.64390100	-0.80817800	-1.62450600
C	-5.26707200	-0.29568600	-0.24634000
H	-5.84196400	0.02489300	-2.30573400
H	-4.82608400	-1.40445000	-2.03899200
H	-6.53873200	-1.43571900	-1.57010500
H	-5.08152400	-1.13256200	0.43462300
H	-6.08198800	0.31089600	0.17387000
O	-4.09065400	0.50523500	-0.38129600
H	-3.71564100	0.72559900	0.49269800

TS-b2S

N	0.53086000	1.13339400	0.71528900
C	1.99324800	0.30628000	2.31969000
C	2.79546200	0.45779600	3.44954700
H	2.57774000	1.28285400	4.12085900
C	3.86174200	-0.41604900	3.67034500
H	4.48885200	-0.29891100	4.54901300
C	4.12982800	-1.43507400	2.75020400
H	4.96693500	-2.10860000	2.91280800
C	3.31344500	-1.60256000	1.63038500
H	3.49721400	-2.42487100	0.94499600
C	2.23129200	-0.73893200	1.40371100
C	1.35656400	0.63111100	-2.56101600
C	2.46973300	1.25633700	-1.84702100
C	3.43278100	0.25784100	-1.55661500
C	2.91462100	-1.00679600	-2.04540700
C	1.66938900	-0.75354400	-2.71664900
Rh	1.45178100	-0.24176100	-0.54076600
C	0.96627200	1.34304800	1.98435000
O	0.62085600	2.25110200	2.74503000
C	0.86454800	-1.75556300	-3.48469800
H	1.17440100	-1.75877500	-4.53741500
H	1.01321400	-2.76683700	-3.09735400
H	-0.19889100	-1.51929900	-3.43525700
C	0.17864400	1.34736500	-3.14156400
H	0.39320000	1.69340100	-4.16125000
H	-0.69210200	0.69086200	-3.16313400
H	-0.07861000	2.21769100	-2.53672200
C	2.54796400	2.71391200	-1.51603900

H	2.84844000	3.29207500	-2.39835300
H	1.57905700	3.08496600	-1.17707600
H	3.27266900	2.90454700	-0.72226700
C	4.74241300	0.44228000	-0.85659900
H	5.57479900	0.40458200	-1.56970000
H	4.78344200	1.40464400	-0.34282300
H	4.90485600	-0.33555800	-0.10571400
C	3.64562700	-2.31414400	-2.02370200
H	4.19966800	-2.46671700	-2.95869300
H	4.36700700	-2.35008800	-1.20488200
H	2.95762900	-3.15550100	-1.90710100
O	-0.25927300	2.21007300	0.23660900
C	-1.50202500	2.29942100	0.76165000
O	-2.03593300	1.41339900	1.40327900
C	-2.13018200	3.65231900	0.42807000
C	-3.54815700	3.69951300	1.01370300
H	-3.53637900	3.51162900	2.08983000
H	-3.98278600	4.68793800	0.83557400
H	-4.19165700	2.95356200	0.54079100
C	-1.25221600	4.75050000	1.06612300
H	-0.25429500	4.75854800	0.62324400
H	-1.71802300	5.72855500	0.90603700
H	-1.13516500	4.58335400	2.13973700
C	-2.19038200	3.83035300	-1.10244800
H	-1.18866900	3.86102700	-1.53698200
H	-2.75073500	3.01226700	-1.56398200
H	-2.69230000	4.77405700	-1.34012500
C	-0.06742600	-1.51721300	-0.05069200
C	0.60496700	-1.86768000	0.98127700
C	0.63119700	-2.83641300	2.10679200
C	-1.30765900	-1.94005700	-0.78482700
H	-1.02025300	-2.81923700	-1.37656200
H	1.43735200	-3.56814000	2.00270700
O	-1.76352600	-0.99349500	-1.73770300
H	-2.36344700	-0.34673300	-1.29940300
C	-2.41638800	-2.36453900	0.16933600
C	-3.28810900	-3.39096000	-0.21012700
C	-2.62579300	-1.70534900	1.38713000
C	-4.35271200	-3.76016000	0.61241500
H	-3.13308200	-3.89822500	-1.15883900
C	-3.69239800	-2.07242500	2.20867400
H	-1.96872500	-0.89326900	1.67693300
C	-4.55657600	-3.10081800	1.82634000
H	-5.01975300	-4.56131300	0.30791200

H	-3.84756200	-1.54975200	3.14783800
H	-5.38344100	-3.38692500	2.46965500
H	0.75681300	-2.32957400	3.06750200
H	-0.32887700	-3.36388700	2.10297500
C	-5.15053300	-0.51322000	-2.13044600
C	-4.92061600	-0.04066900	-0.70608800
H	-5.17012100	0.33622900	-2.82023400
H	-4.34359900	-1.18536600	-2.43402400
H	-6.10342400	-1.04594700	-2.20683200
H	-4.91013500	-0.89400200	-0.01959600
H	-5.72182000	0.64163900	-0.38884200
O	-3.66272800	0.64487300	-0.66253900
H	-3.39214600	0.80551900	0.25997600

II-b2$_S$

N	-0.15763600	0.86423400	-0.88161300
C	-1.89022800	-0.10524300	-2.17830600
C	-3.07317000	0.42069900	-2.73883300
H	-3.03151900	1.43188100	-3.12803500
C	-4.23924700	-0.32491800	-2.80573700
H	-5.13682400	0.10568000	-3.23924900
C	-4.24708300	-1.64202000	-2.32291200
H	-5.15307200	-2.23891600	-2.37337300
C	-3.08528600	-2.18696900	-1.79979800
H	-3.08228900	-3.21364200	-1.44625500
C	-1.87911600	-1.45224600	-1.70873400
C	-1.19848100	0.75089600	2.43915800
C	-2.16491000	1.63661000	1.77637300
C	-3.27289500	0.86301500	1.41574700
C	-3.04622700	-0.51435100	1.88066300
C	-1.82150700	-0.55328600	2.59781300
Rh	-1.38593800	-0.09549800	0.49541000
C	-0.75675600	0.91244300	-2.09971100
O	-0.55980800	1.73524500	-2.99056400
C	-1.28417500	-1.69720300	3.39661900
H	-1.59742500	-1.60222700	4.44408100
H	-1.66253700	-2.65080100	3.02070900
H	-0.19574900	-1.71535400	3.34925200
C	0.06935500	1.22330000	3.07301000
H	-0.15623300	1.83155200	3.95919700
H	0.69538800	0.38301400	3.36655100
H	0.64157800	1.84033000	2.37664500
C	-1.92066200	3.08766600	1.50488300
H	-1.88879800	3.65505000	2.44260700

H	-0.96759300	3.22711100	0.99084100
H	-2.70522600	3.51584400	0.87774900
C	-4.48404700	1.28451200	0.64700900
H	-5.37580500	1.25106100	1.28456500
H	-4.38090100	2.29936100	0.25871000
H	-4.66155500	0.61837000	-0.20338800
C	-4.03818700	-1.62488200	1.72990300
H	-4.84456500	-1.52806900	2.46794500
H	-4.49133700	-1.61523000	0.73525800
H	-3.56475700	-2.59822300	1.87305500
O	0.48116800	2.10433400	-0.57148100
C	1.73016000	2.25702200	-1.06057200
O	2.35621600	1.38117900	-1.62519000
C	2.25308400	3.66380700	-0.76956300
C	3.68749600	3.76481800	-1.30502700
H	3.72310000	3.56356300	-2.37815100
H	4.07695100	4.77119100	-1.12289200
H	4.34244400	3.04456800	-0.80744800
C	1.33924400	4.68462200	-1.47773600
H	0.32064000	4.63689500	-1.08670600
H	1.72876600	5.69615600	-1.32249400
H	1.29333700	4.48970200	-2.55280300
C	2.24793100	3.89726800	0.75614100
H	1.23023200	3.91138500	1.15327900
H	2.80829500	3.10943900	1.26784000
H	2.71290300	4.86299400	0.97979100
C	-0.19398400	-1.67628200	-0.01282500
C	-0.66592100	-2.16415900	-1.16863500
C	-0.17456000	-3.35610600	-1.95933500
C	0.99430300	-2.19692700	0.76882300
H	0.68668000	-3.12881700	1.26331500
H	-1.01069300	-3.99510700	-2.26562600
O	1.38049400	-1.33538000	1.84132800
H	1.91908500	-0.60149100	1.47201400
C	2.21722400	-2.50234600	-0.08783000
C	3.09286700	-3.52116000	0.30292700
C	2.53790400	-1.72190700	-1.20462000
C	4.26777500	-3.76354100	-0.41012800
H	2.85270600	-4.12451800	1.17477200
C	3.71824000	-1.95369100	-1.91069000
H	1.87185900	-0.92470300	-1.51216000
C	4.58506000	-2.97702400	-1.51945100
H	4.93467900	-4.56266100	-0.09920300
H	3.95645800	-1.32946800	-2.76672200

H	5.49988800	-3.16149300	-2.07511400
H	0.33378400	-3.02879700	-2.87544900
H	0.53161600	-3.96147200	-1.39053300
C	4.50733300	-0.44698700	2.70532600
C	4.47738100	-0.07186300	1.23470800
H	4.35557100	0.43733700	3.33260300
H	3.71477900	-1.16834900	2.92070600
H	5.47239500	-0.89360600	2.96433900
H	4.61393300	-0.96293400	0.61222600
H	5.28398100	0.63623300	0.99713700
O	3.20896200	0.53552500	0.94873700
H	3.10673100	0.60631000	-0.01632700

I-a_{2S}

N	1.23699600	1.14614200	0.36655600
C	1.59946000	0.05237300	2.36552500
C	1.80311400	-0.03170600	3.74404200
H	1.96045100	0.88817200	4.29939000
C	1.79003700	-1.27963500	4.36425000
H	1.94203000	-1.36016500	5.43627000
C	1.56591400	-2.42760200	3.59870800
H	1.53360200	-3.40160100	4.07976300
C	1.36667200	-2.33637000	2.21767200
H	1.16998800	-3.24268200	1.65278800
C	1.39230400	-1.09367800	1.58586600
C	2.40839400	-0.47110800	-2.41002000
C	3.34213800	-0.59969500	-1.30710900
C	3.20613300	-1.91237500	-0.75166700
C	2.12529100	-2.56887500	-1.43496600
C	1.66719200	-1.68264700	-2.48536600
Rh	1.29167200	-0.74542900	-0.43745000
C	1.56345900	1.36924100	1.67231400
O	1.74039300	2.47107900	2.19704400
C	0.59000200	-2.03458700	-3.46333500
H	0.93570100	-2.82032200	-4.14492500
H	-0.30145800	-2.40651100	-2.94930900
H	0.29508800	-1.17322600	-4.06495500
C	2.30117800	0.72626700	-3.30343900
H	3.15256400	0.78009600	-3.99231300
H	1.38964100	0.69533400	-3.90382400
H	2.28414100	1.64766600	-2.71618300
C	4.32910700	0.44453800	-0.88699500
H	5.25432800	0.36366400	-1.47067000
H	3.92067600	1.44675900	-1.03144000

H	4.58561700	0.34239300	0.16934600
C	4.07245500	-2.50107800	0.31516400
H	4.95469500	-2.97121000	-0.13632200
H	4.41375700	-1.73615700	1.01506600
H	3.54118700	-3.25715200	0.89425700
C	1.67082000	-3.98321100	-1.24468000
H	2.19961400	-4.66334200	-1.92432700
H	1.85541400	-4.32637600	-0.22463700
H	0.60072400	-4.08230900	-1.44408500
O	1.28424500	2.32364500	-0.43035500
C	0.25105100	3.16372800	-0.23498600
O	-0.71701300	2.88840800	0.45551900
C	0.39613900	4.46180000	-1.02354300
C	-0.47202500	5.53617200	-0.34721800
H	-0.16153000	5.69700200	0.68867000
H	-0.36793300	6.47974900	-0.89122400
H	-1.52671100	5.25266900	-0.34991500
C	1.86766400	4.90903400	-1.06661600
H	2.49013600	4.18990100	-1.60356200
H	1.93899200	5.87472200	-1.57660200
H	2.27165800	5.01664600	-0.05638500
C	-0.13425600	4.19716100	-2.45182300
H	0.46958300	3.44531800	-2.96879600
H	-1.17539800	3.86223000	-2.42783300
H	-0.08633800	5.12479900	-3.03046100
C	-0.78628100	-0.34482600	-0.99919600
C	-0.81130600	-1.28746400	-0.18135400
C	-1.53626100	-2.28745500	0.65266000
O	-1.72987000	-1.85431100	1.97254500
H	-1.68714800	-0.86996900	2.00002700
C	-1.24003000	0.65423400	-1.97613500
H	-1.63691100	0.14769600	-2.86297800
H	-2.03311500	1.28378500	-1.55552400
H	-0.42557800	1.30647000	-2.29124200
H	-0.94778600	-3.21388700	0.68912100
C	-2.84323600	-2.57494600	-0.08396600
C	-2.89158300	-3.55392500	-1.07941800
C	-3.97898800	-1.80700700	0.18312300
C	-4.06238000	-3.76379600	-1.80871900
H	-2.00961500	-4.15980500	-1.27803700
C	-5.15079200	-2.01694100	-0.54369400
H	-3.93285800	-1.05736200	0.96582800
C	-5.19508900	-2.99209700	-1.54294700
H	-4.09352700	-4.53202500	-2.57609300

H	-6.03097800	-1.41806200	-0.33049600
H	-6.10917500	-3.15414200	-2.10631500
C	-5.25172000	1.73655900	-0.66097400
C	-4.20145200	2.45981000	0.16545200
H	-5.67622800	2.40907100	-1.41300700
H	-4.81421700	0.87559400	-1.17451400
H	-6.06503900	1.37796800	-0.02076900
H	-3.74181900	1.77152800	0.88700700
H	-4.67266900	3.27533500	0.73728100
O	-3.20902700	2.98589400	-0.71731800
H	-2.39936700	3.12351800	-0.19731800
C	-1.79729400	0.50564200	4.42485400
C	-1.54978900	1.50685400	3.31012400
H	-2.79639600	0.06751400	4.33452200
H	-1.06161400	-0.30198800	4.38560900
H	-1.72344200	0.99803000	5.39991700
H	-0.53599900	1.91545300	3.37061400
H	-2.25570700	2.34664200	3.38045500
O	-1.72883600	0.84587300	2.04798100
H	-1.23060300	1.34483900	1.37461500

TS-a_{2S}

N	0.92341900	1.23985900	0.98354300
C	0.92779800	-0.57410900	2.41420900
C	1.04398400	-1.09871200	3.69942800
H	0.74937600	-0.47289400	4.53625800
C	1.55302900	-2.38396500	3.88291400
H	1.64207800	-2.79842100	4.88232600
C	1.96155400	-3.13293000	2.77482300
H	2.37106200	-4.12950100	2.91424000
C	1.82220100	-2.61944600	1.48674700
H	2.09064100	-3.23516700	0.63357700
C	1.28207400	-1.33997600	1.28119900
C	2.90972700	1.22198600	-1.77536700
C	3.72858700	1.01394400	-0.57954000
C	4.04143100	-0.36332700	-0.48666900
C	3.37666400	-1.03858000	-1.58577500
C	2.74415800	-0.04490000	-2.41121800
Rh	1.77158300	-0.05969400	-0.38638000
C	0.52292600	0.84993200	2.21980500
O	-0.04870700	1.54667900	3.06573000
C	2.04928900	-0.30805700	-3.71125600
H	2.76871500	-0.30206300	-4.53927000
H	1.55462400	-1.28231200	-3.70830900

H	1.29233300	0.44980700	-3.92234000
C	2.46507200	2.55606200	-2.28869100
H	3.26452300	3.04725600	-2.85809100
H	1.59925500	2.45961200	-2.94878000
H	2.18537600	3.21570800	-1.46468700
C	4.14974600	2.10743000	0.35159000
H	4.96159000	2.69930100	-0.08817600
H	3.31475100	2.77902500	0.56431500
H	4.49917600	1.70589200	1.30442400
C	4.87209700	-1.03772800	0.55959100
H	5.83062800	-1.37007900	0.14346700
H	5.08270000	-0.36423300	1.39237200
H	4.36047200	-1.91333400	0.96929800
C	3.50273100	-2.49530300	-1.91160200
H	4.34514600	-2.67037100	-2.59300800
H	3.68167400	-3.08700000	-1.01155900
H	2.60174100	-2.87976100	-2.39647100
O	0.53782800	2.56459600	0.63313700
C	-0.77559300	2.76390400	0.45259200
O	-1.61750900	1.88795400	0.58301400
C	-1.10468000	4.18083200	-0.00848500
C	-2.43149900	4.60419100	0.64973700
H	-2.35264800	4.58766400	1.74075400
H	-2.67962400	5.62339100	0.33831900
H	-3.24714500	3.94503800	0.34685900
C	0.01080700	5.17508700	0.34832400
H	0.95010200	4.92621200	-0.15086000
H	-0.28781900	6.17935600	0.03219300
H	0.19510600	5.19347100	1.42583700
C	-1.29091000	4.10765900	-1.54329400
H	-0.37155000	3.77601800	-2.03586300
H	-2.10383800	3.42723700	-1.80891800
H	-1.53799800	5.10395700	-1.92330800
C	-0.15313800	-0.45406600	-0.94893100
C	-0.11072900	-1.43600400	-0.11975000
C	-0.84306700	-2.73026600	0.17917500
O	-1.33090500	-2.79632100	1.48639400
H	-1.73832600	-1.92270200	1.69525100
C	-0.99500200	0.14864700	-2.01011300
H	-1.05223300	-0.52934000	-2.86900500
H	-2.01539200	0.32392500	-1.65915800
H	-0.59029500	1.10597600	-2.34690000
H	-0.13554500	-3.55968300	0.06417200
C	-1.91794400	-2.87098300	-0.89786800

C	-1.55453000	-3.26236700	-2.19142200
C	-3.25359800	-2.57648600	-0.62202900
C	-2.51099000	-3.34898700	-3.20140100
H	-0.51370800	-3.49717500	-2.40514400
C	-4.21346700	-2.66559000	-1.63220700
H	-3.53224300	-2.27808400	0.38117200
C	-3.84652100	-3.04593600	-2.92329600
H	-2.21865800	-3.65833000	-4.20086700
H	-5.25045800	-2.43671700	-1.40819900
H	-4.59551200	-3.11333500	-3.70660000
C	-5.85362300	0.56406200	-1.53937700
C	-4.89707200	0.97647100	-0.43369700
H	-6.25849400	1.44793600	-2.04214000
H	-5.33122200	-0.04473300	-2.28265000
H	-6.68934100	-0.01698700	-1.13474400
H	-4.48187600	0.09229900	0.06788500
H	-5.43777400	1.55966400	0.32971600
O	-3.85421400	1.75454100	-1.01381600
H	-3.13854000	1.83301100	-0.35923200
C	-3.07383700	-1.27804400	4.04012900
C	-2.83461000	-0.01752000	3.22695200
H	-3.86553500	-1.88744000	3.59221000
H	-2.16341500	-1.88324300	4.08952000
H	-3.37434500	-1.02020700	5.06075000
H	-2.01115700	0.56854100	3.64516000
H	-3.73800700	0.60935000	3.21630900
O	-2.50993400	-0.39789300	1.88036500
H	-2.04439700	0.34268200	1.45022900

II-a_{2S}

N	0.70943800	1.04098600	1.03311400
C	1.03887800	-1.05269000	1.91131000
C	1.80641800	-1.38243900	3.04295600
H	1.75057400	-0.73363500	3.91123700
C	2.60746300	-2.51414800	3.05203200
H	3.19421300	-2.75862000	3.93229200
C	2.64832000	-3.34966200	1.92328800
H	3.26789200	-4.24157700	1.93050500
C	1.88277600	-3.04729100	0.80949400
H	1.89268100	-3.70609200	-0.05342800
C	1.05402400	-1.90034300	0.76404400
C	3.16621900	1.68900200	-1.24845000
C	3.82001800	1.69716100	0.07071000
C	4.40399600	0.44368300	0.26716300

C	4.14741400	-0.37052400	-0.93087700
C	3.49038400	0.43668900	-1.89845600
Rh	2.12482800	0.16406000	-0.18464900
C	0.21002400	0.22027200	1.95860700
O	-0.70575600	0.41993300	2.77315400
C	3.20001400	0.07051200	-3.31954400
H	4.06003000	0.30769400	-3.95791100
H	2.98952400	-0.99658300	-3.41935700
H	2.33746900	0.61673100	-3.70330300
C	2.51563300	2.88312200	-1.87126100
H	3.26901300	3.59578400	-2.23060500
H	1.89102600	2.59832700	-2.72040700
H	1.88201800	3.39781700	-1.14483200
C	3.74182000	2.84671500	1.02510700
H	4.32051500	3.70139000	0.65532100
H	2.70516800	3.17216200	1.15145900
H	4.12796200	2.57637200	2.00962600
C	5.11130600	-0.06747500	1.48210400
H	6.16142700	-0.29026200	1.25851400
H	5.08639200	0.66129300	2.29451700
H	4.64933900	-0.99007200	1.84943200
C	4.67150200	-1.75908900	-1.12726600
H	5.73784400	-1.73609700	-1.38570100
H	4.56138800	-2.35232500	-0.21616600
H	4.14180200	-2.27488700	-1.93110400
O	0.06317000	2.28715100	0.84875500
C	-1.21688600	2.22950400	0.38654700
O	-1.78344100	1.18845600	0.13211200
C	-1.84245800	3.61664500	0.25547100
C	-2.94086700	3.70066200	1.34065600
H	-2.52102300	3.54197700	2.33884600
H	-3.40054300	4.69387200	1.31283200
H	-3.71577400	2.95490700	1.15268600
C	-0.82213600	4.74864000	0.44489400
H	-0.02775200	4.70269900	-0.30634400
H	-1.33202700	5.71110700	0.33745300
H	-0.35880300	4.71368600	1.43346300
C	-2.48784700	3.70546600	-1.14240500
H	-1.73434700	3.60730400	-1.93160600
H	-3.24312300	2.92952700	-1.27544700
H	-2.97044900	4.68146500	-1.25538300
C	0.49952800	-0.59239800	-1.14108800
C	0.15814200	-1.67495400	-0.43185900
C	-0.94811600	-2.72276500	-0.59734600

O	-1.56050100	-2.97204600	0.65389700
H	-1.97955400	-2.14645200	0.98625200
C	-0.10873700	0.05662300	-2.34597700
H	0.17688800	-0.46208100	-3.26770700
H	-1.19795300	0.05887700	-2.29364300
H	0.22199200	1.09559300	-2.42960300
H	-0.46456100	-3.67343800	-0.86605300
C	-1.92320100	-2.37111900	-1.70323900
C	-1.68893400	-2.81064800	-3.00866600
C	-3.01323100	-1.53169800	-1.45363100
C	-2.51302300	-2.39742000	-4.05662700
H	-0.84715900	-3.47048900	-3.20737100
C	-3.82964700	-1.10262000	-2.49896900
H	-3.20483900	-1.18901900	-0.44505600
C	-3.57951000	-1.53259800	-3.80470400
H	-2.32054800	-2.74656800	-5.06739200
H	-4.63247000	-0.40551900	-2.28207800
H	-4.21352800	-1.19761600	-4.62068700
C	-6.91652700	0.95320600	0.33361100
C	-5.50375700	0.47483600	0.62286300
H	-7.00112000	2.03000400	0.51076600
H	-7.17917200	0.76085400	-0.71151800
H	-7.63955200	0.43632800	0.97303400
H	-5.42986700	-0.60991400	0.46044000
H	-5.24591500	0.65689400	1.67589400
O	-4.61752000	1.17183800	-0.24317800
H	-3.69814600	0.94716800	-0.01804700
C	-4.25578700	-2.72542500	2.60833100
C	-3.35145900	-1.57989400	3.03282400
H	-5.12819100	-2.34562000	2.06817600
H	-3.71476600	-3.41017300	1.94980200
H	-4.60745400	-3.27999200	3.48432000
H	-2.49114900	-1.95895100	3.60098200
H	-3.89557900	-0.88001300	3.68371700
O	-2.89670300	-0.89826400	1.86189400
H	-2.19765600	-0.26522100	2.13363700

I-b1$_{2S}$

N	-0.65432400	1.05748400	0.53560600
C	-2.37592000	1.79060000	-0.83719900
C	-3.09797400	2.75239000	-1.54622800
H	-2.87293800	3.79980900	-1.36946600
C	-4.07340100	2.34691700	-2.45509600
H	-4.63934000	3.08332500	-3.01755200

C	-4.31502600	0.98246800	-2.64187900
H	-5.06992100	0.65834500	-3.35390100
C	-3.59165800	0.02562200	-1.92204700
H	-3.79181800	-1.02787100	-2.09560100
C	-2.61647500	0.42175000	-1.00431300
C	-1.48299300	-1.58699200	2.37168700
C	-2.70678500	-0.86389700	2.07244500
C	-3.43449600	-1.61812100	1.08784100
C	-2.61496000	-2.71758900	0.67878300
C	-1.43205600	-2.71798900	1.52116700
Rh	-1.50578600	-0.79977400	0.23079800
C	-1.31879900	2.18054600	0.13053900
O	-1.06024200	3.33728700	0.47772600
C	-0.40815100	-3.80641200	1.57528000
H	-0.72824600	-4.57404800	2.29156700
H	-0.29198400	-4.29747900	0.60647000
H	0.56157600	-3.42360600	1.89645800
C	-0.48278600	-1.23646900	3.42776400
H	-0.65914600	-1.83102800	4.33326600
H	0.53429000	-1.42210400	3.07637900
H	-0.55577500	-0.18230800	3.69483500
C	-3.18698300	0.37335100	2.76570700
H	-3.76442500	0.12440100	3.66449000
H	-2.34684300	1.00350500	3.06430400
H	-3.82394800	0.96716000	2.10635400
C	-4.83693900	-1.33614300	0.65501400
H	-5.53313900	-1.76235100	1.38815300
H	-5.02979000	-0.26484200	0.58446300
H	-5.06225700	-1.77914300	-0.31548300
C	-2.96922000	-3.78534300	-0.30932000
H	-3.38705400	-4.66972800	0.18795100
H	-3.70809900	-3.42734900	-1.02950700
H	-2.08716300	-4.10430800	-0.87096300
O	0.16601700	1.33249900	1.66773500
C	1.30154500	1.99608900	1.38313200
O	1.76166300	2.10194100	0.25519800
C	1.92310500	2.59501200	2.64410700
C	3.15962000	3.41518800	2.25064100
H	2.90198300	4.19520100	1.52995000
H	3.57684200	3.88996500	3.14398300
H	3.92871600	2.77736200	1.81095900
C	0.86910300	3.51344900	3.30131500
H	0.01640000	2.93519000	3.66281400
H	1.32420200	4.03554400	4.14931600

H	0.48998200	4.24851100	2.58780400
C	2.32599400	1.46414200	3.61290600
H	1.45883900	0.87535100	3.91732300
H	3.05560400	0.79918800	3.14556400
H	2.77445000	1.90234800	4.51057500
C	0.31463700	-1.41868700	-0.80159900
C	-0.47707300	-1.16204700	-1.73008000
C	-0.85631100	-0.91075000	-3.12528000
C	1.59811000	-1.98644700	-0.29753800
H	1.43633300	-3.06510800	-0.19185100
H	-1.81549800	-1.36084900	-3.38815700
O	1.97800800	-1.53605100	0.99046400
H	2.60998700	-0.78726800	0.89965900
C	2.70142300	-1.80963100	-1.33783000
C	3.71542300	-2.77323300	-1.39775000
C	2.75462300	-0.70835400	-2.20081300
C	4.76857700	-2.64550100	-2.30269500
H	3.67660100	-3.62794900	-0.72718800
C	3.80803500	-0.58338800	-3.10879900
H	1.97807800	0.04875500	-2.18794300
C	4.81585400	-1.54770200	-3.16478200
H	5.54566700	-3.40329600	-2.33914300
H	3.83394200	0.27345900	-3.77554800
H	5.63053700	-1.44773100	-3.87593500
H	-0.90572900	0.16743500	-3.29095700
H	-0.07482300	-1.32668600	-3.77107800
C	5.64443100	-1.07302600	1.18087700
C	5.14186400	0.07517700	0.32488400
H	5.74527400	-0.76246100	2.22529800
H	4.93801300	-1.90595900	1.13495400
H	6.61817400	-1.42060300	0.82296700
H	5.08340900	-0.22651800	-0.72536800
H	5.81849500	0.93801400	0.39781200
O	3.84564800	0.43947800	0.81042200
H	3.44020100	1.14298300	0.27477500
C	-0.29205600	3.23166000	-3.98579200
C	0.47182100	3.16105600	-2.67359500
H	0.21665800	2.64331900	-4.75689300
H	-1.30253400	2.83249100	-3.85574400
H	-0.36930400	4.26610100	-4.33697600
H	-0.05944800	3.72003700	-1.89339800
H	1.46676300	3.62125900	-2.79009900
O	0.59263200	1.79363000	-2.29910200
H	0.82441400	1.76253900	-1.35312900

TS-b1$_{2S}$

N	-0.55581300	0.44864000	1.12438400
C	-2.00029800	2.05141100	0.26151700
C	-2.80444500	3.18225100	0.39213800
H	-2.62561500	3.83952500	1.23723000
C	-3.82388100	3.42416400	-0.53043700
H	-4.44930200	4.30624200	-0.43200800
C	-4.04836100	2.51895400	-1.57292900
H	-4.85031000	2.69608400	-2.28436000
C	-3.23445400	1.39383800	-1.71222800
H	-3.38658800	0.71818300	-2.54887100
C	-2.19138100	1.14960900	-0.80611500
C	-1.50900700	-2.81336300	0.68844300
C	-2.60627700	-2.03738800	1.26934700
C	-3.53121600	-1.73161500	0.24213500
C	-3.00192300	-2.26902900	-0.99898500
C	-1.79537100	-2.99120000	-0.69845800
Rh	-1.49786200	-0.81507100	-0.23862000
C	-1.02566500	1.70239200	1.33895800
O	-0.72838100	2.44886800	2.28034400
C	-1.00440300	-3.81959700	-1.66218900
H	-1.36362600	-4.85638800	-1.65029800
H	-1.11056500	-3.44802600	-2.68458400
H	0.05416300	-3.81432300	-1.40022800
C	-0.37866300	-3.42625800	1.45219400
H	-0.66654200	-4.40363600	1.86121800
H	0.49272700	-3.55056000	0.80860000
H	-0.08477900	-2.78474300	2.28401800
C	-2.70399600	-1.66893500	2.71694600
H	-3.05615300	-2.52350800	3.30754800
H	-1.73003000	-1.36531500	3.10527700
H	-3.39740900	-0.84035300	2.87341300
C	-4.81342900	-0.97190800	0.37668300
H	-5.67526200	-1.64743500	0.31629600
H	-4.86376800	-0.44795000	1.33311700
H	-4.91559300	-0.22218700	-0.41235900
C	-3.69995100	-2.24699800	-2.32404100
H	-4.28738300	-3.16237200	-2.47058000
H	-4.38590400	-1.40057400	-2.39451700
H	-2.98763400	-2.17597100	-3.15002400
O	0.20820800	-0.03154800	2.22446000
C	1.41429700	0.53787100	2.38703300
O	1.94884100	1.26439100	1.56116800

C	2.02351200	0.16378600	3.73563400
C	3.45716000	0.70744600	3.80287900
H	3.47786900	1.78722100	3.63930400
H	3.88048500	0.49402700	4.78906300
H	4.08794000	0.23258500	3.04757500
C	1.15036700	0.82303500	4.82713300
H	0.13638300	0.41795400	4.81355800
H	1.59424500	0.63333300	5.80991900
H	1.07871000	1.90271500	4.67338200
C	2.03324000	-1.36771900	3.90636700
H	1.01846300	-1.77029600	3.93268400
H	2.58020400	-1.84178600	3.08700300
H	2.52494200	-1.62425500	4.85028100
C	0.05482800	-0.40439900	-1.50379600
C	-0.55811500	0.65413200	-1.88466800
C	-0.50792800	1.77300000	-2.86041100
C	1.24336000	-1.24056500	-1.87793700
H	0.91030500	-1.88345100	-2.70304500
H	-1.35955000	1.76454100	-3.54474400
O	1.63853500	-2.14567800	-0.85591600
H	2.21124000	-1.66558400	-0.21593900
C	2.43247900	-0.42919500	-2.38047600
C	3.36642100	-1.06584800	-3.20824900
C	2.66401800	0.89264100	-1.98831800
C	4.50994500	-0.39549200	-3.63932100
H	3.19586400	-2.09714500	-3.50603500
C	3.80848300	1.56591200	-2.42077400
H	1.95431600	1.41642000	-1.36259700
C	4.73486100	0.92658200	-3.24512500
H	5.22346700	-0.90179300	-4.28293800
H	3.96296600	2.59404400	-2.10759900
H	5.62341500	1.45222400	-3.58232200
H	-0.47060000	2.72947500	-2.33595400
H	0.41508800	1.65521400	-3.43763200
C	4.99202600	-2.51487900	-0.14114400
C	4.77218700	-1.04349500	0.15937500
H	4.94603100	-3.10776900	0.77773500
H	4.21779700	-2.87416700	-0.82386200
H	5.97126500	-2.66714900	-0.60514900
H	4.83311500	-0.45299200	-0.76013100
H	5.53499200	-0.67107500	0.85762700
O	3.47338900	-0.90125000	0.75133400
H	3.23585800	0.03929900	0.82333700
C	0.11751000	5.30464100	-0.77546000

C	0.83527800	4.42732000	0.23791400
H	0.68095000	5.34771900	-1.71362900
H	-0.87795900	4.90299800	-0.98853100
H	0.00430200	6.32533500	-0.39496200
H	0.24604000	4.34645500	1.15896100
H	1.80787300	4.87746100	0.49791600
O	1.01847400	3.13788400	-0.33445500
H	1.23827100	2.51152000	0.37777500

II-b1$_{2S}$

N	-0.17393500	-0.00804000	1.06333300
C	-1.81482900	1.69340300	0.96633000
C	-2.95082900	2.02512300	1.73180100
H	-2.89467100	1.84932500	2.80019500
C	-4.08792800	2.56457000	1.15124000
H	-4.94971600	2.80953500	1.76458600
C	-4.11066700	2.79929100	-0.23075500
H	-4.99392700	3.22134700	-0.70119700
C	-2.98889900	2.51296600	-0.99308400
H	-2.99554800	2.72224000	-2.05835700
C	-1.80917400	1.96446900	-0.43508500
C	-1.43970400	-2.76444100	-0.65849600
C	-2.37533800	-2.56056100	0.45568700
C	-3.43768400	-1.78579200	-0.01928700
C	-3.21408500	-1.52108700	-1.45065600
C	-2.04381600	-2.21351100	-1.86058200
Rh	-1.47450300	-0.64913000	-0.43387200
C	-0.72770200	1.00262000	1.77249100
O	-0.51439000	1.27495800	2.95672900
C	-1.53574400	-2.38060800	-3.25644900
H	-1.90722400	-3.32239600	-3.67993500
H	-1.87781300	-1.56716700	-3.90055100
H	-0.44619200	-2.39233800	-3.26314800
C	-0.22807200	-3.63524900	-0.58326200
H	-0.52511500	-4.69202600	-0.54784600
H	0.41910000	-3.47465800	-1.44341800
H	0.34681800	-3.41554400	0.31921900
C	-2.13707400	-3.05175900	1.84920400
H	-2.18193800	-4.14667000	1.88614100
H	-1.15161700	-2.74245000	2.20522700
H	-2.88197400	-2.65989900	2.54451000
C	-4.59116200	-1.22530700	0.74956700
H	-5.53635600	-1.65495900	0.39692100
H	-4.50101700	-1.43106600	1.81768700

H	-4.65430200	-0.13943000	0.62396600
C	-4.16410500	-0.75463500	-2.31613500
H	-5.03703400	-1.36678800	-2.57598100
H	-4.52198000	0.14014300	-1.80036000
H	-3.68441200	-0.43761100	-3.24417100
O	0.51767300	-0.93025600	1.90630400
C	1.73179900	-0.52723400	2.32269800
O	2.27261800	0.50565700	1.96358700
C	2.33753900	-1.52498100	3.30661600
C	3.83507000	-1.21913500	3.44621400
H	3.99890200	-0.18852500	3.76727300
H	4.28127900	-1.89396800	4.18309700
H	4.34846600	-1.36190100	2.49122600
C	1.61677200	-1.31653300	4.65728000
H	0.54609200	-1.51243300	4.56305700
H	2.03665900	-1.99770600	5.40463700
H	1.74058400	-0.28986700	5.01271100
C	2.14118000	-2.96925300	2.80861200
H	1.08392400	-3.24092000	2.77184300
H	2.56679600	-3.08788300	1.80882100
H	2.64540900	-3.66061100	3.49150400
C	-0.24557900	0.51925300	-1.56948700
C	-0.63342900	1.78598300	-1.36687300
C	-0.08396100	3.05497700	-1.98044700
C	0.88046600	0.01992500	-2.45114700
H	0.52628200	0.02587500	-3.49110400
H	-0.89580900	3.72748900	-2.27872400
O	1.20912700	-1.35102000	-2.19633800
H	1.73690100	-1.38190800	-1.37036500
C	2.16077000	0.84378700	-2.38339000
C	3.03500100	0.85152200	-3.47597300
C	2.53032900	1.51707600	-1.21576900
C	4.25497100	1.52558400	-3.40367800
H	2.75867500	0.32155300	-4.38400800
C	3.74776700	2.19177300	-1.13835300
H	1.84910800	1.53673200	-0.37772900
C	4.61573600	2.19709000	-2.23242800
H	4.92242300	1.52901100	-4.26083600
H	3.99417700	2.72495100	-0.22565700
H	5.56218800	2.72732100	-2.17863300
H	0.52837600	3.57877700	-1.23794800
H	0.53558500	2.85416400	-2.85524100
C	4.26015800	-2.72410200	-1.71149300
C	4.31675400	-1.49679600	-0.82068600

H	4.06678400	-3.62375100	-1.11828300
H	3.46129400	-2.61213600	-2.44936600
H	5.21059100	-2.85534500	-2.23801700
H	4.48155800	-0.59634300	-1.42108700
H	5.13824100	-1.57935700	-0.09508200
O	3.06827700	-1.39248500	-0.11760400
H	3.01452700	-0.50969600	0.28314000
C	-0.05437800	5.06811900	1.50613200
C	0.83692500	4.04234900	2.18905300
H	0.49048500	5.58078700	0.70644400
H	-0.92861300	4.57953100	1.06548500
H	-0.40090200	5.81965400	2.22362400
H	0.26824500	3.50230200	2.95463400
H	1.67944800	4.55220700	2.68545000
O	1.31589200	3.13572200	1.20216800
H	1.58137300	2.30555100	1.63134800

I-b2$_{2S}$

N	-0.77554300	0.77000800	-0.77060200
C	-0.45882300	-0.86046100	-2.40237900
C	-0.09169900	-1.31620200	-3.67043500
H	0.09939400	-0.58366800	-4.44876500
C	0.00815100	-2.68457700	-3.90358300
H	0.30336500	-3.05454700	-4.88046600
C	-0.27440600	-3.58085500	-2.86948100
H	-0.20101700	-4.65100700	-3.04569900
C	-0.64267700	-3.11713700	-1.60267200
H	-0.84098900	-3.83831700	-0.81594100
C	-0.72911900	-1.74701700	-1.35204500
C	-3.00877700	-0.00139600	1.67214600
C	-3.50032500	-0.46257100	0.38397800
C	-3.32036000	-1.88349100	0.31579900
C	-2.62748300	-2.29567800	1.50329000
C	-2.48157200	-1.12982100	2.35199500
Rh	-1.31188700	-0.84816600	0.40935400
C	-0.64310800	0.58317200	-2.12484900
O	-0.66367400	1.48245700	-2.97046500
C	-1.90521600	-1.15770900	3.73184200
H	-2.57681900	-1.69428000	4.41231400
H	-0.93964500	-1.67198700	3.74836800
H	-1.76586700	-0.14893800	4.12355700
C	-3.09307800	1.39908800	2.19760400
H	-3.94519900	1.50933700	2.87958700
H	-2.17966300	1.68528800	2.72361900

H	-3.22291600	2.10464300	1.37749000
C	-4.18565400	0.38556100	-0.64157800
H	-5.25293100	0.48662900	-0.40943500
H	-3.74514400	1.38227200	-0.67849600
H	-4.09713300	-0.05289200	-1.63766800
C	-3.82404500	-2.77299700	-0.77540900
H	-4.86212500	-3.06203000	-0.56966300
H	-3.79569400	-2.27079700	-1.74390900
H	-3.22980700	-3.68306100	-0.86212300
C	-2.28690900	-3.69756700	1.90376500
H	-3.08960900	-4.14224500	2.50552400
H	-2.13790800	-4.33656100	1.03076100
H	-1.37172500	-3.72492100	2.50065400
O	-1.35399900	2.06053400	-0.52591900
C	-0.47270400	3.06852000	-0.55551900
O	0.74096700	2.91530500	-0.48702100
C	-1.11722300	4.44092200	-0.69569300
C	-0.52320200	5.35779700	0.38920800
H	0.56679100	5.36998800	0.32805300
H	-0.89596100	6.37791200	0.25486700
H	-0.80593000	5.01747500	1.39064500
C	-0.70174800	4.93447200	-2.10225700
H	-1.04704700	4.23862400	-2.87100200
H	-1.13741600	5.92189200	-2.28541500
H	0.38580600	5.00923200	-2.17405200
C	-2.64739100	4.40090900	-0.59021100
H	-3.08190400	3.75037000	-1.35246400
H	-2.97315300	4.05122800	0.39349500
H	-3.04355900	5.41102500	-0.73418700
C	0.51805000	-0.48406700	1.54037800
C	0.68532300	-1.61715500	1.04575200
C	1.38630700	-2.87129800	0.75182600
C	0.88444200	0.61734600	2.47762600
H	0.40042400	0.40338700	3.43626500
H	0.74366000	-3.74209900	0.90897800
O	0.39836100	1.89176700	2.10804100
H	0.75472600	2.11952400	1.23127000
C	2.39162300	0.58646900	2.69733900
C	2.90343100	0.40296500	3.98408600
C	3.27600300	0.73998500	1.62151000
C	4.28196200	0.37496000	4.20280900
H	2.21898300	0.28441700	4.82064500
C	4.65193900	0.71797100	1.84168900
H	2.90624300	0.86522500	0.60878500

C	5.15933400	0.53323600	3.13027700
H	4.66758500	0.23078600	5.20781900
H	5.32768600	0.83593600	0.99993000
H	6.23236300	0.51084700	3.29600600
H	1.74148500	-2.86356000	-0.28304800
H	2.25080300	-2.94676000	1.42121800
C	4.74517500	-3.14494000	-1.26968700
C	4.11752000	-1.77008200	-1.10477400
H	4.09555500	-3.91864100	-0.84725800
H	4.89037000	-3.37065500	-2.33048000
H	5.71521800	-3.19462100	-0.76411300
H	4.79579100	-1.00051100	-1.50456700
H	3.98150400	-1.54605700	-0.03509700
O	2.87830700	-1.75622300	-1.79361100
H	2.51595100	-0.84849300	-1.72471500
C	3.75771400	0.95159400	-3.55550000
C	2.60794400	1.63956700	-2.84038500
H	4.67235400	0.99930000	-2.95578700
H	3.51971400	-0.10141800	-3.73106100
H	3.95187600	1.43601700	-4.51766800
H	1.70461600	1.64160700	-3.46082000
H	2.86070400	2.68472800	-2.61427400
O	2.34357200	0.93833100	-1.61859600
H	1.61526400	1.40334700	-1.16658000

TS-b2$_{2S}$

N	-0.71130400	0.96741000	-0.76453600
C	0.17555500	-0.56555200	-2.25941700
C	0.68355800	-0.89140100	-3.51452900
H	1.14921100	-0.10398000	-4.09797000
C	0.55839200	-2.19350500	-3.99878400
H	0.95732700	-2.45174900	-4.97469400
C	-0.09082400	-3.16339700	-3.22848100
H	-0.20682500	-4.17370700	-3.61106600
C	-0.56450100	-2.84790400	-1.95493500
H	-1.00641800	-3.62490200	-1.33744600
C	-0.42167800	-1.54993000	-1.44027900
C	-3.52007800	0.23621200	0.95159700
C	-3.79545600	0.04564300	-0.47548600
C	-3.75973400	-1.34212000	-0.75401900
C	-3.41666700	-2.03049500	0.47768200
C	-3.34799900	-1.05499100	1.53225300
Rh	-1.72982900	-0.65160700	0.03205700
C	0.11006100	0.86466800	-1.83643800

O	0.67200000	1.80264800	-2.41848400
C	-3.16418600	-1.34772800	2.98837800
H	-4.13448200	-1.55294200	3.45758700
H	-2.53248500	-2.22577800	3.14551400
H	-2.71379200	-0.50043800	3.50851800
C	-3.53098300	1.54278600	1.68342800
H	-4.51315300	1.73700300	2.13276200
H	-2.77420900	1.54891400	2.47141100
H	-3.30301600	2.36423600	1.00280100
C	-4.07796000	1.15488500	-1.43998300
H	-5.11950800	1.48733300	-1.35250500
H	-3.43020400	2.01182300	-1.24590900
H	-3.90795300	0.83825800	-2.47089100
C	-4.00509900	-2.01053600	-2.07009900
H	-4.96099500	-2.54784300	-2.06088900
H	-4.03647300	-1.28421000	-2.88425100
H	-3.21565700	-2.73073200	-2.30341000
C	-3.34965200	-3.51648700	0.65286100
H	-4.32980400	-3.92267100	0.93381400
H	-3.04433200	-4.00949600	-0.27266200
H	-2.63891800	-3.79494600	1.43506600
O	-1.03730600	2.32128500	-0.46971200
C	-0.08271000	3.02843800	0.15032900
O	0.90882500	2.53088400	0.66887700
C	-0.33592900	4.52950400	0.09910900
C	0.10103900	5.14747600	1.43703500
H	1.12946800	4.86925800	1.67435800
H	0.03477100	6.23809100	1.37876700
H	-0.54182400	4.81021300	2.25672300
C	0.57119200	5.03813400	-1.04960900
H	0.34766400	4.51287800	-1.98122100
H	0.41123800	6.11191600	-1.18939500
H	1.62419800	4.86897700	-0.81074500
C	-1.80202800	4.87379400	-0.20253700
H	-2.11880900	4.47048900	-1.16638400
H	-2.47116200	4.48641600	0.57183200
H	-1.91660600	5.96187500	-0.23020700
C	-0.10269600	-0.89073200	1.24594900
C	0.40687600	-1.67528100	0.36880400
C	1.48092200	-2.67947100	0.16399200
C	0.19703800	-0.39444500	2.62970300
H	-0.43797200	-0.94896300	3.32837800
H	1.07094600	-3.68353400	0.02283900
O	-0.15996900	0.96694700	2.80116800

H	0.26925400	1.47372600	2.08909900
C	1.64857000	-0.69912400	2.96550900
C	1.96313700	-1.78006100	3.79319600
C	2.68459100	0.03240200	2.37441900
C	3.29436200	-2.13309000	4.02545000
H	1.16139600	-2.35387800	4.25231500
C	4.01279800	-0.31833400	2.60371300
H	2.46448500	0.86605300	1.72086300
C	4.32265700	-1.40396500	3.42749100
H	3.52602300	-2.97544400	4.67076800
H	4.80153400	0.25156300	2.12287100
H	5.35859100	-1.67957400	3.60107500
H	2.09736300	-2.41378000	-0.69927100
H	2.09738300	-2.67655700	1.06912100
C	5.11854300	-2.94190300	-1.46069400
C	4.68507900	-1.58413900	-0.93129500
H	4.30344500	-3.66765700	-1.37291300
H	5.39043100	-2.86782700	-2.51815900
H	5.98141600	-3.32135500	-0.90332400
H	5.52668900	-0.87560300	-0.99239300
H	4.41453800	-1.66479100	0.13264200
O	3.58680500	-1.12967800	-1.70555000
H	3.30648400	-0.26665300	-1.33145600
C	4.93467300	1.90828400	-2.06858200
C	3.61618100	2.36342500	-1.46740100
H	5.67697100	1.72860100	-1.28399700
H	4.79215400	0.97880700	-2.62677500
H	5.32833700	2.67142000	-2.74742700
H	2.87035900	2.54035700	-2.24867600
H	3.75492400	3.29782600	-0.90272700
O	3.14243000	1.33891800	-0.58354600
H	2.24490000	1.58902900	-0.30516100

II-b2$_{2S}$

N	-0.48318800	0.89657500	-0.73391900
C	-0.49012500	-0.98327800	-2.19398900
C	-1.19725300	-1.37259300	-3.35238800
H	-1.48852800	-0.58754000	-4.04070600
C	-1.49415500	-2.69907300	-3.61026700
H	-2.03662800	-2.97065800	-4.51056900
C	-1.08258400	-3.68862400	-2.70354000
H	-1.30934700	-4.73363000	-2.89298800
C	-0.36225200	-3.32988600	-1.57813800
H	-0.01579600	-4.09857600	-0.89517200

C	-0.02645700	-1.98334200	-1.28416900
C	-3.08415200	0.21824700	1.47489800
C	-3.75793000	0.16686500	0.17310600
C	-3.81610500	-1.17572400	-0.21899100
C	-3.21039800	-1.99702300	0.83900500
C	-2.86329900	-1.14180200	1.92129800
Rh	-1.60026800	-0.64142100	0.19290600
C	-0.36523900	0.52679900	-2.04907100
O	-0.29042300	1.26629900	-3.02460300
C	-2.42885500	-1.54424700	3.29305900
H	-3.30515100	-1.61481800	3.95006900
H	-1.94064600	-2.52135100	3.28875900
H	-1.74127900	-0.80921500	3.71279900
C	-2.91925000	1.44736900	2.30705400
H	-3.81846600	1.62079000	2.91294200
H	-2.05735500	1.35003700	2.96774300
H	-2.77472700	2.32377800	1.67324500
C	-4.21542800	1.37051100	-0.58903800
H	-5.05806000	1.85662500	-0.08330200
H	-3.40883100	2.10109400	-0.67553900
H	-4.53485600	1.10603800	-1.59899300
C	-4.34328400	-1.73966900	-1.49807000
H	-5.23285600	-2.35247200	-1.30927900
H	-4.61491100	-0.95344800	-2.20449400
H	-3.59836700	-2.37870800	-1.98177300
C	-3.14927600	-3.49224500	0.81825300
H	-4.11720300	-3.92769600	1.09718900
H	-2.89100800	-3.85961000	-0.17807900
H	-2.39691400	-3.86418800	1.51698400
O	-0.87945800	2.27884700	-0.69107500
C	-0.24277600	3.02690700	0.22674600
O	0.52259800	2.58311100	1.06301300
C	-0.58087300	4.51115900	0.04751800
C	0.09689400	5.30725100	1.16953900
H	1.17872800	5.15695800	1.15948700
H	-0.10916200	6.37387500	1.03842000
H	-0.27154900	5.00061700	2.15226800
C	-0.05003600	4.95909600	-1.33309400
H	-0.45226100	4.33170300	-2.13156000
H	-0.34202300	5.99838000	-1.51354200
H	1.04091200	4.90412400	-1.37108400
C	-2.10719700	4.72164300	0.09335700
H	-2.60764300	4.19092600	-0.71909200
H	-2.53051200	4.38812900	1.04597000

H	-2.32694400	5.78868700	-0.01100400
C	0.25525700	-1.11651000	0.91742400
C	0.87094500	-1.76490500	-0.08143800
C	2.22118400	-2.43836800	-0.16918400
C	0.68837900	-0.80240400	2.33219800
H	0.25534800	-1.57920400	2.97413400
H	2.10262800	-3.52739100	-0.24038900
O	0.11120000	0.41706500	2.79750100
H	0.30024200	1.10972200	2.13730800
C	2.18890800	-0.82168800	2.56406800
C	2.77146600	-1.85808600	3.29881500
C	3.00981700	0.17706200	2.02845700
C	4.15520500	-1.91997000	3.47214600
H	2.13729200	-2.63227500	3.72458200
C	4.39107100	0.11597300	2.19744700
H	2.58001800	0.98444300	1.44944800
C	4.97011800	-0.93463700	2.91454500
H	4.59436500	-2.73553700	4.03946600
H	5.01750000	0.88641100	1.75792000
H	6.04786300	-0.98223400	3.03940200
H	2.74670500	-2.10867600	-1.07177200
H	2.84302500	-2.22792700	0.69623500
C	6.08494200	-1.93751300	-2.04895600
C	5.19822500	-0.82026200	-1.52301700
H	5.56599900	-2.89910400	-1.98416800
H	6.33764000	-1.76011200	-3.09900300
H	7.01395100	-2.00326700	-1.47275500
H	5.74729300	0.13572900	-1.55423500
H	4.94423500	-1.00670800	-0.46894300
O	4.03006300	-0.75613000	-2.32611500
H	3.41784700	-0.13016500	-1.88863200
C	3.92569200	2.57125600	-2.24314800
C	2.56714300	2.38931900	-1.58850900
H	4.72179700	2.52601700	-1.49324500
H	4.10495500	1.78283500	-2.97899700
H	3.97816600	3.54270000	-2.74478800
H	1.76455200	2.46185900	-2.33177000
H	2.40725500	3.16675500	-0.82944600
O	2.53607000	1.10399400	-0.95872100
H	1.63678300	0.93308100	-0.62588200

I-a1$_{2a}$

N	-0.06416900	-1.48678200	0.41976000
C	-0.07441700	-0.36007600	2.43900300

C	0.44686400	0.03004700	3.67448500
H	1.37252400	-0.42648000	4.01255400
C	-0.22876800	0.98131800	4.43509800
H	0.16867200	1.29778700	5.39450800
C	-1.41633300	1.53488900	3.94980300
H	-1.93854300	2.29077100	4.53051300
C	-1.93319700	1.14101900	2.71196400
H	-2.83777800	1.61461000	2.34229300
C	-1.26867400	0.18222300	1.94911800
C	-3.14150500	-2.18565200	-0.94238200
C	-3.11566200	-2.47283900	0.47748200
C	-3.78183900	-1.40945500	1.16667900
C	-4.14263600	-0.41379100	0.19297400
C	-3.77921900	-0.92312700	-1.11059500
Rh	-1.90903700	-0.61348400	0.16298600
C	0.61636100	-1.36680700	1.59227100
O	1.65543300	-1.96886500	1.88983500
C	-4.06106800	-0.20355100	-2.39205100
H	-5.14180400	-0.13213200	-2.55878900
H	-3.65833500	0.81365600	-2.36596700
H	-3.62357000	-0.71722900	-3.24950000
C	-2.62421700	-3.10360800	-2.00753200
H	-3.26537800	-3.98761200	-2.10783000
H	-2.59099600	-2.60863500	-2.98039600
H	-1.61414100	-3.44481800	-1.77112000
C	-2.54595800	-3.71566500	1.08811600
H	-3.26680900	-4.54070200	1.03380500
H	-1.63649400	-4.01971100	0.56616900
H	-2.28919100	-3.55960300	2.13757800
C	-4.09630400	-1.37669800	2.62793400
H	-5.07687600	-1.83337300	2.81035900
H	-3.35177800	-1.92689700	3.20624400
H	-4.11720000	-0.35672600	3.01328300
C	-4.92609900	0.83986700	0.43391100
H	-5.99425000	0.68167300	0.23837100
H	-4.82769100	1.17817500	1.46724100
H	-4.58500400	1.64831000	-0.21839400
O	0.40314200	-2.56898600	-0.37292100
C	1.56279800	-2.31618400	-1.03307300
O	2.02558400	-1.20355100	-1.18579700
C	2.21379800	-3.59730100	-1.54052700
C	2.84597800	-4.28996300	-0.31112000
H	2.09099600	-4.51827600	0.44323600
H	3.33045400	-5.21837600	-0.63129700

H	3.59427400	-3.64277500	0.15017700
C	1.16773000	-4.52426100	-2.18663900
H	0.66665600	-4.03583200	-3.02946600
H	1.66428400	-5.42235400	-2.56698600
H	0.40916600	-4.83412400	-1.46447800
C	3.30498700	-3.22318100	-2.55342500
H	2.87861700	-2.72669000	-3.43069400
H	4.03593800	-2.54667700	-2.10652400
H	3.81891600	-4.12968700	-2.88849200
C	-0.99562000	0.50272600	-1.46623400
C	-1.25823500	1.33181000	-0.56774900
C	-1.17607800	2.72510000	-0.03626200
O	-0.12657600	2.89829600	0.87655300
H	0.61362500	2.30214000	0.62464800
C	-0.50368700	0.02390200	-2.76354500
H	-0.35770700	0.88940900	-3.42025700
H	0.45609200	-0.48148800	-2.64243500
H	-1.20574500	-0.66592200	-3.23876700
H	-2.10659200	2.96980300	0.49106000
C	-1.05643500	3.61911800	-1.26838100
C	-2.18486700	4.22830200	-1.81996300
C	0.18663400	3.77093400	-1.89382300
C	-2.08044100	4.98409700	-2.98920700
H	-3.14866400	4.11621100	-1.32756600
C	0.29036400	4.52380100	-3.06233800
H	1.06120800	3.29756800	-1.45775900
C	-0.84156400	5.13070600	-3.61419900
H	-2.96217500	5.46162800	-3.40703500
H	1.25720700	4.64075600	-3.54355800
H	-0.75621100	5.71942600	-4.52282000
C	2.96911300	1.11391700	1.04001600
H	2.60207900	0.49942900	1.87041400
O	1.91668200	1.26492100	0.06555900
H	1.74915000	0.38216000	-0.32541000
C	4.17042600	0.41316800	0.42667700
C	4.54399000	-0.85473700	0.87616800
C	4.86520100	1.00666300	-0.63168400
C	5.61553600	-1.52088500	0.27682100
H	3.96906900	-1.32692400	1.66645700
C	5.92635600	0.33762600	-1.23645200
H	4.56322000	1.99151200	-0.97495300
C	6.30607300	-0.92871800	-0.78126000
H	5.90635400	-2.50506200	0.63338400
H	6.46158800	0.80178400	-2.05999200

H	7.13713500	-1.44856200	-1.24948400
C	3.28707400	2.45011800	1.54333500
C	3.51977700	3.56040200	1.95874600
C	3.78510100	4.90386500	2.45871200
H	2.96117500	5.58003800	2.20516400
H	3.89375900	4.90673800	3.54906100
H	4.70446500	5.31814100	2.02970300

TS-a1$_{2a}$

N	-0.50484900	1.33727300	-0.59787900
C	-0.30044900	-0.27002900	-2.24992900
C	0.09263800	-0.66146600	-3.52761300
H	0.89166400	-0.10723700	-4.01028700
C	-0.55649900	-1.72002800	-4.16243100
H	-0.24930200	-2.03110900	-5.15605900
C	-1.61128900	-2.37329200	-3.51858500
H	-2.12555700	-3.19287700	-4.01284700
C	-1.99496300	-1.99485900	-2.23231600
H	-2.78036000	-2.54694000	-1.72450900
C	-1.33691200	-0.94727600	-1.57051200
C	-3.57169000	1.81983200	0.84807800
C	-3.65574700	1.98167200	-0.60432700
C	-4.20871600	0.79926400	-1.15745700
C	-4.42238500	-0.13239700	-0.06757900
C	-4.09375600	0.52977000	1.16471400
Rh	-2.23694100	0.33167500	-0.09467100
C	0.28359700	0.95419900	-1.62751300
O	1.31230200	1.52479500	-2.02005900
C	-4.29690500	-0.04869100	2.53045300
H	-5.35951000	-0.02617900	2.80121200
H	-3.96441000	-1.08932200	2.57935600
H	-3.75252400	0.51610300	3.28954100
C	-3.13007500	2.87529700	1.81415900
H	-3.96322900	3.52981600	2.10054200
H	-2.72293300	2.42941000	2.72510000
H	-2.34723000	3.49765300	1.37822900
C	-3.23115100	3.21333800	-1.34156800
H	-4.00217000	3.99043300	-1.27329900
H	-2.30477900	3.61418900	-0.92486100
H	-3.05254500	3.00292600	-2.39764700
C	-4.49341400	0.51591700	-2.59917800
H	-5.57326500	0.47039900	-2.78377100
H	-4.07515400	1.29060600	-3.24444800
H	-4.05622000	-0.43848000	-2.90747500

C	-5.06490500	-1.48068200	-0.18260800
H	-6.14626200	-1.41319500	-0.00672100
H	-4.91952000	-1.90434200	-1.17827800
H	-4.65516100	-2.18226000	0.54891100
O	-0.07431500	2.53461400	0.02807500
C	1.04748200	2.42404900	0.78028200
O	1.57109100	1.36797300	1.07550100
C	1.56608400	3.79610300	1.20009400
C	2.08248500	4.50192000	-0.07363300
H	1.27894300	4.63796700	-0.80043900
H	2.48824700	5.48270700	0.19623700
H	2.87228200	3.91466500	-0.54555500
C	0.43054800	4.62187600	1.83428200
H	0.00494800	4.11244300	2.70540500
H	0.82474700	5.58695600	2.16771400
H	-0.37147800	4.81010400	1.11709300
C	2.71251000	3.60037800	2.20121400
H	2.36404200	3.09175100	3.10499300
H	3.51609800	3.00283600	1.76797700
H	3.11553800	4.57658300	2.48894900
C	-1.05052000	-0.70310200	1.21593600
C	-0.87078000	-1.56178800	0.27942100
C	-0.34195800	-2.96654600	0.05667200
O	0.68797800	-3.02986400	-0.88334500
H	1.31986400	-2.30320900	-0.68468300
C	-0.69175800	-0.42194200	2.62428700
H	-0.30841200	-1.32147200	3.11561200
H	0.09111800	0.34178600	2.64106100
H	-1.54927500	-0.04480300	3.18725500
H	-1.15917700	-3.58448800	-0.33180500
C	0.03731300	-3.49098300	1.44046900
C	-0.94614200	-4.06474500	2.25247500
C	1.33743200	-3.34774000	1.93296600
C	-0.64082200	-4.48877800	3.54500400
H	-1.95751400	-4.17663900	1.86759900
C	1.64282100	-3.77117500	3.22757700
H	2.09737300	-2.88944500	1.31050500
C	0.65801100	-4.33977000	4.03726900
H	-1.41118600	-4.93807400	4.16522500
H	2.65434100	-3.65311900	3.60534900
H	0.90036900	-4.66849000	5.04357900
C	3.33858800	-0.60716300	-1.08123400
H	2.83591000	-0.14652100	-1.93900700
O	2.34601200	-0.99275300	-0.11175700

H	1.94190800	-0.17732800	0.25217700
C	4.29914400	0.41606700	-0.49690700
C	4.48913800	1.64173300	-1.13740700
C	4.97945500	0.14600900	0.69456900
C	5.37063400	2.58397000	-0.60224100
H	3.92320500	1.86024100	-2.03704300
C	5.84994200	1.08969000	1.23499400
H	4.81457900	-0.80449200	1.19227400
C	6.05236100	2.31045900	0.58403100
H	5.51646900	3.53465400	-1.10714700
H	6.37380100	0.87519300	2.16210900
H	6.73375100	3.04498400	1.00349200
C	4.02534400	-1.82708300	-1.50804500
C	4.57234100	-2.84242600	-1.86864000
C	5.22608200	-4.07232700	-2.29971300
H	4.64054400	-4.94872100	-2.00044000
H	5.33521400	-4.10287000	-3.38964200
H	6.22528900	-4.17070200	-1.86057100

II-a1$_{2a}$

N	0.54489700	-1.30959300	-0.53482600
C	0.78747100	0.24151500	-2.22590200
C	1.21509300	-0.00273700	-3.54381400
H	0.82915200	-0.88158600	-4.04996500
C	2.09424300	0.85811800	-4.18372700
H	2.41175400	0.65437000	-5.20187200
C	2.56300100	1.99839500	-3.51260700
H	3.24905900	2.67914600	-4.00798200
C	2.13073100	2.26566600	-2.22397100
H	2.47331300	3.16030400	-1.71301700
C	1.23209700	1.41053600	-1.54170900
C	3.47763900	-1.47927000	1.31682100
C	3.73860800	-2.15332200	0.03219200
C	4.33955000	-1.22835400	-0.82437200
C	4.48962200	0.03634700	-0.08908500
C	4.06770500	-0.15833200	1.25240200
Rh	2.30567000	-0.35653100	-0.05880800
C	-0.10032500	-0.83354500	-1.60886700
O	-1.14826200	-1.23438900	-2.12317500
C	4.22994200	0.80491700	2.38628500
H	5.24336100	0.73807500	2.80108600
H	4.06617700	1.83577600	2.06321000
H	3.52614400	0.59256800	3.19204800
C	2.96264900	-2.15929000	2.54486900

H	3.77288300	-2.68042700	3.07153000
H	2.51908400	-1.44076600	3.23740200
H	2.19918700	-2.89661500	2.29104500
C	3.31421800	-3.55630700	-0.26911900
H	3.90096200	-4.27450900	0.31570500
H	2.25892000	-3.70147100	-0.02247500
H	3.44327800	-3.79409300	-1.32669000
C	4.70800700	-1.39836300	-2.26464000
H	5.79212600	-1.31366100	-2.40573600
H	4.39355800	-2.37206300	-2.64506600
H	4.23318000	-0.63071300	-2.88529700
C	5.14304000	1.26069900	-0.64835800
H	6.23513600	1.15328100	-0.63634500
H	4.83388600	1.43407400	-1.68163900
H	4.88484300	2.14744700	-0.06576800
O	-0.02594300	-2.44725000	0.08656000
C	-1.07333600	-2.21142600	0.91481000
O	-1.51067900	-1.10784100	1.16144900
C	-1.59311100	-3.51698500	1.51596800
C	-1.93019100	-4.50317800	0.37966300
H	-1.04399900	-4.74770300	-0.20986600
H	-2.33220400	-5.42667300	0.80901000
H	-2.68283800	-4.07901900	-0.28794100
C	-0.49110600	-4.11220000	2.41743100
H	-0.20258300	-3.41019800	3.20686600
H	-0.86358200	-5.02310300	2.89650700
H	0.39821400	-4.37145100	1.83704600
C	-2.84652300	-3.20406000	2.34341300
H	-2.61933600	-2.50652200	3.15362900
H	-3.62553800	-2.75702700	1.72420000
H	-3.23598900	-4.12972900	2.77881800
C	1.06917000	0.99779300	0.80936900
C	0.71529800	1.82496400	-0.18301300
C	-0.08645800	3.13189900	-0.19541600
O	-1.20001700	3.02678100	-1.05177500
H	-1.75672000	2.28224600	-0.73153800
C	0.70058300	0.96423200	2.25776400
H	-0.26492800	1.43649200	2.44504900
H	0.63796600	-0.07067700	2.60438400
H	1.44420200	1.48567900	2.87028200
H	0.56251900	3.88222800	-0.67102200
C	-0.40999000	3.66163200	1.19182900
C	0.61231000	4.22577500	1.96355500
C	-1.69979800	3.58613200	1.72332900

C	0.36259200	4.68152800	3.25620800
H	1.61484100	4.29607200	1.54656900
C	-1.95117600	4.03925900	3.02011600
H	-2.49632800	3.15217700	1.13052100
C	-0.92386300	4.58328100	3.79202500
H	1.16640300	5.11625200	3.84405800
H	-2.95553000	3.96659500	3.42781000
H	-1.12400500	4.93537600	4.79982300
C	-3.54659600	0.47801400	-1.15383500
H	-2.89215500	0.12456400	-1.95873800
O	-2.73687600	1.00129800	-0.08385200
H	-2.21144400	0.26504200	0.28894200
C	-4.39197600	-0.69332600	-0.67770100
C	-4.31288500	-1.92661900	-1.32764200
C	-5.25840600	-0.53986300	0.41021000
C	-5.11703100	-2.99138000	-0.91157100
H	-3.60713900	-2.04942100	-2.14272400
C	-6.05082100	-1.60474600	0.83277200
H	-5.30138300	0.41960600	0.91588600
C	-5.98770800	-2.83287800	0.16672300
H	-5.05836900	-3.94560500	-1.42751800
H	-6.72127300	-1.47912200	1.67815400
H	-6.60988800	-3.66154000	0.49217900
C	-4.38073100	1.57547300	-1.64670400
C	-5.06183100	2.48278900	-2.06232100
C	-5.87394500	3.58545600	-2.56270300
H	-5.41517300	4.54964900	-2.31695500
H	-5.97925000	3.53680600	-3.65238600
H	-6.88024900	3.57268000	-2.12880800

I-a1i$_{2a}$

N	-0.80098300	1.34860700	-0.52510500
C	-0.08285500	0.15523500	-2.37552800
C	0.66674200	-0.05167400	-3.53551100
H	1.29559500	0.75742500	-3.89524500
C	0.59035800	-1.27829700	-4.19250600
H	1.17223400	-1.45477200	-5.09197100
C	-0.23172400	-2.28494700	-3.67826800
H	-0.28209800	-3.24978300	-4.17619500
C	-0.98285500	-2.06966100	-2.51904800
H	-1.58837900	-2.87954900	-2.12350400
C	-0.92095900	-0.84111500	-1.86258500
C	-3.94058900	0.59211700	0.64245200
C	-3.92757500	0.73469300	-0.79848500

C	-3.94102400	-0.57229600	-1.38285400
C	-3.88241200	-1.53336600	-0.31314400
C	-3.92301900	-0.80412500	0.93300000
Rh	-2.02126800	-0.27893600	-0.21559400
C	-0.03030100	1.44778200	-1.64476100
O	0.62759500	2.43785400	-1.98366200
C	-3.96987500	-1.45600300	2.27949100
H	-4.89231100	-2.03795200	2.38589000
H	-3.12699000	-2.13979100	2.41872800
H	-3.94583200	-0.72036000	3.08486000
C	-4.01593800	1.73193300	1.61178200
H	-5.01361100	2.18716100	1.60702300
H	-3.80536800	1.40425200	2.63178300
H	-3.29067500	2.50669100	1.35333500
C	-3.96418200	2.03983300	-1.53083900
H	-4.99220100	2.41665900	-1.59749800
H	-3.35664100	2.78792100	-1.01803400
H	-3.57634200	1.93562700	-2.54588300
C	-4.05583800	-0.87127500	-2.84339500
H	-5.11158500	-0.89784400	-3.13983300
H	-3.55163300	-0.11124600	-3.44324300
H	-3.60560400	-1.83217000	-3.09396200
C	-3.96711100	-3.02374500	-0.43577900
H	-5.00118400	-3.37041800	-0.31391500
H	-3.62028500	-3.36311400	-1.41360900
H	-3.35938400	-3.51775400	0.32685900
O	-1.01888300	2.61626100	0.08359400
C	0.00198800	3.04466600	0.86347500
O	0.88392600	2.32295400	1.28649100
C	-0.04529500	4.54722500	1.11082000
C	0.86912800	5.14954900	0.01445100
H	0.50173000	4.89185600	-0.98086300
H	0.89957400	6.23850100	0.12593500
H	1.88315600	4.75084700	0.10194600
C	-1.46456400	5.12270400	0.99035400
H	-2.14221600	4.67557900	1.72551300
H	-1.43430600	6.20090500	1.17628700
H	-1.87884900	4.95810100	-0.00608400
C	0.54002900	4.83389500	2.50206600
H	-0.10051900	4.42996700	3.29361800
H	1.52856000	4.38244200	2.60373500
H	0.62407000	5.91450700	2.65274400
C	-0.84346300	-0.64582800	1.57929600
C	-0.53624300	-1.54325900	0.76438700

C	0.34369400	-2.69234000	0.39193000
O	1.38444300	-2.31891500	-0.46995400
H	1.70639700	-1.42467900	-0.21866400
C	-0.80325900	0.09119000	2.84770800
H	-0.17583000	-0.47010700	3.55009800
H	-0.35832300	1.07702800	2.70433900
H	-1.79816700	0.20905200	3.28490600
H	-0.24687300	-3.45152500	-0.13442400
C	0.83249700	-3.27275400	1.71714900
C	0.17802000	-4.35853900	2.30181300
C	1.90241500	-2.66793300	2.38780000
C	0.58242100	-4.84154500	3.54771400
H	-0.64812400	-4.83256400	1.77588100
C	2.30461100	-3.14975000	3.63264800
H	2.41379800	-1.82611400	1.93048900
C	1.64623400	-4.23536100	4.21692200
H	0.07246700	-5.69219000	3.99092600
H	3.13749600	-2.67927700	4.14730600
H	1.96511400	-4.60990500	5.18519100
C	3.22769100	0.86632100	-0.52625900
H	2.69271100	1.26353900	-1.39845200
O	2.27807900	0.15941600	0.30445100
H	1.61145800	0.80986500	0.60782600
C	4.25052800	-0.15440300	-0.99398300
C	3.88084000	-1.06028200	-1.99427700
C	5.52026200	-0.24799000	-0.42032200
C	4.77042200	-2.04745900	-2.41309600
H	2.88928700	-1.00405600	-2.43083800
C	6.41371300	-1.23263700	-0.84340300
H	5.80433500	0.46042500	0.35106100
C	6.04077100	-2.13480900	-1.84038300
H	4.46947400	-2.74909100	-3.18542200
H	7.40039800	-1.29550300	-0.39325900
H	6.73589100	-2.90225600	-2.16878200
C	3.80607400	2.00387600	0.19733000
C	4.23049900	2.96506200	0.79513600
C	4.73270000	4.12734700	1.51939800
H	5.59867600	4.56737200	1.01205800
H	3.96496300	4.90554800	1.59960000
H	5.04324200	3.85983300	2.53566400

TS-a1i$_{2a}$

N	-0.84805000	1.23716600	-0.75808300
C	-0.09236900	-0.48420000	-2.10935100

C	0.48655200	-0.93792700	-3.29284700
H	1.14330900	-0.26303600	-3.83328400
C	0.19915900	-2.22049300	-3.76033300
H	0.65359200	-2.58060100	-4.67815000
C	-0.68389800	-3.03779800	-3.04793700
H	-0.91571200	-4.03448700	-3.41298500
C	-1.25709000	-2.58796200	-1.85859100
H	-1.90633300	-3.24802800	-1.29077700
C	-0.96208900	-1.30852900	-1.36493100
C	-4.04361900	1.09785600	0.40522600
C	-4.02829300	0.97066800	-1.05282700
C	-4.20481500	-0.39453600	-1.38612200
C	-4.27564800	-1.14141000	-0.14472700
C	-4.25149200	-0.20545100	0.94650100
Rh	-2.28930200	-0.11948500	-0.16420100
C	0.10030700	0.92903100	-1.67203900
O	0.97615300	1.68988600	-2.10923200
C	-4.44888800	-0.56260500	2.38660000
H	-5.51304900	-0.72829500	2.59482900
H	-3.91475900	-1.47919100	2.65105800
H	-4.10456700	0.23356300	3.04939100
C	-3.98303600	2.39693500	1.14855700
H	-4.94705200	2.91994500	1.11138700
H	-3.72670900	2.24207200	2.19939500
H	-3.22582300	3.05412500	0.71551200
C	-3.87023900	2.12535100	-1.99230100
H	-4.80945500	2.68580800	-2.07508600
H	-3.09608500	2.80894800	-1.63727800
H	-3.58522500	1.79249600	-2.99202200
C	-4.27468000	-0.98942400	-2.75722400
H	-5.30053800	-1.28994200	-3.00181000
H	-3.94366700	-0.27572400	-3.51393600
H	-3.63467700	-1.87232400	-2.84033500
C	-4.53593900	-2.61127100	-0.02014000
H	-5.60878500	-2.80994000	0.09850400
H	-4.19803000	-3.14851400	-0.90846600
H	-4.02347200	-3.03418100	0.84804300
O	-0.78830600	2.59169100	-0.33674900
C	0.23221800	2.88510300	0.50329600
O	0.91271500	2.05059300	1.06825300
C	0.46964900	4.38653800	0.61007700
C	1.44764600	4.71785700	-0.54519400
H	1.01955900	4.43768500	-1.50986400
H	1.66073200	5.79212800	-0.54017100

H	2.38434600	4.16727400	-0.42521400
C	-0.82924400	5.19327300	0.45398400
H	-1.55435300	4.93700300	1.23389200
H	-0.60580900	6.26120000	0.54217400
H	-1.29337500	5.01977300	-0.51883700
C	1.13504100	4.68316200	1.96185900
H	0.45603700	4.47220600	2.79478200
H	2.02806200	4.06934400	2.09008300
H	1.41515800	5.74005800	2.01098900
C	-1.00410400	-0.58805600	1.36238000
C	-0.49688300	-1.47609900	0.58830300
C	0.43962000	-2.66933000	0.60991400
O	1.52069200	-2.54312200	-0.26450400
H	1.91608600	-1.65216500	-0.14100100
C	-0.89036500	-0.03201500	2.72937600
H	-0.25280500	-0.66445700	3.35446600
H	-0.44036400	0.96256900	2.66871800
H	-1.87128600	0.06309600	3.20116500
H	-0.11999900	-3.55361000	0.28646600
C	0.83214700	-2.85861400	2.07357000
C	0.01606300	-3.62753200	2.90914700
C	1.95599500	-2.22078500	2.60761900
C	0.31276400	-3.76048500	4.26492800
H	-0.85761700	-4.12400900	2.49241600
C	2.25232200	-2.35396200	3.96514000
H	2.58171900	-1.60713400	1.96888100
C	1.43408900	-3.12012100	4.79725500
H	-0.32502500	-4.36532800	4.90316100
H	3.12550900	-1.85352000	4.37347000
H	1.66975900	-3.22148000	5.85255100
C	3.46280000	0.65680400	-0.57986400
H	2.91858500	1.07351900	-1.43683400
O	2.50281900	-0.03004600	0.25476000
H	1.82443600	0.62159500	0.52737100
C	4.44672300	-0.38607600	-1.08058100
C	3.98166500	-1.35578900	-1.97756800
C	5.77771300	-0.42590400	-0.66216300
C	4.83530800	-2.35321300	-2.44211500
H	2.94488300	-1.33909800	-2.29670600
C	6.63646700	-1.42023700	-1.13423100
H	6.13668700	0.32905900	0.02963900
C	6.16752300	-2.38662900	-2.02375800
H	4.45981800	-3.10452900	-3.13056500
H	7.67105300	-1.44041800	-0.80362500

H	6.83490700	-3.16196400	-2.38891700
C	4.07958900	1.76950700	0.15052200
C	4.53846700	2.71873600	0.74323200
C	5.08899300	3.86575600	1.45738400
H	6.05768500	4.16359400	1.04069800
H	4.41893500	4.73051800	1.39339100
H	5.23927300	3.63829500	2.51868500

II-a1i$_{2a}$

N	-0.62427800	1.15140400	-0.62992100
C	-0.68946800	-0.61217000	-2.13640500
C	-1.13783000	-0.66045200	-3.46859400
H	-0.88100800	0.16787400	-4.12033500
C	-1.87671600	-1.73698600	-3.93692900
H	-2.21460900	-1.75665200	-4.96865200
C	-2.18102600	-2.80164400	-3.07456700
H	-2.75837000	-3.64795600	-3.43477400
C	-1.71962900	-2.78077400	-1.76821500
H	-1.92325100	-3.61741500	-1.10658600
C	-0.95786200	-1.70154600	-1.25860200
C	-3.59814600	1.31478100	1.08227600
C	-3.95728000	1.61609500	-0.31392500
C	-4.41110200	0.43314400	-0.90176900
C	-4.37262900	-0.62849800	0.11652800
C	-3.98553400	-0.05332200	1.35706700
Rh	-2.27804200	0.06450300	-0.02308600
C	-0.00750100	0.68358700	-1.72657700
O	0.87465200	1.22490900	-2.40239000
C	-4.00760000	-0.72006200	2.69569800
H	-5.00815100	-0.64412900	3.13942600
H	-3.75388400	-1.77964100	2.61769100
H	-3.30078200	-0.25598300	3.38484200
C	-3.16584900	2.33426300	2.08672200
H	-4.03091600	2.87234600	2.49574600
H	-2.63311800	1.86890800	2.91845600
H	-2.50103000	3.06980200	1.62905900
C	-3.74727900	2.95098100	-0.95765500
H	-4.44974200	3.69255000	-0.55900300
H	-2.73287300	3.31320400	-0.77099800
H	-3.88718000	2.89845000	-2.03901900
C	-4.78491900	0.19272600	-2.32993300
H	-5.82825600	-0.13341700	-2.41251200
H	-4.66284800	1.09429100	-2.93295100
H	-4.15698800	-0.58971600	-2.76996200

C	-4.84325900	-2.03166500	-0.10726700
H	-5.93722600	-2.09013800	-0.04139100
H	-4.54717800	-2.39215100	-1.09504300
H	-4.42368800	-2.71078100	0.63816300
O	-0.32696900	2.51111900	-0.34610100
C	0.54715000	2.71890200	0.66533500
O	0.98560300	1.83880600	1.37876600
C	0.94145800	4.19226600	0.74679000
C	1.86780700	4.46529100	-0.46335300
H	1.37601400	4.20230900	-1.40257100
H	2.13132000	5.52796200	-0.48376000
H	2.78985900	3.88374500	-0.38127900
C	-0.30118300	5.09786400	0.67243200
H	-0.99213900	4.89413100	1.49770600
H	0.00809000	6.14500300	0.74809700
H	-0.83612100	4.96612300	-0.27039400
C	1.70450100	4.42370900	2.05720900
H	1.06332500	4.25179800	2.92718900
H	2.55638800	3.74498700	2.12660500
H	2.06448300	5.45680000	2.09430100
C	-0.88113900	-0.97709400	1.02295700
C	-0.37138000	-1.83258300	0.12926000
C	0.71432200	-2.90928800	0.23381900
O	1.80088900	-2.57857900	-0.60208700
H	2.11294300	-1.68537300	-0.34129400
C	-0.55981800	-0.72808100	2.46125700
H	0.46605300	-1.00814300	2.70684300
H	-0.68264600	0.33202200	2.69531600
H	-1.21857300	-1.30731200	3.11736900
H	0.28862700	-3.82371000	-0.20481200
C	1.10416800	-3.24761400	1.66278400
C	0.19438700	-3.92975000	2.47911900
C	2.34606500	-2.88208200	2.18647800
C	0.50424100	-4.21734100	3.80645700
H	-0.76947000	-4.22443500	2.06939800
C	2.65661300	-3.16555700	3.51826100
H	3.05339600	-2.35769900	1.55563400
C	1.73849400	-3.82835100	4.33330900
H	-0.21240900	-4.74556200	4.42938800
H	3.62133700	-2.86726000	3.91883900
H	1.98374800	-4.04785300	5.36837600
C	3.39301000	0.71665700	-0.47916800
H	2.71486700	1.29509000	-1.11731600
O	2.60686000	-0.14369600	0.37118500

H	1.91339700	0.40347300	0.78888800
C	4.21894300	-0.18750500	-1.37365100
C	3.71054500	-0.54938100	-2.62528500
C	5.43186100	-0.72568600	-0.93501400
C	4.41753000	-1.44110200	-3.43200300
H	2.76198700	-0.13191700	-2.95074500
C	6.13594600	-1.61743000	-1.74231000
H	5.82099300	-0.43396000	0.03575900
C	5.62935800	-1.97623000	-2.99318600
H	4.01969900	-1.72000200	-4.40341600
H	7.07863400	-2.03241000	-1.39710600
H	6.17788500	-2.67116600	-3.62271400
C	4.20151100	1.64356800	0.32466300
C	4.84285700	2.43159700	0.98166400
C	5.62175400	3.37802300	1.77302800
H	6.52222100	3.69593700	1.23568300
H	5.03809700	4.27555500	2.00725000
H	5.94043200	2.93192800	2.72172300

I-b1$_{2a}$

N	0.63303500	0.47718800	-1.11291000
C	0.30964300	2.59441300	-0.20566300
C	-0.25326000	3.87034000	-0.13256900
H	-0.88587400	4.20650400	-0.94586300
C	0.00504000	4.67481800	0.97436800
H	-0.43693800	5.66372700	1.04591000
C	0.82812100	4.19666000	1.99781400
H	1.02776900	4.81695500	2.86800400
C	1.39752200	2.92174600	1.91506100
H	2.02454000	2.56547500	2.72727300
C	1.14919900	2.11197400	0.80580200
C	3.69496900	-0.86811500	-0.53013900
C	3.80504100	0.55780600	-0.77249500
C	4.02928000	1.21076400	0.48615200
C	3.95815700	0.21803200	1.51952600
C	3.79680800	-1.06618300	0.87436100
Rh	1.97443300	0.26023700	0.44307100
C	0.06953700	1.70174900	-1.36779500
O	-0.55589800	2.00058400	-2.39001000
C	3.84681300	-2.38045500	1.58566700
H	4.87055200	-2.57761400	1.92656900
H	3.20253100	-2.38723900	2.46919600
H	3.54991600	-3.19980300	0.92943700
C	3.53773900	-1.94244900	-1.56396000

H	4.44212300	-2.55950400	-1.62556700
H	2.68340300	-2.58372700	-1.33159900
H	3.36285200	-1.50516600	-2.54697700
C	3.79195900	1.22656700	-2.11220600
H	4.80187700	1.26441900	-2.53839400
H	3.14346300	0.69355500	-2.80881100
H	3.41972700	2.25034800	-2.03319500
C	4.36297100	2.65755900	0.66073400
H	5.43995900	2.80539300	0.51267100
H	3.83185400	3.28159600	-0.06001100
H	4.10633700	3.01647900	1.65768400
C	4.19905000	0.41888100	2.98363700
H	5.24635800	0.22105200	3.24545100
H	3.97203500	1.44290200	3.28819700
H	3.57536000	-0.25365000	3.57856600
O	0.78374700	-0.26348300	-2.32617500
C	-0.28193600	-1.00557000	-2.65951400
O	-1.20365400	-1.25280300	-1.89383700
C	-0.25091600	-1.47764100	-4.10650500
C	-0.81006300	-2.90876100	-4.16081700
H	-1.80271300	-2.95227600	-3.70890600
H	-0.87964400	-3.23896900	-5.20178400
H	-0.15916000	-3.60535200	-3.62228100
C	-1.19066000	-0.50068600	-4.85597200
H	-0.85746000	0.53209800	-4.72640900
H	-1.19838300	-0.74923600	-5.92209900
H	-2.21040800	-0.57949300	-4.47040000
C	1.15582800	-1.42438700	-4.71960000
H	1.56017000	-0.41004500	-4.70789200
H	1.84762600	-2.08116900	-4.18470100
H	1.10707800	-1.76195000	-5.75956600
C	0.68027600	-1.29270000	1.27888400
C	0.42607700	-0.27705900	1.95867200
C	-0.34851900	0.50480000	2.93059600
C	0.51263500	-2.73459000	0.94083700
H	1.39452700	-3.27822500	1.28699700
H	0.28450400	1.11260300	3.58021100
O	0.46236000	-2.99134700	-0.45545800
H	-0.29730800	-2.50152100	-0.81719600
C	-0.69782300	-3.29725500	1.67801000
C	-0.60228700	-4.55448000	2.28358600
C	-1.91403600	-2.60424400	1.72188200
C	-1.70426100	-5.11804800	2.92675100
H	0.33960600	-5.09646400	2.24606900

C	-3.01399700	-3.16777700	2.36847100
H	-2.01186800	-1.62457400	1.26643900
C	-2.91427200	-4.42308000	2.97163800
H	-1.61727700	-6.09454500	3.39425500
H	-3.94619200	-2.61275200	2.39887900
H	-3.77205300	-4.85618100	3.47814800
H	-1.03804400	1.16061500	2.39355300
H	-0.93322600	-0.19261800	3.54039000
C	-3.27474300	0.56601400	-0.50570600
H	-2.99866200	0.63804800	-1.56429700
O	-2.07942600	0.36310900	0.26129700
H	-1.45992500	-0.11500600	-0.32003500
C	-3.86611400	1.89627700	-0.08265900
C	-3.50819000	3.04904200	-0.78765300
C	-4.69292100	2.00263000	1.03831800
C	-3.97263800	4.29729100	-0.37368000
H	-2.84717200	2.95844200	-1.64521800
C	-5.15460300	3.25094000	1.45509400
H	-4.97621500	1.10100700	1.57305000
C	-4.79574200	4.40118700	0.74904100
H	-3.69266400	5.18906200	-0.92760800
H	-5.79732200	3.32692900	2.32766400
H	-5.15902900	5.37303800	1.07094500
C	-4.19300500	-0.57185600	-0.34449300
C	-4.89267600	-1.55077200	-0.22037200
C	-5.71948500	-2.74513200	-0.08640300
H	-6.59828700	-2.55939900	0.54174500
H	-6.07613000	-3.09197300	-1.06275500
H	-5.14705100	-3.56076300	0.36971600

TS-b1$_{2a}$

N	-0.68289400	-0.01825000	-1.29344800
C	-0.39821100	-2.29938400	-0.96584100
C	-0.07204500	-3.57425400	-1.42331800
H	0.56050200	-3.66025800	-2.30080000
C	-0.58490200	-4.69924300	-0.77450100
H	-0.33032200	-5.69352900	-1.12855700
C	-1.43439900	-4.54494700	0.32583900
H	-1.84126600	-5.41962000	0.82575400
C	-1.74459600	-3.26866300	0.79783600
H	-2.35909200	-3.15339000	1.68625900
C	-1.22714700	-2.12996100	0.16324400
C	-3.65832800	1.33876500	-0.42418200
C	-3.88834800	0.17820800	-1.28818800

C	-4.28748800	-0.90927600	-0.47533400
C	-4.26755000	-0.46020900	0.90521000
C	-3.95258300	0.94509400	0.91354100
Rh	-2.19540100	-0.21026000	0.12951900
C	0.00799000	-1.09271600	-1.75055700
O	0.81796800	-1.11184700	-2.68753700
C	-3.98280900	1.84886200	2.10568300
H	-4.97089100	2.31757700	2.19399900
H	-3.79939900	1.29600300	3.03004100
H	-3.23367200	2.63720300	2.01799400
C	-3.30504400	2.71728500	-0.88824600
H	-4.20543500	3.30077800	-1.11979800
H	-2.73482000	3.24487500	-0.12090200
H	-2.69502700	2.67262900	-1.79230200
C	-3.73569100	0.18819700	-2.77693500
H	-4.62019700	0.63063600	-3.25137500
H	-2.86328400	0.77261200	-3.07521000
H	-3.60874200	-0.82140000	-3.17261200
C	-4.64295400	-2.28992100	-0.93000000
H	-5.72854900	-2.44231900	-0.90079000
H	-4.30521600	-2.46748300	-1.95274000
H	-4.17791000	-3.04984300	-0.29654800
C	-4.70993300	-1.26534700	2.08845500
H	-5.77755700	-1.11056100	2.29042400
H	-4.56048400	-2.33314300	1.91584300
H	-4.15904800	-0.98870800	2.99115100
O	-0.50553200	1.10634800	-2.15655200
C	0.36986800	2.02269200	-1.72459000
O	0.84192100	2.02721900	-0.59603700
C	0.77706500	3.00071600	-2.81786900
C	1.29485100	4.28974600	-2.16524200
H	2.09763200	4.06531300	-1.46035800
H	1.67733400	4.96410700	-2.93741100
H	0.49872600	4.80927200	-1.62203100
C	1.92801400	2.28622300	-3.57327100
H	1.60437500	1.30893900	-3.94029900
H	2.24122500	2.90465900	-4.42060900
H	2.78765800	2.14194900	-2.91268300
C	-0.38099000	3.29846700	-3.78380700
H	-0.73827600	2.38896000	-4.27041300
H	-1.22228100	3.76972600	-3.26523700
H	-0.03546800	3.99059100	-4.55778000
C	-0.84635100	0.24852600	1.60475700
C	-0.42196300	-0.95822100	1.61870800

C	0.52432400	-1.90720100	2.25077600
C	-0.63109400	1.52417200	2.37735500
H	-1.43337200	1.58441600	3.12102900
H	0.00742800	-2.72576400	2.75788700
O	-0.78341300	2.67584000	1.56700600
H	-0.23040400	2.53820000	0.77739000
C	0.69119500	1.46036300	3.12852800
C	0.70203000	0.99979000	4.44899400
C	1.90441500	1.76487200	2.50265100
C	1.90561200	0.83384900	5.13560100
H	-0.23929500	0.76242400	4.93986600
C	3.10720500	1.59289100	3.18481800
H	1.92221000	2.11845500	1.48011300
C	3.11361500	1.12658900	4.50060500
H	1.89908500	0.47676900	6.16137600
H	4.03987500	1.80045900	2.66996200
H	4.05333700	0.98955100	5.02745200
H	1.21179900	-2.31167100	1.50625000
H	1.10258200	-1.33215400	2.98115700
C	3.20237300	-0.18022700	-0.77153200
H	2.73653200	-0.10515900	-1.76260200
O	2.18147500	-0.40259100	0.20519000
H	1.51106400	0.28942200	0.07959800
C	4.08063500	-1.41652900	-0.77099600
C	3.69421200	-2.50489900	-1.56097900
C	5.20650400	-1.52204000	0.04766900
C	4.43261300	-3.68727700	-1.53175200
H	2.81224200	-2.40625400	-2.18746400
C	5.94548200	-2.70520500	0.07601500
H	5.50118700	-0.67182800	0.65518900
C	5.55987700	-3.79003100	-0.71337600
H	4.13138600	-4.52828500	-2.15022700
H	6.82228700	-2.78055100	0.71306100
H	6.13700500	-4.71023400	-0.69301900
C	3.92520300	1.07438300	-0.50203600
C	4.43404400	2.14910600	-0.27624000
C	5.04133500	3.44523300	0.00853600
H	6.13550700	3.38696600	-0.00267800
H	4.74018900	4.19692700	-0.72991700
H	4.73658600	3.81158300	0.99562400

II-b1$_{2a}$

N	0.22563100	0.49321500	-0.82074700
C	0.71644700	2.31775500	0.61411600

C	1.19540800	3.63718600	0.46251700
H	0.90376100	4.16796300	-0.43655200
C	1.99018700	4.23553200	1.42429500
H	2.34435000	5.25209000	1.28320200
C	2.32642300	3.52180100	2.58586600
H	2.94994600	3.97890100	3.34854000
C	1.83776200	2.24004300	2.76745000
H	2.07029700	1.69804900	3.67876700
C	1.01201300	1.59649600	1.81045000
C	3.34415100	-1.04619300	-1.28720300
C	3.55131600	0.31941800	-1.78222600
C	4.11485200	1.06631200	-0.74188100
C	4.29806300	0.18161700	0.41822500
C	3.92182000	-1.13662400	0.03902700
Rh	2.13620300	0.14170800	0.02305400
C	-0.05292000	1.80966400	-0.59344500
O	-0.72777700	2.56344200	-1.29353800
C	4.13705200	-2.39819500	0.81083200
H	5.09451700	-2.84922400	0.52061200
H	4.17354200	-2.20668500	1.88546000
H	3.33815800	-3.11248100	0.60960900
C	2.89183400	-2.19690300	-2.12552400
H	3.74412900	-2.62217800	-2.67210500
H	2.44397800	-2.97242400	-1.50480500
H	2.15391900	-1.87669000	-2.86384400
C	3.15622200	0.78913300	-3.14695100
H	3.78914600	0.32800500	-3.91442000
H	2.11977400	0.52455500	-3.36580700
H	3.24911100	1.87292400	-3.23967800
C	4.45508900	2.52121000	-0.73127200
H	5.54245800	2.65993000	-0.69799100
H	4.07357600	3.03106700	-1.61756600
H	4.03213200	3.01899900	0.14641800
C	4.93686800	0.60031000	1.70507900
H	6.02792300	0.65290200	1.59943300
H	4.58261100	1.58624900	2.01636600
H	4.70831200	-0.10592800	2.50595100
O	-0.14427700	0.18586400	-2.17058900
C	-0.64655400	-1.04382400	-2.37476300
O	-0.68005600	-1.92555800	-1.53773800
C	-1.18596700	-1.16880200	-3.80201000
C	-1.66407700	-2.60911400	-4.02055500
H	-2.43778900	-2.87509300	-3.29849500
H	-2.07595900	-2.70882400	-5.02945400

H	-0.84276100	-3.32239000	-3.90821200
C	-2.36268100	-0.17908700	-3.95502700
H	-2.03684700	0.84639200	-3.76562500
H	-2.75823800	-0.24100100	-4.97399100
H	-3.16781100	-0.42250000	-3.25689600
C	-0.08019100	-0.81355700	-4.81587500
H	0.24439200	0.22289700	-4.70175700
H	0.79073300	-1.46886200	-4.70693500
H	-0.46641200	-0.94053100	-5.83209200
C	0.99506600	-0.76316600	1.46787800
C	0.47927600	0.23327500	2.20246800
C	-0.45434800	0.21908600	3.39429700
C	0.86143200	-2.26552800	1.61453600
H	1.70051500	-2.60388900	2.23652700
H	-0.11064900	0.92787900	4.15562000
O	1.03700300	-2.93499300	0.36825000
H	0.42762400	-2.52314700	-0.27368100
C	-0.42030000	-2.71884700	2.29074200
C	-0.38130800	-3.35085900	3.53635600
C	-1.65953500	-2.49488400	1.68063500
C	-1.56169200	-3.72887500	4.17983000
H	0.57903100	-3.53555800	4.01223700
C	-2.83850000	-2.86247700	2.32294600
H	-1.70908600	-2.02812300	0.70532200
C	-2.79445500	-3.47712900	3.57692000
H	-1.51742300	-4.21551800	5.15006100
H	-3.78891000	-2.64578000	1.84606300
H	-3.71488500	-3.75792000	4.08055000
H	-1.45418400	0.53397600	3.07608500
H	-0.53540400	-0.76601500	3.84821400
C	-3.19384400	0.68421100	-0.28504000
H	-2.61061400	1.04543700	-1.14248900
O	-2.33874500	0.62310300	0.86383500
H	-1.52390500	0.16678900	0.59612000
C	-4.25978100	1.72480900	0.00306100
C	-3.88977100	3.07409000	-0.05534200
C	-5.56416900	1.38145100	0.35924100
C	-4.82136600	4.06680300	0.24090100
H	-2.87192100	3.32866200	-0.33734300
C	-6.49748300	2.37697800	0.65441300
H	-5.84461200	0.33348800	0.39688400
C	-6.12788200	3.72068000	0.59641300
H	-4.53094300	5.11240500	0.19034200
H	-7.51196500	2.10233700	0.92928200

H	-6.85441700	4.49574000	0.82361200
C	-3.71771700	-0.65113400	-0.61348600
C	-4.03996300	-1.78941800	-0.86784500
C	-4.37576800	-3.18005600	-1.15225400
H	-5.16927200	-3.54590300	-0.49153700
H	-4.71708300	-3.30712100	-2.18562000
H	-3.49664200	-3.81721400	-1.00509500

I-b1i$_{2a}$

N	-0.71734200	0.59580500	-1.13086700
C	-0.74575600	-1.56185300	-1.97749600
C	-0.34650600	-2.58764300	-2.83513200
H	0.35359100	-2.35368300	-3.63083200
C	-0.84937900	-3.87397600	-2.64970500
H	-0.54527200	-4.68060200	-3.30994500
C	-1.74662100	-4.11872300	-1.60666100
H	-2.14194700	-5.12005400	-1.45448700
C	-2.13681200	-3.08625200	-0.74614100
H	-2.81294700	-3.30855300	0.07427700
C	-1.64058700	-1.79437600	-0.92474600
C	-3.46907900	1.65424400	0.51637600
C	-3.84293700	0.92028200	-0.67948800
C	-4.29882500	-0.38087100	-0.28503700
C	-4.12068000	-0.49949300	1.13485000
C	-3.65141200	0.78017900	1.62291200
Rh	-2.10516800	-0.13517800	0.21171700
C	-0.25594100	-0.17173700	-2.15790200
O	0.46842100	0.22327200	-3.08051300
C	-3.47492200	1.11709400	3.06903700
H	-4.45490000	1.20982800	3.55249600
H	-2.92139300	0.33477000	3.59555400
H	-2.94653300	2.06290400	3.19563500
C	-3.03140100	3.08594500	0.57079600
H	-3.87709000	3.74315600	0.80860400
H	-2.24604000	3.23132500	1.31510600
H	-2.62281800	3.39754500	-0.39124700
C	-3.83770700	1.46600700	-2.07360800
H	-4.77794700	1.98734200	-2.29082400
H	-3.01478700	2.16878400	-2.21269800
H	-3.71594500	0.66606200	-2.80680000
C	-4.91530900	-1.39618700	-1.19321400
H	-5.98818000	-1.19341800	-1.29985200
H	-4.46398100	-1.37123500	-2.18653100
H	-4.80039700	-2.40910300	-0.80666500

C	-4.52360800	-1.65440100	1.99867300
H	-5.54390100	-1.52694000	2.38218800
H	-4.49529400	-2.59492900	1.44414900
H	-3.85510500	-1.75221900	2.85781300
O	-0.56365000	1.98378000	-1.42468100
C	0.67341600	2.45787500	-1.22174200
O	1.52378600	1.87236400	-0.56209100
C	0.92503100	3.79980300	-1.89388300
C	1.64073200	4.71418700	-0.88364800
H	2.54506500	4.23474400	-0.50379000
H	1.91737400	5.65478700	-1.36950300
H	0.99208600	4.94606300	-0.03249200
C	1.86205600	3.48000700	-3.08377400
H	1.40580600	2.74005700	-3.74617100
H	2.06176100	4.39733000	-3.64651000
H	2.81103600	3.07672300	-2.72177600
C	-0.36457000	4.45884500	-2.40252300
H	-0.87377100	3.82750000	-3.13381200
H	-1.05750100	4.66643300	-1.58172800
H	-0.11675500	5.41100300	-2.88196700
C	-0.61345800	0.01732200	1.79797500
C	-0.67731800	-1.20698000	1.56529200
C	-0.22736700	-2.59838000	1.67703500
C	-0.06306000	1.17121900	2.57372700
H	-0.76805700	1.41554000	3.37419300
H	-1.05716900	-3.30624100	1.73648600
O	0.07056300	2.35765900	1.82289800
H	0.64934300	2.16030400	1.06752400
C	1.23265100	0.68458600	3.21754200
C	1.17259500	0.02706600	4.45010600
C	2.46393500	0.81279300	2.56788600
C	2.32740900	-0.49561600	5.03202800
H	0.21496500	-0.07508000	4.95599400
C	3.61936100	0.29459600	3.15088700
H	2.53369400	1.30494700	1.60521400
C	3.55494900	-0.36179200	4.38103100
H	2.26922200	-0.99977900	5.99237600
H	4.56517600	0.39196800	2.62859400
H	4.45672400	-0.76695900	4.83068300
H	0.39523000	-2.84616200	0.81408600
H	0.38531100	-2.67864100	2.58208500
C	2.67681300	-1.34896300	-1.12482800
H	2.28131000	-1.01618000	-2.09400900
O	1.77457500	-0.96477000	-0.08418900

H	1.54673000	-0.02928300	-0.22942400
C	4.02619700	-0.68268500	-0.91133500
C	4.34155200	0.46829100	-1.63776300
C	4.90788600	-1.13517200	0.07490300
C	5.52452500	1.16363400	-1.38232800
H	3.64557000	0.82045600	-2.39364000
C	6.09174700	-0.44483800	0.32953400
H	4.65489500	-2.02828400	0.63796800
C	6.40152300	0.70898700	-0.39687900
H	5.76145400	2.05795400	-1.95183900
H	6.77574300	-0.80559500	1.09293400
H	7.32380000	1.24687400	-0.19708600
C	2.72206700	-2.81339500	-1.13478700
C	2.67315100	-4.02070200	-1.15609400
C	2.57559100	-5.47452300	-1.20441500
H	2.80880800	-5.92622300	-0.23359900
H	1.56031900	-5.78084500	-1.48222700
H	3.26751400	-5.89687200	-1.94187000

TS-b1i$_{2a}$

N	-0.81703300	0.77669300	-1.05829100
C	-0.56596700	-1.35133900	-1.94609500
C	-0.26611700	-2.20766300	-3.00262100
H	0.37433100	-1.83774800	-3.79620100
C	-0.80615900	-3.49498200	-3.02854500
H	-0.57842500	-4.16316300	-3.85377900
C	-1.65547800	-3.91719700	-1.99961100
H	-2.08953600	-4.91298200	-2.02677600
C	-1.92893600	-3.07090000	-0.92485900
H	-2.53775800	-3.42608900	-0.09780700
C	-1.37597200	-1.78139900	-0.87230000
C	-3.65113000	1.55961900	0.55013000
C	-4.01062800	0.98358500	-0.74917100
C	-4.42965800	-0.35135500	-0.54157200
C	-4.29247600	-0.64405200	0.87516300
C	-3.88782600	0.56557300	1.54370700
Rh	-2.26432400	-0.09998400	0.14606800
C	-0.14326000	0.07994500	-2.00333900
O	0.66021800	0.54522900	-2.82458600
C	-3.76439700	0.75588300	3.02271800
H	-4.71840300	1.09913800	3.44181800
H	-3.50296900	-0.17901200	3.52441900
H	-3.00155300	1.49950200	3.25999100
C	-3.23521300	2.97836700	0.78664200

H	-4.10947000	3.62556100	0.93327700
H	-2.59265900	3.05253500	1.66613900
H	-2.67229600	3.35956200	-0.06746400
C	-3.94182400	1.72263600	-2.04898300
H	-4.80478700	2.39038900	-2.16088300
H	-3.03497400	2.32832800	-2.10302300
H	-3.93267300	1.03599000	-2.89773100
C	-4.90526100	-1.32109600	-1.57729400
H	-5.98914200	-1.47013100	-1.50233500
H	-4.68334400	-0.96481800	-2.58497400
H	-4.42191700	-2.29517500	-1.46213700
C	-4.70776800	-1.91951700	1.54138200
H	-5.76017100	-1.87720600	1.85023300
H	-4.59883600	-2.77035100	0.86500000
H	-4.10865900	-2.11906000	2.43351800
O	-0.61268400	2.18039500	-1.20770500
C	0.53194700	2.64829300	-0.69324800
O	1.23026100	2.02414000	0.09723100
C	0.90896200	4.02509500	-1.21899000
C	1.40962500	4.87876000	-0.04154600
H	2.20991600	4.36592600	0.49538900
H	1.79149100	5.83381800	-0.41467800
H	0.60104800	5.08963600	0.66642300
C	2.06667900	3.74963300	-2.21200900
H	1.74390000	3.05664000	-2.99319700
H	2.38361400	4.69214800	-2.66970900
H	2.91921000	3.30552000	-1.69138300
C	-0.25115600	4.72214300	-1.94325300
H	-0.59774600	4.13571400	-2.79640500
H	-1.09955700	4.88965800	-1.27231400
H	0.08692000	5.69725300	-2.30750300
C	-0.78131200	-0.47201900	1.50927200
C	-0.49760200	-1.57099800	0.91819600
C	0.31808600	-2.80594700	1.00258600
C	-0.37176400	0.31876700	2.71898600
H	-1.14083000	0.16826000	3.48394500
H	-0.30290400	-3.69173600	1.16495100
O	-0.37048100	1.71206100	2.45705300
H	0.14536400	1.84336700	1.64257200
C	0.94494100	-0.20043700	3.27943200
C	0.92526700	-1.25774600	4.19529400
C	2.17409800	0.31795400	2.86366000
C	2.11471300	-1.79828700	4.68426100
H	-0.02984300	-1.66103600	4.52505600

C	3.36397000	-0.21573700	3.35683100
H	2.20792500	1.13668400	2.15564400
C	3.33943900	-1.27688600	4.26322600
H	2.08486400	-2.61812600	5.39616600
H	4.31015700	0.19246800	3.01751900
H	4.26825900	-1.69213600	4.64327600
H	0.91633100	-2.93764800	0.09973600
H	0.99309400	-2.67691100	1.85448400
C	2.99490300	-0.75655000	-1.26492800
H	2.62671600	-0.17389700	-2.11906300
O	2.05830000	-0.67364900	-0.19123400
H	1.78039500	0.25447900	-0.09894600
C	4.34827300	-0.21102000	-0.83787600
C	4.93751800	0.84965800	-1.52736000
C	4.98528300	-0.73258100	0.29384300
C	6.15475900	1.38514600	-1.09729900
H	4.43829400	1.25833400	-2.40219600
C	6.19831400	-0.20120400	0.72440800
H	4.50950000	-1.54240400	0.83707500
C	6.78692800	0.86052900	0.02922100
H	6.60478700	2.21158100	-1.63996200
H	6.68863000	-0.61274600	1.60250800
H	7.73219900	1.27537400	0.36700200
C	3.04581800	-2.16438300	-1.67513200
C	3.00821600	-3.32217100	-2.02050700
C	2.92580200	-4.71394600	-2.44686200
H	3.32237400	-5.39391800	-1.68445700
H	1.88334300	-4.99499900	-2.63826600
H	3.49284400	-4.88256300	-3.36938900

II-b1i$_{2a}$

N	-0.53202900	1.03287000	-0.58981900
C	-0.94989500	-0.45569800	-2.32177100
C	-1.47565600	-0.25115900	-3.61035600
H	-1.13296400	0.61789900	-4.16179200
C	-2.39550900	-1.13177700	-4.16028600
H	-2.79064400	-0.95442200	-5.15597000
C	-2.81101800	-2.25150200	-3.42408800
H	-3.53430900	-2.94434600	-3.84388400
C	-2.27485500	-2.48435500	-2.16737200
H	-2.56607300	-3.36862400	-1.60834100
C	-1.32495400	-1.61306300	-1.57969400
C	-3.33348100	1.53177500	1.24867600
C	-3.71002700	1.97284300	-0.10058600

C	-4.38248000	0.91284500	-0.71789000
C	-4.47689500	-0.20070300	0.24028000
C	-3.92955900	0.23108600	1.47893100
Rh	-2.31560800	0.14595800	-0.01011400
C	-0.07307500	0.67205700	-1.80164700
O	0.81025400	1.21194500	-2.47243300
C	-4.00516000	-0.46611200	2.79805500
H	-4.90860300	-0.14797200	3.33377300
H	-4.05562500	-1.55084700	2.67926700
H	-3.14251400	-0.22231900	3.41960300
C	-2.66426800	2.38718900	2.27497200
H	-3.40770000	2.95726300	2.84749500
H	-2.07717900	1.77130000	2.95771300
H	-1.98904400	3.09823700	1.79569200
C	-3.31991900	3.29294200	-0.68920100
H	-3.84452300	4.11420600	-0.18704400
H	-2.24546100	3.46357800	-0.57963100
H	-3.55760300	3.34195100	-1.75366600
C	-4.87495600	0.82852500	-2.12685600
H	-5.96109900	0.68139300	-2.14857900
H	-4.64304500	1.73501300	-2.68848200
H	-4.41654400	-0.01584700	-2.65275900
C	-5.19098900	-1.48830600	-0.02999000
H	-6.27624100	-1.36755100	0.08010200
H	-4.99367200	-1.83569900	-1.04713900
H	-4.86666400	-2.27025100	0.66002200
O	-0.01306200	2.28432000	-0.15038200
C	1.08667300	2.19967000	0.62215400
O	1.52875400	1.14363600	1.04566400
C	1.70108800	3.57060200	0.87711800
C	2.86139600	3.41241500	1.86801200
H	3.61571300	2.72401200	1.48456100
H	3.32995700	4.38697900	2.03682900
H	2.50994600	3.02704700	2.82946600
C	2.21906200	4.10175800	-0.47863700
H	1.40993100	4.17697500	-1.20772500
H	2.66332800	5.09141700	-0.33100300
H	2.98493700	3.43762000	-0.88470200
C	0.63025700	4.52359600	1.44421800
H	-0.19205300	4.66555000	0.73894300
H	0.22097900	4.14503900	2.38669800
H	1.08351000	5.49969700	1.64273500
C	-1.08829600	-1.28885600	0.77413200
C	-0.70804800	-2.04723600	-0.26280900

C	0.16605200	-3.27975700	-0.35083300
C	-0.76837900	-1.35077100	2.24923600
H	-1.67367400	-1.68113100	2.76992300
H	-0.26097200	-3.98951200	-1.06808500
O	-0.51442400	-0.03716200	2.76071600
H	0.14604500	0.36521500	2.17183200
C	0.33761200	-2.31727000	2.63170000
C	0.01130200	-3.55665000	3.18977700
C	1.68364300	-2.00540600	2.40985100
C	1.00601600	-4.48672600	3.49532400
H	-1.03283400	-3.79974300	3.37389900
C	2.67806300	-2.93125800	2.71567400
H	1.95656300	-1.04793900	1.98555000
C	2.34449100	-4.17680800	3.25263100
H	0.73676400	-5.44771700	3.92429000
H	3.71879400	-2.68249800	2.52912200
H	3.12275100	-4.89763100	3.48517400
H	1.15608800	-2.98465200	-0.71256800
H	0.28259200	-3.78280700	0.60628400
C	3.30542200	-0.41345300	-1.53609700
H	2.78860900	0.25080600	-2.24176200
O	2.34995100	-1.01853900	-0.66946900
H	1.89689400	-0.30666200	-0.18589900
C	4.33242700	0.40879300	-0.76163700
C	4.87965000	1.56543200	-1.32161500
C	4.74244200	0.00406800	0.51160500
C	5.82846500	2.31102000	-0.61882700
H	4.55864800	1.88149300	-2.31080300
C	5.68773800	0.74737700	1.21624200
H	4.30236400	-0.89030600	0.93842500
C	6.23477000	1.90352500	0.65267500
H	6.24363400	3.21216200	-1.06099500
H	5.99604500	0.42833100	2.20782800
H	6.96779700	2.48522400	1.20383800
C	3.97148100	-1.47973600	-2.29157700
C	4.53842600	-2.33694800	-2.92742000
C	5.22381100	-3.37559300	-3.68832900
H	5.78810000	-4.04575600	-3.02987300
H	4.51462700	-3.98712700	-4.25774100
H	5.93196600	-2.93910500	-4.40199400

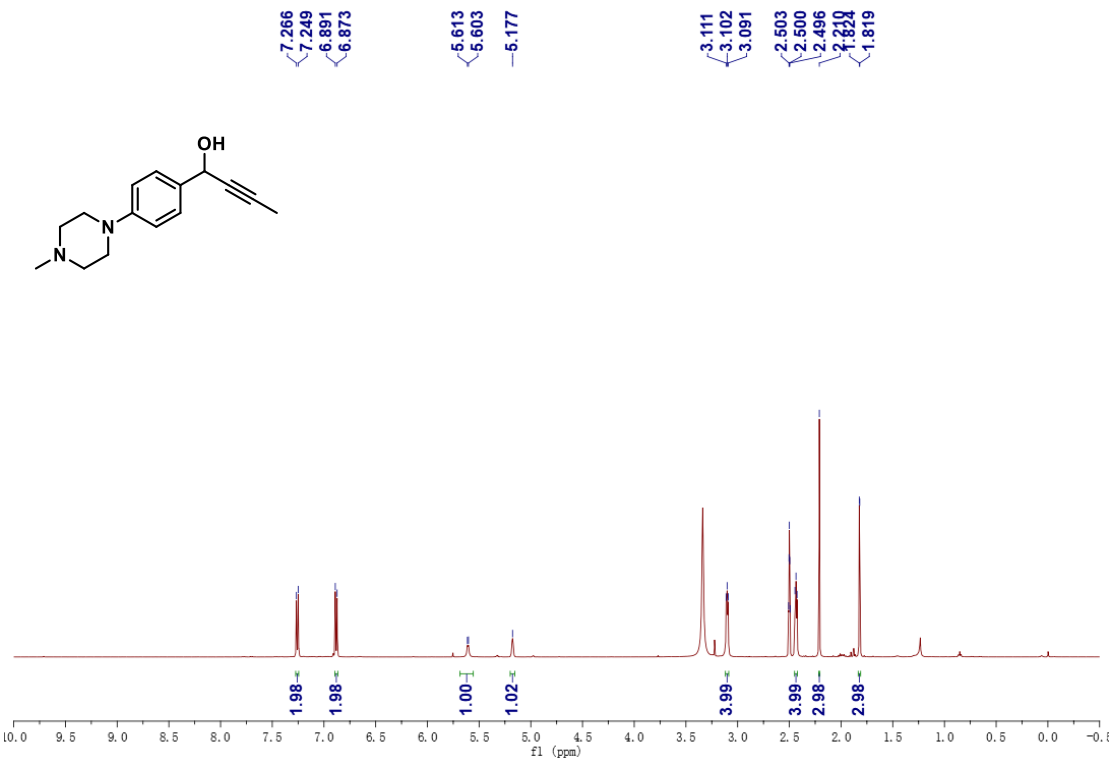
References

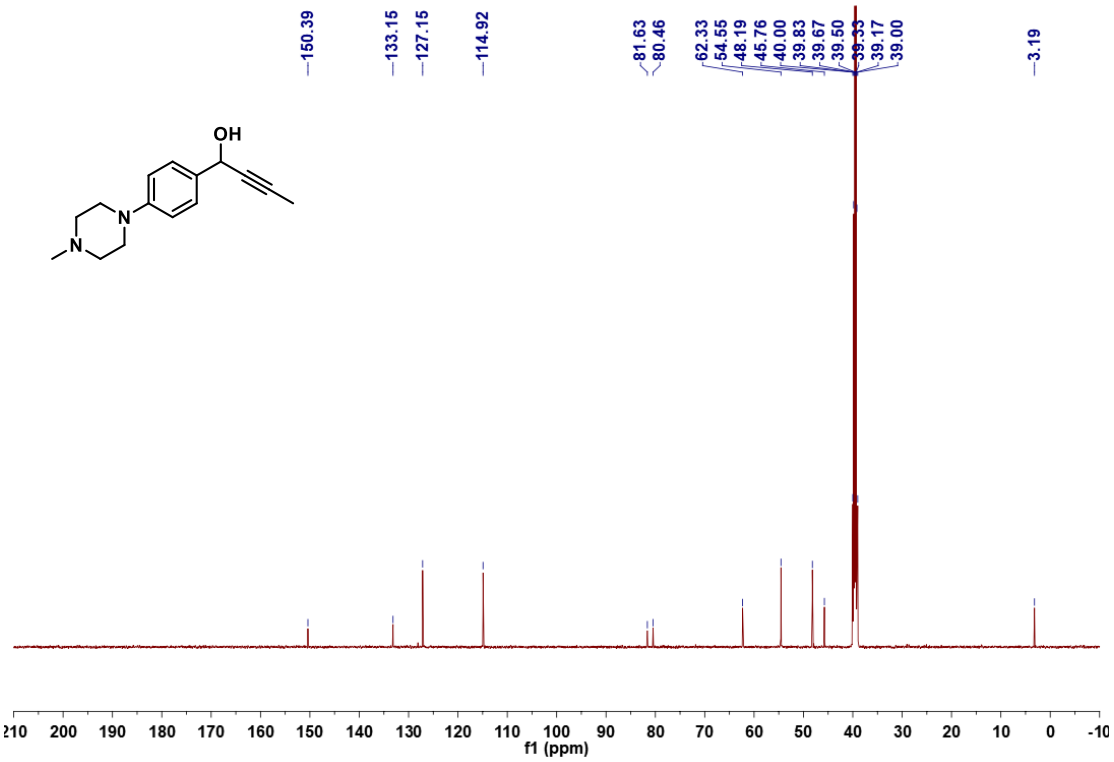
1. Rakshit, S., Grohmann, C., Besset, T., Glorius, F. Rh(III)-catalyzed directed C-H olefination using an oxidizing directing group: mild, efficient, and versatile. *J. Am. Chem. Soc.* 2011, 133, 2350.
2. Presset, M., Oehlrich, D., Rombouts, F., Molander, G. A. Complementary regioselectivity in Rh(III)-catalyzed insertions of potassium vinyltrifluoroborate via C-H activation: preparation and use of 4-trifluoroboratotetrahydroisoquinolones. *Org. Lett.* 2013, 15, 1528.
3. Guimond, N., Gorelsky, S. I., Fagnou, K. Rhodium(III)-catalyzed heterocycle synthesis using an internal oxidant: improved reactivity and mechanistic studies. *J. Am. Chem. Soc.* 2011, 133, 6449.
4. Wang, H., Glorius, F. Mild rhodium(III)-catalyzed C-H activation and intermolecular annulation with allenes. *Angew. Chem. Int. Ed.* 2012, 51, 7318.
5. Webb, N. J., Marsden, S. P., Raw, S. A. Rhodium(III)-catalyzed C-H activation/annulation with vinyl esters as an acetylene equivalent. *Org. Lett.* 2014, 16, 4718.
6. Xiaowei, W., Bao, W., Shengbin, Z., Yu, Z., Hong, L. Ruthenium-Catalyzed Redox-Neutral [4 + 1] Annulation of Benzamides and Propargyl Alcohols via C−H Bond Activation. *ACS Catal.* 2017, 7, 2494.
7. Erenler, R., Uno, M., Goud, T. V., Biellmann, J-F. Preparation of Some heterocyclic enones and ynones by isomerisation of the propargylic alcohols. *J. Chem. Res.* 2009, 459.
8. Yan, W., Wang, Q., Chen, Y., Petersen, J. L., Shi, X. Iron-catalyzed C-O bond activation for the synthesis of propargyl-1,2,3-triazoles and 1,1-bis-triazoles. *Org. Lett.* 2010, 12, 3308.
9. Tian, Q., Chen, B., Zhang, G. Silver-initiated radical ring expansion/fluorination of ethynyl cyclobutanols: efficient synthesis of monofluoroethenyl cyclopentanones. *Green Chem.* 2016, 18, 6236.
10. González-Granda, S., Lavandera, I., Gotor-Fernández, V. Alcohol Dehydrogenases and N-Heterocyclic Carbene Gold(I) Catalysts: Design of a Chemoenzymatic Cascade towards Optically Active β,β-Disubstituted Allylic Alcohols. *Angew. Chem. Int. Ed.* 2021, 60, 13945.
11. Galler, D. J., Bermudez, G. C., Parker, K. A. Multi-gram-scale synthesis of a versatile syn-anti stereotriad by a short and cost-effective route. *Arkivoc* 2019, 3, 93.
12. Das, A., Chaudhuri, R., Liu, R. S. Gold-catalyzed oxidative cleavage of aryl-substituted alkynyl ethers using molecular oxygen. Simultaneous degradation of C-H and single and triple carbon-carbon bonds under ambient conditions. *Chem. Commun.* 2009, 27, 4046.
13. Parr, R. G.; Yang, W. Density Functional Theory of Atoms and Molecules. Oxford University Press: New York, 1989.
14. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, Jr., J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J.J.; Brothers, E.; Kudin, K.N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G.A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.;

Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski J.; Fox, D. J. Gaussian 09, Revision E.01, Gaussian, Inc.: Wallingford CT, 2013.
15. (a) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B: Condens. Matter Mater. Phys.* 1988, 37, 785. (b) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys*. 1993, 98, 5648.
16. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys*. 2010, 132, 154104.
17. Andrae, D.; Häußermann, U.; Dolg, M.; Stoll, H.; Preuß, H. Energy-adjustedab initio pseudopotentials for the second and third row transition elements. *Theor. Chim. Acta* 1990, 77, 123.
18. Ditchfield, R.; Hehre, W. J.; Pople, J. A. Self-Consistent Molecular-Orbital Methods. IX. An Extended Gaussian-Type Basis for Molecular-Orbital Studies of Organic Molecules. *J. Chem. Phys*. 1971, 54, 724-728.
19. (a) Gonzalez, C.; Schlegel, H. B. An improved algorithm for reaction path following. *J. Chem. Phys*. 1989, 90, 2154. (b) Gonzalez, C.; Schlegel, H. B. Reaction Path Following in Mass-Weighted Internal Coordinates. *J. Phys. Chem*. 1990, 94, 5523.
20. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phys. Chem. B* 2009, 113, 6378.
21. Zhao, Y.; Truhlar, D. G. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. *J. Chem. Phys.* 2006, 125, 194101.

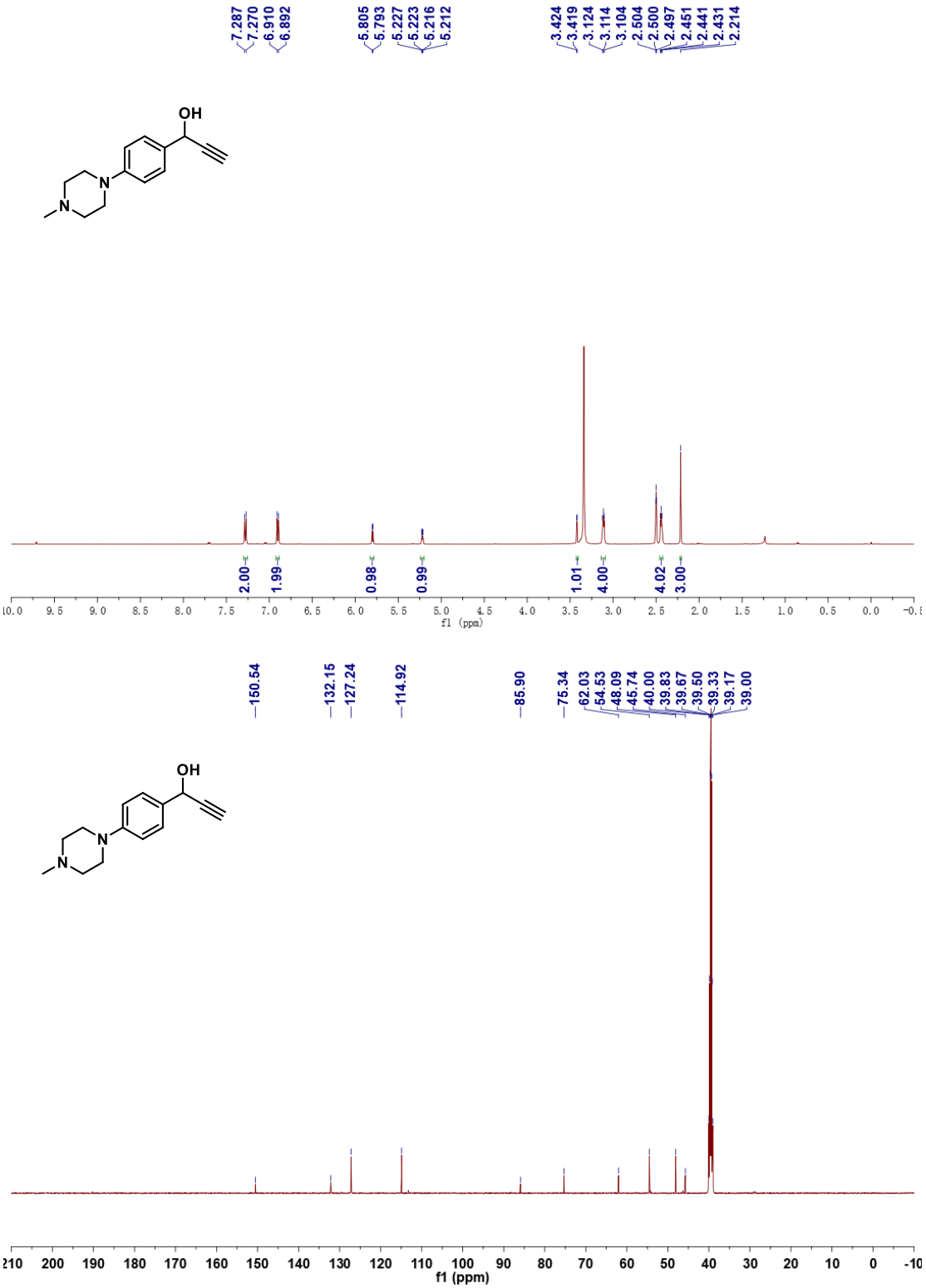
Copies of ^{1}H, ^{13}C NMR and ^{19}F NMR spectra

1-(4-(4-methylpiperazin-1-yl)phenyl)but-2-yn-1-ol (2am)

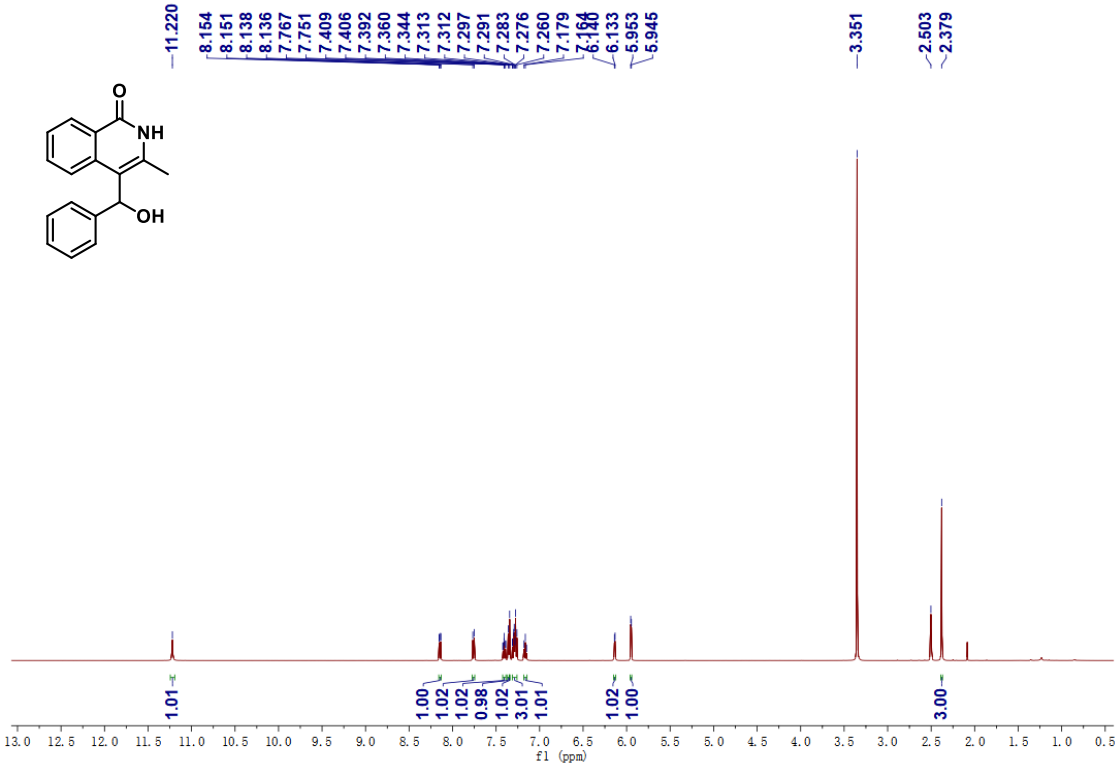


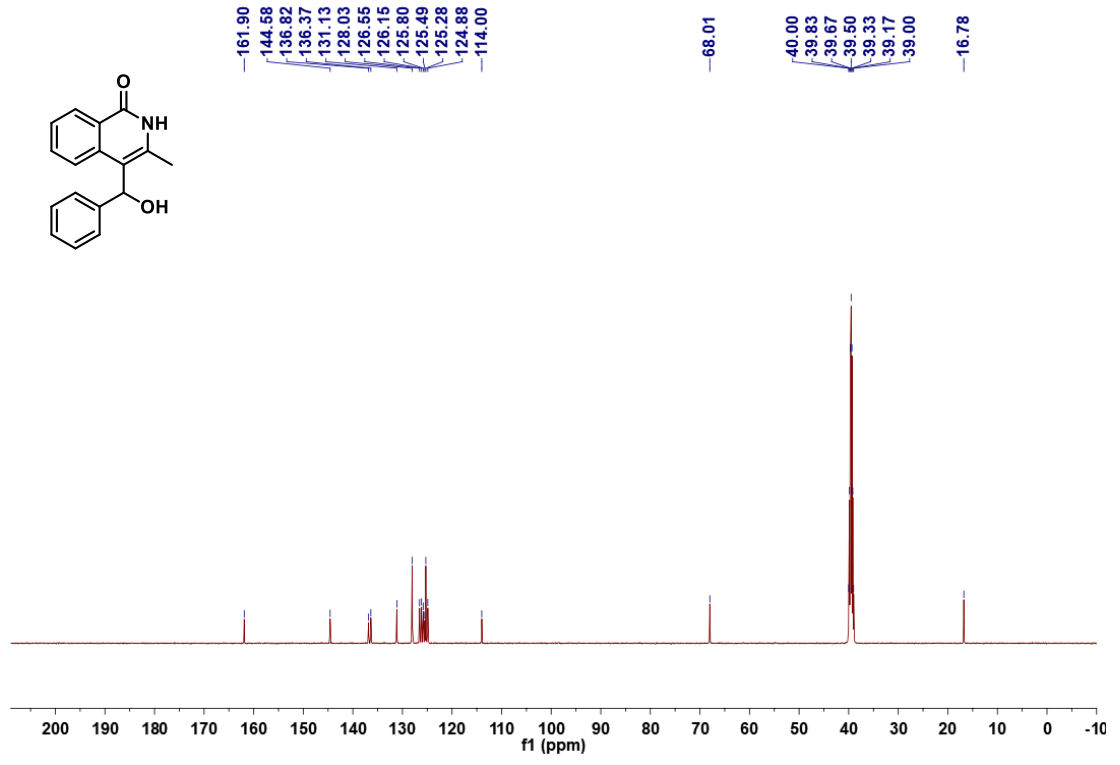


1-(4-(4-methylpiperazin-1-yl)phenyl)prop-2-yn-1-ol (2an)

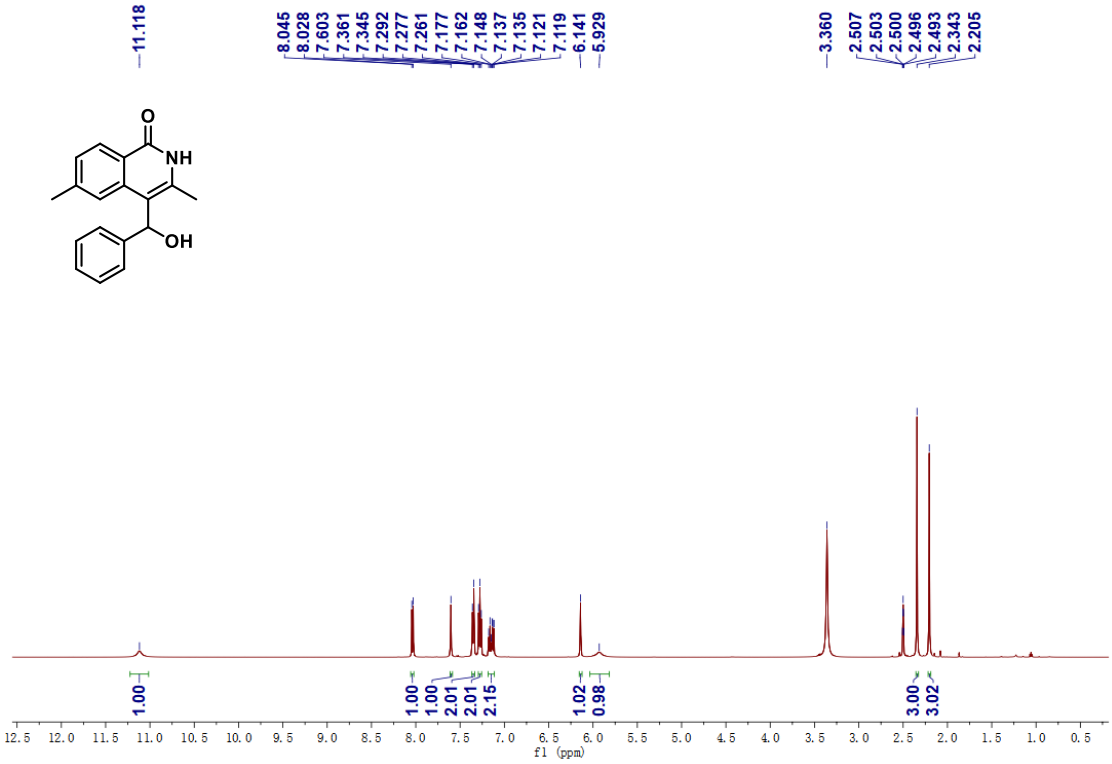


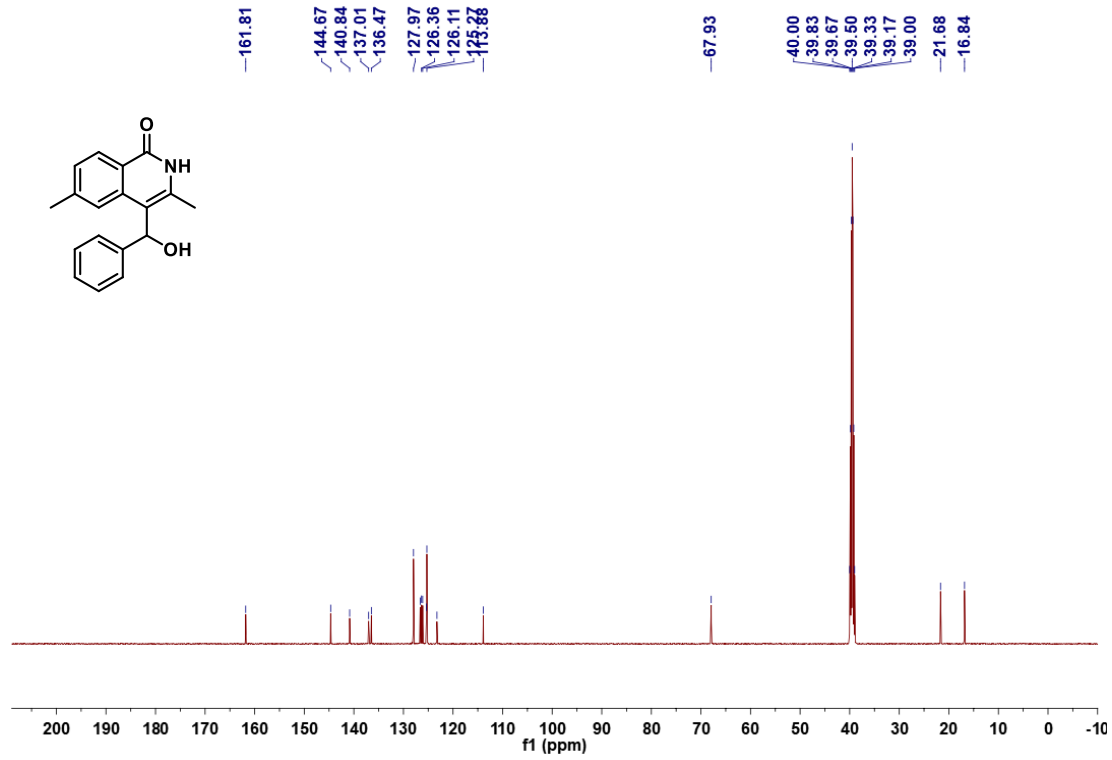
4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3aa)



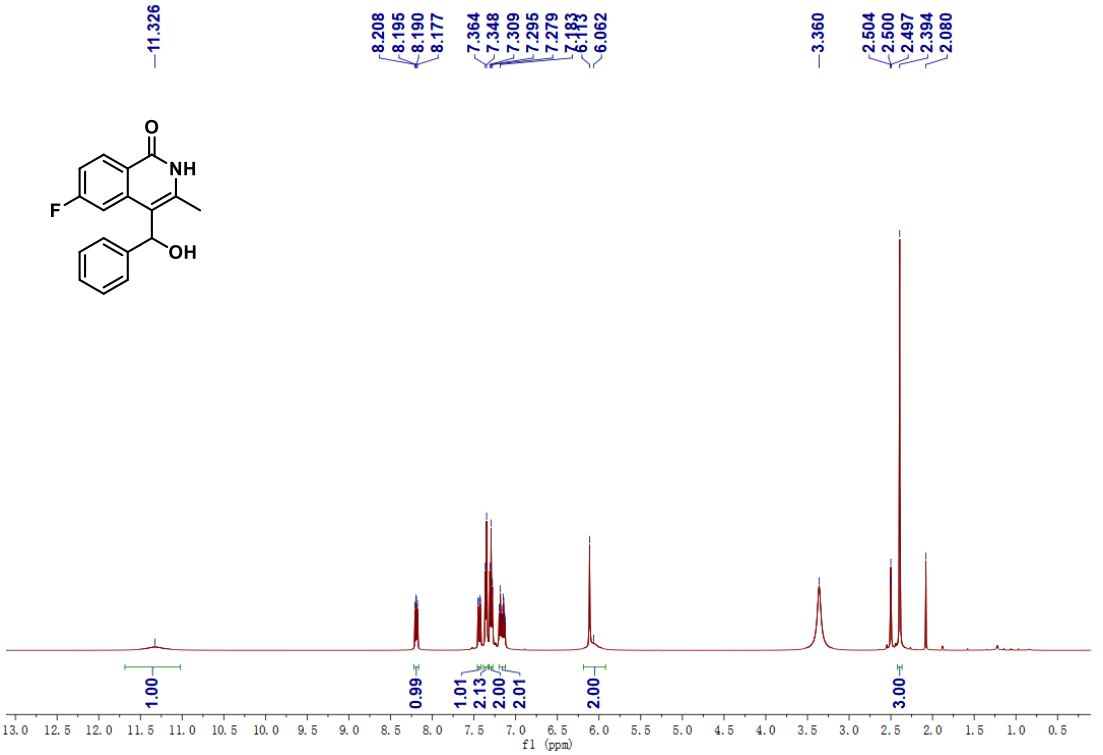


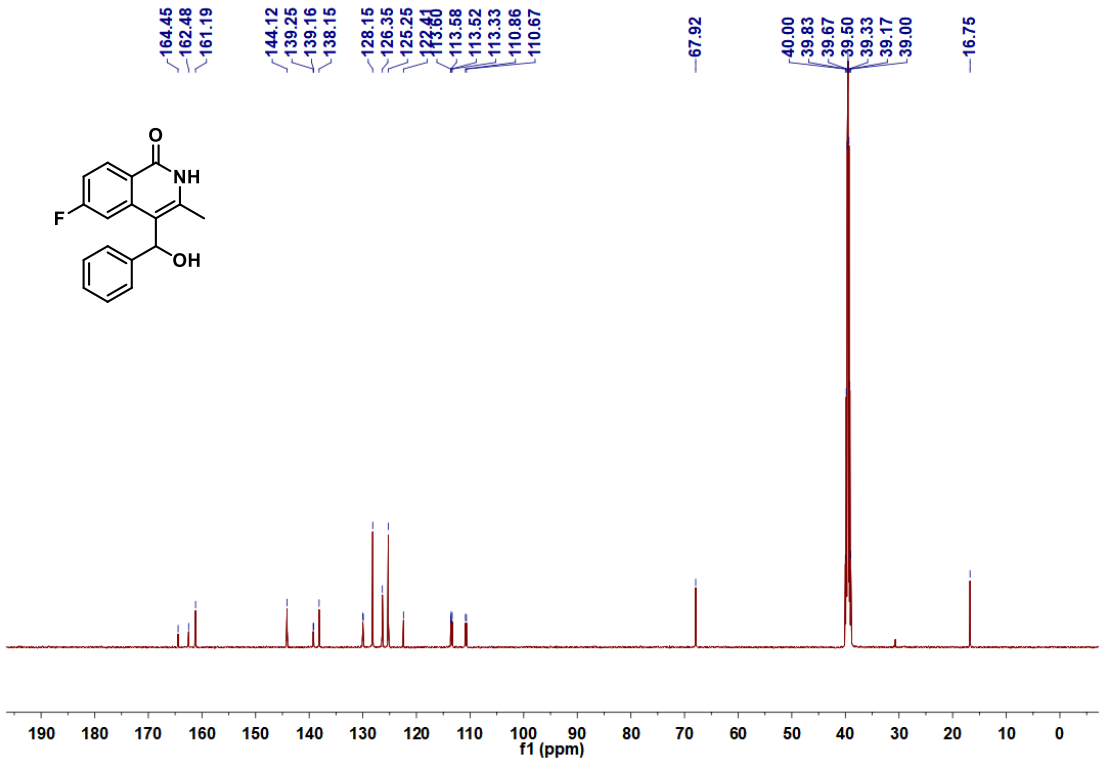
4-(hydroxy(phenyl)methyl)-3,6-dimethylisoquinolin-1(2H)-one (3ab)

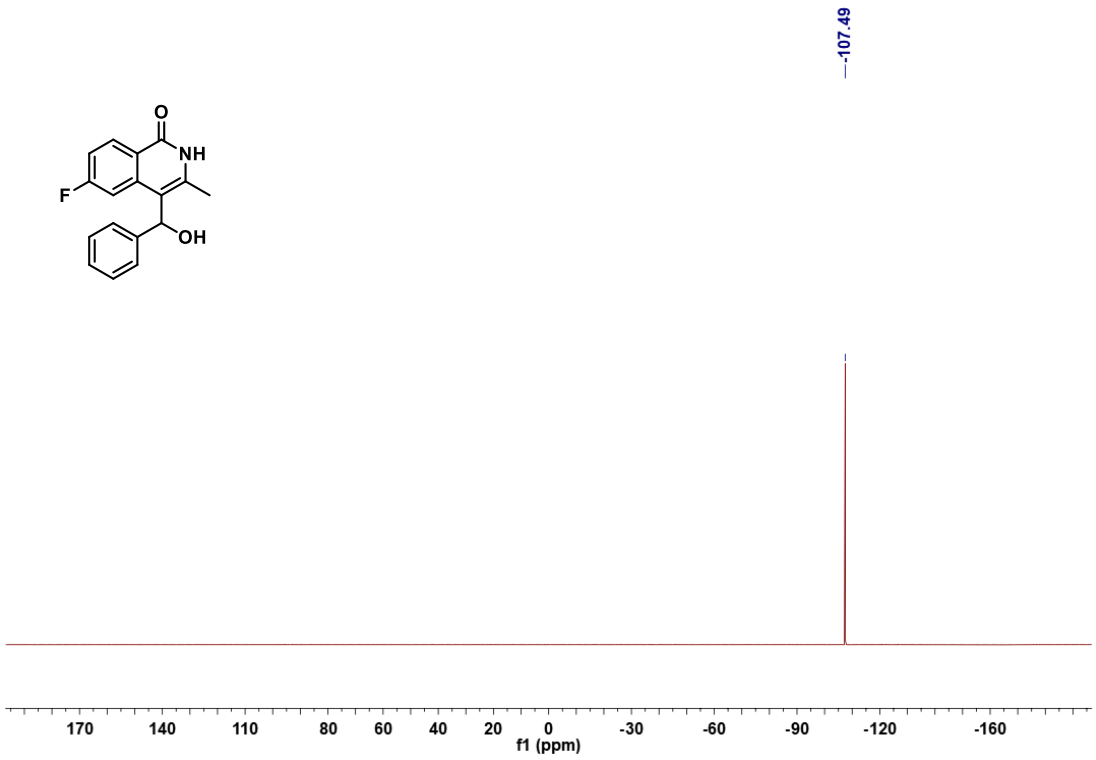




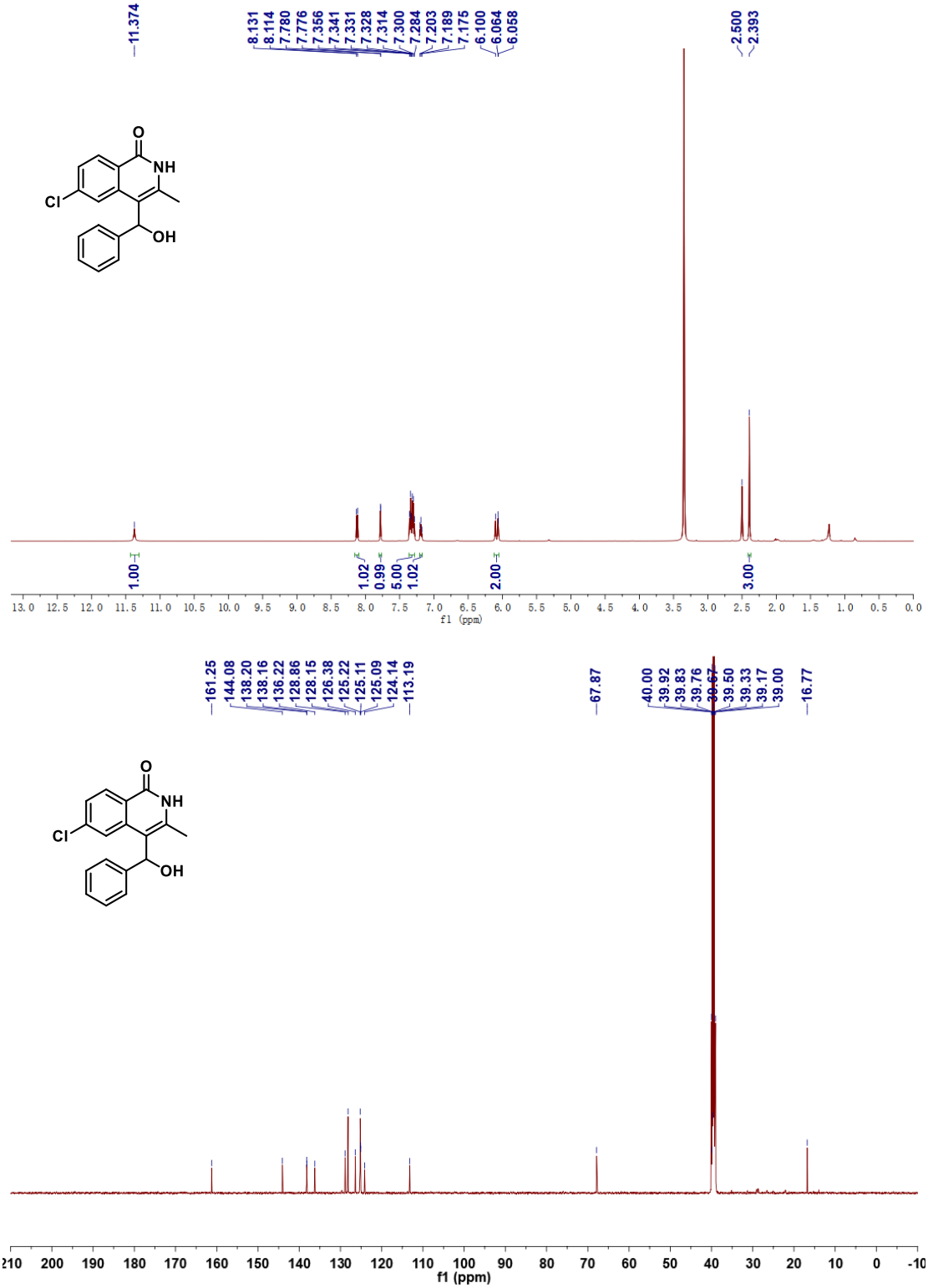
6-fluoro-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3ac)



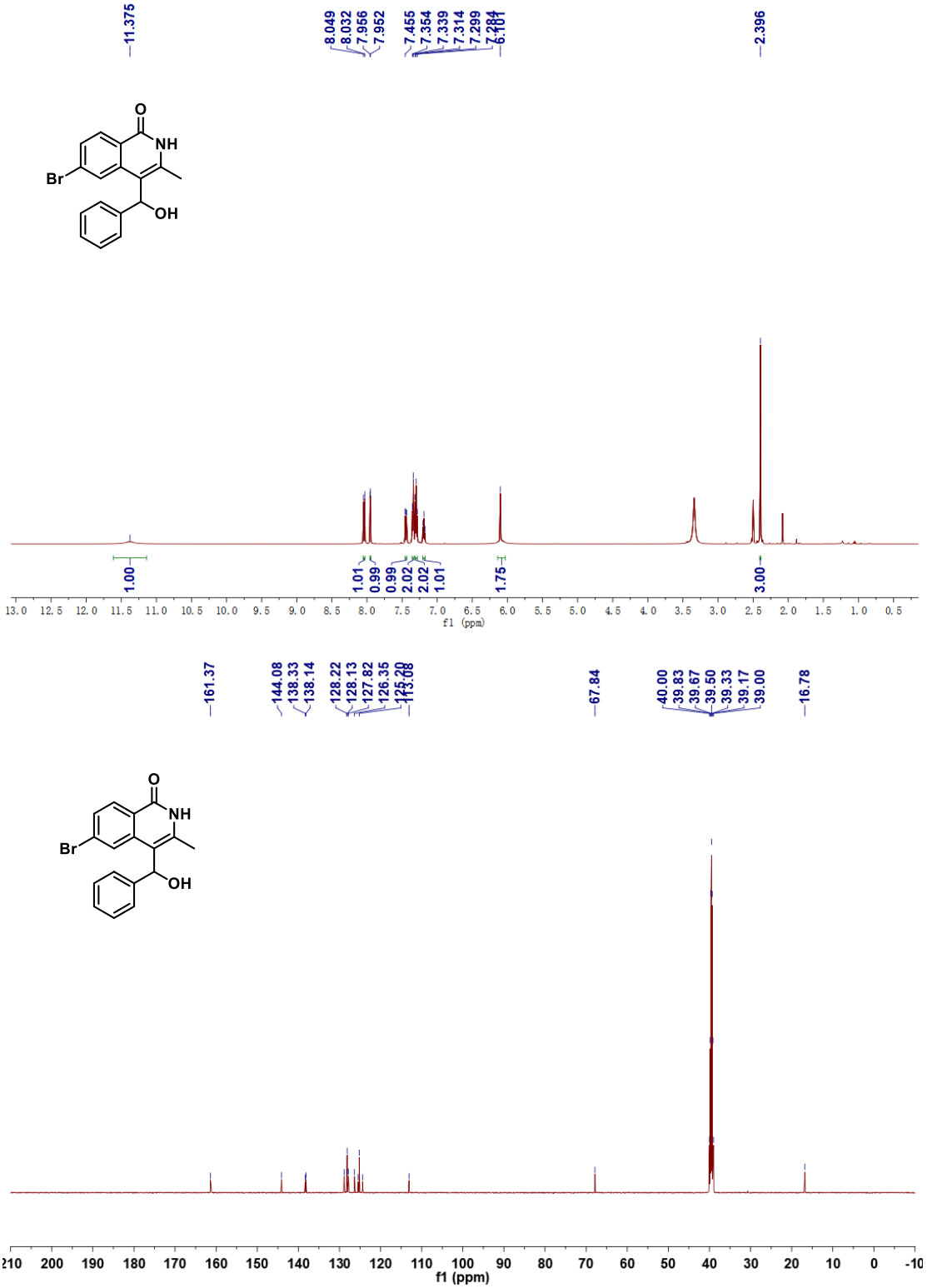



-107.49
O
NH
F
OH
170
140
110
80
60
40
20
0
-30
-60
-90
-120
-160
f1 (ppm)

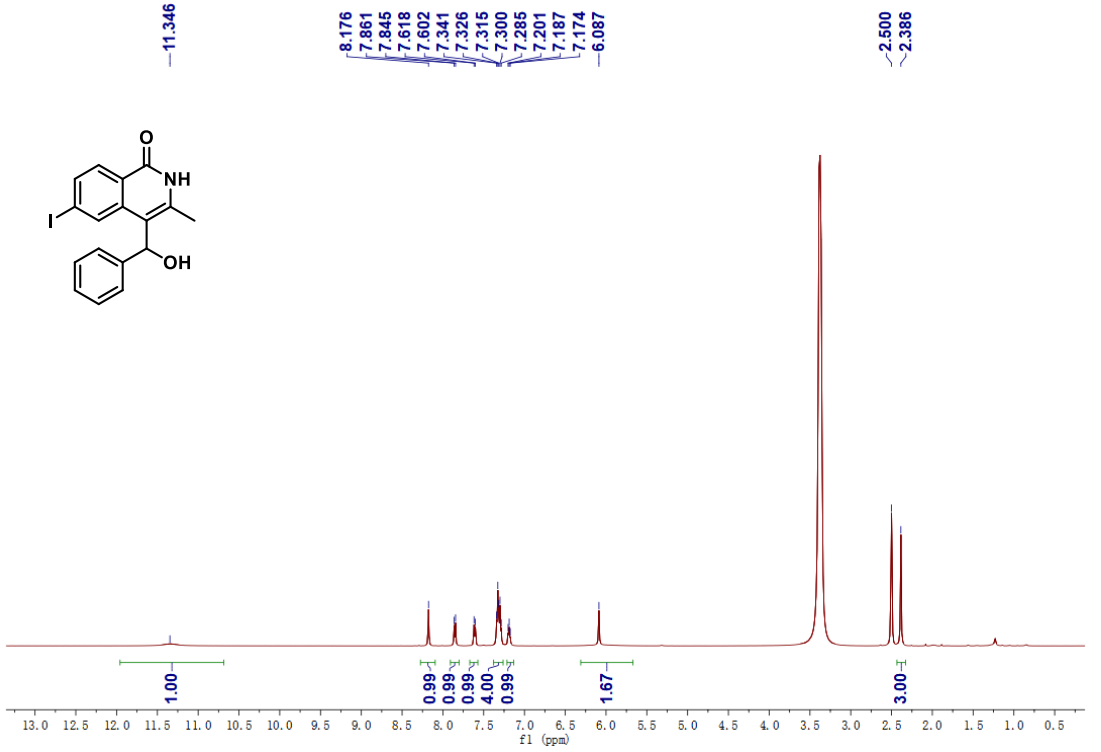
6-chloro-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3ad)

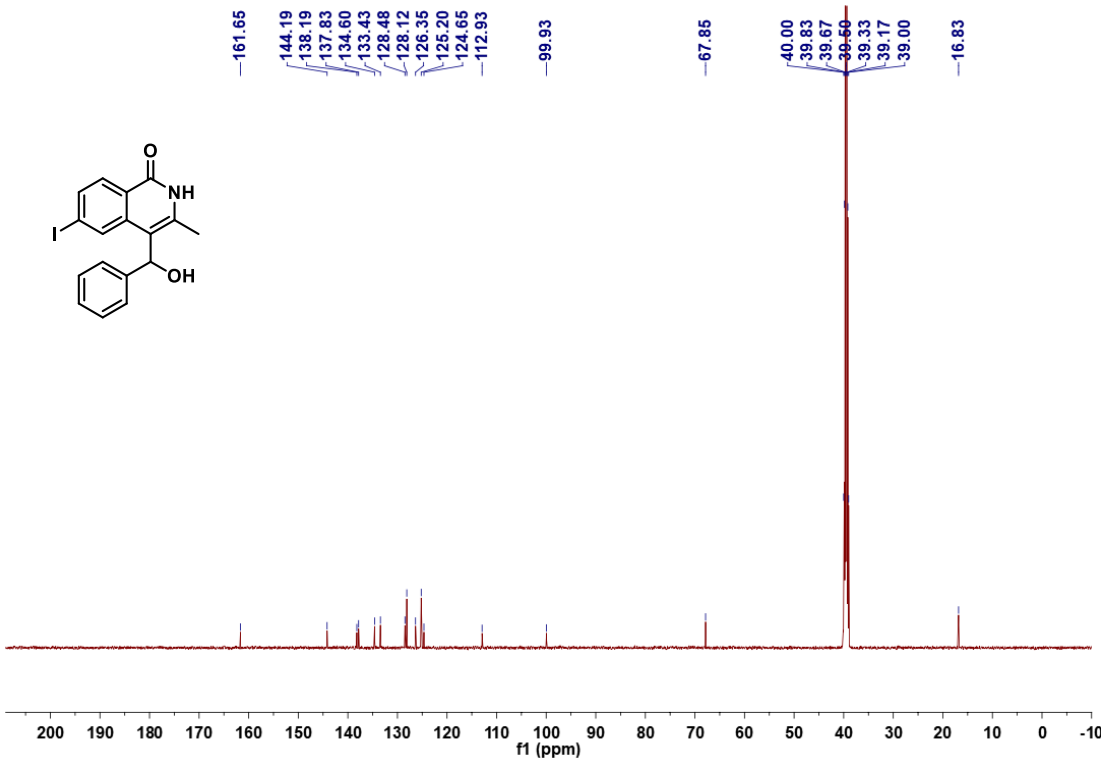


6-bromo-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3ae)

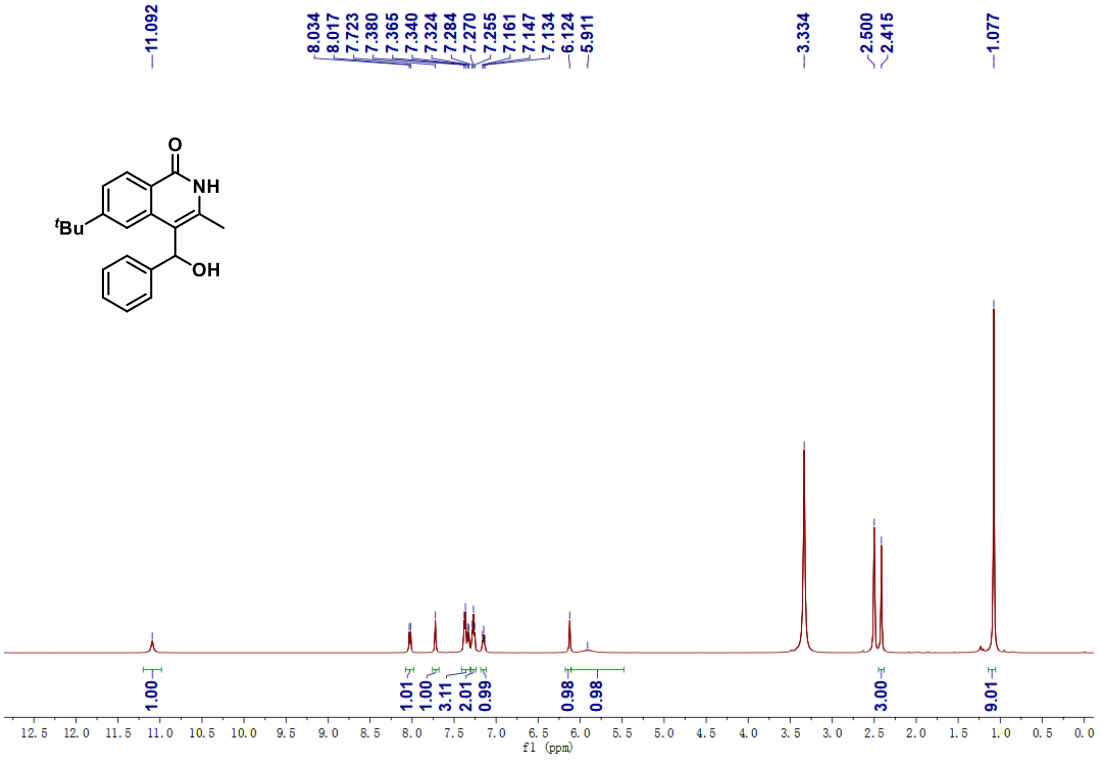


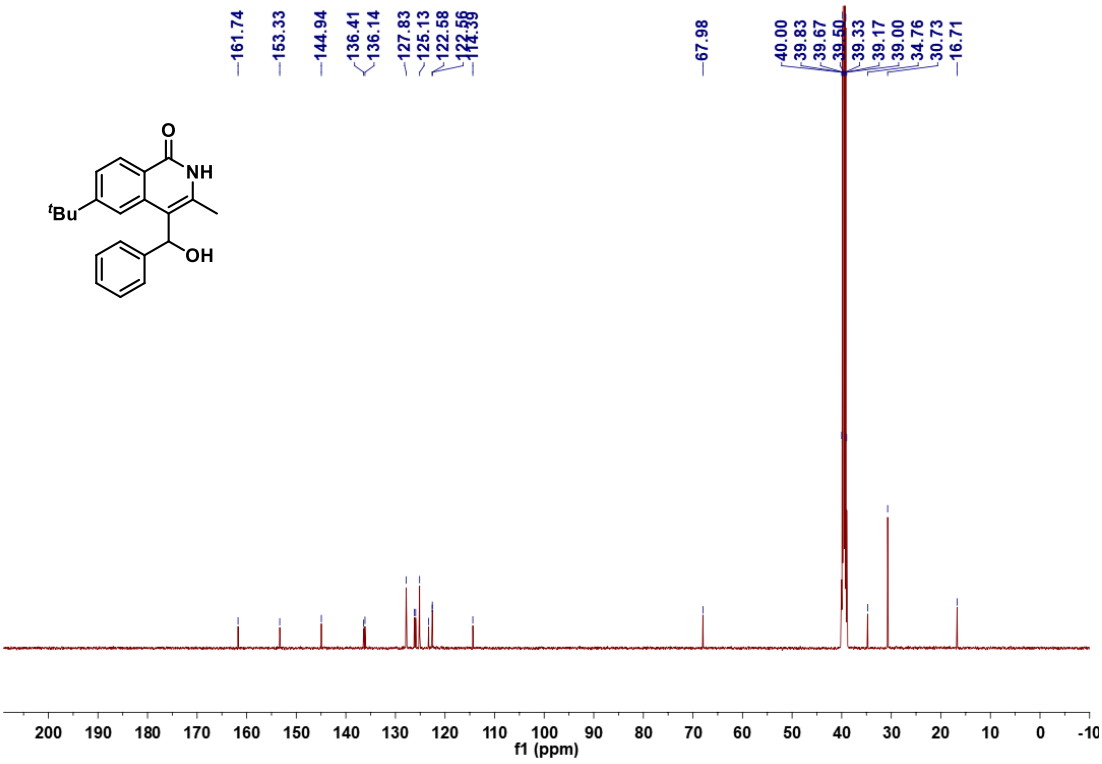
4-(hydroxy(phenyl)methyl)-6-iodo-3-methylisoquinolin-1(2H)-one (3af)



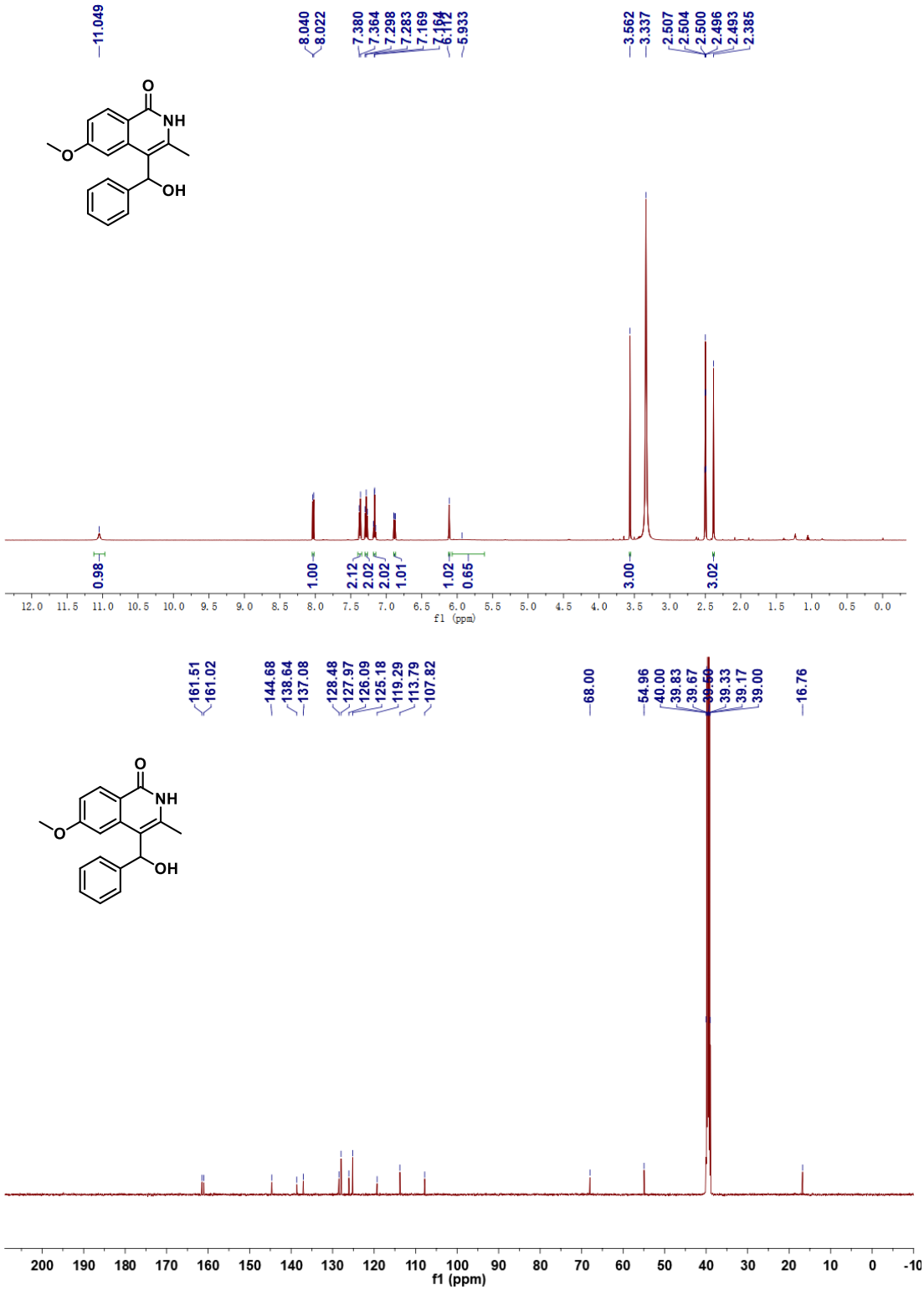


6-(tert-butyl)-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3ag)

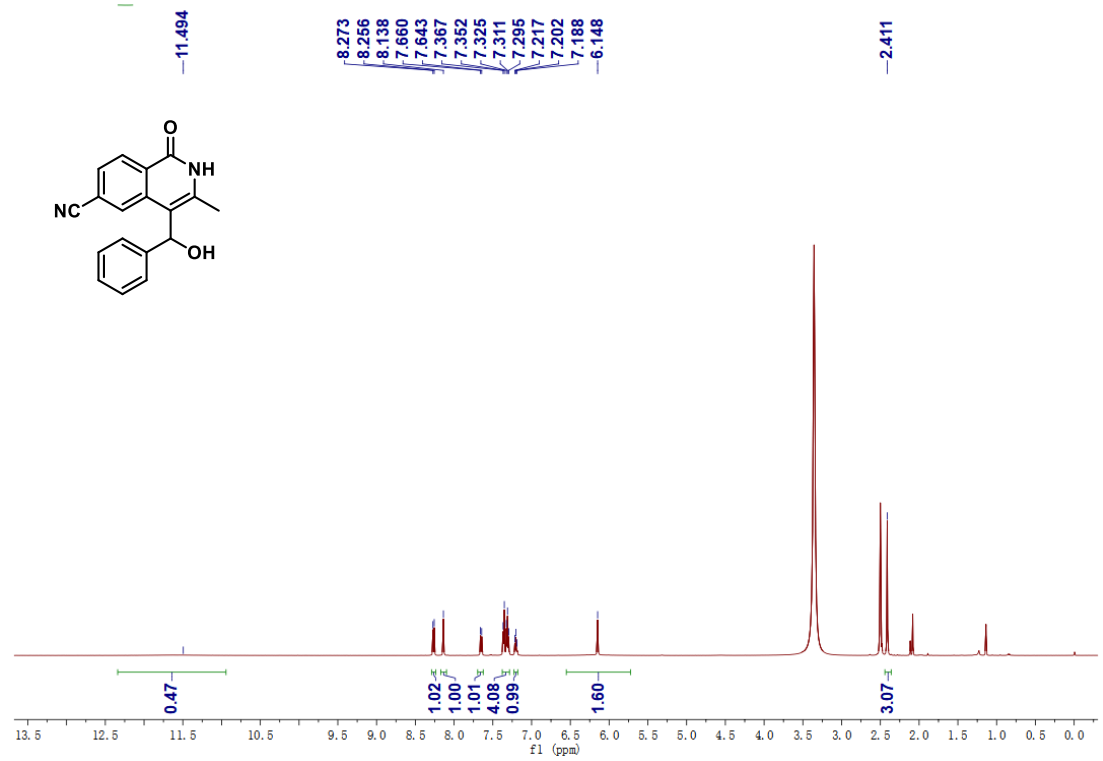


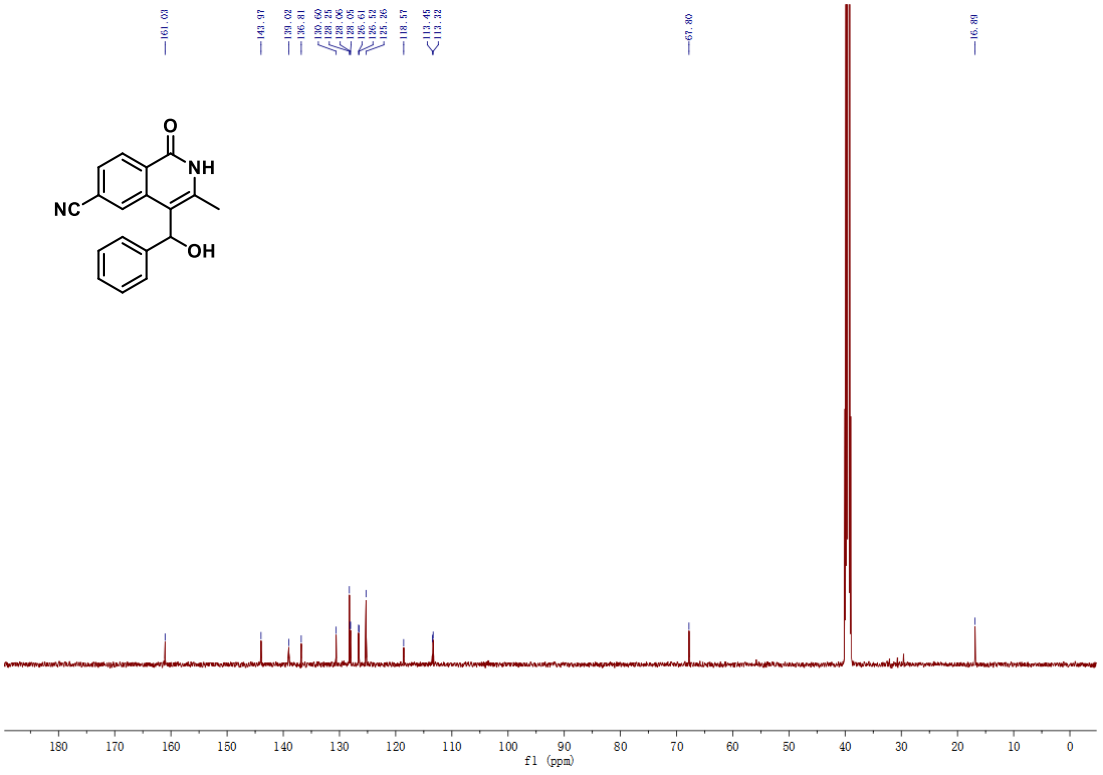


4-(hydroxy(phenyl)methyl)-6-methoxy-3-methylisoquinolin-1(2H)-one (3ah)

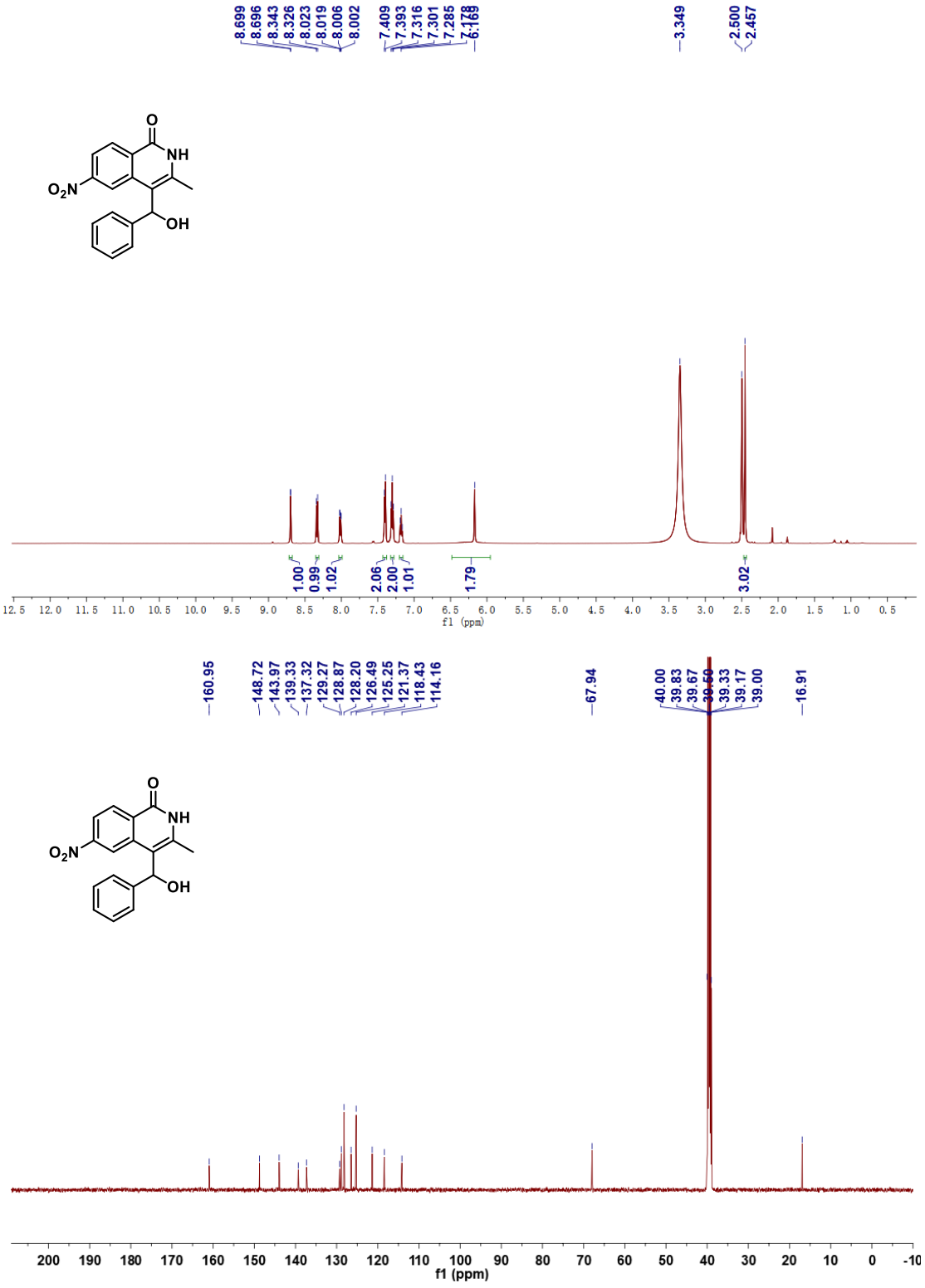


4-(hydroxy(phenyl)methyl)-3-methyl-1-oxo-1,2-dihydroisoquinoline-6-carbonitrile (3ai)

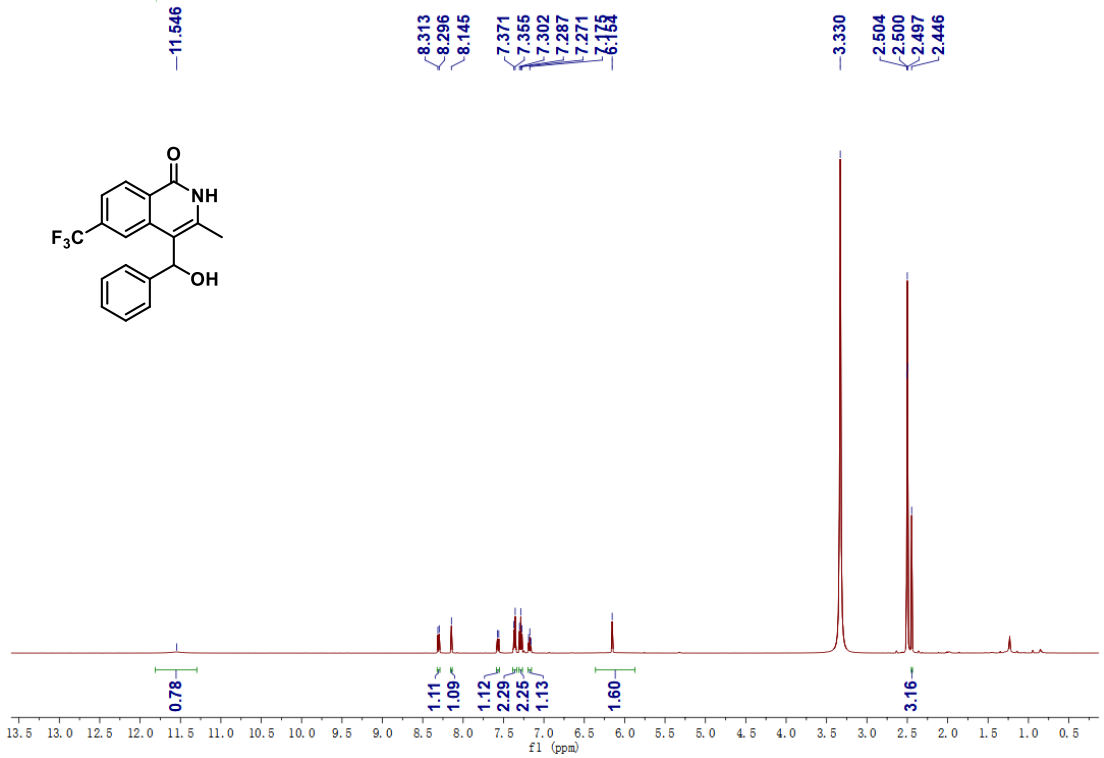


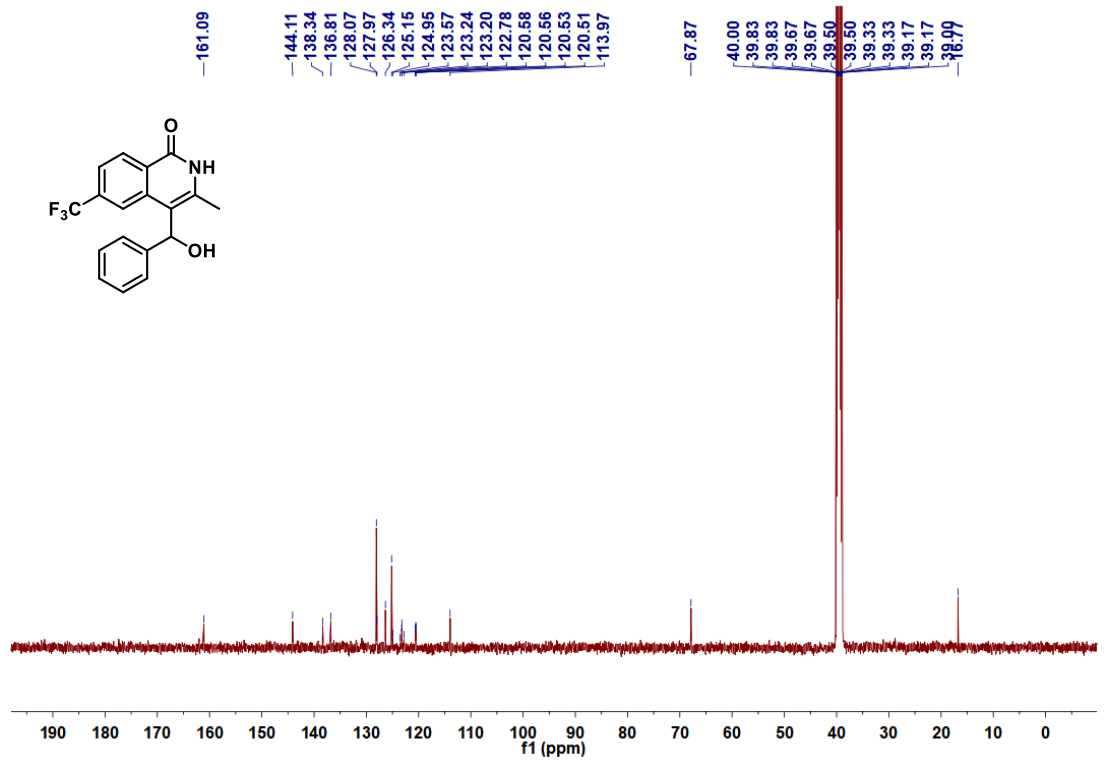


4-(hydroxy(phenyl)methyl)-3-methyl-6-nitroisoquinolin-1(2H)-one (3aj)

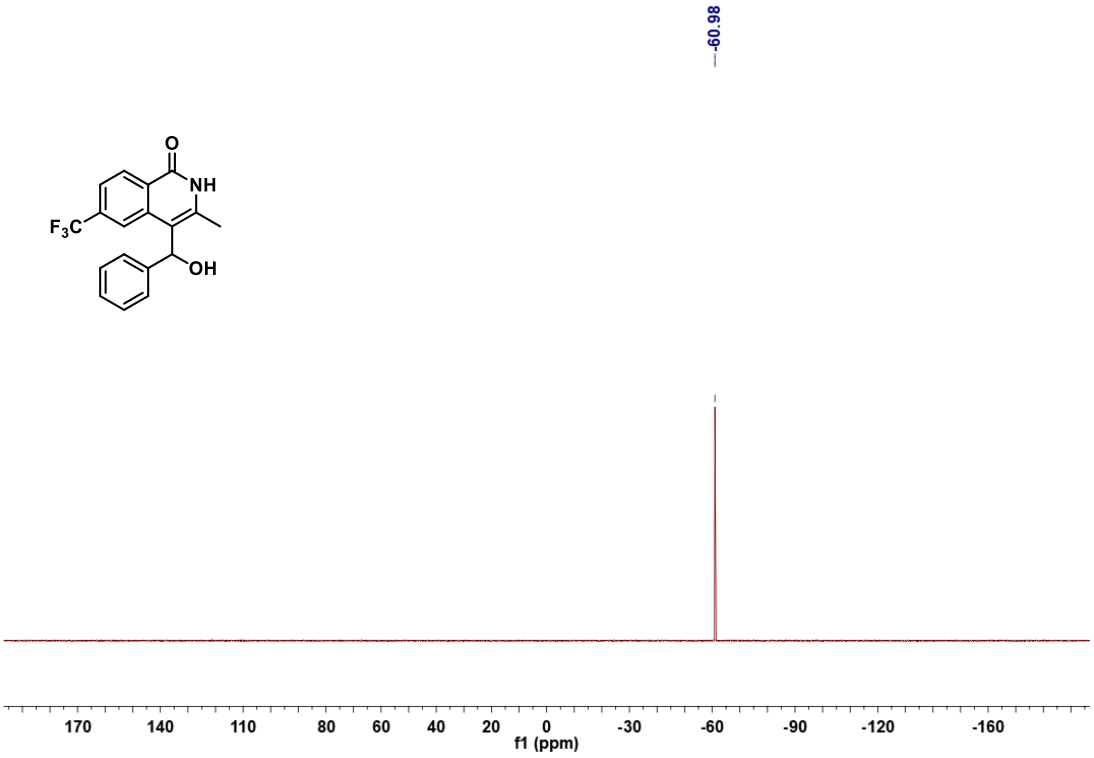


4-(hydroxy(phenyl)methyl)-3-methyl-6-(trifluoromethyl)isoquinolin-1(2H)-one (3ak)

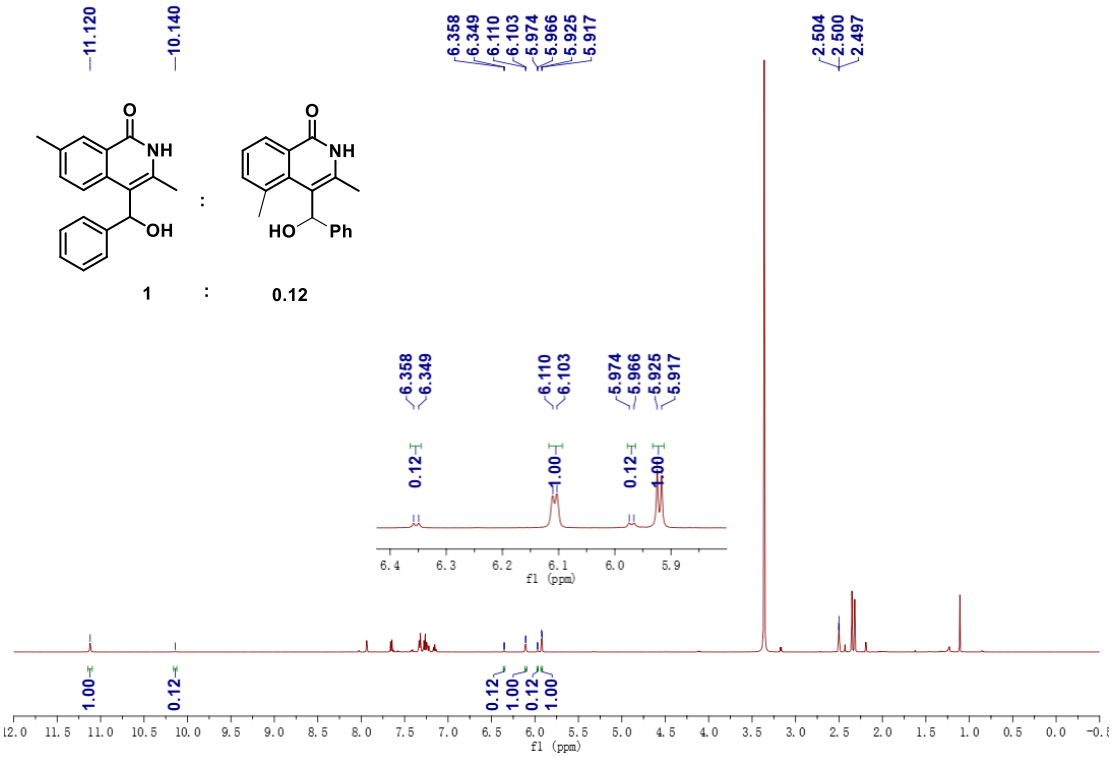




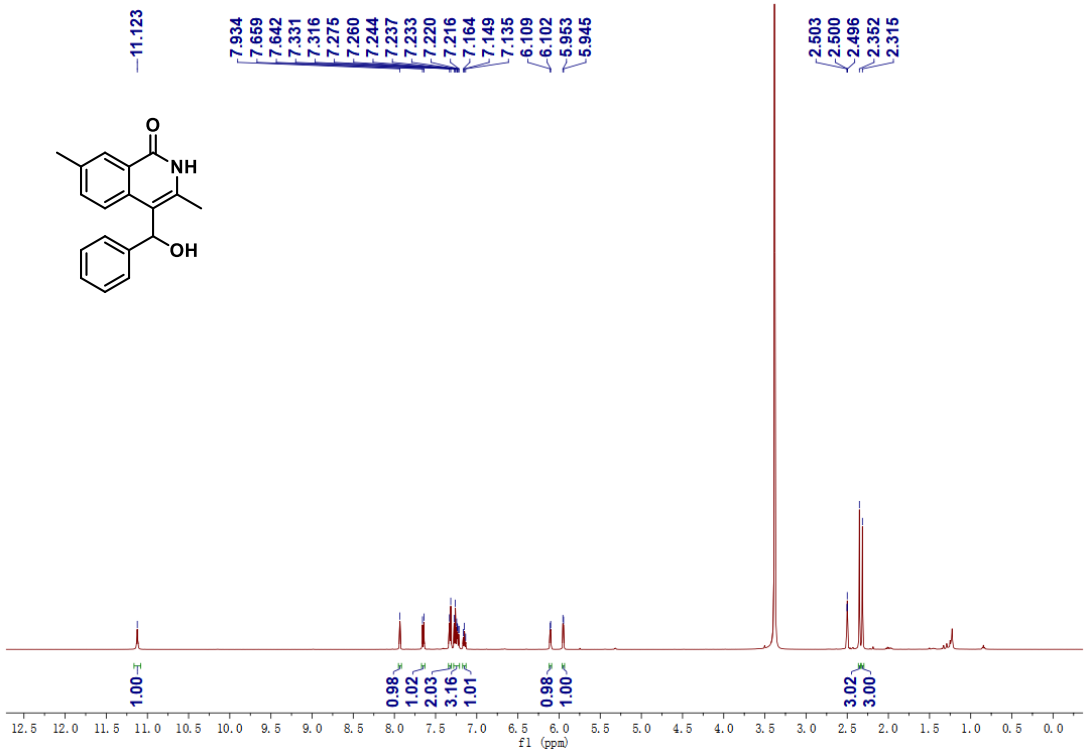
O
NH
F3C
OH

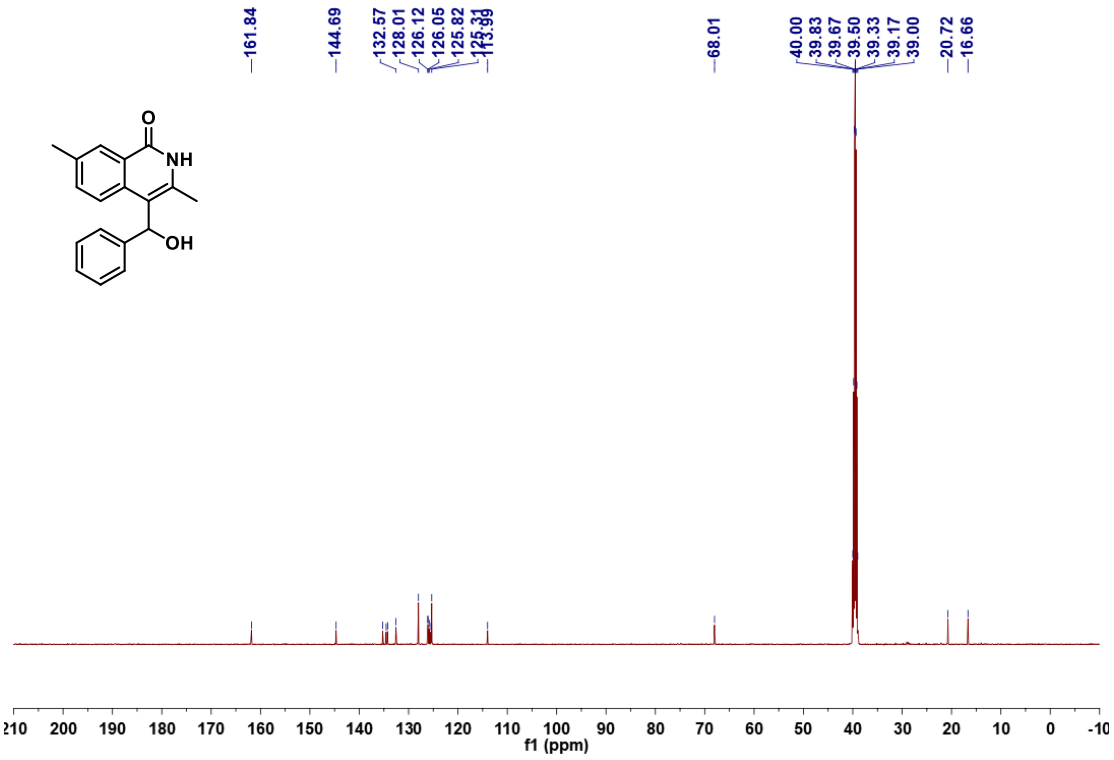

-60.98
170
140
110
80
60
40
20
0
-30
-60
-90
-120
-160
f1 (ppm)

4-(hydroxy(phenyl)methyl)-3,7-dimethylisoquinolin-1(2H)-one (3al) and
4-(hydroxy(phenyl)methyl)-3,5-dimethylisoquinolin-1(2H)-one (3al')

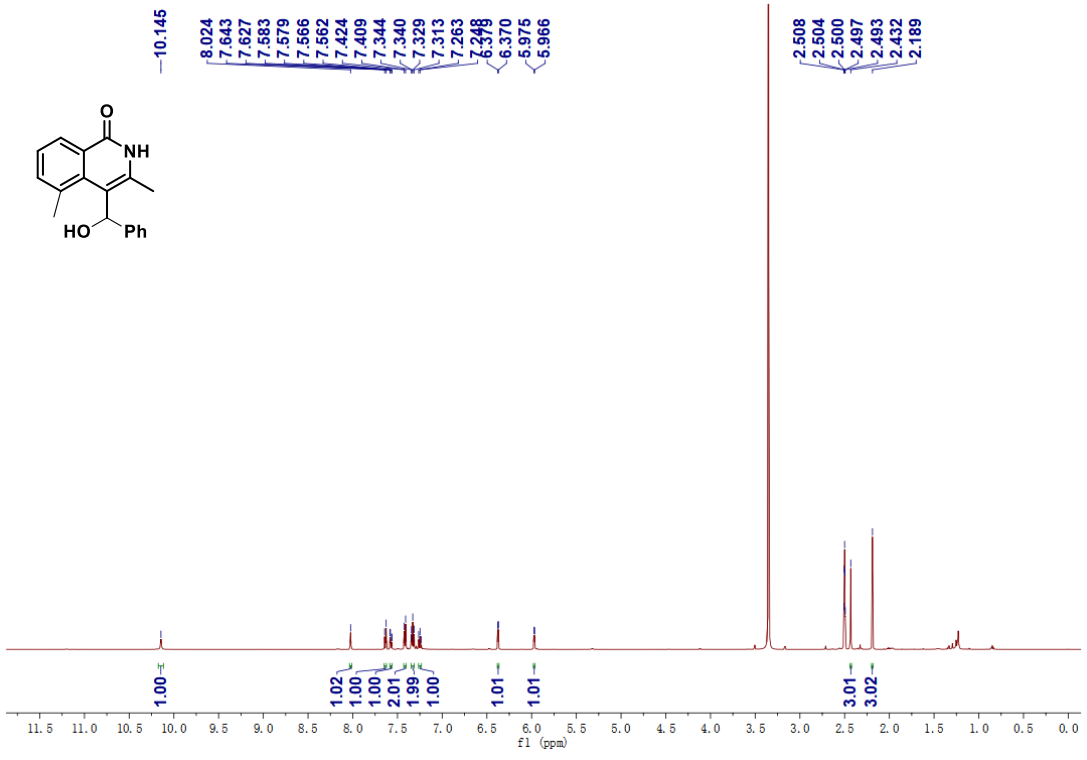


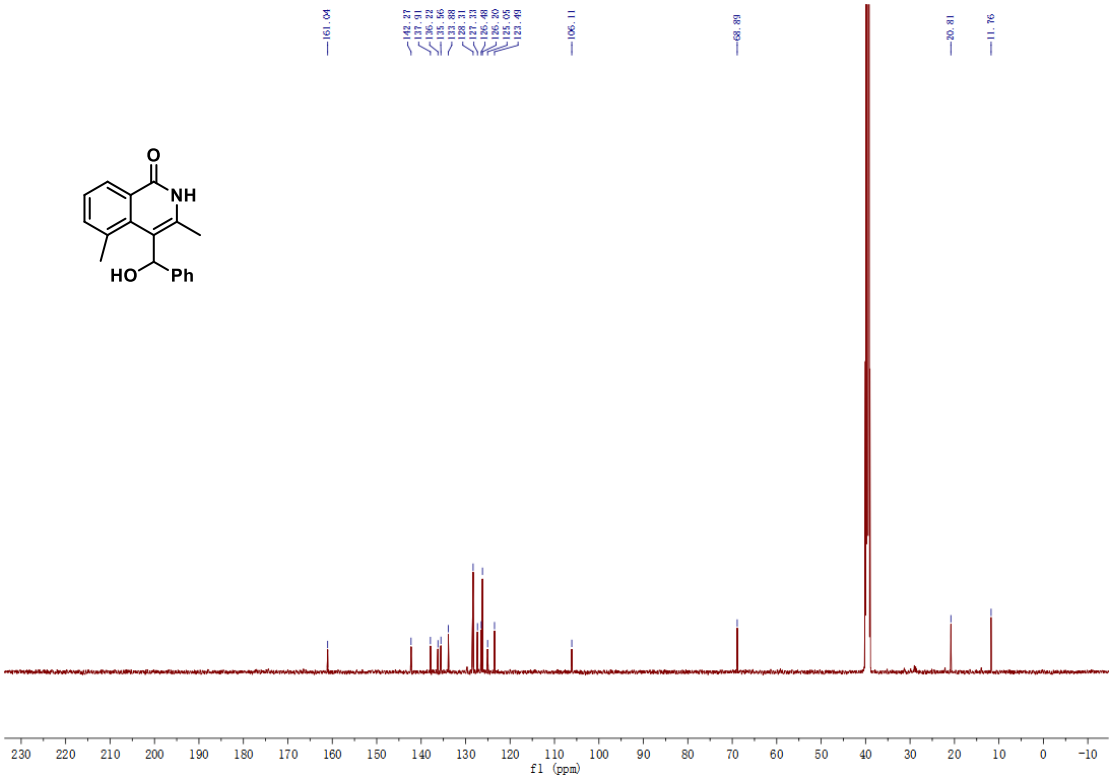
4-(hydroxy(phenyl)methyl)-3,7-dimethylisoquinolin-1(2H)-one (3al)



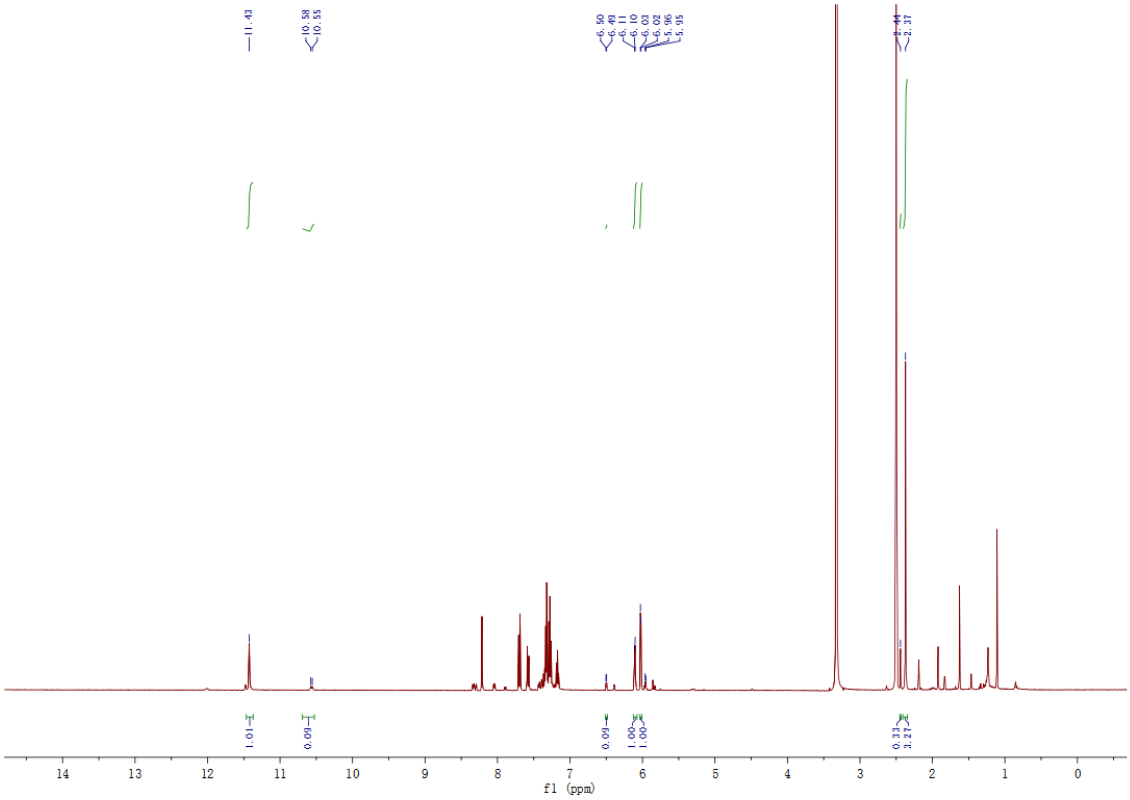


3-(hydroxy(phenyl)methyl)-4,7-dimethylisoquinolin-1(2H)-one (3al')

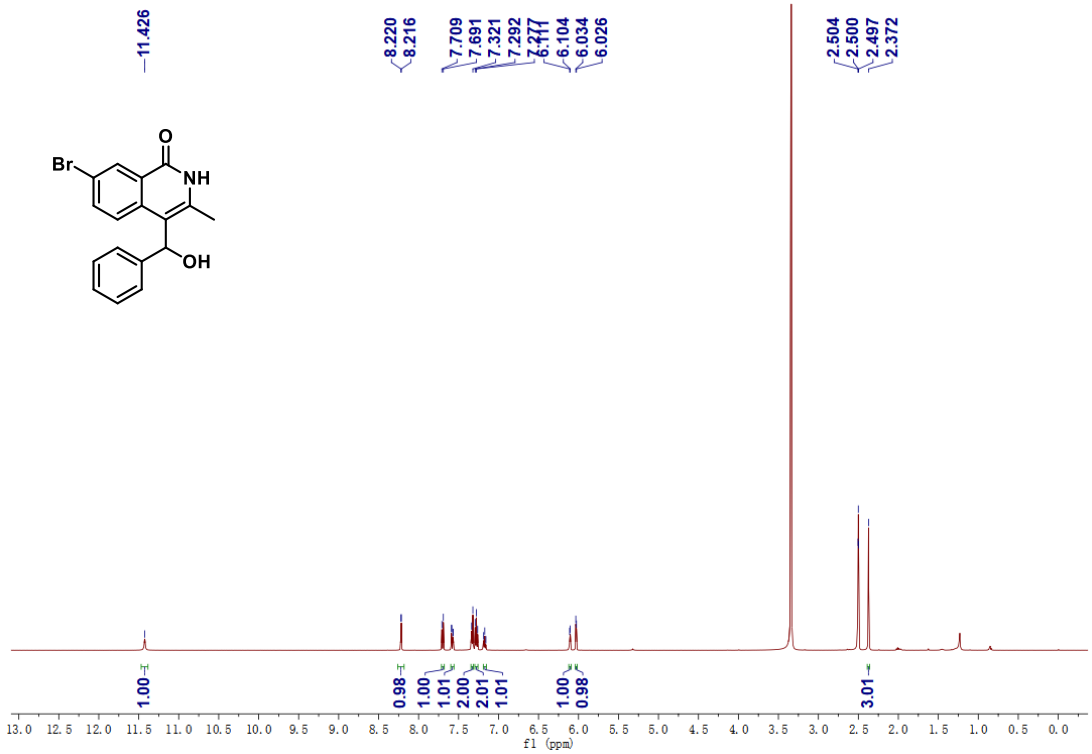


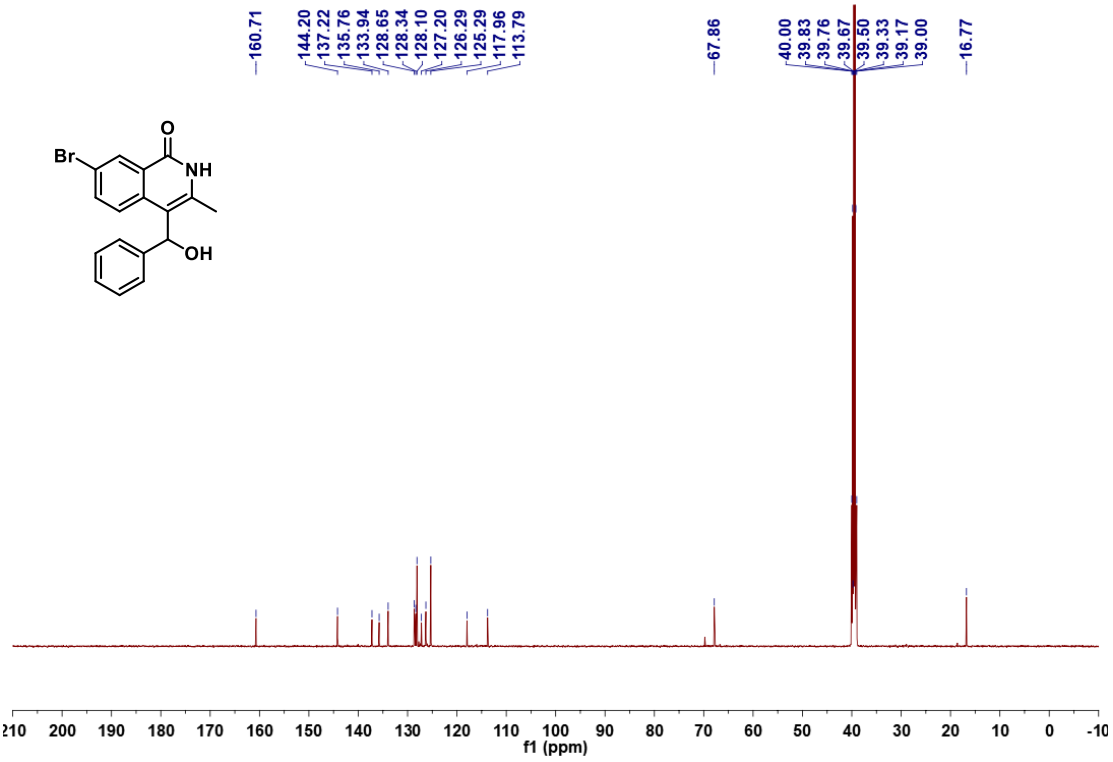

O
NH
HO
Ph
161.04
142.27
137.91
136.22
135.56
132.88
132.31
128.31
127.33
126.48
126.20
125.65
123.49
106.11
68.89
20.81
11.76
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Crude ^{1}H-NMR spectra of
7-bromo-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3am) and
7-bromo-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3am')

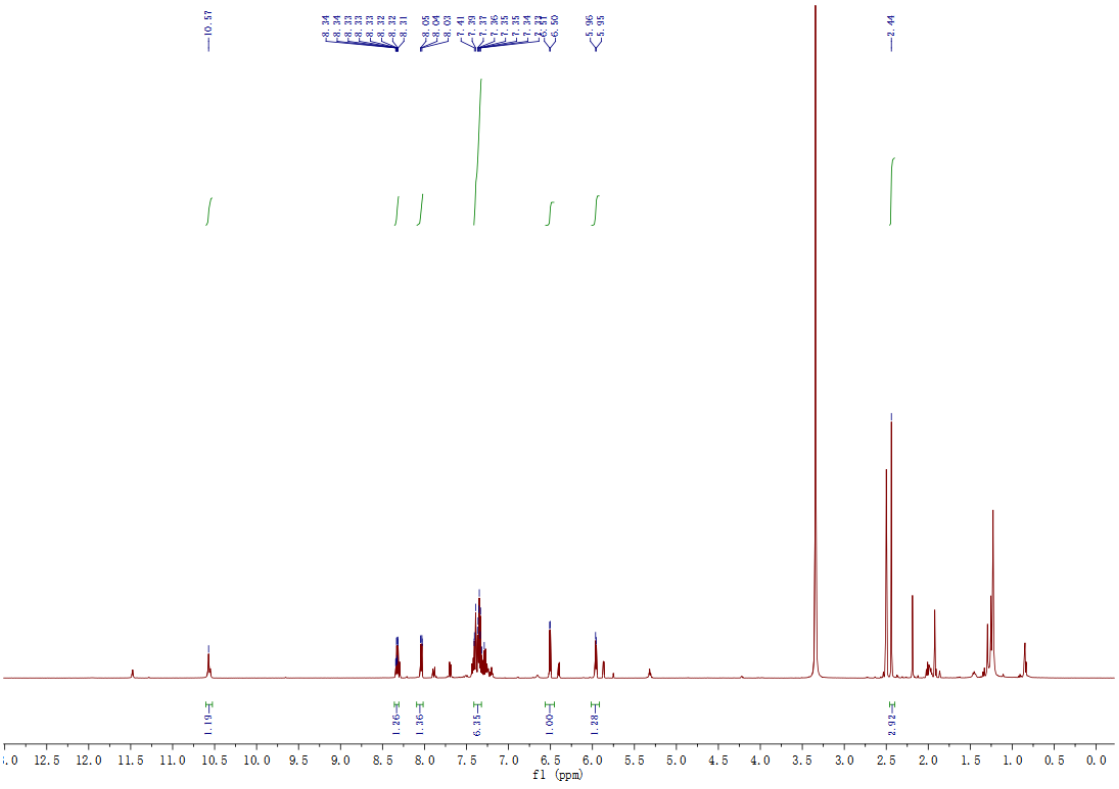


7-bromo-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3am)

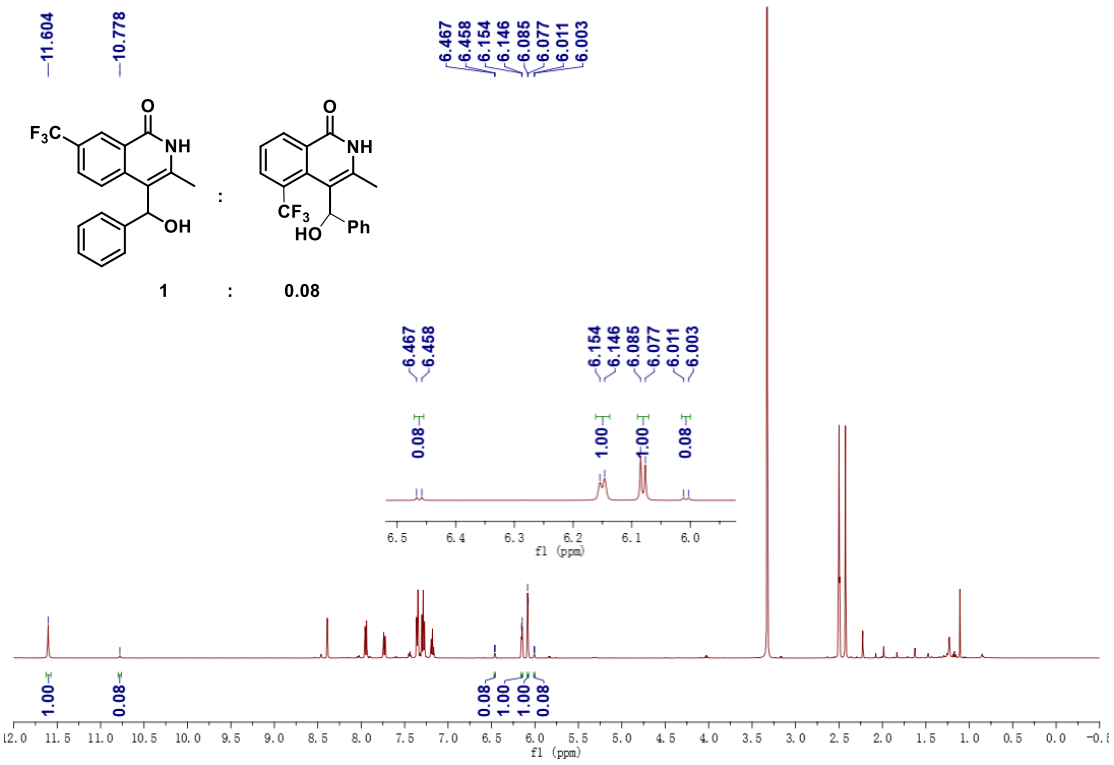




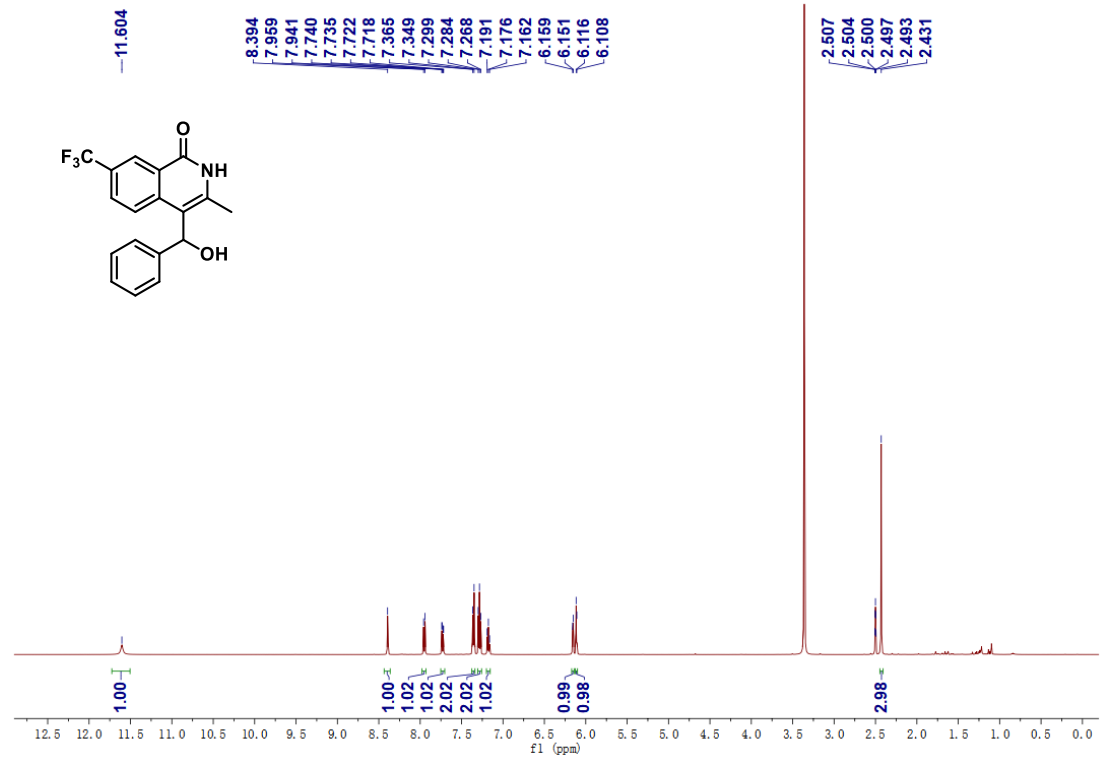
7-bromo-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3am')

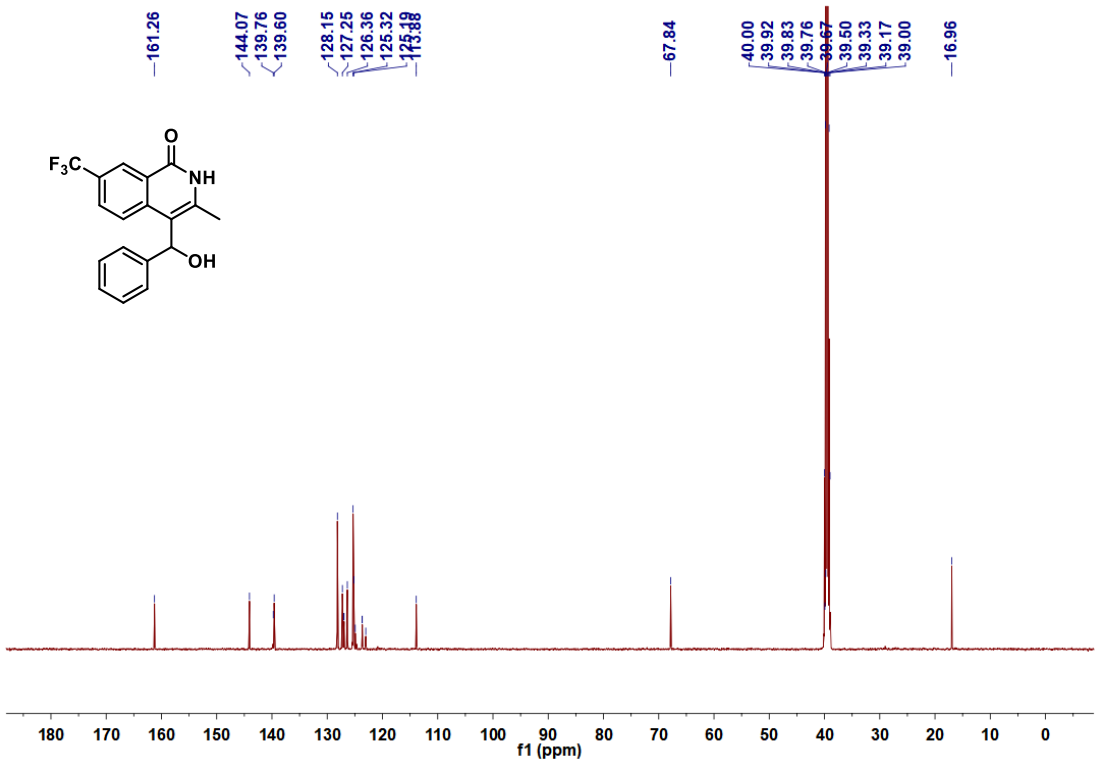


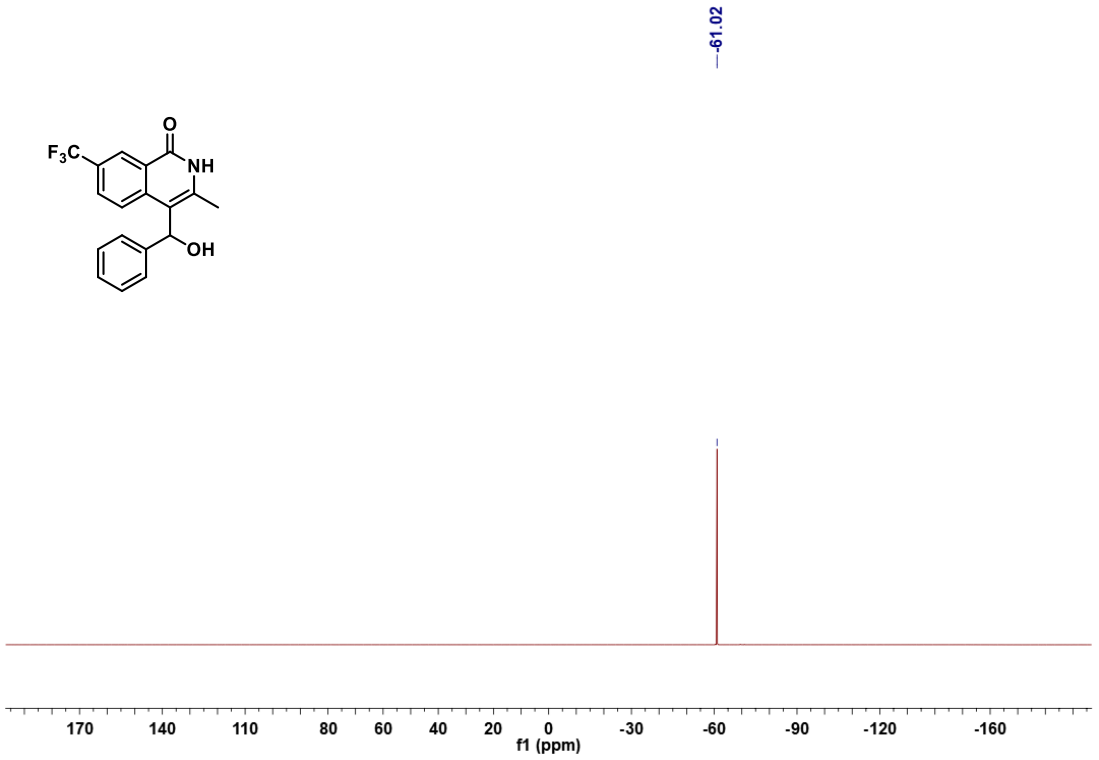
Crude ^{1}H-NMR spectra of
4-(hydroxy(phenyl)methyl)-3-methyl-7-(trifluoromethyl)isoquinolin-1(2H)-one (3an) and
4-(hydroxy(phenyl)methyl)-3-methyl-5-(trifluoromethyl)isoquinolin-1(2H)-one (3an')



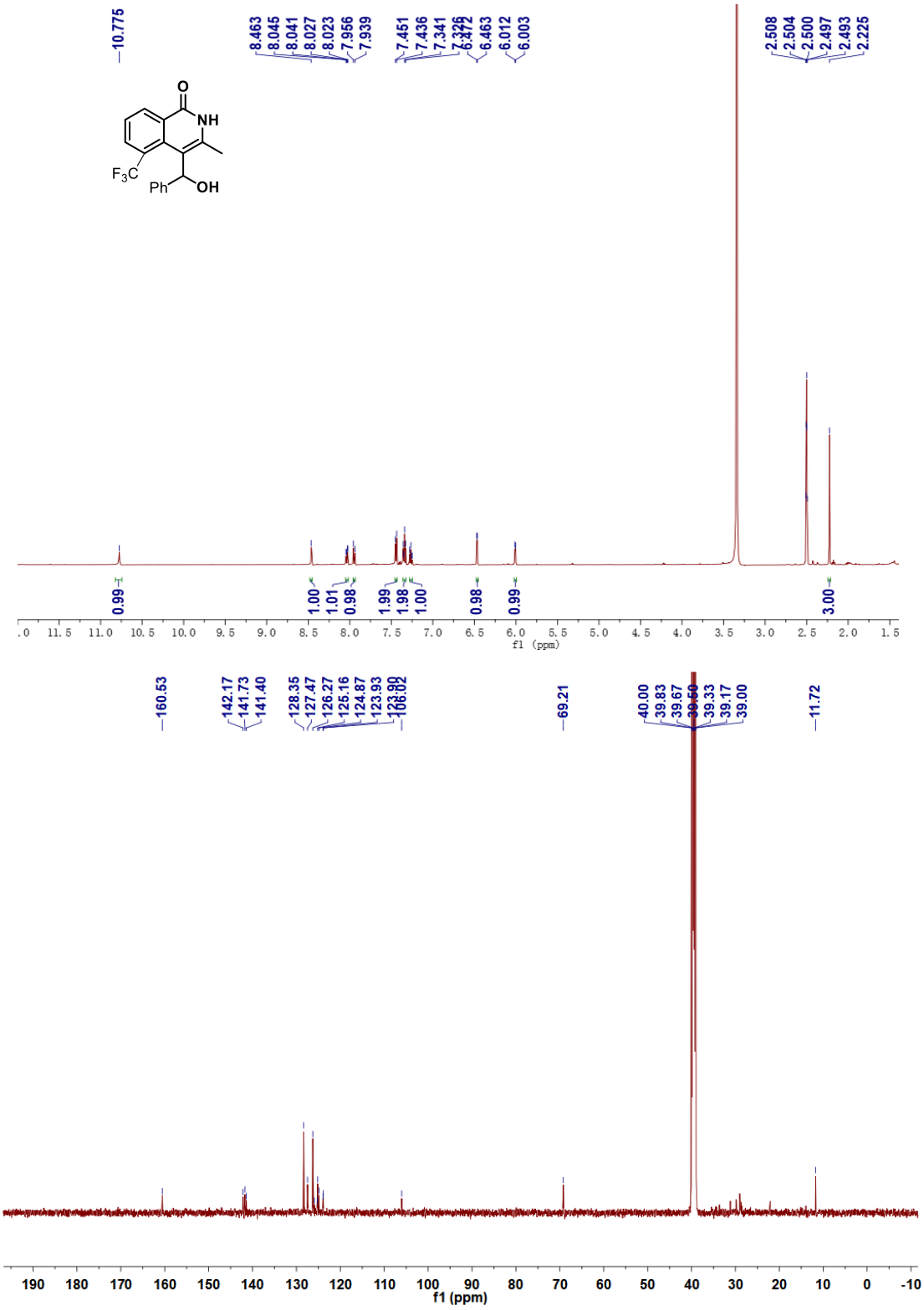
4-(hydroxy(phenyl)methyl)-3-methyl-7-(trifluoromethyl)isoquinolin-1(2H)-one (3an)

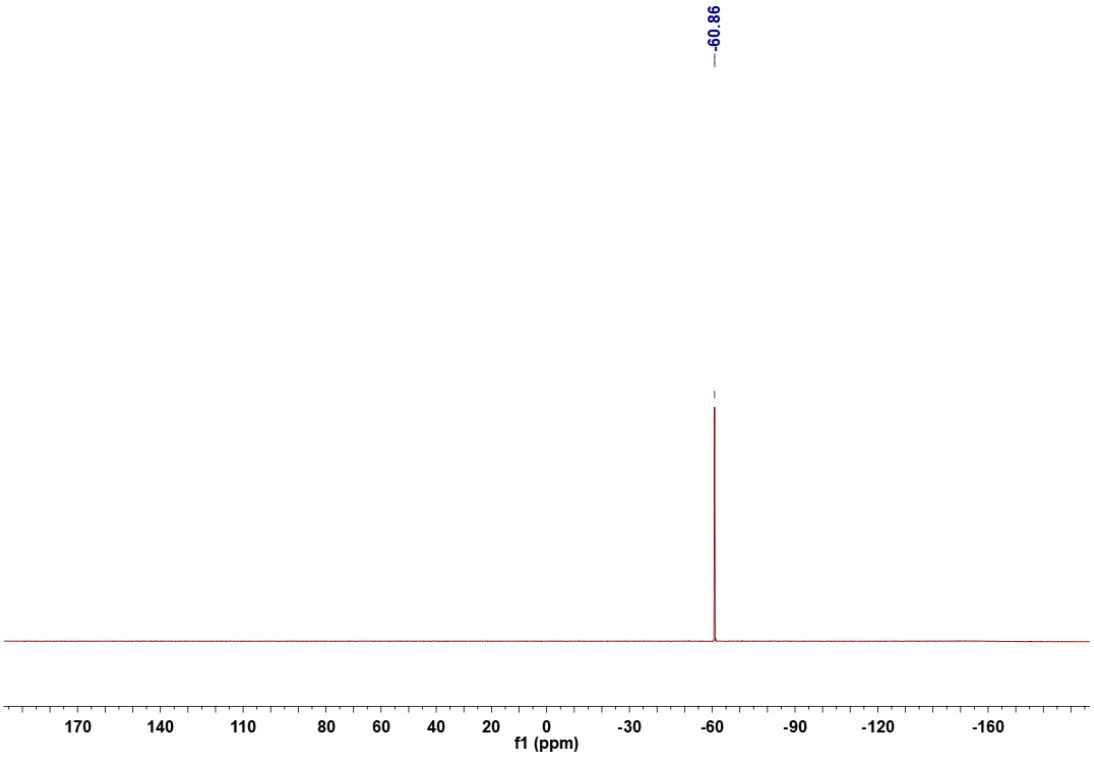



161.26
144.07
139.76
139.60
128.15
127.25
126.36
125.32
67.84
40.00
39.92
39.83
39.76
39.67
39.50
39.33
39.17
39.00
16.96
O
NH
OH
F3C
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

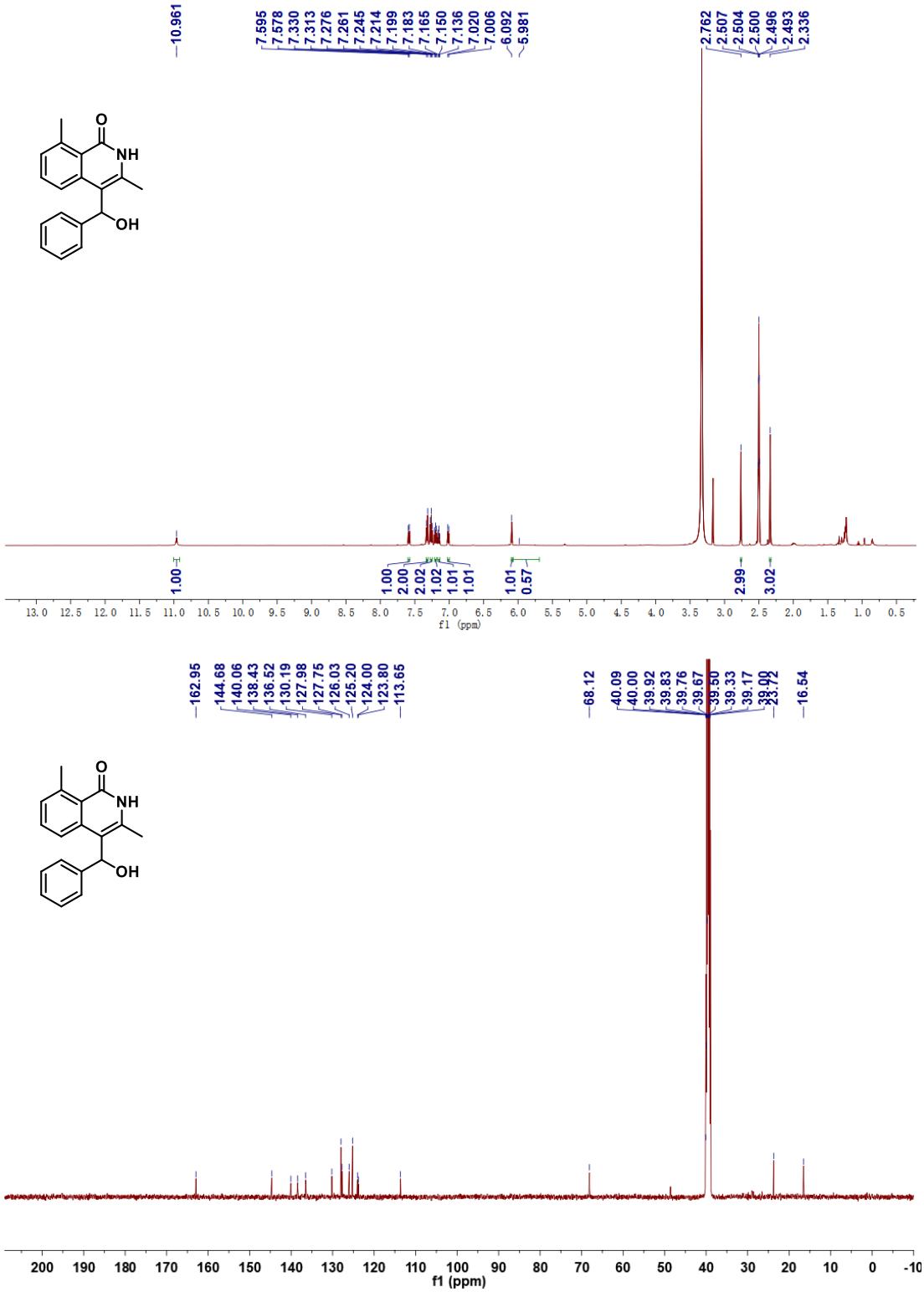

-61.02
O
NH
OH
F3C
170 140 110 80 60 40 20 0 -30 -60 -90 -120 -160
f1 (ppm)

4-(hydroxy(phenyl)methyl)-3-methyl-5-(trifluoromethyl)isoquinolin-1(2H)-one (3an')

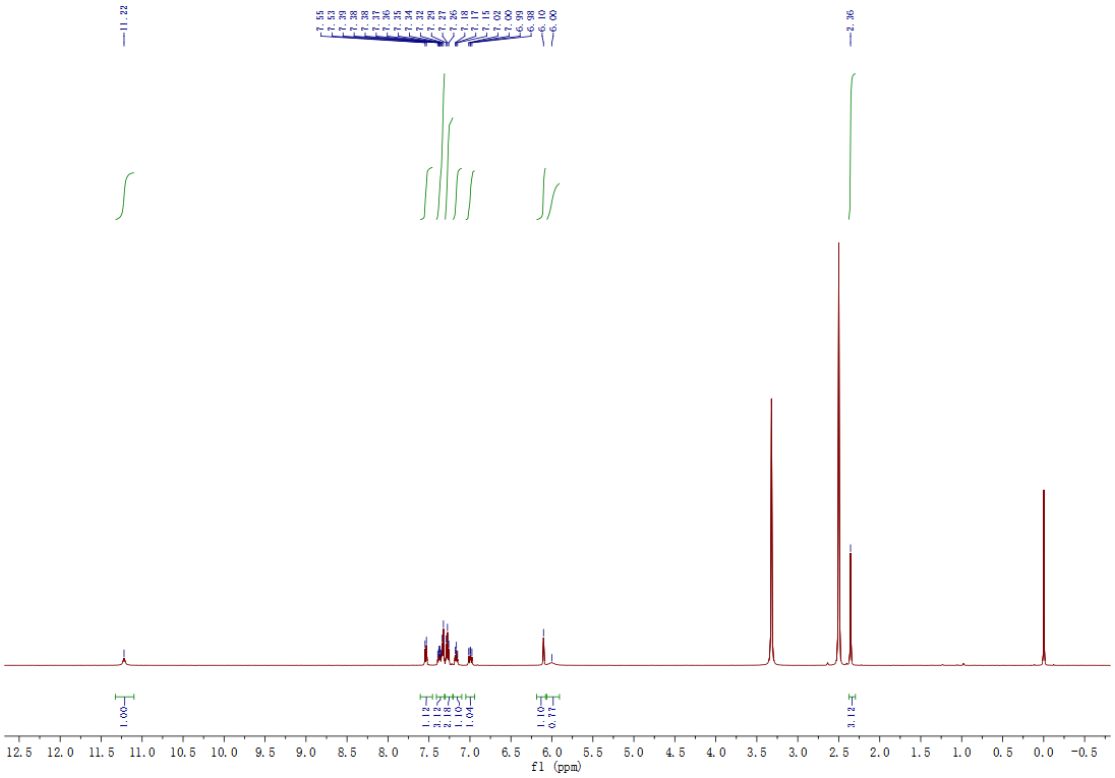


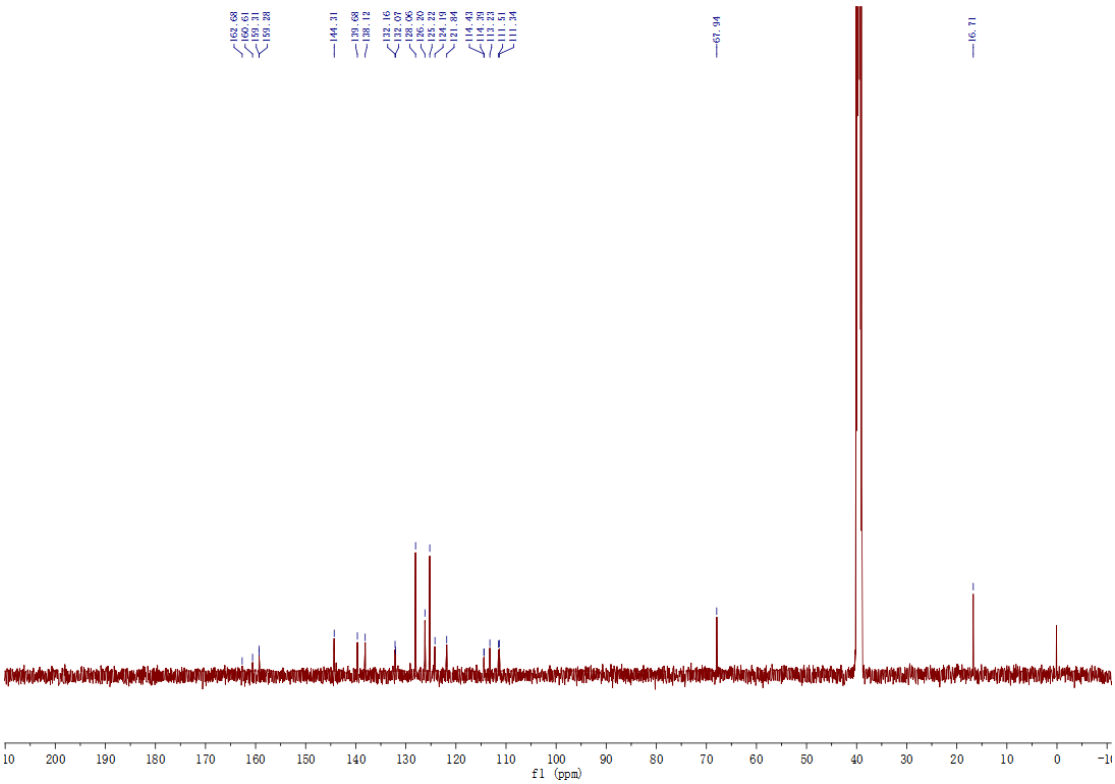

-60.86
170
140
110
80
60
40
20
0
-30
-60
-90
-120
-160
f1 (ppm)

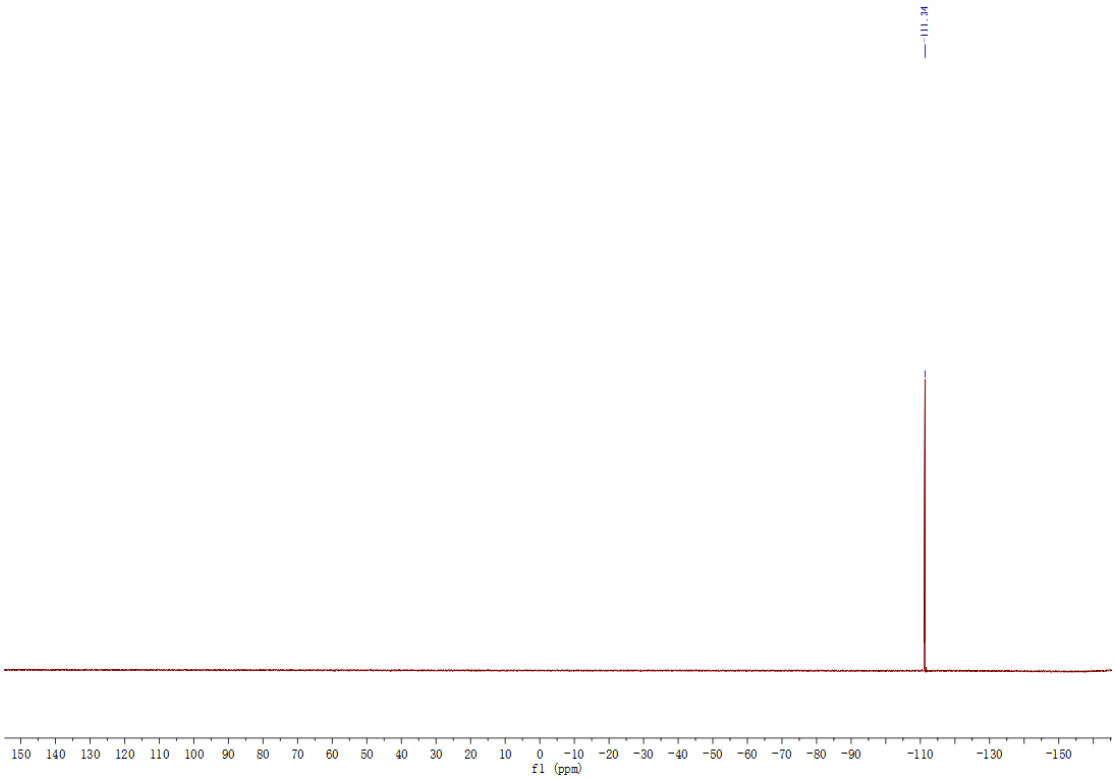
4-(hydroxy(phenyl)methyl)-3,8-dimethylisoquinolin-1(2H)-one (3ao)



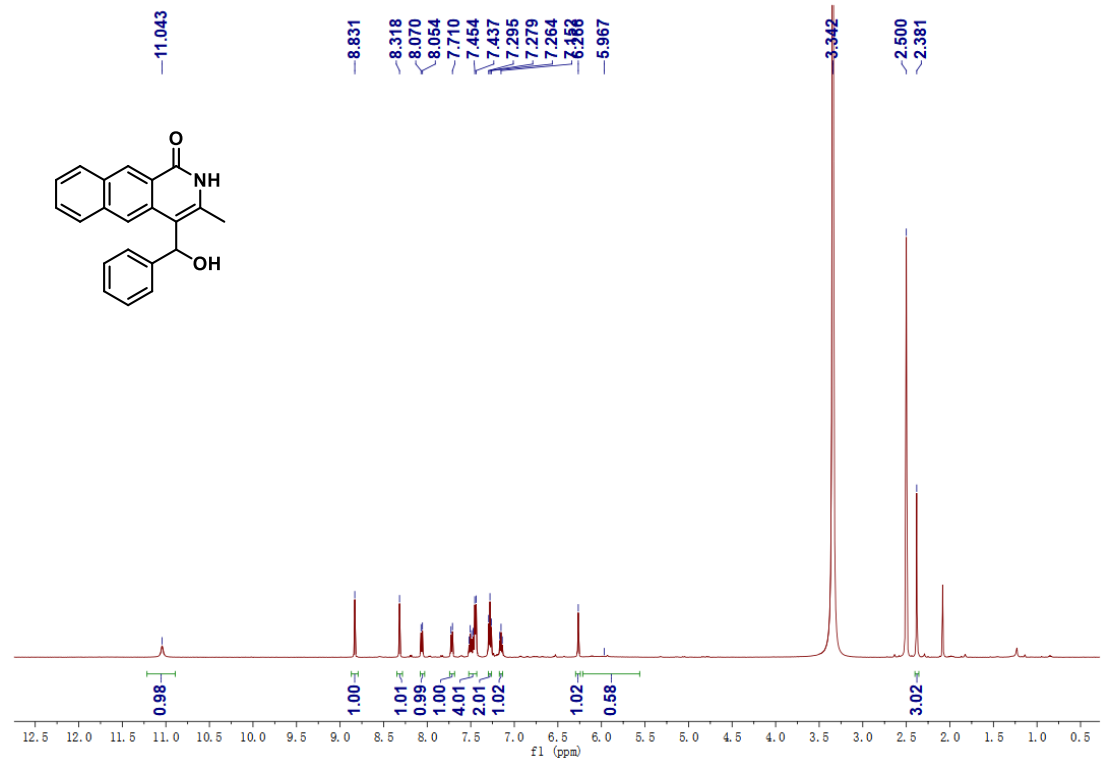
8-fluoro-4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3ap)

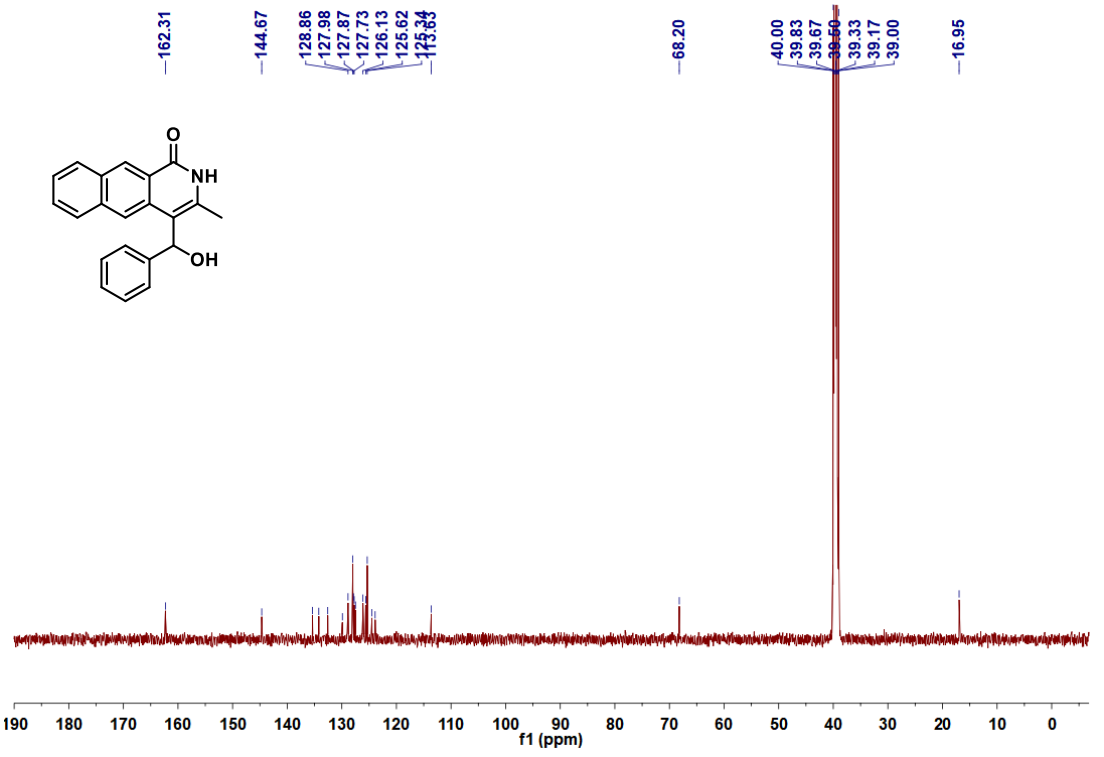




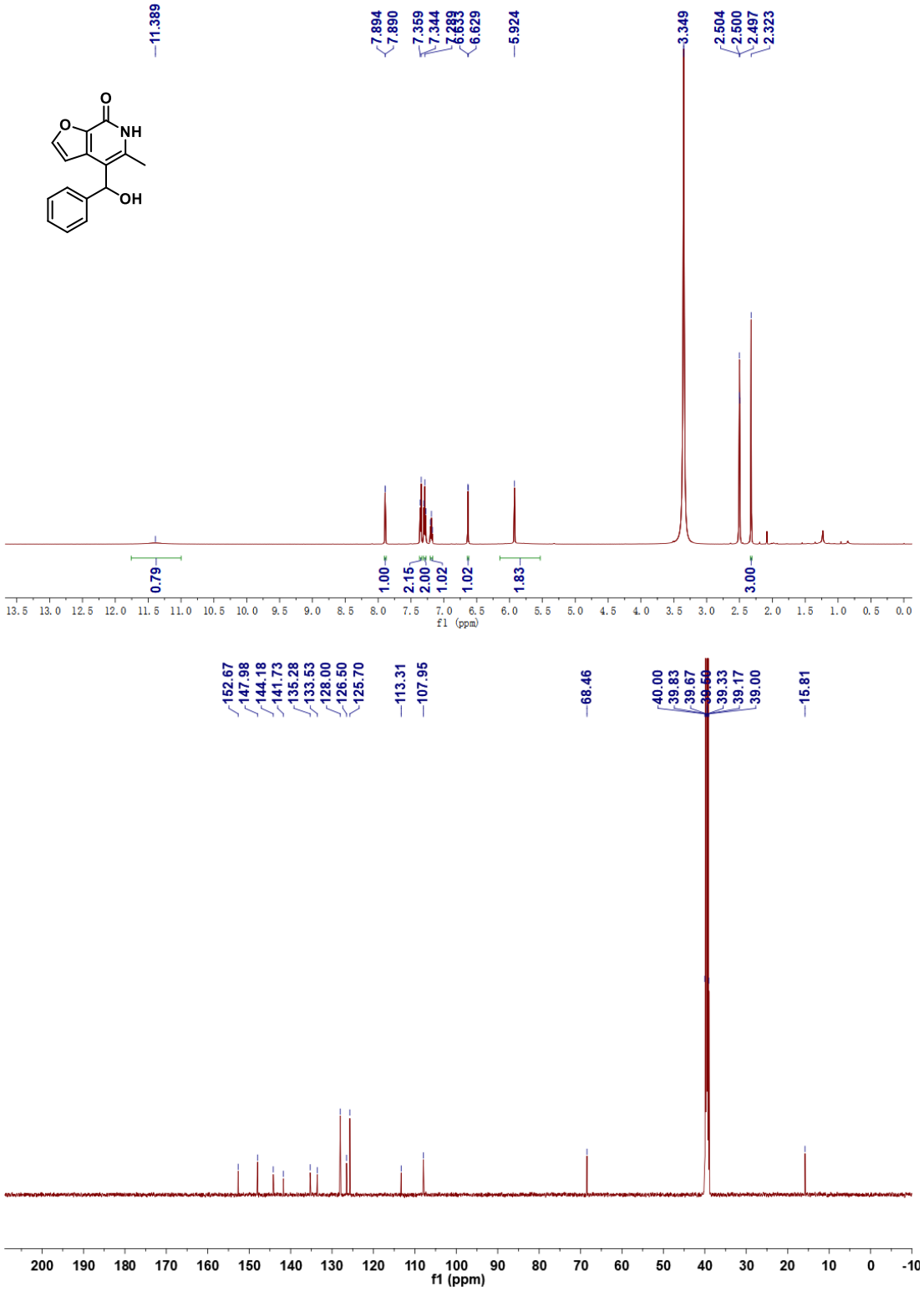

-111.34
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150
f1 (ppm)

4-(hydroxy(phenyl)methyl)-3-methylbenzo[g]isoquinolin-1(2H)-one (3aq)

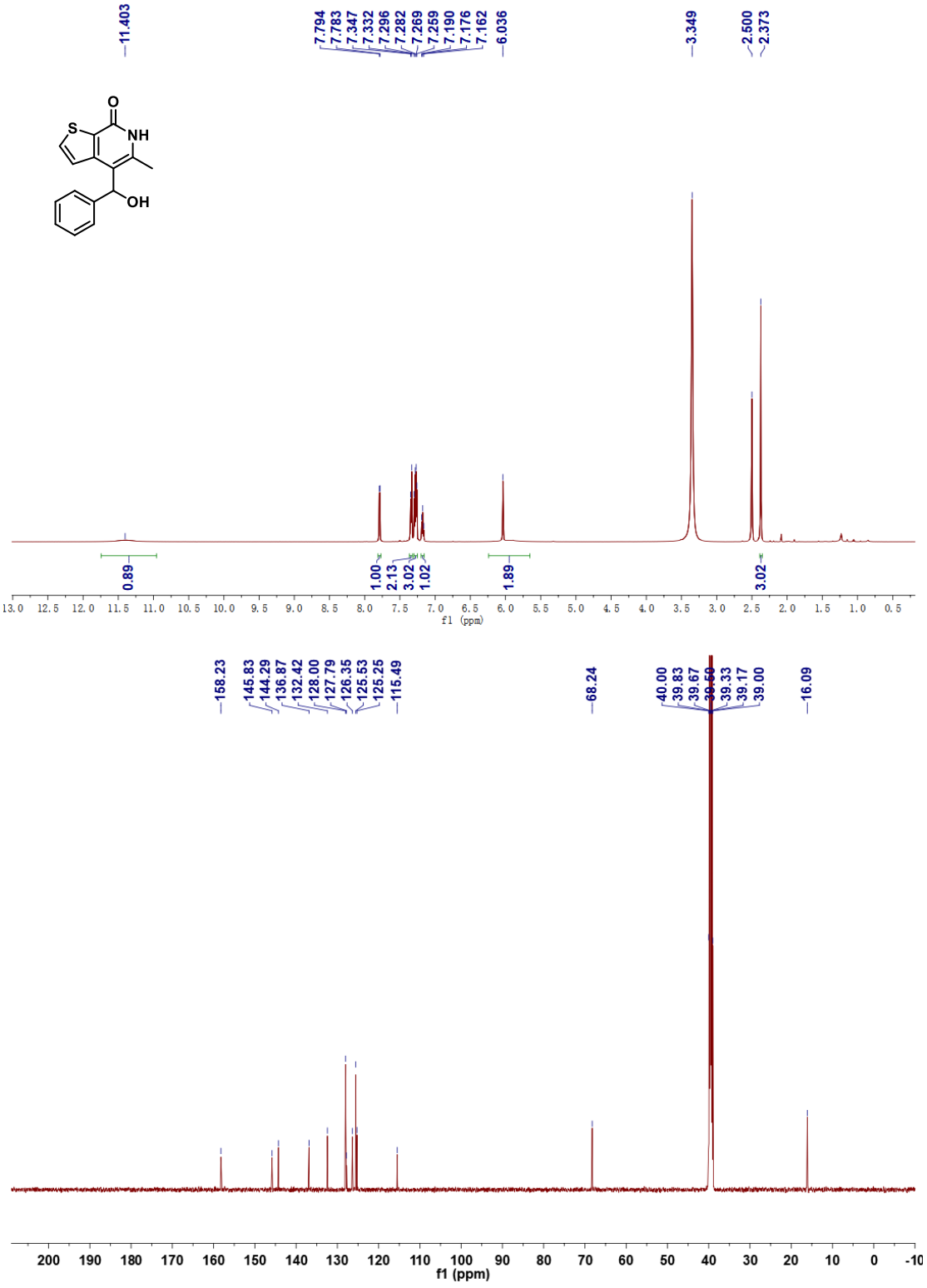




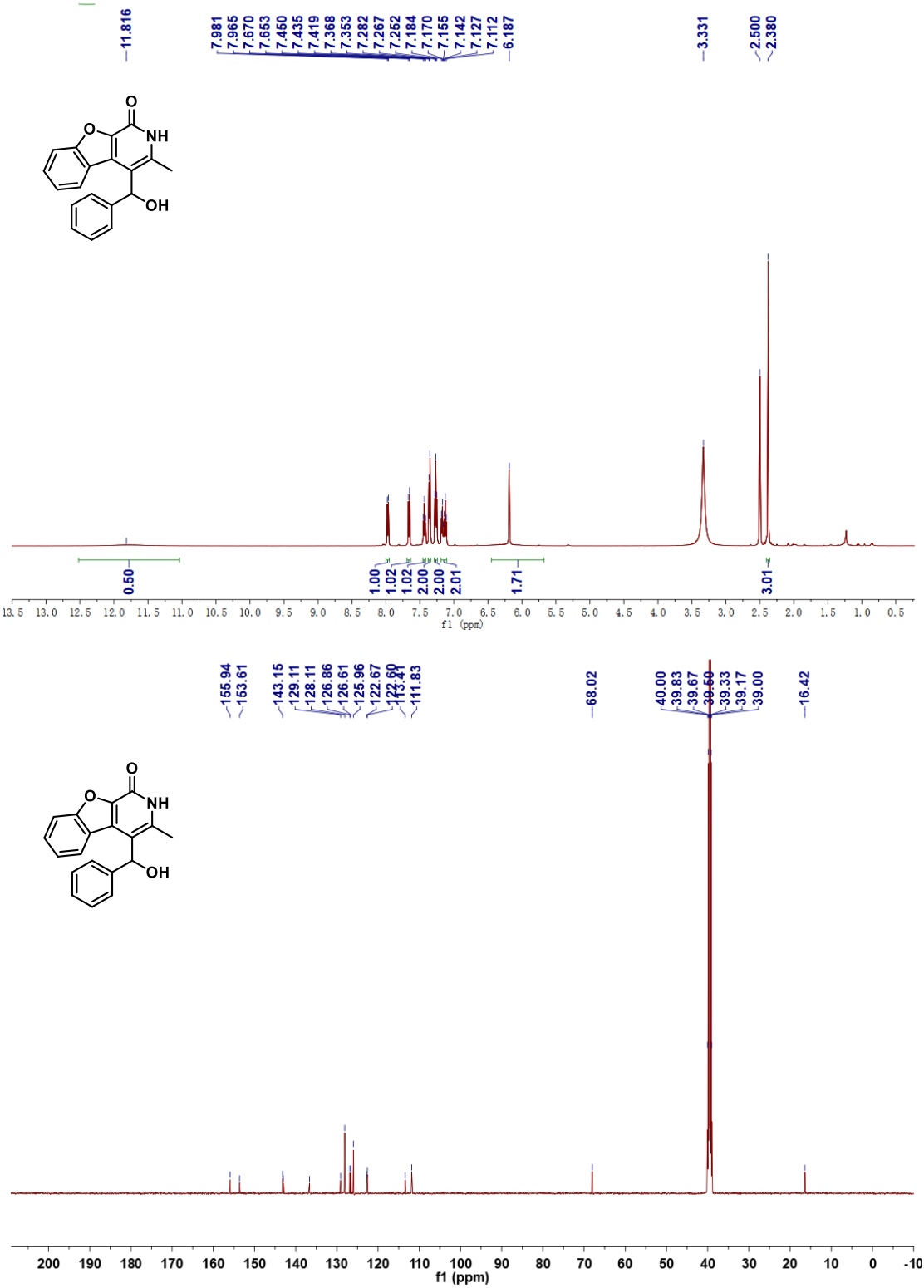
4-(hydroxy(phenyl)methyl)-5-methylfuro[2,3-c]pyridin-7(6H)-one (3ar)



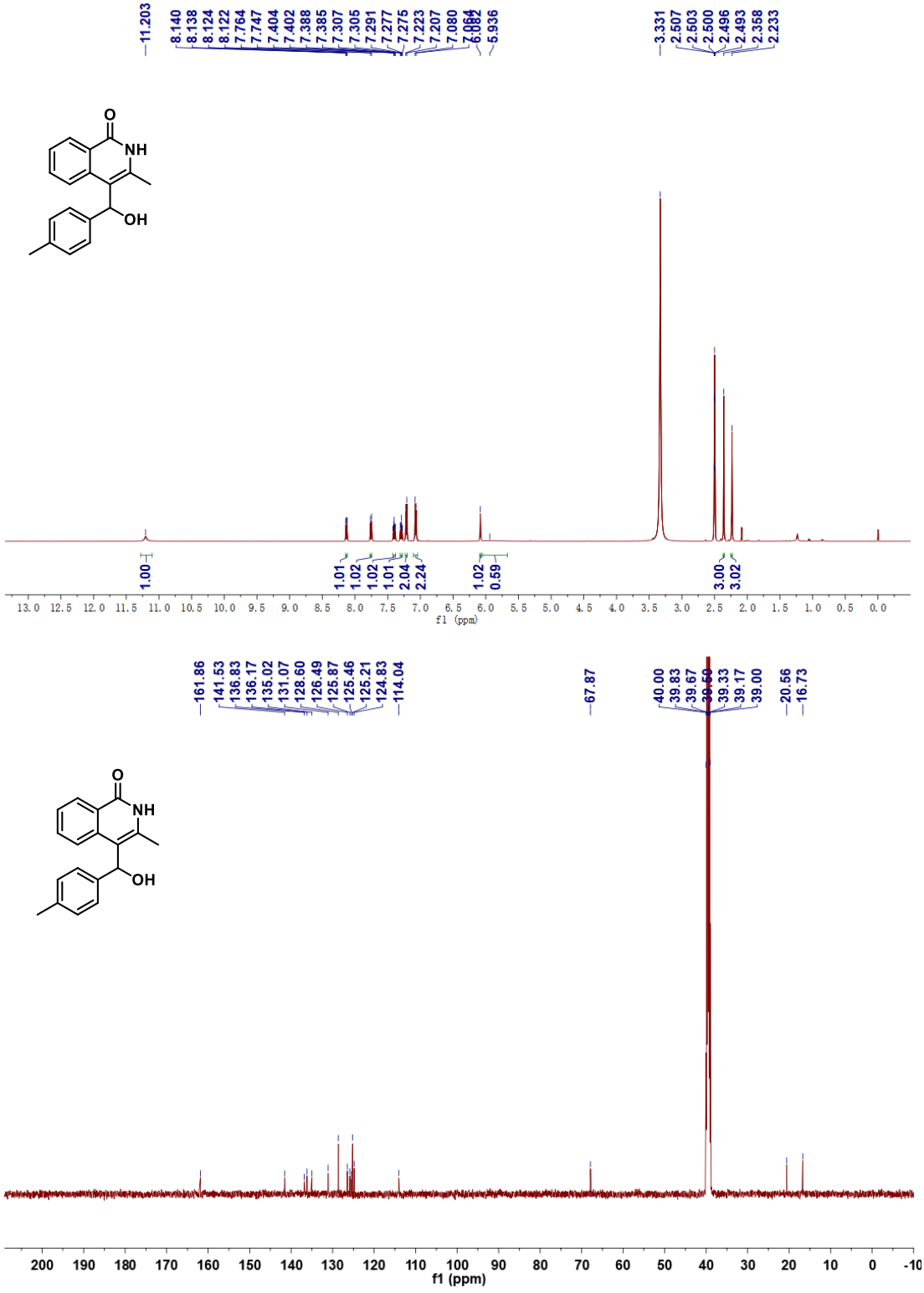
4-(hydroxy(phenyl)methyl)-5-methylthieno[2,3-c]pyridin-7(6H)-one (3as)



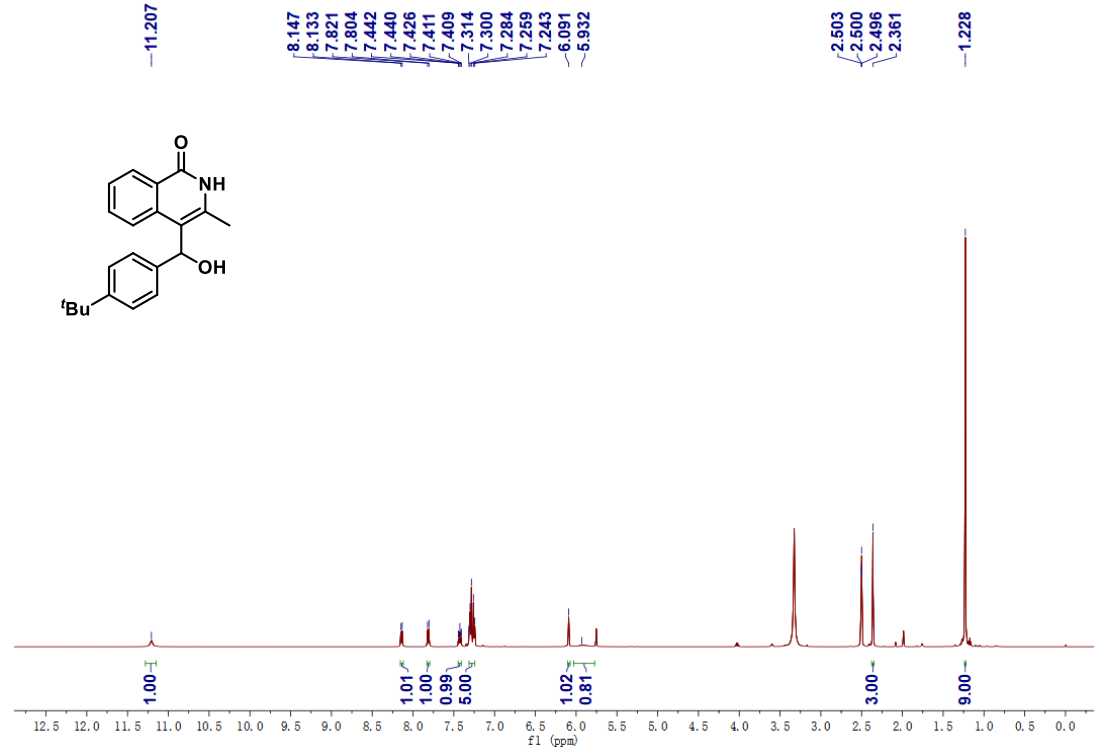
4-(hydroxy(phenyl)methyl)-3-methylbenzofuro[2,3-c]pyridin-1(2H)-one (3at)

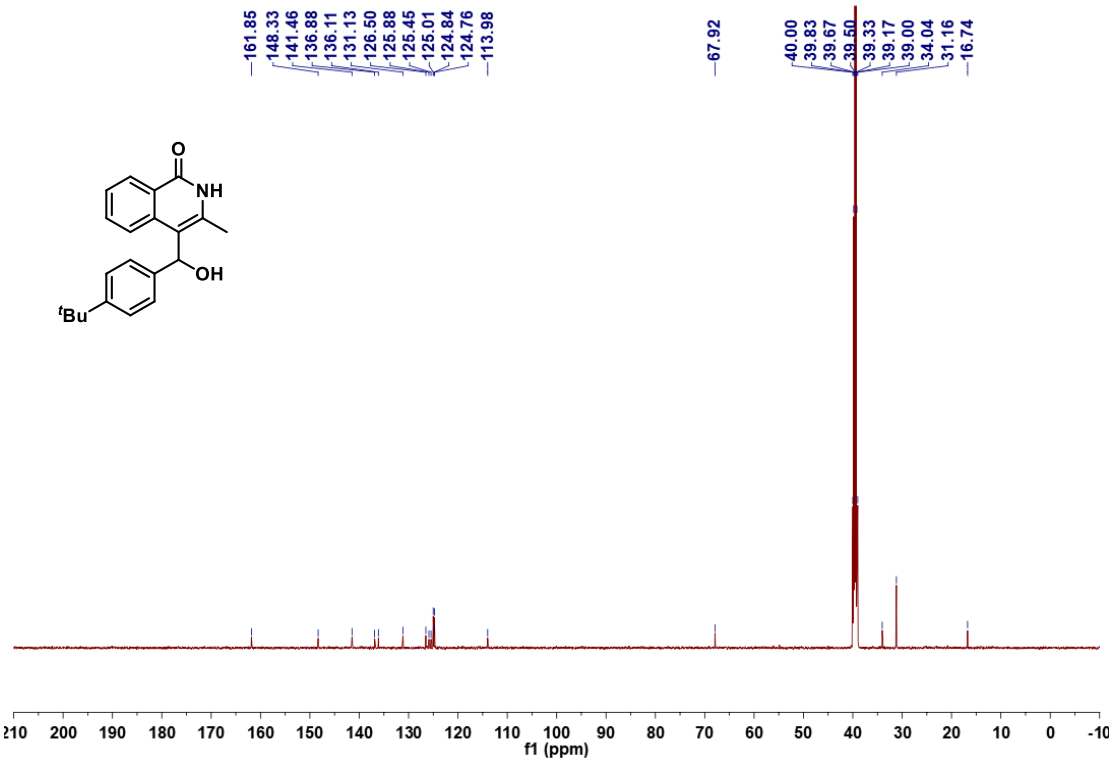


4-(hydroxy(p-tolyl)methyl)-3-methylisoquinolin-1(2H)-one (3au)

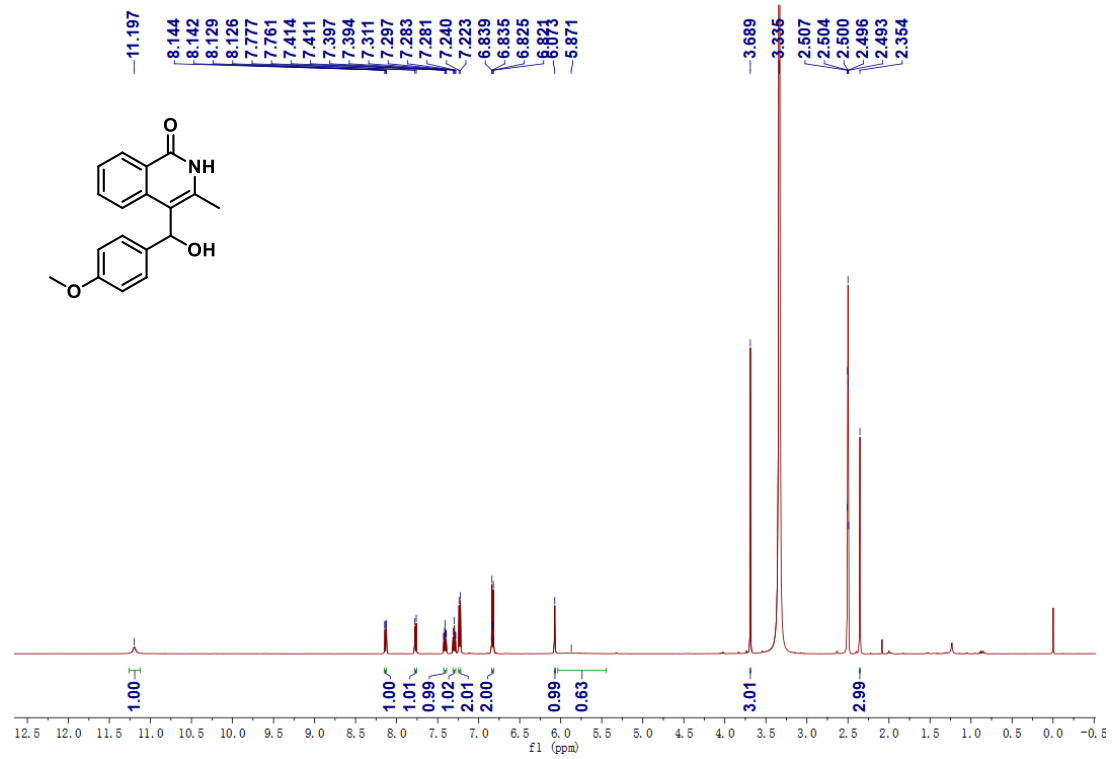


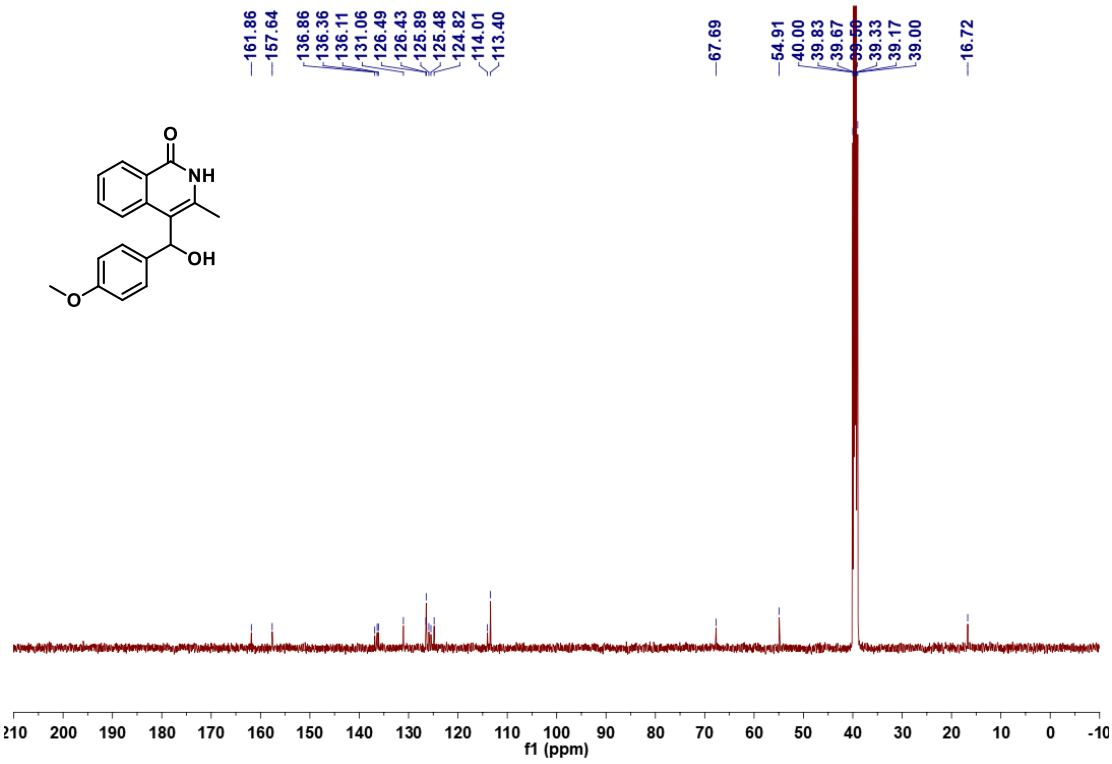
4-((4-(tert-butyl)phenyl)(hydroxy)methyl)-3-methylisoquinolin-1(2H)-one (3av)



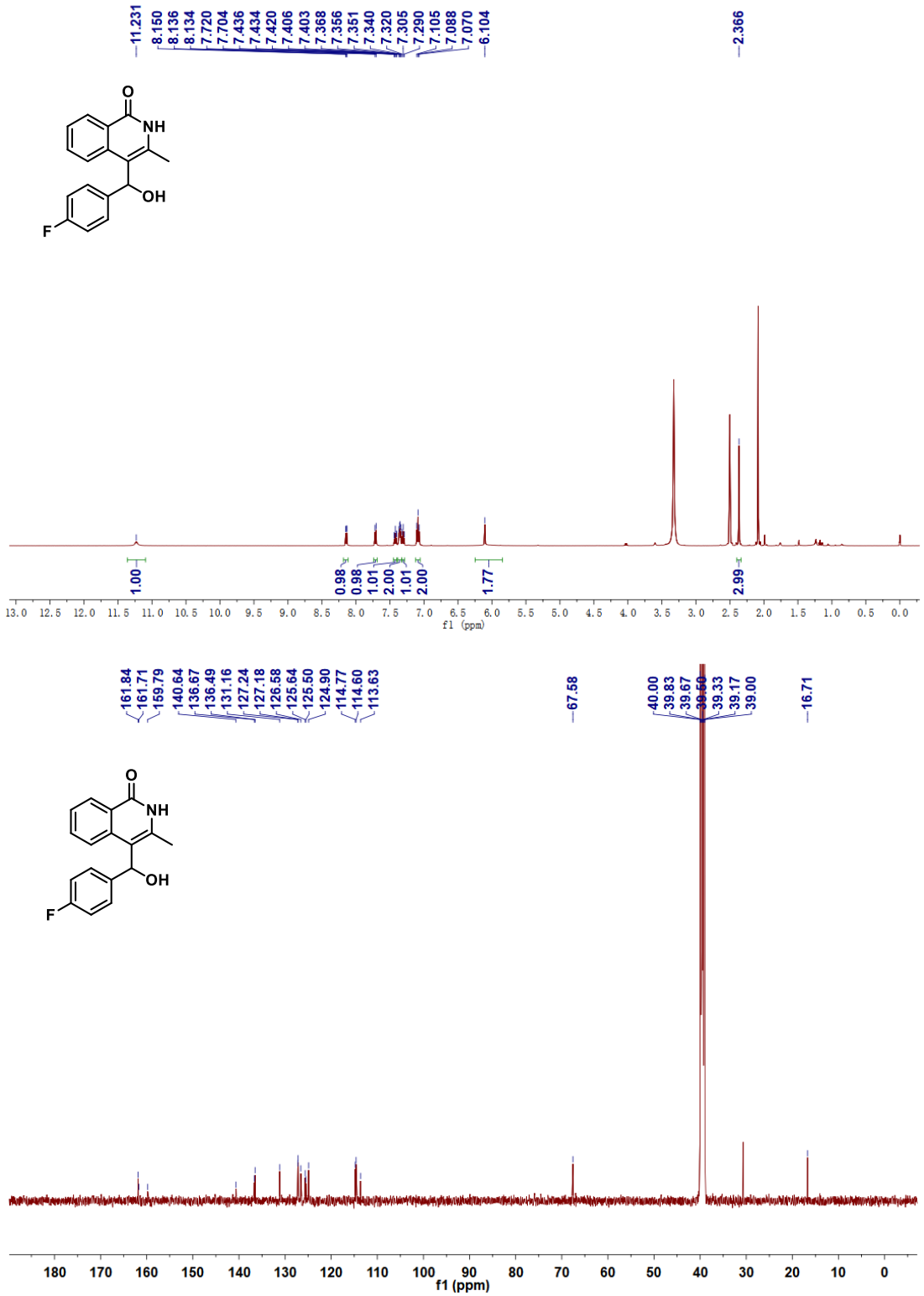


4-(hydroxy(4-methoxyphenyl)methyl)-3-methylisoquinolin-1(2H)-one (3aw)

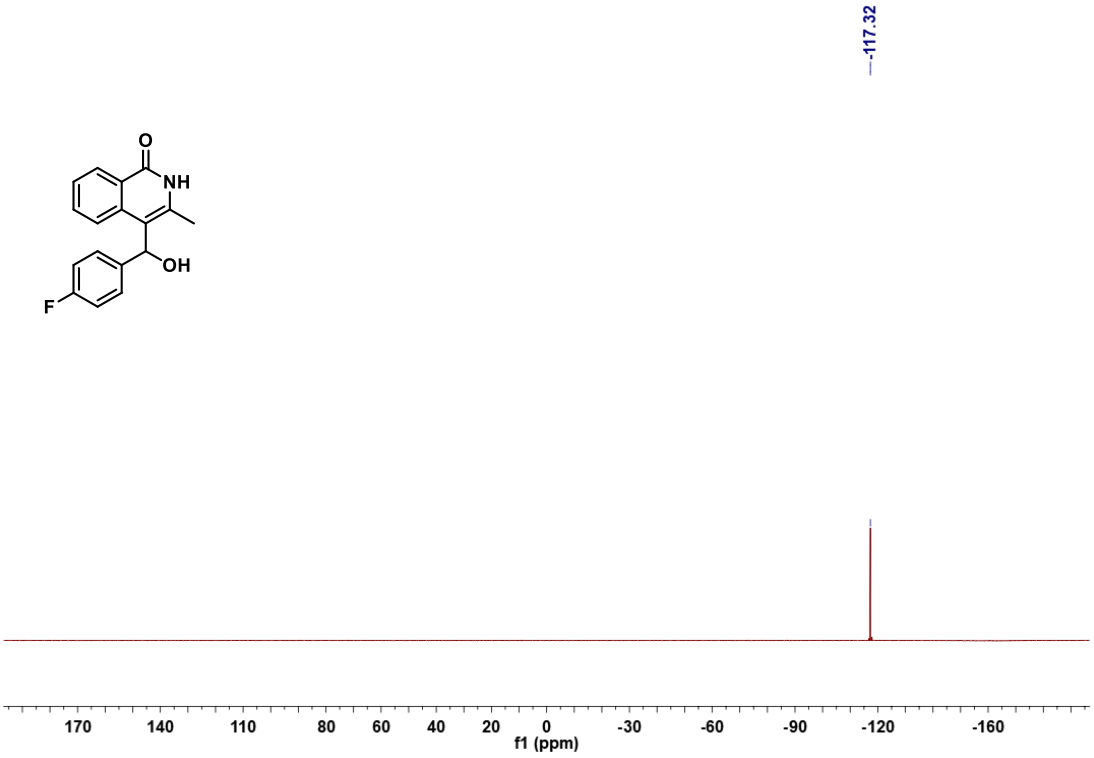




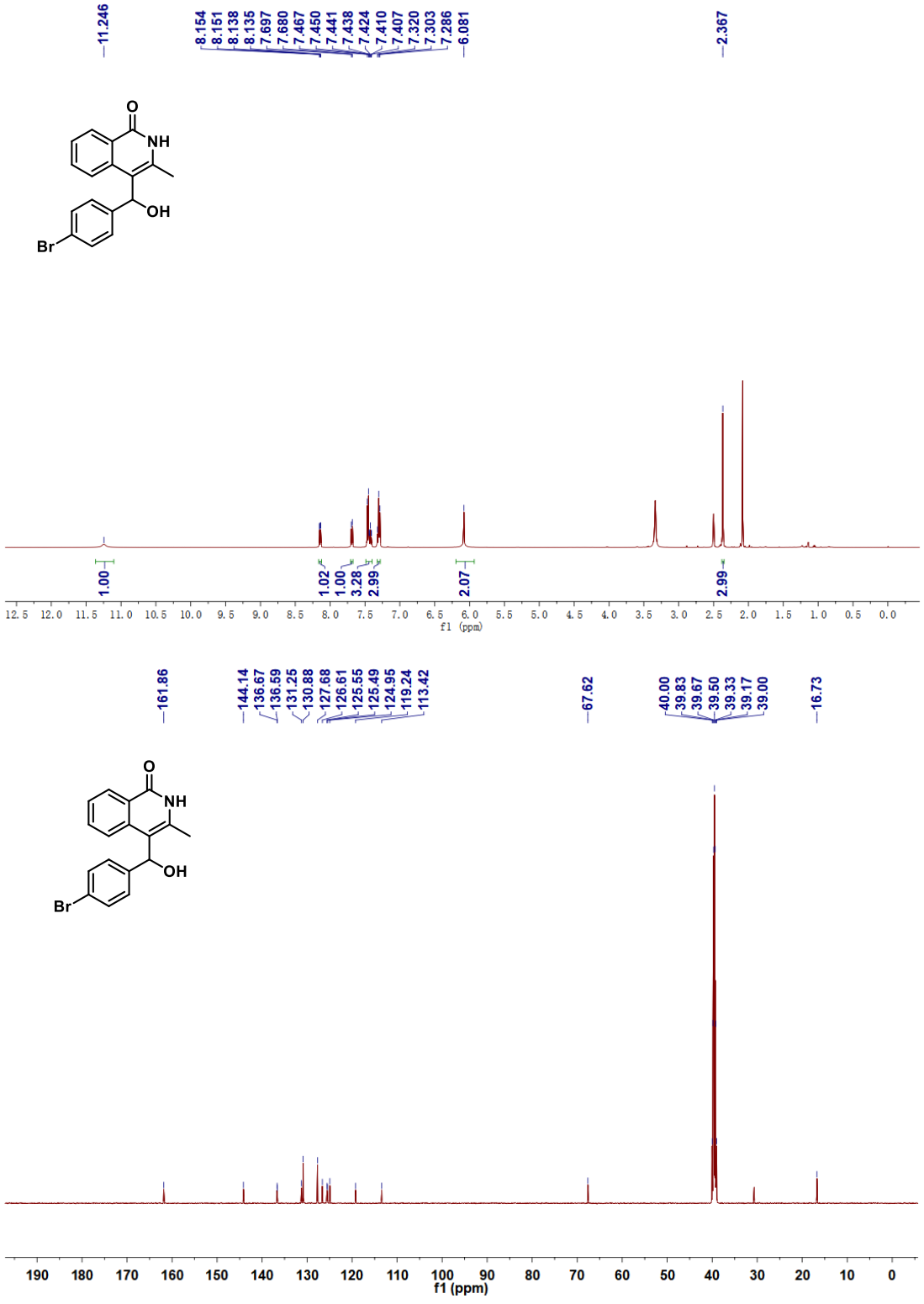
4-((4-fluorophenyl)(hydroxy)methyl)-3-methylisoquinolin-1(2H)-one (3ax)



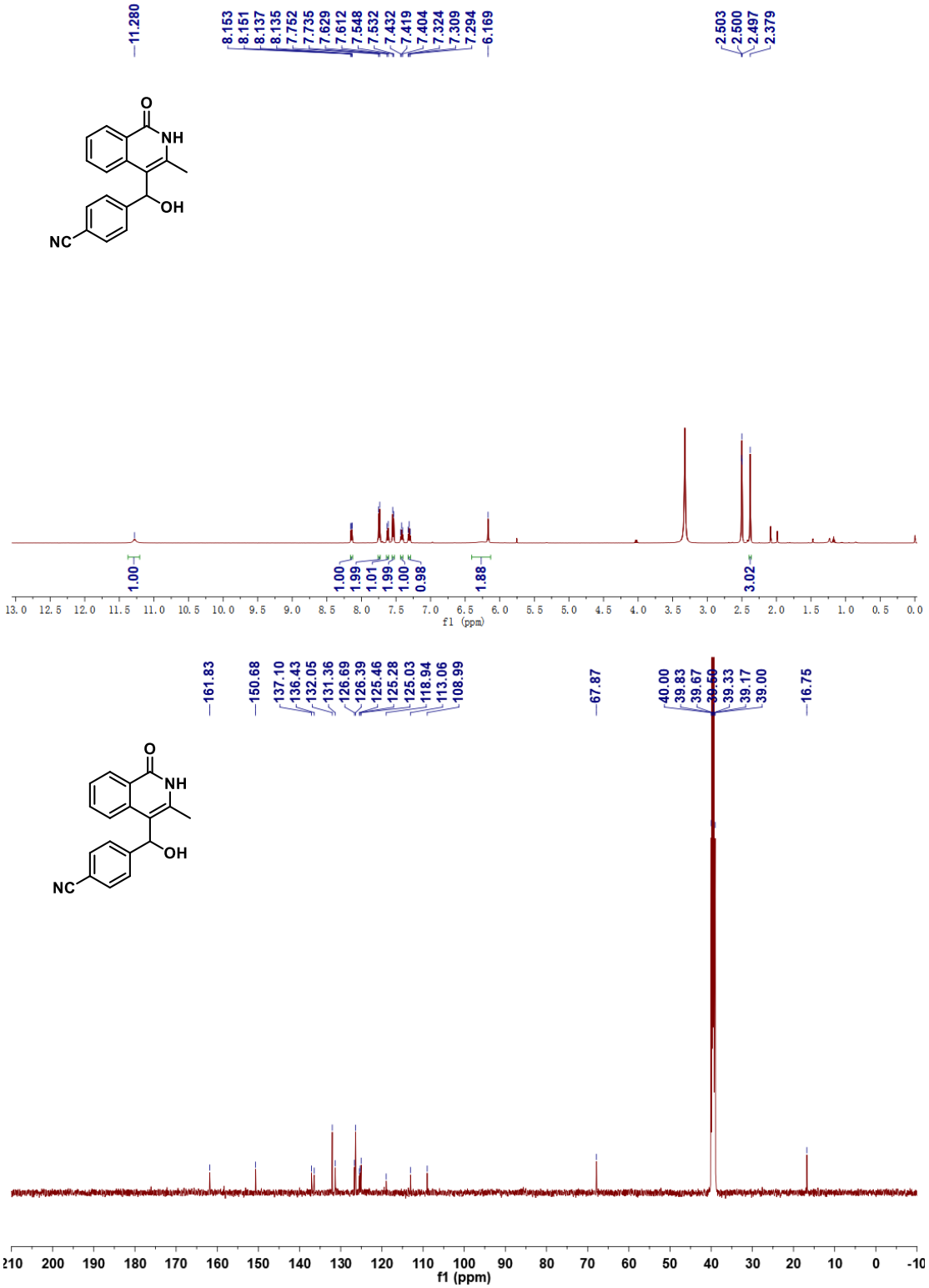
O
NH
OH
F


-117.32
170
140
110
80
60
40
20
0
-30
-60
-90
-120
-160
f1 (ppm)

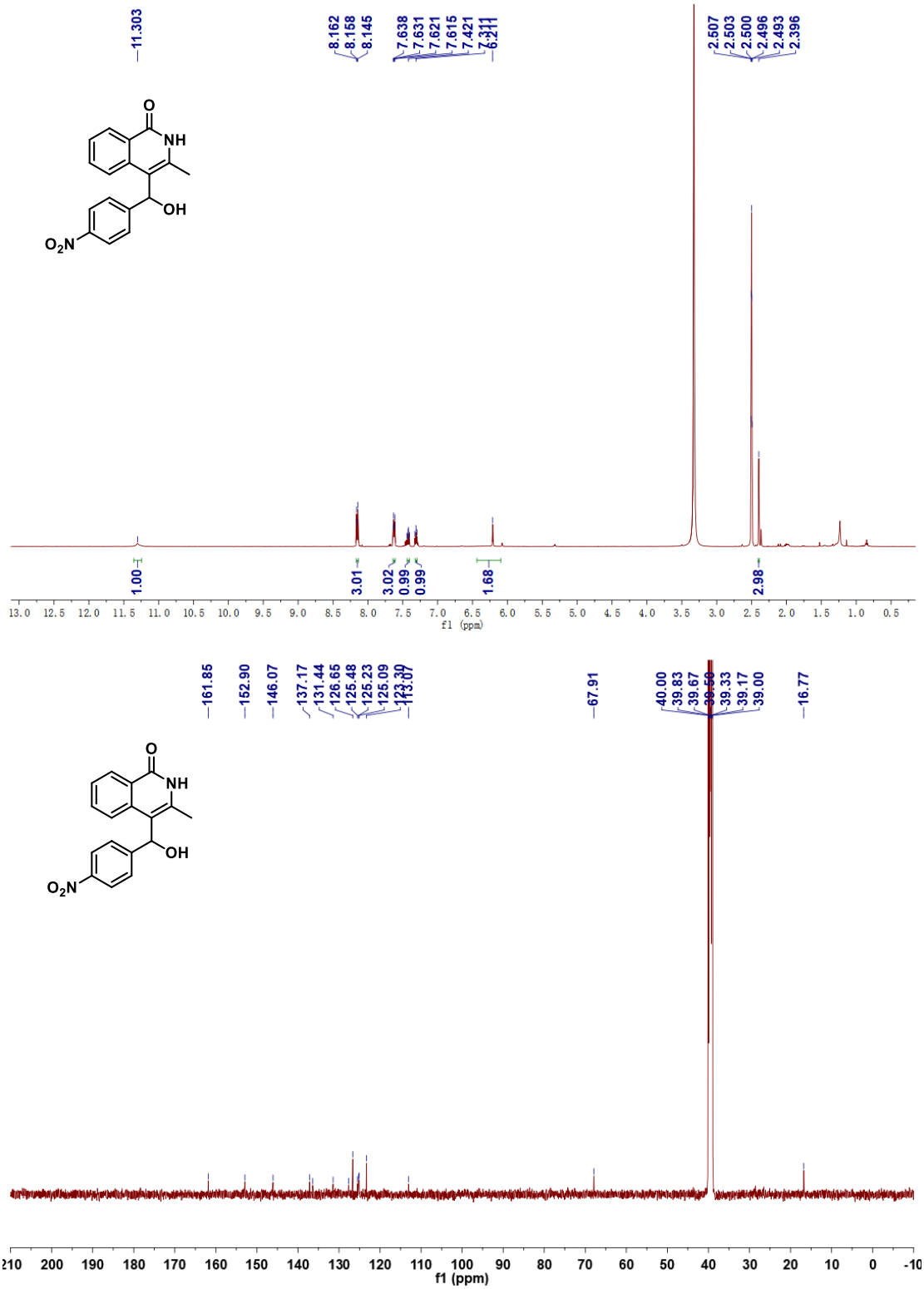
4-((4-bromophenyl)(hydroxy)methyl)-3-methylisoquinolin-1(2H)-one (3ay)



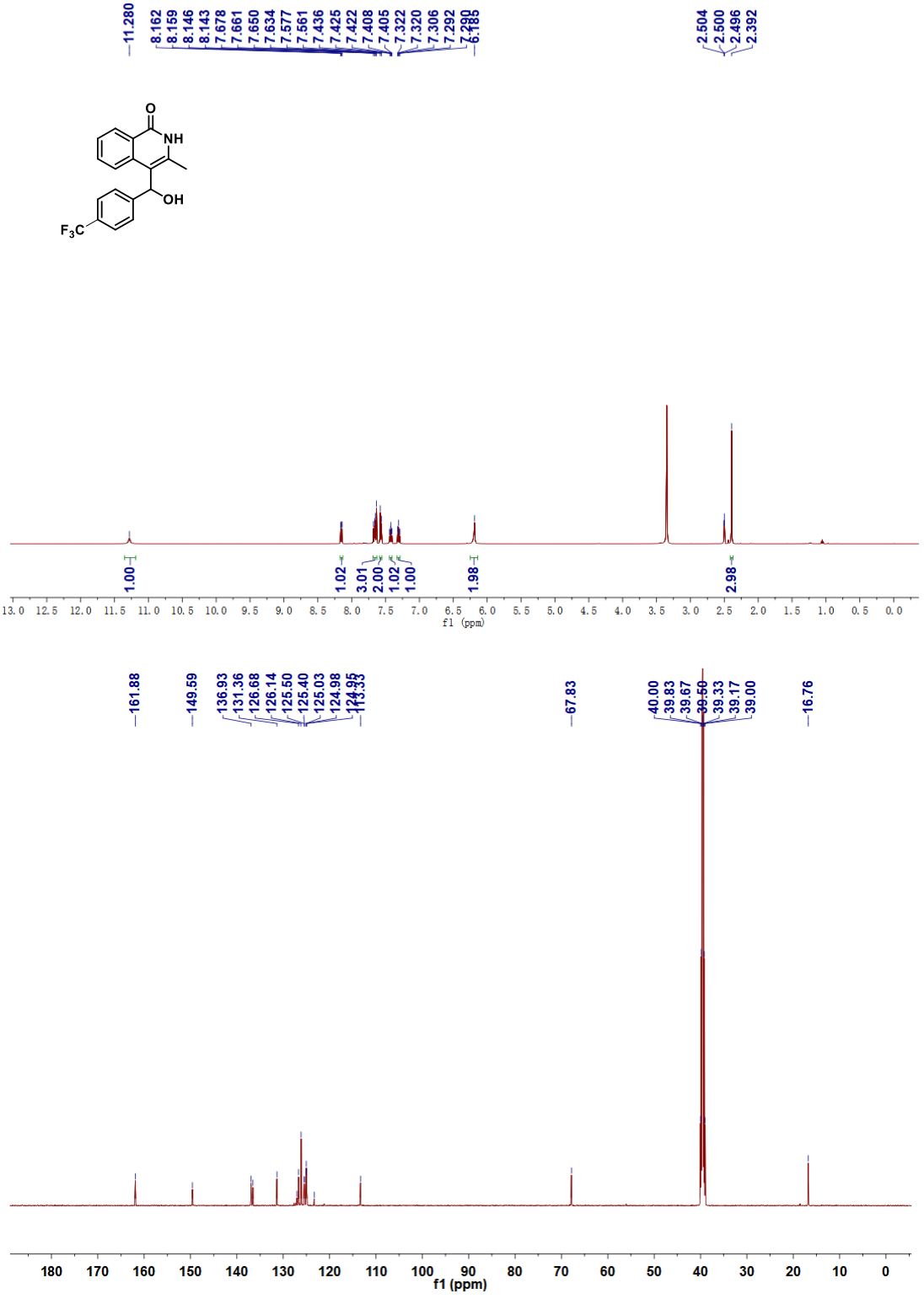
4-(hydroxy(3-methyl-1-oxo-1,2-dihydroisoquinolin-4-yl)methyl)benzonitrile (3az)

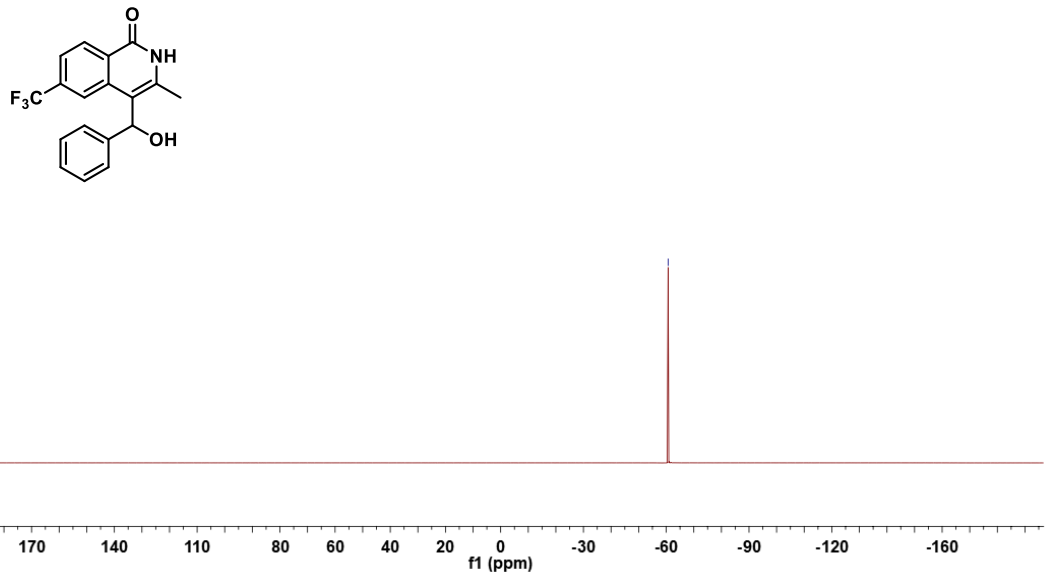


4-(hydroxy(3-methyl-1-oxo-1,2-dihydroisoquinolin-4-yl)methyl)benzonitrile (3ba)

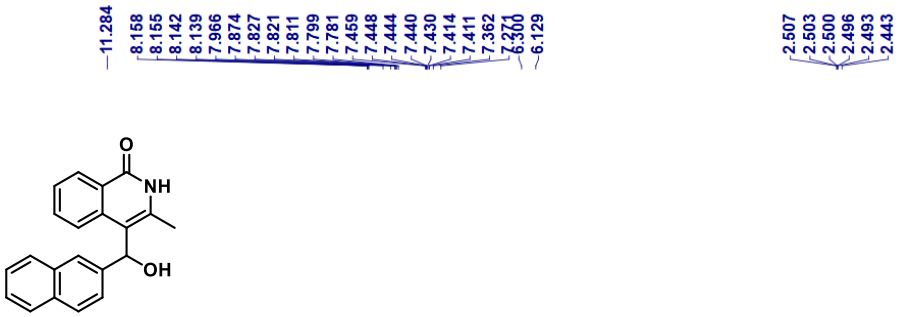


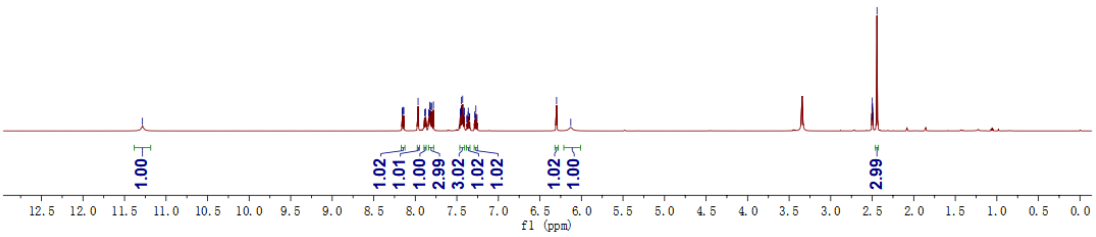
4-(hydroxy(4-(trifluoromethyl)phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3bb)

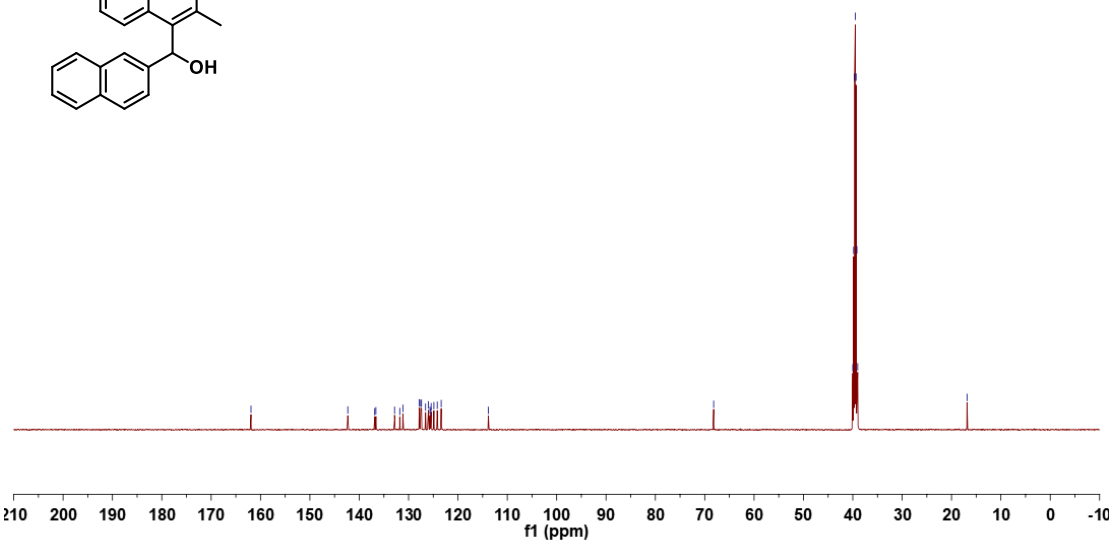



-60.69
O
NH
F3C
OH
170
140
110
80
60
40
20
0
-30
-60
-90
-120
-160
f1 (ppm)

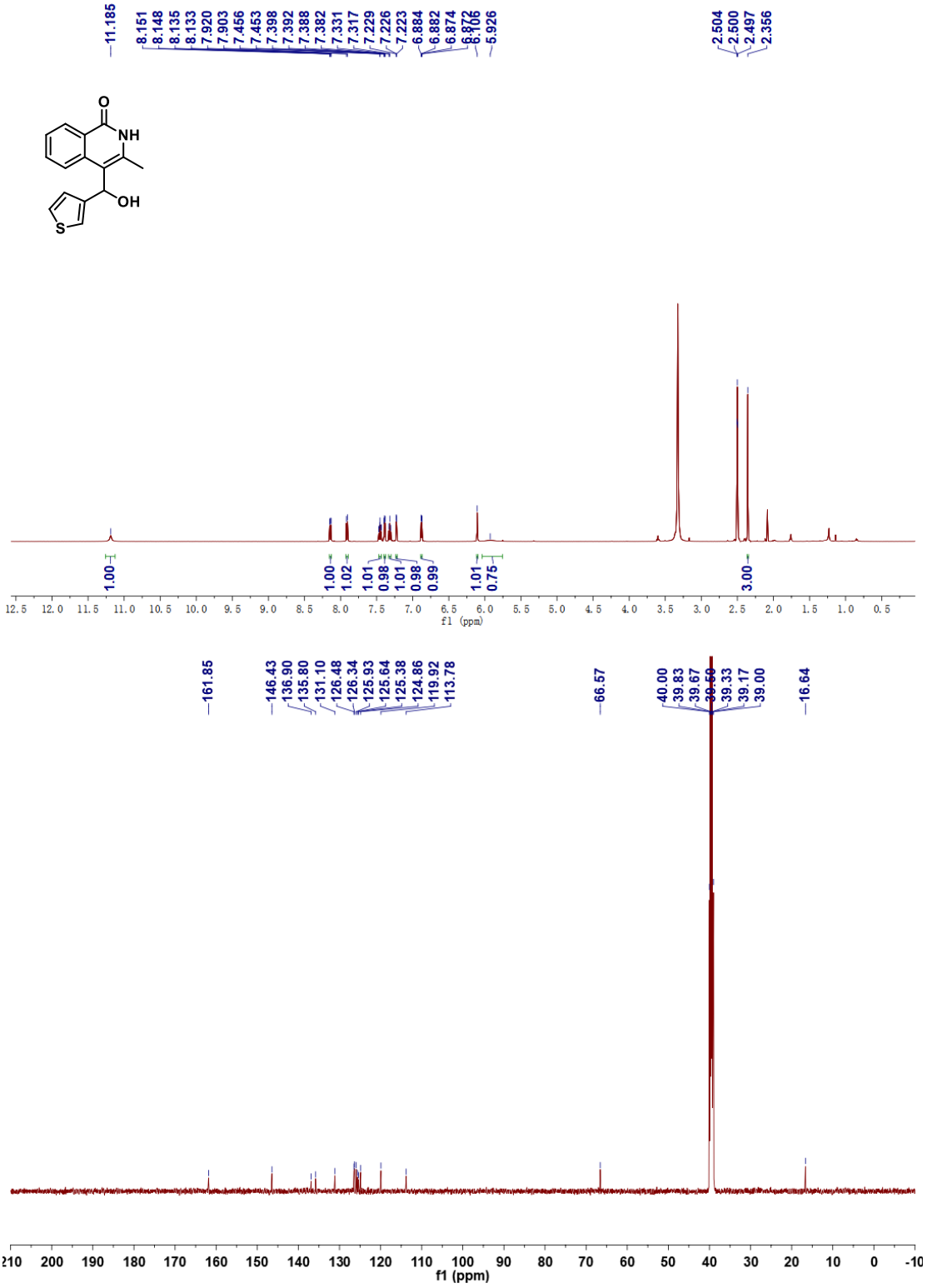
4-(hydroxy(naphthalen-2-yl)methyl)-3-methylisoquinolin-1(2H)-one (3bc)



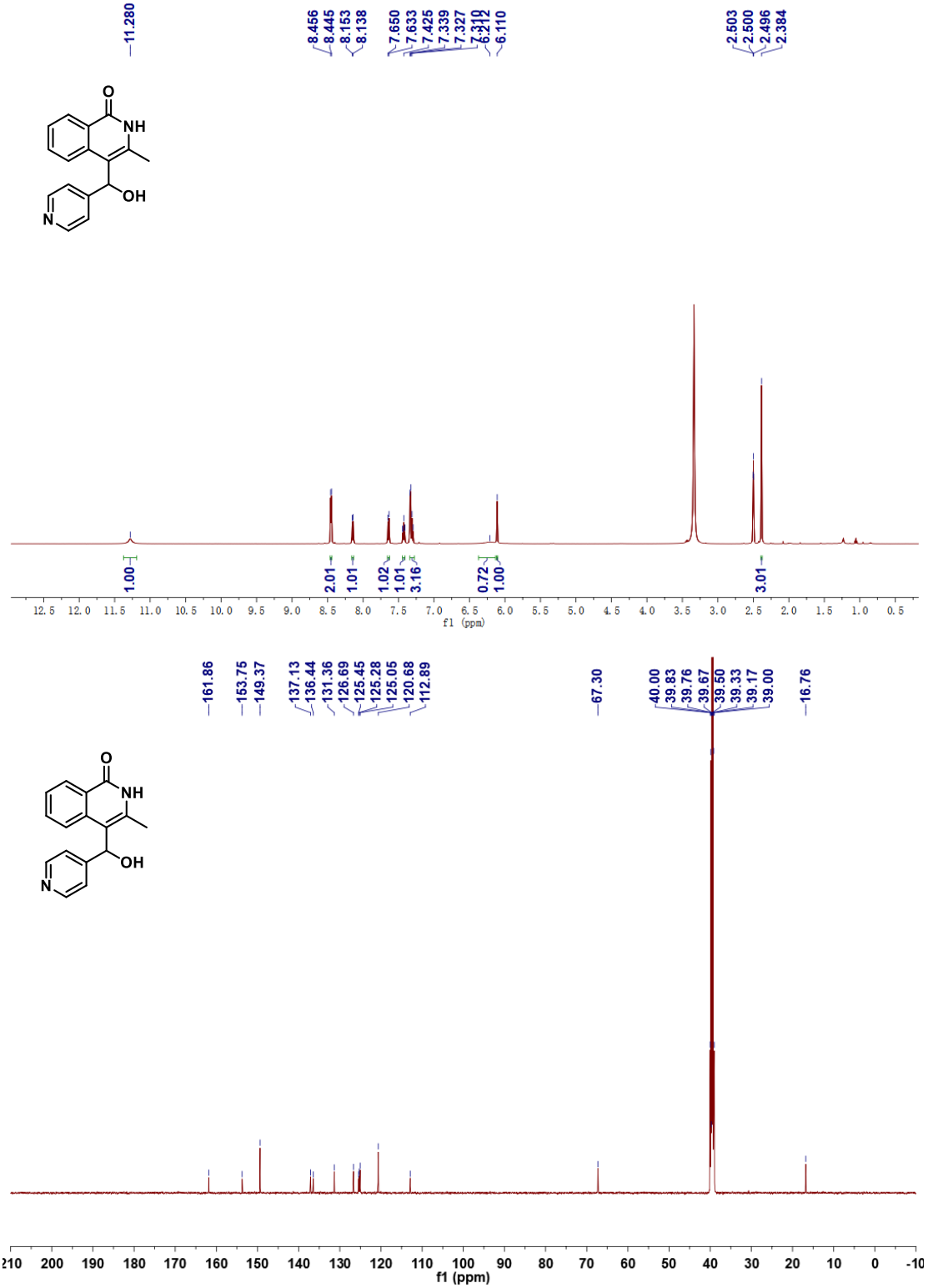




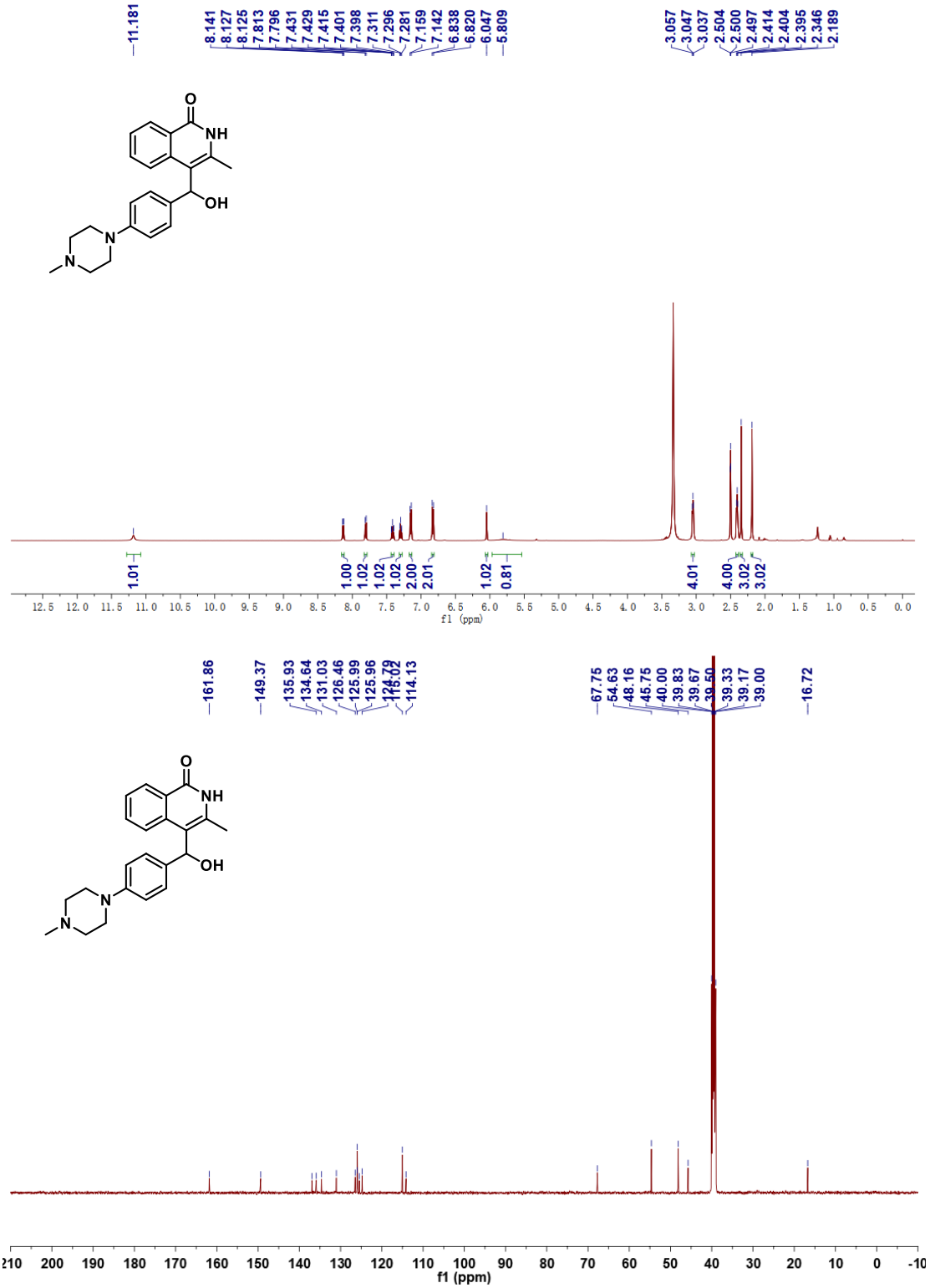
4-(hydroxy(thiophen-3-yl)methyl)-3-methylisoquinolin-1(2H)-one (3bd)



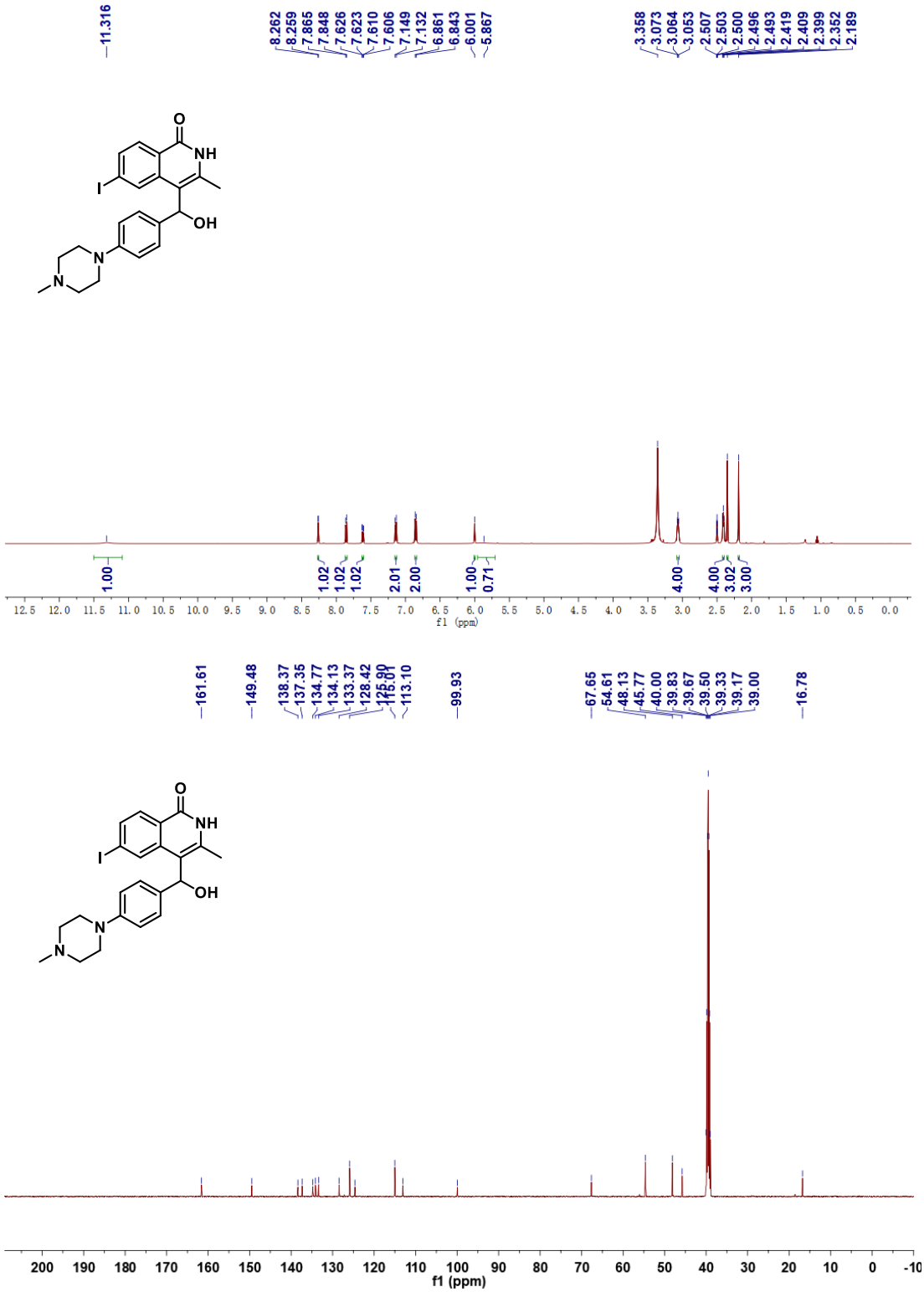
4-(hydroxy(pyridin-4-yl)methyl)-3-methylisoquinolin-1(2H)-one (3be)



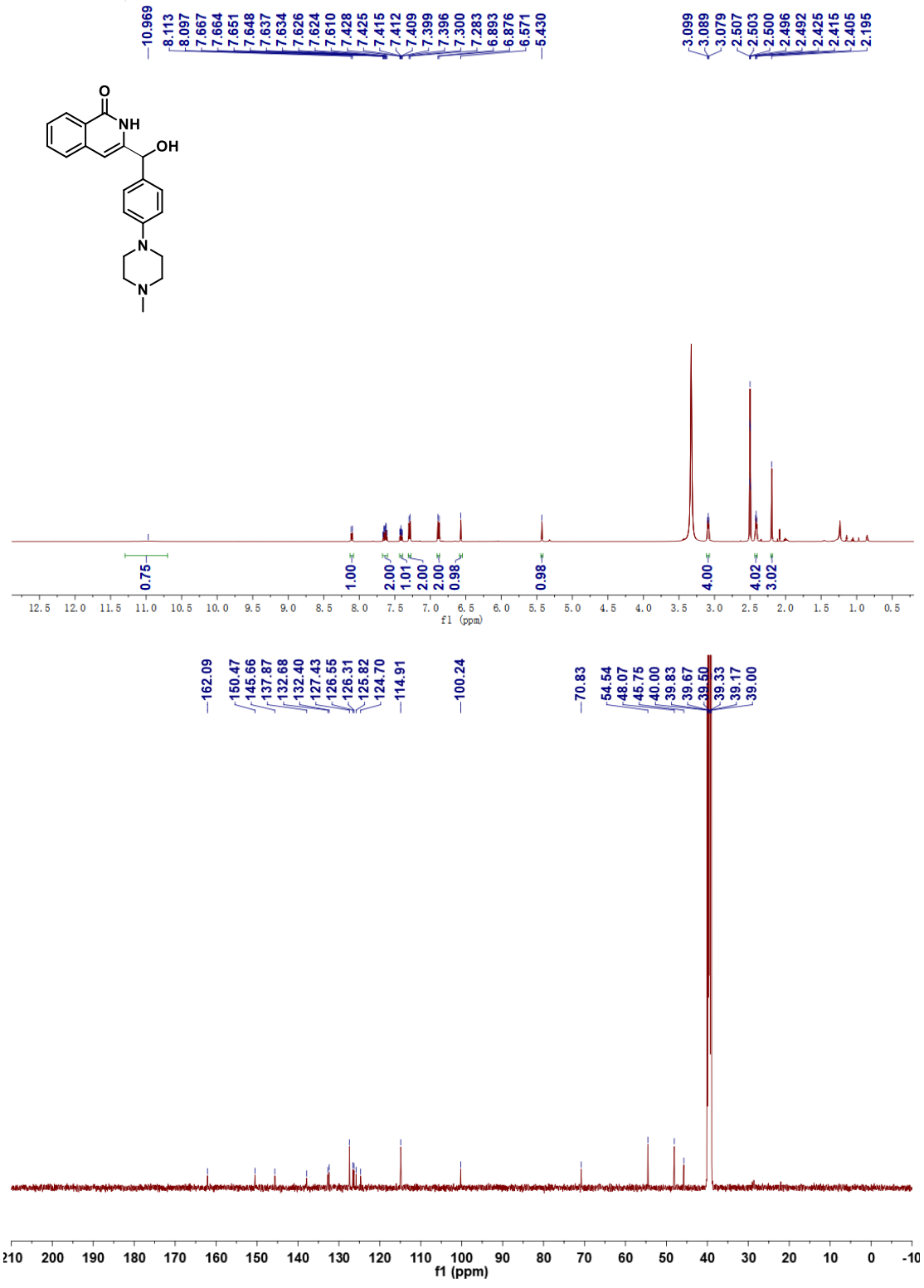
4-(hydroxy(4-(4-methylpiperazin-1-yl)phenyl)methyl)-3-methylisoquinolin-1(2H)-one (3bf)



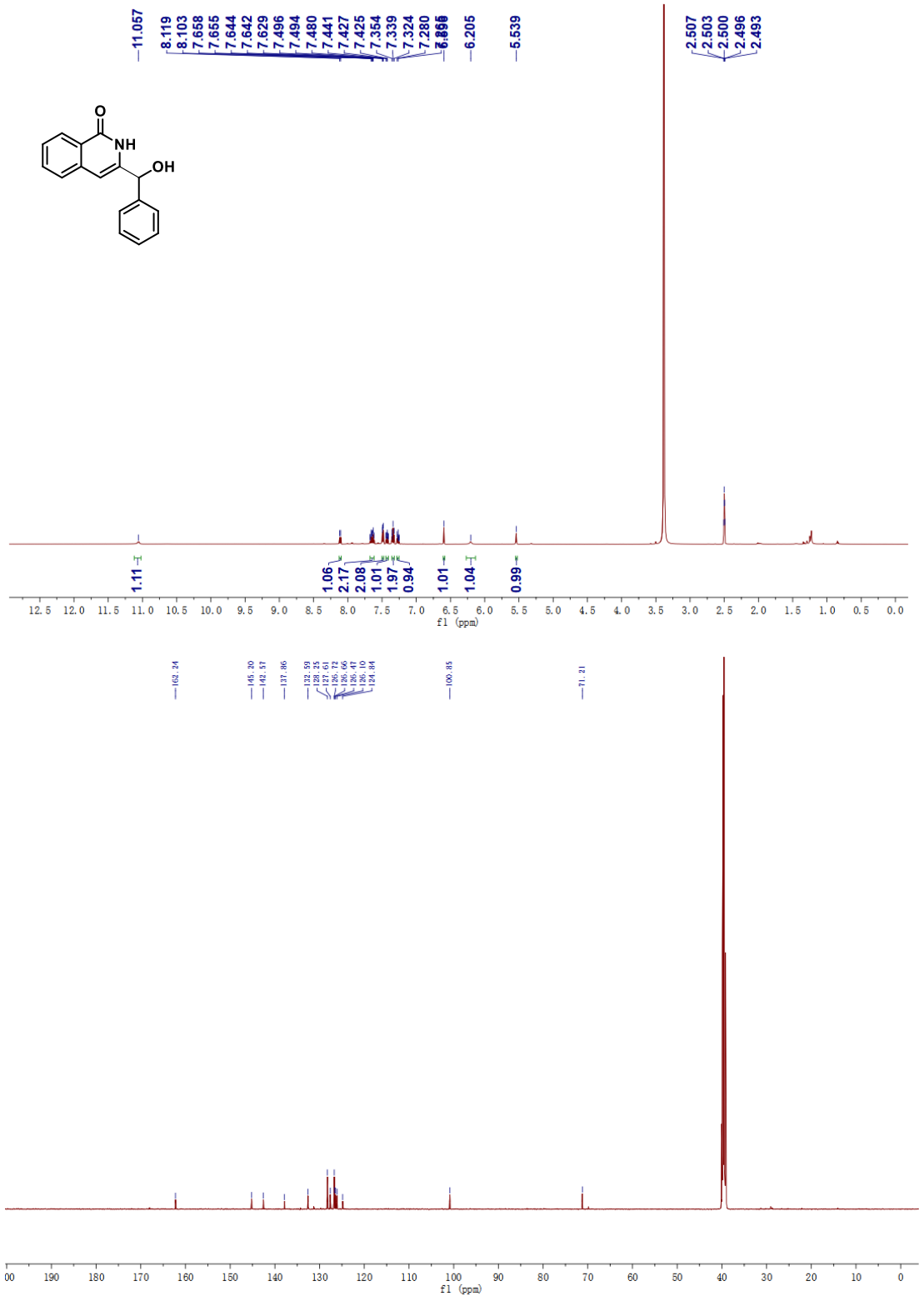
4-(hydroxy(4-(4-methylpiperazin-1-yl)phenyl)methyl)-6-iodo-3-methylisoquinolin-1(2H)-one (3bg)



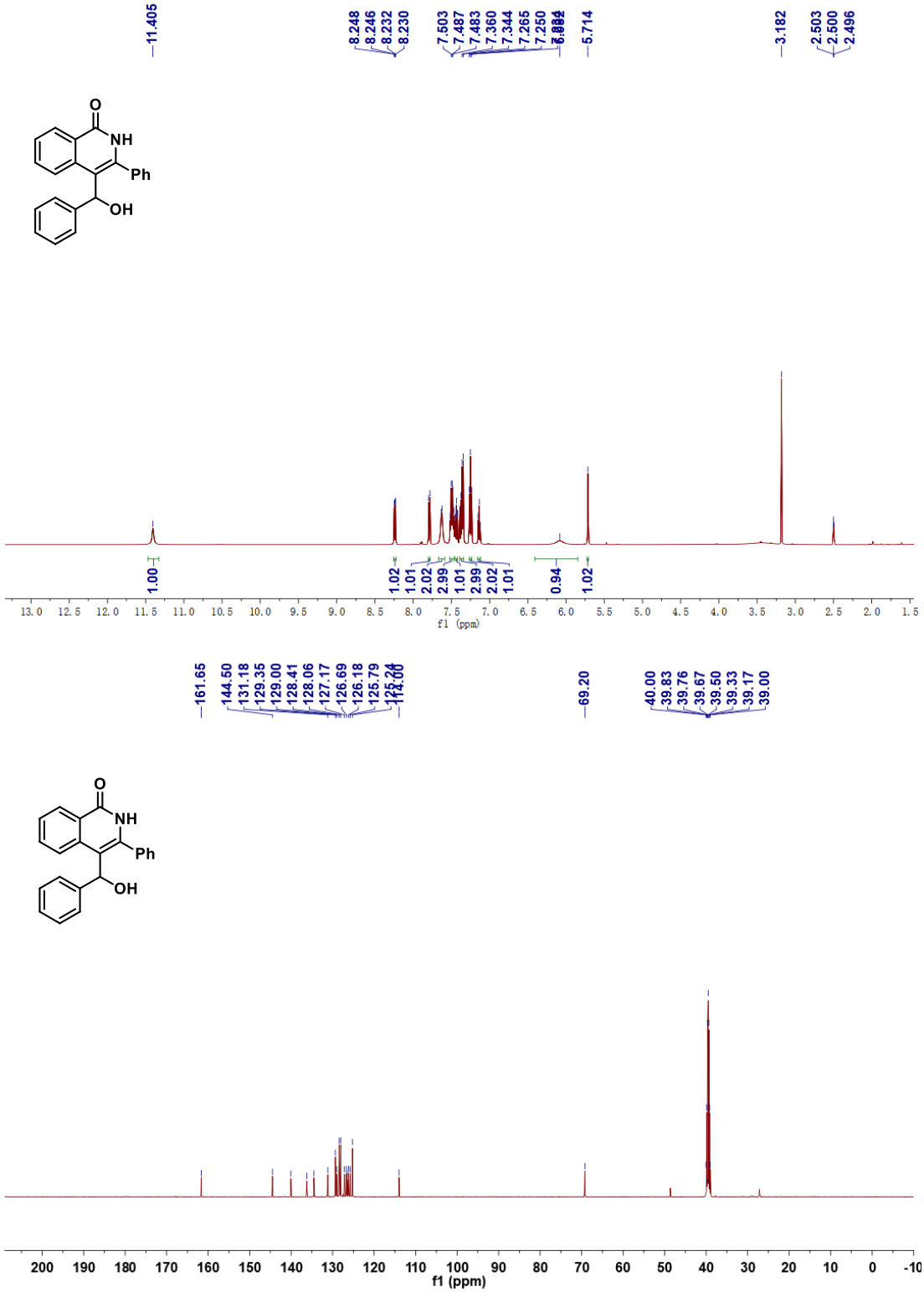
3-(hydroxy(4-(4-methylpiperazin-1-yl)phenyl)methyl)isoquinolin-1(2H)-one (3bh)



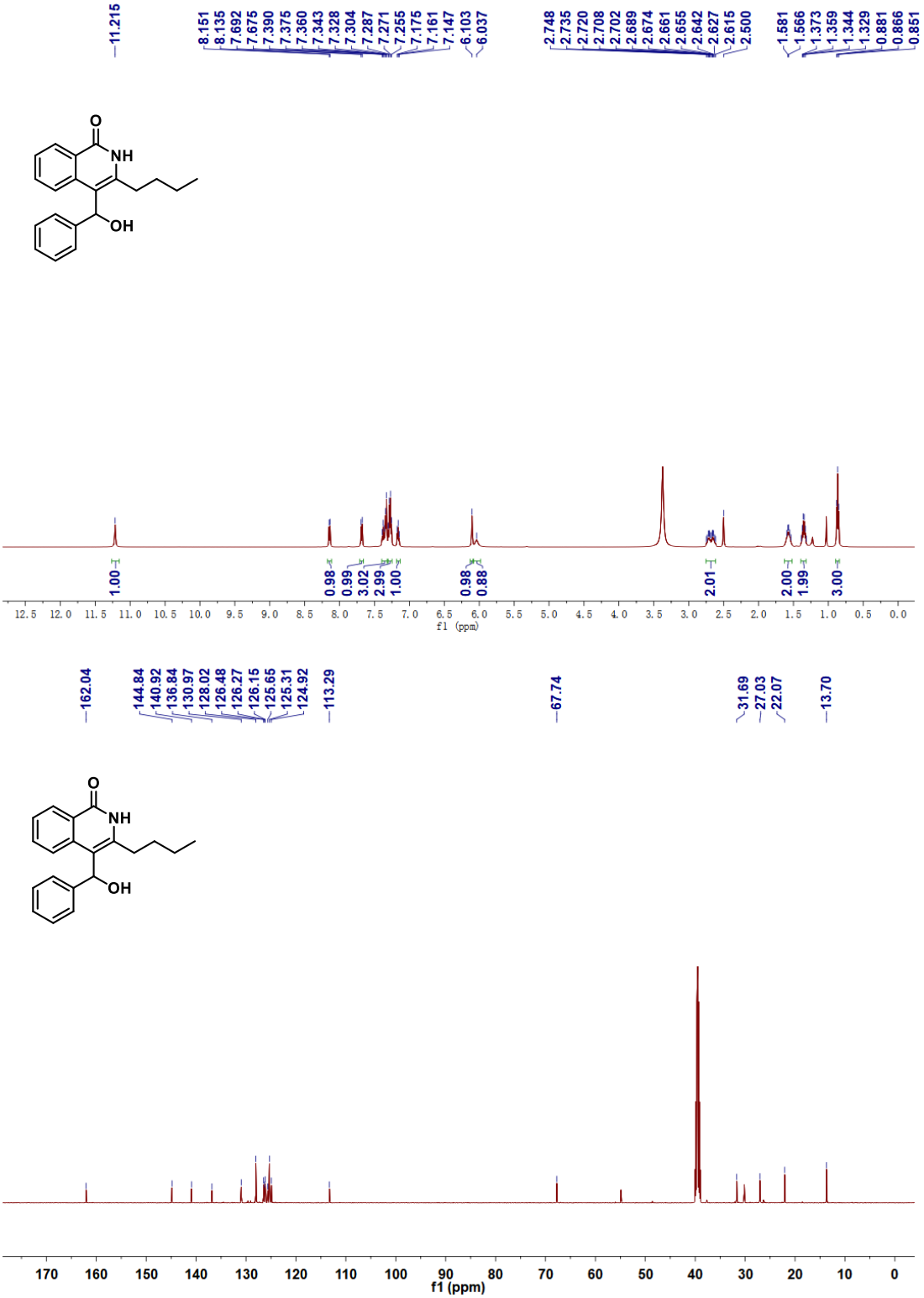
3-(hydroxy(phenyl)methyl)isoquinolin-1(2H)-one (3bi)



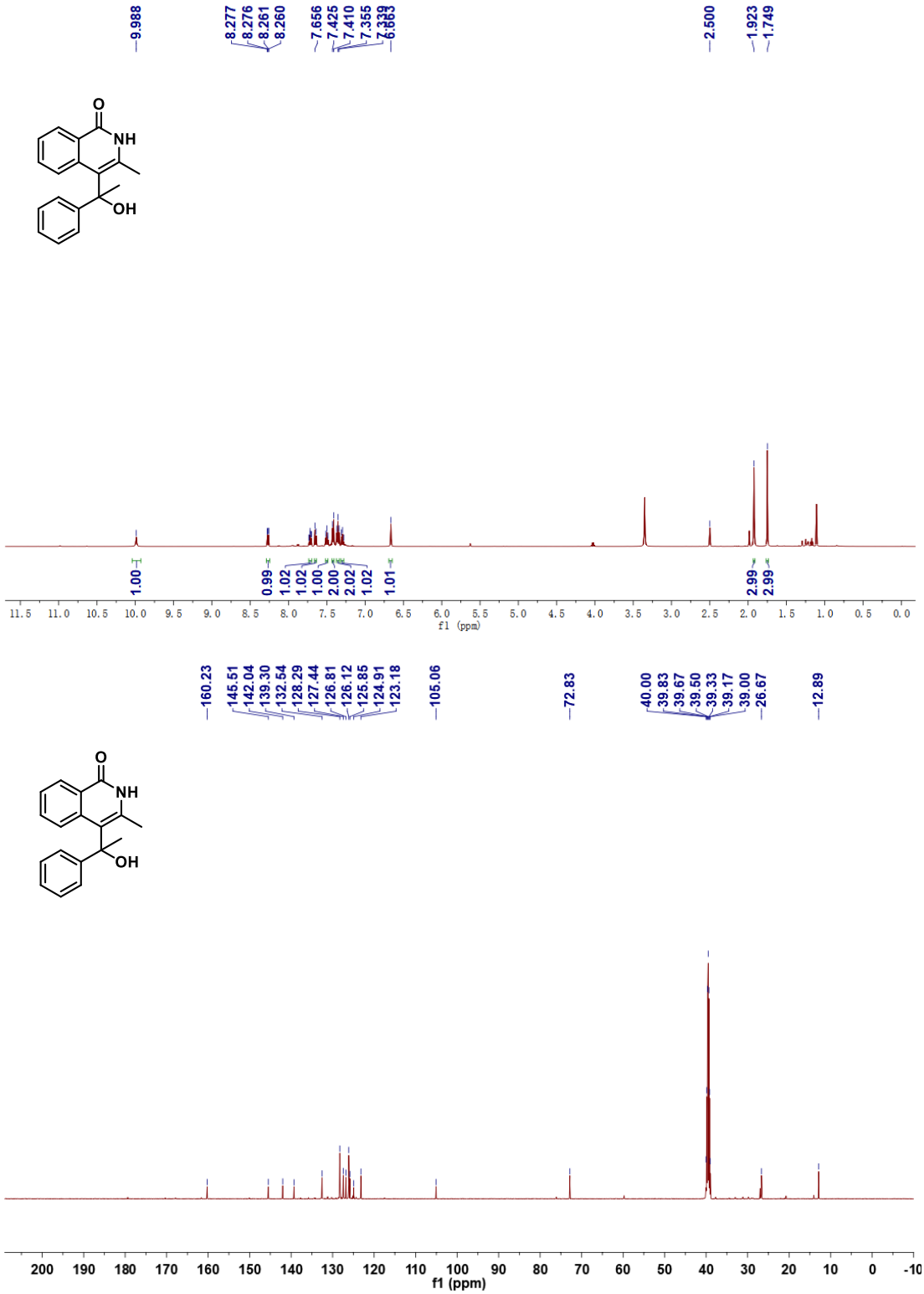
4-(hydroxy(phenyl)methyl)-3-phenylisoquinolin-1(2H)-one (3bj)



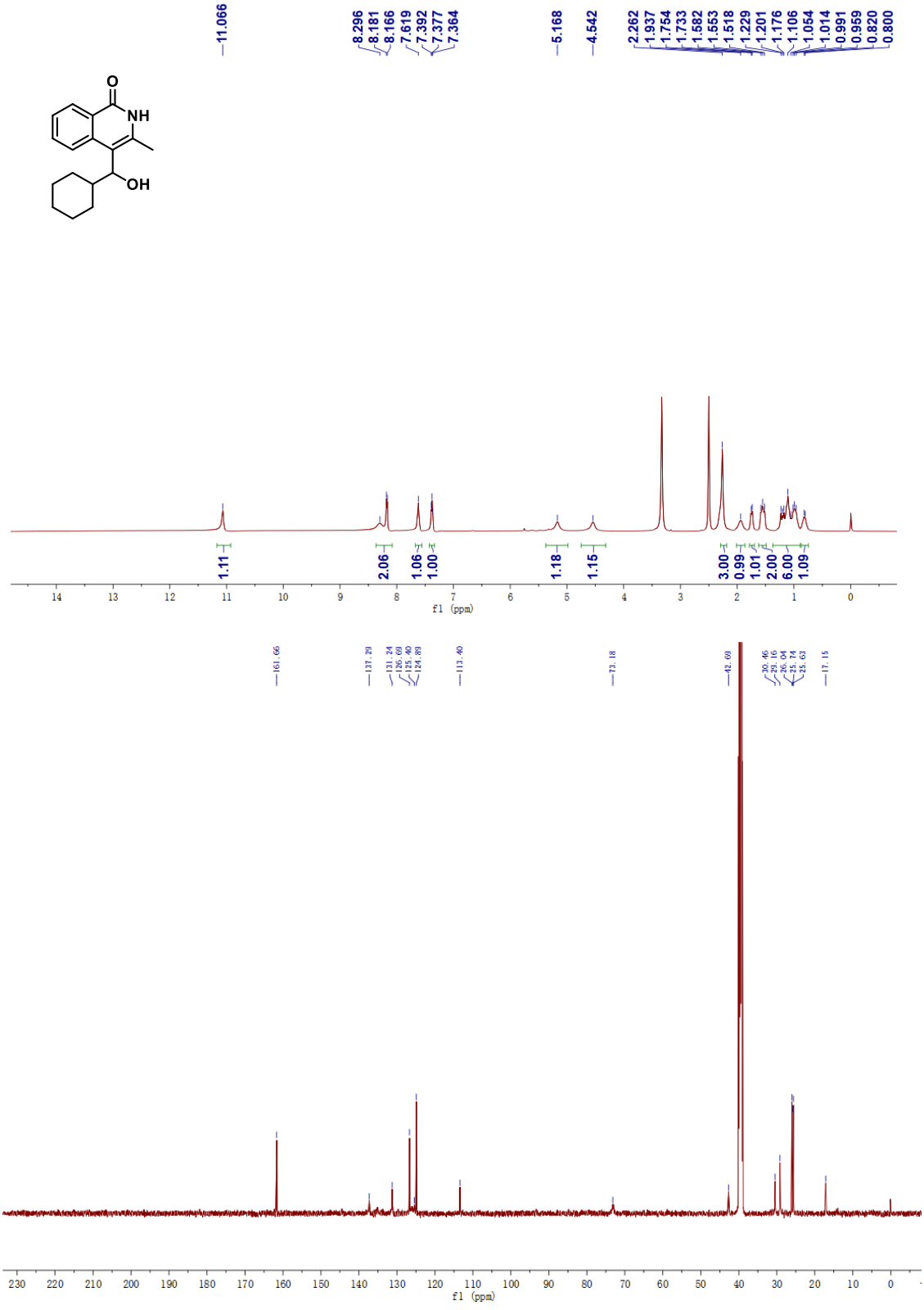
3-butyl-4-(hydroxy(phenyl)methyl)isoquinolin-1(2H)-one (3bk)



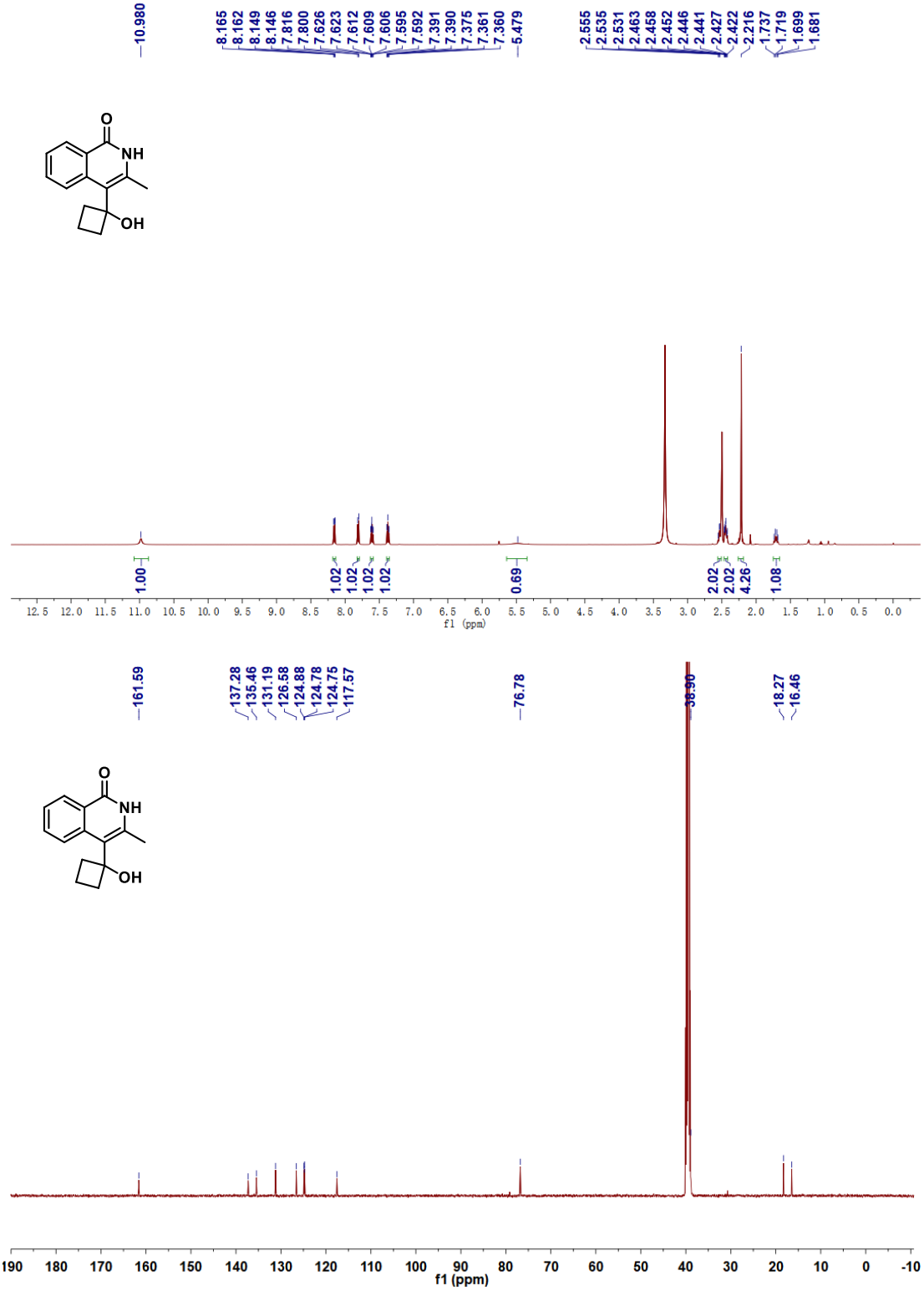
4-(1-hydroxy-1-phenylethyl)-3-methylisoquinolin-1(2H)-one (3bl)



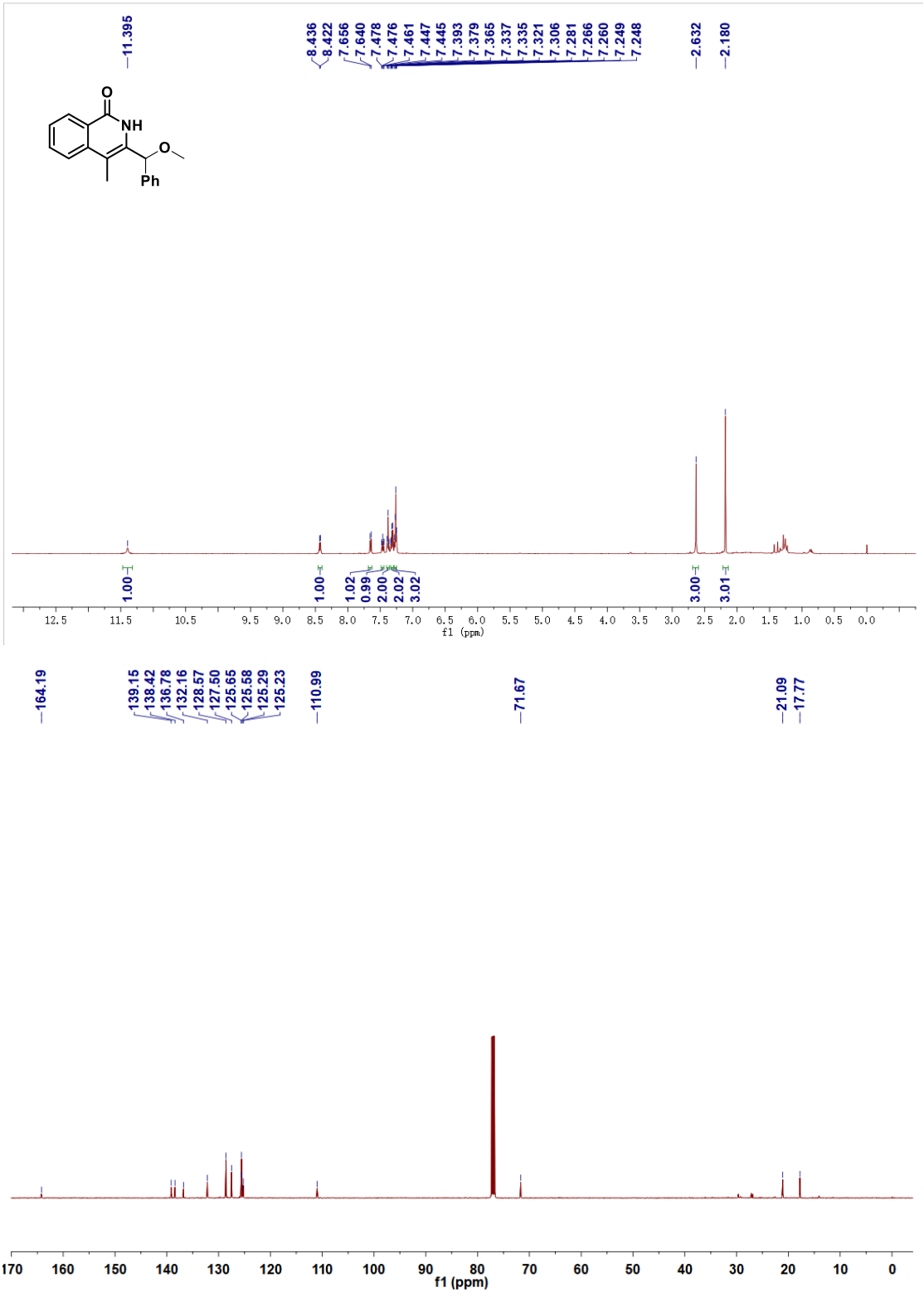
4-(cyclohexyl(hydroxy)methyl)-3-methylisoquinolin-1(2H)-one (3bm)



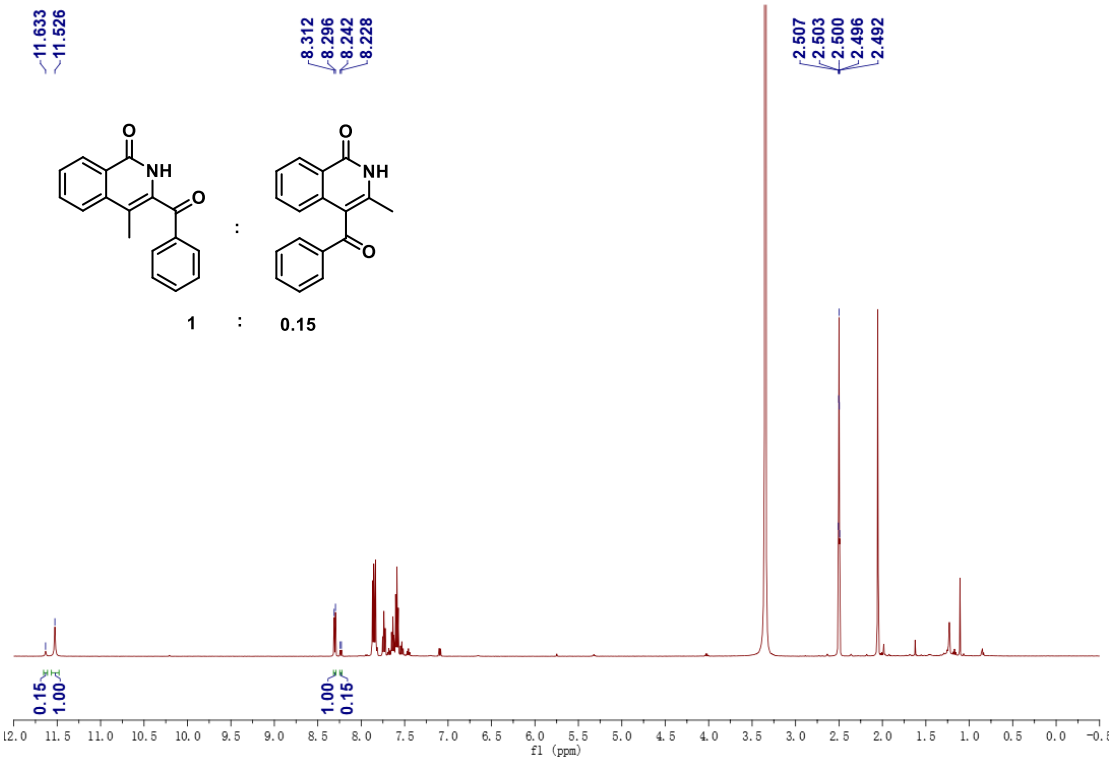
4-(1-hydroxycyclobutyl)-3-methylisoquinolin-1(2H)-one (3bn)



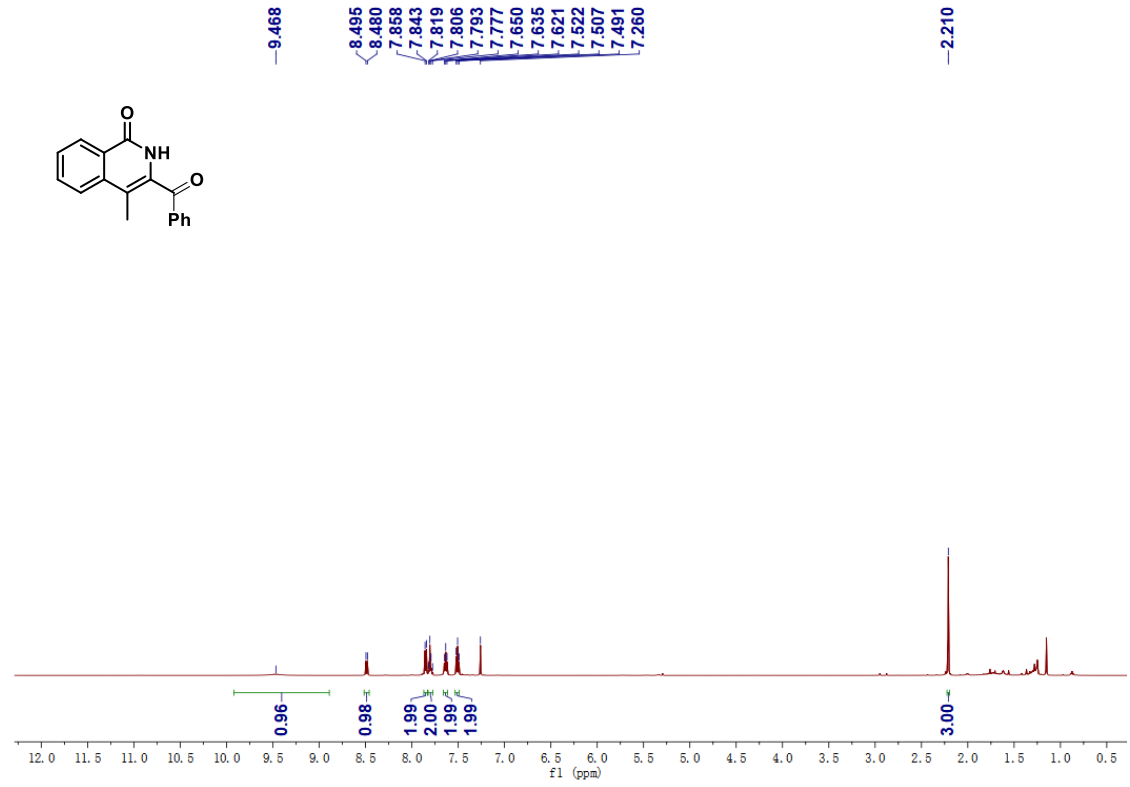
3-(methoxy(phenyl)methyl)-4-methylisoquinolin-1(2H)-one (4a)

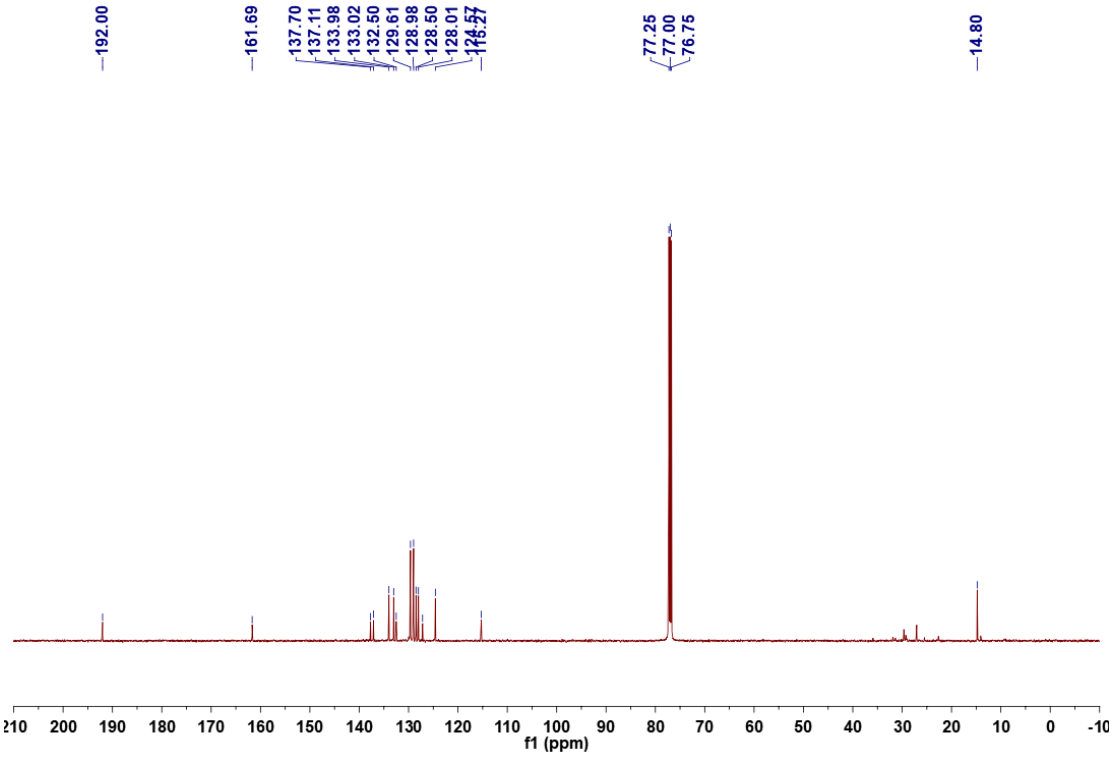


A mixture of 3-benzoyl-4-methylisoquinolin-1(2H)-one (4b) and 4-benzoyl-3-methylisoquinolin-1(2H)-one (4b')

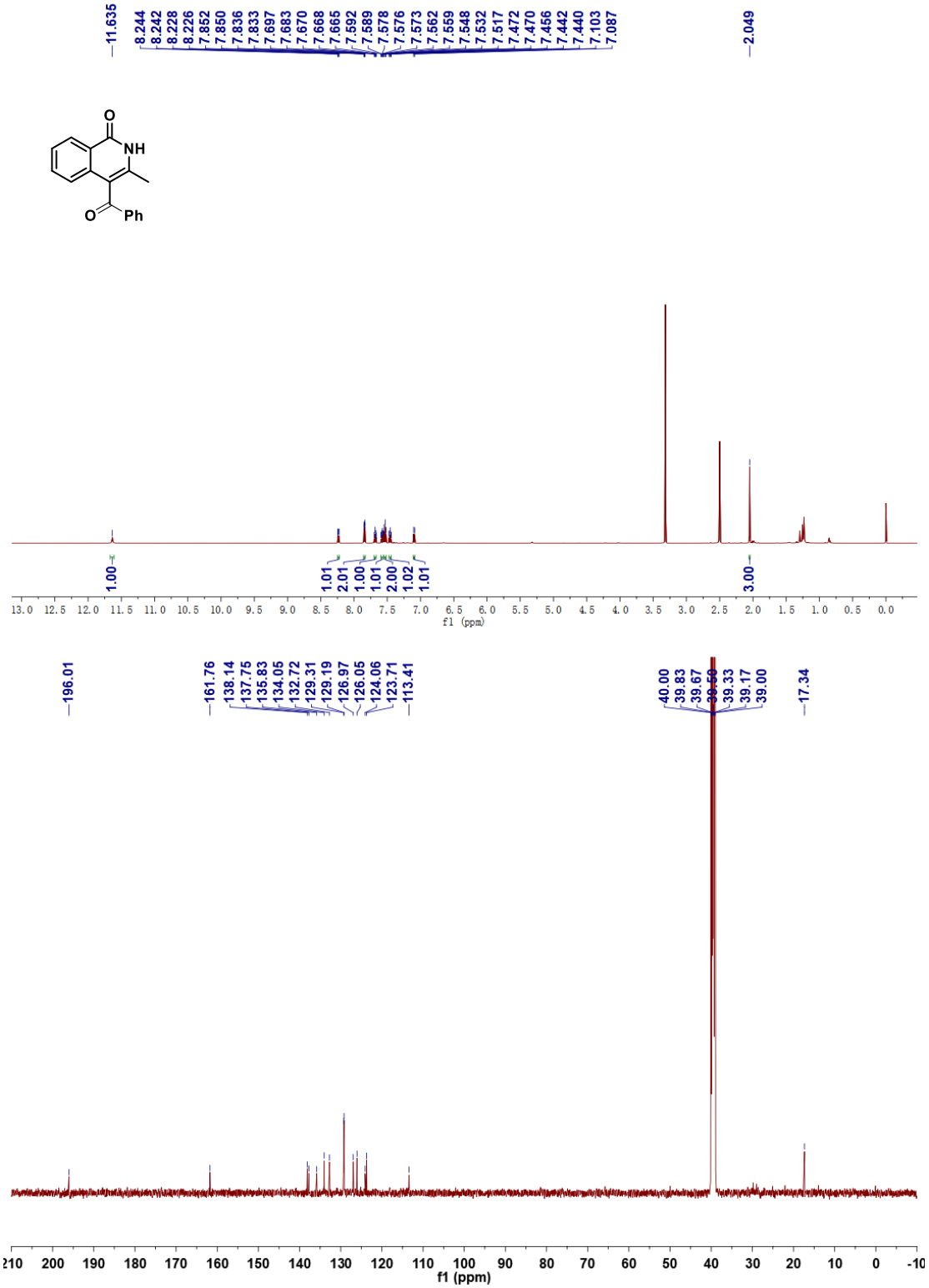


3-benzoyl-4-methylisoquinolin-1(2H)-one (4b)

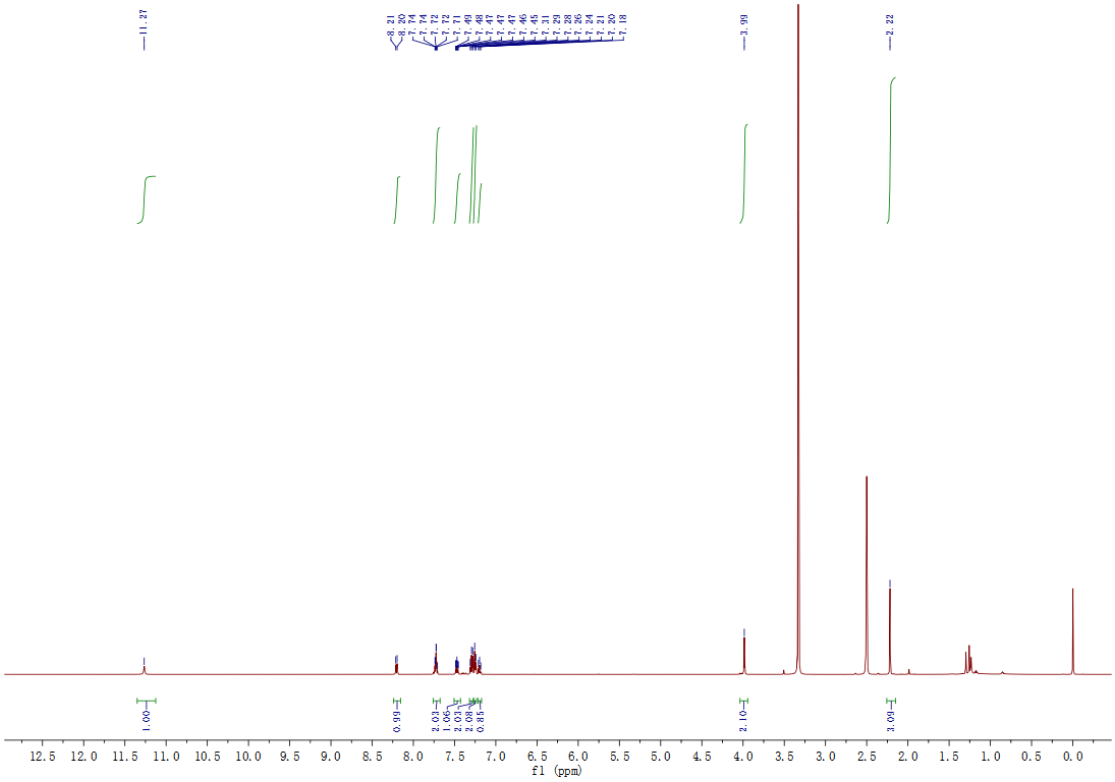


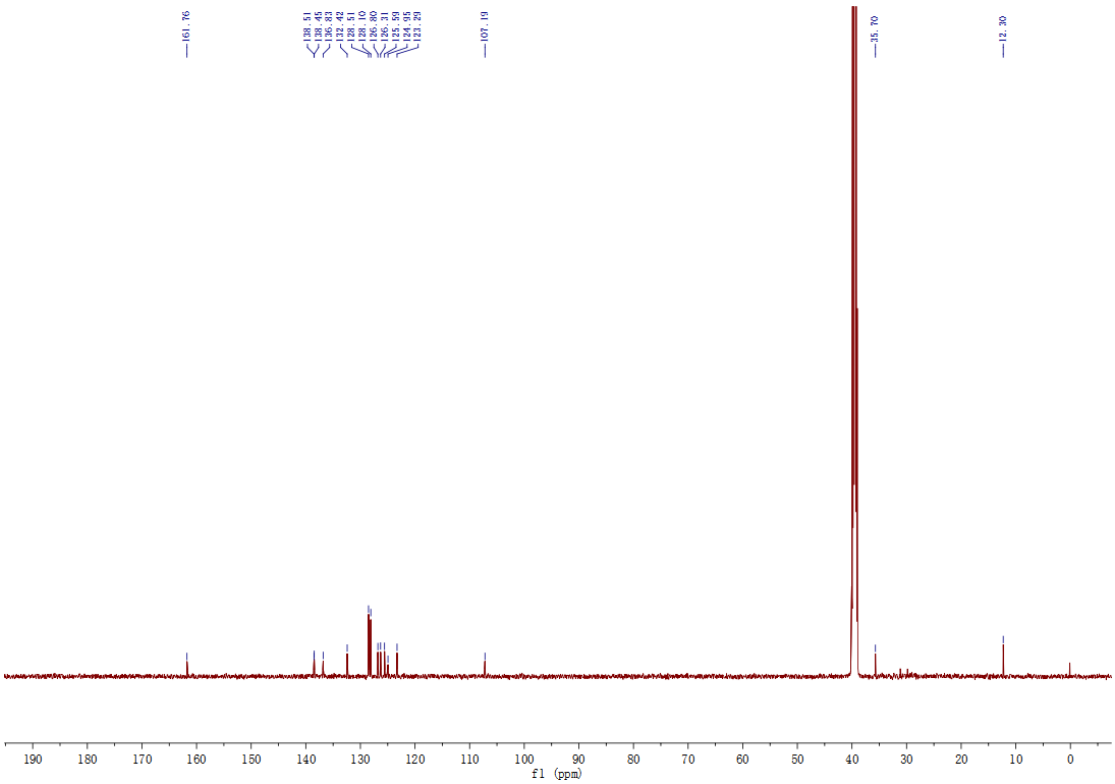

192.00
161.69
137.70
137.11
133.98
133.02
132.50
129.61
128.98
128.50
128.01
77.25
77.00
76.75
14.80
f1 (ppm)

4-benzoyl-3-methylisoquinolin-1(2H)-one (4b')

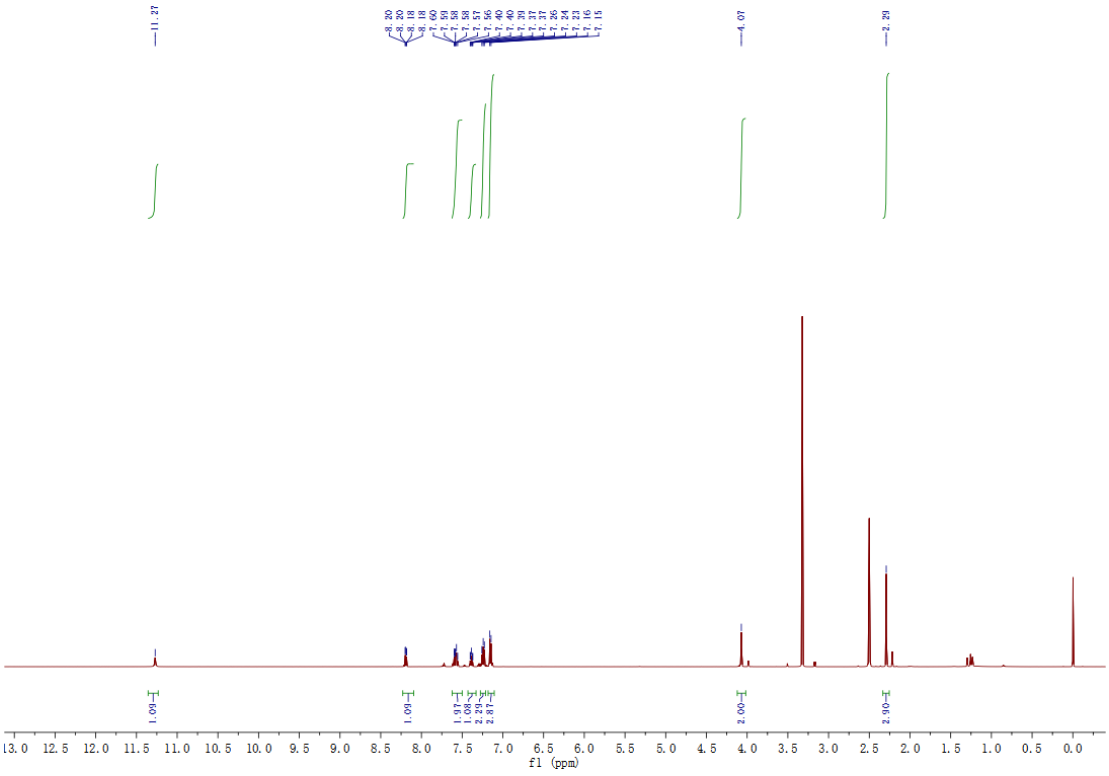


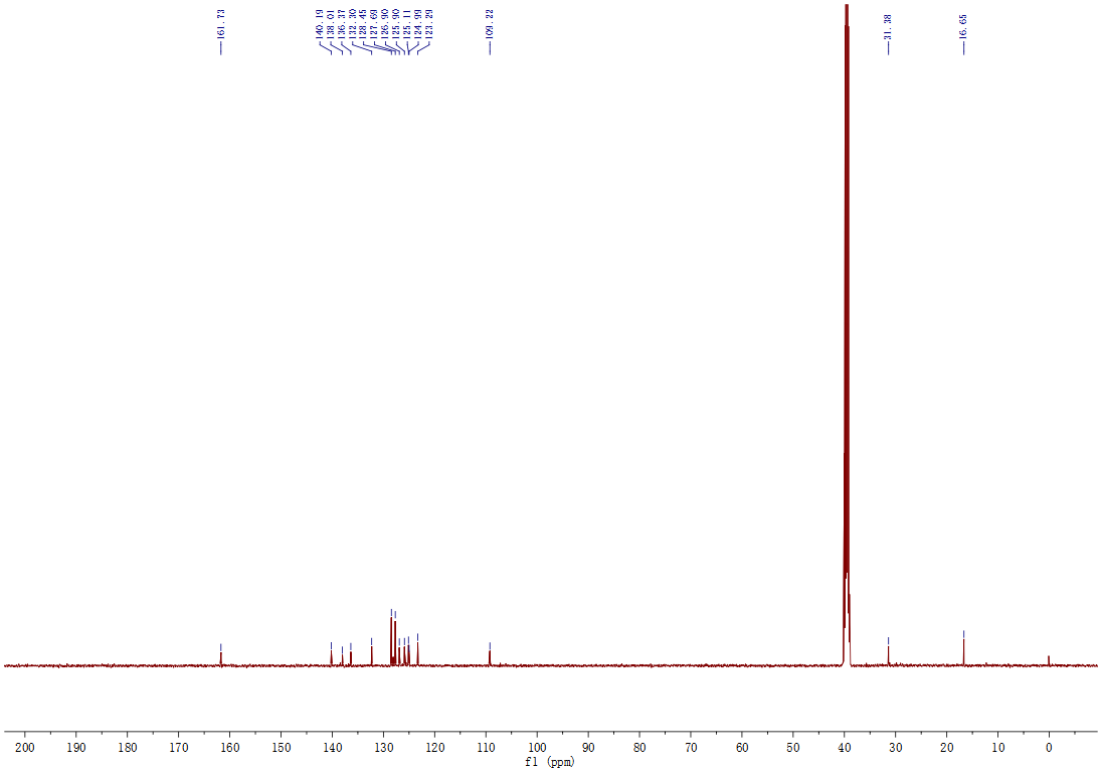
3-benzyl-4-methylisoquinolin-1(2H)-one (4c)



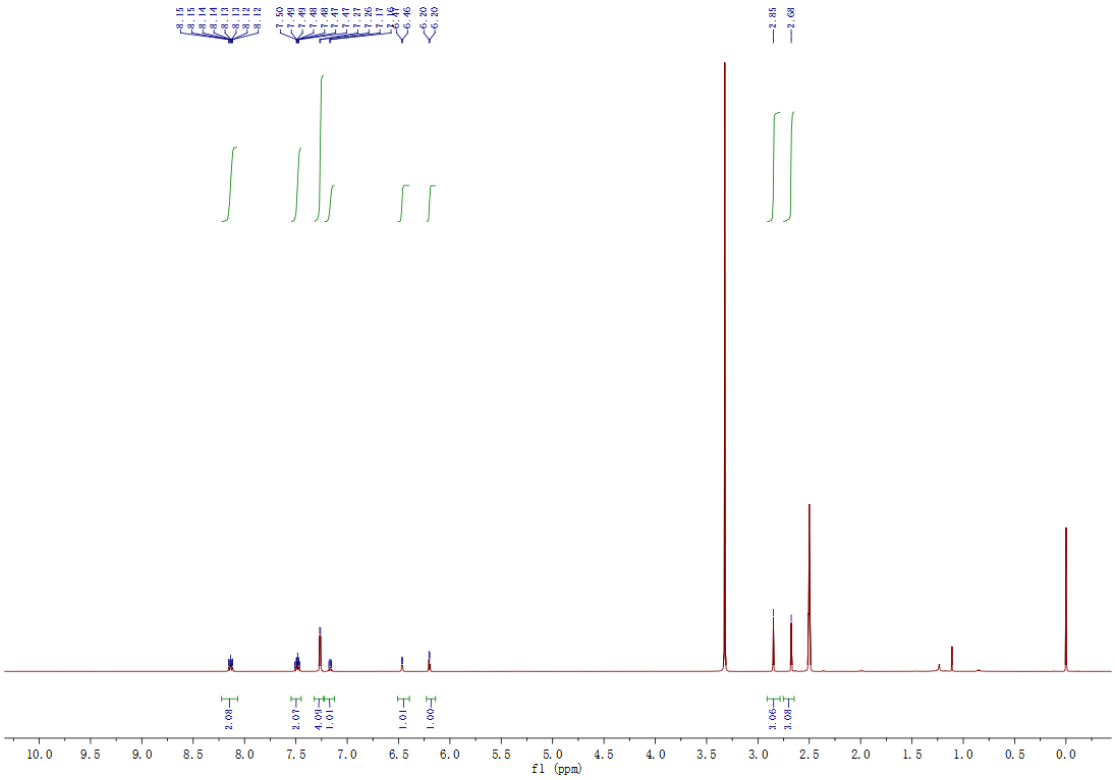


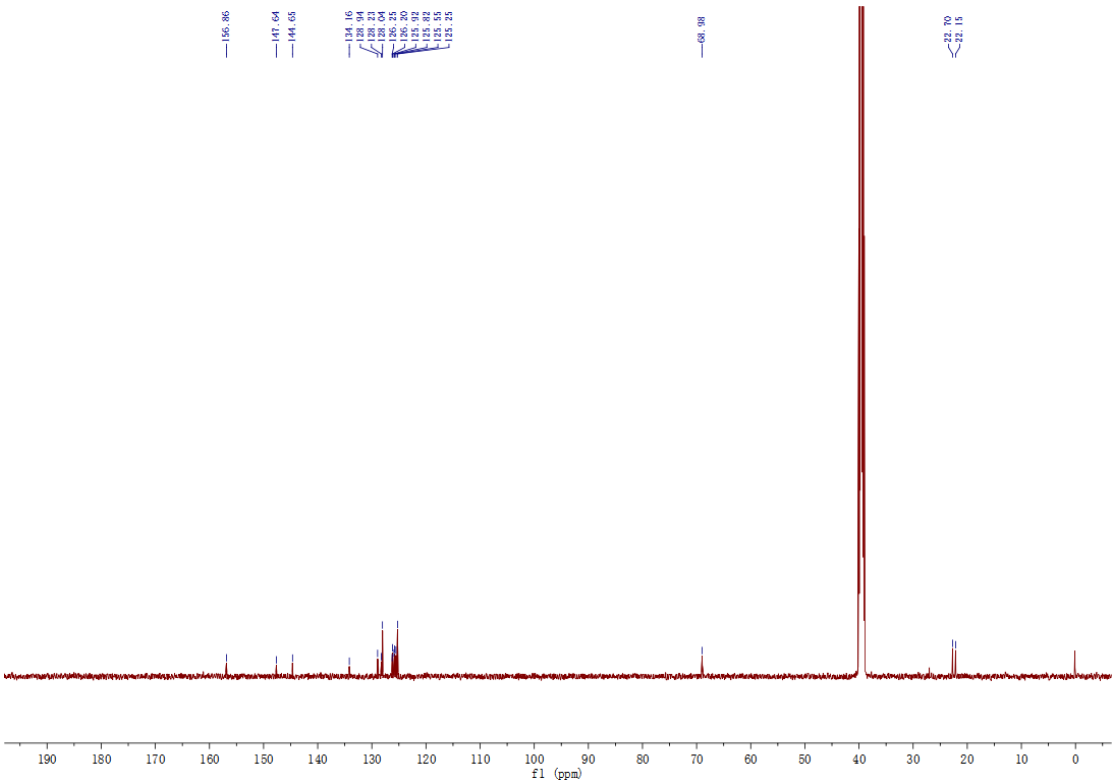
4-benzyl-3-methylisoquinolin-1(2H)-one (4c')





(1,3-dimethylisoquinolin-4-yl)(phenyl)methanol (4d)





4-(hydroxy(phenyl)methyl)-3-methylisoquinolin-1(2H)-one-5,6,7,8-d$_4$ (3aa-D$_n$)