# Site-Selective Coupling of Remote C($sp^3$)−H/*meta*-C($sp^2$)−H Bonds Enabled by Ru/Photoredox Dual Catalysis and Mechanistic Studies

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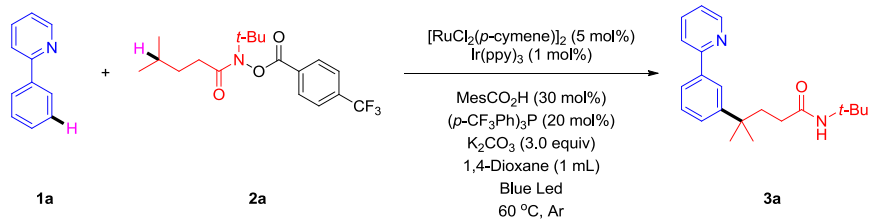
## 1. General information

Unless otherwise noted, all of these reactions were carried out under an argon atmosphere. For column chromatography, silica gel (200-300 mesh) was employed. Solvent was freshly distilled prior to use unless otherwise noted. Organic solvents were concentrated under reduced pressure using a rotary evaporator.

**Instrumentation.** Deuterated solvents were purchased from Cambridge Isotope Laboratories. $^{1}$H NMR spectra were recorded on Bruker AVANCE III 400 or Bruker AVANCE III HD 400 with a 400 MHz frequencies, and $^{13}$C NMR spectra were recorded on Bruker AVANCE III 400 or Bruker AVANCE III HD 400 with 101 MHz frequencies. $^{19}$F NMR spectra were recorded on a Bruker AVANCE III HD 400 spectrometer with a $^{19}$F operating frequency of 376 MHz. Chemical shifts (ppm) were recorded with TMS (tetramethylsilane) as the internal reference standard. Chemical shifts (δ) were reported in ppm relative to the residual solvent signal (TMS $\delta = 0$ for $^{1}$H NMR and $CDCl_3$ $\delta = 77.0$ for $^{13}$C NMR). Multiplicities are given as s (singlet), d (doublet), t (triplet), dd (doublet of doublets), td (triplet of doublets) or m (multiplet). Data collection for crystal structure was performed using Mo Kα radiation on a Bruker APEXII diffractometer. HRMS obtained using a Q-TOF instrument equipped with an ESI source. All photochemical reactions were conducted using a blue light-emitting diode (LED) as the visible-light source (440 nm, Kessil LEDs lights).

**Materials**. Unless otherwise noted below, all other compounds have been reported in the literature or are commercially available. Commercial reagents were used without further purification. $[Ru(O_2CMes)_2(p\text{-cymene})]$[1], cyclometalated complex **6**[2], Ruthenium(II) phosphine complexas **7**[3], hydroxamide compounds[4] and $[D_5]$-**1a**[5] were synthesized according to previously described methods.

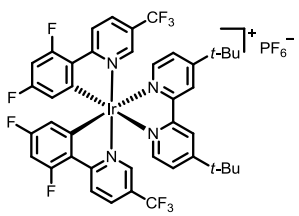
## 2. The optimization of the reaction



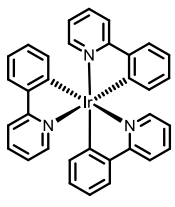

1a 2a 3a

| entry | deviation from standard condition | yield (%) |
|---|---|---|
| 1 | none | 84 |
| 2 | No ($p$-$CF_3Ph)_3P$ | <10 |
| 3 | No $MesCO_2H$ | 65 |
| 4 | 4CzIPN instead of $Ir(ppy)_3$ | 0 |
| 5 | Eosin instead of $Ir(ppy)_3$ | 0 |
| 6 | $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ instead of $Ir(ppy)_3$ | 0 |
| 7 | DME instead of 1,4-dioxane | 40% |
| 8 | DCE instead of 1,4-dioxane | trace |
| 9 | DMSO instead of 1,4-dioxane | trace |
| 10 | DMF instead of 1,4-dioxane | trace |
| 11 | PhMe instead of 1,4-dioxane | 19 |
| 12 | MTBE instead of 1,4-dioxane | 12 |
| 13 | THF instead of 1,4-dioxane | 60 |
| 14 | 2-Me-THF instead of 1,4-dioxane | 55 |
| 15 | $Et_2O$ instead of 1,4-dioxane | 38 |
| 16 | $1\text{-}AdCO_2H$ instead of $MesCO_2H$ | 27 |
| 17 | KOAc instead of $K_2CO_3$ | trace |
| 18 | $Na_2CO_3$ instead of $K_2CO_3$ | 14 |
| 19 | $Ru_3(CO)_{12}$ instead of $[RuCl_2(p\text{-cymene})]_2$ | <10 |
| 20 | $RuCl_3$ instead of $[RuCl_2(p\text{-cymene})]_2$ | trace |
| 21 | 50 °C | 76% |
| 22 | 70 °C | 70% |
| 23 | No $[RuCl_2(p\text{-cymene})]_2$ | 0 |
| 24 | No $Ir(ppy)_3$ | 0 |
| 25 | No light (100 °C) | 0 |

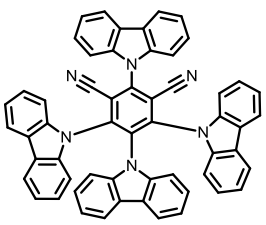
Reaction conditions: **1a** (0.2 mmol), **2a** (0.5 mmol, 2.5 equiv), $[RuCl_2(p\text{-cymene})]_2$ (0.01 mmol, 5 mol%), $Ir(ppy)_3$ (1 mol%), $MesCO_2H$ (30 mol%), $(p\text{-}CF_3Ph)_3P$ (20 mol%), $K_2CO_3$ (3.0 equiv), 1,4-dioxane (1 mL), blue led, 60 °C, Ar, 36h.



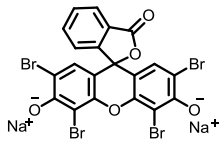
$Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$



$Ir(ppy)_3$



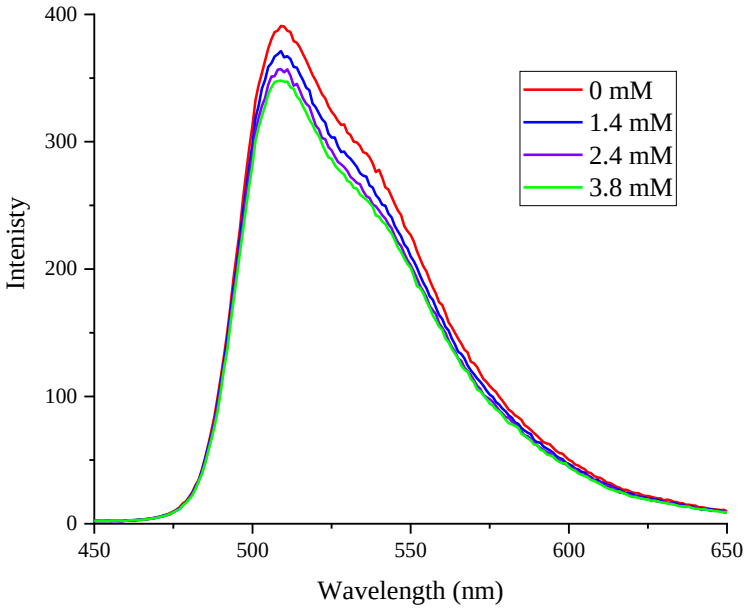
4CzIPN



Eosin

### 3. Stern-volmer quenching studies

All $Ir(ppy)_3$ solutions were excited at 378 nm and the emission intensity was collected at 509 nm. In a typical experiment, the emission spectrum of a solution of $Ir(ppy)_3$ in 1,4-dioxane ($1\times10^{-4}$ M) was collected. The decrease of $Ir(ppy)_3$ luminescence could be observed in the presence of the substrate **2a**.



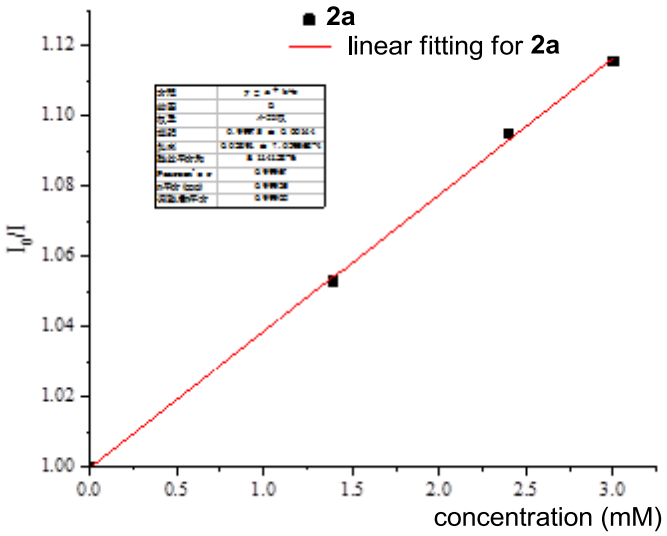




**Figure S1.** $Ir(ppy)_3$ Emission Quenching by **2a**.

**4. Cyclic voltammetry experiments**

Cyclic voltammetry (CV) measurement was performed in a 25 mL glass vial fitted with a glassy carbon working electrode (3 mm in diameter), a saturated calomel reference electrode, and a platinum wire counter electrode. A solution of **2a** in MeCN (1 mM) was tested with *n*-$Bu_4NPF_6$ (0.1 M) as electrolyte.

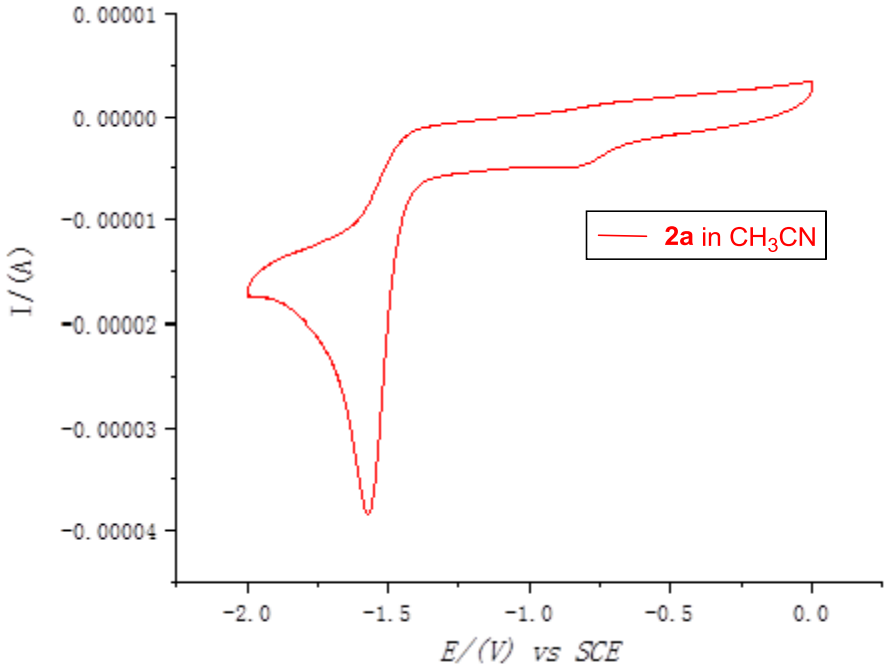



**Figure S2.**Cyclic voltammogram of **2a** (1 mM) in MeCN, $E_{p/2}$ = -1.56 V vs SCE

**5. Synthesis and characterization of products**

**(1), General Procedures I (GPI)**

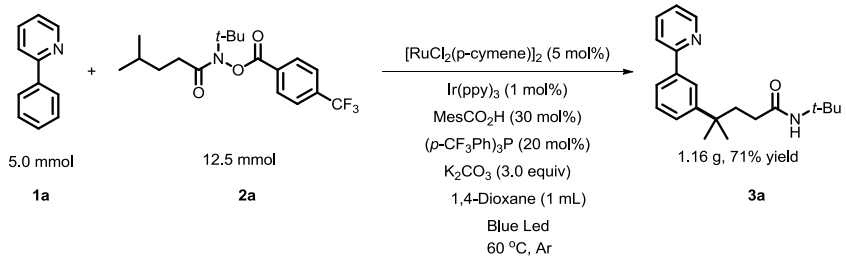
In an oven-dried 10 ml tube equipped with a stirring bar, hydroxamide compounds (0.5 mmol, 2.5 equiv), arenes (0.2 mmol, 1.0 equiv), $K_2CO_3$ (0.6 mmol, 3.0 equiv), $MesCO_2H$ (0.06 mmol, 30 mol%), P(*p*-$CF_3Ph)_3$ (0.04 mmol, 20 mol%), $[RuCl_2$(*p*-cymene)$]_2$ (0.01 mmol, 5 mol%) and $Ir(ppy)_3$ (0.002 mmol, 1 mol%) were added. The tube was charged with argon (repeated three times), then 1,4-dioxane (1 mL) was injected. The resulting suspension was stirred at room temperature for 10 mins, and then was placed in a preheated oil bath at 60 ℃ and irradiated with blue LEDs (2*20W) for 36 h. The resulting mixture was filtered through a short plug of

silica gel (rinsed with ethyl acetate). After the removal of solvents under reduced pressure, the crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:5, v:v) as the eluent to give the pure products.

**(2), General Procedures II (GPII)**

In an oven-dried 10 ml tube equipped with a stirring bar, hydroxamide compounds (0.5 mmol, 2.5 equiv), arenes (0.2 mmol, 1.0 equiv), $K_2CO_3$ (0.6 mmol, 3.0 equiv), $MesCO_2H$ (0.06 mmol, 30 mol%), P(*p*-$CF_3Ph)_3$ (0.04 mmol, 20 mol%), $[RuCl_2(p\text{-cymene})]_2$ (0.01 mmol, 5 mol%) and $Ir(ppy)_3$ (0.004 mmol, 2 mol%) were added. The tube was charged with argon (repeated three times), then 1,4-dioxane (1 mL) was injected. The resulting suspension was stirred at room temperature for 10 mins, and then was placed in a preheated oil bath at 60 ℃ and irradiated with blue LEDs (2*20W) for 5 days. The resulting mixture was filtered through a short plug of silica gel (rinsed with ethyl acetate). After the removal of solvents under reduced pressure, the crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:5, v:v) as the eluent to give the pure products.

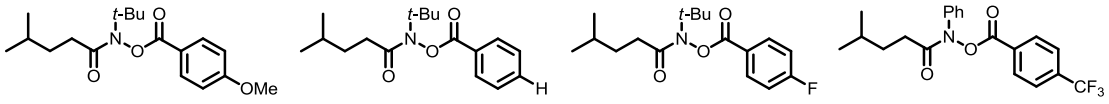
**(3), Gram-scale reaction procedures**




In an oven-dried 50 ml tube equipped with a stirring bar, **2a** (12.5 mmol, 2.5 equiv), **1a** (5.0 mmol, 1.0 equiv), $K_2CO_3$ (15.0 mmol, 3.0 equiv), $MesCO_2H$ (1.5 mmol, 30 mol%), P(*p*-$CF_3Ph)_3$ (1.0 mmol, 20 mol%), $[RuCl_2(p\text{-cymene})]_2$ (0.25 mmol, 5 mol%) and $Ir(ppy)_3$ (0.025 mmol, 0.5 mol%) were added. The tube was charged with argon (repeated three times), then 1,4-dioxane (25.0 mL) was injected. The resulting suspension was stirred at room temperature for 10 mins, and then was placed in a

preheated oil bath at 60 ℃ and irradiated with blue LEDs (2*20W) for 48 h. The resulting mixture was filtered through a short plug of silica gel (rinsed with ethyl acetate). After the removal of solvents under reduced pressure, the crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:5, v:v) as the eluent to give the pure product (**3aa**, 1.16 g, 71% yield).

**(4), Unsuccessful substrates**

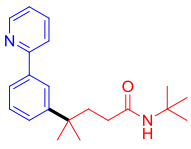



No reaction　　No reaction　　No reaction　　No product

**(5), Photo for the reaction setup**

**(6), Characterization of products**

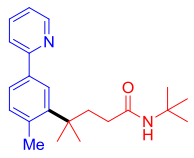
***N*-(*tert*-butyl)-4-methyl-4-(3-(pyridin-2-yl)phenyl)pentanamide (3a)**



**GP I**, 55.1 mg, 84% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.7 Hz, 1H), 7.96 (s, 1H), 7.78 – 7.69 (m, 3H), 7.44 – 7.38 (m, 2H), 7.25 – 7.20 (m, 1H), 5.21 (s, 1H), 2.04 – 1.99 (m, 2H),

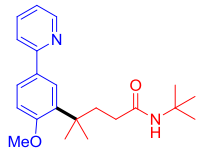
1.87 – 1.82 (m, 2H), 1.38 (s, 6H), 1.27 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 157.8, 149.5, 148.9, 139.3, 136.7, 128.6, 126.6, 124.5, 124.3, 122.0, 120.7, 50.9, 39.6, 37.5, 33.2, 28.8, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{28}N_2OH$ ($[M + H]^+$): 325.2274; found: 325.2274.

***N*-(*tert*-butyl)-4-methyl-4-(2-methyl-5-(pyridin-2-yl)phenyl)pentanamide (3b)**



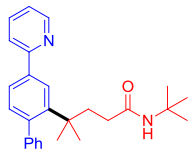

**GP I**, 60.7 mg, 89% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.68 – 8.65 (m, 1H), 7.95 (d, *J* = 1.9 Hz, 1H), 7.75 – 7.66 (m, 3H), 7.23 – 7.18 (m, 2H), 5.18 (s, 1H), 2.58 (s, 3H), 2.19 – 2.13 (m, 2H), 1.84 – 1.78 (m, 2H), 1.48 (s, 6H), 1.27 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 157.8, 149.5, 145.6, 137.5, 136.8, 136.6, 133.4, 126.0, 124.4, 121.7, 120.4, 50.9, 39.1, 36.7, 33.6, 29.5, 28.7, 23.2; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{30}N_2OH$ ($[M + H]^+$): 339.2431; found: 339.2429.

***N*-(*tert*-butyl)-4-(2-methoxy-5-(pyridin-2-yl)phenyl)-4-methylpentanamide (3c)**



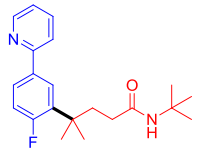

**GP I**, 57.2 mg, 80% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.66 – 8.63 (m, 1H), 7.87 (d, *J* = 2.3 Hz, 1H), 7.80 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.73 – 7.68 (m, 1H), 7.67 – 7.64 (m, 1H), 7.18 – 7.14 (m, 1H), 6.96 (d, *J* = 8.5 Hz, 1H), 5.13 (s, 1H), 3.89 (s, 3H), 2.22 – 2.16 (m, 2H), 1.81 – 1.75 (m, 2H), 1.43 (s, 6H), 1.27 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 173.0, 159.3, 157.6, 149.4, 136.6, 135.7, 131.4, 126.6, 126.0, 121.2, 119.9, 111.6, 55.2, 50.8, 38.1, 36.1, 34.0, 28.7, 28.3; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{30}N_2O_2H$ ($[M + H]^+$): 355.2380; found: 355.2379.

***N*-(*tert*-butyl)-4-methyl-4-(4-(pyridin-2-yl)-[1,1'-biphenyl]-2-yl)pentanamide (3d)**



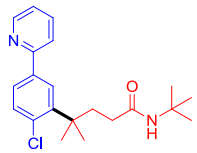

**GP I**, 66.3 mg, 82% yield, white solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.72 – 8.69 (m, 1H), 8.09 (d, *J* = 1.9 Hz, 1H), 7.79 – 7.73 (m, 3H), 7.38 – 7.33 (m, 3H), 7.31 – 7.27 (m, 2H), 7.26 – 7.21 (m, 1H), 7.13 (d, *J* = 7.9 Hz, 1H), 5.17 (s, 1H), 1.93 – 1.87 (m, 2H), 1.84 – 1.78 (m, 2H), 1.28 (s, 9H), 1.27 (s, 6H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 157.5, 149.6, 145.2, 144.5, 142.8, 138.1, 136.7, 133.3, 129.4, 127.4, 126.8, 126.3, 123.6, 122.0, 120.6, 50.8, 39.7, 38.9, 33.7, 30.8, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{27}H_{32}N_2OH$ ($[M + H]^+$): 401.2587; found: 401.2591.

***N*-(*tert*-butyl)-4-(2-fluoro-5-(pyridin-2-yl)phenyl)-4-methylpentanamide (3e)**



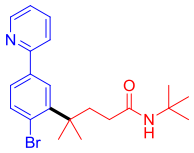
**GP I**, 52.3 mg, 76% yield, yellow oil; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.68 – 8.66 (m, 1H), 7.90 (dd, *J* = 8.0, 2.3 Hz, 1H), 7.80 – 7.72 (m, 2H), 7.68 – 7.65 (m, 1H), 7.24 – 7.20 (m, 1H), 7.09 (dd, *J* = 12.2, 8.4 Hz, 1H), 5.20 (s, 1H), 2.15 – 2.10 (m, 2H), 1.89 – 1.83 (m, 2H), 1.44 (s, 6H), 1.29 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 162.4 (d, *J* = 250.9 Hz), 156.8, 149.6, 136.7, 135.2 (d, *J* = 3.1 Hz), 134.8 (d, *J* = 12.0 Hz), 127.2 (d, *J* = 6.4 Hz), 126.5 (d, *J* = 9.4 Hz), 121.9, 120.4, 116.7 (d, *J* = 25.1 Hz), 50.9, 37.5 (d, *J* = 3.2 Hz), 37.1 (d, *J* = 4.4 Hz), 33.7, 28.7, 28.1 (d, *J* = 2.9 Hz); $^{19}$F NMR (376 MHz, $CDCl_3$) δ -109.07; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{27}FN_2OH$ ($[M + H]^+$): 343.2180; found: 343.2179.

***N*-(*tert*-butyl)-4-(2-chloro-5-(pyridin-2-yl)phenyl)-4-methylpentanamide (3f)**



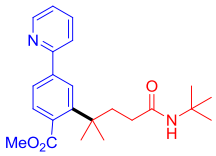
**GP I**, 59.2 mg, 82% yield, white solid; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.66 (m, 1H), 8.03 (s, 1H), 7.79 – 7.66 (m, 3H), 7.44 (d, *J* = 8.2 Hz, 1H), 7.27 – 7.22 (m, 1H), 5.19 (s, 1H), 2.38 – 2.32 (m, 2H), 1.83 – 1.77 (m, 2H), 1.54 (s, 6H), 1.28 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 156.6, 149.7, 144.3, 137.8, 136.8, 134.4, 132.2, 127.7, 125.7, 122.3, 120.5, 50.9, 39.4, 35.6, 33.8, 28.7, 28.5; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{27}ClN_2OH$ ($[M + H]^+$): 359.1885; found: 359.1883.

**4-(2-bromo-5-(pyridin-2-yl)phenyl)-*N*-(*tert*-butyl)-4-methylpentanamide (3g)**



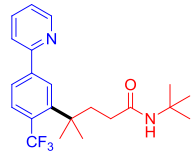
**GP I**, 60.5 mg, 74% yield, white solid; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.8 Hz, 1H), 8.03 (s, 1H), 7.79 – 7.73 (m, 1H), 7.68 (d, *J* = 8.9 Hz, 2H), 7.64 – 7.60 (m, 1H), 7.28 – 7.23 (m, 1H), 5.18 (s, 1H), 2.43 – 2.38 (m, 2H), 1.82 – 1.76 (m, 2H), 1.56 (s, 6H), 1.29 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 156.6, 149.7, 145.6, 138.3, 136.9, 136.1, 128.0, 125.9, 123.3, 122.3, 120.5, 50.9, 39.9, 35.5, 33.9, 28.7, 28.6; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{27}BrN_2OH$ ($[M + H]^+$): 403.1380; found: 403.1378.

**methyl 2-(5-(*tert*-butylamino)-2-methyl-5-oxopentan-2-yl)-4-(pyridin-2-yl)benzoate (3h)**



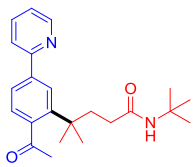
**GP I**, 63.0 mg, 82% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 4.7 Hz, 1H), 8.06 (d, *J* = 1.7 Hz, 1H), 7.82 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.78 – 7.71 (m, 2H), 7.38 (d, *J* = 7.9 Hz, 1H), 7.29 – 7.24 (m, 1H), 5.51 (s, 1H), 3.93 (s, 3H), 2.10 – 2.05 (m, 2H), 1.93 – 1.88 (m, 2H), 1.45 (s, 6H), 1.29 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.6, 172.5, 156.6, 149.7, 145.1, 140.6, 136.8, 133.3, 129.0, 126.6, 124.1, 122.5, 120.8, 52.5, 50.8, 39.1, 39.1, 33.9, 29.7, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{23}H_{30}N_2O_3H$ ($[M + H]^+$): 383.2329; found: 383.2328.

***N*-(*tert*-butyl)-4-methyl-4-(5-(pyridin-2-yl)-2-(trifluoromethyl)phenyl)pentanamide (3i)**



**GP I**, 57.3 mg, 73% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.74 – 8.71 (m, 1H), 8.26 (s, 1H), 7.91 – 7.84 (m, 2H), 7.82 – 7.75 (m, 2H), 7.32 – 7.27 (m, 1H), 5.20 (s, 1H), 2.21 – 2.15 (m, 2H), 1.92 – 1.87 (m, 2H), 1.54 (s, 6H), 1.29 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.2, 156.0, 149.9, 147.2 (d, *J* = 1.8 Hz), 142.1, 136.9, 129.0 (q, *J* = 7.5 Hz), 128.6, 128.1 (q, *J* = 30.5 Hz), 125.0 (q, *J* = 273.8 Hz), 124.4, 122.9, 121.0, 50.9, 39.9, 38.8 (q, *J* = 3.2 Hz), 33.7, 30.4 (q, *J* = 3.3 Hz), 28.7; $^{19}$F NMR (376 MHz, $CDCl_3$) δ -53.07; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{27}F_3N_2OH$ ($[M + H]^+$): 393.2148; found: 393.2146.

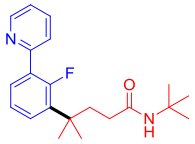
**4-(2-acetyl-5-(pyridin-2-yl)phenyl)-*N*-(*tert*-butyl)-4-methylpentanamide (3j)**



**GP I**, 43.5 mg, 59% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.72 – 8.69 (m, 1H), 8.03 (d, *J* = 1.6 Hz, 1H), 7.83 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.80 – 7.75 (m, 1H), 7.74 – 7.71 (m, 1H), 7.29 – 7.23 (m, 2H), 5.57 (s, 1H), 2.66 (s, 3H), 2.08 – 2.03 (m, 2H), 1.94 – 1.89 (m, 2H), 1.41 (s, 6H), 1.28 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 207.9, 172.6, 156.7, 149.7, 144.5, 142.7, 140.0, 136.8, 127.1, 126.5, 124.1, 122.5, 120.8, 50.8, 39.9, 39.3, 34.0, 32.4, 29.9, 28.6; HRMS (ESI-TOF) (m/z): Calcd for $C_{23}H_{30}N_2O_2H$ ($[M + H]^+$): 367.2380; found: 367.2382.

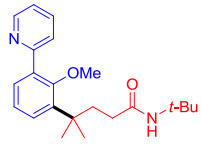
***N*-(*tert*-butyl)-4-(2-fluoro-3-(pyridin-2-yl)phenyl)-4-methylpentanamide (3k)**

**GP I**, 49.1 mg, 71% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.74 – 8.70 (m,



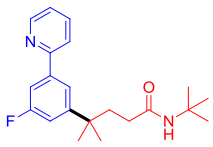
1H), 7.79 – 7.69 (m, 3H), 7.32 – 7.24 (m, 2H), 7.19 (t, *J* = 7.7 Hz, 1H), 5.19 (s, 1H), 2.16 – 2.10 (m, 2H), 1.88 – 1.82 (m, 2H), 1.43 (s, 6H), 1.28 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 159.2 (d, *J* = 252.2 Hz), 154.1, 149.6, 136.1, 135.0 (d, *J* = 12.8 Hz), 129.4 (d, *J* = 3.5 Hz), 128.8 (d, *J* = 6.3 Hz), 128.5 (d, *J* = 14.7 Hz), 124.9 (d, *J* = 8.1 Hz), 123.9 (d, *J* = 4.0 Hz), 122.3, 50.9, 37.6 (d, *J* = 2.5 Hz), 37.1 (d, *J* = 4.7 Hz), 33.7, 28.7, 28.3 (d, *J* = 3.0 Hz); $^{19}$F NMR (376 MHz, $CDCl_3$) δ -115.28; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{27}FN_2OH$ ($[M + H]^+$): 343.2180; found: 343.2180.

***N*-(*tert*-butyl)-4-(2-methoxy-3-(pyridin-2-yl)phenyl)-4-methylpentanamide (3l)**



**GP I**, 34.5 mg, 48% yield, white solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.73 – 8.71 (m, 1H), 7.76 – 7.70 (m, 2H), 7.47 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.29 – 7.22 (m, 2H), 7.12 (t, *J* = 7.7 Hz, 1H), 5.24 (s, 1H), 3.33 (s, 3H), 2.20 – 2.15 (m, 2H), 1.88 – 1.82 (m, 2H), 1.43 (s, 6H), 1.29 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.7, 157.6, 149.7, 140.1, 136.2, 134.1, 130.1, 128.5, 124.6, 123.4, 121.8, 61.2, 50.8, 38.3, 37.6, 34.0, 29.2, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{30}N_2O_2H$ ($[M + H]^+$): 355.2380; found: 355.2380.

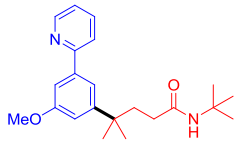
***N*-(*tert*-butyl)-4-(3-fluoro-5-(pyridin-2-yl)phenyl)-4-methylpentanamide (3m)**



**GP I**, 31.4 mg, 45% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.69 – 8.67 (m, 1H), 7.79 – 7.73 (m, 2H), 7.71 – 7.68 (m, 1H), 7.53 – 7.49 (m, 1H), 7.28 – 7.23 (m, 1H), 7.10 – 7.05 (m, 1H), 5.28 (s, 1H), 2.03 – 1.97 (m, 2H), 1.88 – 1.83 (m, 2H), 1.36 (s, 6H), 1.28 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.1, 163.3 (d, *J* = 244.3 Hz), 156.4 (d, *J* = 2.9 Hz), 151.7 (d, *J* = 6.7 Hz), 149.6, 141.2 (d, *J* = 7.9 Hz), 136.8, 122.5, 120.7, 120.0 (d, *J* = 2.3 Hz), 113.5 (d, *J* = 21.8 Hz), 111.2 (d, *J* = 23.0 Hz), 50.9, 39.4, 37.7 (d, *J* = 1.7 Hz), 33.0, 28.7, 28.7; $^{19}$F NMR (376 MHz, $CDCl_3$) δ -113.24; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{27}FN_2OH$ ($[M + H]^+$): 343.2180; found: 343.2179.

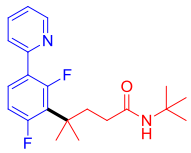
***N*-(*tert*-butyl)-4-(3-methoxy-5-(pyridin-2-yl)phenyl)-4-methylpentanamide (3n)**

**GP I**, 26.5 mg, 37% yield, white solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.68 (m, 1H), 7.78 – 7.70 (m, 2H), 7.51 (t, *J* = 1.6 Hz, 1H), 7.38 (dd, *J* = 2.4, 1.4 Hz, 1H), 7.26 – 7.22 (m, 1H), 6.95 (t, *J* = 2.0 Hz, 1H), 5.14 (s, 1H), 3.90 (s, 3H), 2.02 – 1.97 (m,



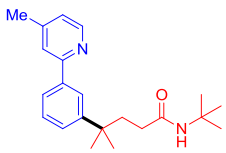
2H), 1.88 – 1.83 (m, 2H), 1.37 (s, 6H), 1.27 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 160.0, 157.7, 150.6, 149.5, 140.6, 136.7, 122.2, 120.9, 117.3, 113.7, 108.7, 55.3, 50.9, 39.5, 37.7, 33.2, 28.8, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{30}N_2O_2H$ ($[M + H]^+$): 355.2380; found: 355.2380.

***N*-(*tert*-butyl)-4-(2,6-difluoro-3-(pyridin-2-yl)phenyl)-4-methylpentanamide (3o)**



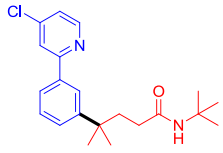
**GP I**, 54.6 mg, 75% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 4.4 Hz, 1H), 7.78 – 7.64 (m, 3H), 7.29 – 7.23 (m, 1H), 6.97 – 6.90 (m, 1H), 5.23 (s, 1H), 2.12 (dd, *J* = 10.9, 5.9 Hz, 2H), 1.97 (dd, *J* = 10.7, 5.9 Hz, 2H), 1.53 (s, 6H), 1.29 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.1, 163.3 (d, *J* = 10.0 Hz), 160.7 (t, *J* = 10.5 Hz), 158.2 (d, *J* = 10.2 Hz), 153.5, 149.6, 136.2, 129.4 (dd, *J* = 11.7, 5.7 Hz), 125.1 (dd, *J* = 16.8, 3.5 Hz), 124.6 (d, *J* = 8.3 Hz), 122.3, 122.2 (dd, *J* = 16.0, 14.5 Hz), 112.8 (dd, *J* = 27.2, 3.4 Hz), 50.9, 39.3 (t, *J* = 3.0 Hz), 38.3 (t, *J* = 3.8 Hz), 34.0, 29.6 (t, *J* = 6.2 Hz), 28.7; $^{19}$F NMR (376 MHz, $CDCl_3$) δ -104.52 (d, *J* = 8.2 Hz, 1F), -110.35 (d, *J* = 8.1 Hz, 1F); HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{26}F_2N_2OH$ ($[M + H]^+$): 361.2086; found: 361.2087.

***N*-(*tert*-butyl)-4-methyl-4-(3-(4-methylpyridin-2-yl)phenyl)pentanamide (3p)**



**GP I**, 61.5 mg, 90% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.9 Hz, 1H), 7.93 (s, 1H), 7.76 (d, *J* = 6.6 Hz, 1H), 7.53 (s, 1H), 7.43 – 7.36 (m, 2H), 7.05 (d, *J* = 5.0 Hz, 1H), 5.21 (s, 1H), 2.42 (s, 3H), 2.04 – 1.98 (m, 2H), 1.87 – 1.81 (m, 2H), 1.38 (s, 6H), 1.27 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 157.7, 149.3, 148.8, 147.6, 139.4, 128.5, 126.4, 124.5, 124.4, 123.0, 121.7, 50.9, 39.6, 37.5, 33.2, 28.8, 28.7, 21.2; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{30}N_2OH$ ($[M + H]^+$): 339.2431; found: 339.2434.

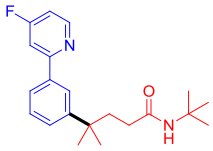
***N*-(*tert*-butyl)-4-(3-(4-chloropyridin-2-yl)phenyl)-4-methylpentanamide (3q)**



**GP I**, 58.4 mg, 81% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 5.3 Hz, 1H), 7.95 – 7.93 (m, 1H), 7.76 – 7.73 (m, 1H), 7.72 (d, *J* = 1.8 Hz, 1H), 7.44 – 7.41 (m, 2H), 7.24 (dd, *J* = 5.3, 1.9 Hz, 1H), 5.15 (s, 1H), 2.04 – 1.99 (m, 2H), 1.87 – 1.82 (m, 2H), 1.38

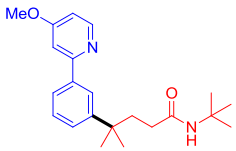
(s, 6H), 1.28 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 159.4, 150.4, 149.2, 144.6, 138.0, 128.7, 127.2, 124.6, 124.4, 122.2, 121.0, 50.9, 39.5, 37.6, 33.2, 28.8, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{27}ClN_2OH$ ([M + H]$^+$): 359.1885; found: 359.1885.

***N*-(*tert*-butyl)-4-(3-(4-fluoropyridin-2-yl)phenyl)-4-methylpentanamide (3r)**



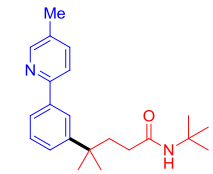
**GP I**, 60.2 mg, 87% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.65 (dd, *J* = 8.8, 5.6 Hz, 1H), 7.97 – 7.95 (m, 1H), 7.77 – 7.73 (m, 1H), 7.46 – 7.42 (m, 3H), 7.00 – 6.95 (m, 1H), 5.13 (s, 1H), 2.05 – 1.99 (m, 2H), 1.87 – 1.82 (m, 2H), 1.39 (s, 6H), 1.28 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.2 (d, *J* = 261.4 Hz), 161.0 (d, *J* = 7.0 Hz), 151.8 (d, *J* = 7.3 Hz), 149.1, 138.1 (d, *J* = 3.5 Hz), 128.7, 127.2, 124.5, 124.3, 109.8 (d, *J* = 16.4 Hz), 108.2 (d, *J* = 17.3 Hz), 50.9, 39.5, 37.5, 33.1, 28.8, 28.6; $^{19}$F NMR (376 MHz, $CDCl_3$) δ -102.50; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{27}FN_2OH$ ([M + H]$^+$): 343.2180; found: 343.2179.

***N*-(*tert*-butyl)-4-(3-(4-methoxypyridin-2-yl)phenyl)-4-methylpentanamide (3s)**



**GP I**, 58.5 mg, 82% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 5.7 Hz, 1H), 7.92 (s, 1H), 7.74 – 7.70 (m, 1H), 7.41 – 7.38 (m, 2H), 7.22 (d, *J* = 2.4 Hz, 1H), 6.78 (dd, *J* = 5.7, 2.4 Hz, 1H), 5.24 (s, 1H), 3.91 (s, 3H), 2.04 – 1.99 (m, 2H), 1.87 – 1.82 (m, 2H), 1.38 (s, 6H), 1.27 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.5, 166.3, 159.6, 150.7, 148.9, 139.3, 128.5, 126.6, 124.6, 124.4, 107.9, 107.2, 55.1, 50.9, 39.6, 37.6, 33.2, 28.8, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{30}N_2O_2H$ ([M + H]$^+$): 355.2380; found: 355.2378.

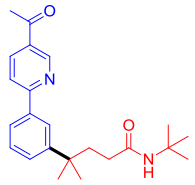
***N*-(*tert*-butyl)-4-methyl-4-(3-(5-methylpyridin-2-yl)phenyl)pentanamide (3t)**



**GP I**, 60.2 mg, 88% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H), 7.93 – 7.91 (m, 1H), 7.75 – 7.71 (m, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 7.1 Hz, 1H), 7.44 – 7.33 (m, 2H), 5.21 (s, 1H), 2.37 (s, 3H), 2.04 – 1.98 (m, 2H), 1.87 – 1.81 (m, 2H), 1.38 (s, 6H), 1.27 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.5, 155.1, 149.9, 148.9, 139.3, 137.2, 131.4, 128.5, 126.2, 124.2, 124.1, 120.2, 50.9, 39.6, 37.5, 33.2, 28.8,

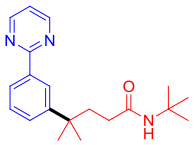
28.7, 18.1; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{30}N_2OH$ ([M + H]$^+$): 339.2431; found: 339.2430.

**4-(3-(5-acetylpyridin-2-yl)phenyl)-*N*-(*tert*-butyl)-4-methylpentanamide (3u)**



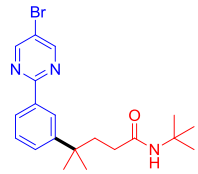
**GP I**, 63.5 mg, 86% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 9.23 (d, *J* = 2.2 Hz, 1H), 8.29 (dd, *J* = 8.4, 2.2 Hz, 1H), 8.06 (s, 1H), 7.86 – 7.82 (m, 2H), 7.49 – 7.42 (m, 2H), 5.19 (s, 1H), 2.66 (s, 3H), 2.07 – 2.00 (m, 2H), 1.90 – 1.84 (m, 2H), 1.40 (s, 6H), 1.28 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 196.4, 172.3, 161.3, 150.0, 149.3, 138.0, 136.3, 130.4, 128.8, 127.7, 124.9, 124.8, 120.3, 50.9, 39.5, 37.6, 33.2, 28.8, 28.7, 26.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{23}H_{30}N_2O_2H$ ([M + H]$^+$): 367.2380; found: 367.2377.

***N*-(*tert*-butyl)-4-methyl-4-(3-(pyrimidin-2-yl)phenyl)pentanamide (3v)**



**GP I**, 57.2 mg, 87% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.81 (d, *J* = 4.8 Hz, 2H), 8.43 (t, *J* = 1.9 Hz, 1H), 8.28 – 8.25 (m, 1H), 7.50 – 7.44 (m, 2H), 7.19 (t, *J* = 4.8 Hz, 1H), 5.13 (s, 1H), 2.06 – 2.01 (m, 2H), 1.88 – 1.82 (m, 2H), 1.40 (s, 6H), 1.27 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 164.9, 157.2, 148.9, 137.4, 128.5, 128.4, 125.6, 125.6, 119.0, 50.9, 39.6, 37.6, 33.3, 28.8, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{20}H_{27}N_3OH$ ([M + H]$^+$): 326.2227; found: 326.2227.

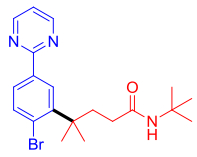
**4-(3-(5-bromopyrimidin-2-yl)phenyl)-*N*-(*tert*-butyl)-4-methylpentanamide (3w)**



**GP I**, 67.7 mg, 83% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.82 (s, 2H), 8.39 (s, 1H), 8.22 (d, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 1H), 5.14 (s, 1H), 2.05 – 1.99 (m, 2H), 1.88 – 1.82 (m, 2H), 1.39 (s, 6H), 1.27 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 163.0, 157.7, 149.0, 136.3, 128.8, 128.6, 125.6, 125.6, 118.1, 50.9, 39.6, 37.6, 33.2, 28.8, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{20}H_{26}BrN_3OH$ ([M + H]$^+$): 404.1332; found: 404.1330.

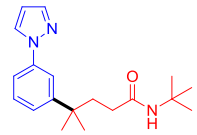
**4-(2-bromo-5-(pyrimidin-2-yl)phenyl)-*N*-(*tert*-butyl)-4-methylpentanamide (3x)**

**GP I**, 66.8 mg, 82% yield, white solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 4.8 Hz, 2H), 8.49 (d, *J* = 2.2 Hz, 1H), 8.11 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.70 (d, *J* = 8.3 Hz,



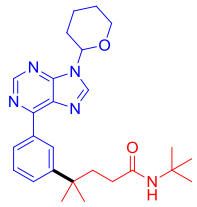
1H), 7.21 (t, *J* = 4.8 Hz, 1H), 5.19 (s, 1H), 2.45 – 2.38 (m, 2H), 1.83 – 1.76 (m, 2H), 1.58 (s, 6H), 1.29 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 164.0, 157.2, 145.5, 136.5, 136.1, 129.1, 127.2, 125.4, 119.2, 50.9, 39.9, 35.5, 33.9, 28.7, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{20}H_{26}BrN_3OH$ ($[M + H]^+$): 404.1332; found: 404.1330.

**4-(3-(1*H*-pyrazol-1-yl)phenyl)-*N*-(*tert*-butyl)-4-methylpentanamide (3y)**



**GP I**, 48.1 mg, 76% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 2.4 Hz, 1H), 7.72 (d, *J* = 1.8 Hz, 1H), 7.68 (t, *J* = 2.0 Hz, 1H), 7.48 – 7.44 (m, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 7.29 – 7.26 (m, 1H), 6.47 (t, *J* = 2.1 Hz, 1H), 5.20 (s, 1H), 2.03 – 1.97 (m, 2H), 1.86 – 1.81 (m, 2H), 1.36 (s, 6H), 1.28 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.2, 150.3, 140.9, 140.1, 129.2, 126.9, 124.2, 117.2, 116.6, 107.5, 51.0, 39.4, 37.6, 33.1, 28.8, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{19}H_{27}N_3OH$ ($[M + H]^+$): 314.2227; found: 314.2227.

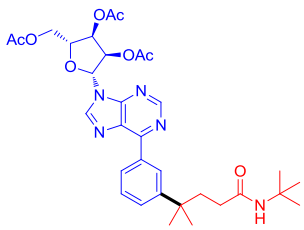
***N*-(*tert*-butyl)-4-methyl-4-(3-(9-(tetrahydro-2*H*-pyran-2-yl)-9*H*-purin-6-yl)phenyl )pentanamide (3z)**



**GP I**, 80.4 mg, 89% yield, white solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 9.02 (s, 1H), 8.71 – 8.70 (m, 1H), 8.64 – 8.60 (m, 1H), 8.33 (s, 1H), 7.53 – 7.50 (m, 2H), 5.85 (dd, *J* = 10.2, 2.7 Hz, 1H), 5.19 (s, 1H), 4.23 – 4.18 (m, 1H), 3.85 – 3.78 (m, 1H), 2.20 – 2.15 (m, 1H), 2.12 – 2.06 (m, 2H), 2.06 – 2.02 (m, 2H), 1.91 – 1.86 (m, 2H), 1.83 – 1.75 (m, 2H), 1.70 – 1.64 (m, 1H), 1.42 (s, 6H), 1.26 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.5, 155.3, 152.3, 151.6, 148.9, 142.0, 135.4, 131.1, 128.6, 128.5, 127.5, 127.1, 81.9, 68.8, 50.9, 39.6, 37.6, 33.3, 31.8, 28.8, 28.7, 24.8, 22.8; HRMS (ESI-TOF) (m/z): Calcd for $C_{26}H_{35}N_5O_2H$ ($[M + H]^+$): 450.2864; found: 450.2867.

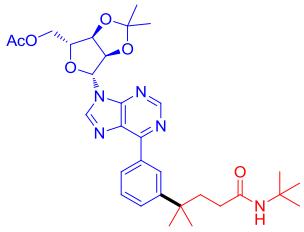
**(2*R*,3*R*,4*R*,5*R*)-2-(acetoxymethyl)-5-(6-(3-(5-(*tert*-butylamino)-2-methyl-5-oxopen tan-2-yl)phenyl)-9*H*-purin-9-yl)tetrahydrofuran-3,4-diyl diacetate (3aa)**

**GP I**, 91.8 mg, 73% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.71 (s, 1H), 8.61 – 8.58 (m, 1H), 8.29 (s, 1H), 7.55 – 7.49 (m, 2H), 6.31 (d, *J* = 5.3 Hz, 1H), 6.03 (t, *J* = 5.4 Hz, 1H), 5.72 (dd, *J* = 5.6, 4.4 Hz, 1H), 5.22 (s, 1H), 4.52 –



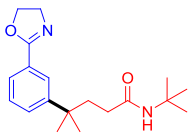
4.45 (m, 2H), 4.44 – 4.36 (m, 1H), 2.17 (s, 3H), 2.15 (s, 3H), 2.10 (s, 3H), 2.07 – 2.02 (m, 2H), 1.91 – 1.86 (m, 2H), 1.43 (s, 6H), 1.27 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 170.2, 169.5, 169.3, 155.7, 152.5, 151.9, 148.9, 142.4, 135.1, 131.6, 128.8, 128.5, 127.4, 127.2, 86.2, 80.3, 72.9, 70.6, 63.0, 50.8, 39.6, 37.6, 33.2, 28.8, 28.8, 28.6, 20.7, 20.5, 20.3; HRMS (ESI-TOF) (m/z): Calcd for $C_{32}H_{41}N_5O_8H$ ([M + H]$^+$): 624.3028; found: 624.3021.

**((3*aR*,4*R*,6*R*,6*aR*)-6-(6-(3-(5-(tert-butylamino)-2-methyl-5-oxopentan-2-yl)phenyl)-9*H*-purin-9-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)methyl acetate (3ab)**



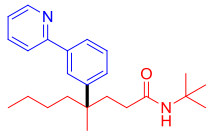
**GP I**, 75.3 mg, 64% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.70 – 8.69 (m, 1H), 8.62 – 8.59 (m, 1H), 8.22 (s, 1H), 7.54 – 7.50 (m, 2H), 6.24 (d, *J* = 2.1 Hz, 1H), 5.54 (dd, *J* = 6.3, 2.1 Hz, 1H), 5.19 (s, 1H), 5.11 (dd, *J* = 6.3, 3.5 Hz, 1H), 4.56 – 4.52 (m, 1H), 4.39 (dd, *J* = 12.0, 4.3 Hz, 1H), 4.25 (dd, *J* = 12.0, 6.1 Hz, 1H), 2.07 – 2.02 (m, 2H), 2.00 (s, 3H), 1.90 – 1.86 (m, 2H), 1.66 (s, 3H), 1.43 (s, 3H), 1.42 (s, 6H), 1.27 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 170.3, 155.7, 152.4, 151.5, 148.9, 143.2, 135.1, 131.8, 128.8, 128.6, 127.5, 127.1, 114.7, 91.1, 84.9, 84.2, 81.5, 64.0, 50.9, 39.6, 37.6, 33.2, 28.8, 28.8, 28.7, 27.1, 25.3, 20.6; HRMS (ESI-TOF) (m/z): Calcd for $C_{31}H_{41}N_5O_6H$ ([M + H]$^+$): 580.3130; found: 580.3126.

***N*-(*tert*-butyl)-4-(3-(4,5-dihydrooxazol-2-yl)phenyl)-4-methylpentanamide (3ac)**



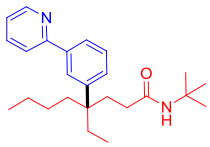
**GP I**, 36.7 mg, 57% yield， yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.91 (t, *J* = 1.9 Hz, 1H), 7.78 – 7.74 (m, 1H), 7.48 – 7.45 (m, 1H), 7.36 (t, *J* = 7.7 Hz, 1H), 5.13 (s, 1H), 4.44 (t, *J* = 9.5 Hz, 2H), 4.06 (t, *J* = 9.5 Hz, 2H), 2.00 – 1.94 (m, 2H), 1.83 – 1.77 (m, 2H), 1.34 (s, 6H), 1.28 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.2, 164.9, 148.8, 129.0, 128.3, 127.5, 125.6, 125.6, 67.5, 54.9, 51.0, 39.5, 37.5, 33.2, 28.7, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{19}H_{28}N_2O_2H$ ([M + H]$^+$): 317.2224; found: 317.2225.

**N-(*tert*-butyl)-4-methyl-4-(3-(pyridin-2-yl)phenyl)octanamide (3ae)**



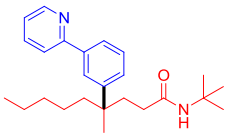
**GP I**, 65.6 mg, 89% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.71 – 8.67 (m, 1H), 7.92 – 7.89 (m, 1H), 7.80 – 7.70 (m, 3H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 7.6 Hz, 1H), 7.22 (t, *J* = 5.8 Hz, 1H), 5.19 (s, 1H), 2.16 – 2.05 (m, 1H), 1.97 – 1.87 (m, 2H), 1.82 – 1.69 (m, 2H), 1.63 – 1.54 (m, 1H), 1.35 (s, 3H), 1.29 – 1.17 (m, 12H), 1.03 – 0.91 (m, 1H), 0.81 (t, *J* = 6.8 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.6, 157.9, 149.5, 147.7, 139.2, 136.6, 128.5, 127.1, 125.0, 124.2, 121.9, 120.7, 50.9, 43.3, 40.7, 38.5, 32.8, 28.7, 26.4, 23.5, 23.3, 14.0; HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{34}N_2OH$ ($[M + H]^+$): 367.2744; found: 367.2743.

***N*-(*tert*-butyl)-4-ethyl-4-(3-(pyridin-2-yl)phenyl)octanamide (3af)**



**GP I**, 55.6mg, 73% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.68 (m, 1H), 7.94 (s, 1H), 7.80 – 7.72 (m, 3H), 7.45 – 7.36 (m, 2H), 7.25 – 7.20 (m, 1H), 5.16 (s, 1H), 2.06 – 2.00 (m, 2H), 1.83 – 1.74 (m, 4H), 1.73 – 1.65 (m, 2H), 1.30 – 1.24 (m, 11H), 1.16 – 1.01 (m, 2H), 0.86 (t, *J* = 7.3 Hz, 3H), 0.74 (t, *J* = 7.4 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.6, 158.0, 149.5, 147.5, 139.1, 136.6, 128.5, 127.3, 125.2, 124.2, 121.9, 120.8, 50.9, 43.1, 36.0, 33.4, 32.2, 29.0, 28.7, 25.6, 23.4, 14.1, 8.0; HRMS (ESI-TOF) (m/z): Calcd for $C_{25}H_{36}N_2OH$ ($[M + H]^+$): 381.2900; found: 381.2895.

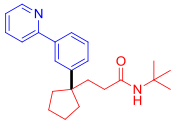
***N*-(*tert*-butyl)-4-methyl-4-(3-(pyridin-2-yl)phenyl)nonanamide (3ag)**



**GP I**, 63.7 mg, 83% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.67 (m, 1H), 7.90 (t, *J* = 1.8 Hz, 1H), 7.79 – 7.70 (m, 3H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.37 – 7.33 (m, 1H), 7.24 – 7.20 (m, 1H), 5.19 (s, 1H), 2.15 – 2.05 (m, 1H), 1.97 – 1.88 (m, 2H), 1.80 – 1.69 (m, 2H), 1.62 – 1.53 (m, 1H), 1.35 (s, 3H), 1.27 (s, 9H), 1.24 – 1.14 (m, 5H), 1.05 – 0.93 (m, 1H), 0.81 (t, *J* = 6.9 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.6, 157.9, 149.5, 147.7, 139.2, 136.7, 128.5, 127.1, 125.0, 124.2, 121.9, 120.7, 50.9, 43.5, 40.7, 38.5, 32.8, 32.5, 28.7, 23.8, 23.5, 22.5, 14.0; HRMS (ESI-TOF) (m/z): Calcd for $C_{25}H_{36}N_2OH$ ($[M + H]^+$): 381.2900; found: 381.2901.

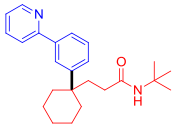
***N*-(*tert*-butyl)-3-(1-(3-(pyridin-2-yl)phenyl)cyclopentyl)propanamide (3ah)**

**GP I**, 56.4 mg, 80% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.4



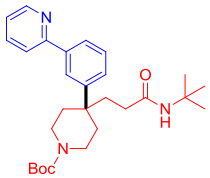
Hz, 1H), 7.90 – 7.88 (m, 1H), 7.78 – 7.69 (m, 3H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.32 (d, *J* = 7.7 Hz, 1H), 7.25 – 7.20 (m, 1H), 5.16 (s, 1H), 2.04 – 1.87 (m, 6H), 1.83 – 1.74 (m, 4H), 1.72 – 1.62 (m, 2H), 1.25 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.4, 157.8, 149.5, 148.6, 139.1, 136.6, 128.4, 127.6, 125.4, 124.3, 122.0, 120.7, 50.8, 50.7, 37.5, 36.9, 33.7, 28.7, 23.1; HRMS (ESI-TOF) (m/z): Calcd for $C_{23}H_{30}N_2OH$ ($[M + H]^+$): 351.2431; found: 351.2430.

**_N_-(*tert*-butyl)-3-(1-(3-(pyridin-2-yl)phenyl)cyclohexyl)propanamide (3ai)**



**GP I**, 59.1 mg, 81% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.66 (m, 1H), 7.94 (t, *J* = 1.9 Hz, 1H), 7.79 – 7.69 (m, 3H), 7.43 (t, *J* = 7.7 Hz, 1H), 7.39 – 7.35 (m, 1H), 7.24 – 7.20 (m, 1H), 5.15 (s, 1H), 2.14 (dd, *J* = 12.5, 5.7 Hz, 2H), 1.95 – 1.88 (m, 2H), 1.76 – 1.71 (m, 2H), 1.69 – 1.55 (m, 4H), 1.48 – 1.37 (m, 4H), 1.24 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.6, 157.9, 149.5, 146.8, 139.3, 136.6, 128.6, 127.5, 125.5, 124.2, 121.9, 120.7, 50.8, 40.9, 38.7, 36.1, 32.0, 28.6, 26.4, 22.2; HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{32}N_2OH$ ($[M + H]^+$): 365.2587; found: 365.2584.

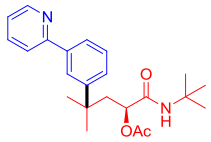
***tert*-butyl 4-(3-(*tert*-butylamino)-3-oxopropyl)-4-(3-(pyridin-2-yl)phenyl)piperidine-1-carboxylate (3aj)**



**GP I**, 69.3 mg, 74% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.67 (m, 1H), 7.92 (t, *J* = 1.8 Hz, 1H), 7.80 – 7.74 (m, 2H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.35 – 7.31 (m, 1H), 7.27 – 7.23 (m, 1H), 5.24 (s, 1H), 3.74 – 3.62 (m, 2H), 3.26 – 3.14 (m, 2H), 2.24 – 2.16 (m, 2H), 2.01 – 1.94 (m, 2H), 1.83 – 1.73 (m, 4H), 1.43 (s, 9H), 1.24 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.0, 157.5, 154.9, 149.5, 144.8, 139.5, 136.8, 129.0, 127.4, 125.5, 124.7, 122.2, 120.8, 79.2, 50.9, 40.7, 39.6, 37.8, 35.1, 31.8, 28.6, 28.4; HRMS (ESI-TOF) (m/z): Calcd for $C_{28}H_{39}N_3O_3H$ ($[M + H]^+$): 466.3064; found: 466.3066.

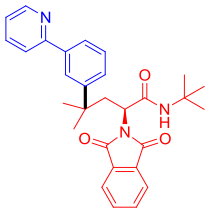
**(S)-1-(tert-butylamino)-4-methyl-1-oxo-4-(3-(pyridin-2-yl)phenyl)pentan-2-yl acetate (3ak)**

**GP I**, 57.6mg, 75% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.72 – 8.68 (m, 1H), 7.96 – 7.94 (m, 1H), 7.80 – 7.77 (m, 1H), 7.75 (dd, *J* = 7.0, 1.8 Hz, 1H), 7.74 –



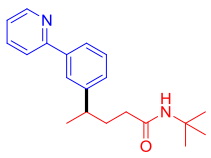
7.71 (m, 1H), 7.45 – 7.38 (m, 2H), 7.26 – 7.22 (m, 1H), 5.52 (s, 1H), 4.97 (dd, *J* = 6.9, 5.0 Hz, 1H), 2.29 – 2.27 (m, 2H), 1.64 (s, 3H), 1.46 (s, 3H), 1.42 (s, 3H), 1.28 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 169.7, 169.4, 157.7, 149.6, 148.5, 139.3, 136.7, 128.6, 126.6, 124.6, 124.4, 122.0, 120.7, 72.1, 51.1, 45.4, 37.1, 30.4, 28.5, 28.0, 20.4; HRMS (ESI-TOF) (m/z): Calcd for $C_{23}H_{30}N_2O_3H$ ($[M + H]^+$): 383.2329; found: 383.2326.

**(*S*)-*N*-(*tert*-butyl)-2-(1,3-dioxoisoindolin-2-yl)-4-methyl-4-(3-(pyridin-2-yl)phenyl) pentanamide (3al)**



**GP II**, 65.9 mg, 70% yield, yellow solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.64 – 8.61 (m, 1H), 7.79 – 7.73 (m, 1H), 7.68 (t, *J* = 1.9 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.41 (m, 2H), 7.36 – 7.31 (m, 2H), 7.23 – 7.16 (m, 2H), 7.15 – 7.11 (m, 1H), 6.93 (t, *J* = 7.8 Hz, 1H), 6.02 (s, 1H), 4.81 (dd, *J* = 11.8, 2.4 Hz, 1H), 3.09 (dd, *J* = 14.8, 11.8 Hz, 1H), 2.26 (dd, *J* = 14.8, 2.4 Hz, 1H), 1.55 (s, 3H), 1.34 (s, 3H), 1.29 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$*d*) δ 168.5, 167.9, 157.1, 149.4, 146.8, 138.6, 136.5, 133.5, 131.0, 128.4, 126.2, 124.1, 123.5, 122.8, 121.9, 120.3, 52.7, 51.4, 41.5, 36.9, 33.3, 28.5, 25.3; HRMS (ESI-TOF) (m/z): Calcd for $C_{29}H_{31}N_3O_3H$ ($[M + H]^+$): 470.2438; found: 470.2440.

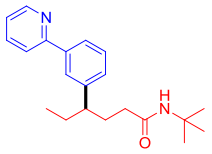
***N*-(*tert*-butyl)-4-(3-(pyridin-2-yl)phenyl)pentanamide (3am)**



**GP I**, 35.4 mg, 57% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.67 (m, 1H), 7.83 – 7.77 (m, 2H), 7.76 – 7.70 (m, 2H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.26 – 7.21 (m, 2H), 5.19 (s, 1H), 2.85 – 2.76 (m, 1H), 2.07 – 2.00 (m, 1H), 2.00 – 1.92 (m, 2H), 1.92 – 1.83 (m, 1H), 1.35 – 1.28 (m, 12H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.1, 157.5, 149.6, 147.1, 139.5, 136.7, 128.9, 127.6, 125.9, 124.7, 122.0, 120.7, 51.0, 39.6, 35.6, 33.7, 28.7, 22.5; HRMS (ESI-TOF) (m/z): Calcd for $C_{20}H_{26}N_2OH$ ($[M + H]^+$): 311.2118; found: 311.2117.

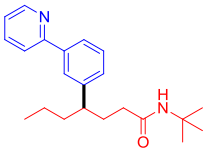
***N*-(*tert*-butyl)-4-(3-(pyridin-2-yl)phenyl)hexanamide (3an)**

**GP I**, 39.7 mg, 61% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.67 (m, 1H), 7.81 – 7.77 (m, 2H), 7.76 – 7.71 (m, 2H), 7.43 – 7.38 (m, 1H), 7.25 – 7.19 (m,



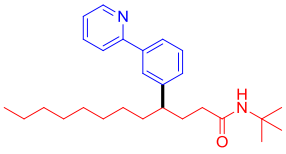
2H), 5.16 (s, 1H), 2.56 – 2.47 (m, 1H), 2.16 – 2.09 (m, 1H), 1.99 – 1.79 (m, 3H), 1.78 – 1.61 (m, 2H), 1.29 (s, 9H), 0.81 (t, *J* = 7.3 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.2, 157.6, 149.6, 145.4, 139.4, 136.7, 128.8, 128.3, 126.6, 124.8, 122.0, 120.7, 50.9, 47.4, 35.6, 31.9, 29.9, 28.7, 12.2; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{28}N_2OH$ ($[M + H]^+$): 325.2274; found: 325.2274.

***N*-(*tert*-butyl)-4-(3-(pyridin-2-yl)phenyl)heptanamide (3ao)**



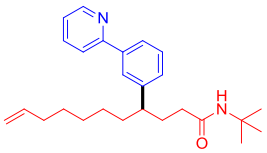
**GP I**, 46.3 mg, 68% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.67 (m, 1H), 7.81 – 7.77 (m, 2H), 7.76 – 7.71 (m, 2H), 7.42 – 7.38 (m, 1H), 7.25 – 7.19 (m, 2H), 5.17 (s, 1H), 2.67 – 2.58 (m, 1H), 2.15 – 2.07 (m, 1H), 1.98 – 1.77 (m, 3H), 1.69 – 1.59 (m, 2H), 1.29 (s, 9H), 1.25 – 1.13 (m, 2H), 0.84 (t, *J* = 7.3 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.2, 157.6, 149.5, 145.7, 139.4, 136.7, 128.8, 128.2, 126.5, 124.7, 122.0, 120.7, 50.9, 45.3, 39.2, 35.6, 32.2, 28.7, 20.7, 14.0; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{30}N_2OH$ ($[M + H]^+$): 339.2431; found: 339.2430.

***N*-(*tert*-butyl)-4-(3-(pyridin-2-yl)phenyl)dodecanamide (3ap)**



**GP I**, 58.6 mg, 71% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.67 (m, 1H), 7.81 – 7.77 (m, 2H), 7.76 – 7.71 (m, 2H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.25 – 7.18 (m, 2H), 5.13 (s, 1H), 2.64 – 2.55 (m, 1H), 2.15 – 2.07 (m, 1H), 2.04 – 1.76 (m, 4H), 1.71 – 1.60 (m, 2H), 1.29 (s, 9H), 1.26 – 1.18 (m, 11H), 0.85 (t, *J* = 6.9 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.2, 157.6, 149.6, 145.8, 139.4, 136.7, 128.8, 128.2, 126.5, 124.7, 122.0, 120.7, 51.0, 45.6, 37.1, 35.6, 32.3, 31.8, 29.7, 29.4, 29.2, 28.7, 27.6, 22.6, 14.1; HRMS (ESI-TOF) (m/z): Calcd for $C_{27}H_{40}N_2OH$ ($[M + H]^+$): 409.3213; found: 409.3215.

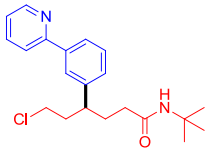
***N*-(*tert*-butyl)-4-(3-(pyridin-2-yl)phenyl)undec-10-enamide (3aq)**



**GP I**, 42.8 mg, 54% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.7 Hz, 1H), 7.82 – 7.71 (m, 4H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.25 – 7.18 (m, 2H), 5.82 – 5.69 (m, 1H), 5.13 (s, 1H), 4.98 – 4.85 (m, 2H), 2.65 – 2.54 (m, 1H), 2.18 – 2.01 (m, 2H), 2.01 – 1.77 (m,

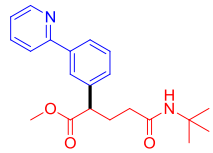
6H), 1.70 – 1.60 (m, 2H), 1.29 (s, 13H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.1, 157.6, 149.6, 145.7, 139.4, 139.1, 136.7, 128.8, 128.2, 126.5, 124.8, 122.0, 120.7, 114.1, 51.0, 45.6, 37.0, 35.6, 33.7, 32.3, 29.1, 28.7, 28.7, 27.4; HRMS (ESI-TOF) (m/z): Calcd for $C_{26}H_{36}N_2OH$ ($[M + H]^+$): 393.2900; found: 393.2902.

***N*-(*tert*-butyl)-6-chloro-4-(3-(pyridin-2-yl)phenyl)hexanamide (3ar)**



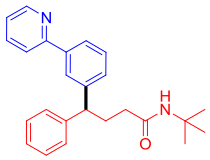
**GP I**, 35.7 mg, 49% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.5 Hz, 1H), 7.85 – 7.80 (m, 2H), 7.79 – 7.71 (m, 2H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.28 – 7.21 (m, 2H), 5.16 (s, 1H), 3.48 – 3.41 (m, 1H), 3.33 – 3.25 (m, 1H), 2.95 – 2.86 (m, 1H), 2.17 – 2.07 (m, 3H), 1.97 – 1.89 (m, 3H), 1.29 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.7, 157.3, 149.6, 143.5, 139.8, 136.8, 129.1, 128.3, 126.4, 125.4, 122.2, 120.7, 51.0, 43.0, 42.6, 39.5, 35.3, 31.8, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{27}ClN_2OH$ ($[M + H]^+$): 359.1885; found: 359.1887.

**methyl 5-(*tert*-butylamino)-5-oxo-2-(3-(pyridin-2-yl)phenyl)pentanoate (3as)**



**GP I**, 34.2 mg, 48% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.67 (m, 1H), 7.92 – 7.86 (m, 2H), 7.78 – 7.70 (m, 2H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.38 – 7.34 (m, 1H), 7.26 – 7.22 (m, 1H), 5.23 (s, 1H), 3.73 (t, *J* = 7.7 Hz, 1H), 3.66 (s, 3H), 2.48 – 2.38 (m, 1H), 2.21 – 2.11 (m, 1H), 2.08 – 1.97 (m, 2H), 1.32 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 174.0, 171.1, 157.1, 149.6, 139.8, 138.9, 136.7, 129.2, 128.4, 126.9, 126.0, 122.2, 120.7, 52.0, 51.1, 50.5, 34.8, 29.0, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{26}N_2O_3H$ ($[M + H]^+$): 355.2016; found: 355.2018.

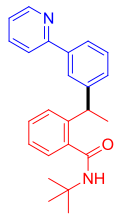
***N*-(*tert*-butyl)-4-phenyl-4-(3-(pyridin-2-yl)phenyl)butanamide (3at)**



**GP I**, 41.9 mg, 56% yield, yellow solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.8 Hz, 1H), 7.90 (s, 1H), 7.78 (d, *J* = 7.8 Hz, 1H), 7.75 – 7.66 (m, 2H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.30 – 7.27 (m, 5H), 7.22 – 7.16 (m, 2H), 5.17 (s, 1H), 4.01 (t, *J* = 8.0 Hz, 1H), 2.47 – 2.40 (m, 2H), 2.08 – 2.02 (m, 2H), 1.31 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.7, 157.4, 149.6, 144.9, 144.2, 139.6, 136.7, 128.9, 128.5, 127.9, 126.7, 126.3, 124.9, 122.1, 120.7, 51.1, 50.6, 35.8, 31.1, 28.8; HRMS (ESI-TOF) (m/z): Calcd for $C_{25}H_{28}N_2OH$ ([M +

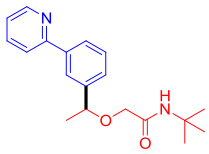
H]$^+$): 373.2274; found: 373.2277.

***N*-(*tert*-butyl)-2-(1-(3-(pyridin-2-yl)phenyl)ethyl)benzamide (3au)**



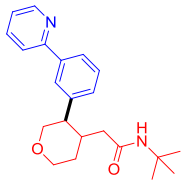
**GP I**, 41.6 mg, 58% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.66 – 8.63 (m, 1H), 7.85 (t, *J* = 1.9 Hz, 1H), 7.80 – 7.76 (m, 1H), 7.74 – 7.69 (m, 1H), 7.68 – 7.65 (m, 1H), 7.39 – 7.33 (m, 3H), 7.32 – 7.25 (m, 2H), 7.22 – 7.17 (m, 2H), 5.49 (s, 1H), 4.82 (q, *J* = 7.2 Hz, 1H), 1.70 (d, *J* = 7.2 Hz, 3H), 1.32 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 169.8, 157.4, 149.5, 146.8, 143.0, 139.4, 137.9, 136.6, 129.5, 128.7, 128.4, 127.8, 126.8, 126.3, 126.0, 124.6, 122.0, 120.6, 51.6, 40.3, 28.6, 22.2; HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{26}N_2OH$ ([M + H]$^+$): 359.2118; found: 359.2120.

***N*-(*tert*-butyl)-2-(1-(3-(pyridin-2-yl)phenyl)ethoxy)acetamide (3av)**



**GP I**, 17.0 mg, 27% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 4.9 Hz, 1H), 7.97 – 7.95 (m, 1H), 7.91 – 7.87 (m, 1H), 7.79 – 7.72 (m, 2H), 7.47 (t, *J* = 7.7 Hz, 1H), 7.38 – 7.33 (m, 1H), 7.27 – 7.23 (m, 1H), 6.47 (s, 1H), 4.55 (q, *J* = 6.5 Hz, 1H), 3.77 (s, 2H), 1.56 (d, *J* = 6.5 Hz, 3H), 1.36 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 168.9, 157.0, 149.7, 142.9, 139.8, 136.8, 129.1, 126.6, 126.4, 124.8, 122.3, 120.6, 79.1, 68.7, 50.8, 28.7, 23.6; HRMS (ESI-TOF) (m/z): Calcd for $C_{19}H_{24}N_2O_2H$ ([M + H]$^+$): 313.1911; found: 313.1912.

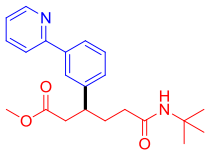
***N*-(*tert*-butyl)-2-(3-(3-(pyridin-2-yl)phenyl)tetrahydro-2*H*-pyran-4-yl)acetamide (3aw)**



**GP I**, 28.9 mg, 40% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.66 (m, 1H), 7.97 (s, 0.5H), 7.86 – 7.79 (m, 1.5H), 7.78 – 7.70 (m, 2H), 7.62 (d, *J* = 7.8 Hz, 0.5H), 7.44 – 7.38 (m, 1H), 7.29 – 7.22 (m, 1.5H), 5.26 (d, *J* = 9.4 Hz, 1H), 4.17 – 4.02 (m, 1.5H), 3.96 – 3.87 (m, 1H), 3.67 – 3.55 (m, 1H), 3.45 (t, *J* = 11.3 Hz, 0.5H), 2.99 – 2.94 (m, 0.5H), 2.68 – 2.56 (m, 1H), 2.48 – 2.37 (m, 0.5H), 2.13 (dd, *J* = 14.3, 3.6 Hz, 0.5H), 1.95 – 1.84 (m, 1H), 1.73 – 1.63 (m, 1.5H), 1.53 – 1.43 (m, 1H), 1.25 (d, *J* = 5.4 Hz, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.9, 170.8, 157.6, 157.1, 149.5, 149.5, 142.2, 140.6, 139.7, 139.0, 136.8, 136.7, 130.2, 129.1, 128.4, 128.4, 125.6, 125.1, 122.2, 122.0, 120.8, 120.7, 73.5, 71.5,

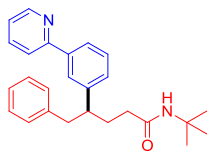
68.1, 67.6, 51.0, 49.5, 43.6, 41.9, 41.0, 37.2, 34.8, 31.9, 28.7, 28.6, 27.6; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{28}N_2O_2H$ ([M + H]$^+$): 353.2224; found: 353.2222.

**methyl 6-(*tert*-butylamino)-6-oxo-3-(3-(pyridin-2-yl)phenyl)hexanoate (3ax)**



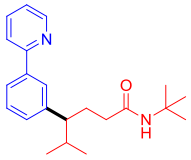
**GP I**, 37.1 mg, 50% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.67 (m, 1H), 7.84 – 7.80 (m, 2H), 7.78 – 7.70 (m, 2H), 7.44 – 7.39 (m, 1H), 7.28 – 7.22 (m, 2H), 5.21 (s, 1H), 3.58 (s, 3H), 3.26 – 3.16 (m, 1H), 2.75 – 2.64 (m, 2H), 2.16 – 2.06 (m, 1H), 1.97 – 1.88 (m, 3H), 1.29 (s, 9H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.5, 171.6, 157.3, 149.6, 143.6, 139.7, 136.7, 129.0, 128.1, 126.3, 125.4, 122.2, 120.7, 51.5, 51.0, 41.6, 41.5, 35.2, 31.5, 28.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{28}N_2O_3H$ ([M + H]$^+$): 369.2173; found: 369.2173.

***N*-(*tert*-butyl)-5-phenyl-4-(3-(pyridin-2-yl)phenyl)pentanamide (3ay)**



**GP I**, 44.3 mg, 57% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.69 – 8.66 (m, 1H), 7.80 – 7.64 (m, 4H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.28 – 7.25 (m, 1H), 7.24 – 7.10 (m, 5H), 7.07 – 7.04 (m, 1H), 5.17 (d, *J* = 59.5 Hz, 1H), 4.00 (t, *J* = 7.8 Hz, 0.24H), 2.99 – 2.90 (m, 2.35H), 2.18 – 2.07 (m, 2.0H), 1.99 – 1.82 (m, 2.54H), 1.30 (s, 2.12H), 1.25 (s, 6.97H); $^{13}$C NMR (101 MHz, $CDCl_3$) major：δ 171.9, 157.5, 149.5, 144.7, 140.2, 139.4, 136.7, 129.1, 128.8, 128.4, 128.1, 126.5, 125.8, 125.0, 122.1, 120.7, 50.9, 47.5, 43.8, 35.5, 31.0, 28.7；minor：$^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.0, 157.5, 149.5, 145.3, 144.7, 139.5, 136.6, 128.8, 128.4, 128.4, 127.8, 126.6, 126.1, 124.8, 122.0, 120.7, 51.3, 51.0, 37.5, 35.2, 28.8, 24.3; HRMS (ESI-TOF) (m/z): Calcd for $C_{26}H_{30}N_2OH$ ([M + H]$^+$): 387.2431; found: 387.2433.

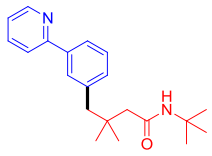
***N*-(*tert*-butyl)-5-methyl-4-(3-(pyridin-2-yl)phenyl)hexanamide (3az)**



**GPI**, 42.1 mg, 62% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.67 (m, 1H), 7.82 – 7.76 (m, 1H), 7.76 – 7.70 (m, 3H), 7.43 – 7.37 (m, 1H), 7.25 – 7.20 (m, 1H), 7.20 – 7.16 (m, 1H), 5.21 (d, *J* = 41.3 Hz, 1H), 2.37 – 2.29 (m, 1.2H), 2.28 – 2.21 (m, 0.93H), 1.98 (t, *J* = 7.5 Hz, 0.42H), 1.91 – 1.85 (m, 1.56H), 1.83 – 1.76 (m, 1.29H), 1.70 – 1.64 (m, 0.46H), 1.37 (s, 1.2H), 1.28 (d, *J* = 5.7 Hz, 9H), 1.01 (d, *J* = 6.6 Hz, 2.58H), 0.75 (d, *J* = 6.7 Hz,

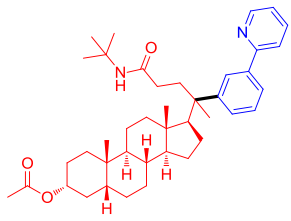
2.56H). major: $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.3, 157.6, 149.5, 144.5, 139.2, 136.7, 128.9, 128.6, 127.2, 124.7, 122.0, 120.7, 52.7, 50.9, 35.8, 33.6, 28.7, 28.6, 21.0, 20.9, minor: $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.2, 157.9, 149.8, 149.5, 139.1, 136.6, 128.4, 126.5, 124.5, 124.2, 121.9, 120.8, 50.9, 43.9, 38.0, 37.8, 28.8, 28.7, 21.1; HRMS (ESI-TOF) (m/z): Calcd for $C_{22}H_{30}N_2OH$ ($[M + H]^+$): 339.2431; found: 339.2433.

***N*-(*tert*-butyl)-3,3-dimethyl-4-(3-(pyridin-2-yl)phenyl)butanamide (3ba)**



**GP I**, 14.5 mg, 22% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.67 (m, 1H), 7.85 – 7.81 (m, 1H), 7.80 – 7.78 (m, 1H), 7.77 – 7.70 (m, 2H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.28 – 7.25 (m, 1H), 7.24 – 7.20 (m, 1H), 5.19 (s, 1H), 2.76 (s, 2H), 1.97 (s, 2H), 1.35 (s, 9H), 1.06 (s, 6H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.0, 157.7, 149.6, 139.2, 138.9, 136.7, 131.5, 129.3, 128.2, 124.7, 122.0, 120.7, 51.2, 48.8, 48.4, 34.5, 28.8, 27.4; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{28}N_2OH$ ($[M + H]^+$): 325.2274; found: 325.2276.

**(3*R*,5*R*,8*R*,9*S*,10*S*,13*S*,14*S*,17*S*)-17-(5-(*tert*-butylamino)-5-oxo-2-(3-(pyridin-2-yl) phenyl)pentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthre n-3-yl acetate (3bb)**



**GP I**, 60.9 mg, 48% yield, yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.72 – 8.66 (m, 1H), 7.93 (d, *J* = 17.8 Hz, 1H), 7.84 – 7.71 (m, 3H), 7.42 – 7.31 (m, 2H), 7.26 – 7.20 (m, 1H), 5.11 (d, *J* = 18.3 Hz, 1H), 4.76 – 4.60 (m, 1H), 2.56 – 2.34 (m, 1H), 2.29 – 2.07 (m, 2H), 2.05 – 1.97 (m, 4H), 1.90 – 1.73 (m, 6H), 1.68 – 1.49 (m, 5H), 1.47 – 1.32 (m, 9H), 1.27 (d, *J* = 10.6 Hz, 9H), 1.20 – 1.15 (m, 2H), 1.04 – 0.93 (m, 4H), 0.91 – 0.79 (m, 4H), 0.71 (d, *J* = 32.2 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.8, 172.7, 170.6, 170.5, 157.9, 157.9, 149.6, 148.7, 147.4, 139.0, 138.9, 136.7, 128.3, 128.3, 127.8, 127.4, 125.6, 125.3, 124.3, 124.0, 121.9, 120.7, 120.6, 74.3, 63.3, 62.7, 56.8, 56.4, 50.9, 44.4, 44.1, 44.0, 43.2, 41.8, 40.9, 40.4, 40.2, 39.4, 38.6, 35.8, 35.3, 35.2, 35.0, 34.9, 34.5, 34.4, 33.0, 32.2, 32.2, 32.1, 28.8, 28.7, 27.0, 26.5, 26.5, 26.1, 26.1, 23.9, 23.6, 23.5, 23.3, 23.3, 23.2, 21.5, 21.4, 20.7, 20.5, 18.8, 14.8, 14.7; HRMS (ESI-TOF) (m/z): Calcd for $C_{41}H_{58}N_2O_3H$ ($[M + H]^+$):

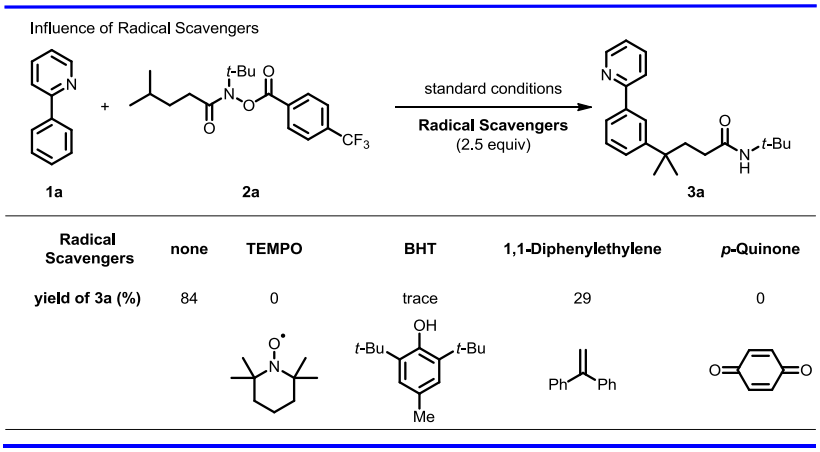
627.4520; found: 627.4523.

***N*-(*tert*-butyl)-5-(3,4-dihydronaphthalen-1-yl)-4,4-dimethylpentanamide (5)**

**Procedure of Radical clock experiment**, 31.4 mg, 20% yield, yellow oil; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 7.5 Hz, 1H), 7.17 – 7.09 (m, 3H), 5.84 (t, *J* = 4.6 Hz, 1H), 5.08 (s, 1H), 2.71 (t, *J* = 7.9 Hz, 2H), 2.41 (s, 2H), 2.25 – 2.19 (m, 2H), 2.10 – 2.05 (m, 2H), 1.58 – 1.52 (m, 2H), 1.31 (s, 9H), 0.82 (s, 6H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.9, 136.6, 136.2, 134.1, 129.1, 127.5, 126.3, 125.9, 123.3, 51.0, 43.0, 38.4, 34.0, 33.1, 28.9, 28.8, 27.3, 23.3; HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{31}NOH$ ($[M + H]^+$): 314.2478; found: 314.2478.

**6. Control experiments**

**(1), Influence of radical scavengers**

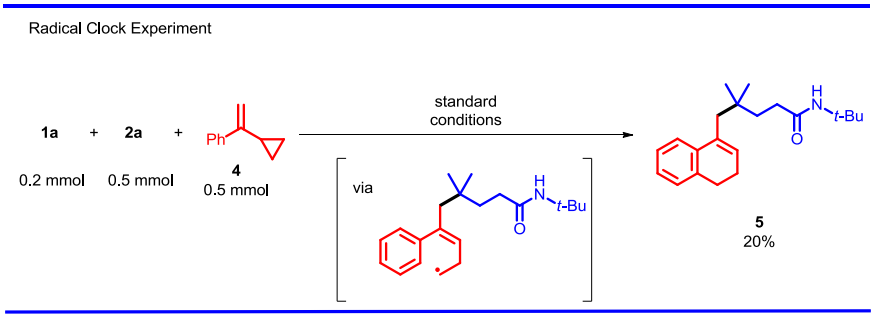



| Radical Scavengers | none | TEMPO | BHT | 1,1-Diphenylethylene | *p*-Quinone |
|---|---|---|---|---|---|
| yield of 3a (%) | 84 | 0 | trace | 29 | 0 |

In an oven-dried 10 ml tube equipped with a stirring bar, **2a** (0.5 mmol, 2.5 equiv), **1a** (0.2 mmol, 1.0 equiv), $K_2CO_3$ (0.6 mmol, 3.0 equiv), $MesCO_2H$ (0.06 mmol, 30 mol%), P(*p*-$CF_3$Ph)$_3$ (0.04 mmol, 20 mol%), radical scavengers (0.5 mmol, 2.5 equiv), $[RuCl_2(p\text{-cymene})]_2$ (0.01 mmol, 5 mol%) and $Ir(ppy)_3$ (0.002 mmol, 1 mol%) were added. The tube was charged with argon (repeated three times), then 1,4-dioxane (1 mL) was injected. The resulting suspension was stirred at room temperature for 10 mins, and then was placed in a preheated oil bath at 60 ℃ and irradiated with blue LEDs (2*20W) for 36 h. The resulting mixture was filtered through a short plug of silica gel (rinsed with ethyl acetate). After the removal of solvents under reduced

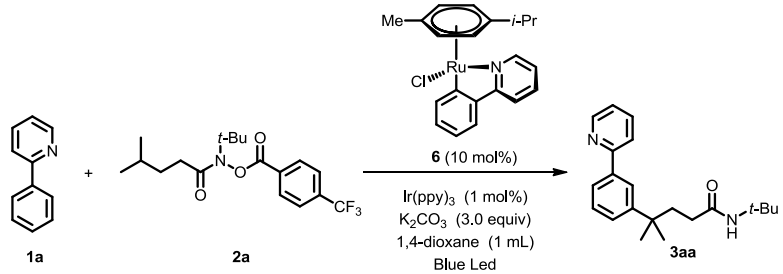
pressure, the crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:5, v:v) as the eluent to give the pure product.

**(2), Procedure of radical clock experiment**



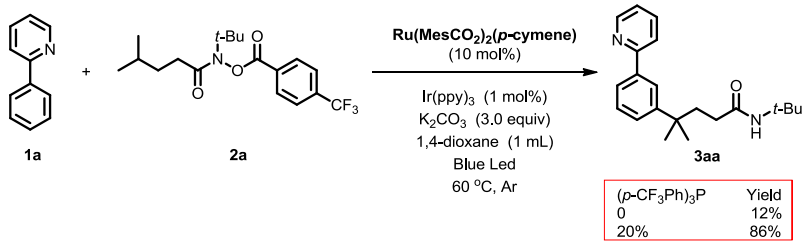

In an oven-dried 10 ml tube equipped with a stirring bar, **2a** (0.5 mmol, 2.5 equiv), **1a** (0.2 mmol, 1.0 equiv), $K_2CO_3$ (0.6 mmol, 3.0 equiv), $MesCO_2H$ (0.06 mmol, 30 mol%), P(*p*-$CF_3Ph)_3$ (0.04 mmol, 20 mol%), (1-cyclopropylvinyl)benzene (0.5 mmol, 2.5 equiv), $[RuCl_2(p\text{-cymene})]_2$ (0.01 mmol, 5 mol%) and $Ir(ppy)_3$ (0.002 mmol, 1 mol%) were added. The tube was charged with argon (repeated three times), then 1,4-dioxane (1 mL) was injected. The resulting suspension was stirred at room temperature for 10 mins, and then was placed in a preheated oil bath at 60 ℃ and irradiated with blue LEDs (2*20W) for 36 h. The resulting mixture was filtered through a short plug of silica gel (rinsed with ethyl acetate). After the removal of solvents under reduced pressure, the crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:5, v:v) as the eluent to give the pure product **5** (31.4 mg, 20% yield).

**(3), Cyclometalated complexes or phosphine complex as catalyst**

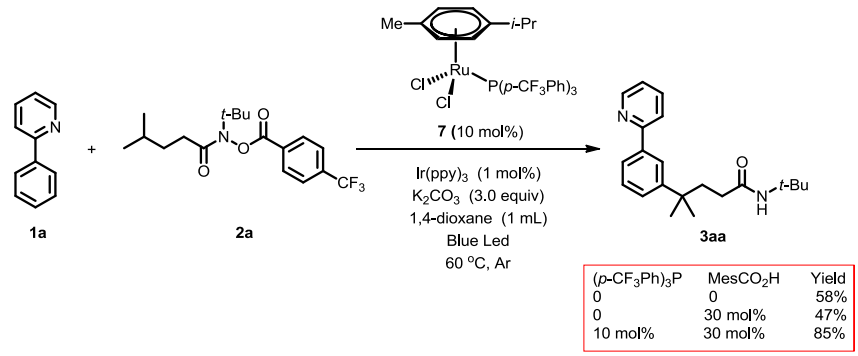



| (*p*-$CF_3Ph)_3P$ | $MesO_2H$ | Yield |
|---|---|---|
| 0 | 30 mol% | 8% |
| 20 mol% | 0 | 63% |
| 20 mol% | 30 mmol% | 83% |

In an oven-dried 10 ml tube equipped with a stirring bar, **2a** (0.5 mmol, 2.5 equiv), **1a** (0.2 mmol, 1.0 equiv), $K_2CO_3$ (0.6 mmol, 3.0 equiv), $MesCO_2H$ (0.06 mmol, 30 mol%), P(*p*-$CF_3$Ph)$_3$ (0.04 mmol, 20 mol%), cyclometalated complexes **6** (0.02 mmol, 10 mol%) and Ir(ppy)$_3$ (0.002 mmol, 1 mol%) were added. The tube was charged with argon (repeated three times), then 1,4-dioxane (1 mL) was injected. The resulting suspension was stirred at room temperature for 10 mins, and then was placed in a preheated oil bath at 60 ℃ and irradiated with blue LEDs (2*20W) for 36 h. The resulting mixture was filtered through a short plug of silica gel (rinsed with ethyl acetate). After the removal of solvents under reduced pressure, the crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:5, v:v) as the eluent to give the pure product.



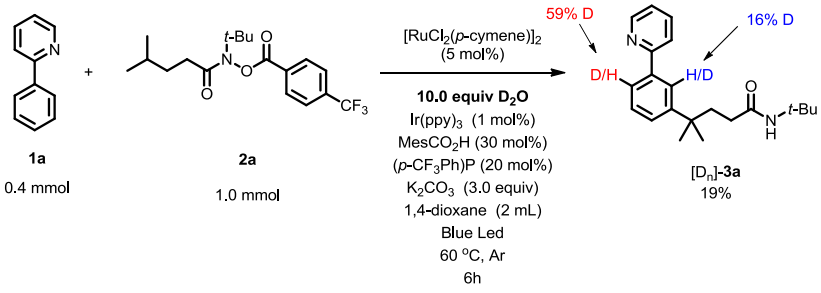

In an oven-dried 10 ml tube equipped with a stirring bar, **2a** (0.5 mmol, 2.5 equiv), **1a** (0.2 mmol, 1.0 equiv), $K_2CO_3$ (0.6 mmol, 3.0 equiv), $MesCO_2H$ (0.06 mmol, 30 mol%), P(*p*-$CF_3$Ph)$_3$ (0.04 mmol, 20 mol%), Ru($MesCO_2$)$_2$(*p*-cymene) (0.02 mmol, 10 mol%) and Ir(ppy)$_3$ (0.002 mmol, 1 mol%) were added. The tube was charged with argon (repeated three times), then 1,4-dioxane (1 mL) was injected. The resulting suspension was stirred at room temperature for 10 mins, and then was placed in a preheated oil bath at 60 ℃ and irradiated with blue LEDs (2*20W) for 36 h. The resulting mixture was filtered through a short plug of silica gel (rinsed with ethyl acetate). After the removal of solvents under reduced pressure, the crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:5, v:v) as the eluent to give the pure product.




In an oven-dried 10 ml tube equipped with a stirring bar, **2a** (0.5 mmol, 2.5 equiv), **1a** (0.2 mmol, 1.0 equiv), $K_2CO_3$ (0.6 mmol, 3.0 equiv), $MesCO_2H$ (0.06 mmol, 30 mol%), P(*p*-$CF_3Ph)_3$ (0.04 mmol, 20 mol%), Ru-complex **7** (0.02 mmol, 10 mol%) and $Ir(ppy)_3$ (0.002 mmol, 1 mol%) were added. The tube was charged with argon (repeated three times), then 1,4-dioxane (1 mL) was injected. The resulting suspension was stirred at room temperature for 10 mins, and then was placed in a preheated oil bath at 60 ℃ and irradiated with blue LEDs (2*20W) for 36 h. The resulting mixture was filtered through a short plug of silica gel (rinsed with ethyl acetate). After the removal of solvents under reduced pressure, the crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:5, v:v) as the eluent to give the pure product.

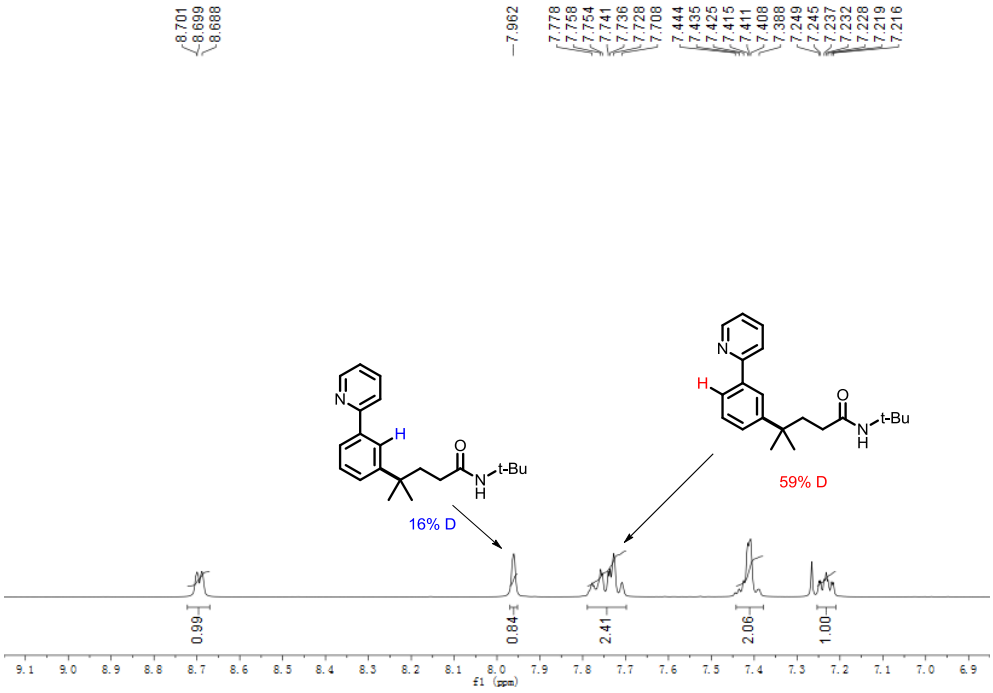
## 7. Mechanistic studies by isotopic labeling

### (1), H/D-Exchange study by adding $D_2O$

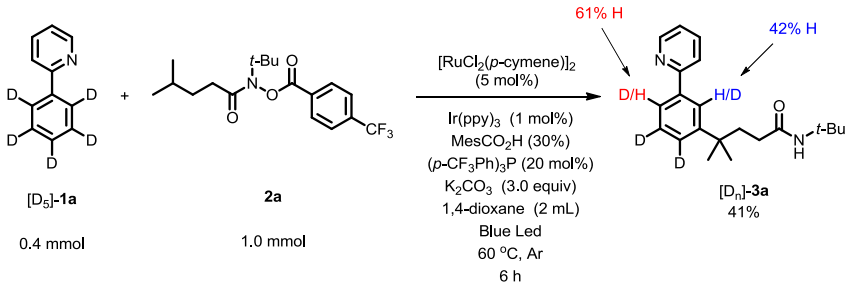



In an oven-dried 10 ml tube equipped with a stirring bar, **2a** (1.0 mmol, 2.5 equiv), **1a** (0.4 mmol, 1.0 equiv), $K_2CO_3$ (1.2 mmol, 3.0 equiv), $MesCO_2H$ (0.12 mmol, 30 mol%), P(*p*-$CF_3Ph)_3$ (0.08 mmol, 20 mol%), $[RuCl_2(p\text{-cymene})]_2$ (0.02 mmol, 5 mol%) and $Ir(ppy)_3$ (0.004 mmol, 1 mol%) were added. The tube was charged with

argon (repeated three times), then 1,4-dioxane (2 mL) and $D_2O$ (4.0 mmol, 10.0 equiv) were injected. The resulting suspension was stirred at room temperature for 10 mins, and then was placed in a preheated oil bath at 60 ℃ and irradiated with blue LEDs (2*20W) for 6 h. The resulting mixture was filtered through a short plug of silica gel (rinsed with ethyl acetate). After the removal of solvents under reduced pressure, the crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:5, v:v) as the eluent to give the pure product (25.3 mg, 19%).

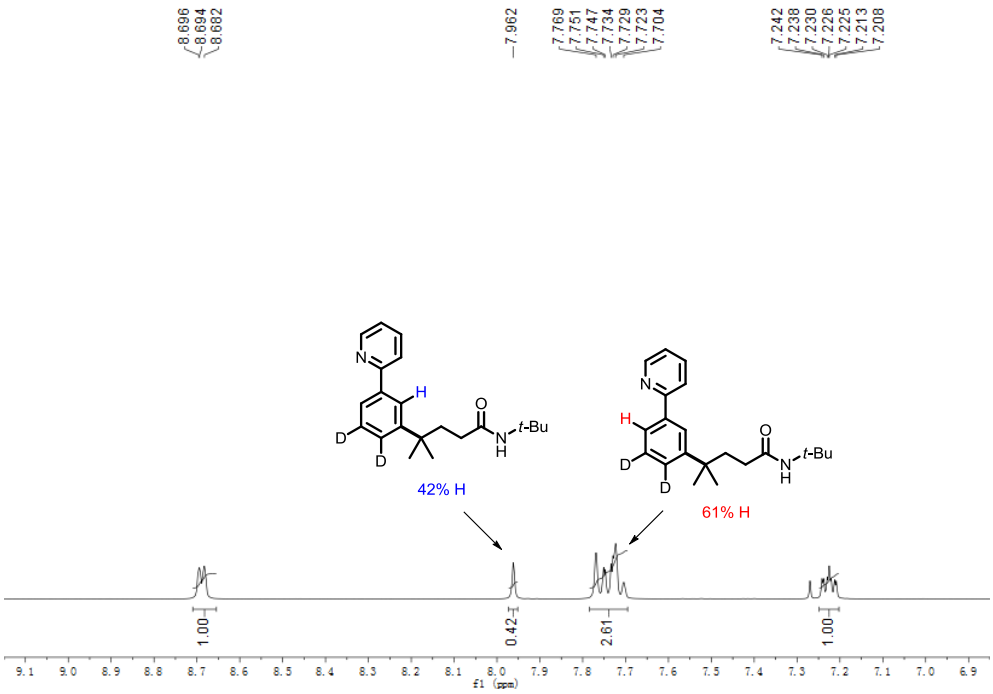



**(2), [$D_5$]-1a was used for H/D-Exchange study**

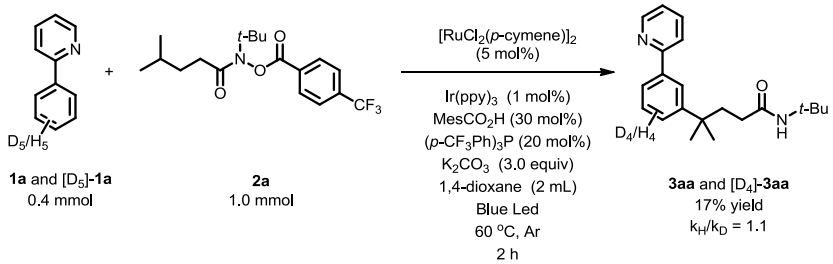



In an oven-dried 10 ml tube equipped with a stirring bar, **2a** (1.0 mmol, 2.5 equiv), [$D_5$]-**1a** (0.4 mmol, 1.0 equiv), $K_2CO_3$ (1.2 mmol, 3.0 equiv), $MesCO_2H$ (0.12 mmol,

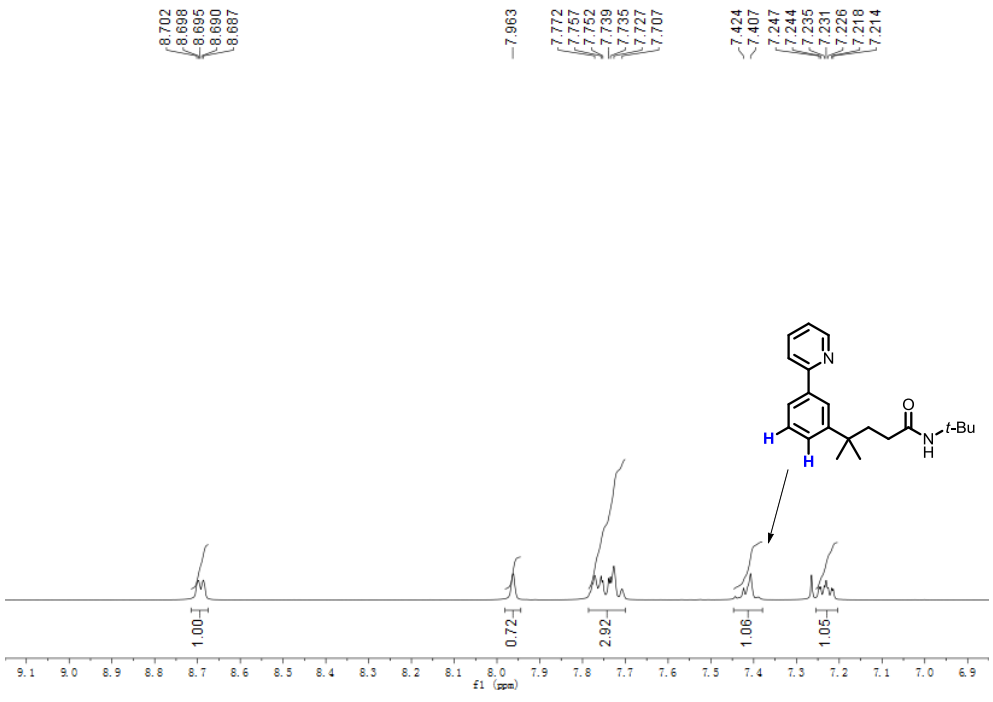
30 mol%), P(*p*-$CF_3Ph)_3$ (0.08 mmol, 20 mol%), $[RuCl_2(p\text{-cymene})]_2$ (0.02 mmol, 5 mol%) and $Ir(ppy)_3$ (0.004 mmol, 1 mol%) were added. The tube was charged with argon (repeated three times), then 1,4-dioxane (2 mL) was injected. The resulting suspension was stirred at room temperature for 10 mins, and then was placed in a preheated oil bath at 60 ℃ and irradiated with blue LEDs (2*20W) for 6 h. The resulting mixture was filtered through a short plug of silica gel (rinsed with ethyl acetate). After the removal of solvents under reduced pressure, the crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:5, v:v) as the eluent to give the pure product. The H incorporation was determined by $^1$H-NMR spectroscopy (54.2 mg, 41%).




## (3), Intermolecular KIE competition

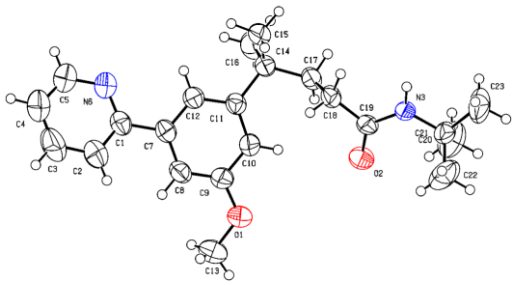


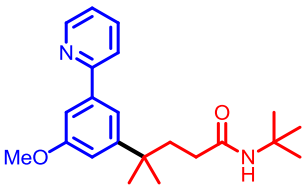
In an oven-dried 10 ml tube equipped with a stirring bar, **2a** (1.0 mmol, 2.5 equiv), **1a** (0.2 mmol) and [$D_5$]-**1a** (0.2 mmol), $K_2CO_3$ (1.2 mmol, 3.0 equiv), $MesCO_2H$ (0.12 mmol, 30 mol%), P(*p*-$CF_3$Ph)$_3$ (0.08 mmol, 20 mol%), [$RuCl_2$(*p*-cymene)]$_2$ (0.02 mmol, 5 mol%) and Ir(ppy)$_3$ (0.004 mmol, 1 mol%) were added. The tube was charged with argon (repeated three times), then 1,4-dioxane (2 mL) was injected. The resulting suspension was stirred at room temperature for 10 mins, and then was placed in a preheated oil bath at 60 ℃ and irradiated with blue LEDs (2*20W) for 2 h. The resulting mixture was filtered through a short plug of silica gel (rinsed with ethyl acetate). After the removal of solvents under reduced pressure, the crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:5, v:v) as the eluent to give the pure product. The $k_H/k_D$ (1.1) was determined by $^1$H-NMR spectroscopy (22.6 mg, 17%).



## 8. X-ray single crystal diffraction data

### (1), X-ray single crystal diffraction data of 3n






The ellipsoid contour percent probability level is 30% in the caption of the thermal ellipsoid plot.

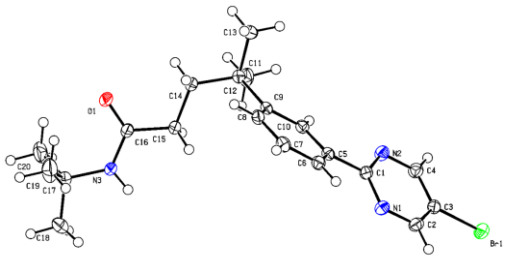
| | | | |
|---|---|---|---|
| Bond precision: | C-C = 0.0054 A | | Wavelength= 1.54184 |
| Cell: | a=19.4831(8) | b=10.8800(4) | c=9.8987(3) |
| | alpha=90 | beta=99.028(3) | gamma=90 |
| Temperature: | 303 K | | |

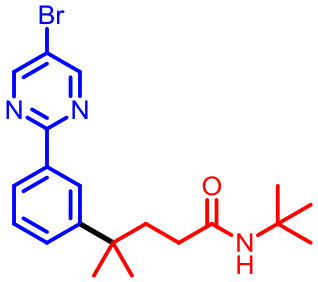
| | Calculated | Reported |
|---|---|---|
| Volume | 2072.29(13) | 2072.29(13) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | $C_{22}$ $H_{30}$ $N_2$ $O_2$ | $C_{22}$ $H_{30}$ $N_2$ $O_2$ |
| Sum formula | $C_{22}$ $H_{30}$ $N_2$ $O_2$ | $C_{22}$ $H_{30}$ $N_2$ $O_2$ |
| Mr | 354.48 | 354.48 |
| Dx,g cm$^{-3}$ | 1.136 | 1.136 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.570 | 0.570 |
| F000 | 768.0 | 768.0 |
| F000’ | 770.11 | |
| h,k,lmax | 24,13,12 | 24,13,12 |
| Nref | 4346 | 15890 |
| Tmin,Tmax | 0.953,0.972 | 0.680,1.000 |
| Tmin’ | 0.918 | |

Correction method= # Reported T Limits: Tmin= 0.680 Tmax=1.000
AbsCorr = MULTI-SCAN

| | |
|---|---|
| Data completeness= 3.656 | Theta(max)= 76.210 |
| R(reflections)= 0.0771( 11742) | wR2(reflections)= 0.2523( 15890) |
| S = 1.085 | Npar= 242 |

**(2), X-ray single crystal diffraction data of 3w**






The ellipsoid contour percent probability level is 30% in the caption of the thermal ellipsoid plot.

| | | | |
|---|---|---|---|
| Bond precision: | C-C = 0.0023 A | | Wavelength= 1.54184 |
| Cell: | a=6.36816(5) | b=31.0073(3) | c=10.01092(9) |
| | alpha=90 | beta=97.3165(8) | gamma=90 |
| Temperature: | 150 K | | |

| | Calculated | Reported |
|---|---|---|
| Volume | 1960.66(3) | 1960.65(3) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | $C_{20}$ $H_{26}$ Br $N_3$ O | $C_{20}$ $H_{26}$ Br $N_3$ O |
| Sum formula | $C_{20}$ $H_{26}$ Br $N_3$ O | $C_{20}$ $H_{26}$ Br $N_3$ O |
| Mr | 404.34 | 404.35 |
| Dx,g cm$^{-3}$ | 1.370 | 1.370 |
| Z | 4 | 4 |
| Mu (mm-1) | 2.946 | 2.946 |
| F000 | 840.0 | 840.0 |
| F000' | 839.17 | |
| h,k,lmax | 8,39,12 | 8,39,12 |
| Nref | 4108 | 3894 |
| Tmin,Tmax | 0.838,0.915 | 0.530,1.000 |
| Tmin' | 0.767 | |

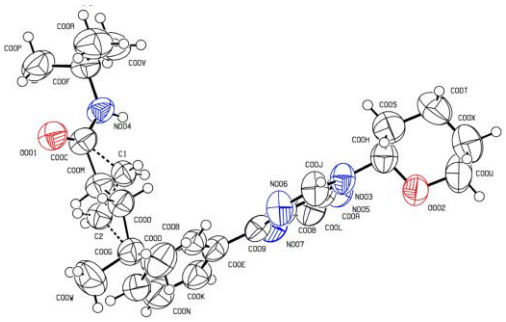
Correction method= # Reported T Limits: Tmin= 0.530 Tmax=1.000
AbsCorr = MULTI-SCAN

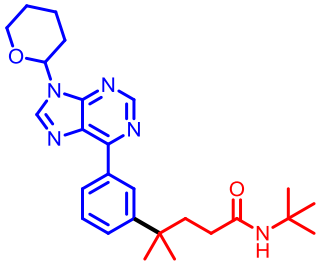
Data completeness= 0.948 Theta(max)= 76.447

R(reflections)= 0.0272( 3729) wR2(reflections)= 0.0663( 3894)

S = 1.067 Npar= 232

**(3), X-ray single crystal diffraction data of 3z**





The ellipsoid contour percent probability level is 30% in the caption of the thermal ellipsoid plot.

| | | | |
|---|---|---|---|
| Bond precision: | C-C = 0.0041 A | | Wavelength= 1.54184 |
| Cell: | a=10.3083(3) | b=24.7520(7) | c=10.4153(4) |
| | alpha=90 | beta=108.265(4) | gamma=90 |
| Temperature: | 303 K | | |

| | Calculated | Reported |
|---|---|---|
| Volume | 2523.58(15) | 2523.58(16) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | $C_{26}$ $H_{35}$ $N_5$ $O_2$ | $C_{26}$ $H_{35}$ $N_5$ $O_2$ |
| Sum formula | $C_{26}$ $H_{35}$ $N_5$ $O_2$ | $C_{26}$ $H_{35}$ $N_5$ $O_2$ |
| Mr | 449.59 | 449.59 |
| Dx,g $cm^{-3}$ | 1.183 | 1.183 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.608 | 0.608 |
| F000 | 968.0 | 968.0 |
| F000’ | 970.70 | |
| h,k,lmax | 12,31,13 | 12,31,13 |
| Nref | 5281 | 5281 |
| Tmin,Tmax | 0.950,0.970 | 0.950,0.970 |
| Tmin’ | 0.935 | |

Correction method= # Reported T Limits: Tmin= 0.900 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.966 Theta(max)= 76.252

R(reflections)= 0.0625( 3610) wR2(reflections)= 0.2029( 5099)

S = 1.046 Npar= 321

## 9. Computational details

All the structures were optimized by the B3LYP hybrid functional with the Grimme's dispersion correction at the D3 level (B3LYP-D3) including solvation effects via integral equation formalism model by using the Gaussian 09 program as our previous study.[6] The 6-31G* basis set was used to C, H, O, N, F, and P atoms, while Lanl2DZ basis set was employed to Ru and Ir atom.[7] All of the energy minima and transition states have been verified by vibrational frequency analyses at the same level with no or only one imaginary frequency, respectively. The solvation free energy was calculated at the M05-2X level with same basis sets, which was proved to be a good choice to obtain solvation free energy by previous studies.[8] Radical Fukui indices were calculated as our past studies.[6f] The minimum energy crossing points (MECPs) were found by using the program developed by J. Rodr ǵuez-Guerra, et al.[9] All of the above computations were performed at the standard conditions.

The overall zero-value of the energy scale in scheme 9 is sum of Gibbs free energies of **8**, **1a** and Ir(IV), which could be considered as reactants. From **8** to **9**, Ir(IV) does not take part in the reaction, and has not been included in the ΔG. From **10**, the free energy of Ir(IV) is considered.

Comparing with employing phosphine as ligand (scheme 9), the kinetics and thermodynamics of every elementary process of this reaction that proceeded without phosphine ligand are more unfavorable. For example, from **M** to **O** (Figure S3) for 1,4-dioxane as ligand, the energy barrier of this step is 10.7 kcal/mol, absorbing 5.3 kcal/mol; while the corresponding step with phosphine as ligand (Scheme 9, **I** to **K**), the energy barrier is 9.2 kcal/mol, absorbing 2.6 kcal/mol. Hence, the use of phosphine as the ligand is necessary in our experiment.

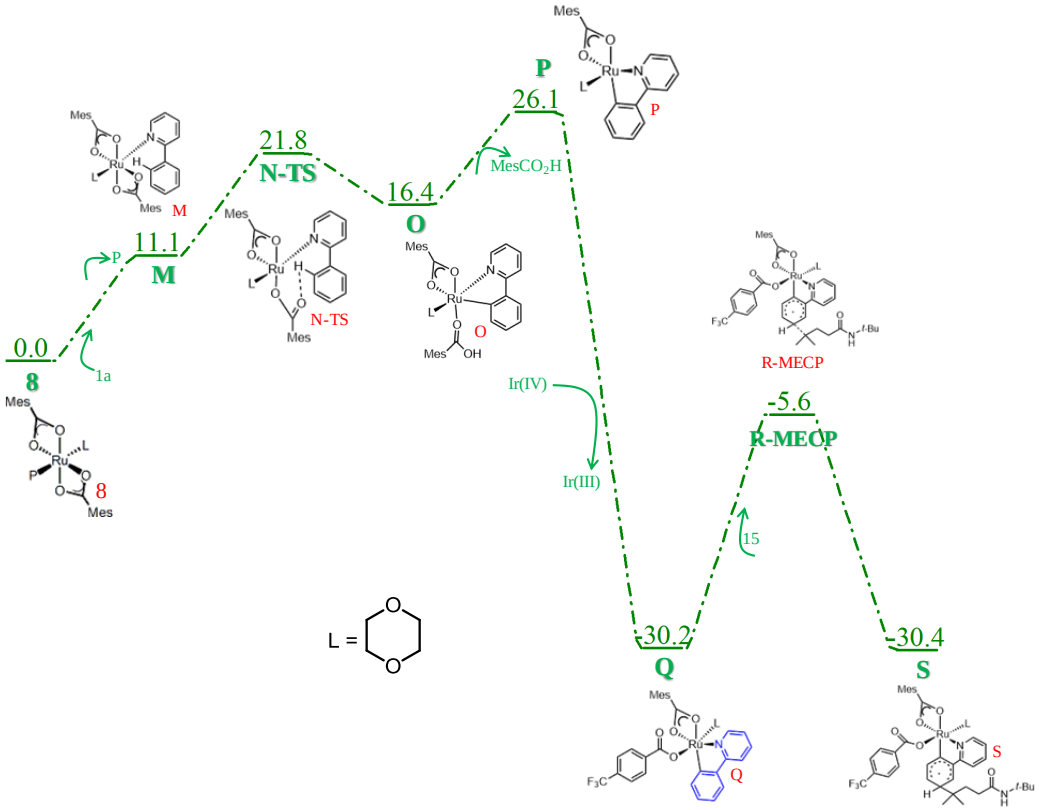



**Figure S3.** Computed free energy profile of this reaction without phosphine ligand

**Cartesian Coordinates**

| | A | | |
|---|---|---|---|
| Ru | -1.15350400 | -0.66960200 | 0.08579600 |
| O | 0.90020600 | -0.61047200 | -0.38218000 |
| O | 1.52820300 | -1.01958600 | 1.75586700 |
| C | 1.76711800 | -0.72542100 | 0.57529500 |
| C | 3.18667600 | -0.43310300 | 0.13642000 |
| C | 3.82601800 | -1.24991000 | -0.81284400 |
| C | 3.86245000 | 0.66386300 | 0.70450000 |
| C | 5.14852100 | -0.96430000 | -1.16980300 |
| C | 5.17833500 | 0.92406400 | 0.30971500 |
| C | 5.84088400 | 0.12100000 | -0.62462800 |
| H | 5.64881400 | -1.60409200 | -1.89489400 |
| H | 5.70073400 | 1.77502400 | 0.74397900 |
| C | 7.25469000 | 0.43867300 | -1.05510000 |
| H | 7.26547400 | 1.16892700 | -1.87579700 |
| H | 7.83776300 | 0.86877900 | -0.23277400 |
| H | 7.77757300 | -0.45634800 | -1.40984500 |
| C | 3.10990200 | -2.42979100 | -1.43156300 |
| H | 2.79566200 | -3.14675900 | -0.66289700 |
| H | 2.20373200 | -2.10457300 | -1.95169800 |
| H | 3.75626800 | -2.95808300 | -2.13977800 |
| C | 3.17571300 | 1.55943000 | 1.71073600 |

| | | | |
|---|---|---|---|
| H | 2.27091100 | 2.01141300 | 1.28600000 |
| H | 2.85624100 | 0.98921200 | 2.58775600 |
| H | 3.83653100 | 2.37021000 | 2.03463200 |
| C | -1.27995600 | 0.70077200 | -1.41973800 |
| C | -1.04020300 | 2.04787000 | -1.04719700 |
| C | -1.54399300 | 0.44190300 | -2.77305600 |
| C | -1.60401300 | 1.47489200 | -3.71240300 |
| H | -1.69637300 | -0.58133800 | -3.10797500 |
| C | -1.38858200 | 2.80251200 | -3.32275800 |
| H | -1.81627500 | 1.24562200 | -4.75451000 |
| H | -1.43688700 | 3.60477100 | -4.05375600 |
| C | -0.45860200 | 1.15233200 | 2.42081500 |
| C | -0.72298900 | 2.25365600 | 0.36477600 |
| C | -0.16620200 | 2.33869800 | 3.08021100 |
| H | -0.43840000 | 0.19576300 | 2.92501400 |
| C | -0.41074700 | 3.47739600 | 0.97637800 |
| C | -0.14175000 | 3.52325600 | 2.33863500 |
| H | 0.05444300 | 2.32590900 | 4.14180400 |
| H | -0.37977600 | 4.38276300 | 0.38136200 |
| H | 0.09599000 | 4.46925800 | 2.81629300 |
| N | -0.74740100 | 1.11216600 | 1.10833600 |
| C | -1.09963800 | 3.08663800 | -1.99177800 |
| H | -0.91811700 | 4.11656800 | -1.69490600 |
| C | -2.67291500 | -1.38808500 | 1.58378700 |
| C | -1.61056400 | -2.32452400 | 1.74652900 |
| C | -1.08270300 | -2.97958400 | 0.61905000 |
| C | -1.70311000 | -2.75754600 | -0.65388000 |
| C | -2.82233700 | -1.89847400 | -0.77186300 |
| C | -3.36069200 | -1.19534200 | 0.34953400 |
| H | -2.99122200 | -0.81962700 | 2.45263300 |
| H | -1.12855100 | -2.43429100 | 2.71092200 |
| H | -1.29578300 | -3.23314400 | -1.53922900 |
| H | -3.24394400 | -1.73975500 | -1.75631200 |
| C | -4.57490000 | -0.27342500 | 0.26373700 |
| C | -5.12374400 | -0.13036900 | -1.16313000 |
| C | -4.28514500 | 1.12312700 | 0.84705400 |
| H | -5.35960200 | -0.73935200 | 0.87966500 |
| H | -5.42978500 | -1.09361200 | -1.58680100 |
| H | -6.00321700 | 0.52221400 | -1.15807600 |
| H | -4.37403600 | 0.31972900 | -1.82457400 |
| H | -3.90409600 | 1.08093900 | 1.87219500 |
| H | -3.53800100 | 1.63547700 | 0.23370500 |
| H | -5.20203900 | 1.72336100 | 0.85748100 |
| C | 0.12823900 | -3.86455800 | 0.73759000 |

| | | | |
|---|---|---|---|
| H | -0.15724100 | -4.84526200 | 1.13884600 |
| H | 0.59652900 | -4.01927000 | -0.23786800 |
| H | 0.86080800 | -3.40653400 | 1.40640300 |

B

| | | | |
|---|---|---|---|
| Ru | -0.57271800 | 0.74404200 | -0.24885500 |
| O | 1.37357800 | 1.11674800 | 0.56682900 |
| O | 1.57505500 | 0.72043000 | -1.59779800 |
| P | -0.43345200 | -1.49697400 | 0.12517300 |
| C | -1.86085600 | -2.18381100 | 1.07097600 |
| C | -1.81208600 | -2.35450700 | 2.46101900 |
| C | -3.08679500 | -2.36250700 | 0.40890600 |
| C | -2.96469400 | -2.68984000 | 3.17365500 |
| H | -0.87697400 | -2.22154700 | 2.99413900 |
| C | -4.23531900 | -2.70512300 | 1.12124700 |
| H | -3.14733500 | -2.22621600 | -0.66656400 |
| C | -4.17929800 | -2.86472100 | 2.50774800 |
| H | -2.91127000 | -2.81247200 | 4.25209700 |
| H | -5.17564500 | -2.83492700 | 0.59192200 |
| C | 1.08511200 | -2.03004300 | 1.02847200 |
| C | 1.94149900 | -3.02928900 | 0.54414000 |
| C | 1.45515000 | -1.31861300 | 2.18241300 |
| C | 3.14579700 | -3.30605200 | 1.19595600 |
| H | 1.68144700 | -3.58197800 | -0.35247900 |
| C | 2.64865000 | -1.60912300 | 2.84120600 |
| H | 0.81892500 | -0.52033000 | 2.54546500 |
| C | 3.50278800 | -2.59660800 | 2.34330300 |
| H | 3.80704100 | -4.07185000 | 0.79938800 |
| H | 2.92385000 | -1.04624000 | 3.72908900 |
| C | -0.40580400 | -2.53354200 | -1.40596400 |
| C | -0.86464400 | -3.86073600 | -1.42284500 |
| C | 0.13269500 | -1.98398400 | -2.58115700 |
| C | -0.79948500 | -4.61814300 | -2.59370600 |
| H | -1.27776100 | -4.30285700 | -0.52144800 |
| C | 0.19980100 | -2.74612100 | -3.74982300 |
| H | 0.52341300 | -0.97152400 | -2.56793500 |
| C | -0.26999100 | -4.06134000 | -3.76089500 |
| H | 0.62357000 | -2.31023100 | -4.65079100 |
| H | -1.16117700 | -5.64301200 | -2.59289100 |
| C | 2.10547100 | 0.87789700 | -0.45933500 |
| C | 3.58255600 | 0.71876100 | -0.24679100 |
| C | 4.24326300 | 1.45078600 | 0.76925600 |
| C | 4.30817000 | -0.22029700 | -1.02013700 |
| C | 5.60965200 | 1.24062600 | 0.97890900 |

| | | | |
|---|---|---|---|
| C | 5.66793600 | -0.40999200 | -0.75170800 |
| C | 6.33967100 | 0.30707700 | 0.23997300 |
| H | 6.11621200 | 1.81887600 | 1.74960200 |
| H | 6.21876400 | -1.14207300 | -1.33911700 |
| C | 7.80199000 | 0.05954200 | 0.52639600 |
| H | 7.92594600 | -0.70185100 | 1.30850100 |
| H | 8.33104100 | -0.29934000 | -0.36314400 |
| H | 8.30233000 | 0.96871400 | 0.87778200 |
| C | 3.53959300 | 2.46061200 | 1.64996500 |
| H | 2.89282500 | 3.12881600 | 1.07480500 |
| H | 2.88994900 | 1.95883800 | 2.37314000 |
| H | 4.27132400 | 3.06746400 | 2.19394800 |
| C | 3.67648100 | -1.05869800 | -2.10930100 |
| H | 2.80761500 | -1.60746800 | -1.73734500 |
| H | 3.31835800 | -0.43882000 | -2.93493100 |
| H | 4.39960000 | -1.78428100 | -2.49692000 |
| C | -1.73255600 | 1.04831000 | 1.34051100 |
| C | -3.13710200 | 1.01972800 | 1.12335100 |
| C | -1.28210000 | 1.34963800 | 2.63944700 |
| C | -2.18196000 | 1.57829900 | 3.68217200 |
| H | -0.21148400 | 1.40442800 | 2.82926300 |
| C | -3.56428400 | 1.51993900 | 3.45550000 |
| H | -1.80930400 | 1.80093800 | 4.68040300 |
| H | -4.26207000 | 1.69123200 | 4.27066100 |
| C | -2.71451500 | 0.19935500 | -2.38794200 |
| C | -3.53308900 | 0.71776100 | -0.25125500 |
| C | -3.99515300 | 0.06801100 | -2.90958500 |
| H | -1.83337800 | 0.03474200 | -2.99889000 |
| C | -4.84745800 | 0.60519400 | -0.72748100 |
| C | -5.08399900 | 0.27847400 | -2.05699800 |
| H | -4.13016800 | -0.19381000 | -3.95356300 |
| H | -5.67698500 | 0.76605700 | -0.04812600 |
| H | -6.10153900 | 0.18583600 | -2.42563700 |
| N | -2.47743600 | 0.51330800 | -1.10021300 |
| C | -4.03926200 | 1.24719800 | 2.17530700 |
| H | -5.11253100 | 1.21088200 | 2.00320500 |
| C | -0.43379400 | 3.27970300 | -2.12059400 |
| C | -0.08044900 | 3.88462200 | 0.17278300 |
| C | -0.20143800 | 4.78882700 | -2.27613300 |
| H | 0.42802500 | 2.70128200 | -2.47363200 |
| C | -0.74680000 | 5.25091100 | -0.02346700 |
| H | -0.25527700 | 3.50068600 | 1.17802400 |
| H | -0.45163300 | 5.10007600 | -3.29448500 |
| H | -0.09153400 | 6.04029200 | 0.37935200 |

| | | | |
|---|---|---|---|
| O | -0.68643000 | 2.95339100 | -0.73273300 |
| O | -1.05249500 | 5.50712700 | -1.39849400 |
| H | 1.00189300 | 3.91180000 | 0.00161500 |
| H | -1.70152400 | 5.28422400 | 0.51010200 |
| H | -1.33338800 | 2.96104400 | -2.65277100 |
| H | 0.85532100 | 5.04622000 | -2.10141400 |
| H | 4.44531300 | -2.80464300 | 2.84241500 |
| H | -0.22023200 | -4.65179500 | -4.67198800 |
| H | -5.07587500 | -3.12219800 | 3.06525000 |

C (9)

| | | | |
|---|---|---|---|
| Ru | 0.34718800 | -0.77908000 | -1.01232000 |
| O | -1.58395000 | -1.42748800 | -0.35340200 |
| O | -1.71460400 | 0.21487600 | -1.82500500 |
| P | 0.68639300 | 0.71861600 | 0.60614000 |
| C | 2.31302300 | 0.53996500 | 1.45700800 |
| C | 2.43833300 | -0.21586800 | 2.63088300 |
| C | 3.47392100 | 1.02599500 | 0.83433000 |
| C | 3.69812400 | -0.48027600 | 3.16979900 |
| H | 1.55496400 | -0.60772800 | 3.12342200 |
| C | 4.73135700 | 0.76672000 | 1.37857800 |
| H | 3.39893400 | 1.60298300 | -0.08205200 |
| C | 4.84768400 | 0.00912300 | 2.54598600 |
| H | 3.77957900 | -1.07257600 | 4.07704000 |
| H | 5.61935200 | 1.14867300 | 0.88206500 |
| C | -0.57561700 | 0.68806100 | 1.95105800 |
| C | -1.14725200 | 1.85875500 | 2.47242300 |
| C | -1.00321900 | -0.55689600 | 2.44120400 |
| C | -2.12431100 | 1.78372300 | 3.46771700 |
| H | -0.84089800 | 2.83027800 | 2.10004200 |
| C | -1.96969300 | -0.62715200 | 3.44374100 |
| H | -0.58988600 | -1.46697200 | 2.02497500 |
| C | -2.53647500 | 0.54256000 | 3.95584800 |
| H | -2.56480900 | 2.69764500 | 3.85705500 |
| H | -2.29165900 | -1.59720300 | 3.81229800 |
| C | 0.68025300 | 2.48174400 | 0.04933400 |
| C | 1.40091200 | 3.48103800 | 0.72472600 |
| C | -0.11856500 | 2.84048800 | -1.04873100 |
| C | 1.33434100 | 4.80955500 | 0.30113100 |
| H | 2.01565500 | 3.22452900 | 1.58152800 |
| C | -0.18354600 | 4.17128600 | -1.46721100 |
| H | -0.69990500 | 2.08008200 | -1.55926800 |
| C | 0.54421200 | 5.15731400 | -0.79746400 |
| H | -0.80738900 | 4.43526700 | -2.31700700 |

| | | | |
|---|---|---|---|
| H | 1.89878200 | 5.57193800 | 0.83142200 |
| C | -2.28331100 | -0.59380300 | -1.03291900 |
| C | -3.76794200 | -0.58576200 | -0.84838600 |
| C | -4.48808100 | -1.79844800 | -0.88892800 |
| C | -4.43485600 | 0.63695300 | -0.62186800 |
| C | -5.87541900 | -1.76154900 | -0.71985300 |
| C | -5.82062500 | 0.61992700 | -0.43506400 |
| C | -6.55995100 | -0.56538700 | -0.48403800 |
| H | -6.43650600 | -2.69290300 | -0.77019100 |
| H | -6.33672200 | 1.55984400 | -0.24870900 |
| C | -8.05390500 | -0.55992800 | -0.25782800 |
| H | -8.29313500 | -0.73457300 | 0.79994600 |
| H | -8.49949400 | 0.40072600 | -0.53800800 |
| H | -8.54991700 | -1.34747000 | -0.83595300 |
| C | -3.80279100 | -3.12709000 | -1.12203000 |
| H | -3.11663700 | -3.08632900 | -1.97545000 |
| H | -3.19814300 | -3.41128100 | -0.25544400 |
| H | -4.53897500 | -3.91486600 | -1.31156400 |
| C | -3.69108700 | 1.95218600 | -0.55085400 |
| H | -2.85385300 | 1.90154600 | 0.15326900 |
| H | -3.26699400 | 2.21905300 | -1.52300700 |
| H | -4.35914300 | 2.75639600 | -0.22592600 |
| C | 1.59574900 | -2.12198400 | -0.20010000 |
| C | 2.95034400 | -2.07065700 | -0.63149300 |
| C | 1.23909800 | -3.14905500 | 0.69166900 |
| C | 2.18568000 | -4.06218600 | 1.16169500 |
| H | 0.20398500 | -3.23578500 | 1.01581900 |
| C | 3.52088800 | -3.97949500 | 0.74505400 |
| H | 1.88619100 | -4.84351300 | 1.85749300 |
| H | 4.25653300 | -4.68770700 | 1.11655600 |
| C | 2.32099900 | 0.81828100 | -2.74248200 |
| C | 3.25257500 | -0.99217400 | -1.57402000 |
| C | 3.54642500 | 1.16118200 | -3.30026100 |
| H | 1.42281400 | 1.39139700 | -2.94506500 |
| C | 4.51077800 | -0.69562600 | -2.11565200 |
| C | 4.66316200 | 0.38365000 | -2.97814400 |
| H | 3.61793200 | 2.01534000 | -3.96482000 |
| H | 5.36566100 | -1.30576800 | -1.84689700 |
| H | 5.63923100 | 0.61933300 | -3.39230900 |
| N | 2.16794600 | -0.22346200 | -1.90337900 |
| C | 3.90017600 | -2.98923700 | -0.15803600 |
| H | 4.93524300 | -2.93837600 | -0.48763800 |
| H | 5.82779400 | -0.20025200 | 2.96592800 |
| H | 0.49404700 | 6.19193900 | -1.12625500 |

| | | | |
|---|---|---|---|
| H | -3.30034600 | 0.48615100 | 4.72667400 |

D

| | | | |
|---|---|---|---|
| Ru | -0.32604300 | -0.00769700 | -0.03647100 |
| O | 1.72332700 | 0.29441900 | 0.91304300 |
| O | 1.86429100 | -0.05174400 | -1.26919900 |
| P | -0.54225000 | 2.36220100 | -0.15972300 |
| P | -0.18809300 | -2.40144100 | 0.09268100 |
| C | 0.56723900 | 3.19033400 | -1.38377500 |
| C | 0.89121000 | 2.48412500 | -2.55313100 |
| C | 1.09402500 | 4.47821900 | -1.20146700 |
| C | 1.70798000 | 3.05936400 | -3.52718700 |
| H | 0.52574500 | 1.47206700 | -2.68222400 |
| C | 1.92205900 | 5.04699500 | -2.17093400 |
| H | 0.87173500 | 5.03572200 | -0.29766300 |
| C | 2.22823300 | 4.34123700 | -3.33684100 |
| H | 1.95237500 | 2.49768700 | -4.42476500 |
| H | 2.33022400 | 6.04167500 | -2.01212300 |
| C | -0.29112900 | 3.32632500 | 1.39181600 |
| C | -0.87066400 | 4.59080700 | 1.59255500 |
| C | 0.52728100 | 2.78655700 | 2.39495100 |
| C | -0.63628100 | 5.29844000 | 2.77239500 |
| H | -1.51349200 | 5.02078300 | 0.83064000 |
| C | 0.76174300 | 3.49824500 | 3.57326200 |
| H | 0.98811700 | 1.81895100 | 2.23853100 |
| C | 0.18025600 | 4.75272300 | 3.76643100 |
| H | 1.39870800 | 3.06755400 | 4.34148800 |
| C | -2.23218300 | 2.87671200 | -0.69860600 |
| C | -2.53728500 | 3.05407100 | -2.05588600 |
| C | -3.27314000 | 2.93805500 | 0.24297100 |
| C | -3.85099800 | 3.29283200 | -2.46258700 |
| H | -1.74888200 | 3.00669400 | -2.80062700 |
| C | -4.58370600 | 3.18617600 | -0.16480800 |
| H | -3.06211100 | 2.78133400 | 1.29532500 |
| C | -4.87811000 | 3.36073000 | -1.51879800 |
| H | -4.06982200 | 3.42660200 | -3.51874700 |
| H | -5.37550000 | 3.22979900 | 0.57835500 |
| C | -1.75331900 | -3.14911300 | 0.72402500 |
| C | -1.93877300 | -3.36794600 | 2.09673100 |
| C | -2.84055200 | -3.33914200 | -0.14389000 |
| C | -3.17985700 | -3.77203100 | 2.58825700 |
| H | -1.11643100 | -3.21226500 | 2.78722400 |
| C | -4.07892300 | -3.75101300 | 0.34865500 |
| H | -2.72558900 | -3.15642500 | -1.20791800 |

| | | | |
|---|---|---|---|
| C | -4.25387600 | -3.96612300 | 1.71683900 |
| H | -3.30803000 | -3.92889200 | 3.65580600 |
| H | -4.90914800 | -3.88995100 | -0.33894600 |
| C | 1.10222500 | -3.08708600 | 1.21830100 |
| C | 1.74642400 | -4.31325800 | 0.99134200 |
| C | 1.44684300 | -2.33559200 | 2.35296700 |
| C | 2.71630000 | -4.77651800 | 1.88149600 |
| H | 1.50651600 | -4.90198200 | 0.11195000 |
| C | 2.40947300 | -2.80690700 | 3.24694700 |
| H | 0.97579300 | -1.37502100 | 2.51912300 |
| C | 3.04934800 | -4.02539000 | 3.01145200 |
| H | 3.21455000 | -5.72300600 | 1.68886100 |
| H | 2.66952700 | -2.21243300 | 4.11861900 |
| C | 0.07860600 | -3.29925300 | -1.50107100 |
| C | -0.36268700 | -4.61824000 | -1.70551000 |
| C | 0.76386200 | -2.64506600 | -2.53710900 |
| C | -0.12922700 | -5.26470800 | -2.92024400 |
| H | -0.89857600 | -5.13897600 | -0.91807100 |
| C | 0.99685200 | -3.29603500 | -3.75109300 |
| H | 1.13274600 | -1.63833200 | -2.37598900 |
| C | 0.54887400 | -4.60359700 | -3.94786400 |
| H | 1.53209200 | -2.77752300 | -4.54246500 |
| H | -1.09286000 | 6.27439300 | 2.91471900 |
| H | -0.47825200 | -6.28402100 | -3.06315600 |
| C | 2.41708100 | 0.15801100 | -0.15256700 |
| C | 3.91470200 | 0.24036700 | -0.06075900 |
| C | 4.52886100 | 1.40488900 | 0.43904900 |
| C | 4.69652700 | -0.84769100 | -0.50069700 |
| C | 5.92601200 | 1.45970200 | 0.49336800 |
| C | 6.08847000 | -0.75617000 | -0.40872500 |
| C | 6.72380300 | 0.38764800 | 0.08510300 |
| H | 6.40202800 | 2.36574000 | 0.86432300 |
| H | 6.69330100 | -1.59920300 | -0.73827100 |
| C | 8.22976800 | 0.45143000 | 0.19523300 |
| H | 8.57491700 | 0.03161300 | 1.14992700 |
| H | 8.71548200 | -0.12029000 | -0.60355600 |
| H | 8.59271400 | 1.48380800 | 0.14394000 |
| C | 3.71679700 | 2.59291600 | 0.89993500 |
| H | 2.91328500 | 2.83482800 | 0.19792600 |
| H | 3.24169000 | 2.39748000 | 1.86595100 |
| H | 4.34976500 | 3.48010800 | 1.00649100 |
| C | 4.06268000 | -2.09973500 | -1.06127500 |
| H | 3.29892700 | -2.50055900 | -0.38808800 |
| H | 3.56442300 | -1.89672100 | -2.01386000 |

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|---|---|---|---|
| H | 4.81393300 | -2.88014100 | -1.22035500 |
| C | -1.75508700 | 0.01592100 | 1.39867900 |
| C | -3.09952100 | -0.12721300 | 0.95029100 |
| C | -1.55980000 | 0.14176200 | 2.78658400 |
| C | -2.63111800 | 0.12705600 | 3.68045200 |
| H | -0.55214200 | 0.26175000 | 3.17526800 |
| C | -3.94619900 | -0.01853800 | 3.21654600 |
| H | -2.44411000 | 0.22886400 | 4.74779500 |
| H | -4.77794700 | -0.03486600 | 3.91566000 |
| C | -2.06120200 | -0.41833500 | -2.51293900 |
| C | -3.25061800 | -0.25976400 | -0.49562200 |
| C | -3.22508200 | -0.55864000 | -3.25435600 |
| H | -1.08224100 | -0.43252700 | -2.97988400 |
| C | -4.45797700 | -0.38146400 | -1.19934100 |
| C | -4.45040400 | -0.53140300 | -2.57860200 |
| H | -3.16903100 | -0.67985500 | -4.33076000 |
| H | -5.39534600 | -0.35787200 | -0.65605600 |
| H | -5.38473800 | -0.62606500 | -3.12427100 |
| N | -2.06422700 | -0.26705900 | -1.17486800 |
| C | -4.17609800 | -0.14773900 | 1.85119000 |
| H | -5.19479300 | -0.26776400 | 1.49083900 |
| H | 0.72819900 | -5.10712900 | -4.89423600 |
| H | -5.22075500 | -4.27851400 | 2.10236600 |
| H | 0.36013100 | 5.30324700 | 4.68615000 |
| H | 2.87597000 | 4.78457800 | -4.08843600 |
| H | 3.80875100 | -4.38517700 | 3.70061000 |
| H | -5.90049700 | 3.54786400 | -1.83654400 |
| | E (Q) | | |
| Ru | 1.62489700 | 0.23227200 | -0.01999600 |
| O | 0.07804500 | -0.78569600 | -1.06383100 |
| O | -0.24900800 | -0.66383000 | 1.10245200 |
| C | -0.70071700 | -0.96162400 | -0.04944800 |
| C | -2.10133800 | -1.42420200 | -0.25750000 |
| C | -2.64002200 | -1.52460100 | -1.57041000 |
| C | -2.93987800 | -1.67825300 | 0.86390300 |
| C | -3.99284000 | -1.84977100 | -1.71954700 |
| C | -4.28130100 | -1.99921000 | 0.64825400 |
| C | -4.83464100 | -2.07569100 | -0.63115000 |
| H | -4.40421500 | -1.91440600 | -2.72438300 |
| H | -4.92159500 | -2.17337500 | 1.50935400 |
| C | -6.30501100 | -2.35735600 | -0.81665800 |
| H | -6.64766200 | -3.15645500 | -0.14929100 |
| H | -6.89020100 | -1.46089800 | -0.57969700 |
| H | -6.53558200 | -2.64744200 | -1.84682800 |

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|---|---|---|---|
| C | -1.85270500 | -1.28053300 | -2.84046100 |
| H | -1.42885800 | -0.27349100 | -2.86770300 |
| H | -1.00479600 | -1.96550800 | -2.92973100 |
| H | -2.50299200 | -1.41411900 | -3.71132400 |
| C | -2.47623800 | -1.60554700 | 2.30218700 |
| H | -1.58742800 | -2.21737700 | 2.47891900 |
| H | -2.19931800 | -0.58314700 | 2.57219200 |
| H | -3.27624100 | -1.94285900 | 2.96934500 |
| C | 3.09991700 | 0.44401400 | -1.34352200 |
| C | 4.30617200 | 1.00028300 | -0.85347200 |
| C | 3.02110000 | 0.03093000 | -2.67756600 |
| C | 4.13467500 | 0.15245400 | -3.51363500 |
| H | 2.08632100 | -0.37568800 | -3.05504200 |
| C | 5.33019900 | 0.69231200 | -3.02159800 |
| H | 4.07356700 | -0.16642000 | -4.55113000 |
| H | 6.19276400 | 0.78561600 | -3.67553300 |
| C | 2.85721600 | 1.59404500 | 2.41815400 |
| C | 4.25982500 | 1.43686200 | 0.54419100 |
| C | 3.84570800 | 2.21740800 | 3.17115700 |
| H | 1.87032400 | 1.39082200 | 2.82264000 |
| C | 5.29443200 | 2.05541200 | 1.25631700 |
| C | 5.08913200 | 2.44567700 | 2.57565500 |
| H | 3.64066900 | 2.51614500 | 4.19326000 |
| H | 6.24818400 | 2.23441600 | 0.77300600 |
| H | 5.88670200 | 2.92884900 | 3.13199900 |
| N | 3.05751400 | 1.20496900 | 1.14807300 |
| C | 5.41929900 | 1.12058200 | -1.69664500 |
| H | 6.35178200 | 1.54529700 | -1.33429800 |
| C | -0.23956700 | 2.09066600 | -1.24671100 |
| O | 0.74034800 | 1.97902100 | -0.35017400 |
| O | -0.05079900 | 2.22336600 | -2.44712300 |
| C | -1.63192700 | 2.04591100 | -0.67316800 |
| C | -1.85618700 | 1.98812600 | 0.70876300 |
| C | -2.71704900 | 1.95974800 | -1.55317400 |
| C | -3.14430600 | 1.80187800 | 1.20023800 |
| H | -1.01227400 | 2.04691700 | 1.38428600 |
| C | -4.00521200 | 1.75501500 | -1.06722200 |
| H | -2.52579500 | 2.01416900 | -2.61902400 |
| C | -4.21330700 | 1.65869500 | 0.31053800 |
| H | -3.31822500 | 1.72801700 | 2.26888000 |
| H | -4.83880400 | 1.63923400 | -1.75074400 |
| C | -5.59165900 | 1.42503400 | 0.85884600 |
| F | -5.57761600 | 0.57730000 | 1.91537200 |
| F | -6.16366200 | 2.57387500 | 1.29648500 |

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|---|---|---|---|
| F | -6.43187100 | 0.90008100 | -0.06601900 |
| C | 2.41477600 | -2.77557300 | -0.41866600 |
| C | 2.36449200 | -2.10627800 | 1.91157300 |
| C | 2.66261500 | -4.11468600 | 0.27526200 |
| H | 1.42751100 | -2.73443900 | -0.88711800 |
| C | 3.47947700 | -3.09777500 | 2.25114300 |
| H | 2.44812000 | -1.20968100 | 2.52667000 |
| H | 2.94102400 | -4.86255800 | -0.47239900 |
| H | 3.20083500 | -3.64803200 | 3.16370500 |
| O | 2.52578200 | -1.68231000 | 0.54294000 |
| O | 3.74916700 | -4.00455700 | 1.18004100 |
| H | 1.75441000 | -4.47513700 | 0.78209200 |
| H | 3.18153300 | -2.56376900 | -1.16625800 |
| H | 1.35735800 | -2.51217100 | 2.04506100 |
| H | 4.41409600 | -2.56022200 | 2.44166800 |

F

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|---|---|---|---|
| Ru | -1.08269800 | 0.23471600 | 0.85202600 |
| O | 0.41752900 | 1.63731100 | 0.13669300 |
| O | 0.21752700 | 2.07882300 | -2.06313200 |
| P | -1.31754800 | -1.03269500 | -1.09357500 |
| C | -1.59372600 | -2.83743800 | -0.82934100 |
| C | -0.61228100 | -3.77041000 | -1.19929300 |
| C | -2.76492100 | -3.30344000 | -0.20762800 |
| C | -0.79783700 | -5.13151900 | -0.95306800 |
| H | 0.30685900 | -3.44073700 | -1.66878300 |
| C | -2.94922000 | -4.66414300 | 0.03056000 |
| H | -3.53592900 | -2.61030100 | 0.10298500 |
| C | -1.96477300 | -5.58328700 | -0.33687700 |
| H | -0.02372200 | -5.83705100 | -1.24318500 |
| H | -3.86066900 | -5.00054500 | 0.51687400 |
| C | 0.16910800 | -1.01672300 | -2.17007200 |
| C | 1.43749300 | -0.86549000 | -1.59632900 |
| C | 0.05981100 | -1.28386100 | -3.54230400 |
| C | 2.58607800 | -0.99776700 | -2.37726900 |
| H | 1.52561300 | -0.63371600 | -0.54461500 |
| C | 1.20898000 | -1.39648100 | -4.32564900 |
| H | -0.91784900 | -1.40362400 | -3.99898800 |
| C | 2.47257200 | -1.26183500 | -3.74395800 |
| H | 3.56578300 | -0.90611900 | -1.91749400 |
| H | 1.11648100 | -1.59601300 | -5.38985000 |
| C | -2.68442100 | -0.46630700 | -2.19409000 |
| C | -3.84481100 | -1.21192600 | -2.44518700 |
| C | -2.54871800 | 0.80719700 | -2.77511600 |

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|---|---|---|---|
| C | -4.86607400 | -0.68111900 | -3.23760500 |
| H | -3.95822100 | -2.21130700 | -2.04434000 |
| C | -3.57084000 | 1.32839400 | -3.56638100 |
| H | -1.64014700 | 1.37765400 | -2.60502600 |
| C | -4.73675000 | 0.59208400 | -3.79316000 |
| H | -3.45392100 | 2.31610200 | -4.00423800 |
| H | -5.75957000 | -1.27142200 | -3.42267300 |
| C | 0.73561600 | 2.26374200 | -0.95489100 |
| C | 1.75750700 | 3.36896200 | -0.76709000 |
| C | 2.91964800 | 3.16159100 | 0.00844000 |
| C | 1.52655900 | 4.63082700 | -1.36110600 |
| C | 3.81427300 | 4.22039900 | 0.19365600 |
| C | 2.43986100 | 5.66648700 | -1.12918900 |
| C | 3.58716100 | 5.48625200 | -0.35330900 |
| H | 4.71623900 | 4.04838100 | 0.77833000 |
| H | 2.25274400 | 6.64053000 | -1.57766100 |
| C | 4.54394200 | 6.62744500 | -0.09871100 |
| H | 4.52939600 | 7.35435300 | -0.91813200 |
| H | 4.27970600 | 7.16777900 | 0.82061900 |
| H | 5.57241400 | 6.26933300 | 0.02090800 |
| C | 3.23984400 | 1.81758800 | 0.61633600 |
| H | 2.53580200 | 1.56551100 | 1.41145900 |
| H | 3.17079900 | 1.01891100 | -0.12826500 |
| H | 4.25506700 | 1.80950900 | 1.02775200 |
| C | 0.33260800 | 4.91340700 | -2.24917700 |
| H | 0.38183700 | 4.32472100 | -3.16890400 |
| H | -0.61491600 | 4.64469600 | -1.77033200 |
| H | 0.29076900 | 5.97669700 | -2.50722100 |
| C | -2.75665700 | -0.63762300 | 1.64230800 |
| C | -3.99355400 | -0.03578500 | 1.31047500 |
| C | -2.77096000 | -1.75191500 | 2.49666900 |
| C | -3.97917700 | -2.26592000 | 2.97414300 |
| H | -1.84441500 | -2.26145800 | 2.72879800 |
| C | -5.20073100 | -1.69405300 | 2.60007400 |
| H | -3.96649300 | -3.13736200 | 3.62475600 |
| H | -6.13780600 | -2.11049400 | 2.95896000 |
| C | -2.39997100 | 2.80287000 | -0.27145000 |
| C | -3.89912500 | 1.20218800 | 0.54250600 |
| C | -3.42950100 | 3.64299400 | -0.67156500 |
| H | -1.36892300 | 3.07550400 | -0.41388800 |
| C | -4.97744100 | 1.99491900 | 0.12804200 |
| C | -4.74583000 | 3.21681800 | -0.49001200 |
| H | -3.19339900 | 4.59776100 | -1.12839900 |
| H | -5.99046500 | 1.65366200 | 0.30462300 |

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|---|---|---|---|
| H | -5.57936700 | 3.83292200 | -0.81373300 |
| N | -2.61905900 | 1.60263100 | 0.29260200 |
| C | -5.20661300 | -0.57588900 | 1.77201900 |
| H | -6.15378100 | -0.11775300 | 1.50070500 |
| H | -2.10613600 | -6.64296800 | -0.14249700 |
| H | -5.53380800 | 1.00356900 | -4.40693800 |
| H | 3.36600300 | -1.36210900 | -4.35432900 |
| C | 0.65309800 | -2.27366000 | 1.67427900 |
| O | 0.26956400 | -1.01626800 | 1.68164200 |
| O | -0.05019800 | -3.23997300 | 1.94741600 |
| C | 2.10020800 | -2.44745500 | 1.30049200 |
| C | 3.03076600 | -1.42596000 | 1.52639100 |
| C | 2.48855000 | -3.61454700 | 0.63355900 |
| C | 4.32772100 | -1.54699400 | 1.03710600 |
| H | 2.72072400 | -0.53170200 | 2.05398100 |
| C | 3.77780700 | -3.72713800 | 0.11843000 |
| H | 1.75660000 | -4.40204800 | 0.48961700 |
| C | 4.68920500 | -2.68451300 | 0.30764900 |
| H | 5.04945700 | -0.75248700 | 1.19515800 |
| H | 4.07408600 | -4.60924500 | -0.43920600 |
| C | 6.02641300 | -2.71889600 | -0.37238200 |
| F | 5.98044300 | -2.06199700 | -1.56368300 |
| F | 6.99013900 | -2.11676700 | 0.36065800 |
| F | 6.44262900 | -3.97657800 | -0.63803400 |
| C | -0.22377900 | 2.77639000 | 2.80806300 |
| C | -0.73055700 | 0.82918200 | 4.06917500 |
| C | 1.08920600 | 2.72435500 | 3.62177500 |
| H | -0.01933900 | 2.99759000 | 1.76377600 |
| C | 0.75440900 | 0.50786000 | 4.33273400 |
| H | -1.14932200 | 1.48938200 | 4.84151500 |
| H | 0.93412300 | 3.07740100 | 4.65440000 |
| H | 1.00055800 | -0.48618800 | 3.96235400 |
| O | -0.87032400 | 1.48596000 | 2.80260300 |
| O | 1.61046100 | 1.40544600 | 3.62852300 |
| H | -1.33431000 | -0.07722400 | 4.02507900 |
| H | 0.95698800 | 0.55500400 | 5.41542400 |
| H | -0.91992500 | 3.51607900 | 3.22786800 |
| H | 1.84332400 | 3.36189700 | 3.15259000 |

G (10)

| | | | |
|---|---|---|---|
| Ru | -1.00338400 | -0.93610900 | 0.11121200 |
| O | 0.62233300 | -0.42134900 | -1.22555500 |
| O | 1.02703800 | 0.58344100 | 0.69107800 |
| P | -1.96119000 | 1.28211600 | 0.00776900 |

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|---|---|---|---|
| C | -3.71713300 | 1.25808400 | -0.53899700 |
| C | -4.07128600 | 1.47261100 | -1.87828400 |
| C | -4.70867000 | 0.86004900 | 0.37362200 |
| C | -5.38915100 | 1.28345400 | -2.29740300 |
| H | -3.32332000 | 1.78627600 | -2.59823400 |
| C | -6.02471200 | 0.67717100 | -0.04792500 |
| H | -4.45482700 | 0.69036000 | 1.41526900 |
| C | -6.36782600 | 0.88172400 | -1.38630800 |
| H | -5.64866200 | 1.45041900 | -3.33903300 |
| H | -6.77845900 | 0.36627700 | 0.67022900 |
| C | -1.05680900 | 2.40195300 | -1.12614900 |
| C | -0.61791700 | 3.67071200 | -0.72157300 |
| C | -0.71058100 | 1.92747500 | -2.40260000 |
| C | 0.15574000 | 4.45200400 | -1.58194000 |
| H | -0.86306600 | 4.04435800 | 0.26709300 |
| C | 0.05318700 | 2.71647200 | -3.26172500 |
| H | -1.00876900 | 0.93173700 | -2.70943600 |
| C | 0.49358300 | 3.97683800 | -2.85068000 |
| H | 0.50000600 | 5.42934200 | -1.25546700 |
| H | 0.32279500 | 2.33593300 | -4.24282400 |
| C | -1.99962400 | 2.14288400 | 1.63218000 |
| C | -2.98112600 | 3.10799300 | 1.91525300 |
| C | -1.01412000 | 1.86463500 | 2.59418000 |
| C | -2.98801100 | 3.76761100 | 3.14493800 |
| H | -3.74422400 | 3.34238400 | 1.18016300 |
| C | -1.02746000 | 2.52819000 | 3.82255500 |
| H | -0.22325800 | 1.16030800 | 2.36692100 |
| C | -2.01472300 | 3.47510900 | 4.10333300 |
| H | -0.25942500 | 2.30593500 | 4.55826100 |
| H | -3.75352000 | 4.51035900 | 3.35168400 |
| C | 1.40214900 | 0.28743500 | -0.47992600 |
| C | 2.74864200 | 0.67553900 | -0.99099000 |
| C | 3.27422300 | 0.07978000 | -2.16852100 |
| C | 3.55796100 | 1.56756300 | -0.23591300 |
| C | 4.60357600 | 0.34159100 | -2.51977300 |
| C | 4.87415100 | 1.79541800 | -0.64227500 |
| C | 5.42791700 | 1.17259100 | -1.76212900 |
| H | 5.01013700 | -0.13483600 | -3.40931700 |
| H | 5.49651500 | 2.45914800 | -0.04699500 |
| C | 6.88243300 | 1.37268800 | -2.10898200 |
| H | 7.16943000 | 2.42893900 | -2.04608300 |
| H | 7.51440400 | 0.82249000 | -1.40074200 |
| H | 7.11351700 | 1.01360300 | -3.11713000 |
| C | 2.49450700 | -0.84732200 | -3.07639300 |

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|---|---|---|---|
| H | 2.11710500 | -1.72282100 | -2.54260900 |
| H | 1.61577400 | -0.34625400 | -3.49336300 |
| H | 3.13126100 | -1.18216300 | -3.90244100 |
| C | 3.08565800 | 2.29346200 | 1.00495600 |
| H | 2.11966800 | 2.78056700 | 0.84855700 |
| H | 2.95152700 | 1.59720300 | 1.83699000 |
| H | 3.82315500 | 3.04900900 | 1.29637500 |
| C | -2.29790000 | -1.69959300 | -1.19007700 |
| C | -3.53321000 | -2.17741500 | -0.67905500 |
| C | -2.04017300 | -1.78260900 | -2.56687200 |
| C | -3.01753900 | -2.28279800 | -3.42895300 |
| H | -1.07522300 | -1.46043500 | -2.94866300 |
| C | -4.24773600 | -2.72396700 | -2.92365200 |
| H | -2.82122100 | -2.33874700 | -4.49663800 |
| H | -5.00422900 | -3.11173400 | -3.59995900 |
| C | -2.62894600 | -1.33811200 | 2.73373800 |
| C | -3.67960400 | -2.08555900 | 0.77400100 |
| C | -3.70859700 | -1.72170400 | 3.51978100 |
| H | -1.75195900 | -0.86595600 | 3.16261600 |
| C | -4.79083100 | -2.50119100 | 1.51810300 |
| C | -4.80867000 | -2.31720100 | 2.89539500 |
| H | -3.68127200 | -1.55881100 | 4.59145900 |
| H | -5.63346200 | -2.95947600 | 1.01341600 |
| H | -5.66872200 | -2.63394900 | 3.47772800 |
| N | -2.60983800 | -1.51085200 | 1.40085400 |
| C | -4.50353700 | -2.68264100 | -1.55332900 |
| H | -5.45758000 | -3.04101900 | -1.17706600 |
| H | -7.39197200 | 0.73207100 | -1.71662200 |
| H | -2.02262600 | 3.98793800 | 5.06123200 |
| H | 1.10502200 | 4.58229500 | -3.51384800 |
| C | 1.05784600 | -3.09909600 | -0.01716200 |
| O | -0.02465300 | -2.69098300 | 0.62529200 |
| O | 1.02907000 | -3.84272400 | -0.99251500 |
| C | 2.37398000 | -2.58348900 | 0.51461100 |
| C | 2.44954500 | -1.84934200 | 1.70486300 |
| C | 3.52864700 | -2.76039800 | -0.25706300 |
| C | 3.64676400 | -1.25231100 | 2.08625100 |
| H | 1.55419900 | -1.71337200 | 2.29837500 |
| C | 4.72578900 | -2.15177200 | 0.10940900 |
| H | 3.45712500 | -3.34216900 | -1.16906400 |
| C | 4.77562200 | -1.37715600 | 1.27036200 |
| H | 3.69672100 | -0.65216300 | 2.98926600 |
| H | 5.60341700 | -2.24086500 | -0.52060400 |
| C | 6.04043800 | -0.67630200 | 1.67239100 |

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|---|---|---|---|
| F | 5.79667500 | 0.57866900 | 2.12539200 |
| F | 6.68270300 | -1.32446500 | 2.67717500 |
| F | 6.92401900 | -0.57004800 | 0.65150200 |

H

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|---|---|---|---|
| Ru | -0.75781800 | -0.35224900 | 0.08331100 |
| O | 0.21039600 | 1.62172400 | -0.12745300 |
| O | -1.58675900 | 2.88713800 | -0.59452400 |
| P | -2.30164000 | 0.17925400 | -1.76492400 |
| C | -2.61685200 | -1.34768900 | -2.75522200 |
| C | -1.86148800 | -1.64909300 | -3.89705100 |
| C | -3.57742000 | -2.27462900 | -2.31862200 |
| C | -2.06619500 | -2.84371900 | -4.58817900 |
| H | -1.10986100 | -0.95461200 | -4.25397600 |
| C | -3.78842200 | -3.46302500 | -3.01615900 |
| H | -4.16255000 | -2.07283400 | -1.42723800 |
| C | -3.03086500 | -3.75351800 | -4.15248500 |
| H | -1.46699600 | -3.06178700 | -5.46798300 |
| H | -4.53500400 | -4.16701800 | -2.65862200 |
| C | -1.59635500 | 1.34280800 | -3.00792700 |
| C | -0.22423000 | 1.28587300 | -3.29922500 |
| C | -2.39373100 | 2.29069800 | -3.66249900 |
| C | 0.33473400 | 2.16125100 | -4.23142000 |
| H | 0.40182900 | 0.56400800 | -2.79054700 |
| C | -1.82920400 | 3.16703200 | -4.59075500 |
| H | -3.45230200 | 2.36314200 | -3.43763700 |
| C | -0.46401800 | 3.10730500 | -4.87745200 |
| H | 1.39922200 | 2.10595900 | -4.44425800 |
| H | -2.45888900 | 3.90258100 | -5.08443800 |
| C | -4.00753600 | 0.79586400 | -1.42298200 |
| C | -5.07786800 | 0.49410300 | -2.28455700 |
| C | -4.25646600 | 1.60173700 | -0.30194000 |
| C | -6.36344700 | 0.96611200 | -2.01649100 |
| H | -4.91201300 | -0.11342500 | -3.16739500 |
| C | -5.54464500 | 2.06420700 | -0.03074600 |
| H | -3.43597500 | 1.90081200 | 0.33040900 |
| C | -6.60350400 | 1.74469300 | -0.88213200 |
| H | -5.71377200 | 2.68122300 | 0.84777500 |
| H | -7.17607000 | 0.72269400 | -2.69571700 |
| C | -0.39146400 | 2.76346700 | -0.30037000 |
| C | 0.44204800 | 3.99104100 | 0.01167900 |
| C | 1.81189500 | 4.06611100 | -0.32644800 |
| C | -0.16322300 | 5.07027400 | 0.70552200 |
| C | 2.55582200 | 5.18589700 | 0.06351400 |

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|---|---|---|---|
| C | 0.63036100 | 6.15408600 | 1.09762900 |
| C | 1.99236700 | 6.23141200 | 0.79686900 |
| H | 3.60619600 | 5.23915700 | -0.21725400 |
| H | 0.16466600 | 6.97145000 | 1.64500800 |
| C | 2.82766500 | 7.40231300 | 1.25843300 |
| H | 2.24098600 | 8.32706200 | 1.28895100 |
| H | 3.21861200 | 7.23268700 | 2.27089400 |
| H | 3.68812600 | 7.56529000 | 0.60065800 |
| C | 2.52637800 | 2.98813100 | -1.10791000 |
| H | 2.89563900 | 2.21148200 | -0.43139000 |
| H | 1.87551400 | 2.50097400 | -1.83443300 |
| H | 3.38994500 | 3.40660900 | -1.63624200 |
| C | -1.64043500 | 5.12740500 | 1.03434900 |
| H | -2.23541100 | 5.24210700 | 0.12389000 |
| H | -2.00277200 | 4.21265300 | 1.50860700 |
| H | -1.84752400 | 5.97192300 | 1.70053300 |
| C | -1.93766800 | -1.96321800 | 0.52764600 |
| C | -2.97966400 | -1.72912200 | 1.45533300 |
| C | -1.81824700 | -3.24174500 | -0.03601300 |
| C | -2.69540400 | -4.26164000 | 0.33813500 |
| H | -1.06535100 | -3.43004400 | -0.79427300 |
| C | -3.73084500 | -4.02138700 | 1.24986900 |
| H | -2.58482200 | -5.24773400 | -0.10696200 |
| H | -4.41708300 | -4.81725900 | 1.52548400 |
| C | -1.74115400 | 1.57308500 | 2.28153000 |
| C | -2.98199000 | -0.40628600 | 2.06688400 |
| C | -2.58616300 | 2.05654600 | 3.26931000 |
| H | -0.86343000 | 2.11934200 | 1.97189400 |
| C | -3.88466200 | 0.05107400 | 3.03824800 |
| C | -3.69794200 | 1.28974800 | 3.63302900 |
| H | -2.37417700 | 3.01338800 | 3.73282600 |
| H | -4.71614100 | -0.57875200 | 3.33051900 |
| H | -4.39366900 | 1.64619200 | 4.38669200 |
| N | -1.95382700 | 0.39565400 | 1.66318600 |
| C | -3.87696800 | -2.75380400 | 1.80274300 |
| H | -4.67542200 | -2.57069600 | 2.51628300 |
| H | -3.18922600 | -4.68320200 | -4.69265900 |
| H | -7.60635000 | 2.10598300 | -0.66984600 |
| H | -0.02564400 | 3.79390600 | -5.59677300 |
| C | 1.09220000 | -2.12528800 | -1.85302500 |
| O | 0.26353500 | -1.20010100 | -1.44799300 |
| O | 0.75609900 | -3.26843800 | -2.15882200 |
| C | 2.53096200 | -1.69062200 | -1.95620800 |
| C | 2.94543800 | -0.45174800 | -1.45426500 |

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|---|---|---|---|
| C | 3.47596800 | -2.58026600 | -2.47963500 |
| C | 4.29829500 | -0.12262100 | -1.43457500 |
| H | 2.20622000 | 0.22851000 | -1.05018200 |
| C | 4.82821100 | -2.25361600 | -2.46823400 |
| H | 3.13368600 | -3.53591300 | -2.86036800 |
| C | 5.23783700 | -1.03123900 | -1.92731700 |
| H | 4.62812500 | 0.82594400 | -1.02524900 |
| H | 5.56701500 | -2.94772100 | -2.85541900 |
| C | 6.70222200 | -0.75060300 | -1.76234700 |
| F | 6.97766400 | 0.57322800 | -1.74790200 |
| F | 7.16648500 | -1.25617000 | -0.58628600 |
| F | 7.44853200 | -1.31051800 | -2.74148900 |
| P | 0.79945300 | -1.08306700 | 1.87930700 |
| C | -0.14495800 | -1.86193400 | 3.27207500 |
| C | -0.70357900 | -1.02161400 | 4.25051200 |
| C | -0.43241800 | -3.23308000 | 3.32710400 |
| C | -1.53516800 | -1.53647700 | 5.24432900 |
| H | -0.49352700 | 0.04232800 | 4.24005100 |
| C | -1.26619100 | -3.74658200 | 4.32111900 |
| H | -0.01317400 | -3.91387400 | 2.59895200 |
| C | -1.82558100 | -2.90151000 | 5.28046800 |
| H | -1.96001500 | -0.86509000 | 5.98560600 |
| H | -1.48003300 | -4.81156600 | 4.33817300 |
| H | -2.47839500 | -3.30297500 | 6.05081900 |
| C | 2.06398300 | -2.32214300 | 1.37006500 |
| C | 3.43817100 | -2.04227100 | 1.46016800 |
| C | 1.66040200 | -3.53867000 | 0.79702900 |
| C | 4.38102000 | -2.96811600 | 1.01490500 |
| H | 3.77807400 | -1.09276600 | 1.85668300 |
| C | 2.60564000 | -4.47481100 | 0.37907700 |
| H | 0.61032600 | -3.74493500 | 0.63352800 |
| C | 3.96748000 | -4.19364500 | 0.48851500 |
| H | 5.43641600 | -2.71342900 | 1.04738800 |
| H | 2.27025300 | -5.40537400 | -0.06886000 |
| H | 4.70333600 | -4.91198100 | 0.13777900 |
| C | 1.79558200 | 0.17497400 | 2.79107300 |
| C | 2.40157300 | -0.15479600 | 4.01851400 |
| C | 1.99863500 | 1.45174000 | 2.25253100 |
| C | 3.18788300 | 0.78078300 | 4.68801100 |
| H | 2.25776500 | -1.14153500 | 4.44835600 |
| C | 2.78354300 | 2.39053500 | 2.93011700 |
| H | 1.52940900 | 1.71113300 | 1.31211200 |
| C | 3.37909100 | 2.05760100 | 4.14622000 |
| H | 3.65201300 | 0.51431200 | 5.63379400 |

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|---|---|---|---|
| H | 2.91850600 | 3.37778700 | 2.49533200 |
| H | 3.99041000 | 2.78476500 | 4.67426300 |

Ir(III)

| | | | |
|---|---|---|---|
| Ir | -0.00092400 | 0.00266900 | 0.03363200 |
| C | 1.66915400 | -0.46369000 | 1.07243000 |
| C | 2.40826700 | -1.58267400 | 0.58619900 |
| C | 2.18704300 | 0.19337800 | 2.20537200 |
| C | 3.36261500 | -0.22761100 | 2.82639700 |
| H | 1.65080700 | 1.04848200 | 2.60703400 |
| C | 4.07385200 | -1.32998300 | 2.33369800 |
| H | 3.73095200 | 0.30367800 | 3.70184200 |
| H | 4.99014800 | -1.65751800 | 2.81750500 |
| C | 0.09994700 | -2.26912800 | -2.14650300 |
| C | 1.85711200 | -2.26605300 | -0.58864500 |
| C | 0.60018300 | -3.38568500 | -2.80315900 |
| H | -0.81628200 | -1.78252300 | -2.46341800 |
| C | 2.40676600 | -3.39820400 | -1.21382700 |
| C | 1.78188200 | -3.95750100 | -2.32092900 |
| H | 0.07596100 | -3.79452400 | -3.66020900 |
| H | 3.31834800 | -3.83885500 | -0.82708400 |
| H | 2.20750200 | -4.83358800 | -2.80190600 |
| N | 0.70745100 | -1.72073400 | -1.08120700 |
| C | 3.59481000 | -2.00223600 | 1.21561100 |
| H | 4.14910200 | -2.85736600 | 0.83727800 |
| C | -0.43082900 | 1.68284200 | 1.07171200 |
| C | 0.16456100 | 2.88275500 | 0.58111300 |
| C | -1.24612800 | 1.80211700 | 2.21340200 |
| C | -1.46270900 | 3.03003100 | 2.83803000 |
| H | -1.71177600 | 0.90951000 | 2.62045300 |
| C | -0.86934000 | 4.19766500 | 2.33976300 |
| H | -2.09686000 | 3.08231100 | 3.72089300 |
| H | -1.03862400 | 5.15457000 | 2.82620600 |
| C | 1.91501700 | 1.21985600 | -2.14547300 |
| C | 1.02678800 | 2.74605500 | -0.59728900 |
| C | 2.62400600 | 2.21109000 | -2.81091900 |
| H | 1.95793900 | 0.18089700 | -2.45495200 |
| C | 1.72240600 | 3.78849600 | -1.23306900 |
| C | 2.51891500 | 3.52376800 | -2.33973200 |
| H | 3.24099200 | 1.95911600 | -3.66670800 |
| H | 1.63969800 | 4.80067700 | -0.85473000 |
| H | 3.05707900 | 4.33065400 | -2.82897000 |
| N | 1.13592200 | 1.47516700 | -1.08133000 |
| C | -0.05886900 | 4.11976900 | 1.21340400 |

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|---|---|---|---|
| H | 0.40188800 | 5.02777200 | 0.83248000 |
| C | -1.24700300 | -1.21005200 | 1.06426900 |
| C | -2.58026300 | -1.29896600 | 0.56489200 |
| C | -0.94834900 | -1.97430200 | 2.20867000 |
| C | -1.90464400 | -2.77957700 | 2.82659100 |
| H | 0.05408700 | -1.92760000 | 2.62389300 |
| C | -3.20847400 | -2.85491000 | 2.31880400 |
| H | -1.63693900 | -3.35342800 | 3.71168200 |
| H | -3.95354800 | -3.48295900 | 2.79981100 |
| C | -2.00188400 | 1.04623900 | -2.16070600 |
| C | -2.88717700 | -0.48512800 | -0.61608300 |
| C | -3.21017300 | 1.16009600 | -2.83535000 |
| H | -1.12246600 | 1.60329200 | -2.46640800 |
| C | -4.13343500 | -0.40781200 | -1.26072600 |
| C | -4.29632300 | 0.41176700 | -2.37017500 |
| H | -3.29546500 | 1.81754700 | -3.69385500 |
| H | -4.96983600 | -0.98705100 | -0.88736700 |
| H | -5.26083000 | 0.47140200 | -2.86635300 |
| N | -1.83961900 | 0.24753900 | -1.09271400 |
| C | -3.54103300 | -2.11506100 | 1.19019100 |
| H | -4.55481700 | -2.17399200 | 0.80202200 |

Ir(IV)

| | | | |
|---|---|---|---|
| Ir | -1.51821700 | 0.12168800 | -0.08891600 |
| C | -0.15531900 | -0.66068200 | -1.36273400 |
| C | -0.64852600 | -1.62806600 | -2.28395700 |
| C | 1.21288800 | -0.35257100 | -1.42840200 |
| C | 2.06096100 | -0.98117000 | -2.33895800 |
| H | 1.62451200 | 0.37195100 | -0.73537700 |
| C | 1.56196500 | -1.93635600 | -3.23377500 |
| H | 3.12094000 | -0.73873900 | -2.34063300 |
| H | 2.22473000 | -2.43007700 | -3.93893400 |
| C | -4.07227300 | -1.44939600 | -1.04900400 |
| C | -2.07863800 | -1.93609000 | -2.19874100 |
| C | -4.80731700 | -2.34024700 | -1.81872200 |
| H | -4.52520500 | -0.86973000 | -0.25108500 |
| C | -2.77518400 | -2.85172100 | -3.00636500 |
| C | -4.13614200 | -3.05278900 | -2.81890100 |
| H | -5.86789700 | -2.47396800 | -1.63598200 |
| H | -2.24577500 | -3.40268800 | -3.77473700 |
| H | -4.67168700 | -3.76182500 | -3.44360900 |
| N | -2.75680300 | -1.24838600 | -1.23494500 |
| C | 0.20980800 | -2.25430400 | -3.20753700 |
| H | -0.17189100 | -2.99826400 | -3.90191100 |

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|---|---|---|---|
| C | -0.29824400 | 1.52960500 | 0.71293000 |
| C | -0.21460500 | 2.75711700 | -0.00344000 |
| C | 0.43540200 | 1.43653500 | 1.90927900 |
| C | 1.22606800 | 2.49175200 | 2.36616900 |
| H | 0.40979000 | 0.51112200 | 2.47164500 |
| C | 1.31367000 | 3.68515300 | 1.63823800 |
| H | 1.78648200 | 2.38148200 | 3.29230800 |
| H | 1.93425200 | 4.50408400 | 1.99148900 |
| C | -2.55293600 | 1.73402500 | -2.60109500 |
| C | -1.01303400 | 2.85695500 | -1.22994900 |
| C | -2.62947100 | 2.79642800 | -3.49146900 |
| H | -3.11899300 | 0.82149700 | -2.75219200 |
| C | -1.04667700 | 3.95879900 | -2.10071900 |
| C | -1.85485800 | 3.93086200 | -3.22987600 |
| H | -3.27000900 | 2.73071900 | -4.36416600 |
| H | -0.43559300 | 4.82927300 | -1.89339600 |
| H | -1.87848100 | 4.78252000 | -3.90356500 |
| N | -1.77758900 | 1.76261500 | -1.50468100 |
| C | 0.59097100 | 3.81452800 | 0.45845000 |
| H | 0.65574200 | 4.74463500 | -0.09970500 |
| C | -1.30183200 | -1.24874900 | 1.32682600 |
| C | -2.09125300 | -1.08045300 | 2.50636000 |
| C | -0.46973400 | -2.41661800 | 1.27171100 |
| C | -0.45060000 | -3.36239200 | 2.32957200 |
| H | -0.02601900 | -2.69912400 | 0.32679100 |
| C | -1.20393300 | -3.14599400 | 3.46637100 |
| H | 0.19345800 | -4.22951700 | 2.22808100 |
| H | -1.18155500 | -3.85326900 | 4.29036500 |
| C | -3.80143200 | 1.86861200 | 1.23653800 |
| C | -2.99551300 | 0.07756500 | 2.51852200 |
| C | -4.63864200 | 2.29982700 | 2.25763600 |
| H | -3.73967000 | 2.38926200 | 0.28671700 |
| C | -3.81261000 | 0.47223100 | 3.58849500 |
| C | -4.63709500 | 1.58353300 | 3.45833600 |
| H | -5.26331600 | 3.17519500 | 2.11698100 |
| H | -3.79376400 | -0.08420500 | 4.51848200 |
| H | -5.26866600 | 1.89263500 | 4.28603200 |
| N | -3.01035100 | 0.79114300 | 1.35848100 |
| C | -2.02790000 | -2.00647800 | 3.55186400 |
| H | -2.63206700 | -1.87076800 | 4.44498700 |
| C | 2.37254300 | -2.19562000 | 1.02557800 |
| O | 2.26859800 | -3.35477500 | 0.61188600 |
| O | 1.47678100 | -1.50443200 | 1.65791100 |
| C | 3.65936700 | -1.41866700 | 0.78294400 |

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|---|---|---|---|
| C | 4.74656700 | -2.08602300 | 0.20826400 |
| C | 3.76140700 | -0.05379400 | 1.07991700 |
| C | 5.92501300 | -1.39854700 | -0.07332900 |
| H | 4.64328500 | -3.14105700 | -0.02040600 |
| C | 4.93493400 | 0.63932700 | 0.79452600 |
| H | 2.91307000 | 0.46110600 | 1.51436100 |
| C | 6.01731000 | -0.03404200 | 0.21945000 |
| H | 6.77093200 | -1.91468500 | -0.51563300 |
| H | 5.01246900 | 1.69842400 | 1.01907800 |
| C | 7.25627900 | 0.73255200 | -0.14433400 |
| F | 7.50641900 | 1.73722800 | 0.72864100 |
| F | 8.35645800 | -0.05485800 | -0.17830700 |
| F | 7.15106800 | 1.30566100 | -1.37031700 |

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|---|---|---|---|
| Ru | -0.10775200 | 0.61288600 | 0.06651200 |
| O | -1.92743400 | 0.95748000 | -1.03232500 |
| O | -2.00641100 | 0.71552300 | 1.13336900 |
| P | -0.17050400 | -1.65215500 | -0.02443700 |
| C | 1.35269800 | -2.45127600 | -0.70106000 |
| C | 1.39074700 | -3.08706700 | -1.94916800 |
| C | 2.53121700 | -2.37673100 | 0.06162500 |
| C | 2.58407800 | -3.63837800 | -2.42454600 |
| H | 0.49171700 | -3.15930300 | -2.55275000 |
| C | 3.72017000 | -2.92549400 | -0.41607400 |
| H | 2.51920900 | -1.87536300 | 1.02407800 |
| C | 3.74991500 | -3.55969900 | -1.66108000 |
| H | 2.59860100 | -4.12963500 | -3.39390000 |
| H | 4.62526700 | -2.84416700 | 0.17907200 |
| C | -1.53903400 | -2.34287600 | -1.05064900 |
| C | -2.33833100 | -3.42004100 | -0.63979300 |
| C | -1.79872000 | -1.73542300 | -2.29070500 |
| C | -3.37690500 | -3.87939200 | -1.45328400 |
| H | -2.16059800 | -3.89643300 | 0.31850700 |
| C | -2.82685600 | -2.20577100 | -3.10728100 |
| H | -1.20595000 | -0.88225300 | -2.60232100 |
| C | -3.62184500 | -3.27586400 | -2.68808600 |
| H | -3.99450100 | -4.70865700 | -1.11867100 |
| H | -3.01652000 | -1.72598700 | -4.06358500 |
| C | -0.35600300 | -2.51443100 | 1.59980600 |
| C | 0.08831100 | -3.83509600 | 1.78305300 |
| C | -0.98366600 | -1.85187600 | 2.66606700 |
| C | -0.09273400 | -4.47970100 | 3.00736400 |
| H | 0.57999800 | -4.35967500 | 0.96952700 |

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|---|---|---|---|
| C | -1.16260600 | -2.50101200 | 3.89007600 |
| H | -1.33795100 | -0.83667600 | 2.53301600 |
| C | -0.71790500 | -3.81290300 | 4.06446500 |
| H | -1.64837600 | -1.97641700 | 4.70863000 |
| H | 0.25722800 | -5.50058600 | 3.13583700 |
| C | -2.61992100 | 0.95564100 | 0.03937000 |
| C | -4.08416600 | 1.21572200 | 0.01443400 |
| C | -4.57651100 | 2.34638800 | -0.66981300 |
| C | -4.96266000 | 0.32528600 | 0.66669900 |
| C | -5.95518100 | 2.57316600 | -0.68187700 |
| C | -6.33540300 | 0.58461300 | 0.60979600 |
| C | -6.85121900 | 1.70366700 | -0.05117400 |
| H | -6.34006500 | 3.45011100 | -1.19886300 |
| H | -7.02079800 | -0.10722400 | 1.09523800 |
| C | -8.33574900 | 1.98403800 | -0.05912700 |
| H | -8.91887500 | 1.06219900 | 0.03952000 |
| H | -8.61641800 | 2.63895200 | 0.77676800 |
| H | -8.64456300 | 2.48649000 | -0.98236800 |
| C | -3.64791400 | 3.31696600 | -1.36614200 |
| H | -2.81486300 | 3.60697000 | -0.71652800 |
| H | -3.20261300 | 2.86465200 | -2.25777600 |
| H | -4.18563900 | 4.22249500 | -1.66442700 |
| C | -4.46031600 | -0.90325900 | 1.39199000 |
| H | -3.79232500 | -1.49900100 | 0.76108500 |
| H | -3.88757000 | -0.63149200 | 2.28354600 |
| H | -5.29636200 | -1.54064500 | 1.69685100 |
| H | 4.67755900 | -3.98414600 | -2.03536900 |
| H | -0.85522500 | -4.31411000 | 5.01903900 |
| H | -4.43165200 | -3.63323700 | -3.31856600 |
| O | 1.71525300 | 0.78977000 | -1.02870900 |
| O | 1.78141000 | 0.58430100 | 1.13307000 |
| C | 2.42497200 | 0.75004600 | 0.03651400 |
| C | 3.90467000 | 0.84202400 | -0.00938800 |
| C | 4.60066000 | 0.46487100 | -1.18726900 |
| C | 4.62601300 | 1.27690200 | 1.13193800 |
| C | 5.99879900 | 0.50165000 | -1.17872200 |
| C | 6.02123900 | 1.30954600 | 1.07521300 |
| C | 6.72918400 | 0.91445000 | -0.06281300 |
| H | 6.53303200 | 0.20120700 | -2.07756400 |
| H | 6.57212100 | 1.65667900 | 1.94697100 |
| C | 8.23916300 | 0.91491100 | -0.07553900 |
| H | 8.64474200 | 1.73389400 | 0.52863800 |
| H | 8.63461700 | -0.02148800 | 0.34072200 |
| H | 8.63288100 | 1.01200000 | -1.09284400 |

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|---|---|---|---|
| C | 3.91643600 | 0.01458700 | -2.45928200 |
| H | 3.17645900 | -0.76494300 | -2.27082800 |
| H | 3.38009600 | 0.84254800 | -2.93275800 |
| H | 4.65785100 | -0.37054600 | -3.16694500 |
| C | 3.95313200 | 1.74673100 | 2.40203900 |
| H | 3.18281200 | 2.48816900 | 2.17685400 |
| H | 3.45446200 | 0.92461800 | 2.92261900 |
| H | 4.68934700 | 2.19675900 | 3.07603400 |
| C | 0.28395300 | 3.49723400 | 1.45780800 |
| C | 0.11477100 | 3.66585600 | -0.93837800 |
| C | 1.39666500 | 4.51799600 | 1.18674100 |
| H | -0.58521300 | 3.96629700 | 1.93717900 |
| C | 1.62393200 | 3.92509600 | -1.08497000 |
| H | -0.27902000 | 3.10015800 | -1.78357600 |
| H | 0.98680900 | 5.49655600 | 0.88989900 |
| H | 1.78172800 | 4.85514600 | -1.65472100 |
| H | -0.45593800 | 4.60054800 | -0.85407900 |
| H | 2.10165300 | 3.09449900 | -1.60438500 |
| H | 1.99078100 | 4.66841700 | 2.09261200 |
| O | 2.26855300 | 4.01024700 | 0.19076700 |
| O | -0.14089100 | 2.86987800 | 0.22573200 |
| H | 0.65439100 | 2.68379800 | 2.08266800 |

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|---|---|---|---|
| Ru | -0.15398700 | 0.47016500 | -0.43586300 |
| O | 1.74781900 | 0.98246000 | 0.41532000 |
| O | 1.66591000 | 0.16610600 | -1.59485800 |
| P | 0.01335700 | -1.72459900 | 0.27948800 |
| C | -1.33823300 | -2.32822300 | 1.38491100 |
| C | -1.17315000 | -2.54358400 | 2.75936000 |
| C | -2.60659600 | -2.52697800 | 0.81190100 |
| C | -2.25549200 | -2.95030500 | 3.54494500 |
| H | -0.20032900 | -2.40616300 | 3.22025100 |
| C | -3.68364900 | -2.93442800 | 1.59731200 |
| H | -2.75170900 | -2.35270100 | -0.24971800 |
| C | -3.51118600 | -3.14741700 | 2.96766500 |
| H | -2.11234800 | -3.11649100 | 4.60946700 |
| H | -4.65991600 | -3.06950400 | 1.14038700 |
| C | 1.59065600 | -2.07775000 | 1.16652300 |
| C | 2.50860600 | -3.04459400 | 0.73285400 |
| C | 1.94643200 | -1.23490800 | 2.23465000 |
| C | 3.75719100 | -3.16296100 | 1.34873300 |
| H | 2.26176800 | -3.69602400 | -0.09858200 |
| C | 3.18291900 | -1.37139900 | 2.86289300 |

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|---|---|---|---|
| H | 1.27121100 | -0.44314200 | 2.54204600 |
| C | 4.09674300 | -2.32905900 | 2.41412600 |
| H | 4.46600200 | -3.90263200 | 0.98656000 |
| H | 3.44501700 | -0.70829200 | 3.68285900 |
| C | -0.03827800 | -2.98325500 | -1.06980300 |
| C | -0.29693300 | -4.33766300 | -0.79904300 |
| C | 0.19891900 | -2.58515900 | -2.39355600 |
| C | -0.31244100 | -5.27525000 | -1.83167000 |
| H | -0.49284100 | -4.65746000 | 0.22033500 |
| C | 0.18237300 | -3.52643600 | -3.42613200 |
| H | 0.40732400 | -1.54352100 | -2.60719300 |
| C | -0.07301200 | -4.87045900 | -3.14846700 |
| H | 0.36845300 | -3.20595000 | -4.44777400 |
| H | -0.51448900 | -6.31977700 | -1.60961600 |
| C | 2.38395400 | 0.52861500 | -0.59545800 |
| C | 3.85724200 | 0.33298400 | -0.56314800 |
| C | 4.64497000 | 1.03352200 | 0.38658700 |
| C | 4.46846800 | -0.61981600 | -1.42099000 |
| C | 6.01810100 | 0.77751900 | 0.44517900 |
| C | 5.84337300 | -0.84372500 | -1.30515500 |
| C | 6.63854900 | -0.15601400 | -0.38611000 |
| H | 6.61949000 | 1.32115200 | 1.17100800 |
| H | 6.30707100 | -1.58484000 | -1.95302700 |
| C | 8.12722300 | -0.39840200 | -0.31309700 |
| H | 8.37665300 | -1.43716500 | -0.55621700 |
| H | 8.66458100 | 0.23986600 | -1.02747700 |
| H | 8.52212400 | -0.17528200 | 0.68392700 |
| C | 4.07603300 | 2.04819100 | 1.35042500 |
| H | 3.40567900 | 2.75438200 | 0.85957200 |
| H | 3.47545000 | 1.55925300 | 2.12262600 |
| H | 4.88458700 | 2.60673000 | 1.83452200 |
| C | 3.71039500 | -1.44693500 | -2.43541100 |
| H | 2.88850900 | -1.99634200 | -1.96983900 |
| H | 3.25842300 | -0.82361500 | -3.21157000 |
| H | 4.38449600 | -2.16732800 | -2.91061900 |
| C | -0.12178100 | 3.19381100 | 1.63420900 |
| C | 0.49519300 | 3.84638300 | 0.55637900 |
| C | 0.35158400 | 3.38217900 | 2.93202800 |
| C | 1.43586200 | 4.22897800 | 3.17691200 |
| H | -0.13527100 | 2.86728600 | 3.75616300 |
| C | 2.04355900 | 4.89692300 | 2.11184900 |
| H | 1.80271200 | 4.37023200 | 4.19016600 |
| C | -0.78765000 | 2.39988800 | -2.60016300 |
| C | -0.00139000 | 3.69768600 | -0.83587600 |

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|---|---|---|---|
| C | -0.92274600 | 3.49815800 | -3.43953800 |
| H | -1.04873600 | 1.40524000 | -2.93935200 |
| C | -0.12565500 | 4.84875500 | -1.63474700 |
| C | -0.58260700 | 4.75591700 | -2.94295400 |
| H | -1.28877100 | 3.36144300 | -4.45160600 |
| H | 0.11799100 | 5.81342200 | -1.20389200 |
| H | -0.68195300 | 5.64644900 | -3.55685900 |
| N | -0.33747100 | 2.47754800 | -1.32908400 |
| C | 1.57481400 | 4.70805400 | 0.81166600 |
| H | 2.07245000 | 5.20682100 | -0.01568600 |
| H | -4.35128100 | -3.46073100 | 3.58159200 |
| H | -0.08820200 | -5.60081300 | -3.95322800 |
| H | 5.07246400 | -2.41404800 | 2.88457500 |
| H | 2.89139100 | 5.55316600 | 2.28863000 |
| H | -0.96930100 | 2.54530200 | 1.45521400 |
| O | -1.94574400 | 0.86159500 | 0.69738300 |
| O | -2.10746900 | 0.02427300 | -1.29959500 |
| C | -2.70108500 | 0.46631400 | -0.25363200 |
| C | -4.18070900 | 0.48453900 | -0.13334000 |
| C | -4.78776300 | 0.45729200 | 1.15001600 |
| C | -4.98771800 | 0.50210200 | -1.30014100 |
| C | -6.18331200 | 0.40790200 | 1.22775100 |
| C | -6.37742400 | 0.47159400 | -1.15832600 |
| C | -6.99655600 | 0.40908100 | 0.09263800 |
| H | -6.64902100 | 0.37297700 | 2.21035900 |
| H | -6.99536100 | 0.49717300 | -2.05351000 |
| C | -8.49956000 | 0.32497500 | 0.21137100 |
| H | -8.99711500 | 0.86245000 | -0.60323400 |
| H | -8.83777000 | -0.71904200 | 0.16577400 |
| H | -8.85162800 | 0.74041000 | 1.16160500 |
| C | -4.01024400 | 0.47734200 | 2.44796600 |
| H | -3.21466300 | -0.26942000 | 2.46023200 |
| H | -3.52745400 | 1.44763300 | 2.60094600 |
| H | -4.68356300 | 0.28631800 | 3.28997300 |
| C | -4.41992700 | 0.57947400 | -2.70144500 |
| H | -3.67423600 | 1.37504200 | -2.79221800 |
| H | -3.91116400 | -0.34847800 | -2.97759900 |
| H | -5.22182900 | 0.76868000 | -3.42261000 |

J-TS

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|---|---|---|---|
| Ru | -0.16702200 | -0.56767700 | 0.20171600 |
| O | -2.28016300 | -0.54579500 | 0.61540300 |
| O | -1.64262300 | -0.34666900 | -1.47382300 |
| P | 0.10801700 | 1.75703800 | 0.31918800 |

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|---|---|---|---|
| C | 1.44525200 | 2.38836400 | 1.42576600 |
| C | 1.19627600 | 3.15038800 | 2.57498600 |
| C | 2.77073400 | 2.04343300 | 1.10965500 |
| C | 2.25216400 | 3.54997100 | 3.40008200 |
| H | 0.17918600 | 3.42912500 | 2.83199800 |
| C | 3.82218600 | 2.45315200 | 1.92762800 |
| H | 2.97874400 | 1.47061300 | 0.21150900 |
| C | 3.56516100 | 3.20282600 | 3.07997800 |
| H | 2.04445600 | 4.13768900 | 4.29037200 |
| H | 4.84221700 | 2.18811900 | 1.66384600 |
| C | -1.39004900 | 2.68001300 | 0.86012700 |
| C | -1.84641800 | 3.85249600 | 0.23960700 |
| C | -2.11595500 | 2.15014900 | 1.94065200 |
| C | -3.00847700 | 4.48267400 | 0.69138300 |
| H | -1.30519300 | 4.27012100 | -0.60323100 |
| C | -3.26798000 | 2.79023200 | 2.39749900 |
| H | -1.78444200 | 1.23003900 | 2.41033600 |
| C | -3.71982600 | 3.95457300 | 1.77080000 |
| H | -3.35778400 | 5.38485100 | 0.19621500 |
| H | -3.82080600 | 2.36928600 | 3.23286100 |
| C | 0.59535500 | 2.54005500 | -1.28297700 |
| C | 1.22113900 | 3.79785500 | -1.32261000 |
| C | 0.34777300 | 1.86609500 | -2.48879800 |
| C | 1.58562200 | 4.37148500 | -2.54134600 |
| H | 1.43165200 | 4.32805800 | -0.39844000 |
| C | 0.71847100 | 2.44107800 | -3.70685500 |
| H | -0.13666700 | 0.89822400 | -2.47249100 |
| C | 1.33740500 | 3.69226300 | -3.73702900 |
| H | 0.52402900 | 1.90584100 | -4.63257500 |
| H | 2.06852600 | 5.34502300 | -2.55569900 |
| C | -2.58528500 | -0.46296300 | -0.61996200 |
| C | -4.00973300 | -0.52797400 | -1.05027700 |
| C | -4.81129100 | -1.60646700 | -0.62143800 |
| C | -4.53625400 | 0.48410800 | -1.87816100 |
| C | -6.14309900 | -1.65426700 | -1.04341000 |
| C | -5.87873100 | 0.40079100 | -2.25911200 |
| C | -6.69588900 | -0.66159500 | -1.85935100 |
| H | -6.76646100 | -2.48738300 | -0.72439800 |
| H | -6.29760600 | 1.18741000 | -2.88372100 |
| C | -8.13191100 | -0.74990400 | -2.32098500 |
| H | -8.56136000 | 0.24385400 | -2.48822800 |
| H | -8.20784300 | -1.30091500 | -3.26817700 |
| H | -8.75750900 | -1.27337300 | -1.58980300 |
| C | -4.25678300 | -2.70925000 | 0.25524900 |

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|---|---|---|---|
| H | -3.36410700 | -3.16503000 | -0.18977700 |
| H | -3.95269200 | -2.32416300 | 1.23258800 |
| H | -5.00119800 | -3.49818000 | 0.40213400 |
| C | -3.69398400 | 1.65969100 | -2.32187200 |
| H | -3.25814400 | 2.18307900 | -1.46336100 |
| H | -2.85734900 | 1.33722500 | -2.94849000 |
| H | -4.29732400 | 2.37888000 | -2.88476200 |
| C | 0.20539600 | -1.16383700 | 2.21126000 |
| C | -0.32535600 | -2.47487700 | 2.43043400 |
| C | 0.39836800 | -0.35478500 | 3.34873200 |
| C | 0.02417600 | -0.77965100 | 4.62353500 |
| H | 0.85645800 | 0.62067300 | 3.23145400 |
| C | -0.53347600 | -2.04933500 | 4.80957300 |
| H | 0.16983800 | -0.12088000 | 5.47661900 |
| C | -0.51797100 | -3.32280100 | -1.10156500 |
| C | -0.49727300 | -3.32242800 | 1.24506900 |
| C | -0.75554500 | -4.69131900 | -1.15434000 |
| H | -0.43899400 | -2.71402800 | -1.99579600 |
| C | -0.73727800 | -4.70476400 | 1.25364700 |
| C | -0.86960700 | -5.39057700 | 0.05139200 |
| H | -0.84996000 | -5.19034100 | -2.11271000 |
| H | -0.80493000 | -5.23522000 | 2.19651500 |
| H | -1.05419200 | -6.46087200 | 0.05228700 |
| N | -0.39535700 | -2.66189400 | 0.06060000 |
| C | -0.69630700 | -2.89575100 | 3.71472000 |
| H | -1.13888800 | -3.87705900 | 3.86439800 |
| H | 4.38488800 | 3.51731500 | 3.72013100 |
| H | 1.62790400 | 4.13579800 | -4.68577400 |
| H | -4.62546900 | 4.44447000 | 2.11845300 |
| H | -0.83101000 | -2.38031200 | 5.80074500 |
| O | 2.59656900 | -1.53770300 | 1.06491100 |
| O | 1.69959900 | -0.64889600 | -0.76641600 |
| C | 2.69694300 | -1.13406500 | -0.14225300 |
| C | 4.01429900 | -1.18257600 | -0.83826300 |
| C | 5.21649500 | -1.11080400 | -0.08765200 |
| C | 4.06361200 | -1.26369800 | -2.25488700 |
| C | 6.43510900 | -1.10591300 | -0.77416600 |
| C | 5.31237100 | -1.27945600 | -2.88194800 |
| C | 6.50869000 | -1.19667300 | -2.16536200 |
| H | 7.35658000 | -1.03309800 | -0.20053900 |
| H | 5.35093300 | -1.35134800 | -3.96689600 |
| C | 7.84132900 | -1.23411700 | -2.87428600 |
| H | 7.78618500 | -0.75438100 | -3.85761100 |
| H | 8.62078300 | -0.73239300 | -2.29114800 |

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|---|---|---|---|
| H | 8.16920400 | -2.26976700 | -3.03589300 |
| C | 5.25990500 | -1.02330200 | 1.42329300 |
| H | 4.58109600 | -0.26101100 | 1.81288700 |
| H | 4.94953500 | -1.96684400 | 1.88192100 |
| H | 6.27706800 | -0.79216100 | 1.75656300 |
| C | 2.83387400 | -1.34024900 | -3.13537300 |
| H | 2.10603200 | -2.06662900 | -2.76230000 |
| H | 2.31456200 | -0.37756300 | -3.17039900 |
| H | 3.11929900 | -1.62235800 | -4.15422500 |
| H | 1.37817500 | -1.21216500 | 1.41974000 |

K

| | | | |
|---|---|---|---|
| Ru | 0.15289300 | 0.63536900 | 0.03334600 |
| O | 2.25235700 | 0.58967600 | 0.33241800 |
| O | 1.91536100 | 0.27988100 | -1.83979300 |
| P | -0.09187400 | -1.67441700 | 0.42269300 |
| C | -1.50062900 | -2.19955700 | 1.50141900 |
| C | -1.31760600 | -2.79357900 | 2.75742200 |
| C | -2.80879100 | -1.92922400 | 1.06252600 |
| C | -2.41815400 | -3.09294300 | 3.56664400 |
| H | -0.31519600 | -3.01622600 | 3.11004300 |
| C | -3.90508300 | -2.23555800 | 1.86722900 |
| H | -2.96789200 | -1.49290800 | 0.08237300 |
| C | -3.71241600 | -2.81210500 | 3.12712300 |
| H | -2.25952000 | -3.54940900 | 4.54011500 |
| H | -4.90893500 | -2.02494500 | 1.50801000 |
| C | 1.37197300 | -2.49895900 | 1.17947600 |
| C | 1.79770500 | -3.78599400 | 0.81774100 |
| C | 2.09365000 | -1.78575500 | 2.15112500 |
| C | 2.92704800 | -4.34935600 | 1.41537600 |
| H | 1.25679500 | -4.34554800 | 0.06124900 |
| C | 3.21468900 | -2.35703000 | 2.75428300 |
| H | 1.78648600 | -0.78059400 | 2.41724600 |
| C | 3.63687800 | -3.63640400 | 2.38441300 |
| H | 3.25323700 | -5.34318800 | 1.12017800 |
| H | 3.76752200 | -1.79394400 | 3.50125400 |
| C | -0.43362900 | -2.66799700 | -1.10347100 |
| C | -1.15346800 | -3.87435100 | -1.06135100 |
| C | 0.05069500 | -2.20892000 | -2.33918900 |
| C | -1.38758000 | -4.60299300 | -2.22861800 |
| H | -1.53626000 | -4.24511600 | -0.11563000 |
| C | -0.18785900 | -2.94055000 | -3.50534800 |
| H | 0.62784200 | -1.29149300 | -2.38532800 |
| C | -0.90802800 | -4.13578000 | -3.45492600 |

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|---|---|---|---|
| H | 0.19277400 | -2.57222600 | -4.45448100 |
| H | -1.94679000 | -5.53371200 | -2.17903500 |
| C | 2.69483300 | 0.41838000 | -0.85937100 |
| C | 4.18234800 | 0.39123700 | -1.04040600 |
| C | 4.94729300 | 1.51890800 | -0.68635200 |
| C | 4.79433000 | -0.76686000 | -1.55543500 |
| C | 6.33214000 | 1.47242500 | -0.87554600 |
| C | 6.18376200 | -0.77472500 | -1.71252800 |
| C | 6.96877800 | 0.33640400 | -1.38685700 |
| H | 6.92986500 | 2.34323800 | -0.61189800 |
| H | 6.66543700 | -1.67187100 | -2.09732800 |
| C | 8.46410100 | 0.31938800 | -1.60669500 |
| H | 8.87146100 | -0.69363200 | -1.51617900 |
| H | 8.72092800 | 0.68450800 | -2.61047500 |
| H | 8.98342900 | 0.96066700 | -0.88588800 |
| C | 4.29356400 | 2.76113400 | -0.12074600 |
| H | 3.51323900 | 3.14354800 | -0.78974200 |
| H | 3.80419800 | 2.54705300 | 0.83415300 |
| H | 5.02963100 | 3.55741400 | 0.02971400 |
| C | 3.97575400 | -1.99144300 | -1.89847500 |
| H | 3.42444800 | -2.35549000 | -1.02302900 |
| H | 3.23069100 | -1.76575700 | -2.66728100 |
| H | 4.61564200 | -2.80472000 | -2.25543900 |
| C | -0.11214700 | 1.38941900 | 1.89520500 |
| C | 0.24459600 | 2.77764300 | 2.01793200 |
| C | -0.46912800 | 0.73675000 | 3.09675600 |
| C | -0.43930200 | 1.38144500 | 4.33409000 |
| H | -0.78195500 | -0.30002100 | 3.06660000 |
| C | -0.06010100 | 2.72495500 | 4.42838400 |
| H | -0.71551100 | 0.83095300 | 5.23109600 |
| C | 0.69516700 | 3.22416100 | -1.55990300 |
| C | 0.55407000 | 3.48221200 | 0.76901800 |
| C | 1.04547400 | 4.55680100 | -1.74366800 |
| H | 0.62652200 | 2.52670900 | -2.38753100 |
| C | 0.91679900 | 4.83215000 | 0.64486700 |
| C | 1.16339900 | 5.37063900 | -0.61284900 |
| H | 1.23207800 | 4.93762400 | -2.74195900 |
| H | 1.00923000 | 5.45271100 | 1.52867500 |
| H | 1.44795900 | 6.41426800 | -0.71156900 |
| N | 0.45555100 | 2.70449700 | -0.34464900 |
| C | 0.27183900 | 3.41726900 | 3.26833900 |
| H | 0.55441900 | 4.46428600 | 3.34225500 |
| H | -4.56645200 | -3.04573500 | 3.75698700 |
| H | -1.09449500 | -4.70119200 | -4.36428900 |

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|---|---|---|---|
| H | 4.51889300 | -4.07361900 | 2.84494700 |
| H | -0.03527600 | 3.22749500 | 5.39125600 |
| O | -2.85290400 | 1.89262700 | 0.91698600 |
| O | -1.89744600 | 0.65104300 | -0.68487200 |
| C | -2.90881200 | 1.18999000 | -0.20398000 |
| C | -4.23242600 | 1.05751800 | -0.84700000 |
| C | -5.42069300 | 1.04194300 | -0.07051500 |
| C | -4.29033800 | 0.89121600 | -2.25723400 |
| C | -6.64024400 | 0.86168200 | -0.72944600 |
| C | -5.54136100 | 0.73912300 | -2.85730800 |
| C | -6.72613800 | 0.71401300 | -2.11568900 |
| H | -7.55284000 | 0.83753100 | -0.13854300 |
| H | -5.59248700 | 0.63262400 | -3.93850200 |
| C | -8.05673500 | 0.50300700 | -2.79621300 |
| H | -8.09669000 | 1.01810900 | -3.76217400 |
| H | -8.22885300 | -0.56390300 | -2.99075200 |
| H | -8.88650700 | 0.86318600 | -2.17967300 |
| C | -5.44472400 | 1.17677700 | 1.43779600 |
| H | -4.71948800 | 0.51471100 | 1.91914000 |
| H | -5.19714900 | 2.19482600 | 1.75291800 |
| H | -6.44093700 | 0.93182900 | 1.81860600 |
| C | -3.06595100 | 0.88399900 | -3.14790900 |
| H | -2.37727200 | 1.70054500 | -2.91022500 |
| H | -2.49513800 | -0.04229600 | -3.02766400 |
| H | -3.36449700 | 0.97538900 | -4.19674100 |
| H | -1.93680400 | 1.78803300 | 1.29074800 |

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|---|---|---|---|
| N | -1.22451300 | 0.05111600 | -0.75002700 |
| C | -2.36125000 | 0.42674500 | 0.08865700 |
| C | -2.14009600 | 0.13357700 | 1.58444100 |
| H | -3.01267900 | 0.45473200 | 2.16310500 |
| H | -1.98528000 | -0.93460600 | 1.75599000 |
| H | -1.26567900 | 0.67985600 | 1.95624500 |
| C | -3.58002700 | -0.37456700 | -0.44318300 |
| H | -3.41676200 | -1.44429700 | -0.29930900 |
| H | -4.47587000 | -0.06148400 | 0.10582000 |
| H | -3.73405100 | -0.17885600 | -1.50881300 |
| C | -2.59374600 | 1.93203500 | -0.13652100 |
| H | -2.73850400 | 2.14549200 | -1.20011700 |
| H | -3.48259600 | 2.25983100 | 0.41364400 |
| H | -1.73613500 | 2.51387700 | 0.21894400 |
| C | -0.44494300 | -1.05541100 | -0.46957900 |
| O | -0.95367800 | -2.15617300 | -0.25559500 |

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|---|---|---|---|
| C | 1.04968400 | -0.82320000 | -0.56171800 |
| C | 1.51828100 | 0.23667300 | 0.45677200 |
| H | 1.27935700 | -0.49040800 | -1.58115300 |
| H | 1.53933500 | -1.78633700 | -0.39535300 |
| C | 3.02162300 | 0.58188200 | 0.39965200 |
| H | 0.93981000 | 1.15709900 | 0.29713300 |
| H | 1.27314800 | -0.11653400 | 1.46776400 |
| H | 3.18866700 | 1.32427200 | 1.19416200 |
| C | 3.91187500 | -0.63099900 | 0.70802900 |
| H | 3.84628800 | -1.38814500 | -0.08257500 |
| H | 4.96326100 | -0.33069900 | 0.78613900 |
| H | 3.62526200 | -1.10687400 | 1.65361900 |
| C | 3.42028600 | 1.23664900 | -0.93122600 |
| H | 4.46109100 | 1.57915800 | -0.89825100 |
| H | 3.33585800 | 0.53234100 | -1.76764200 |
| H | 2.78637500 | 2.10285500 | -1.15634700 |

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|---|---|---|---|
| C | 3.52180500 | 0.07017400 | 0.03180500 |
| C | 4.63535700 | -0.89608000 | -0.23535100 |
| H | 5.55702200 | -0.60939600 | 0.28698600 |
| H | 4.37044100 | -1.91649100 | 0.06868100 |
| H | 4.88830200 | -0.94530400 | -1.31179800 |
| C | 3.84258700 | 1.53447500 | 0.04462200 |
| H | 3.81102500 | 1.96973800 | -0.97274800 |
| H | 3.13539200 | 2.11501000 | 0.64994800 |
| H | 4.84965000 | 1.72158900 | 0.43582100 |
| C | 2.12093800 | -0.38768700 | -0.26014700 |
| C | 1.01078800 | 0.38577200 | 0.47068500 |
| H | 2.01054000 | -1.44840500 | -0.00725300 |
| H | 1.92202700 | -0.32521600 | -1.34888600 |
| H | 1.22822700 | 0.39939800 | 1.54733600 |
| H | 0.97560200 | 1.43022100 | 0.13975900 |
| C | -0.34872800 | -0.29336400 | 0.29222600 |
| O | -0.46853500 | -1.51699600 | 0.36940600 |
| N | -1.39183500 | 0.55090900 | 0.06483700 |
| H | -1.18755700 | 1.53924100 | 0.01949500 |
| C | -2.80954400 | 0.15451700 | -0.09918100 |
| C | -2.95577200 | -0.75982700 | -1.32888000 |
| H | -2.61674700 | -0.24218000 | -2.23337500 |
| H | -2.35965400 | -1.66535500 | -1.19968500 |
| H | -4.00589300 | -1.04243900 | -1.46518700 |
| C | -3.60484800 | 1.45091200 | -0.31296600 |
| H | -4.66605600 | 1.22020100 | -0.44794700 |

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|---|---|---|---|
| H | -3.51218300 | 2.11998900 | 0.55147000 |
| H | -3.25884400 | 1.98437200 | -1.20691400 |
| C | -3.30555300 | -0.56167700 | 1.16995100 |
| H | -2.72332400 | -1.46830100 | 1.34637000 |
| H | -3.20768100 | 0.09383600 | 2.04278100 |
| H | -4.36134300 | -0.83420100 | 1.05946000 |

L-MECP

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|---|---|---|---|
| Ru | -0.27339100 | -0.10249900 | -0.39238400 |
| O | -1.80760600 | -0.45513300 | 1.02438500 |
| O | -2.54164800 | 0.84606700 | -0.58303500 |
| P | 0.14715700 | 2.10112300 | 0.39676000 |
| C | 1.90145300 | 2.39320500 | 0.88929600 |
| C | 2.32735500 | 2.25065200 | 2.21702800 |
| C | 2.86335500 | 2.60760700 | -0.11238400 |
| C | 3.68529100 | 2.31390400 | 2.53411200 |
| H | 1.60332000 | 2.08918300 | 3.00825600 |
| C | 4.21925500 | 2.67292000 | 0.20726800 |
| H | 2.55481500 | 2.71753900 | -1.14710600 |
| C | 4.63514800 | 2.52120500 | 1.53180500 |
| H | 3.99927900 | 2.19898900 | 3.56820100 |
| H | 4.95007800 | 2.82968300 | -0.58136100 |
| C | -0.87715200 | 2.57013100 | 1.84707400 |
| C | -1.62689800 | 3.75425700 | 1.88860400 |
| C | -0.98053800 | 1.65506100 | 2.90876300 |
| C | -2.45766500 | 4.02272800 | 2.97845400 |
| H | -1.57666100 | 4.46140800 | 1.06729700 |
| C | -1.80192700 | 1.93354700 | 4.00049100 |
| H | -0.44526000 | 0.71340900 | 2.86335700 |
| C | -2.54596000 | 3.11527400 | 4.03579000 |
| H | -3.03976400 | 4.93980900 | 2.99625100 |
| H | -1.87762100 | 1.21613600 | 4.81283300 |
| C | -0.15895100 | 3.41776900 | -0.85506800 |
| C | 0.46897300 | 4.67172900 | -0.76074900 |
| C | -1.04815400 | 3.17802500 | -1.91408100 |
| C | 0.22433700 | 5.65897700 | -1.71579600 |
| H | 1.15606700 | 4.87541500 | 0.05446700 |
| C | -1.28737300 | 4.16784000 | -2.86932900 |
| H | -1.56973600 | 2.23066700 | -1.96738900 |
| C | -0.64961400 | 5.40643400 | -2.77640000 |
| H | -1.97639800 | 3.96862200 | -3.68558700 |
| H | 0.71731300 | 6.62374800 | -1.63209700 |
| C | -2.77870900 | 0.17677300 | 0.46718100 |
| C | -4.15880400 | 0.05631200 | 1.02162000 |

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|---|---|---|---|
| C | -4.48953100 | -0.99876400 | 1.91285800 |
| C | -5.17436200 | 0.94650200 | 0.58110000 |
| C | -5.82818300 | -1.16700700 | 2.28668800 |
| C | -6.49001700 | 0.73390000 | 0.99802600 |
| C | -6.84503800 | -0.32990400 | 1.82959500 |
| H | -6.08429400 | -1.99019300 | 2.95022700 |
| H | -7.26617100 | 1.41021400 | 0.64686100 |
| C | -8.28981500 | -0.57646000 | 2.18902600 |
| H | -8.81633500 | 0.36015000 | 2.40601300 |
| H | -8.80742100 | -1.05640400 | 1.34982900 |
| H | -8.38545700 | -1.23247300 | 3.06072700 |
| C | -3.48454700 | -1.97295000 | 2.49005300 |
| H | -2.89857000 | -2.47357100 | 1.71653100 |
| H | -2.76213400 | -1.45871900 | 3.13197300 |
| H | -4.00314300 | -2.73089800 | 3.08755800 |
| C | -4.91714900 | 2.13181100 | -0.32411200 |
| H | -4.06333400 | 2.72505900 | 0.01414000 |
| H | -4.68090500 | 1.80680400 | -1.34133700 |
| H | -5.80380300 | 2.77456500 | -0.35685000 |
| C | 1.24703900 | -0.83318300 | 0.57243900 |
| C | 2.53314200 | -0.69055300 | -0.03360300 |
| C | 1.16579300 | -1.41670700 | 1.85828400 |
| C | 2.32049700 | -1.75056400 | 2.54987800 |
| H | 0.18460800 | -1.57724300 | 2.29640600 |
| C | 3.58894600 | -1.52759700 | 1.97046300 |
| H | 2.25728400 | -2.18450500 | 3.54507300 |
| C | 1.06701800 | 0.61607700 | -3.07595200 |
| C | 2.49688800 | -0.20824000 | -1.41456800 |
| C | 2.11588400 | 0.74785200 | -3.97901800 |
| H | 0.05155400 | 0.89104100 | -3.33816200 |
| C | 3.59107300 | -0.11956100 | -2.28433700 |
| C | 3.39890700 | 0.36899800 | -3.57292200 |
| H | 1.92259200 | 1.12920900 | -4.97601200 |
| H | 4.57124300 | -0.44657900 | -1.95549800 |
| H | 4.23839700 | 0.44592700 | -4.25823000 |
| N | 1.24586700 | 0.15526500 | -1.82661900 |
| C | 3.68924300 | -0.96594700 | 0.68821300 |
| H | 4.66308200 | -0.77374800 | 0.25525300 |
| H | 5.69241800 | 2.56607900 | 1.77929400 |
| H | -0.83598700 | 6.17343500 | -3.52333200 |
| H | -3.19921100 | 3.32258000 | 4.87894800 |
| C | -1.70560500 | -2.67595000 | -0.92575900 |
| O | -0.89649600 | -1.78460100 | -1.44325800 |
| O | -1.35881000 | -3.60221000 | -0.19190600 |

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|---|---|---|---|
| C | -3.17139400 | -2.50325800 | -1.27231200 |
| C | -3.60420400 | -1.47268500 | -2.11636100 |
| C | -4.12067900 | -3.31818200 | -0.64380300 |
| C | -4.96312800 | -1.21732500 | -2.27410400 |
| H | -2.86515300 | -0.84059400 | -2.59081800 |
| C | -5.48138300 | -3.06603900 | -0.79283600 |
| H | -3.76973200 | -4.11812900 | -0.00096200 |
| C | -5.90004000 | -1.99830600 | -1.59125100 |
| H | -5.29659400 | -0.38735800 | -2.88907400 |
| H | -6.21420900 | -3.66716200 | -0.26559200 |
| C | -7.36073700 | -1.69348300 | -1.74668400 |
| F | -7.59885500 | -0.36211500 | -1.81417400 |
| F | -7.87488300 | -2.23112700 | -2.88297300 |
| F | -8.10302200 | -2.18318100 | -0.72221300 |
| C | 4.17531700 | -3.99092600 | 0.98230600 |
| C | 2.82934800 | -4.23105900 | 0.39333300 |
| H | 2.07712800 | -4.47308100 | 1.14801400 |
| H | 2.47633100 | -3.35665500 | -0.17030900 |
| H | 2.86584200 | -5.06663700 | -0.32721800 |
| C | 4.50602700 | -4.61203400 | 2.29979000 |
| H | 4.71810300 | -5.68966200 | 2.16872400 |
| H | 5.39392400 | -4.17507200 | 2.76935500 |
| H | 3.66697600 | -4.53837000 | 2.99947000 |
| C | 5.27282400 | -3.63117600 | 0.02213000 |
| C | 6.51139700 | -2.94245000 | 0.62257600 |
| H | 4.86545800 | -2.99330600 | -0.76786400 |
| H | 5.59141500 | -4.55664800 | -0.49266300 |
| H | 6.24917400 | -2.44518200 | 1.56441300 |
| H | 7.29875900 | -3.66324000 | 0.87267300 |
| C | 7.08516700 | -1.83754500 | -0.27737800 |
| O | 6.47329800 | -1.39218800 | -1.25181800 |
| N | 8.28181200 | -1.34489500 | 0.13109300 |
| H | 8.68941900 | -1.75308700 | 0.96202000 |
| C | 8.92658800 | -0.11312500 | -0.38966600 |
| C | 9.27479200 | -0.29091000 | -1.87761900 |
| H | 9.95193200 | -1.14143100 | -2.01292600 |
| H | 8.37000900 | -0.46765200 | -2.46189100 |
| H | 9.77127100 | 0.60996200 | -2.25549200 |
| C | 10.21059100 | 0.08428200 | 0.42960300 |
| H | 10.73880900 | 0.97942600 | 0.08786400 |
| H | 9.98619900 | 0.21320400 | 1.49595000 |
| H | 10.88599300 | -0.77196600 | 0.31524900 |
| C | 7.98391000 | 1.09001500 | -0.19148000 |
| H | 7.05941800 | 0.95129600 | -0.75673900 |

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|---|---|---|---|
| H | 7.72944200 | 1.20791900 | 0.86829900 |
| H | 8.46995300 | 2.01035300 | -0.53375700 |
| H | 4.48129500 | -1.67081100 | 2.57057500 |

L-MECP′

| | | | |
|---|---|---|---|
| Ru | 0.15730595 | 0.28546168 | -1.03289707 |
| O | -1.24938964 | -0.08057717 | 0.49629456 |
| O | -2.09935091 | 1.69030779 | -0.51391610 |
| P | 1.12960576 | 2.15838729 | 0.15618659 |
| C | 2.87202461 | 2.12547468 | 0.72720199 |
| C | 3.28435830 | 2.87753265 | 1.83914944 |
| C | 3.82466584 | 1.40290867 | -0.00509794 |
| C | 4.63046907 | 2.90584860 | 2.20302424 |
| H | 2.55582714 | 3.43230301 | 2.42136587 |
| C | 5.17106690 | 1.43512772 | 0.35921927 |
| H | 3.51810435 | 0.80865716 | -0.85493437 |
| C | 5.57562585 | 2.18831065 | 1.46349539 |
| H | 4.94045343 | 3.48425498 | 3.06876205 |
| H | 5.88939454 | 0.83914454 | -0.19577185 |
| C | 0.16366460 | 2.67789096 | 1.62399013 |
| C | -0.27089240 | 3.99801631 | 1.81002856 |
| C | -0.15358289 | 1.70420624 | 2.58394766 |
| C | -1.02705590 | 4.33324898 | 2.93560117 |
| H | -0.03463267 | 4.76087015 | 1.07559357 |
| C | -0.90615956 | 2.04488218 | 3.70650353 |
| H | 0.15356244 | 0.67743228 | 2.43469131 |
| C | -1.34862708 | 3.35843698 | 3.88230706 |
| H | -1.36774711 | 5.35627594 | 3.06777467 |
| H | -1.16055566 | 1.27928015 | 4.43346431 |
| C | 1.07261547 | 3.57207636 | -1.02206978 |
| C | 2.23997522 | 4.21247027 | -1.46210335 |
| C | -0.16883209 | 3.93671552 | -1.57678050 |
| C | 2.16935343 | 5.20107957 | -2.44712072 |
| H | 3.20451002 | 3.94194964 | -1.04592461 |
| C | -0.23022718 | 4.92883225 | -2.55598318 |
| H | -1.07183098 | 3.43145599 | -1.25012970 |
| C | 0.93741669 | 5.55898760 | -2.99774713 |
| H | -1.19303023 | 5.20459139 | -2.97741546 |
| H | 3.07997772 | 5.68934522 | -2.78280534 |
| C | -2.21241872 | 0.77668125 | 0.33988254 |
| C | -3.45630813 | 0.59327762 | 1.14658580 |
| C | -3.75617747 | -0.65414223 | 1.75970285 |
| C | -4.40357928 | 1.64822999 | 1.20746415 |
| C | -5.01994619 | -0.83580866 | 2.33019874 |

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|---|---|---|---|
| C | -5.64443904 | 1.41131389 | 1.80551310 |
| C | -5.98793930 | 0.16981523 | 2.34328646 |
| H | -5.26215884 | -1.80150558 | 2.76695787 |
| H | -6.37004523 | 2.22099316 | 1.84462754 |
| C | -7.36767037 | -0.08855299 | 2.89595489 |
| H | -7.87469931 | 0.84420080 | 3.16485259 |
| H | -7.98125354 | -0.60099248 | 2.14600433 |
| H | -7.33347858 | -0.73064226 | 3.78328493 |
| C | -2.79265858 | -1.81936851 | 1.84264535 |
| H | -2.43686562 | -2.13199433 | 0.86009403 |
| H | -1.90419833 | -1.55213790 | 2.42362523 |
| H | -3.28077898 | -2.67232361 | 2.32528847 |
| C | -4.14161802 | 3.04025596 | 0.67240875 |
| H | -3.15891732 | 3.41036049 | 0.97622869 |
| H | -4.15378739 | 3.05660072 | -0.42103400 |
| H | -4.90704229 | 3.73118527 | 1.04239155 |
| C | 1.29094181 | -1.22036507 | -0.62376296 |
| C | 2.30107276 | -1.56755609 | -1.59312648 |
| C | 1.01761533 | -2.13879923 | 0.43253801 |
| C | 1.66086186 | -3.35268175 | 0.48843829 |
| H | 0.24276548 | -1.88916899 | 1.14919490 |
| C | 2.61870714 | -3.71533615 | -0.50175690 |
| H | 1.41955648 | -4.06888609 | 1.26763510 |
| C | 1.65503996 | 1.42298026 | -3.54093756 |
| C | 2.49150250 | -0.58421387 | -2.66052042 |
| C | 2.61721501 | 1.43637778 | -4.54391129 |
| H | 0.91135256 | 2.20653099 | -3.45431889 |
| C | 3.48813326 | -0.61807707 | -3.64172494 |
| C | 3.55327423 | 0.40034106 | -4.58698402 |
| H | 2.63236343 | 2.24765515 | -5.26308938 |
| H | 4.21041135 | -1.42627055 | -3.64869760 |
| H | 4.32652652 | 0.38644080 | -5.34856920 |
| N | 1.59906512 | 0.44925282 | -2.61635624 |
| C | 2.91776411 | -2.80274265 | -1.54565153 |
| H | 3.61512003 | -3.10529686 | -2.31779426 |
| H | 6.62123912 | 2.20373304 | 1.75737317 |
| H | 0.88574623 | 6.32467657 | -3.76685560 |
| H | -1.94600183 | 3.61949157 | 4.75152585 |
| C | -1.58312674 | -1.92767552 | -2.08742648 |
| O | -1.10901019 | -0.72733287 | -2.34398981 |
| O | -0.90783885 | -2.95040480 | -1.99942141 |
| C | -3.07486355 | -1.97244255 | -1.84253228 |
| C | -3.85111920 | -0.80955327 | -1.87891425 |
| C | -3.66094445 | -3.18308515 | -1.44260358 |

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|---|---|---|---|
| C | -5.18379855 | -0.83938435 | -1.46947820 |
| H | -3.38494817 | 0.12690679 | -2.15908931 |
| C | -4.98674154 | -3.21715293 | -1.02759649 |
| H | -3.04481045 | -4.07560220 | -1.42260519 |
| C | -5.74127641 | -2.03641213 | -1.02256321 |
| H | -5.76841543 | 0.07282768 | -1.44478367 |
| H | -5.43088842 | -4.14524314 | -0.68058539 |
| C | -7.14796623 | -2.08909058 | -0.50284444 |
| F | -7.70862478 | -0.86394109 | -0.38195604 |
| F | -7.95864807 | -2.82215695 | -1.30544000 |
| F | -7.20459163 | -2.67137439 | 0.72346449 |
| N | 4.61322622 | -3.98314966 | 0.61557525 |
| C | 5.36613993 | -5.08687463 | -0.00550795 |
| C | 6.76583686 | -5.12395999 | 0.67065129 |
| H | 7.28030397 | -6.04858524 | 0.38373218 |
| H | 7.36533564 | -4.26690304 | 0.36072662 |
| H | 6.66248458 | -5.11024253 | 1.76123275 |
| C | 5.54814407 | -4.99794382 | -1.53586646 |
| H | 5.97877029 | -4.03399271 | -1.81192780 |
| H | 6.21695133 | -5.79688600 | -1.87760757 |
| H | 4.59396668 | -5.13209617 | -2.05771353 |
| C | 4.63884456 | -6.39458324 | 0.36528199 |
| H | 3.64414127 | -6.45861618 | -0.09022550 |
| H | 5.21348328 | -7.26080006 | 0.01814369 |
| H | 4.51485270 | -6.46558073 | 1.45084642 |
| C | 5.10815082 | -2.69223631 | 0.56516112 |
| O | 6.06601003 | -2.30760194 | -0.12154035 |
| C | 4.42622595 | -1.72858243 | 1.52764760 |
| C | 4.07998832 | -2.33725599 | 2.89590250 |
| H | 3.51859101 | -1.34322103 | 1.04790707 |
| H | 5.09978799 | -0.87616086 | 1.63298741 |
| C | 3.60880477 | -1.31721586 | 3.95283304 |
| H | 3.30740348 | -3.10017849 | 2.75465386 |
| H | 4.96041361 | -2.86822099 | 3.28312456 |
| H | 3.33794617 | -1.90032067 | 4.84602365 |
| C | 4.72220524 | -0.34129893 | 4.36446947 |
| H | 5.00624576 | 0.31578984 | 3.53471764 |
| H | 4.39226006 | 0.30115811 | 5.19001774 |
| H | 5.62007275 | -0.87884517 | 4.69365388 |
| C | 2.35630281 | -0.55570128 | 3.49731736 |
| H | 1.98091665 | 0.10451125 | 4.28791950 |
| H | 2.57273959 | 0.07207135 | 2.62595810 |
| H | 1.55108545 | -1.24639721 | 3.21937960 |
| H | 2.82738369 | -4.76232162 | -0.65292547 |

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|---|---|---|---|
| Ru | -0.34472200 | 0.04099600 | -0.76681100 |
| O | -1.89696000 | -0.38921100 | 0.65167800 |
| O | -2.65507200 | 1.38637300 | -0.42600700 |
| P | 0.43025800 | 1.87844600 | 0.52076500 |
| C | 2.21639700 | 1.75184300 | 0.97102400 |
| C | 2.63254900 | 1.25846100 | 2.21625800 |
| C | 3.18474200 | 1.99202600 | -0.01878400 |
| C | 3.98377000 | 0.99699400 | 2.45800900 |
| H | 1.90691500 | 1.07777600 | 3.00203800 |
| C | 4.53196400 | 1.72654200 | 0.22344600 |
| H | 2.88493100 | 2.37430600 | -0.98948000 |
| C | 4.93634300 | 1.22027800 | 1.46054200 |
| H | 4.28888900 | 0.61752500 | 3.43006500 |
| H | 5.26274800 | 1.89899800 | -0.55999500 |
| C | -0.48094100 | 2.12855000 | 2.09459300 |
| C | -1.03502800 | 3.36722700 | 2.44748500 |
| C | -0.71314000 | 1.01302300 | 2.91724400 |
| C | -1.80591800 | 3.48802500 | 3.60567900 |
| H | -0.88141600 | 4.23439300 | 1.81382900 |
| C | -1.47324000 | 1.14141900 | 4.07905700 |
| H | -0.33022900 | 0.04045500 | 2.63100700 |
| C | -2.02672700 | 2.37729600 | 4.42247100 |
| H | -2.23929300 | 4.45036300 | 3.86394500 |
| H | -1.65386200 | 0.26957600 | 4.70169800 |
| C | 0.31496000 | 3.48758500 | -0.36479400 |
| C | 1.19334200 | 4.54920900 | -0.09099000 |
| C | -0.69982200 | 3.66606500 | -1.31948700 |
| C | 1.06981000 | 5.76093100 | -0.77239000 |
| H | 1.97859900 | 4.43072800 | 0.64908500 |
| C | -0.81857200 | 4.88074600 | -1.99759800 |
| H | -1.41191200 | 2.86875500 | -1.50008200 |
| C | 0.06670900 | 5.92738600 | -1.73068800 |
| H | -1.60903200 | 5.00818900 | -2.73218900 |
| H | 1.75676000 | 6.57382200 | -0.55303600 |
| C | -2.83915500 | 0.45424000 | 0.40150600 |
| C | -4.16814700 | 0.25308800 | 1.06493400 |
| C | -4.50346700 | -0.99047500 | 1.66479400 |
| C | -5.14446400 | 1.28189700 | 1.00048600 |
| C | -5.81805400 | -1.19332300 | 2.10153500 |
| C | -6.43587600 | 1.02509900 | 1.46761100 |
| C | -6.80512500 | -0.21409100 | 1.99305400 |
| H | -6.07966300 | -2.15701400 | 2.53361900 |

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|---|---|---|---|
| H | -7.18220800 | 1.81449400 | 1.40372500 |
| C | -8.23305500 | -0.49535600 | 2.39231000 |
| H | -8.73434700 | 0.40636100 | 2.76141900 |
| H | -8.79949500 | -0.85796200 | 1.52647600 |
| H | -8.29122900 | -1.26447600 | 3.17038000 |
| C | -3.52807600 | -2.12917000 | 1.88094700 |
| H | -3.05384100 | -2.45918400 | 0.95543200 |
| H | -2.71470900 | -1.82510300 | 2.54780600 |
| H | -4.04824900 | -2.98099500 | 2.33303300 |
| C | -4.86944500 | 2.66656400 | 0.45200400 |
| H | -3.93733300 | 3.08126700 | 0.84463300 |
| H | -4.75904400 | 2.64780100 | -0.63615300 |
| H | -5.69433400 | 3.34018500 | 0.71070800 |
| C | 0.94349000 | -1.12765400 | -0.06923000 |
| C | 2.27394000 | -1.12693300 | -0.68221400 |
| C | 0.74695400 | -2.00001900 | 1.07168800 |
| C | 1.79529600 | -2.59097700 | 1.68583700 |
| H | -0.26678800 | -2.12594000 | 1.43941400 |
| C | 3.21954700 | -2.41148000 | 1.24281700 |
| H | 1.62197800 | -3.19755600 | 2.57064600 |
| C | 1.14944500 | 1.11047900 | -3.29642800 |
| C | 2.36189400 | -0.33798300 | -1.91984400 |
| C | 2.23585100 | 1.27737200 | -4.14881800 |
| H | 0.20579700 | 1.61798900 | -3.46402000 |
| C | 3.49059900 | -0.21360400 | -2.73495400 |
| C | 3.42671000 | 0.60531900 | -3.85872700 |
| H | 2.14536900 | 1.92246700 | -5.01608900 |
| H | 4.40629100 | -0.73538100 | -2.47596500 |
| H | 4.29503600 | 0.71911700 | -4.50082000 |
| N | 1.20894900 | 0.32844400 | -2.20531800 |
| C | 3.33191200 | -1.69772200 | -0.06711300 |
| H | 4.32515000 | -1.56950800 | -0.48089100 |
| H | 5.98519100 | 1.00033000 | 1.64073300 |
| H | -0.02709100 | 6.87069400 | -2.26198600 |
| H | -2.63657300 | 2.47120700 | 5.31676100 |
| C | -2.12345000 | -2.14114400 | -1.72188400 |
| O | -1.44586000 | -1.10358000 | -2.14159500 |
| O | -1.63795800 | -3.16838600 | -1.24238700 |
| C | -3.62951200 | -1.99660200 | -1.81014000 |
| C | -4.21932600 | -0.77803700 | -2.16644200 |
| C | -4.44298900 | -3.05699000 | -1.39033600 |
| C | -5.59584000 | -0.60138000 | -2.04554300 |
| H | -3.58193000 | 0.04703900 | -2.45618700 |
| C | -5.81887500 | -2.88933200 | -1.27320800 |

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|---|---|---|---|
| H | -3.96850200 | -3.99168400 | -1.11203600 |
| C | -6.39165300 | -1.65083000 | -1.58109000 |
| H | -6.04576100 | 0.36123600 | -2.26523500 |
| H | -6.44387200 | -3.69851800 | -0.91016300 |
| C | -7.87006000 | -1.44885700 | -1.42734400 |
| F | -8.17961700 | -0.17912600 | -1.07222600 |
| F | -8.54581900 | -1.70138300 | -2.57783600 |
| F | -8.40266200 | -2.26616500 | -0.48324600 |
| C | 4.08903100 | -3.72804000 | 1.31890800 |
| C | 3.39044500 | -4.84626800 | 0.52349900 |
| H | 2.42159900 | -5.10394300 | 0.96394600 |
| H | 3.21303100 | -4.53678100 | -0.51286500 |
| H | 4.00715300 | -5.75268600 | 0.50883600 |
| C | 4.25419300 | -4.15356700 | 2.79019500 |
| H | 4.86062700 | -5.06470400 | 2.85204000 |
| H | 4.75538700 | -3.37582800 | 3.37982600 |
| H | 3.29419700 | -4.37056800 | 3.26958300 |
| C | 5.49439200 | -3.50611300 | 0.69398300 |
| C | 6.31432800 | -2.31477200 | 1.23776500 |
| H | 5.39043900 | -3.38755800 | -0.38794700 |
| H | 6.06678400 | -4.42998200 | 0.84044100 |
| H | 5.66939900 | -1.60182100 | 1.76658500 |
| H | 7.05617400 | -2.64590700 | 1.97292700 |
| C | 6.98012300 | -1.48892600 | 0.12942500 |
| O | 6.45168100 | -1.33926000 | -0.97770500 |
| N | 8.14273500 | -0.88432500 | 0.48159900 |
| H | 8.53117500 | -1.12055400 | 1.38449100 |
| C | 8.96805100 | -0.00996200 | -0.38843100 |
| C | 9.44960800 | -0.80153100 | -1.61781300 |
| H | 10.03809000 | -1.67213000 | -1.30748700 |
| H | 8.59649600 | -1.14745800 | -2.20555100 |
| H | 10.08019400 | -0.16658500 | -2.25021800 |
| C | 10.17004000 | 0.43502300 | 0.45774000 |
| H | 10.81879300 | 1.09010800 | -0.13144400 |
| H | 9.84449400 | 0.98983200 | 1.34601400 |
| H | 10.76705800 | -0.42646600 | 0.78170200 |
| C | 8.15103700 | 1.21951100 | -0.82365000 |
| H | 7.27875000 | 0.90978200 | -1.40224300 |
| H | 7.81316400 | 1.78719200 | 0.05078000 |
| H | 8.76979000 | 1.87867800 | -1.44238500 |
| H | 3.66751600 | -1.71752000 | 1.97957100 |

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|---|---|---|---|
| Ru | 0.17554500 | 0.74328700 | -0.99536300 |

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|---|---|---|---|
| O | -1.23804900 | 0.29808200 | 0.54708300 |
| O | -2.29466300 | 1.76307900 | -0.72678200 |
| P | 0.85855900 | 2.66490900 | 0.18859200 |
| C | 2.59004800 | 2.81782500 | 0.78586600 |
| C | 2.90633900 | 3.54157300 | 1.94559100 |
| C | 3.62863800 | 2.26282600 | 0.02311700 |
| C | 4.23736600 | 3.69877100 | 2.33669800 |
| H | 2.11410900 | 3.97702600 | 2.54585300 |
| C | 4.95782200 | 2.42570300 | 0.41296900 |
| H | 3.39990000 | 1.70699400 | -0.87708700 |
| C | 5.26491900 | 3.14256100 | 1.57218400 |
| H | 4.46969700 | 4.25518200 | 3.24043900 |
| H | 5.75186100 | 1.98676200 | -0.18474700 |
| C | -0.16563600 | 2.93969600 | 1.68534300 |
| C | -1.16081700 | 3.92097600 | 1.75701600 |
| C | -0.03073000 | 2.01794500 | 2.73636500 |
| C | -2.01254700 | 3.97639000 | 2.86375400 |
| H | -1.28653200 | 4.63271700 | 0.94817600 |
| C | -0.87371700 | 2.08195500 | 3.84301500 |
| H | 0.72858000 | 1.24348500 | 2.68050000 |
| C | -1.87403400 | 3.05742600 | 3.90450400 |
| H | -2.78848100 | 4.73563800 | 2.90545800 |
| H | -0.76307200 | 1.36110700 | 4.64831400 |
| C | 0.63520200 | 4.14083800 | -0.89212300 |
| C | 1.65924300 | 5.07678000 | -1.09864900 |
| C | -0.57438200 | 4.27292900 | -1.60147700 |
| C | 1.47915500 | 6.12863900 | -2.00027300 |
| H | 2.59820100 | 4.98760800 | -0.56261500 |
| C | -0.74845500 | 5.33143100 | -2.49421800 |
| H | -1.36937200 | 3.54884300 | -1.44785400 |
| C | 0.27793500 | 6.25814400 | -2.69984900 |
| H | -1.68719300 | 5.42725600 | -3.03302000 |
| H | 2.28033700 | 6.84664000 | -2.15351300 |
| C | -2.30949000 | 0.93842300 | 0.22648500 |
| C | -3.57167300 | 0.61837200 | 0.96893100 |
| C | -3.68454100 | -0.57601200 | 1.72959000 |
| C | -4.70495900 | 1.46121800 | 0.82280000 |
| C | -4.93632600 | -0.92923900 | 2.24732200 |
| C | -5.92310000 | 1.06704700 | 1.38201300 |
| C | -6.07109100 | -0.13787900 | 2.07280000 |
| H | -5.02770100 | -1.86199000 | 2.79879800 |
| H | -6.78761500 | 1.71802200 | 1.26524600 |
| C | -7.41970500 | -0.57314700 | 2.59184200 |
| H | -7.99013300 | 0.27496600 | 2.98752500 |

| | | | |
|---|---|---|---|
| H | -8.00994700 | -1.02233500 | 1.78531700 |
| H | -7.32325200 | -1.32252400 | 3.38441300 |
| C | -2.53092500 | -1.50875700 | 2.03413500 |
| H | -2.03300200 | -1.86151200 | 1.13021200 |
| H | -1.76481600 | -0.99902900 | 2.62693700 |
| H | -2.89307300 | -2.37500000 | 2.59861300 |
| C | -4.67099700 | 2.79041800 | 0.09809300 |
| H | -3.81323900 | 3.39400500 | 0.40628200 |
| H | -4.57559300 | 2.65378700 | -0.98267900 |
| H | -5.59004700 | 3.35107400 | 0.30284200 |
| C | 1.45213900 | -0.49651400 | -0.42302100 |
| C | 2.44666300 | -0.91056200 | -1.42565000 |
| C | 1.36315300 | -1.25242400 | 0.80686600 |
| C | 1.94693500 | -2.46258700 | 0.90865300 |
| H | 0.73338000 | -0.86656700 | 1.60097300 |
| C | 2.66827900 | -3.08171400 | -0.25085200 |
| H | 1.82694200 | -3.08596800 | 1.79027800 |
| C | 1.58235500 | 1.89918400 | -3.54480200 |
| C | 2.56581900 | 0.01918700 | -2.56183600 |
| C | 2.54592300 | 1.93047200 | -4.54823300 |
| H | 0.78385300 | 2.63172700 | -3.49493200 |
| C | 3.56340100 | 0.00023800 | -3.53788000 |
| C | 3.55370200 | 0.96403800 | -4.54362600 |
| H | 2.50258000 | 2.70030300 | -5.31091500 |
| H | 4.34063700 | -0.75572700 | -3.50119200 |
| H | 4.32306900 | 0.96300100 | -5.30963500 |
| N | 1.58920500 | 0.97128500 | -2.57318200 |
| C | 3.05016700 | -2.11514200 | -1.33147600 |
| H | 3.71612800 | -2.49737000 | -2.10124300 |
| H | 6.29936300 | 3.26048500 | 1.88132300 |
| H | 0.14147500 | 7.07680400 | -3.40127100 |
| H | -2.54488400 | 3.09591100 | 4.75807500 |
| C | -1.17116000 | -1.85226100 | -1.73177400 |
| O | -0.87044800 | -0.67819500 | -2.20780300 |
| O | -0.36383900 | -2.71766900 | -1.36540800 |
| C | -2.65655200 | -2.11390400 | -1.58803700 |
| C | -3.58991700 | -1.11146000 | -1.87281200 |
| C | -3.09430400 | -3.32623900 | -1.03555700 |
| C | -4.93770900 | -1.29383800 | -1.56515000 |
| H | -3.23799100 | -0.16541200 | -2.26533700 |
| C | -4.43581700 | -3.51348100 | -0.72423400 |
| H | -2.35684400 | -4.09076000 | -0.81581200 |
| C | -5.35415700 | -2.48506000 | -0.97224100 |
| H | -5.65014000 | -0.49423500 | -1.73291700 |

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|---|---|---|---|
| H | -4.77095100 | -4.43663200 | -0.26070700 |
| C | -6.78475000 | -2.68943700 | -0.57054900 |
| F | -7.51522700 | -1.55158900 | -0.63387300 |
| F | -7.40921500 | -3.60353600 | -1.35551700 |
| F | -6.88448700 | -3.15414900 | 0.70200700 |
| N | 3.72711000 | -4.03328500 | 0.11083500 |
| C | 3.61355100 | -5.49796400 | -0.26908900 |
| C | 3.79407900 | -6.36350600 | 0.99504700 |
| H | 3.69316700 | -7.42219300 | 0.73121400 |
| H | 4.77289800 | -6.20829200 | 1.44652400 |
| H | 3.01928300 | -6.12026400 | 1.73138800 |
| C | 4.67096000 | -5.83823200 | -1.33830500 |
| H | 5.67871400 | -5.67374000 | -0.95761500 |
| H | 4.57296100 | -6.88824900 | -1.63681400 |
| H | 4.52058200 | -5.21800600 | -2.23030500 |
| C | 2.22531900 | -5.81995800 | -0.85175500 |
| H | 2.03249600 | -5.31655300 | -1.80548300 |
| H | 2.18747600 | -6.89621000 | -1.04707100 |
| H | 1.41091800 | -5.58723700 | -0.15674100 |
| C | 4.89024000 | -3.57402900 | 0.70263200 |
| O | 5.86499600 | -4.30012300 | 0.90122900 |
| C | 4.96769200 | -2.13398500 | 1.21304400 |
| C | 4.86626300 | -2.15001400 | 2.75524200 |
| H | 4.22828300 | -1.45868900 | 0.78392600 |
| H | 5.95660300 | -1.77144600 | 0.91726300 |
| C | 4.93152300 | -0.76786500 | 3.43736400 |
| H | 3.92770000 | -2.64058100 | 3.04677100 |
| H | 5.67926000 | -2.78292900 | 3.13054000 |
| H | 4.95438100 | -0.96917200 | 4.51897400 |
| C | 6.21841000 | -0.00762800 | 3.08523700 |
| H | 6.22799600 | 0.29233000 | 2.03134800 |
| H | 6.30376400 | 0.90852900 | 3.68109300 |
| H | 7.10731900 | -0.62232500 | 3.27271200 |
| C | 3.68559000 | 0.08683500 | 3.15813900 |
| H | 3.72764900 | 1.03180500 | 3.71060300 |
| H | 3.59683300 | 0.33973400 | 2.09724500 |
| H | 2.76999400 | -0.44060300 | 3.45182000 |
| H | 1.85730600 | -3.64239100 | -0.73915400 |

M

| | | | |
|---|---|---|---|
| Ru | -0.22154500 | -0.06391900 | -0.27016100 |
| O | 1.74145700 | 0.16219500 | 0.64382800 |
| O | 1.53296100 | -0.54250900 | -1.40702200 |
| C | 2.30048700 | -0.28314000 | -0.41481200 |

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|---|---|---|---|
| C | 3.77248900 | -0.51770500 | -0.47492600 |
| C | 4.64757000 | 0.40514600 | 0.14710200 |
| C | 4.29310100 | -1.66148000 | -1.12773000 |
| C | 6.02363900 | 0.16790000 | 0.09992900 |
| C | 5.67805400 | -1.85734500 | -1.13221900 |
| C | 6.56103300 | -0.95706300 | -0.53112800 |
| H | 6.69495100 | 0.88455400 | 0.56892400 |
| H | 6.07774000 | -2.74349300 | -1.62082200 |
| C | 8.05438400 | -1.17454500 | -0.59006000 |
| H | 8.30289600 | -2.23821300 | -0.67033600 |
| H | 8.48960000 | -0.67077600 | -1.46365900 |
| H | 8.55366600 | -0.77238800 | 0.29825600 |
| C | 4.14581600 | 1.65485800 | 0.83166500 |
| H | 3.43969000 | 2.19998900 | 0.19995800 |
| H | 3.59953600 | 1.42433900 | 1.74977400 |
| H | 4.97859400 | 2.32301000 | 1.07468800 |
| C | 3.41789200 | -2.71235700 | -1.77716900 |
| H | 2.80340800 | -3.23224300 | -1.03282300 |
| H | 2.73895900 | -2.27281700 | -2.51032400 |
| H | 4.03737700 | -3.46575900 | -2.27403900 |
| C | -0.20494000 | 2.44832800 | 1.96514700 |
| C | 0.48592000 | 3.09646200 | 0.92968900 |
| C | 0.23630800 | 2.56655600 | 3.28302700 |
| C | 1.36319300 | 3.33356100 | 3.59014900 |
| H | -0.30982300 | 2.06014700 | 4.07457600 |
| C | 2.04367100 | 3.99836400 | 2.56813900 |
| H | 1.70486200 | 3.41723300 | 4.61844400 |
| C | -0.70619100 | 1.87166300 | -2.36742200 |
| C | 0.03211200 | 3.03571700 | -0.48426900 |
| C | -0.80324100 | 3.02803000 | -3.12632500 |
| H | -0.96631100 | 0.90716200 | -2.78300900 |
| C | -0.05396300 | 4.23694700 | -1.20864800 |
| C | -0.46693500 | 4.24544900 | -2.53433100 |
| H | -1.13909100 | 2.96461500 | -4.15588100 |
| H | 0.18746300 | 5.16398700 | -0.70086200 |
| H | -0.53597800 | 5.17775000 | -3.08673900 |
| N | -0.29533600 | 1.85032200 | -1.07491800 |
| C | 1.60253900 | 3.88570200 | 1.25003500 |
| H | 2.14943100 | 4.38815700 | 0.45690000 |
| H | 2.92211800 | 4.59717600 | 2.79262300 |
| H | -1.08714800 | 1.86318400 | 1.74077900 |
| O | -2.07326900 | 0.20670400 | 0.85089600 |
| O | -2.10443600 | -0.51674500 | -1.20832100 |
| C | -2.74580100 | -0.22900800 | -0.14027000 |

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|---|---|---|---|
| C | -4.21683800 | -0.42506300 | -0.04993500 |
| C | -4.75396400 | -1.10795900 | 1.06177800 |
| C | -5.05487400 | 0.06127100 | -1.07510600 |
| C | -6.13746600 | -1.29822900 | 1.12259000 |
| C | -6.43388600 | -0.13358200 | -0.95733300 |
| C | -6.99403900 | -0.81618600 | 0.12755100 |
| H | -6.55813500 | -1.83453100 | 1.97096500 |
| H | -7.08850500 | 0.25553200 | -1.73467100 |
| C | -8.48384700 | -1.05404400 | 0.20677800 |
| H | -9.04474000 | -0.25590800 | -0.29134400 |
| H | -8.75742900 | -1.99860400 | -0.28248000 |
| H | -8.82605100 | -1.11511900 | 1.24549800 |
| C | -3.87296700 | -1.64821100 | 2.16794900 |
| H | -2.99451800 | -2.16715900 | 1.76861500 |
| H | -3.48920900 | -0.83770200 | 2.79559900 |
| H | -4.43194400 | -2.34485800 | 2.80087100 |
| C | -4.50079000 | 0.79527800 | -2.27683600 |
| H | -3.79065700 | 1.57723300 | -1.98531300 |
| H | -3.95364900 | 0.11206000 | -2.93396800 |
| H | -5.30777800 | 1.26079500 | -2.85138400 |
| C | -0.22806300 | -3.18070900 | -0.46121700 |
| C | 0.30207800 | -2.40814700 | 1.79606700 |
| C | 0.25420700 | -4.46861100 | 0.18664200 |
| H | -1.23596700 | -3.28444200 | -0.87366200 |
| C | 1.62595100 | -3.14039000 | 1.64081700 |
| H | 0.45719600 | -1.45029200 | 2.29288700 |
| H | 0.37576800 | -5.23615600 | -0.58341000 |
| H | 1.98146800 | -3.46052100 | 2.62919000 |
| O | -0.27431100 | -2.10348800 | 0.51093900 |
| O | 1.53025000 | -4.29540100 | 0.79076800 |
| H | -0.48343600 | -4.84045400 | 0.91435900 |
| H | 2.36946000 | -2.45998100 | 1.21307900 |
| H | -0.42266100 | -2.99398200 | 2.37396100 |
| H | 0.45714000 | -2.87214400 | -1.25432300 |

N-TS

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|---|---|---|---|
| Ru | 0.07043900 | 0.03942800 | 0.29981900 |
| O | 2.18420700 | 0.10715100 | 0.69966200 |
| O | 1.51865900 | -0.73146200 | -1.22111100 |
| C | 2.46992100 | -0.36215500 | -0.45592800 |
| C | 3.89158000 | -0.43995400 | -0.89785900 |
| C | 4.71202900 | 0.70220100 | -0.78251000 |
| C | 4.39529800 | -1.63821500 | -1.44511200 |
| C | 6.03737700 | 0.61783500 | -1.22062500 |

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|---|---|---|---|
| C | 5.73183400 | -1.67921700 | -1.85039300 |
| C | 6.56925800 | -0.56330900 | -1.74680200 |
| H | 6.67146000 | 1.49918200 | -1.14883700 |
| H | 6.12919600 | -2.60493800 | -2.26214600 |
| C | 8.01719100 | -0.64300000 | -2.17042200 |
| H | 8.14757500 | -1.31050500 | -3.02938600 |
| H | 8.41191100 | 0.34223800 | -2.44040900 |
| H | 8.64330800 | -1.03451100 | -1.35740900 |
| C | 4.18530900 | 2.01147800 | -0.23407100 |
| H | 3.26472500 | 2.31975500 | -0.74365000 |
| H | 3.93518700 | 1.92384100 | 0.82681100 |
| H | 4.92624700 | 2.80748700 | -0.35812600 |
| C | 3.53015300 | -2.87128000 | -1.58868400 |
| H | 3.04591100 | -3.13563000 | -0.64070800 |
| H | 2.72653300 | -2.70610200 | -2.31212100 |
| H | 4.12664200 | -3.72948900 | -1.91317900 |
| C | -0.35450300 | 1.05262200 | 2.08093300 |
| C | 0.03823600 | 2.42209900 | 1.97195100 |
| C | -0.51217200 | 0.52152000 | 3.37741300 |
| C | -0.24776600 | 1.28647000 | 4.51226000 |
| H | -0.86197900 | -0.50315100 | 3.48338800 |
| C | 0.16221300 | 2.62040000 | 4.38433400 |
| H | -0.36433700 | 0.85017400 | 5.50170400 |
| C | 0.30810500 | 2.29624000 | -1.65807300 |
| C | 0.19964400 | 2.92934100 | 0.60716300 |
| C | 0.45835200 | 3.61355800 | -2.07113800 |
| H | 0.29984400 | 1.46642600 | -2.35569600 |
| C | 0.35266500 | 4.27338300 | 0.24018000 |
| C | 0.48479800 | 4.61974900 | -1.09972400 |
| H | 0.55563300 | 3.83982800 | -3.12739400 |
| H | 0.35503400 | 5.03967200 | 1.00714400 |
| H | 0.60170600 | 5.66071200 | -1.38586600 |
| N | 0.18472700 | 1.96013400 | -0.35927700 |
| C | 0.29852800 | 3.18605600 | 3.11796600 |
| H | 0.63482500 | 4.21602400 | 3.02996300 |
| H | 0.37016900 | 3.21599500 | 5.26881500 |
| O | -2.80714100 | 0.71661100 | 1.03234000 |
| O | -1.76431000 | -0.30797200 | -0.64858500 |
| C | -2.82622000 | 0.12230900 | -0.09528400 |
| C | -4.12578200 | -0.07876600 | -0.79859000 |
| C | -5.24537500 | -0.55152600 | -0.07946500 |
| C | -4.22018300 | 0.20141600 | -2.17976300 |
| C | -6.44580600 | -0.74808300 | -0.76789400 |
| C | -5.45108100 | 0.01213800 | -2.81519300 |

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|---|---|---|---|
| C | -6.57326400 | -0.46404700 | -2.13101900 |
| H | -7.30631000 | -1.13098100 | -0.22304100 |
| H | -5.53416500 | 0.23945200 | -3.87606900 |
| C | -7.89675600 | -0.63871400 | -2.83784400 |
| H | -8.49986300 | 0.27678000 | -2.77185900 |
| H | -7.75841400 | -0.86143500 | -3.90130900 |
| H | -8.48540900 | -1.44795800 | -2.39240500 |
| C | -5.17861800 | -0.87129700 | 1.39802500 |
| H | -4.30683800 | -1.48798500 | 1.64275000 |
| H | -5.08706500 | 0.04209400 | 1.99350200 |
| H | -6.07795000 | -1.40789100 | 1.71601200 |
| C | -3.04552500 | 0.71099900 | -2.98730500 |
| H | -2.51608400 | 1.52068900 | -2.47383200 |
| H | -2.30889100 | -0.08123400 | -3.15381500 |
| H | -3.38262100 | 1.08338900 | -3.95990400 |
| H | -1.53033900 | 0.72636300 | 1.35325600 |
| C | 0.98973400 | -2.41882400 | 2.03406600 |
| C | -0.36755000 | -3.02702900 | 0.14625700 |
| C | 0.43501700 | -3.57174400 | 2.87812000 |
| H | 1.89052900 | -2.69875700 | 1.47506200 |
| C | -0.09202500 | -4.41655500 | 0.73561500 |
| H | -1.42651800 | -2.87791600 | -0.06834000 |
| H | -0.18345200 | -3.18054700 | 3.69229800 |
| H | 0.95484500 | -4.71803100 | 0.57105200 |
| O | -0.03615400 | -2.00100400 | 1.11918200 |
| O | -0.41442500 | -4.43375900 | 2.11676600 |
| H | 1.27143400 | -4.13923700 | 3.31679400 |
| H | 1.23351700 | -1.55212600 | 2.64813300 |
| H | 0.21603800 | -2.85137400 | -0.76466900 |
| H | -0.72884500 | -5.15915900 | 0.24684900 |

O

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|---|---|---|---|
| Ru | 0.08825200 | 0.03792600 | 0.41253600 |
| O | 2.18943400 | 0.24465400 | 0.56862200 |
| O | 1.69786500 | -0.94032700 | -1.24167300 |
| C | 2.54680400 | -0.35736300 | -0.51354700 |
| C | 4.00067600 | -0.33044100 | -0.87583000 |
| C | 4.69602000 | 0.89726900 | -0.89010100 |
| C | 4.65998900 | -1.53144600 | -1.20985800 |
| C | 6.04834400 | 0.89610600 | -1.24806700 |
| C | 6.01757400 | -1.48564700 | -1.53970400 |
| C | 6.72828300 | -0.28157200 | -1.57227200 |
| H | 6.58681300 | 1.84175800 | -1.26936900 |
| H | 6.53344000 | -2.41354200 | -1.77981100 |

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|---|---|---|---|
| C | 8.18412300 | -0.25198500 | -1.97595500 |
| H | 8.70378100 | -1.16734100 | -1.67174800 |
| H | 8.28959600 | -0.16609200 | -3.06595600 |
| H | 8.70725300 | 0.60102100 | -1.53032900 |
| C | 4.01770900 | 2.20638500 | -0.54678000 |
| H | 3.09268800 | 2.34489900 | -1.11766300 |
| H | 3.73337900 | 2.23722600 | 0.50859900 |
| H | 4.68014500 | 3.05161600 | -0.75993800 |
| C | 3.93742800 | -2.86072200 | -1.19781500 |
| H | 3.42830700 | -3.03091400 | -0.24119000 |
| H | 3.16352800 | -2.89254700 | -1.96990600 |
| H | 4.63692500 | -3.68673900 | -1.36057000 |
| C | -0.39353400 | 1.16518400 | 1.98030100 |
| C | -0.33440400 | 2.57882300 | 1.74052100 |
| C | -0.73451700 | 0.75876400 | 3.29172600 |
| C | -0.95341900 | 1.68619400 | 4.31107800 |
| H | -0.83449900 | -0.30321600 | 3.50547100 |
| C | -0.85347700 | 3.06232700 | 4.05871200 |
| H | -1.20701900 | 1.33977100 | 5.31097700 |
| C | 0.31783200 | 2.06544600 | -1.79821600 |
| C | -0.06548700 | 2.94803400 | 0.35067300 |
| C | 0.41647100 | 3.33333600 | -2.35706400 |
| H | 0.45513400 | 1.16287900 | -2.38403700 |
| C | 0.03518400 | 4.24705800 | -0.16484600 |
| C | 0.27526400 | 4.44507200 | -1.52010500 |
| H | 0.61117500 | 3.44105300 | -3.41870600 |
| H | -0.07302600 | 5.09635400 | 0.50069100 |
| H | 0.35553000 | 5.45170700 | -1.91967000 |
| N | 0.07979700 | 1.86995300 | -0.48555600 |
| C | -0.55297700 | 3.50458500 | 2.77327500 |
| H | -0.49342700 | 4.57292700 | 2.57882600 |
| H | -1.02327900 | 3.78014600 | 4.85629400 |
| O | -3.15019900 | 1.00469600 | 0.91096300 |
| O | -1.89828000 | -0.48929400 | -0.20803900 |
| C | -2.99390000 | 0.06245800 | -0.00780600 |
| C | -4.18982300 | -0.27493800 | -0.80954300 |
| C | -5.46292400 | -0.38383700 | -0.20142500 |
| C | -4.02826600 | -0.49129300 | -2.20059100 |
| C | -6.55472600 | -0.72023200 | -1.00552200 |
| C | -5.15967400 | -0.80280700 | -2.95767500 |
| C | -6.42753700 | -0.93033200 | -2.38173100 |
| H | -7.53411900 | -0.82028000 | -0.54317300 |
| H | -5.04802000 | -0.94952800 | -4.02961300 |
| C | -7.62247100 | -1.31390400 | -3.22082300 |

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|---|---|---|---|
| H | -7.53486200 | -0.92920800 | -4.24245100 |
| H | -7.71411600 | -2.40600600 | -3.29078600 |
| H | -8.55479000 | -0.93497300 | -2.78942000 |
| C | -5.68701600 | -0.17956400 | 1.28156300 |
| H | -4.93007300 | -0.68996500 | 1.88556900 |
| H | -5.63688000 | 0.88093600 | 1.54819000 |
| H | -6.67028100 | -0.56078300 | 1.57273100 |
| C | -2.69216300 | -0.36638900 | -2.90154900 |
| H | -2.14823200 | 0.53246000 | -2.59340100 |
| H | -2.03911600 | -1.21361100 | -2.66998600 |
| H | -2.83522600 | -0.32686300 | -3.98561400 |
| H | -2.28735700 | 1.11134300 | 1.39107100 |
| C | -0.06044500 | -3.06713100 | 0.61282000 |
| C | 1.28892900 | -2.14276500 | 2.39094500 |
| C | -0.38872800 | -4.29694800 | 1.46165100 |
| H | -0.91053600 | -2.79664400 | -0.01558200 |
| C | 1.62402600 | -3.62848600 | 2.51695000 |
| H | 2.14672600 | -1.56560500 | 2.03438000 |
| H | -0.28762200 | -5.20066200 | 0.83990300 |
| H | 2.19882100 | -3.79447400 | 3.43269000 |
| O | 0.17035000 | -1.94132700 | 1.48033500 |
| O | 0.43745700 | -4.39793700 | 2.62542500 |
| H | 2.24428100 | -3.97002200 | 1.67329300 |
| H | -1.42187400 | -4.23959600 | 1.82108800 |
| H | 0.80982400 | -3.20991800 | -0.03733900 |
| H | 0.95730200 | -1.73513000 | 3.34839500 |

P

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|---|---|---|---|
| Ru | -0.75435700 | 0.41931500 | -0.59665300 |
| O | 1.18431900 | 0.99186900 | 0.11664100 |
| O | 1.34574600 | -0.66239800 | -1.34821500 |
| C | 1.89390200 | 0.16831400 | -0.57212500 |
| C | 3.38661100 | 0.23249900 | -0.42773000 |
| C | 4.04698200 | 1.47054100 | -0.57210500 |
| C | 4.12212600 | -0.93996700 | -0.15601300 |
| C | 5.44026600 | 1.50785800 | -0.45270300 |
| C | 5.51079100 | -0.85100600 | -0.02487800 |
| C | 6.19085700 | 0.36142000 | -0.17796800 |
| H | 5.95261100 | 2.46015200 | -0.57559800 |
| H | 6.07721700 | -1.75264700 | 0.20055000 |
| C | 7.69726800 | 0.42308800 | -0.07857500 |
| H | 8.08278700 | -0.31271300 | 0.63586700 |
| H | 8.16527100 | 0.20911500 | -1.04894900 |
| H | 8.03893700 | 1.41516900 | 0.23576300 |

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|---|---|---|---|
| C | 3.29200700 | 2.74916100 | -0.86387200 |
| H | 2.60008500 | 2.62620700 | -1.70512900 |
| H | 2.68469200 | 3.05126800 | -0.00565400 |
| H | 3.98441900 | 3.56071200 | -1.10918000 |
| C | 3.44026700 | -2.27700900 | 0.03393200 |
| H | 2.74069500 | -2.24477800 | 0.87993000 |
| H | 2.85859200 | -2.55147300 | -0.84976500 |
| H | 4.17175100 | -3.06453600 | 0.23992000 |
| C | -2.01370000 | 1.53110900 | 0.47416100 |
| C | -3.40271000 | 1.28793900 | 0.27835800 |
| C | -1.65073100 | 2.50116000 | 1.42728900 |
| C | -2.61983700 | 3.19843300 | 2.15219600 |
| H | -0.59535300 | 2.70070100 | 1.60454500 |
| C | -3.98364700 | 2.94265500 | 1.94889100 |
| H | -2.31638900 | 3.94446100 | 2.88413500 |
| H | -4.73373300 | 3.48602000 | 2.51712100 |
| C | -2.74441400 | -1.12951300 | -2.34845700 |
| C | -3.70660000 | 0.28649600 | -0.74417900 |
| C | -3.98532900 | -1.59280800 | -2.76848500 |
| H | -1.82318800 | -1.48302700 | -2.80284800 |
| C | -4.98348500 | -0.15104900 | -1.12375200 |
| C | -5.12767400 | -1.09417600 | -2.13507100 |
| H | -4.04892400 | -2.32382600 | -3.56731500 |
| H | -5.85736600 | 0.25022000 | -0.62263100 |
| H | -6.11635000 | -1.43496500 | -2.42843500 |
| N | -2.59496100 | -0.22428000 | -1.36246500 |
| C | -4.37387900 | 1.98908900 | 1.01182400 |
| H | -5.43343400 | 1.79881600 | 0.85618400 |
| C | -0.35938600 | -0.84133300 | 2.14167900 |
| C | -0.57926300 | -2.47224800 | 0.34810300 |
| C | -0.02762500 | -2.14050600 | 2.87320100 |
| H | 0.51953800 | -0.19956800 | 2.03882200 |
| C | -1.22271000 | -3.46876000 | 1.31198800 |
| H | -1.01948000 | -2.56124300 | -0.64476100 |
| H | 0.03050500 | -1.94142100 | 3.94714000 |
| H | -0.79489400 | -4.46649600 | 1.12788800 |
| O | -0.88107800 | -1.13818300 | 0.80756900 |
| O | -1.05421200 | -3.09935000 | 2.68325700 |
| H | 0.95123100 | -2.53420700 | 2.55784600 |
| H | -1.16178700 | -0.29086200 | 2.63512000 |
| H | 0.50233700 | -2.58945600 | 0.24857100 |
| H | -2.30208700 | -3.51535900 | 1.13258500 |

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|---|---|---|---|
| Ru | -0.22381300 | 1.32709100 | -0.30117800 |
| O | -1.87673500 | 1.05089600 | 1.03084100 |
| O | -2.68274700 | 2.03292300 | -0.78085400 |
| C | -2.87870700 | 1.38662900 | 0.28451400 |
| C | -4.24793200 | 0.90460200 | 0.66750900 |
| C | -4.41080600 | -0.15310500 | 1.60771400 |
| C | -5.38655700 | 1.41305800 | -0.00972300 |
| C | -5.68448000 | -0.69983400 | 1.78937000 |
| C | -6.63859500 | 0.83578700 | 0.22912000 |
| C | -6.80946900 | -0.23517500 | 1.10504500 |
| H | -5.80073800 | -1.52840900 | 2.48482400 |
| H | -7.50443100 | 1.22769100 | -0.30061200 |
| C | -8.15860100 | -0.87777400 | 1.31916400 |
| H | -8.91883700 | -0.44437200 | 0.66166600 |
| H | -8.11175600 | -1.95249300 | 1.11609600 |
| H | -8.49668500 | -0.75350800 | 2.35586500 |
| C | -3.29073400 | -0.74921900 | 2.43536400 |
| H | -2.48846200 | -1.15820400 | 1.81904700 |
| H | -2.82696300 | 0.00470800 | 3.07827100 |
| H | -3.68708900 | -1.55126600 | 3.06755600 |
| C | -5.33652300 | 2.55493900 | -1.00338700 |
| H | -4.74676900 | 3.39716300 | -0.63248000 |
| H | -4.86205700 | 2.24505900 | -1.93907500 |
| H | -6.35168700 | 2.90421700 | -1.22249000 |
| C | 1.15262600 | 0.63689800 | 0.75552800 |
| C | 2.49679200 | 0.57979700 | 0.17599500 |
| C | 0.99764200 | 0.17022000 | 2.11767500 |
| C | 2.03439400 | -0.35494300 | 2.80529700 |
| H | 0.01100200 | 0.24576400 | 2.56541900 |
| C | 3.39533700 | -0.56306700 | 2.20858000 |
| H | 1.88333900 | -0.70084300 | 3.82518100 |
| C | 1.28537600 | 2.03272100 | -2.91004100 |
| C | 2.57563600 | 1.10781200 | -1.19490900 |
| C | 2.38603800 | 2.10635900 | -3.75705000 |
| H | 0.29699800 | 2.35088100 | -3.22697500 |
| C | 3.71854500 | 1.14146000 | -1.99915200 |
| C | 3.62248100 | 1.65211700 | -3.29117500 |
| H | 2.26818500 | 2.50069200 | -4.76071400 |
| H | 4.66136700 | 0.75767400 | -1.62116600 |
| H | 4.49962400 | 1.68607300 | -3.93041000 |
| N | 1.37298900 | 1.55346900 | -1.65697300 |
| C | 3.54454200 | 0.07474500 | 0.86485700 |
| H | 4.53798500 | 0.08404000 | 0.42707900 |
| C | -1.13589300 | -1.45690500 | -0.56899500 |

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|---|---|---|---|
| O | -0.82811100 | -0.37227300 | -1.23527700 |
| O | -0.43252200 | -2.00367900 | 0.28190400 |
| C | -2.51266100 | -1.99530700 | -0.88312900 |
| C | -3.41056500 | -1.25596300 | -1.66208900 |
| C | -2.94551600 | -3.17242400 | -0.25868000 |
| C | -4.73566100 | -1.66684200 | -1.78756600 |
| H | -3.07762000 | -0.32410600 | -2.10285500 |
| C | -4.26739700 | -3.58704800 | -0.37950700 |
| H | -2.24009200 | -3.72271300 | 0.35466900 |
| C | -5.16594300 | -2.82116500 | -1.13156000 |
| H | -5.44489300 | -1.06618700 | -2.34580800 |
| H | -4.61427500 | -4.47918100 | 0.13220400 |
| C | -6.59877500 | -3.25382900 | -1.23593300 |
| F | -7.43034700 | -2.22050600 | -1.50445400 |
| F | -6.78841600 | -4.17230000 | -2.21605700 |
| F | -7.03802600 | -3.82917300 | -0.08550200 |
| C | 3.76652800 | -2.12374100 | 2.15382400 |
| C | 2.58061800 | -2.91307900 | 1.56864300 |
| H | 1.72028200 | -2.90692500 | 2.24304600 |
| H | 2.23758200 | -2.49036300 | 0.61974600 |
| H | 2.87179800 | -3.95695100 | 1.40020900 |
| C | 4.07525800 | -2.61810500 | 3.57793000 |
| H | 4.31409100 | -3.68827400 | 3.55907000 |
| H | 4.93051000 | -2.08931900 | 4.01606200 |
| H | 3.21920900 | -2.48654400 | 4.24788000 |
| C | 4.99211100 | -2.36886600 | 1.23721000 |
| C | 6.29441300 | -1.61676800 | 1.60367100 |
| H | 4.71572700 | -2.11648300 | 0.20902400 |
| H | 5.19774800 | -3.44674900 | 1.24010800 |
| H | 6.07030000 | -0.67366000 | 2.11369200 |
| H | 6.90437500 | -2.20651400 | 2.29650900 |
| C | 7.06354200 | -1.22632700 | 0.34299100 |
| O | 6.55286900 | -0.46649400 | -0.49007500 |
| N | 8.30038900 | -1.76122300 | 0.20664400 |
| H | 8.61673800 | -2.38473000 | 0.93603600 |
| C | 9.22147200 | -1.54622600 | -0.93637500 |
| C | 8.56547600 | -2.04759200 | -2.23560300 |
| H | 8.32181200 | -3.11302100 | -2.15625300 |
| H | 7.64667200 | -1.49327700 | -2.43779100 |
| H | 9.25278600 | -1.91263400 | -3.07831900 |
| C | 10.48667200 | -2.36370100 | -0.63696200 |
| H | 11.20944900 | -2.24274200 | -1.44952100 |
| H | 10.96342000 | -2.02834900 | 0.29221300 |
| H | 10.25609100 | -3.43237500 | -0.54729100 |

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|---|---|---|---|
| C | 9.57414900 | -0.05200700 | -1.04583300 |
| H | 8.67336300 | 0.54042300 | -1.21890200 |
| H | 10.05323400 | 0.29767500 | -0.12438700 |
| H | 10.26867100 | 0.10833700 | -1.87811200 |
| H | 4.14117100 | -0.10961300 | 2.88246000 |
| C | -0.28718200 | 3.60925600 | 1.85156500 |
| C | -0.64230700 | 4.42008700 | -0.40123400 |
| C | -0.70635400 | 5.05324100 | 2.12583700 |
| H | -1.05904700 | 2.89918900 | 2.16249500 |
| C | -0.07182800 | 5.79161900 | -0.03169400 |
| H | -0.38853400 | 4.16642200 | -1.43219000 |
| H | -0.54767900 | 5.28287100 | 3.18342300 |
| H | -0.73675100 | 6.57348300 | -0.43160000 |
| O | -0.01972100 | 3.41896900 | 0.42992900 |
| O | 0.09825600 | 5.95153900 | 1.37898200 |
| H | -1.77569800 | 5.20213800 | 1.91170100 |
| H | 0.92035600 | 5.91993400 | -0.47705900 |
| H | 0.65723700 | 3.36715100 | 2.34465100 |
| H | -1.72908300 | 4.34928300 | -0.29839700 |

R-MECP

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|---|---|---|---|
| Ru | -0.27829697 | -0.10517490 | -0.43056636 |
| O | -1.86135485 | -0.34377160 | 0.99397787 |
| O | -2.59046362 | 0.97268386 | -0.62147059 |
| C | -2.82904601 | 0.28199915 | 0.41067613 |
| C | -4.21968293 | 0.10636782 | 0.94071965 |
| C | -4.50041795 | -0.86560446 | 1.94018736 |
| C | -5.29086073 | 0.85457605 | 0.37927624 |
| C | -5.83153439 | -1.07904102 | 2.31975003 |
| C | -6.59657995 | 0.59882784 | 0.80332771 |
| C | -6.89468256 | -0.37426520 | 1.75823578 |
| H | -6.04165774 | -1.83371638 | 3.07499002 |
| H | -7.41076302 | 1.16387256 | 0.35638174 |
| C | -8.32659881 | -0.66519872 | 2.13542973 |
| H | -8.89568112 | 0.25850299 | 2.29458559 |
| H | -8.82141105 | -1.21959792 | 1.32919874 |
| H | -8.39150520 | -1.26886077 | 3.04672513 |
| C | -3.45528771 | -1.71792542 | 2.63029500 |
| H | -2.87809713 | -2.31274234 | 1.91881841 |
| H | -2.72679135 | -1.10508430 | 3.16842365 |
| H | -3.94120676 | -2.39191792 | 3.34489308 |
| C | -5.11664799 | 1.92119078 | -0.68006477 |
| H | -4.36200765 | 2.65992708 | -0.39904516 |
| H | -4.77644197 | 1.48549046 | -1.62336389 |

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|---|---|---|---|
| H | -6.06940447 | 2.43444542 | -0.85086171 |
| C | 1.22764306 | -0.80011463 | 0.56057758 |
| C | 2.52923579 | -0.55847602 | 0.00808877 |
| C | 1.13058263 | -1.44139957 | 1.81885756 |
| C | 2.27440000 | -1.78815910 | 2.51782356 |
| H | 0.14368741 | -1.64905438 | 2.22231149 |
| C | 3.55371760 | -1.52378710 | 1.97359778 |
| H | 2.19800664 | -2.27955351 | 3.48449118 |
| C | 1.09317689 | 0.61388341 | -3.10249932 |
| C | 2.52004995 | -0.03704770 | -1.36220001 |
| C | 2.16311517 | 0.81848068 | -3.96676180 |
| H | 0.06606675 | 0.77391056 | -3.41540870 |
| C | 3.63797419 | 0.14618819 | -2.18404396 |
| C | 3.45672248 | 0.58026434 | -3.49457351 |
| H | 1.98054797 | 1.14474907 | -4.98506537 |
| H | 4.62893411 | -0.08780914 | -1.81198578 |
| H | 4.31602726 | 0.71748829 | -4.14395143 |
| N | 1.25903113 | 0.20359806 | -1.83293384 |
| C | 3.67152280 | -0.85490691 | 0.74129595 |
| H | 4.65512953 | -0.63041956 | 0.34385669 |
| C | -1.63327905 | -2.67840613 | -0.76239544 |
| O | -0.86800070 | -1.79893233 | -1.38340478 |
| O | -1.23071218 | -3.50523585 | 0.05138831 |
| C | -3.09997591 | -2.59234802 | -1.11940112 |
| C | -3.56058876 | -1.65281505 | -2.05172065 |
| C | -4.02533477 | -3.38082240 | -0.42585692 |
| C | -4.92521715 | -1.47004649 | -2.25086393 |
| H | -2.84160464 | -1.03488943 | -2.57297202 |
| C | -5.39289935 | -3.19361281 | -0.61090331 |
| H | -3.65651687 | -4.10656304 | 0.29056470 |
| C | -5.84127513 | -2.22371067 | -1.51185262 |
| H | -5.27815599 | -0.71458963 | -2.94569180 |
| H | -6.10963558 | -3.76990813 | -0.03678144 |
| C | -7.31032366 | -1.99299653 | -1.71400822 |
| F | -7.60048445 | -0.68097536 | -1.88230716 |
| F | -7.77754662 | -2.63123636 | -2.81724406 |
| F | -8.05161587 | -2.43676652 | -0.66871268 |
| C | 4.07451094 | -3.85879942 | 0.87023155 |
| C | 2.73711515 | -4.06752821 | 0.24844525 |
| H | 1.95445039 | -4.26616402 | 0.98481586 |
| H | 2.42907178 | -3.20004985 | -0.34875062 |
| H | 2.77152592 | -4.92514020 | -0.44643918 |
| C | 4.38234125 | -4.57267716 | 2.14678993 |
| H | 4.58399186 | -5.63976593 | 1.93882429 |

| | | | |
|---|---|---|---|
| H | 5.26847012 | -4.17874466 | 2.65536960 |
| H | 3.53377030 | -4.53960083 | 2.83796056 |
| C | 5.19118286 | -3.48316907 | -0.06307468 |
| C | 6.44993101 | -2.87169458 | 0.57696721 |
| H | 4.81121997 | -2.79433930 | -0.82356574 |
| H | 5.48248031 | -4.39288584 | -0.62017462 |
| H | 6.19665471 | -2.38805260 | 1.52830654 |
| H | 7.19506249 | -3.63927103 | 0.81828823 |
| C | 7.09266131 | -1.77530737 | -0.28770151 |
| O | 6.48986313 | -1.22805871 | -1.21563007 |
| N | 8.34180575 | -1.41651299 | 0.09780290 |
| H | 8.74857985 | -1.91795786 | 0.87580628 |
| C | 9.12314522 | -0.27674951 | -0.44617836 |
| C | 9.44035844 | -0.52654372 | -1.93114197 |
| H | 10.02248808 | -1.44741525 | -2.04893139 |
| H | 8.51667210 | -0.61930622 | -2.50639752 |
| H | 10.02598242 | 0.30716297 | -2.33466739 |
| C | 10.42380743 | -0.21145435 | 0.36777062 |
| H | 11.04471829 | 0.61597654 | 0.01121619 |
| H | 10.21660127 | -0.04233949 | 1.43168790 |
| H | 11.00264594 | -1.13728585 | 0.26537611 |
| C | 8.33360213 | 1.03391443 | -0.27126144 |
| H | 7.39454549 | 0.99476929 | -0.82693570 |
| H | 8.10864210 | 1.20931324 | 0.78704058 |
| H | 8.92610880 | 1.87785372 | -0.64177853 |
| H | 4.43436971 | -1.68534024 | 2.58625304 |
| C | -0.08897291 | 3.04149626 | -0.44997994 |
| C | -0.22719976 | 2.17526485 | 1.76938110 |
| C | 0.63450535 | 4.26348608 | 0.09699079 |
| H | 0.28101377 | 2.76953805 | -1.43995712 |
| C | 0.50719770 | 3.40870930 | 2.27206512 |
| H | -1.31278477 | 2.32477072 | 1.77863658 |
| H | 0.37974691 | 5.14797084 | -0.49452674 |
| H | 1.59052826 | 3.20464472 | 2.30560023 |
| O | 0.19357059 | 1.91214365 | 0.40883977 |
| O | 0.24273917 | 4.53274502 | 1.43823508 |
| H | 1.72400157 | 4.09898032 | 0.04444131 |
| H | 0.16601606 | 3.67029570 | 3.27812670 |
| H | 0.02336915 | 1.28417592 | 2.34555876 |
| H | -1.17474064 | 3.18639794 | -0.48755386 |

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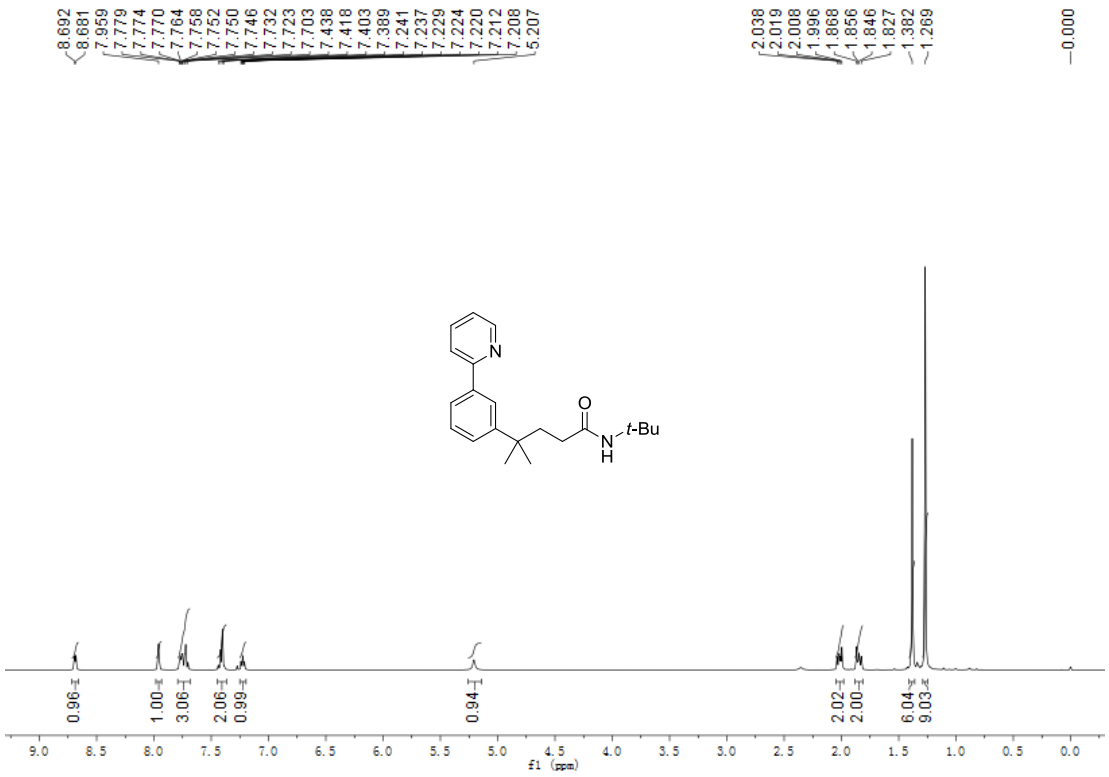
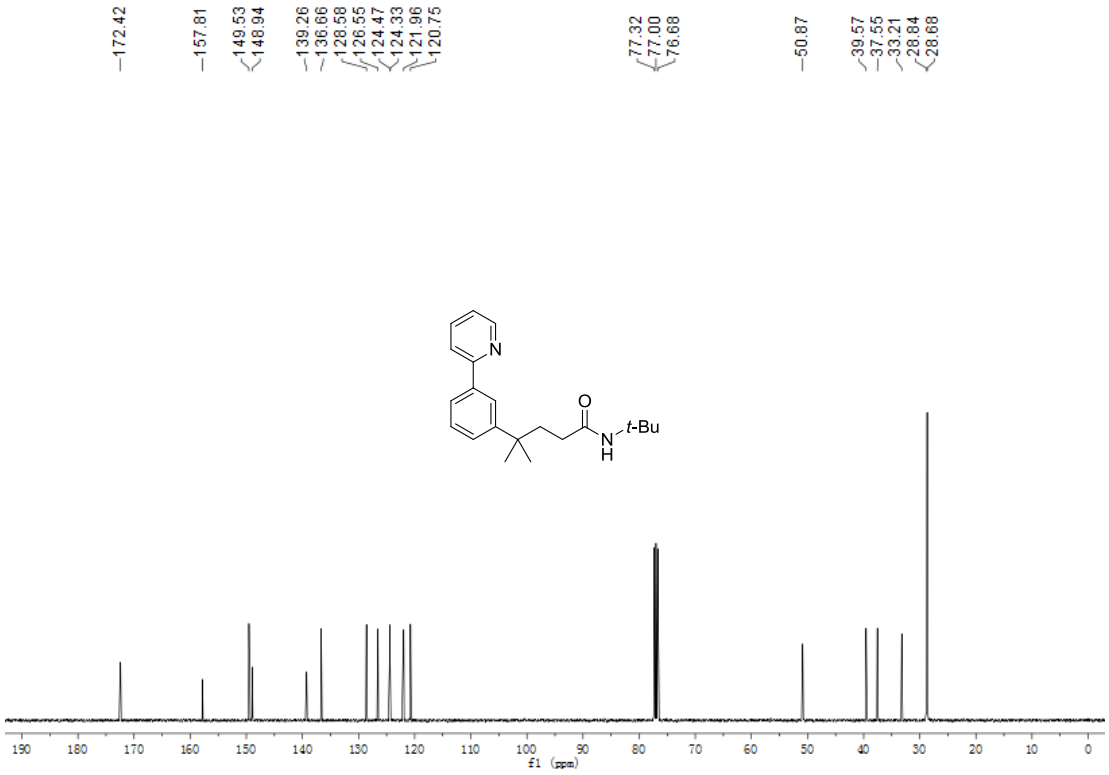
## 11. $^{1}H$, $^{13}C$ and $^{19}F$ NMR spectra of all products

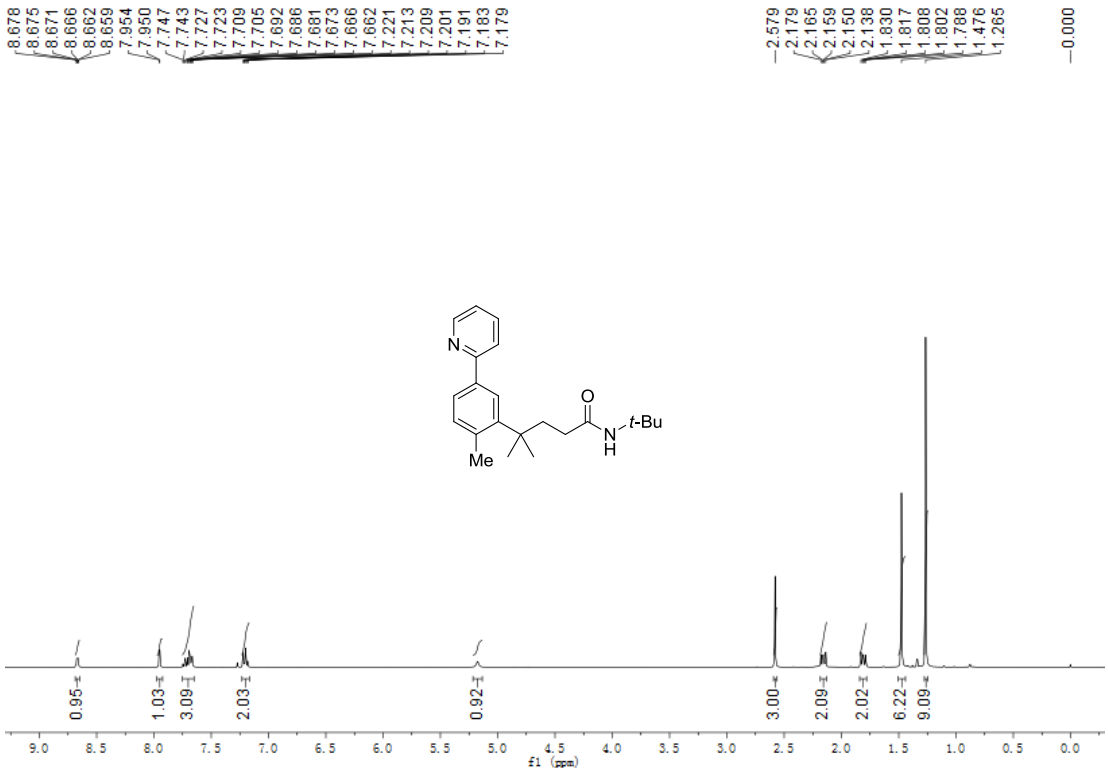
### Compound 3a $^{1}H$ NMR (400 MHz, $CDCl_3$)



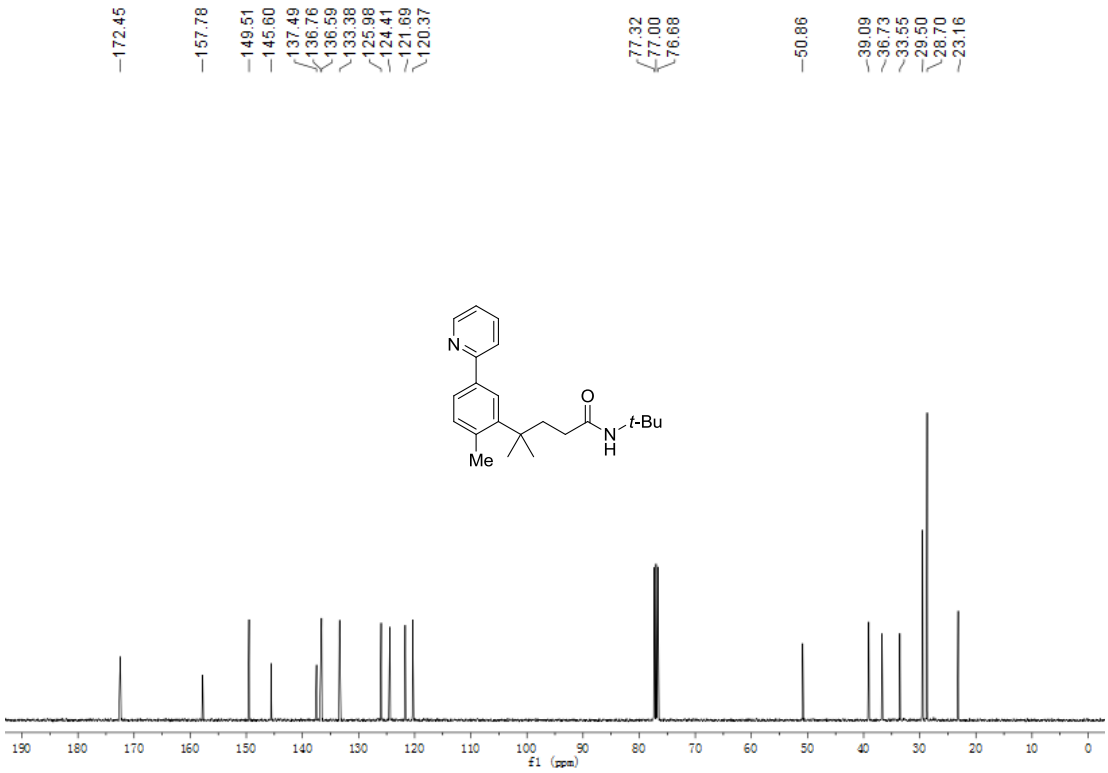

### Compound 3a $^{13}C$ NMR (101 MHz, $CDCl_3$)



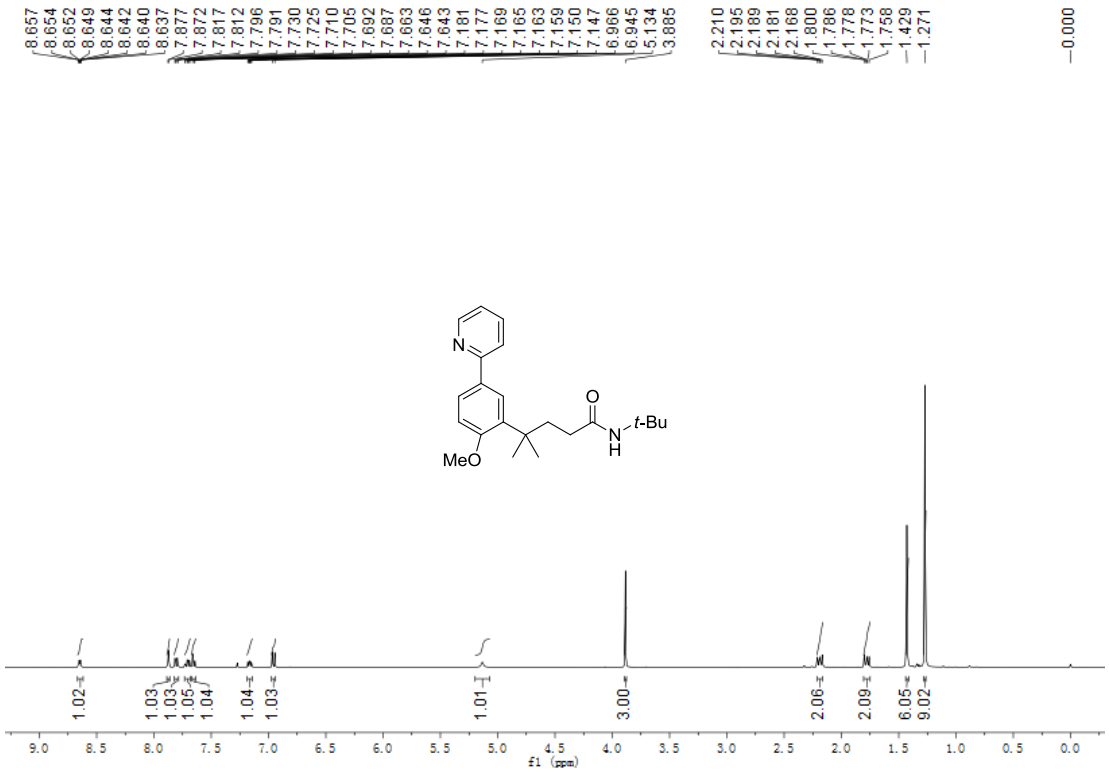
## Compound 3b $^{1}$H NMR (400 MHz, $CDCl_3$)



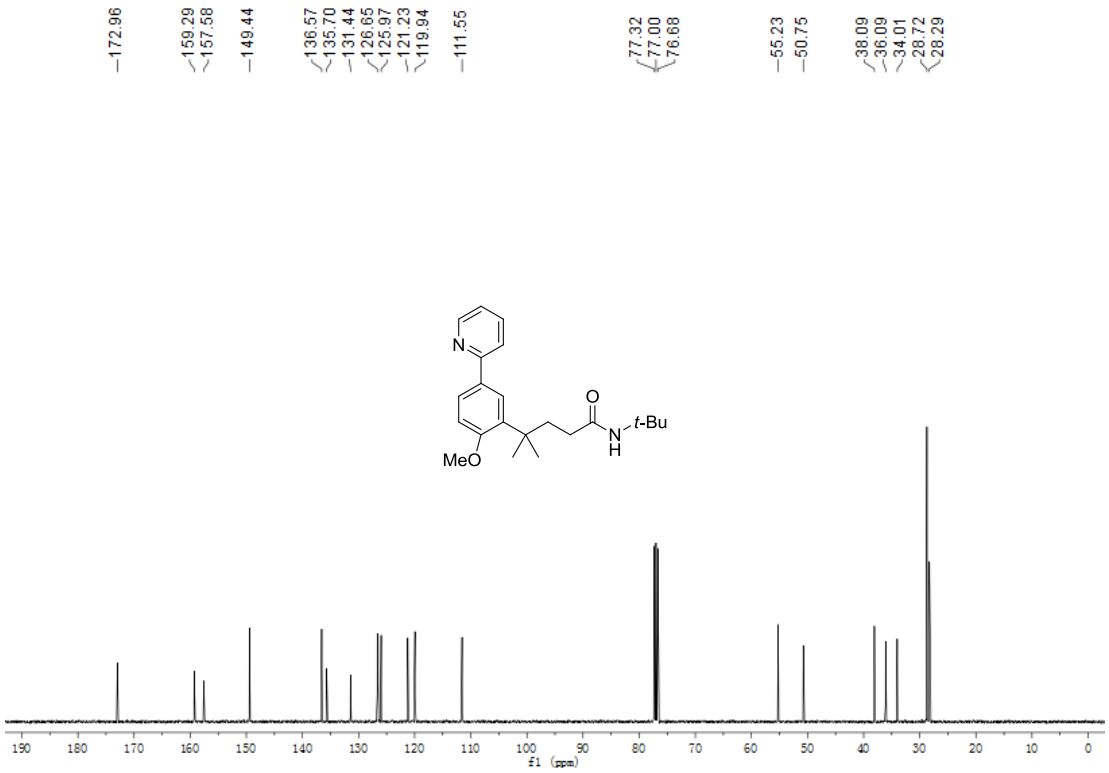

## Compound 3b $^{13}$C NMR (101 MHz, $CDCl_3$)



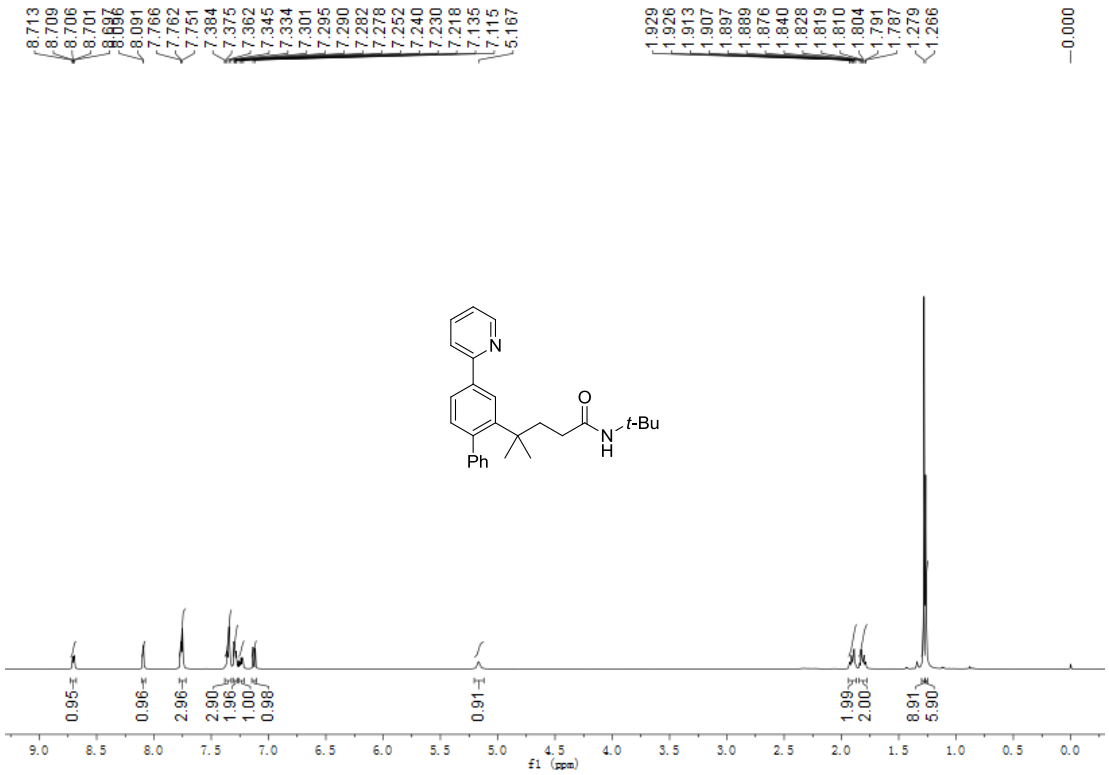
## Compound 3c $^{1}$H NMR (400 MHz, $CDCl_3$)



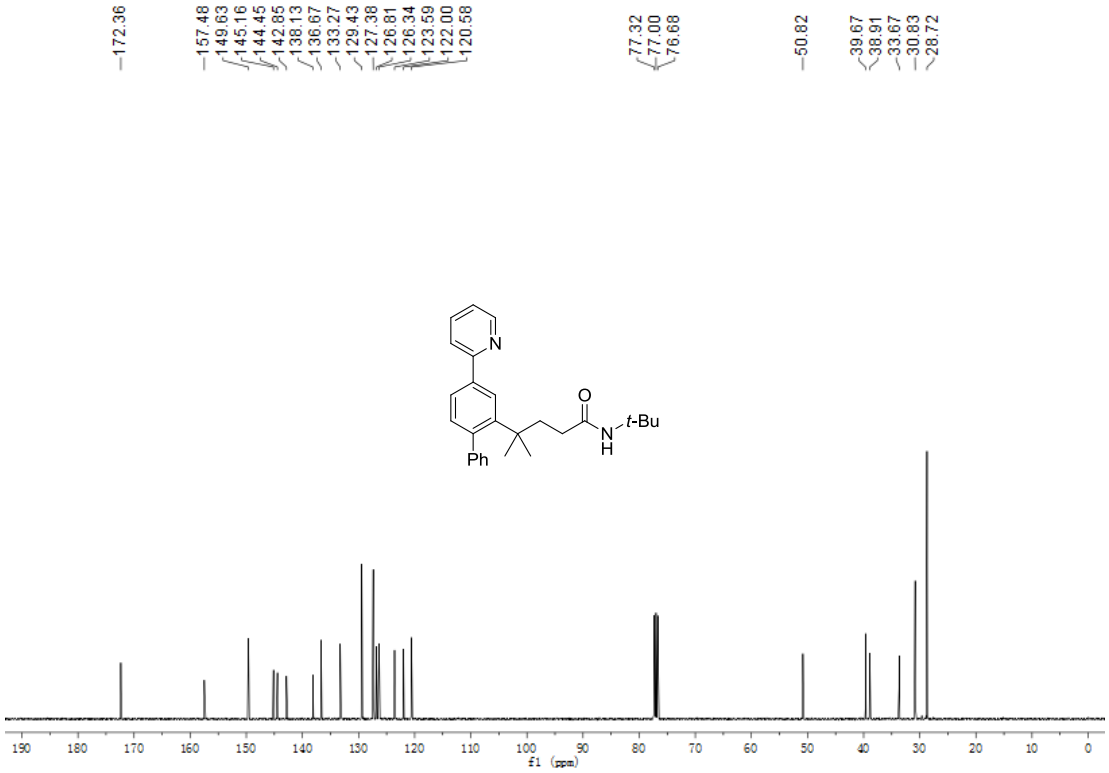

## Compound 3c $^{13}$C NMR (101 MHz, $CDCl_3$)



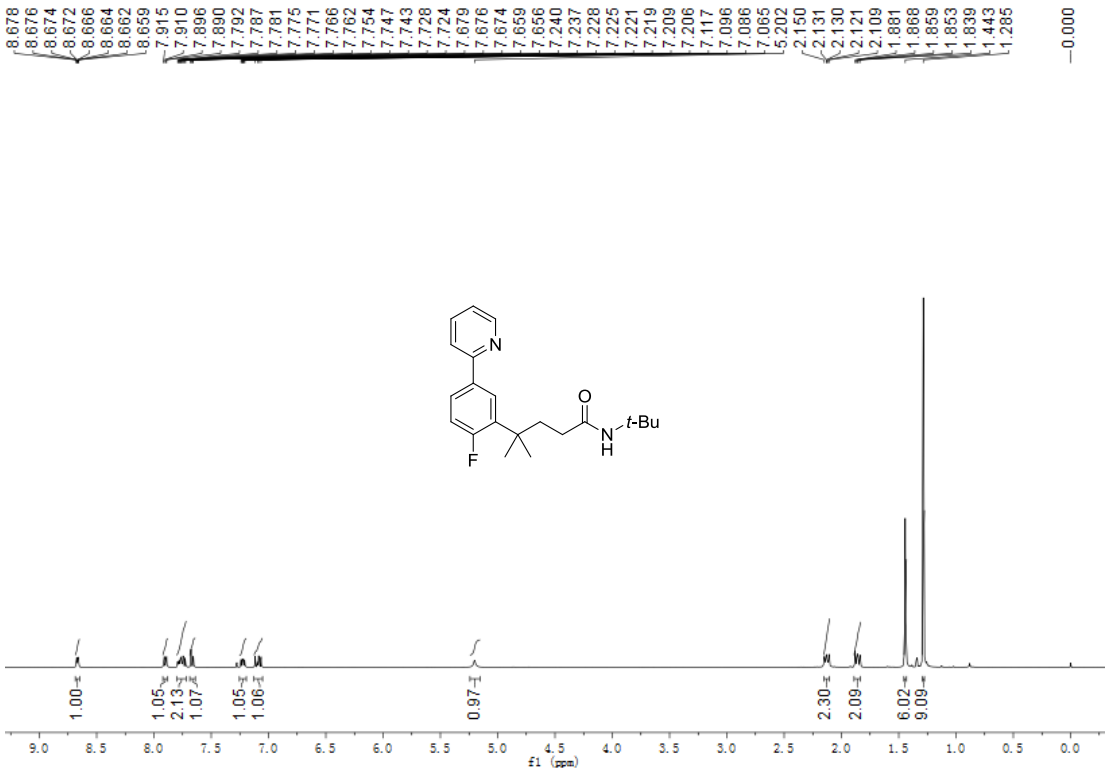
## Compound 3d $^{1}$H NMR (400 MHz, $CDCl_3$)



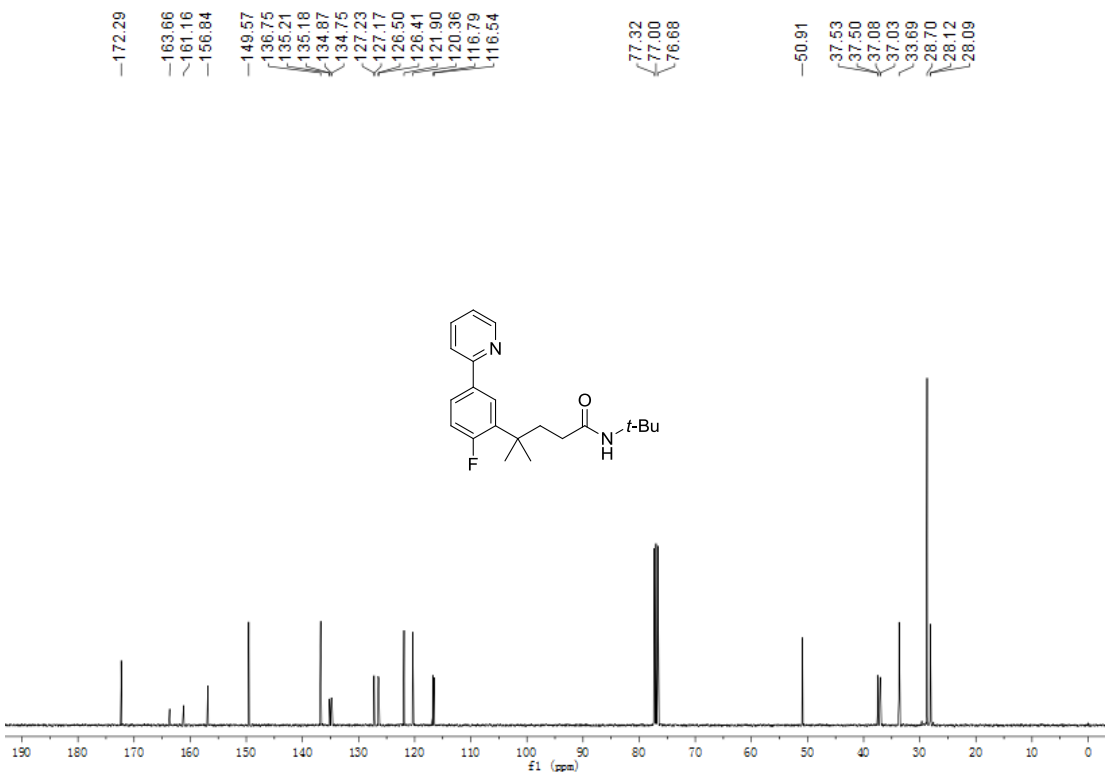

## Compound 3d $^{13}$C NMR (101 MHz, $CDCl_3$)



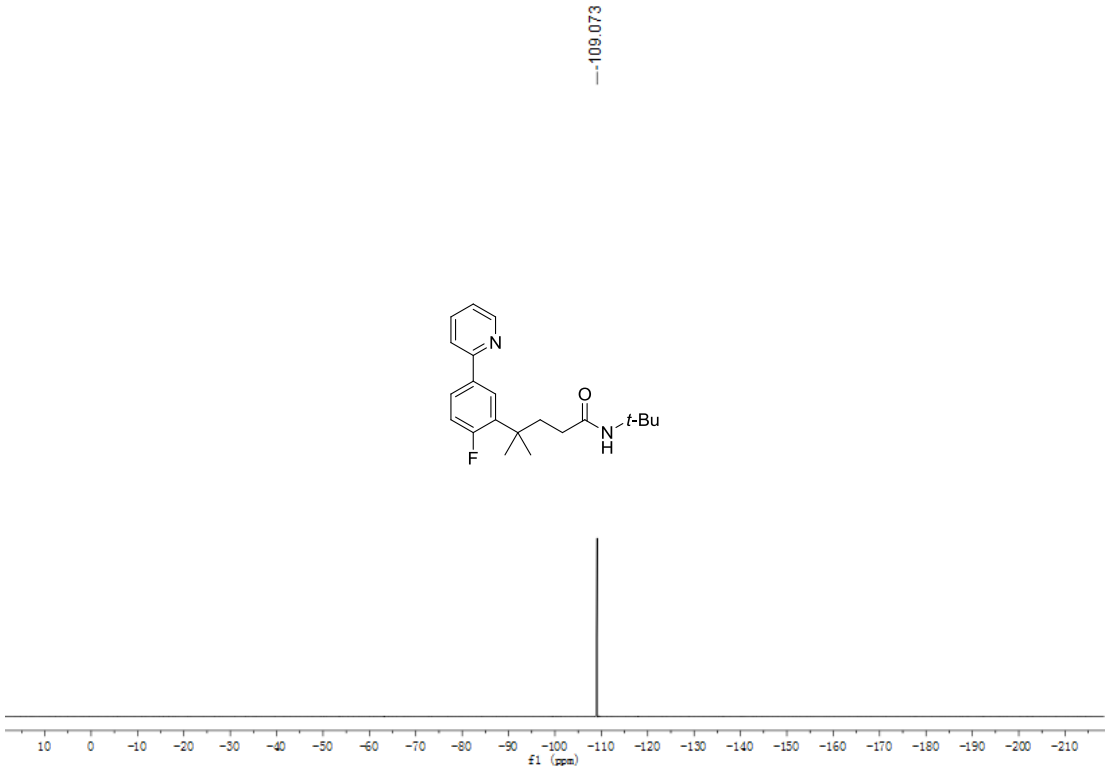
## Compound 3e $^{1}$H NMR (400 MHz, $CDCl_3$)



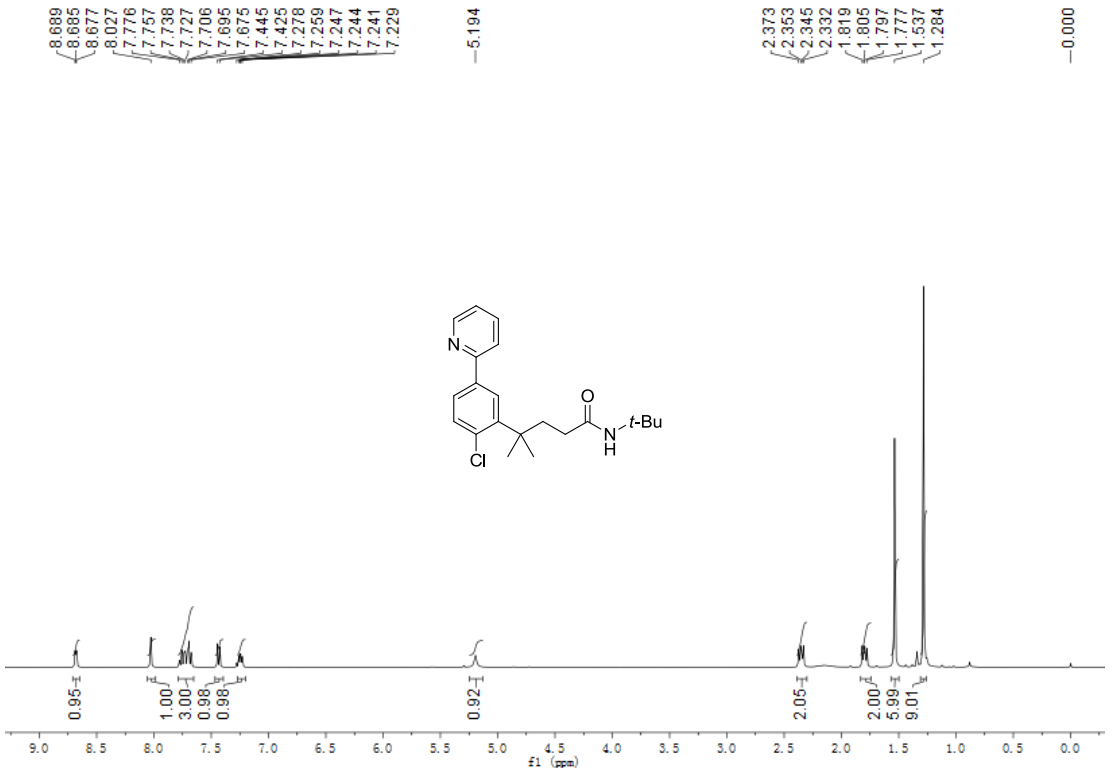

## Compound 3e $^{13}$C NMR (101 MHz, $CDCl_3$)



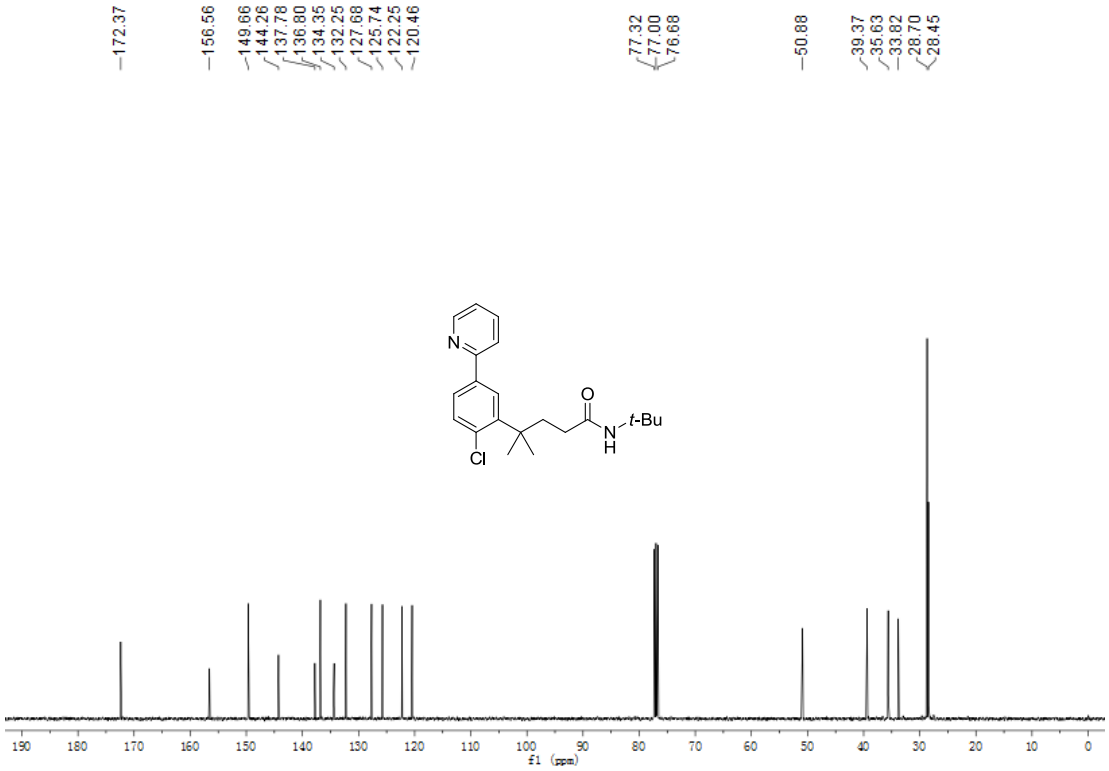
**Compound 3e $^{19}$F NMR (376 MHz, $CDCl_3$)**



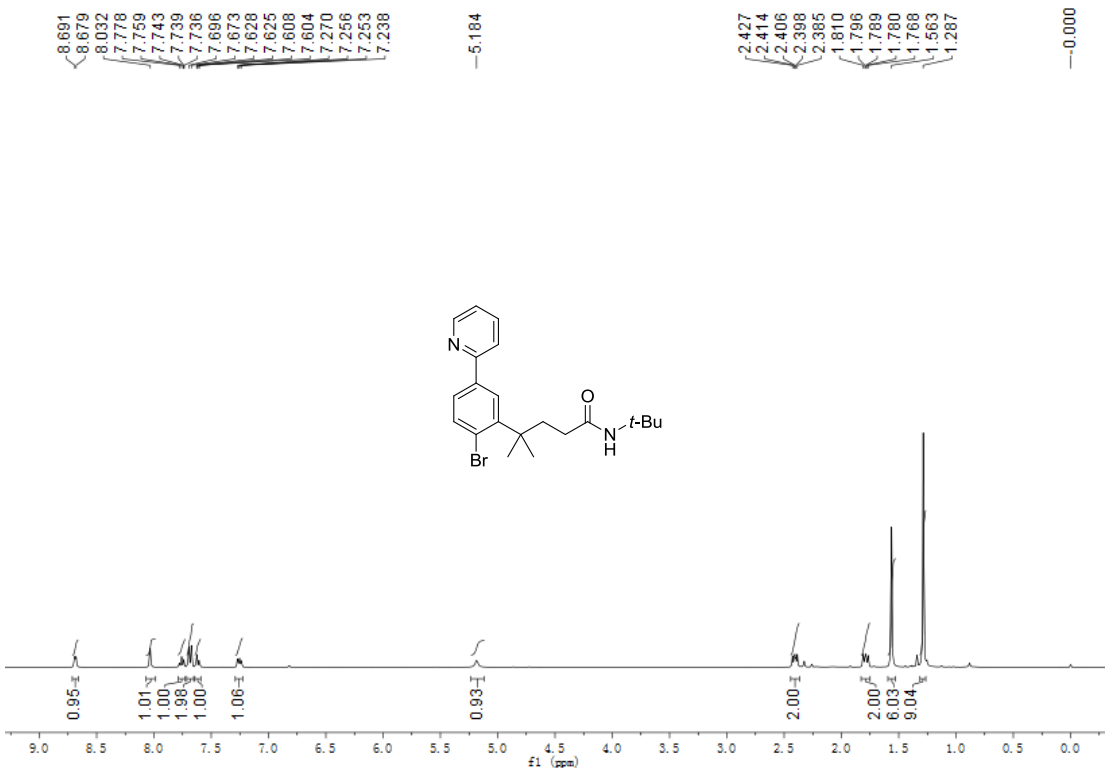

**Compound 3f $^{1}$H NMR (400 MHz, $CDCl_3$)**



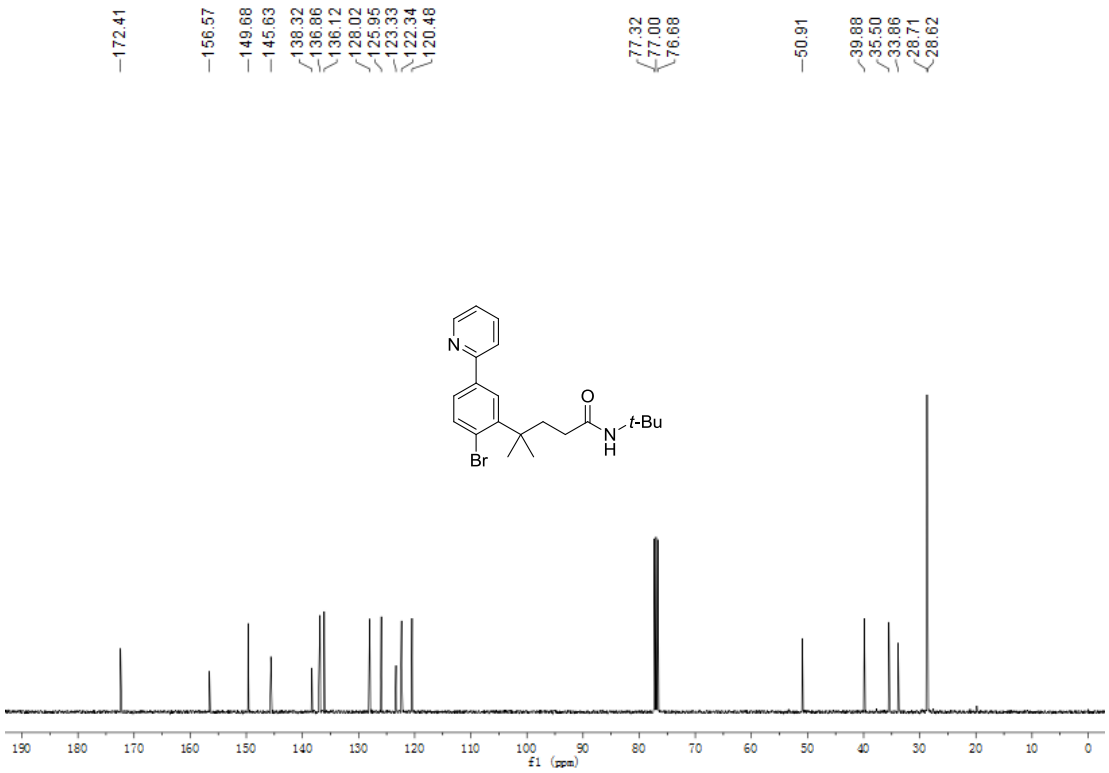
## Compound 3f $^{13}$C NMR (101 MHz, $CDCl_3$)



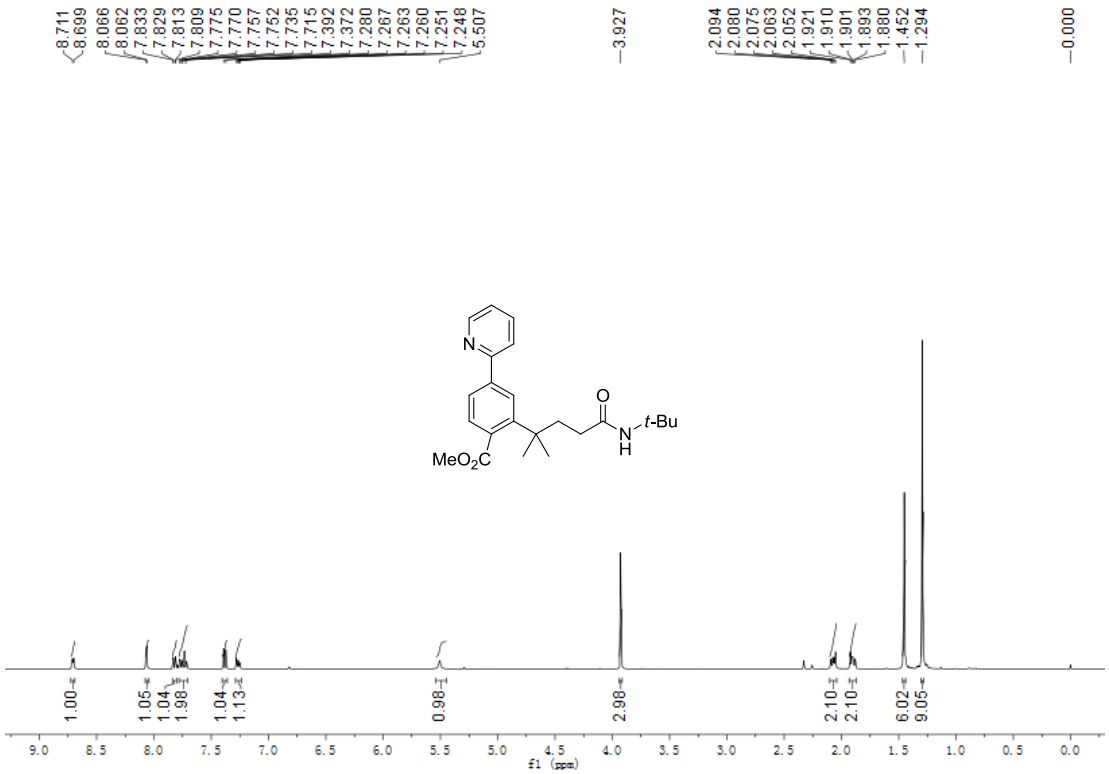

## Compound 3g $^{1}$H NMR (400 MHz, $CDCl_3$)



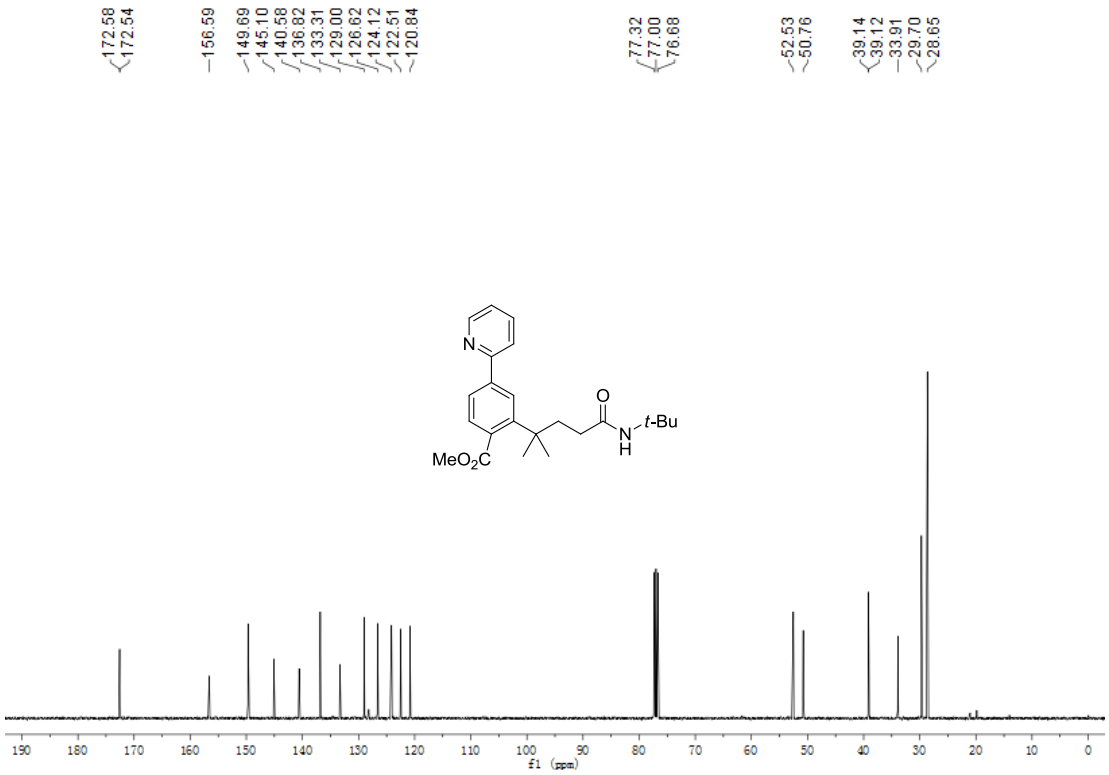
## Compound 3g $^{13}$C NMR (101 MHz, $CDCl_3$)



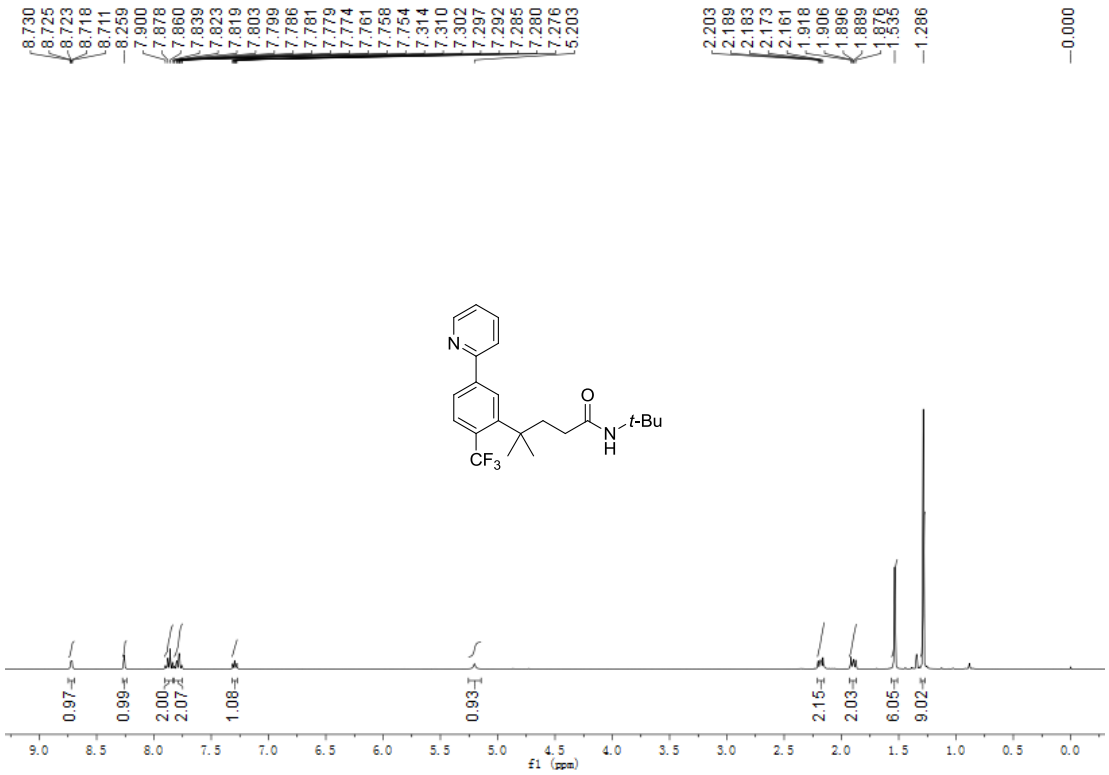

## Compound 3h $^{1}$H NMR (400 MHz, $CDCl_3$)



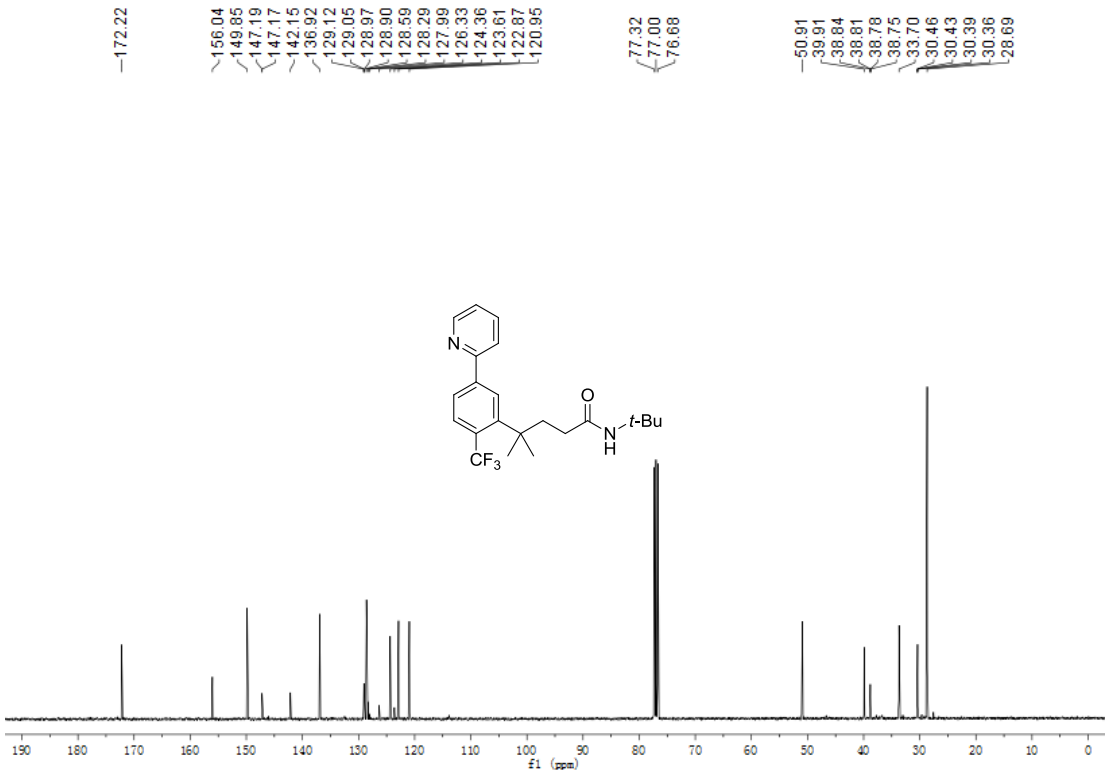
## Compound 3h $^{13}$C NMR (101 MHz, $CDCl_3$)



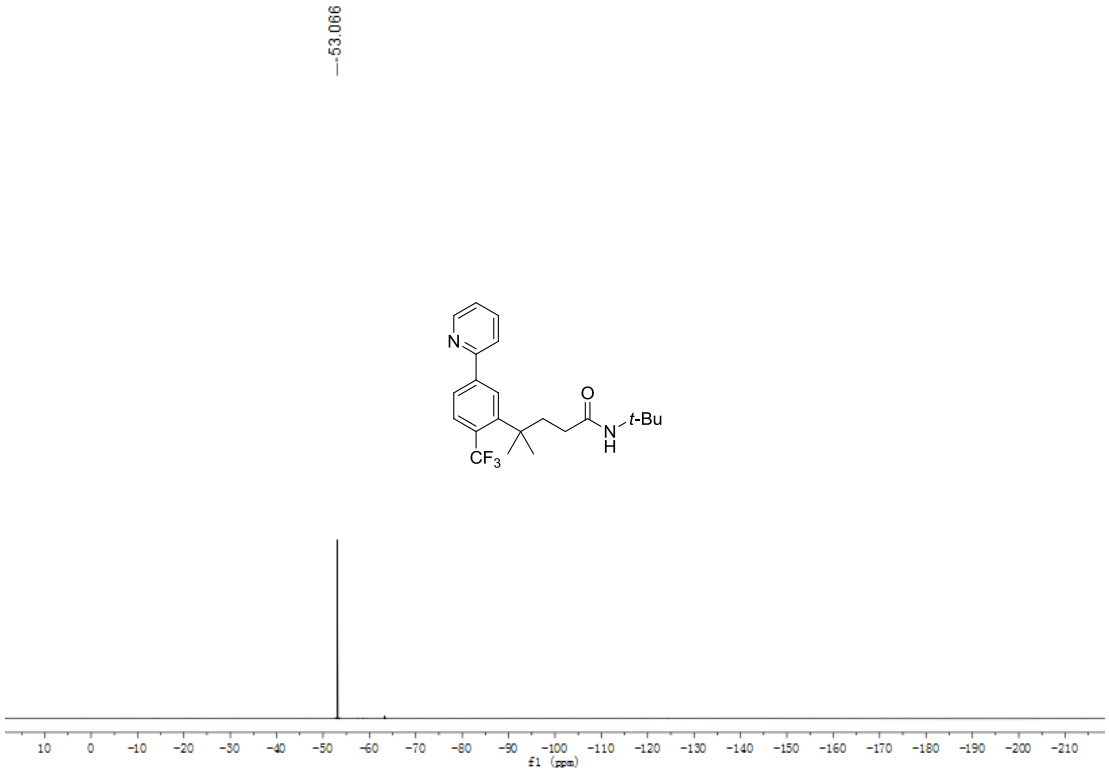

## Compound 3i $^{1}$H NMR (400 MHz, $CDCl_3$)



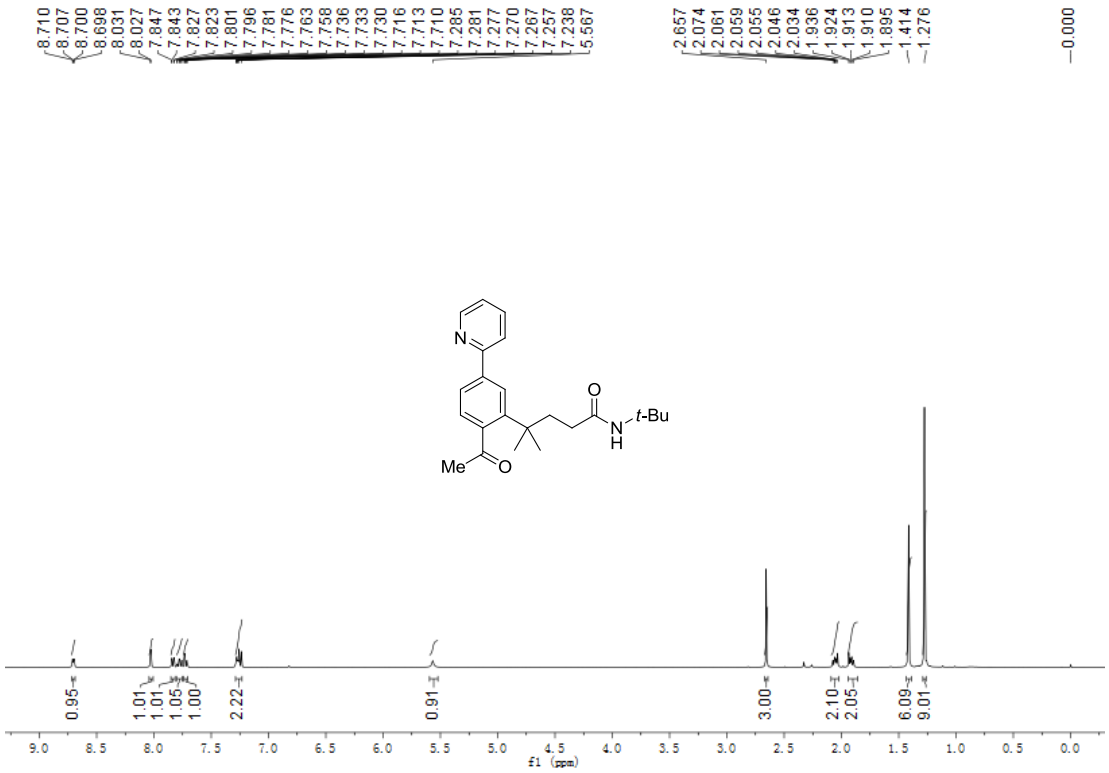
**Compound 3i $^{13}$C NMR (101 MHz, $CDCl_3$)**



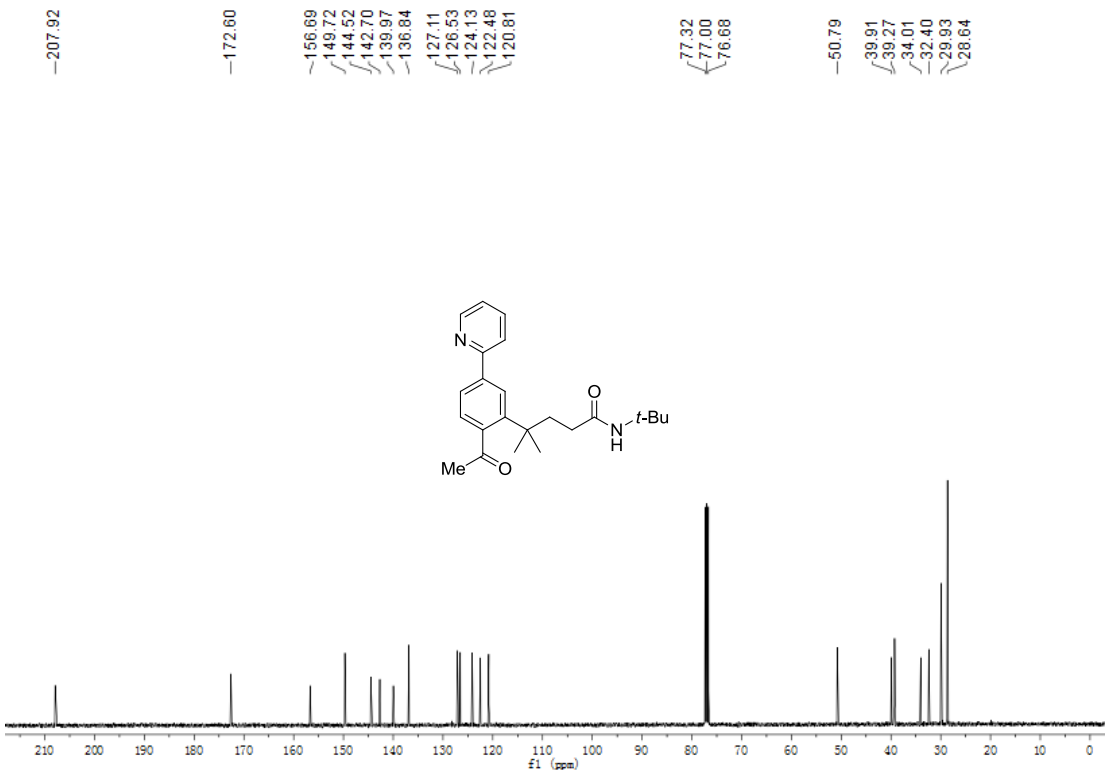

**Compound 3i $^{19}$F NMR (376 MHz, $CDCl_3$)**



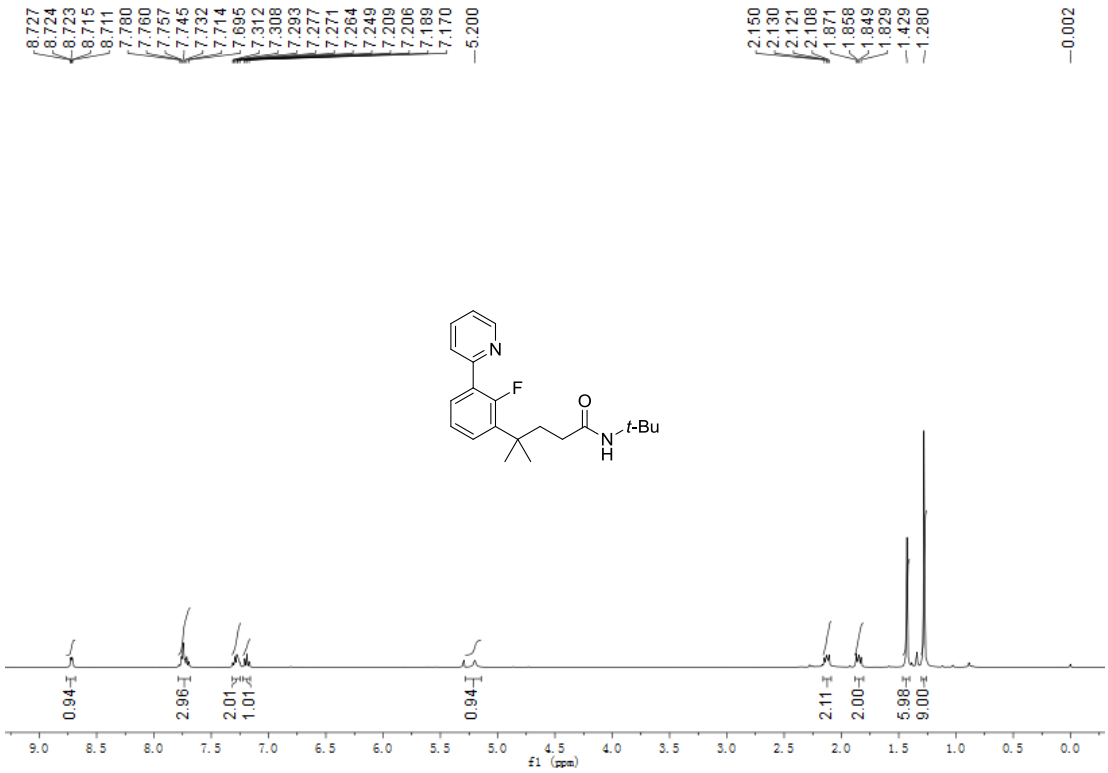
## Compound 3j $^{1}$H NMR (400 MHz, $CDCl_3$)



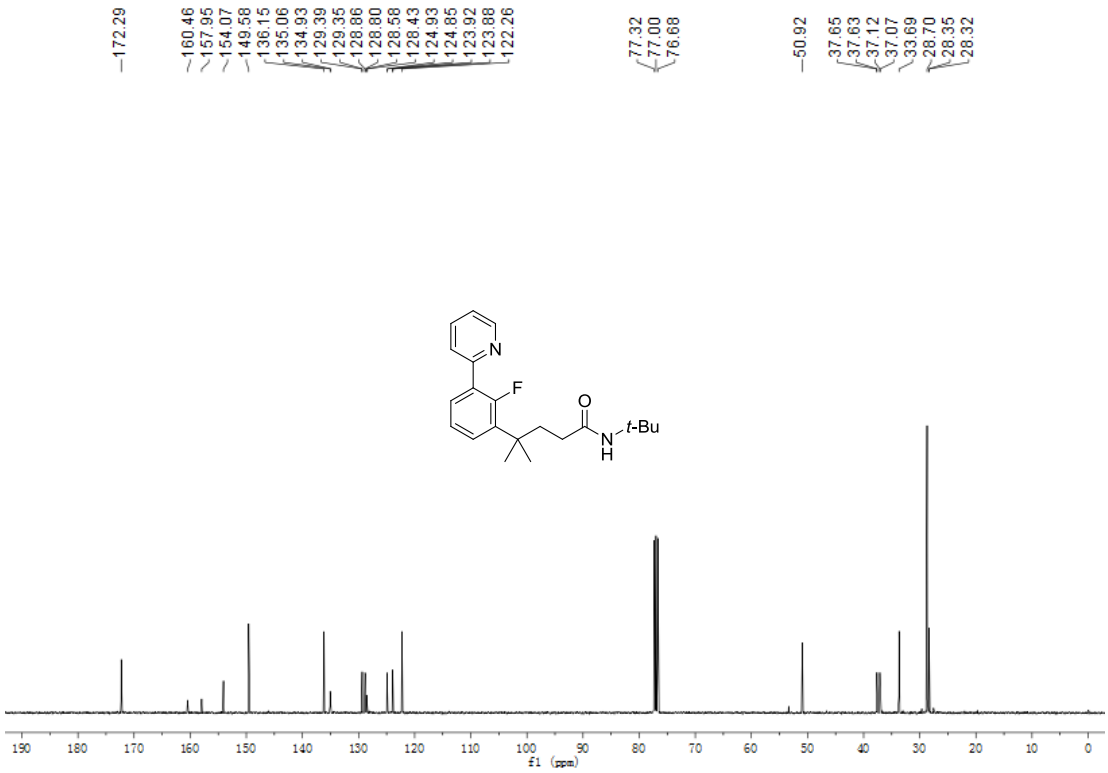

## Compound 3j $^{13}$C NMR (101 MHz, $CDCl_3$)



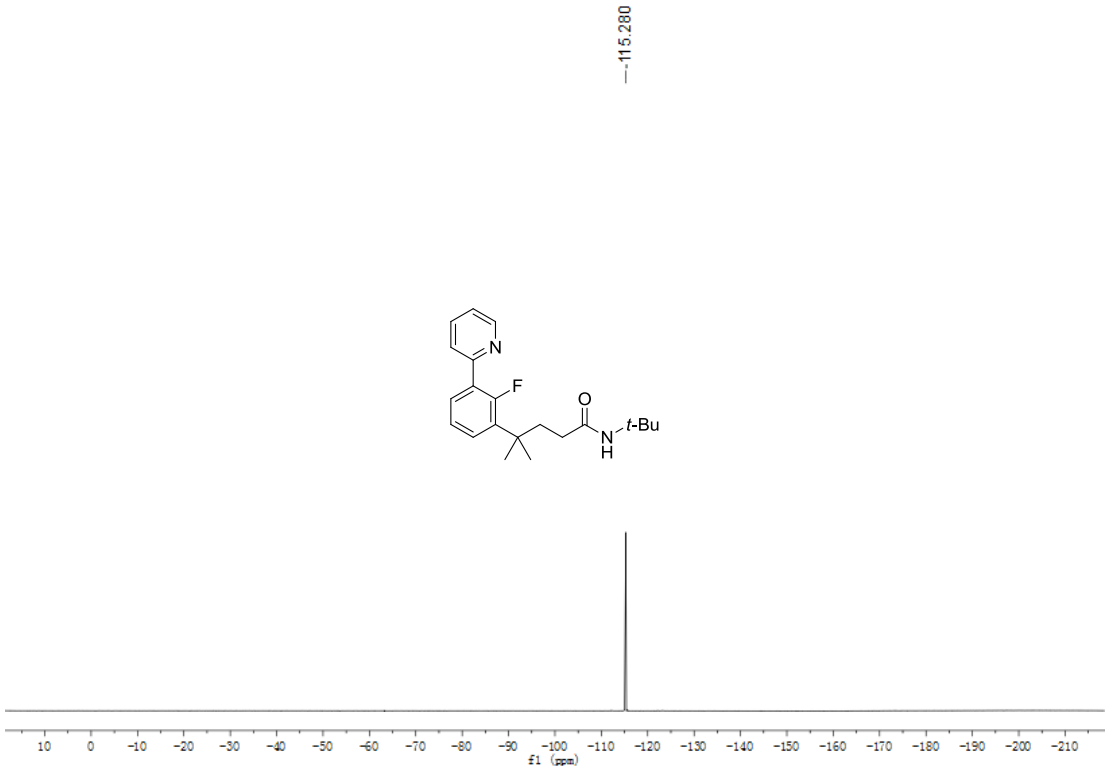
**Compound 3k $^{1}$H NMR (400 MHz, $CDCl_3$)**



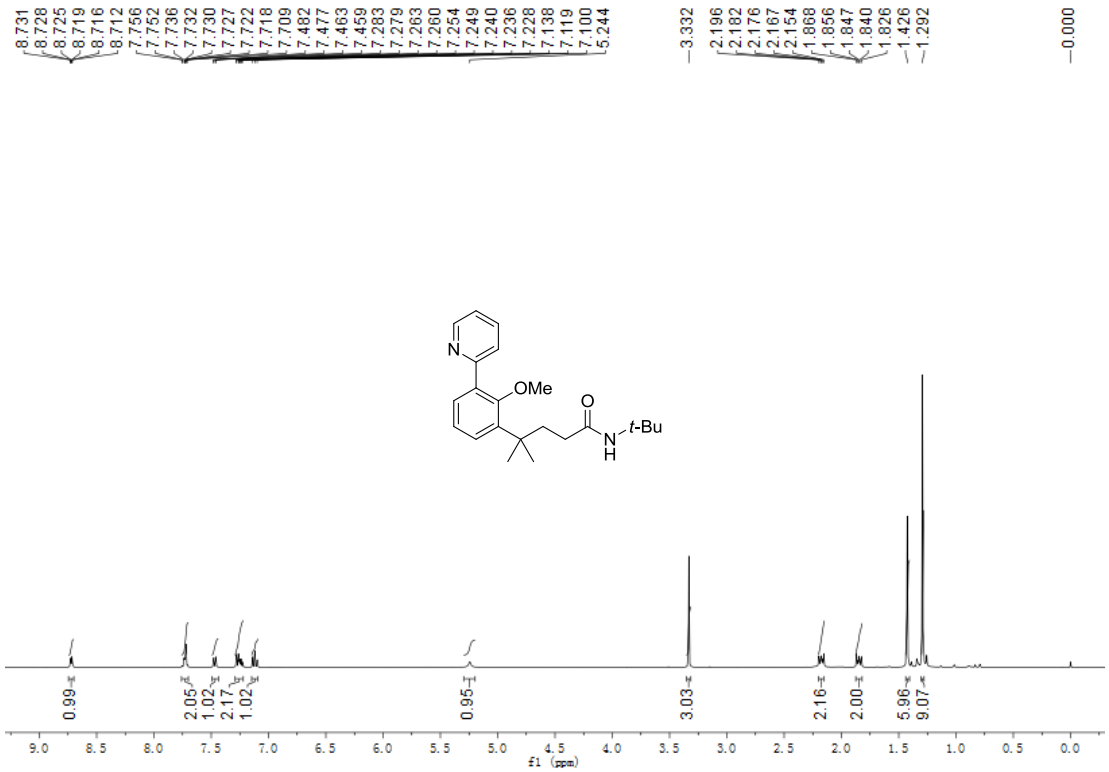

**Compound 3k $^{13}$C NMR (101 MHz, $CDCl_3$)**



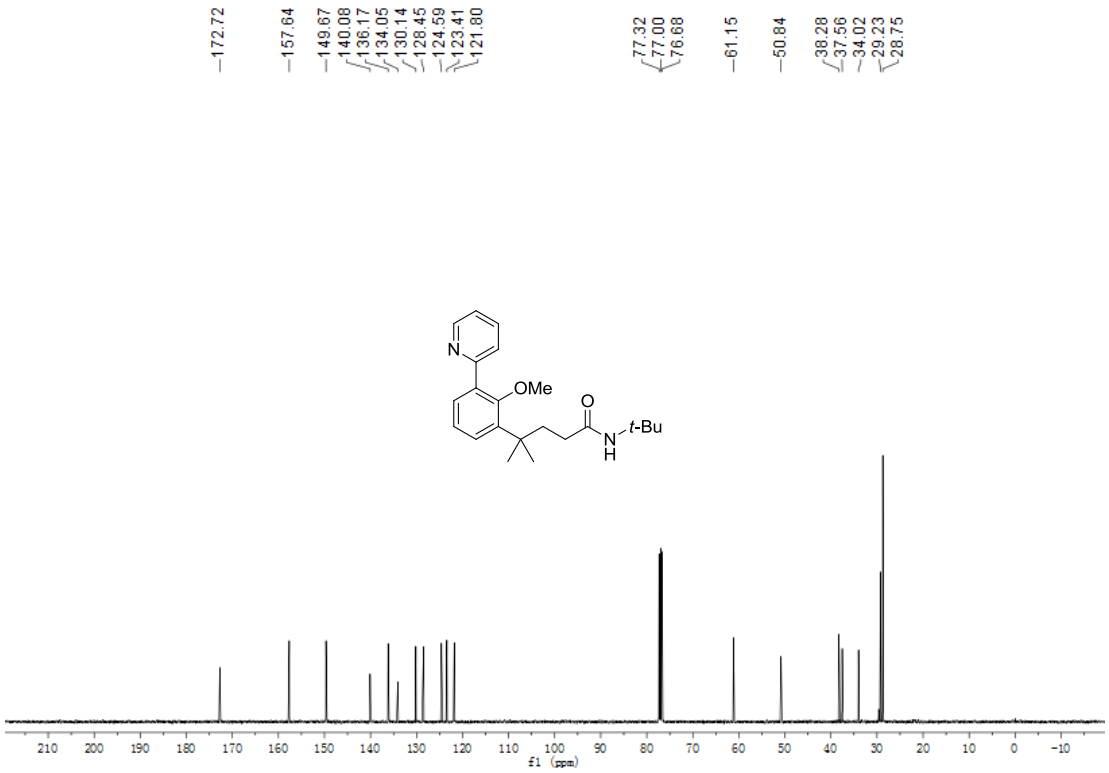
**Compound 3k $^{19}$F NMR (376 MHz, $CDCl_3$)**



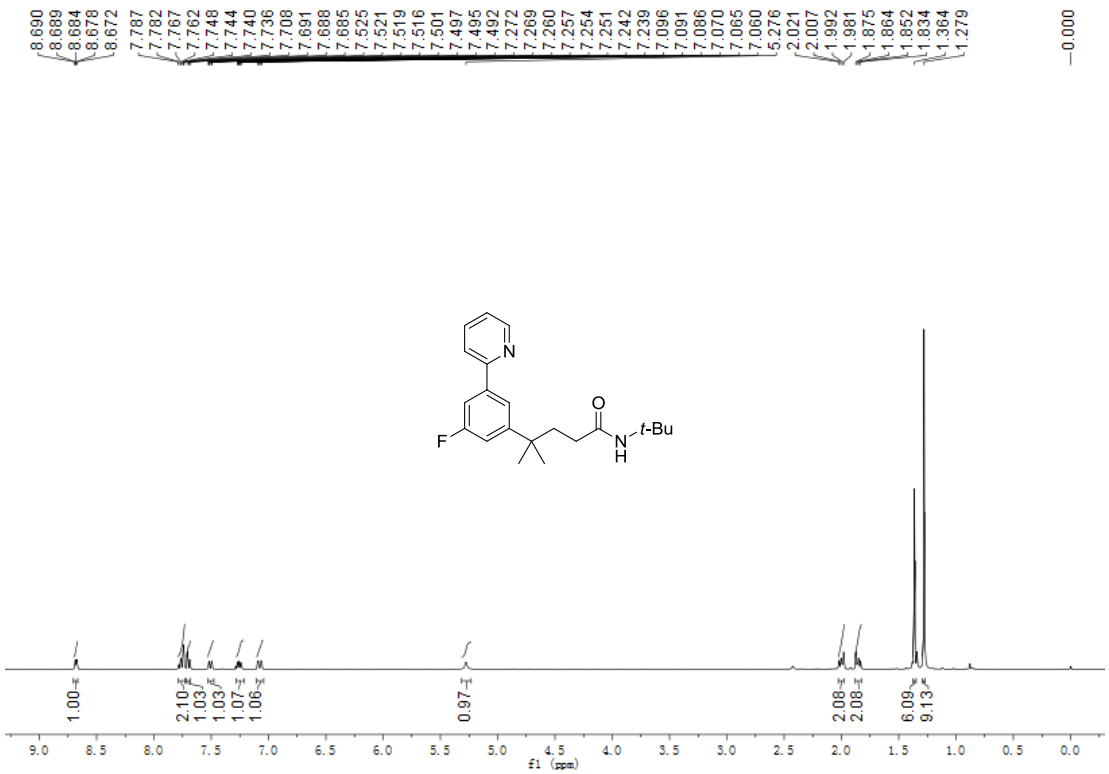

**Compound 3l $^{1}$H NMR (400 MHz, $CDCl_3$)**



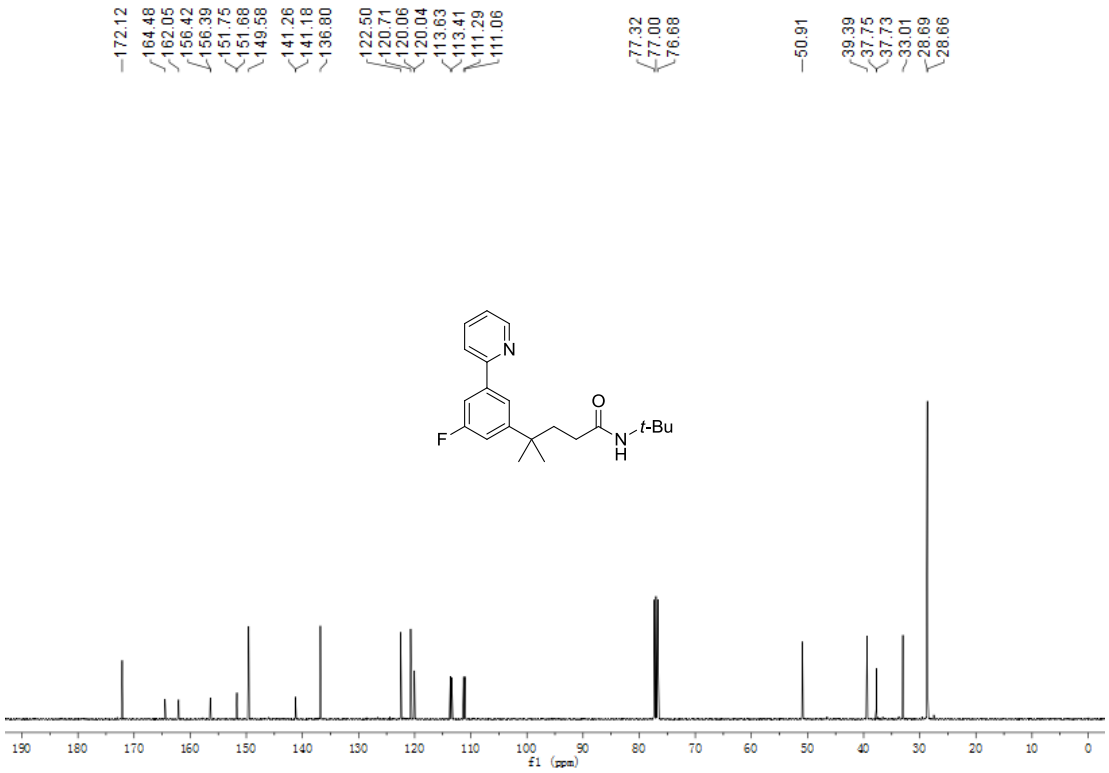
**Compound 3l $^{13}$C NMR (101 MHz, $CDCl_3$)**



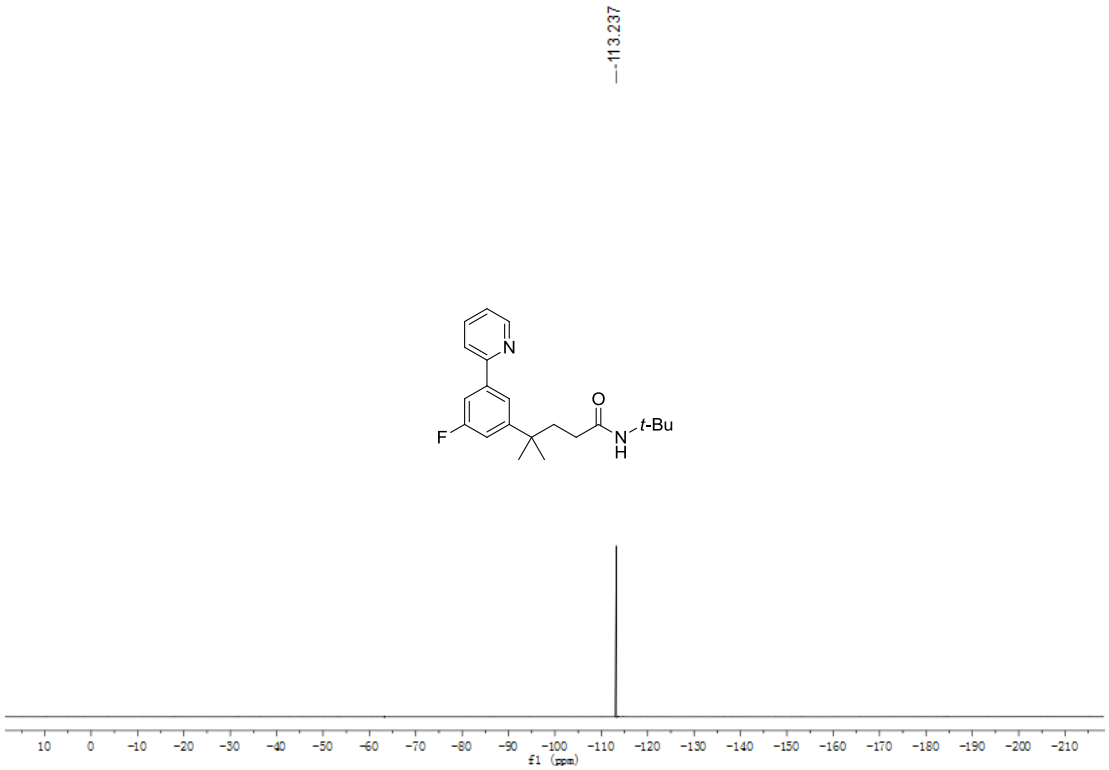

**Compound 3m $^{1}$H NMR (400 MHz, $CDCl_3$)**



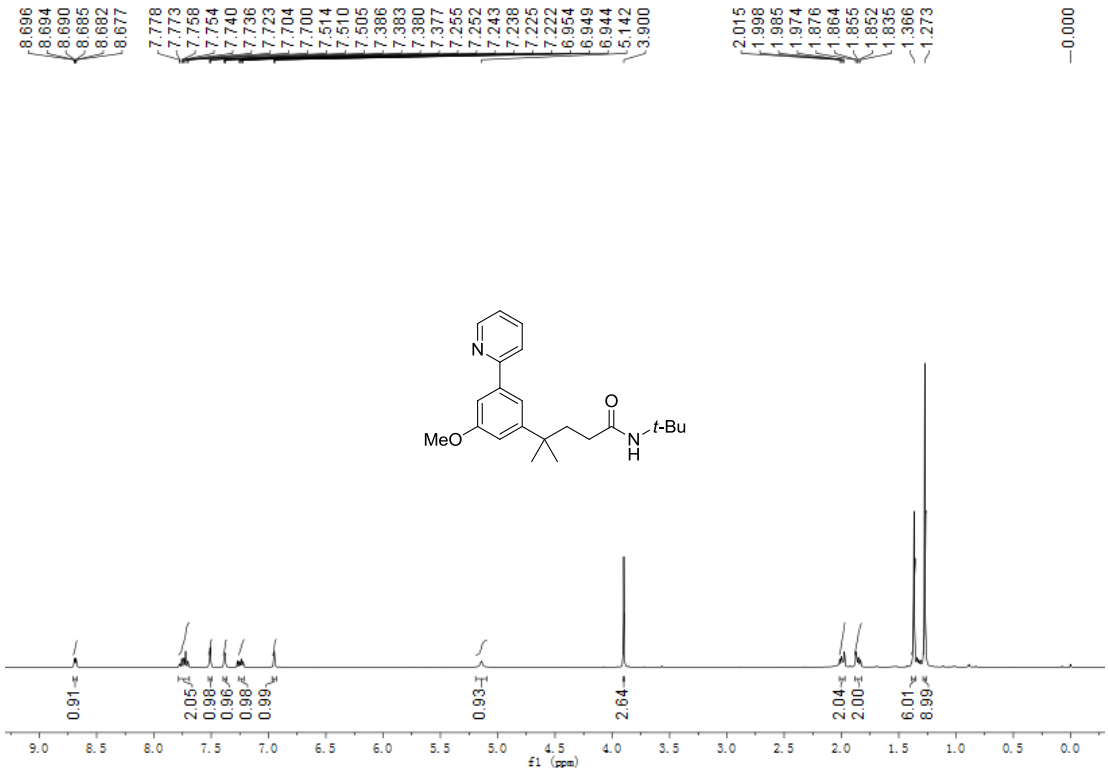
**Compound 3m $^{13}$C NMR (101 MHz, $CDCl_3$)**




**Compound 3m $^{19}$F NMR (376 MHz, $CDCl_3$)**



## Compound 3n $^{1}$H NMR (400 MHz, $CDCl_3$)

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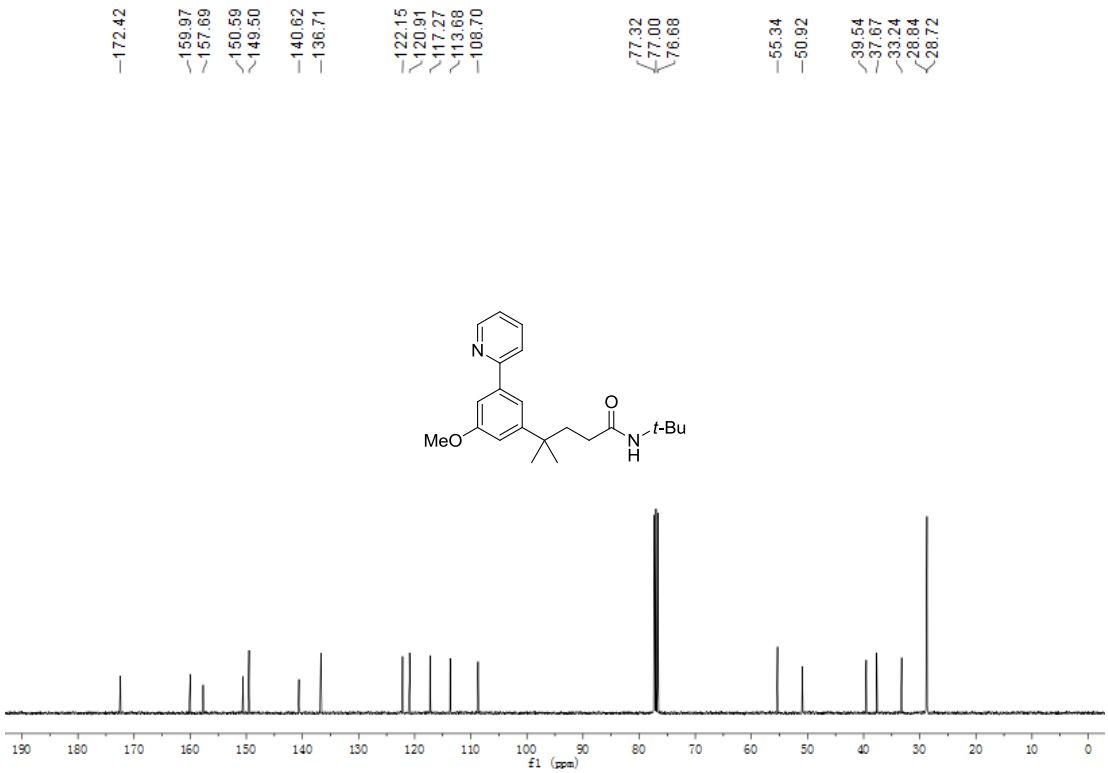

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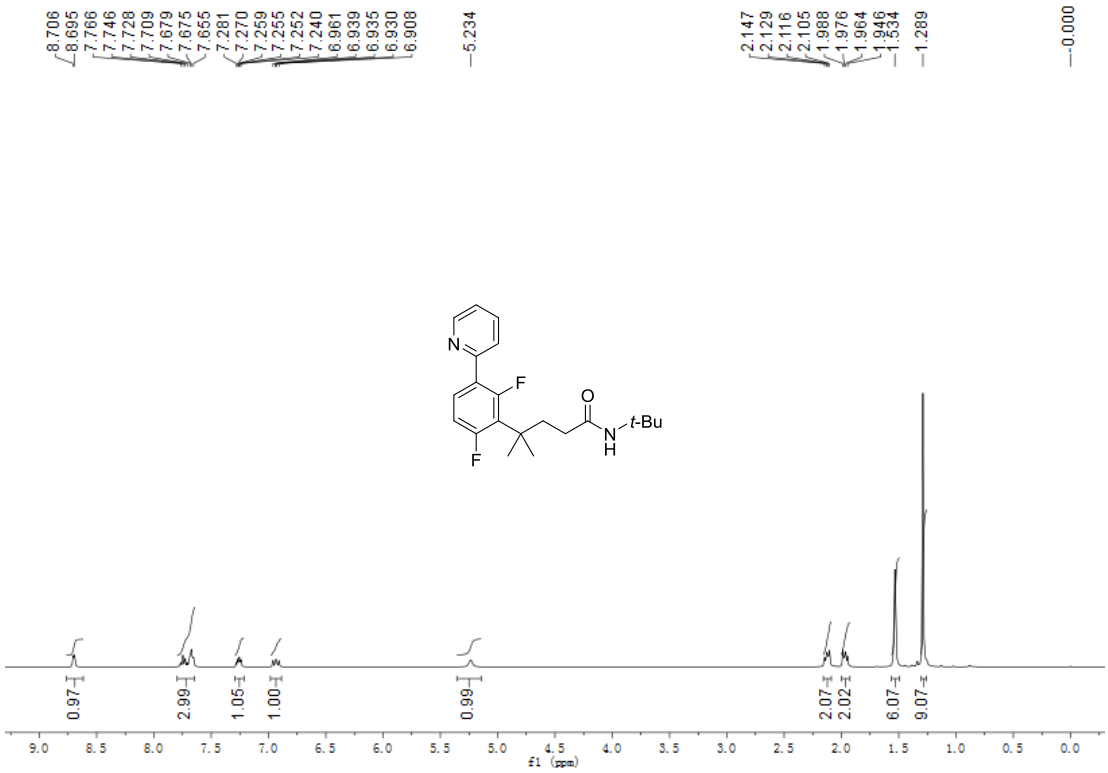
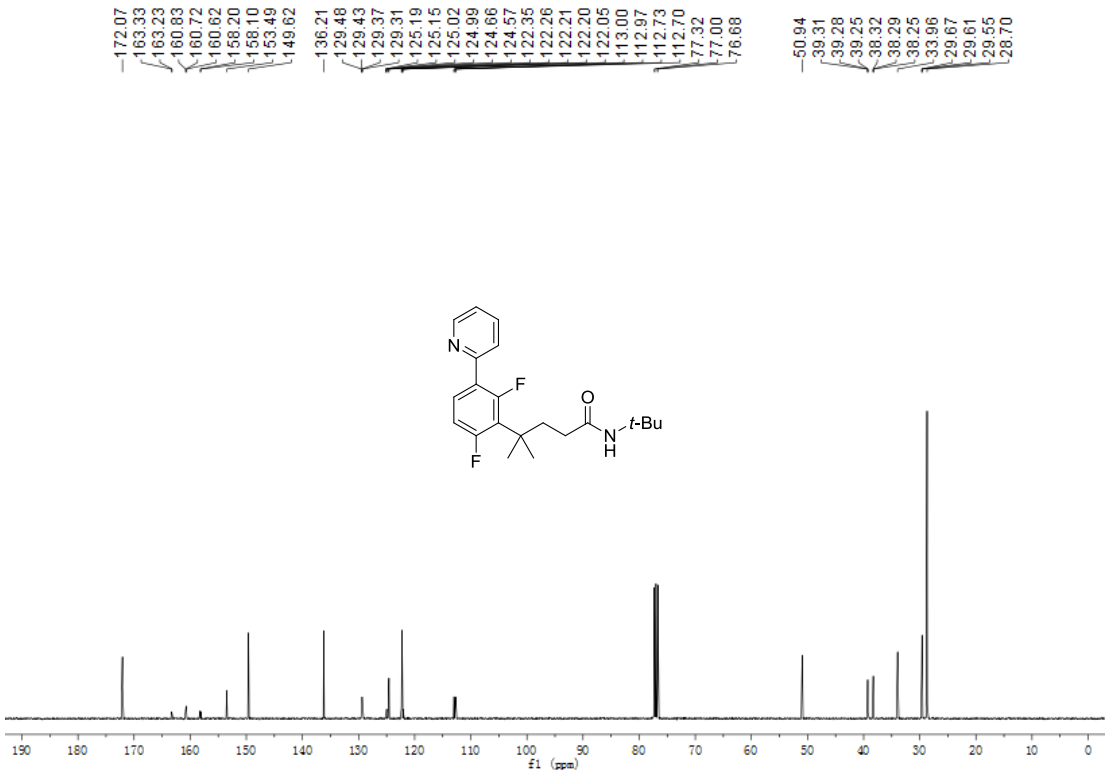
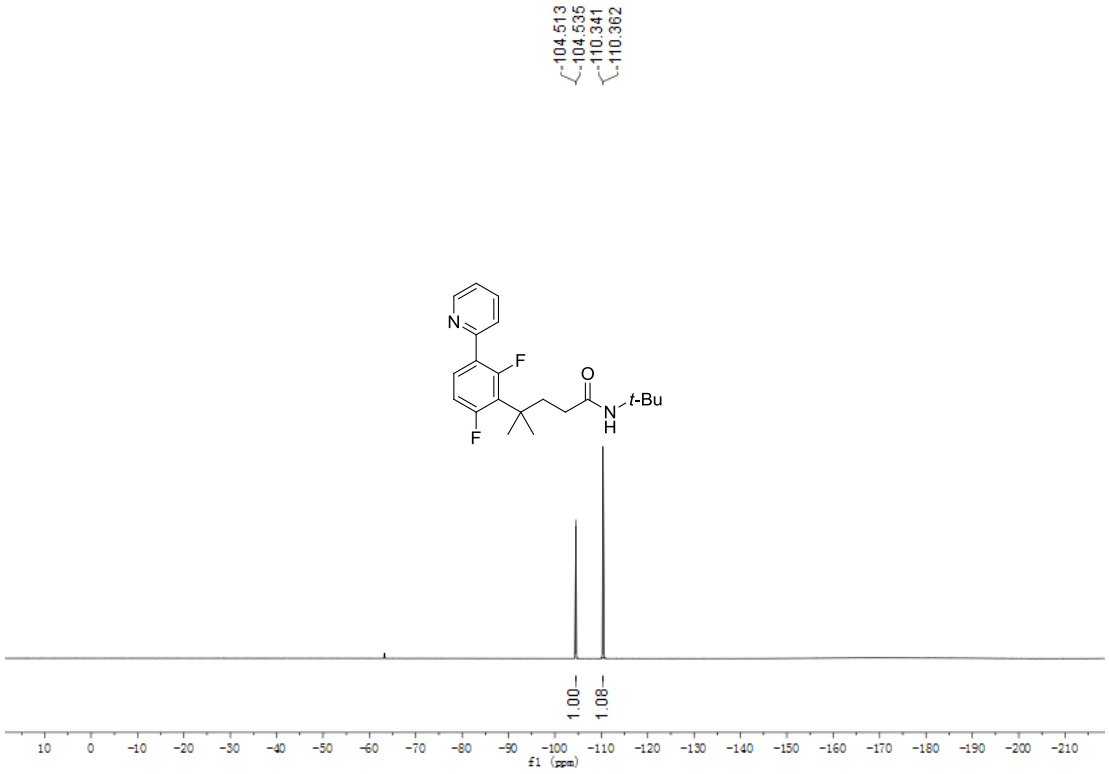


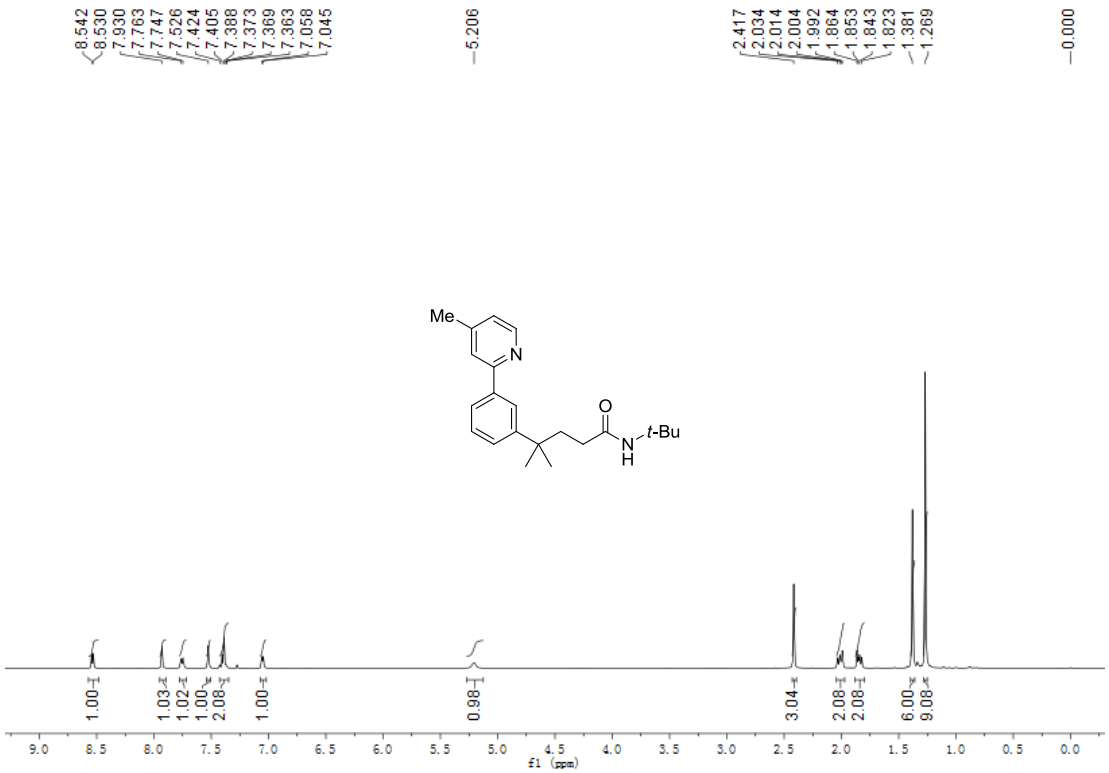

## Compound 3o $^{13}$C NMR (101 MHz, $CDCl_3$)



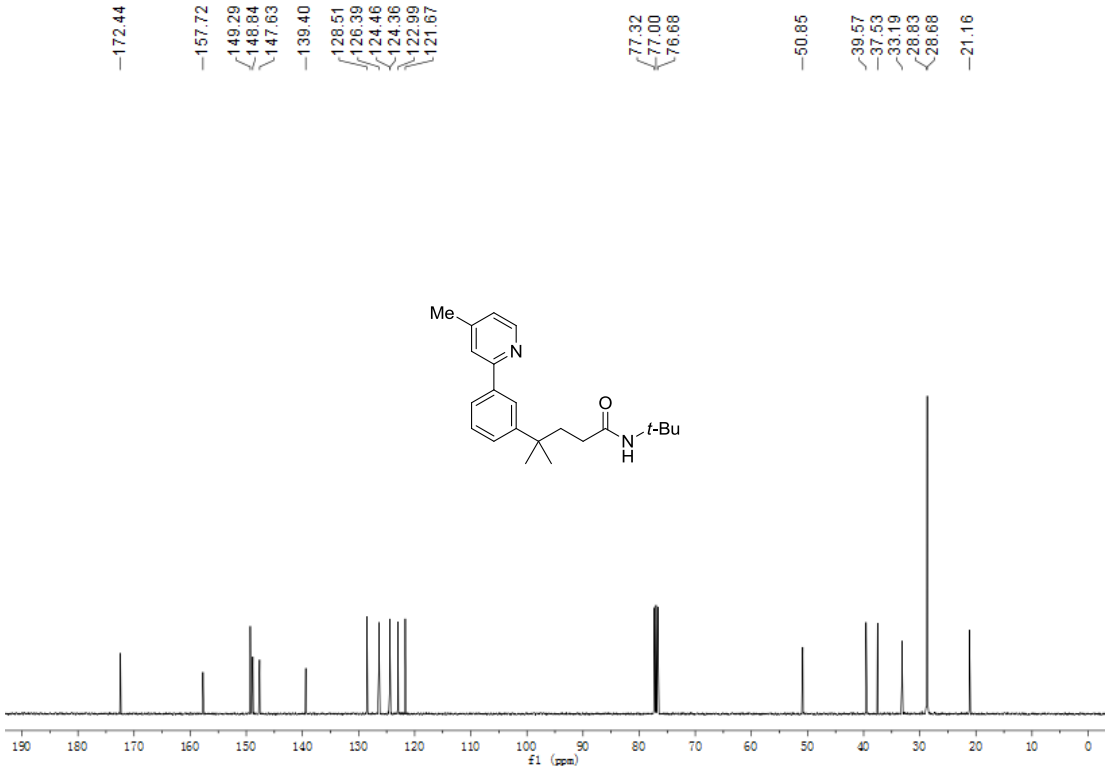
**Compound 3o $^{19}$F NMR (376 MHz, $CDCl_3$)**



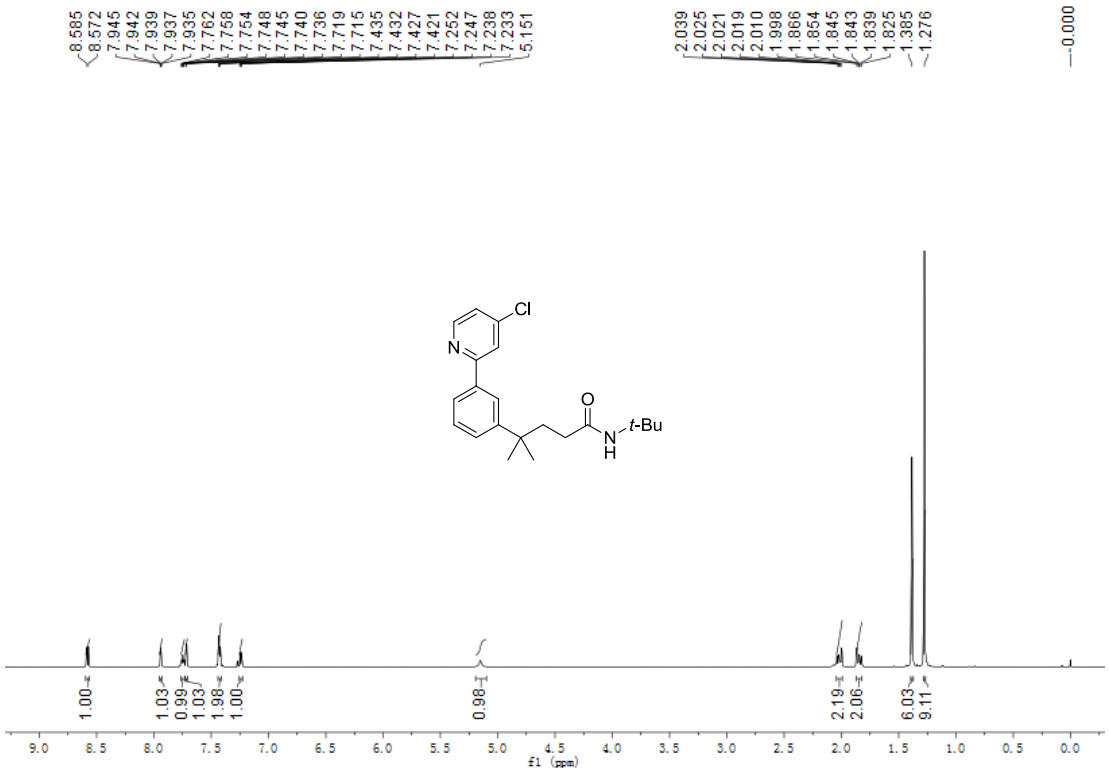

**Compound 3p $^{1}$H NMR (400 MHz, $CDCl_3$)**



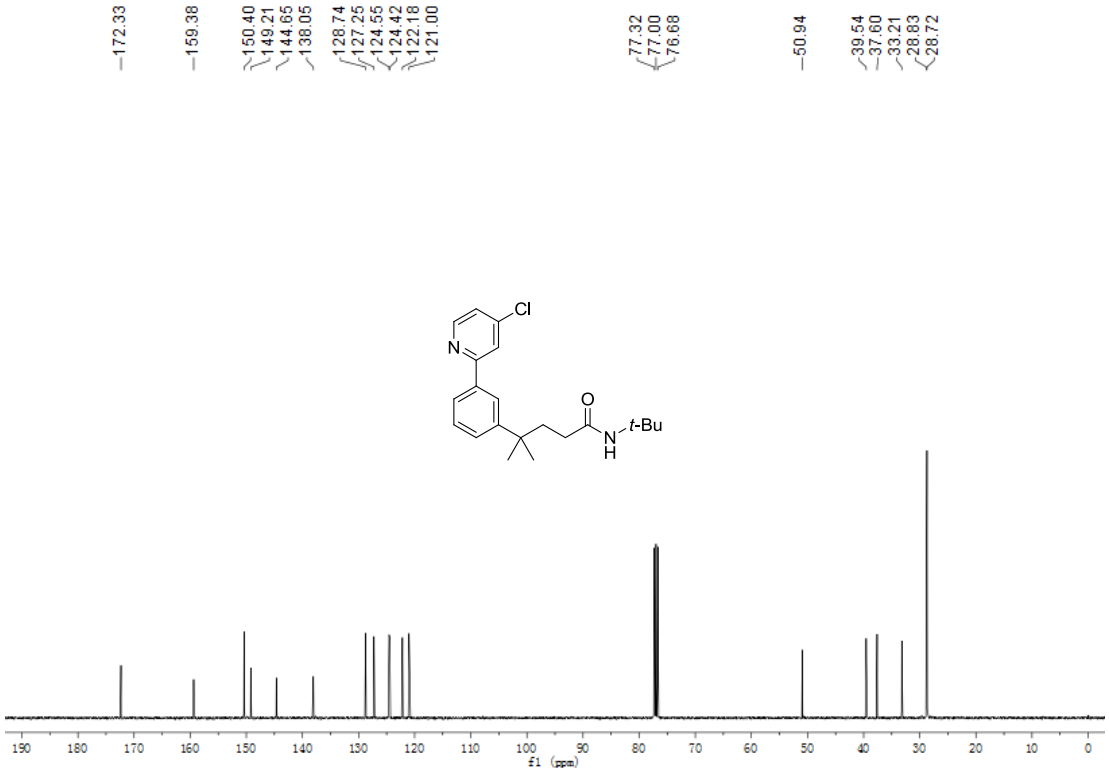
## Compound 3p $^{13}$C NMR (101 MHz, $CDCl_3$)



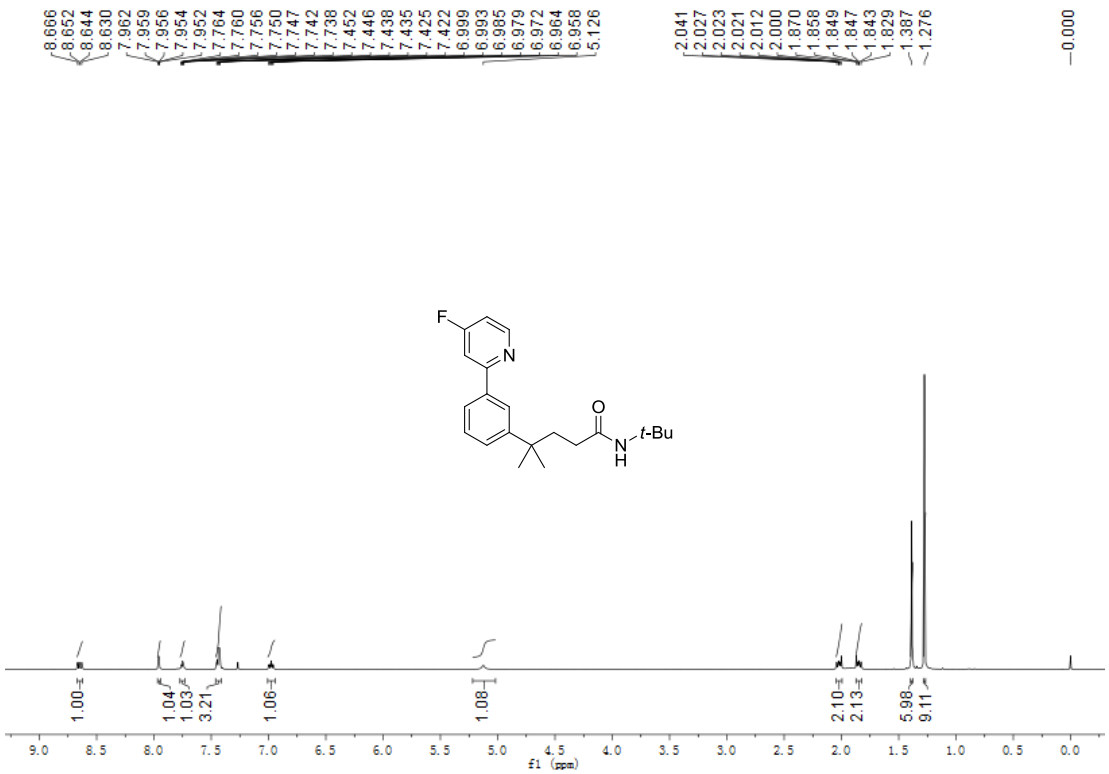

## Compound 3q $^{1}$H NMR (400 MHz, $CDCl_3$)



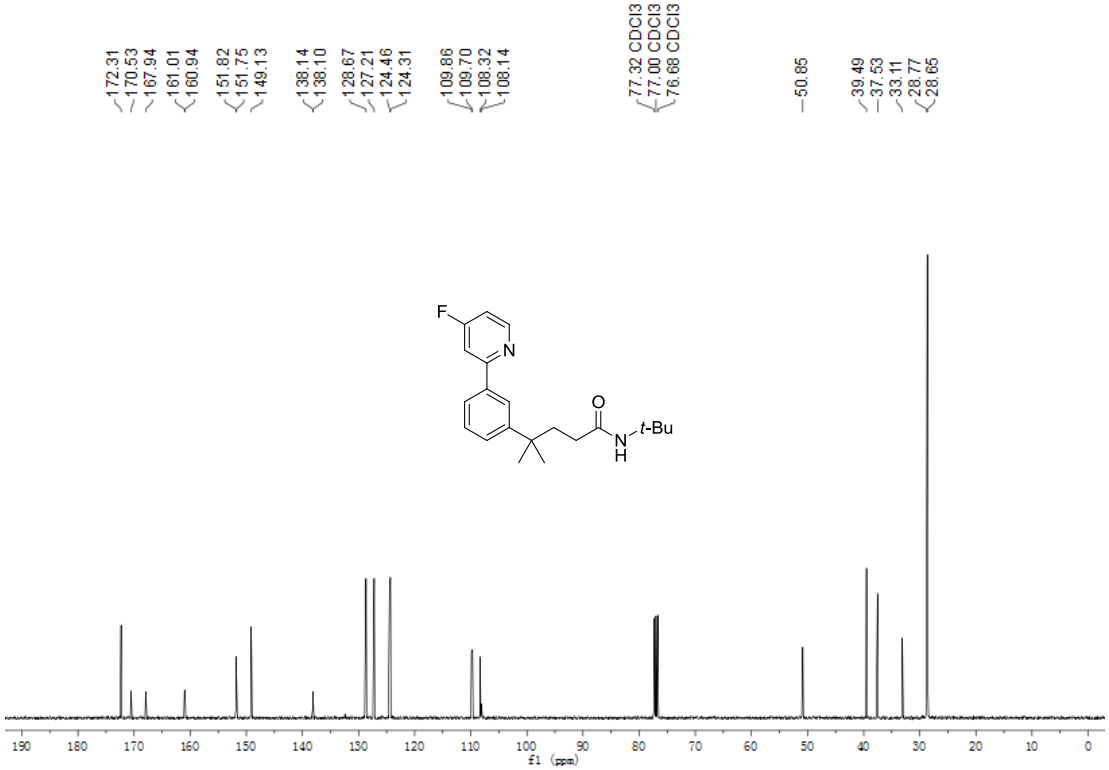
## Compound 3q $^{13}$C NMR (101 MHz, $CDCl_3$)



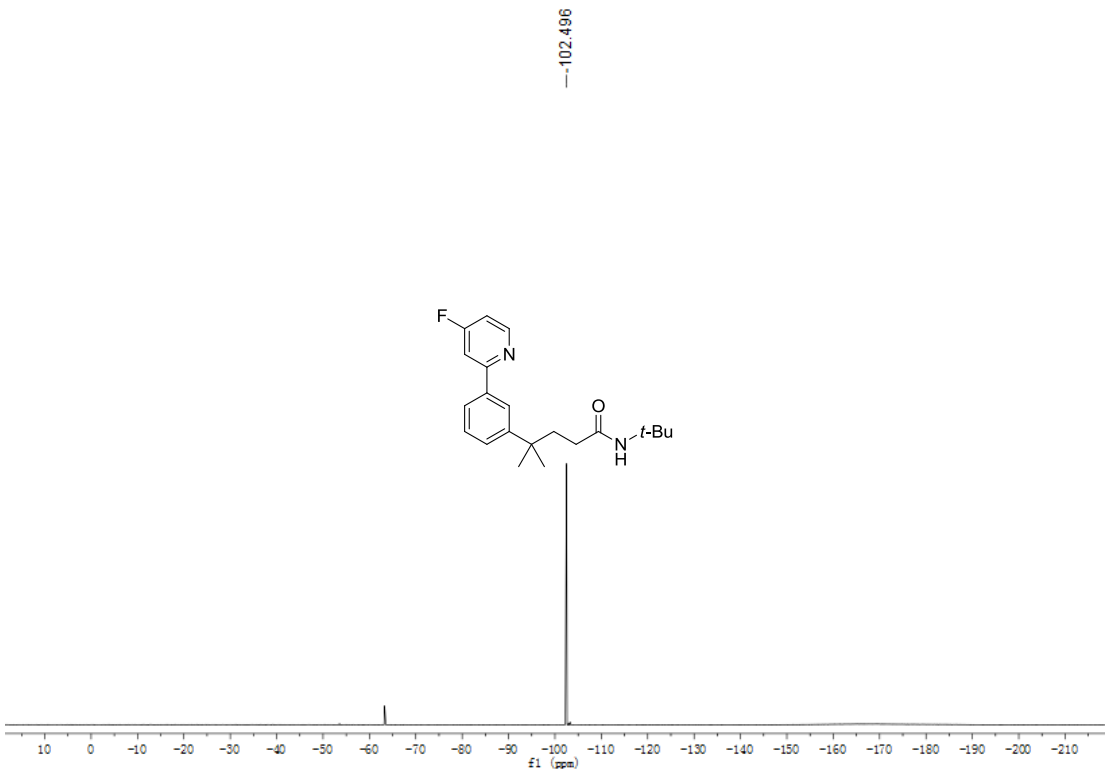

## Compound 3r $^{1}$H NMR (400 MHz, $CDCl_3$)



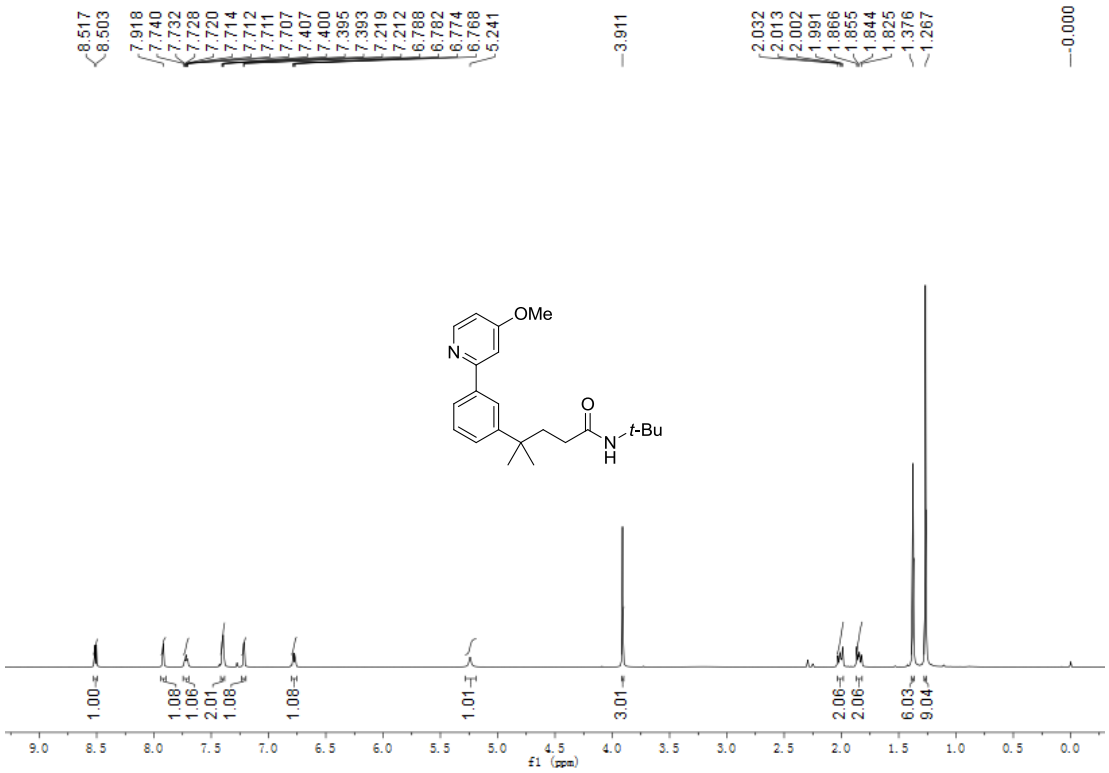
**Compound 3r $^{13}$C NMR (101 MHz, $CDCl_3$)**



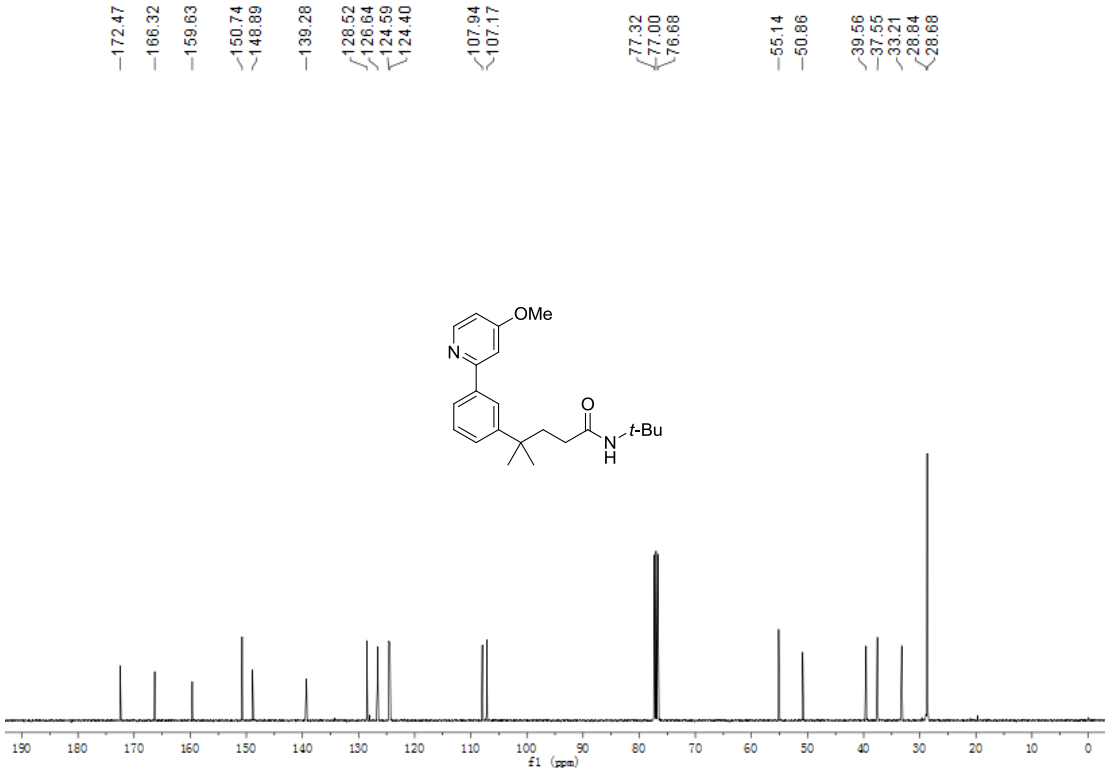

**Compound 3r $^{19}$F NMR (376 MHz, $CDCl_3$)**



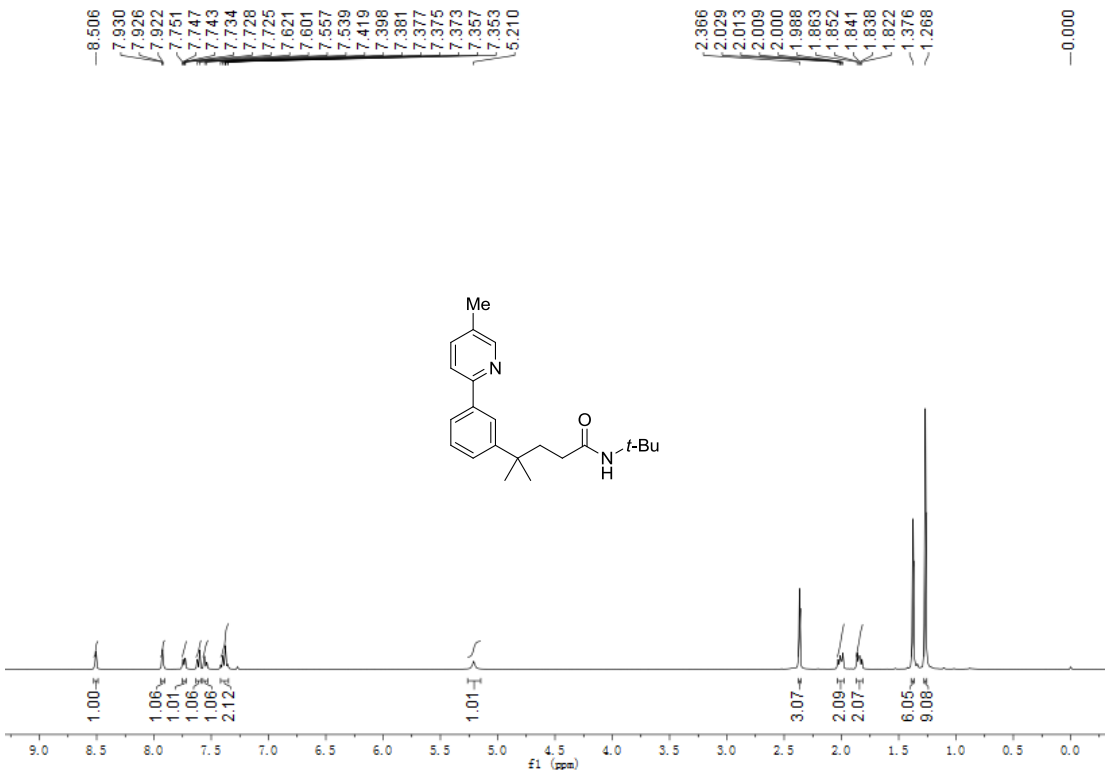
## Compound 3s $^{1}$H NMR (400 MHz, $CDCl_3$)



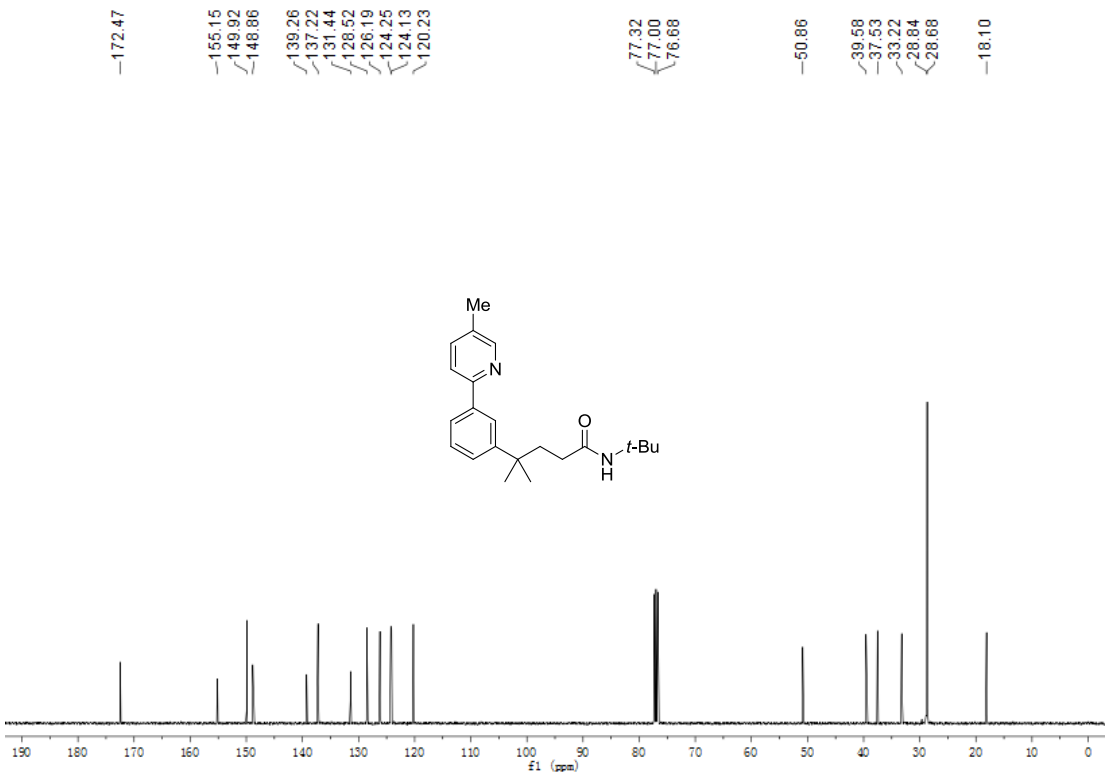

## Compound 3s $^{13}$C NMR (101 MHz, $CDCl_3$)



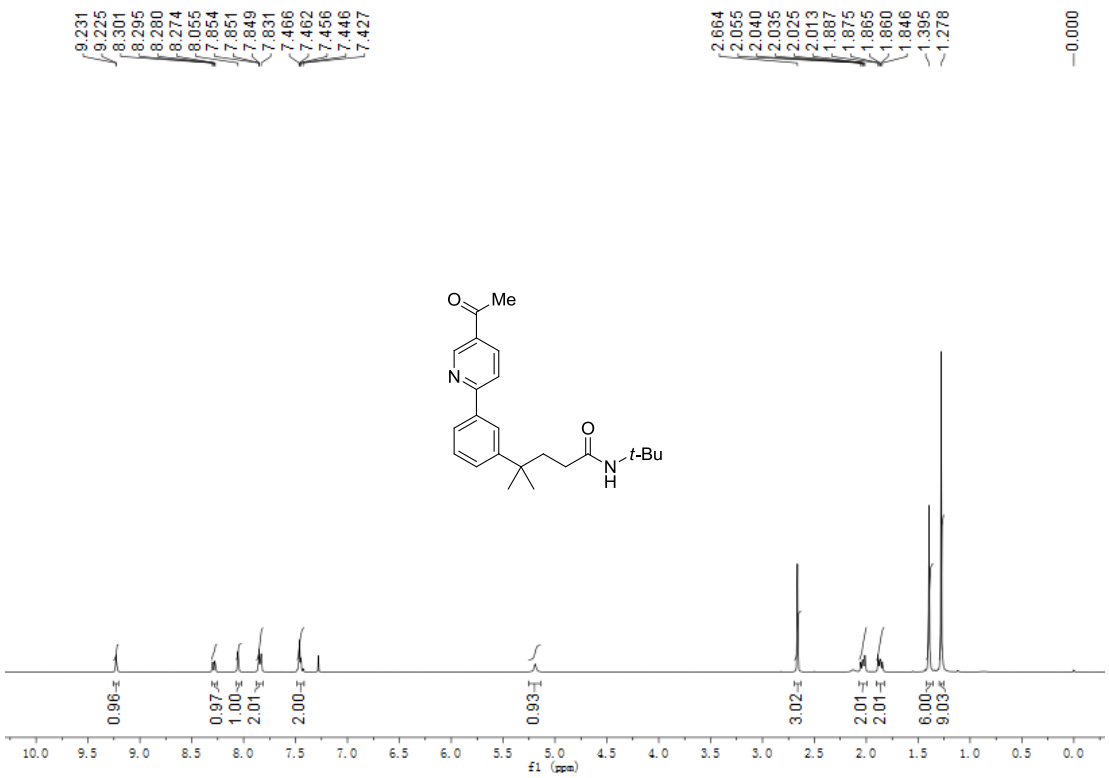
## Compound 3t $^{1}$H NMR (400 MHz, $CDCl_3$)



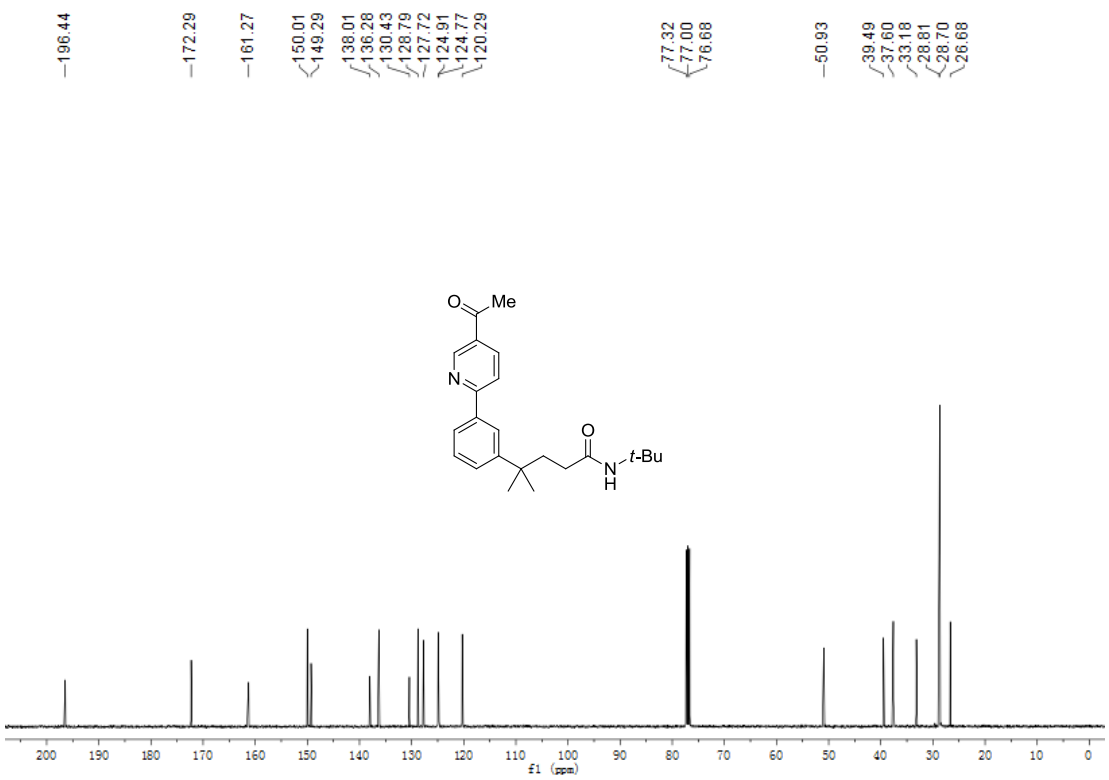

## Compound 3t $^{13}$C NMR (101 MHz, $CDCl_3$)



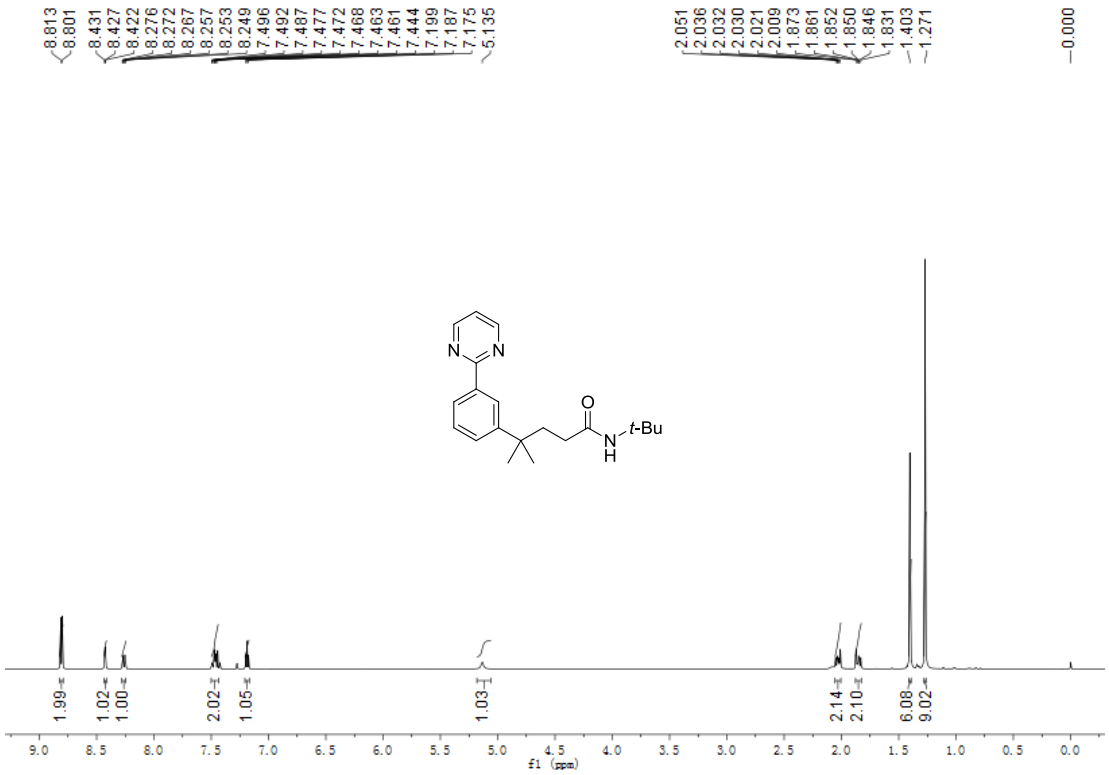
## Compound 3u $^{1}$H NMR (400 MHz, $CDCl_3$)



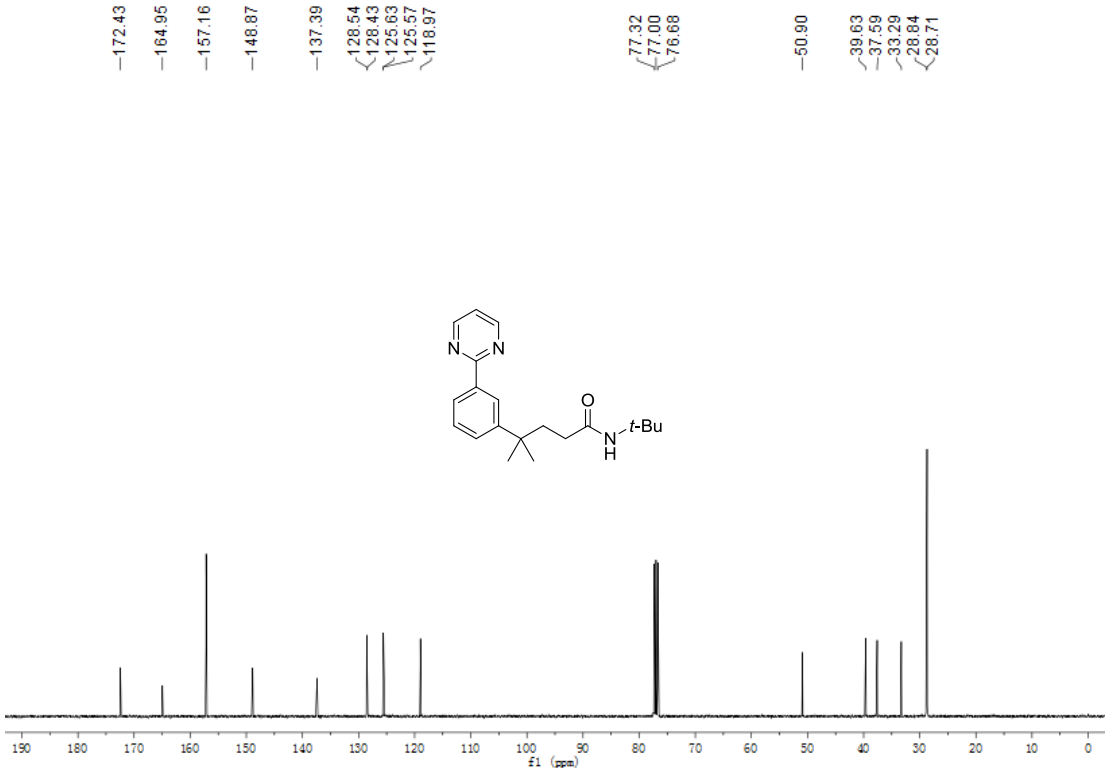

## Compound 3u $^{13}$C NMR (101 MHz, $CDCl_3$)



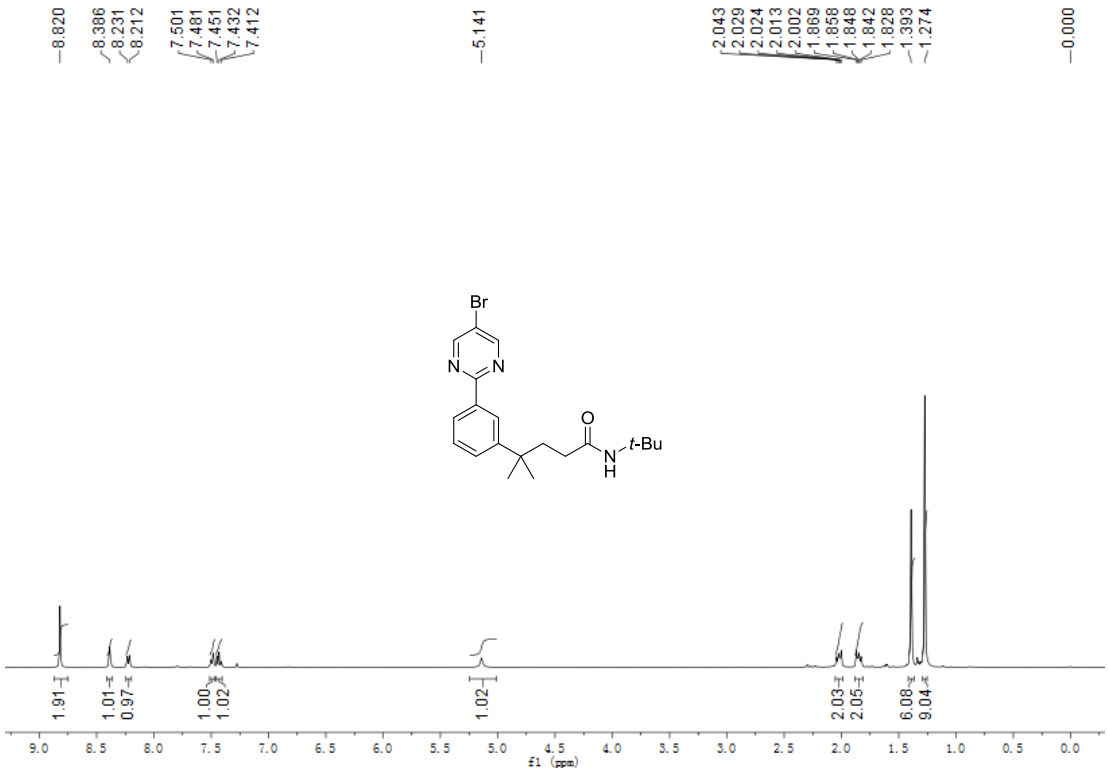
## Compound 3v $^{1}$H NMR (400 MHz, $CDCl_3$)



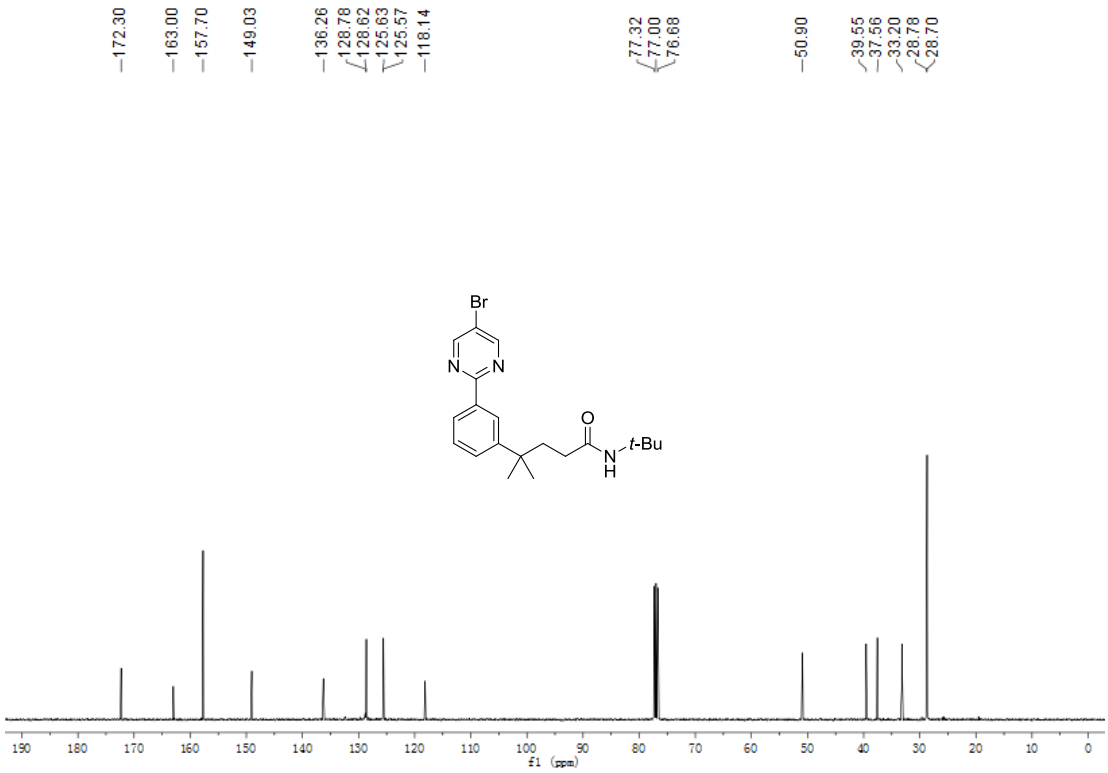

## Compound 3v $^{13}$C NMR (101 MHz, $CDCl_3$)



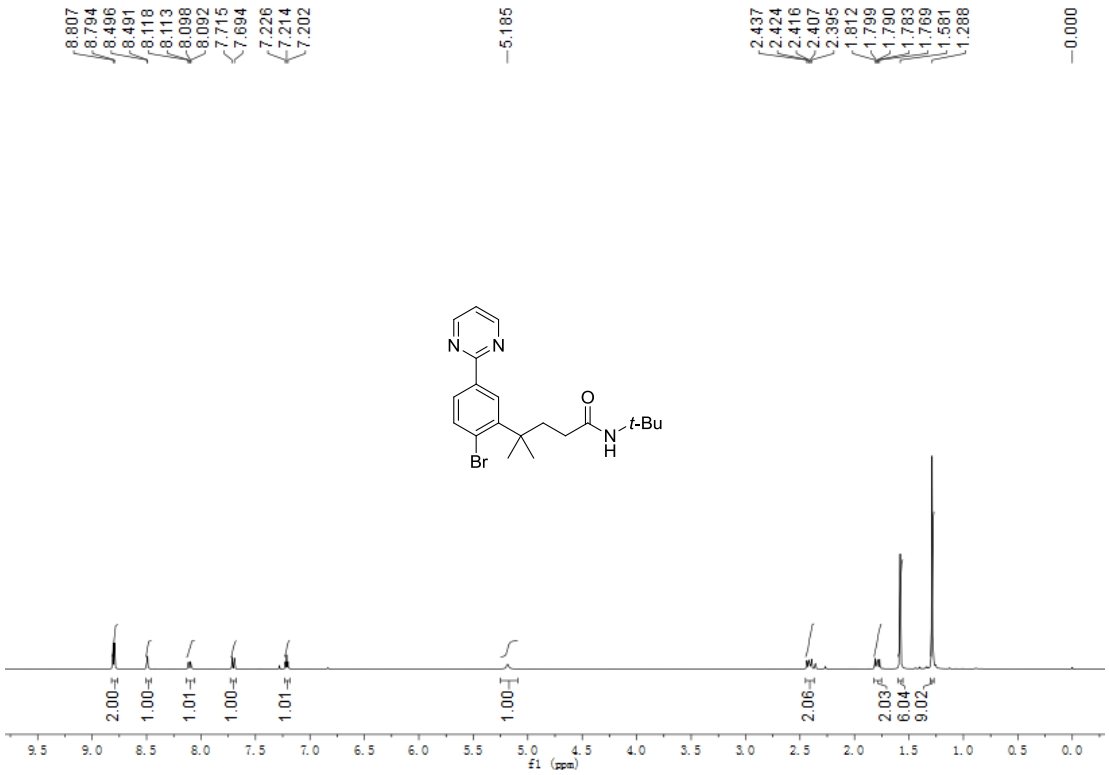
## Compound 3w $^{1}$H NMR (400 MHz, $CDCl_3$)



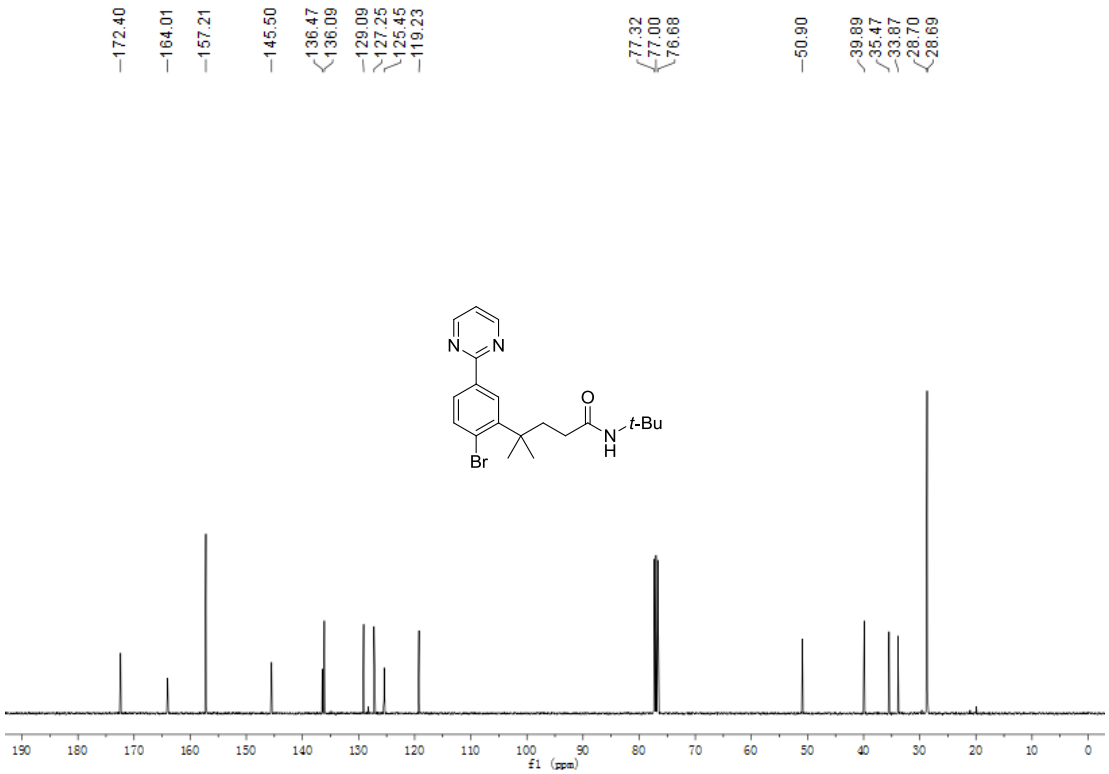

## Compound 3w $^{13}$C NMR (101 MHz, $CDCl_3$)



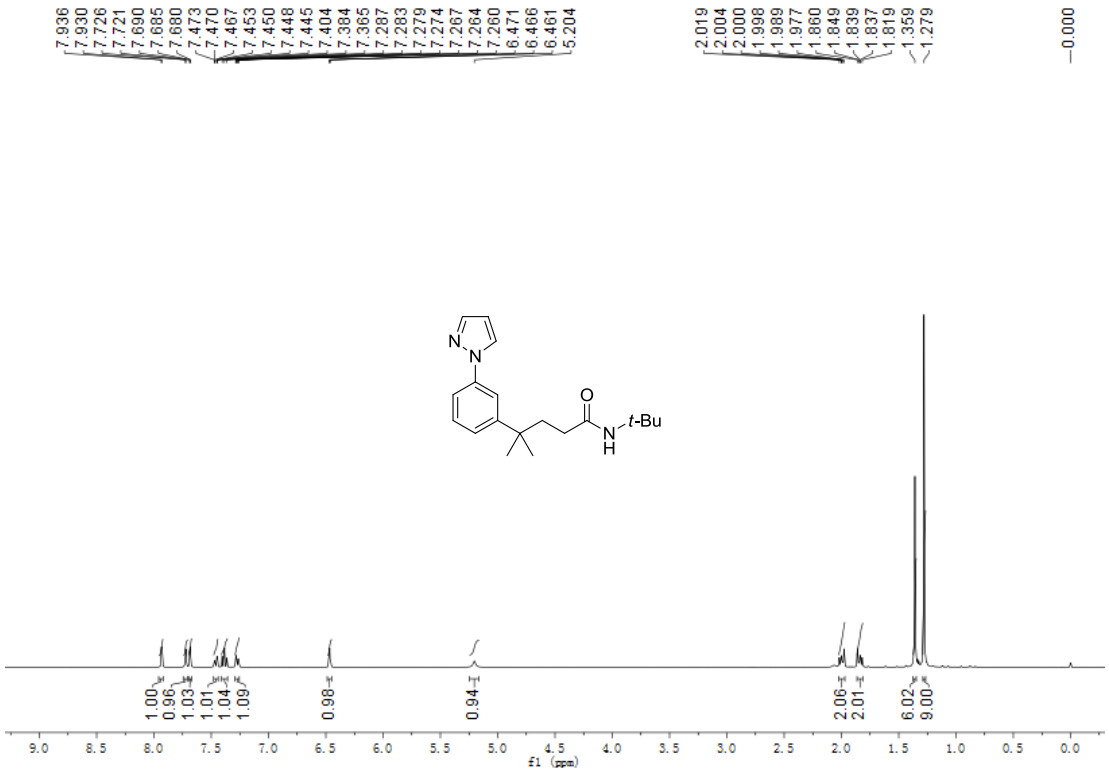
## Compound 3x $^{1}$H NMR (400 MHz, $CDCl_3$)



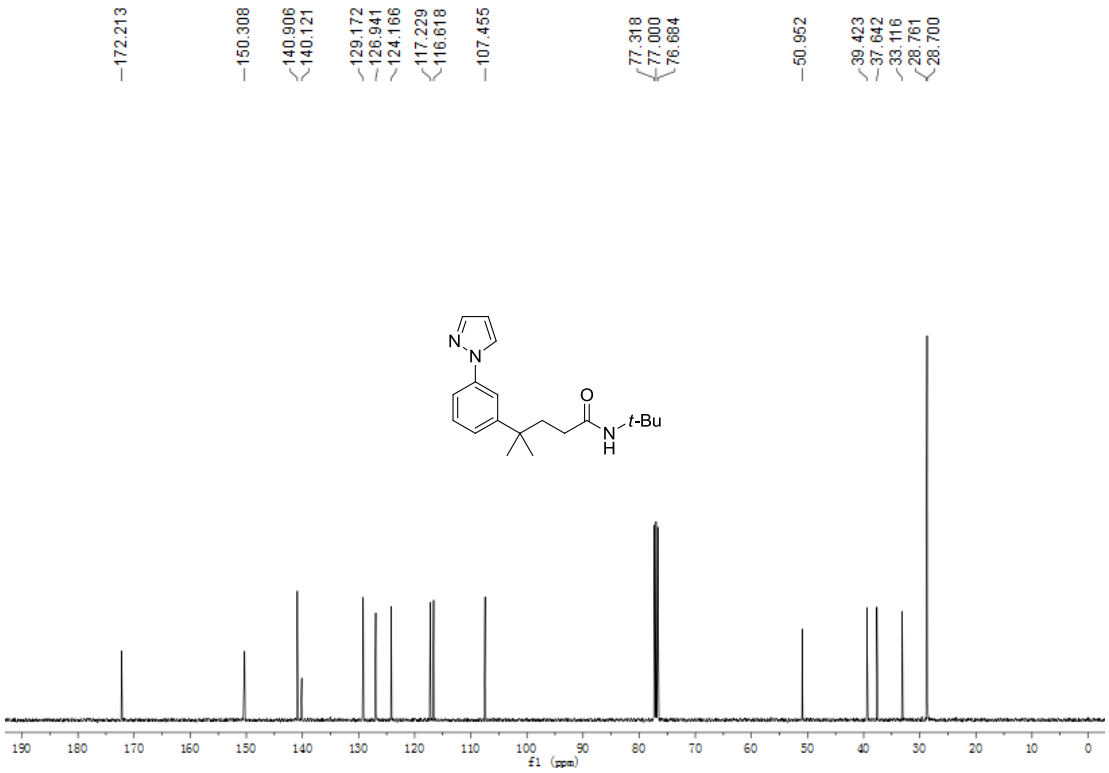

## Compound 3x $^{13}$C NMR (101 MHz, $CDCl_3$)



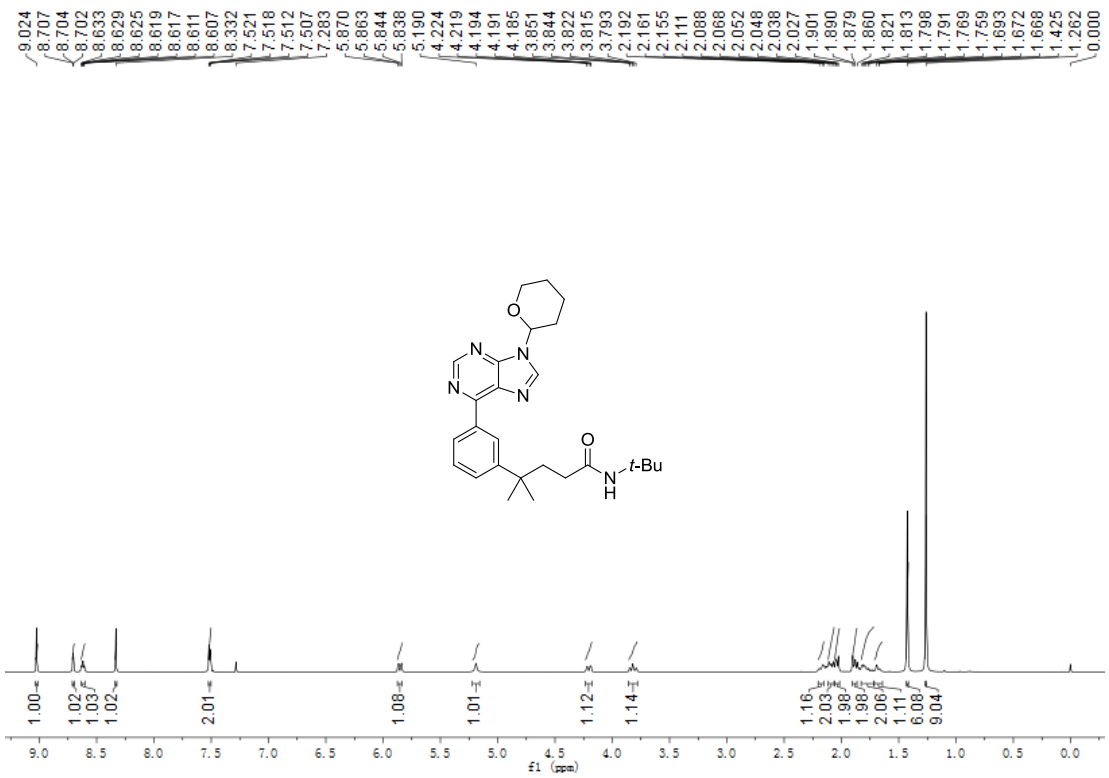
## Compound 3y $^{1}$H NMR (400 MHz, $CDCl_3$)



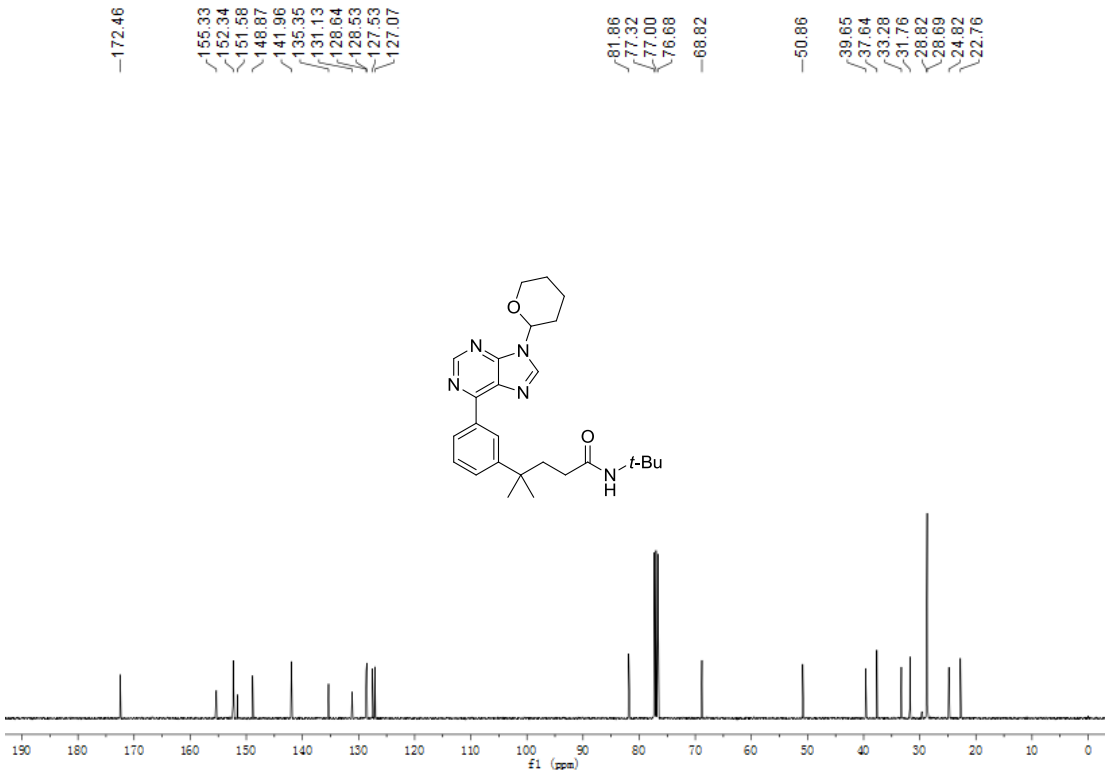

## Compound 3y $^{13}$C NMR (101 MHz, $CDCl_3$)



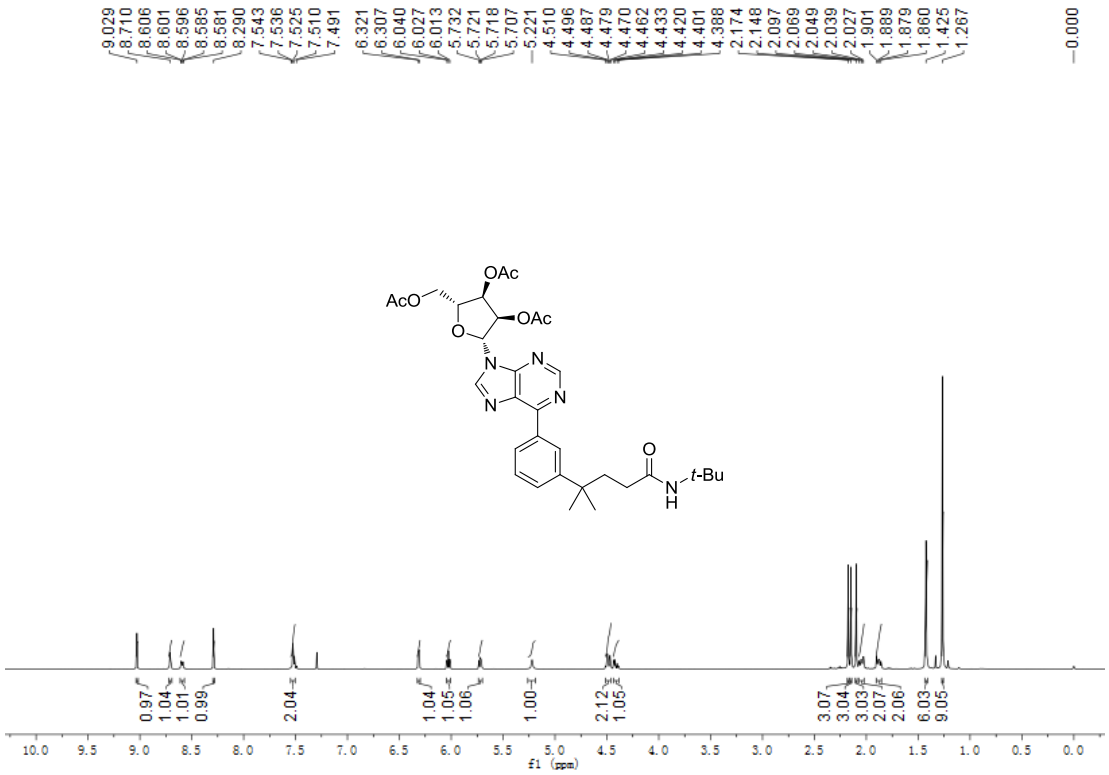
## Compound 3z $^{1}$H NMR (400 MHz, $CDCl_3$)



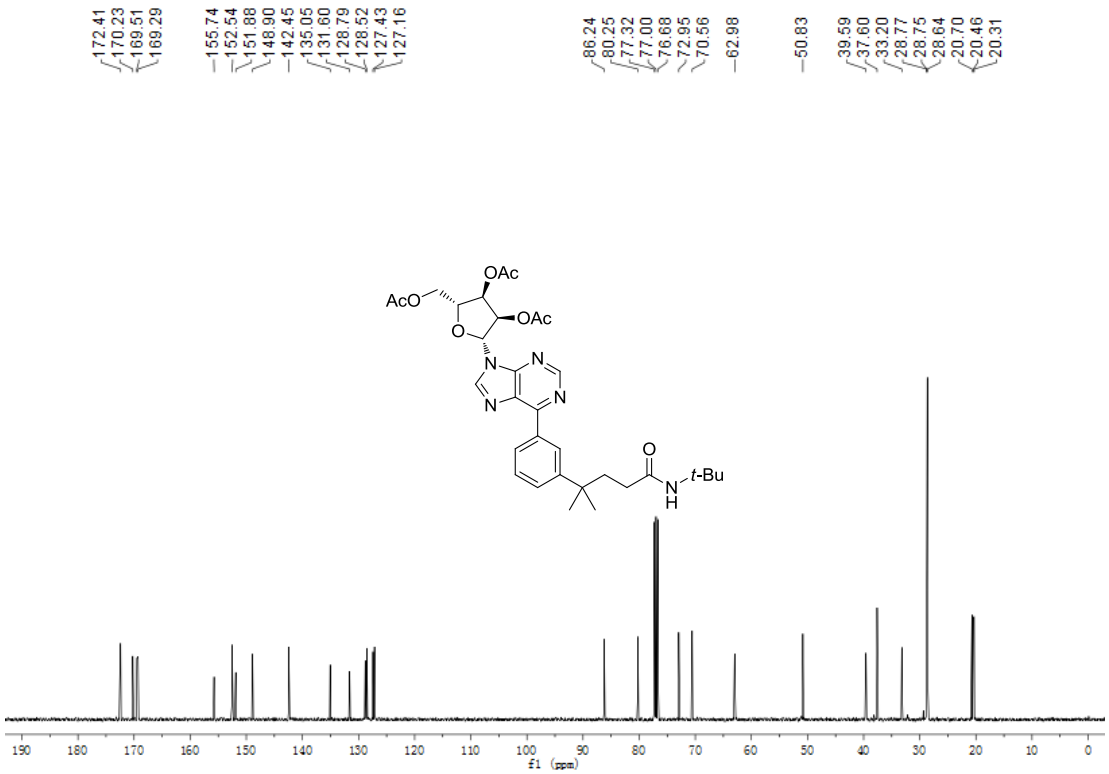

## Compound 3z $^{13}$C NMR (101 MHz, $CDCl_3$)



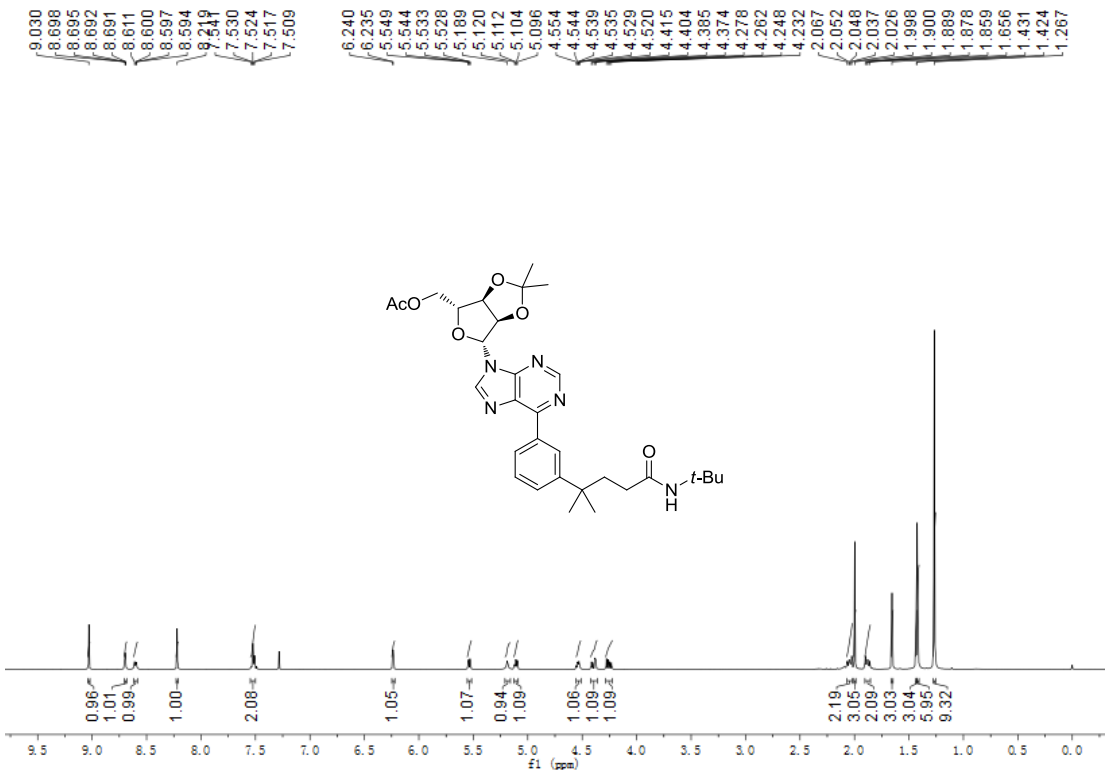
## Compound 3aa $^{1}$H NMR (400 MHz, $CDCl_3$)



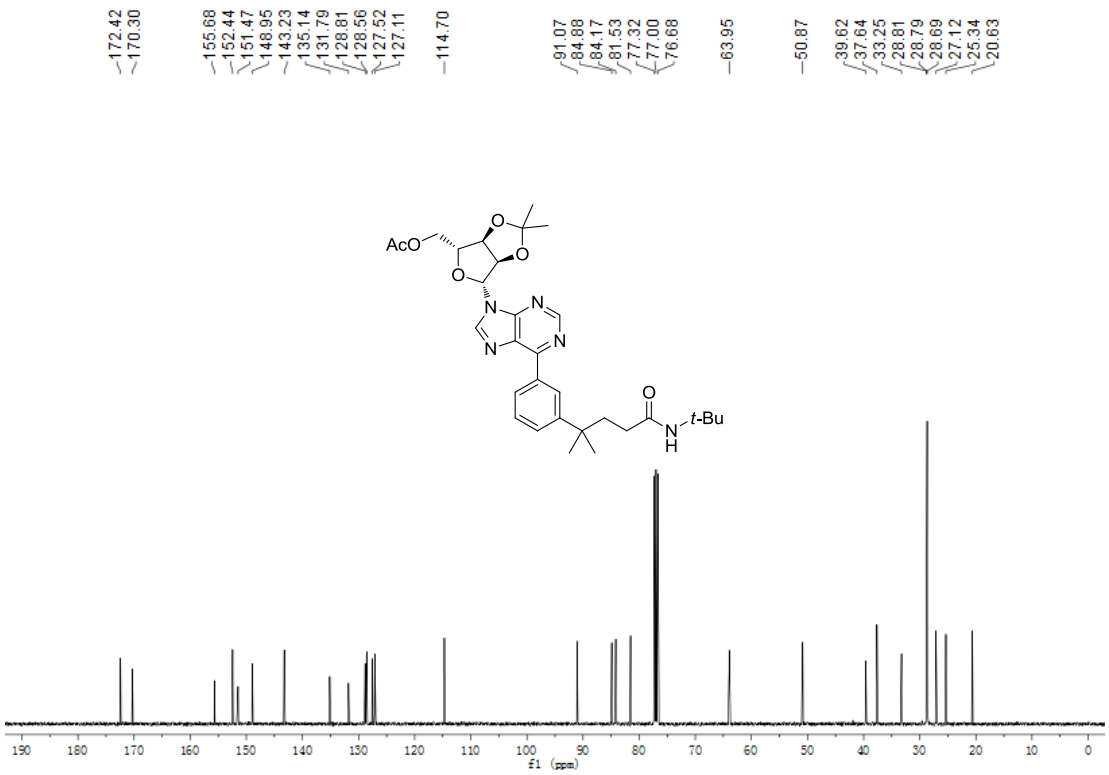

## Compound 3aa $^{13}$C NMR (101 MHz, $CDCl_3$)



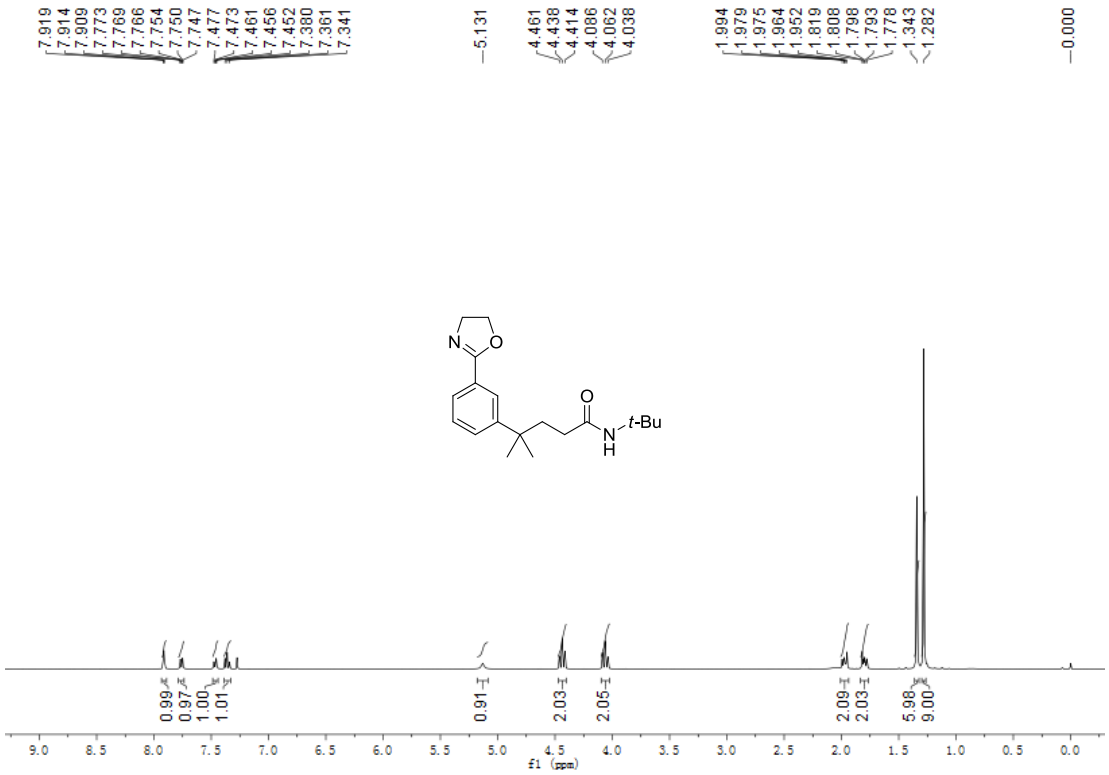
## Compound 3ab $^{1}$H NMR (400 MHz, $CDCl_3$)



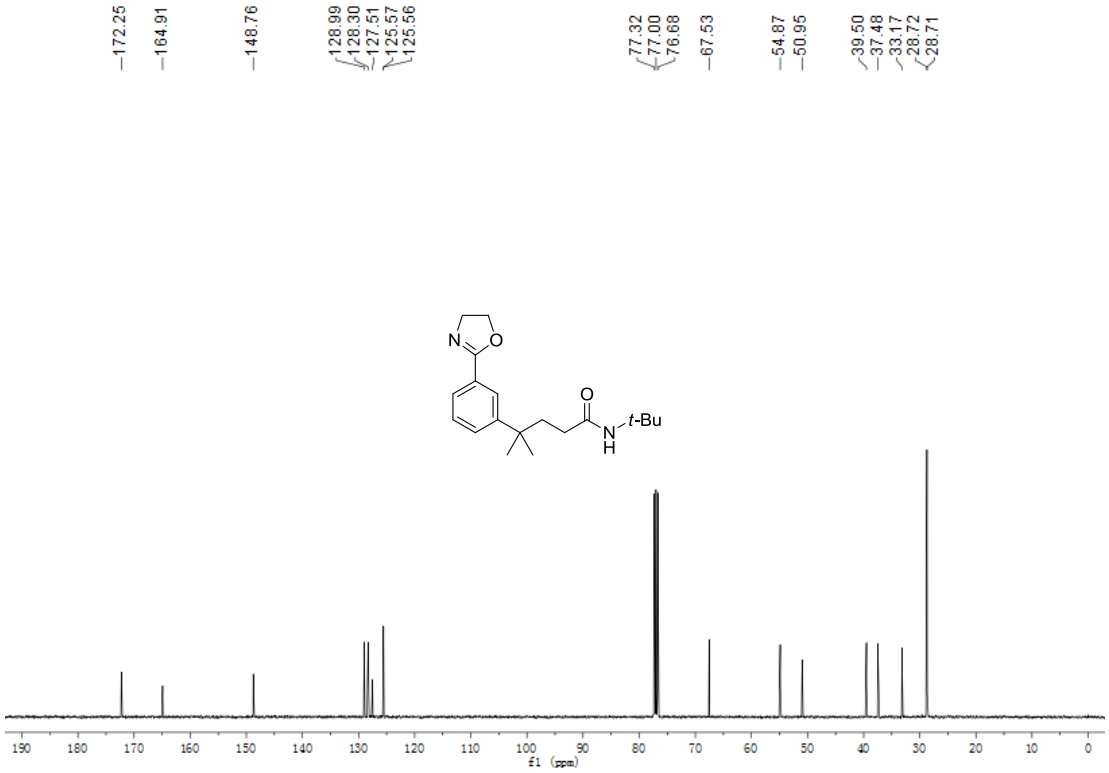

## Compound 3ab $^{13}$C NMR (101 MHz, $CDCl_3$)



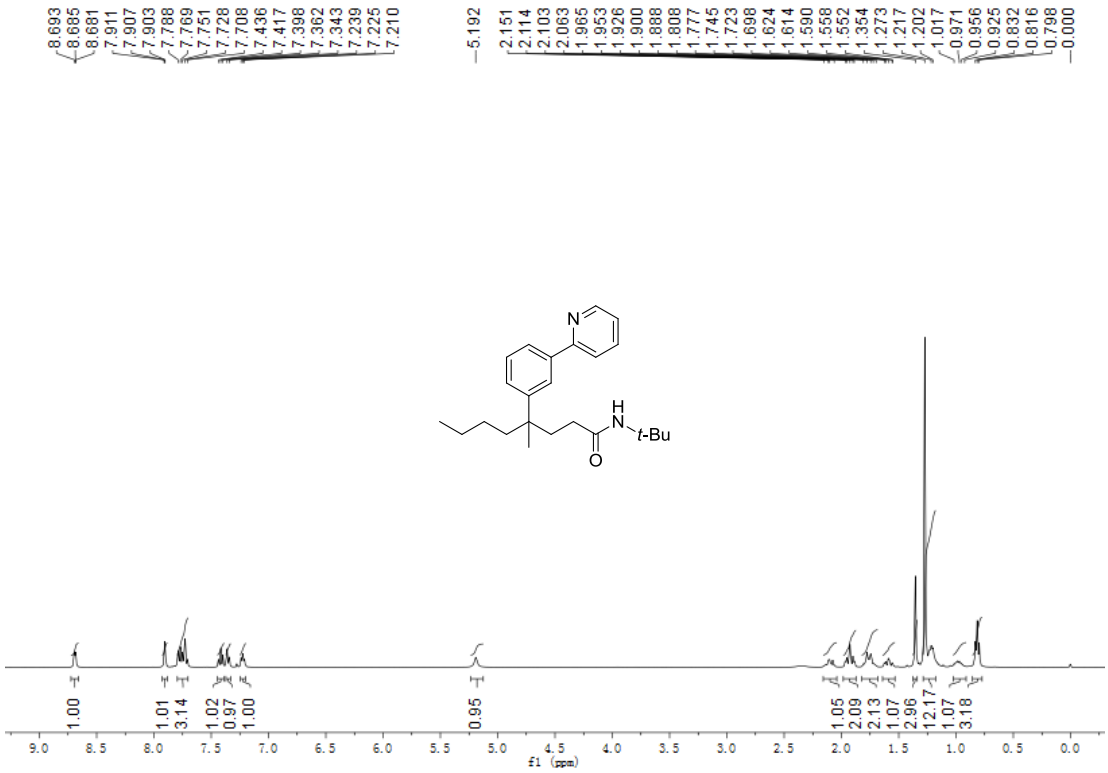
## Compound 3ac $^{1}$H NMR (400 MHz, $CDCl_3$)



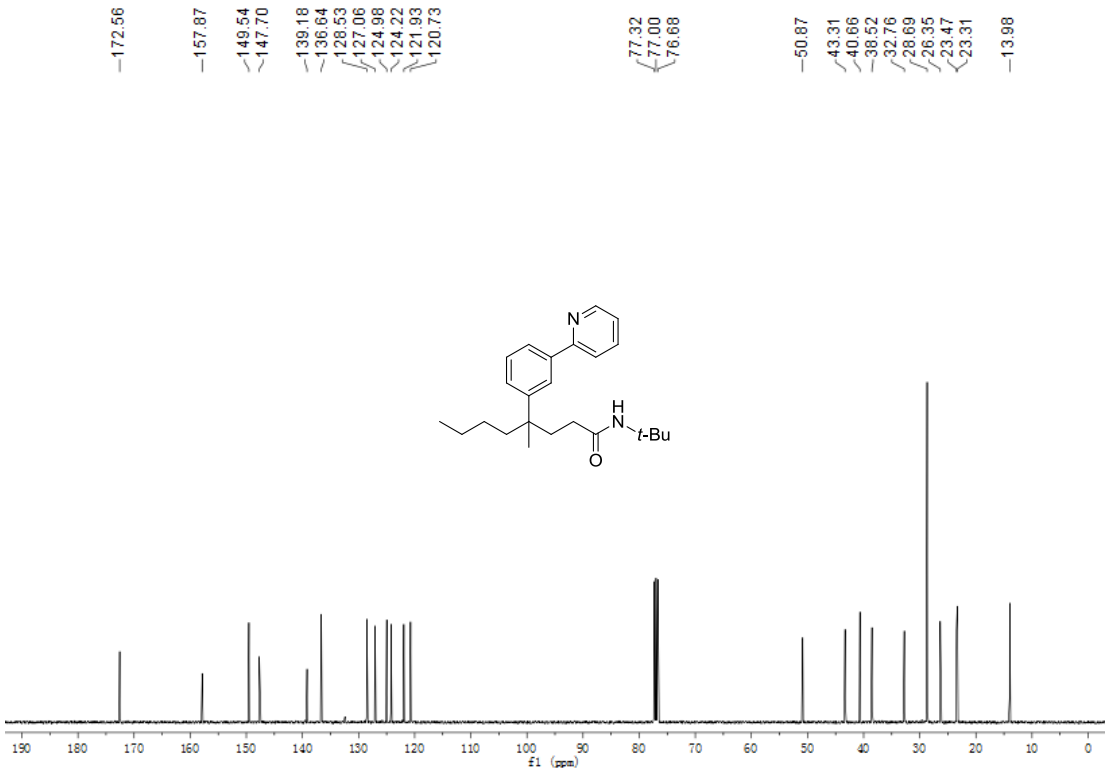

## Compound 3ac $^{13}$C NMR (101 MHz, $CDCl_3$)



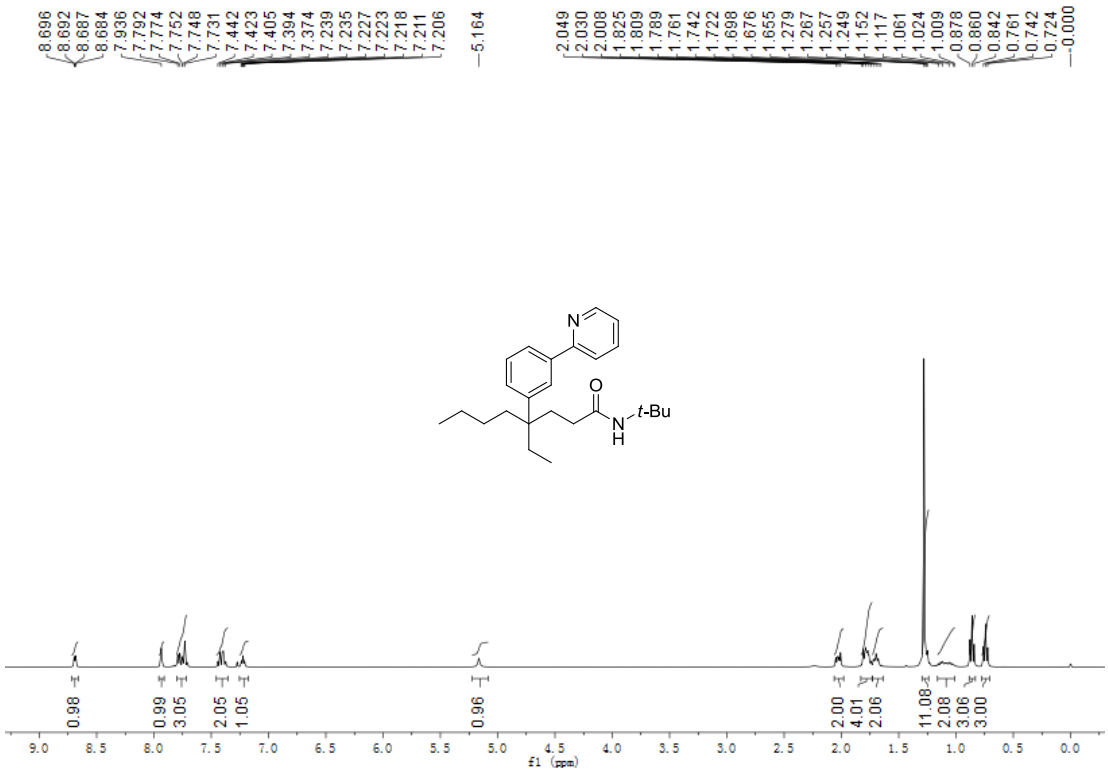
## Compound 3ae $^{1}$H NMR (400 MHz, $CDCl_3$)



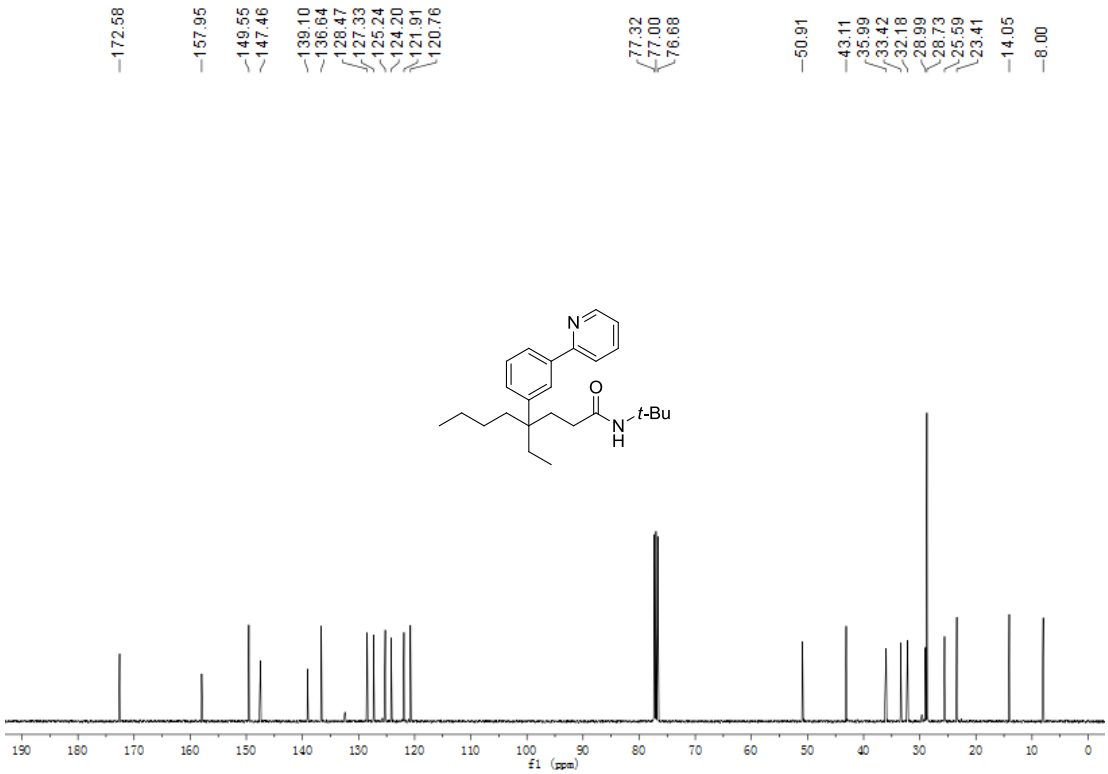

## Compound 3ae $^{13}$C NMR (101 MHz, $CDCl_3$)



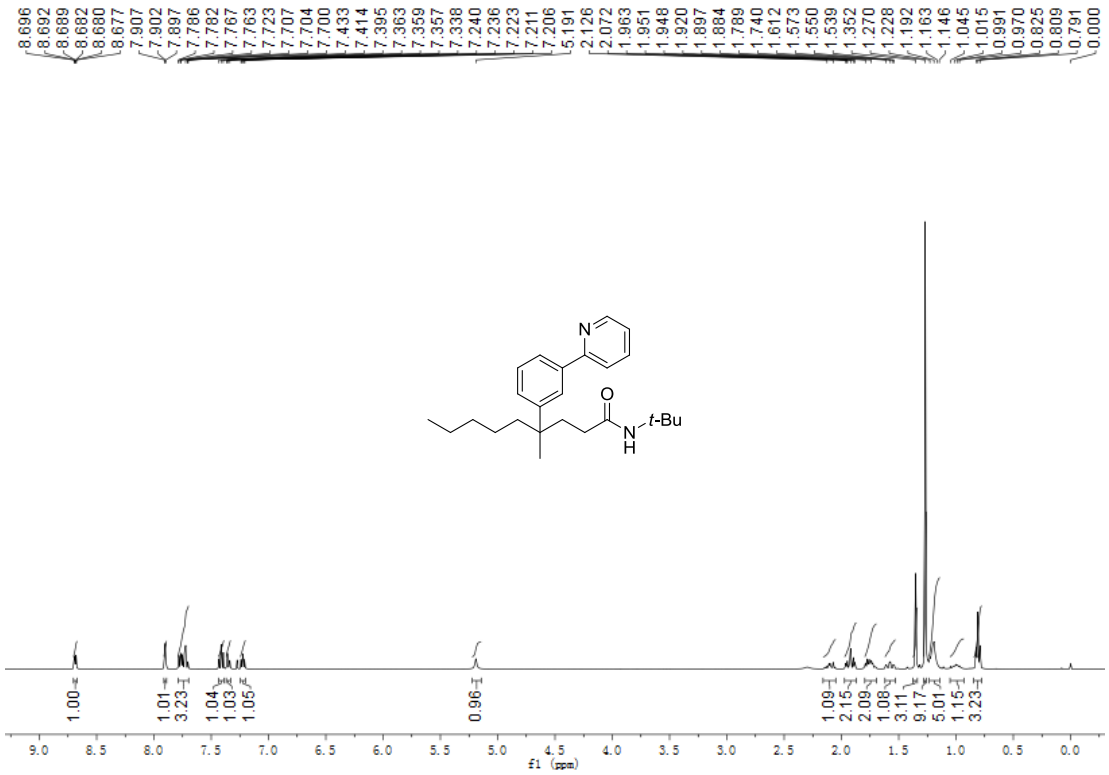
## Compound 3af $^{1}$H NMR (400 MHz, $CDCl_3$)



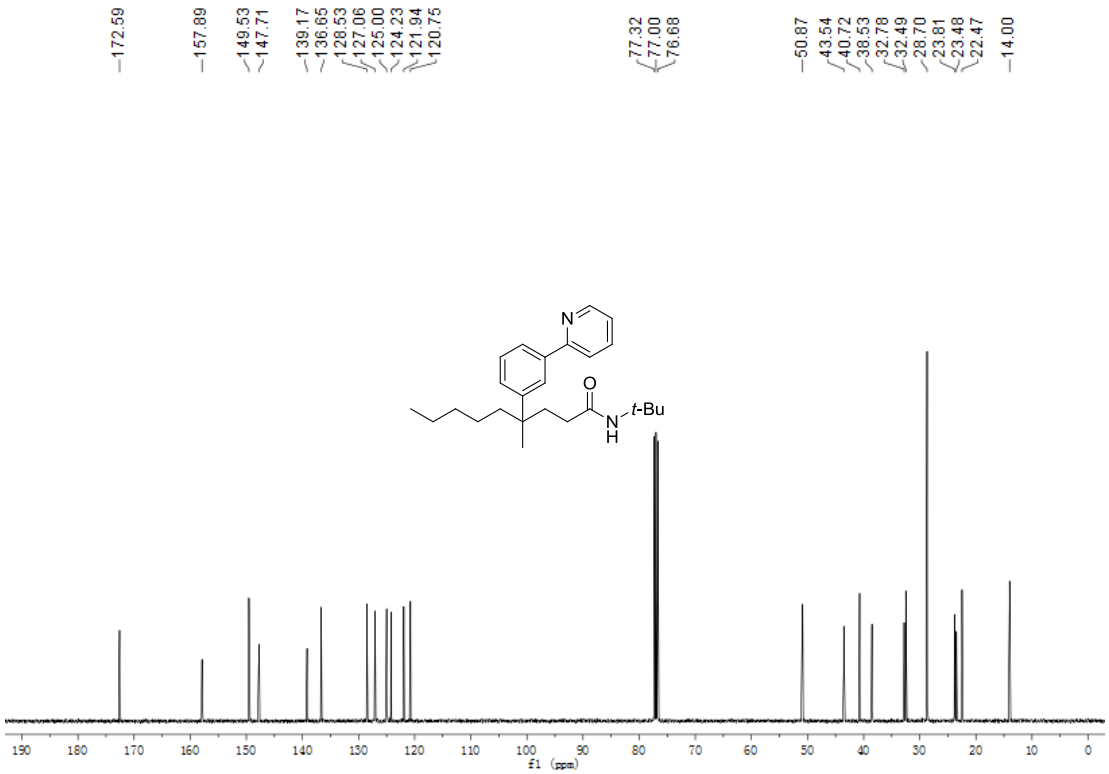

## Compound 3af $^{13}$C NMR (101 MHz, $CDCl_3$)



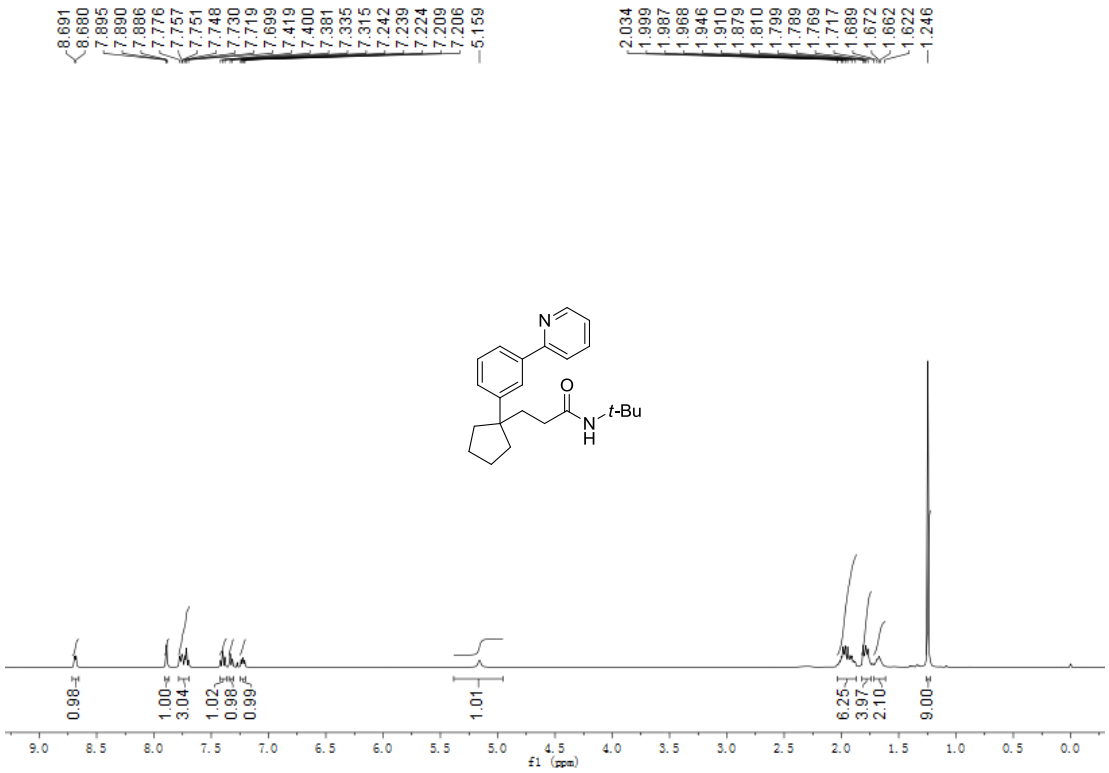
## Compound 3ag $^{1}$H NMR (400 MHz, $CDCl_3$)




## Compound 3ag $^{13}$C NMR (101 MHz, $CDCl_3$)



## Compound 3ah $^{1}$H NMR (400 MHz, $CDCl_3$)

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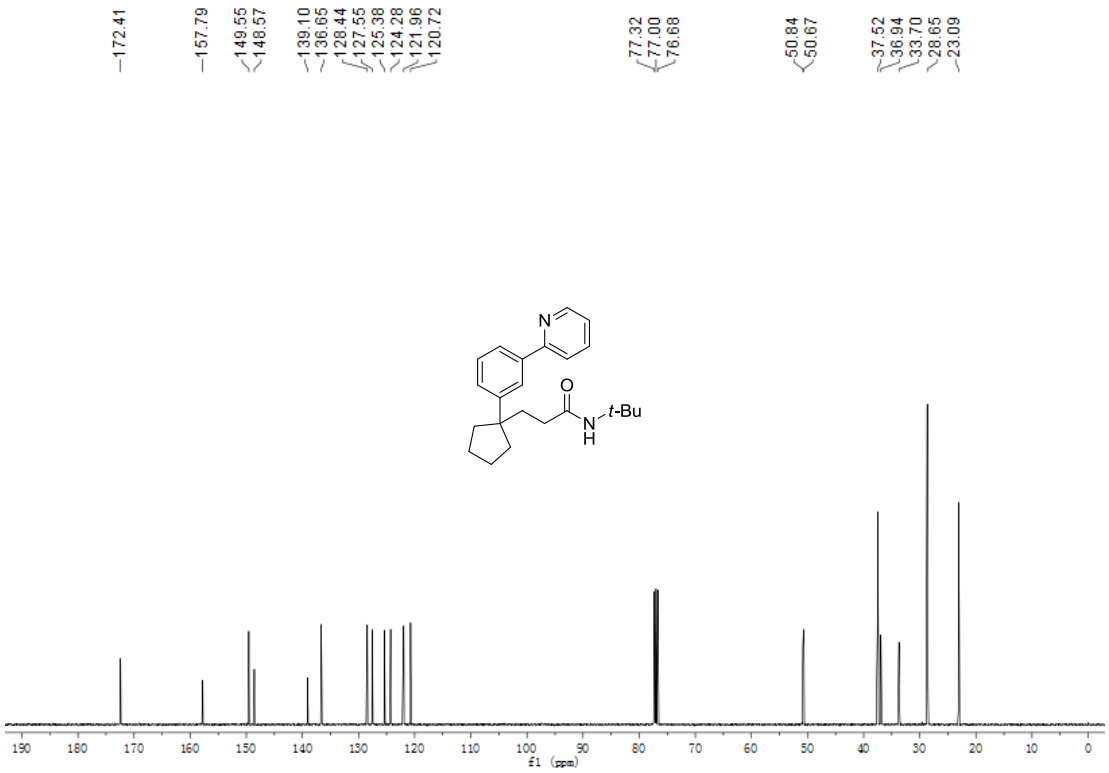

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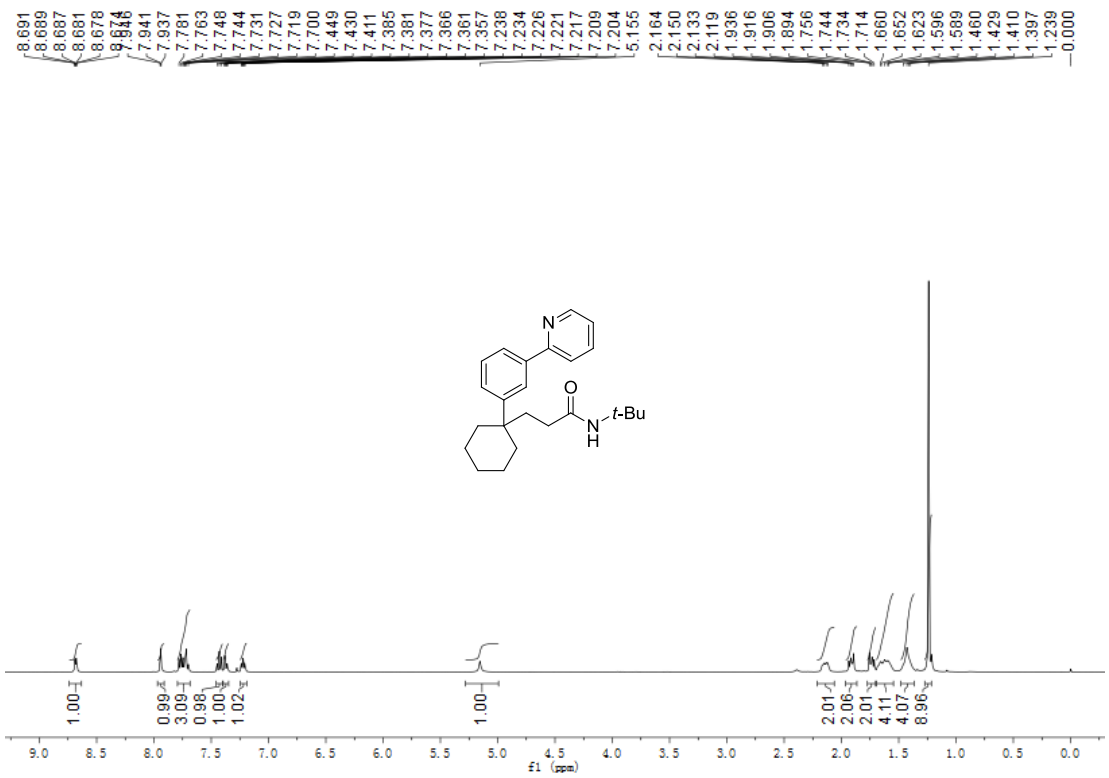


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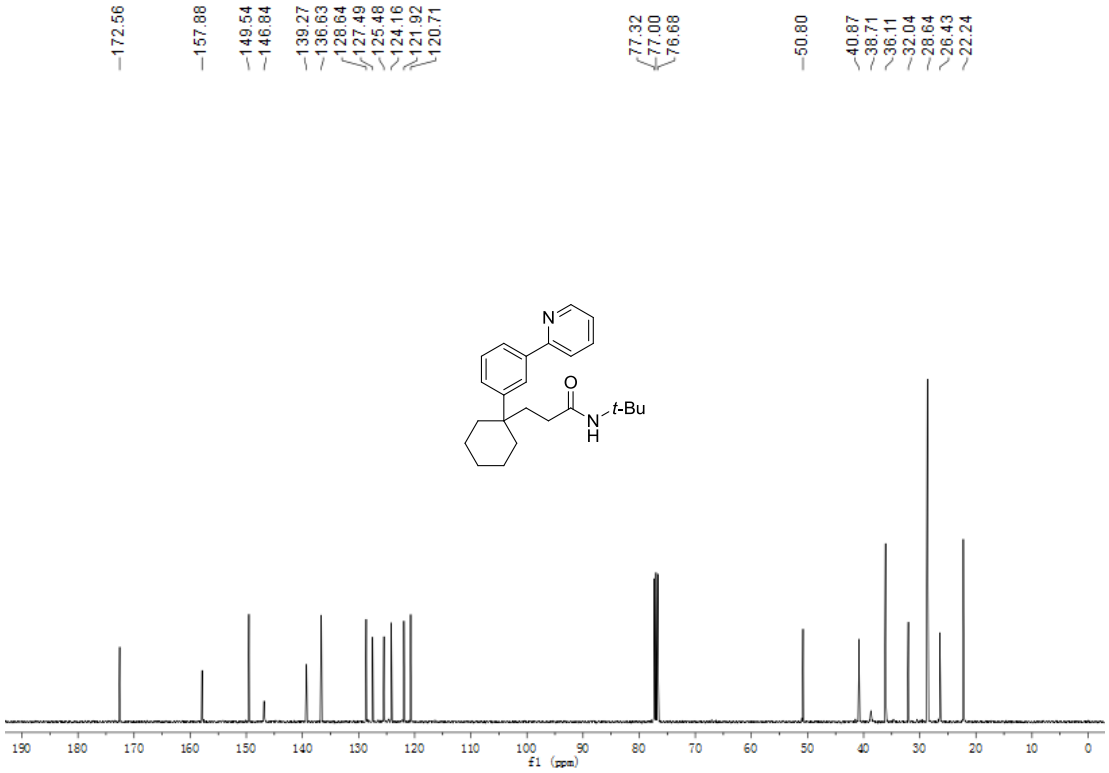

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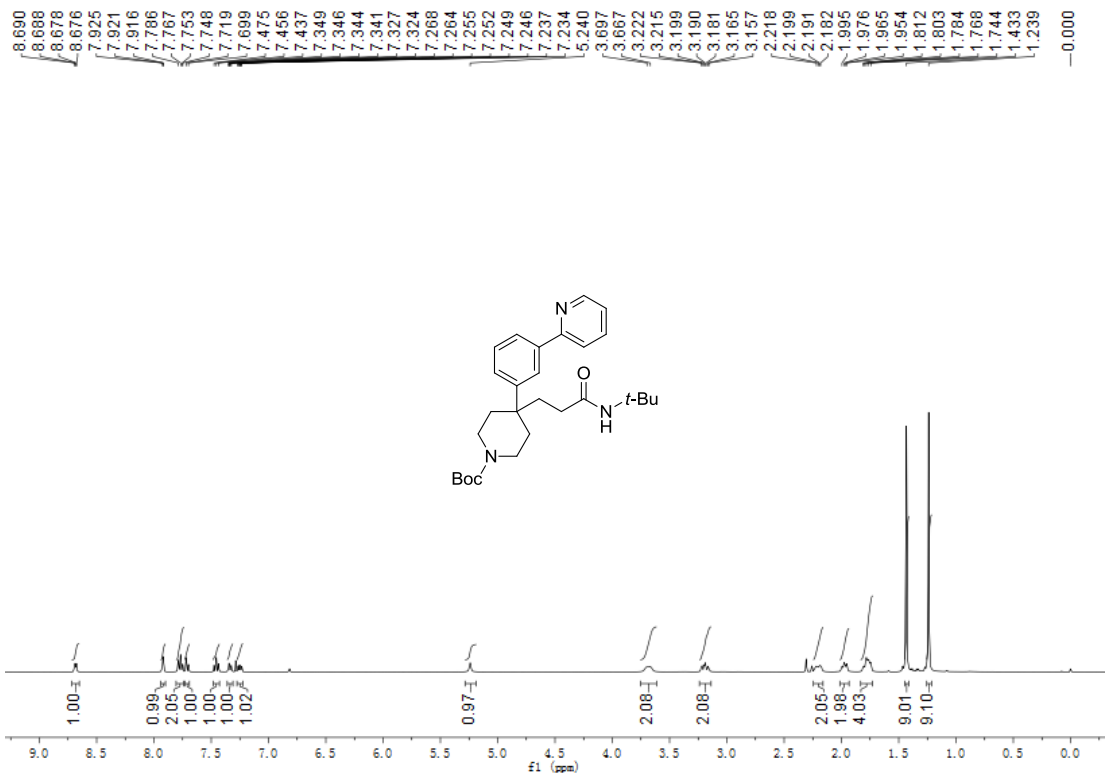
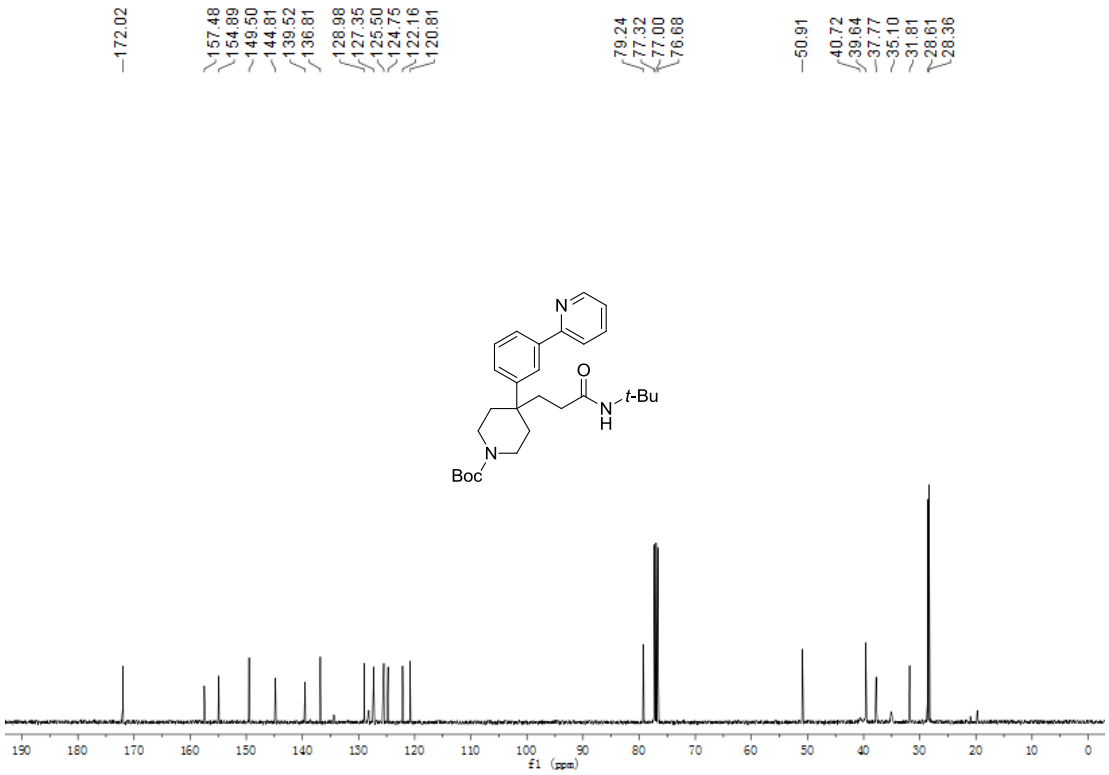
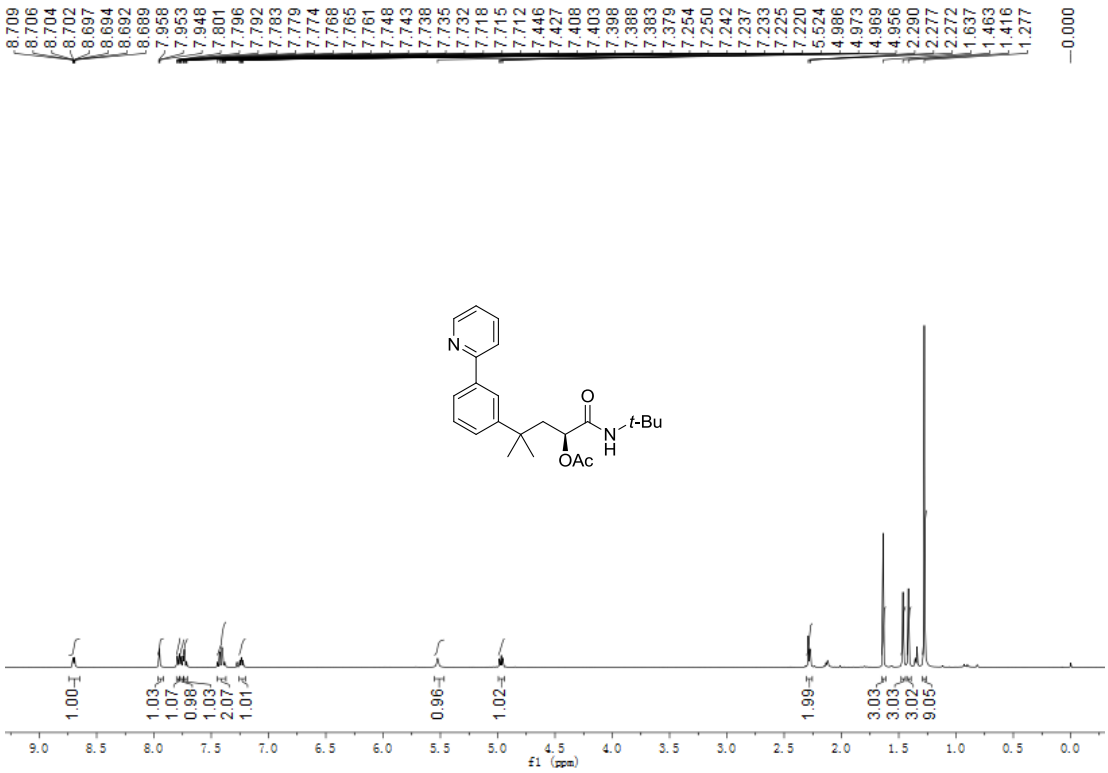


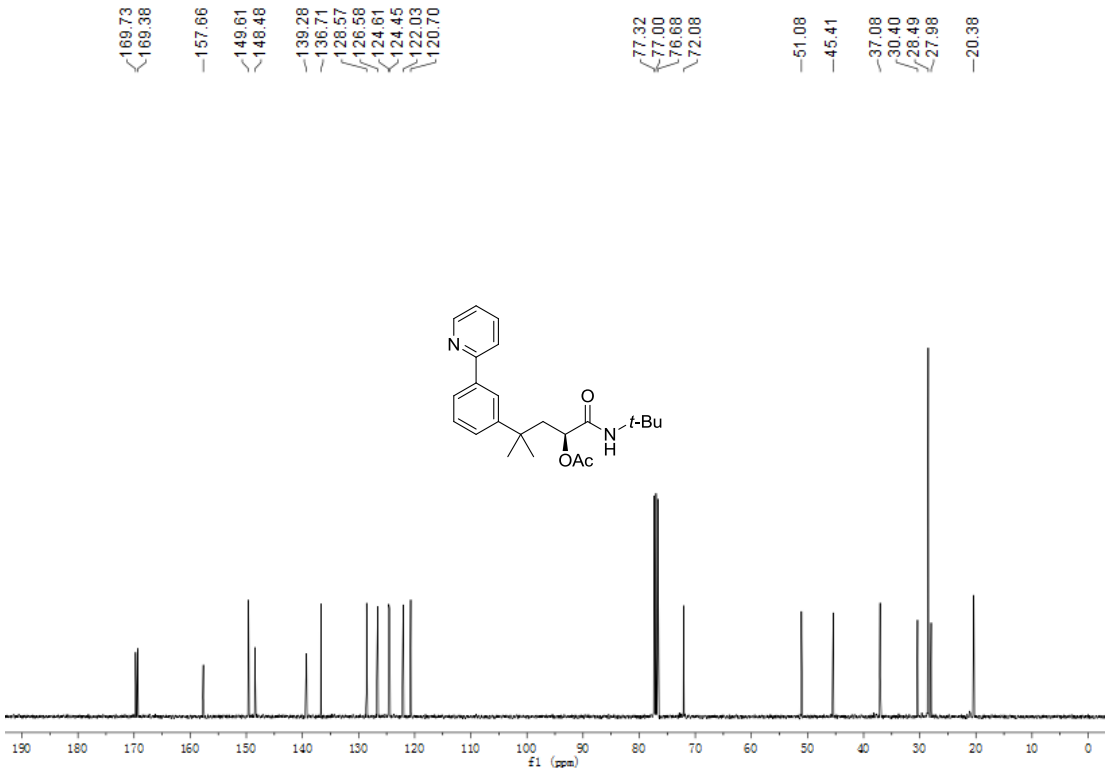

## Compound 3aj $^{13}$C NMR (101 MHz, $CDCl_3$)



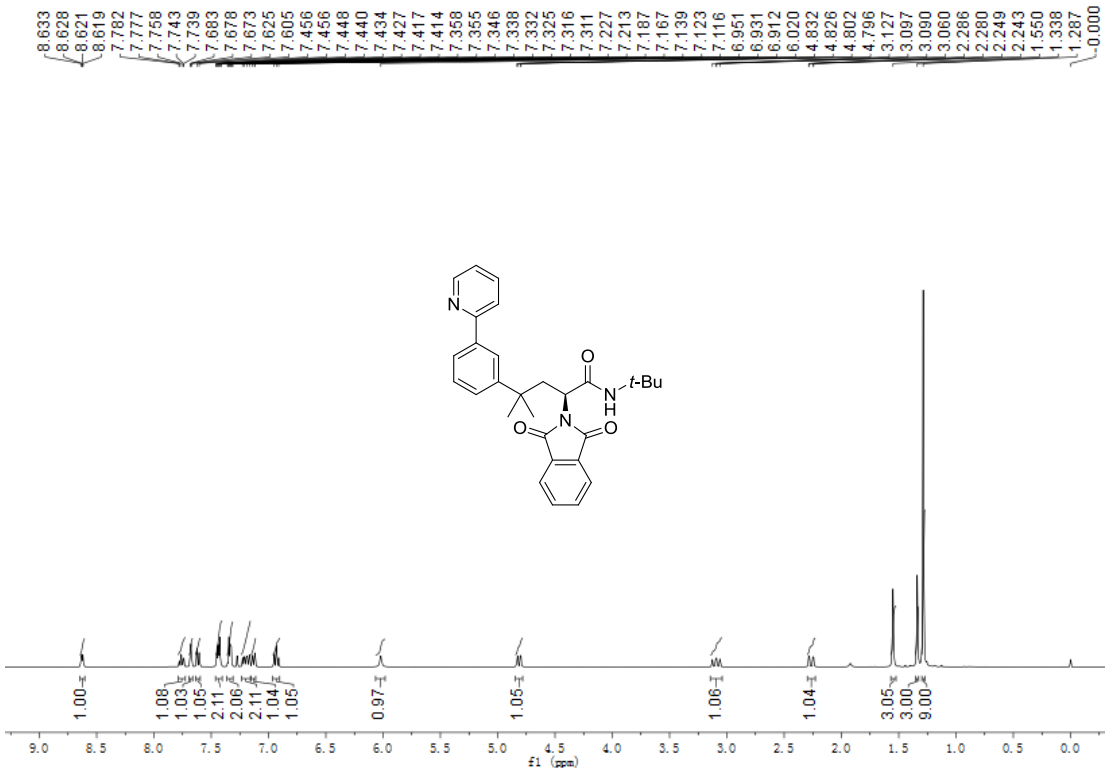
## Compound 3ak $^{1}$H NMR (400 MHz, $CDCl_3$)



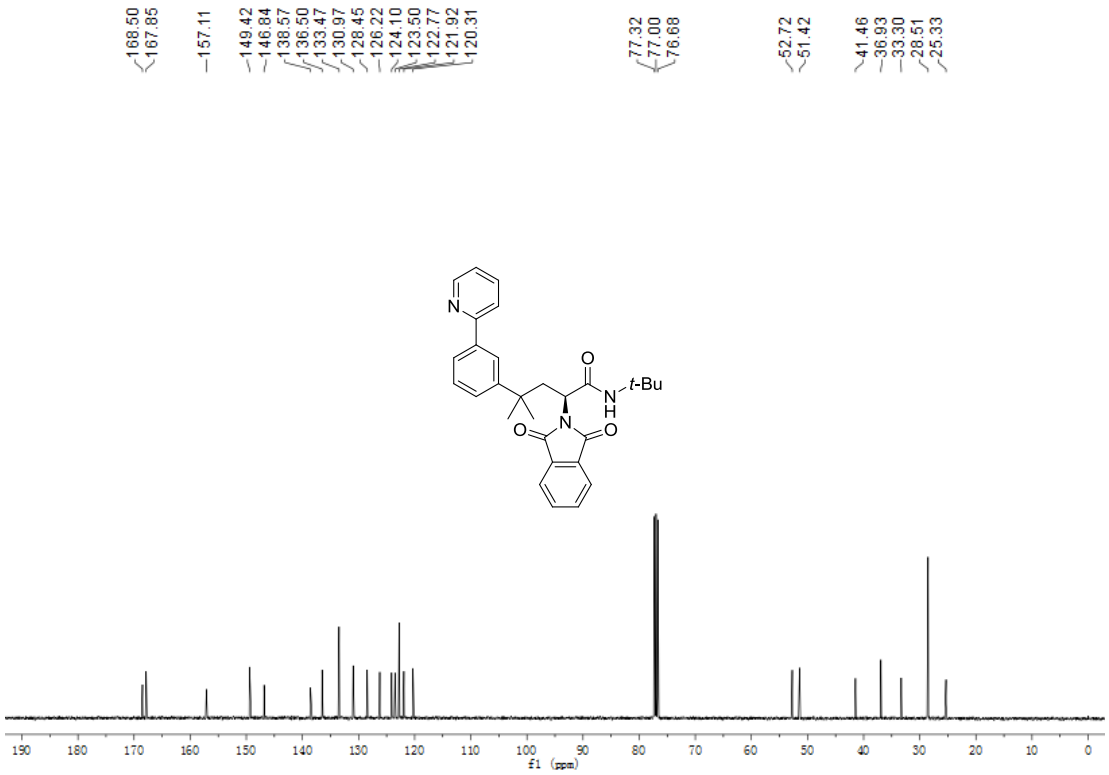

## Compound 3ak $^{13}$C NMR (101 MHz, $CDCl_3$)



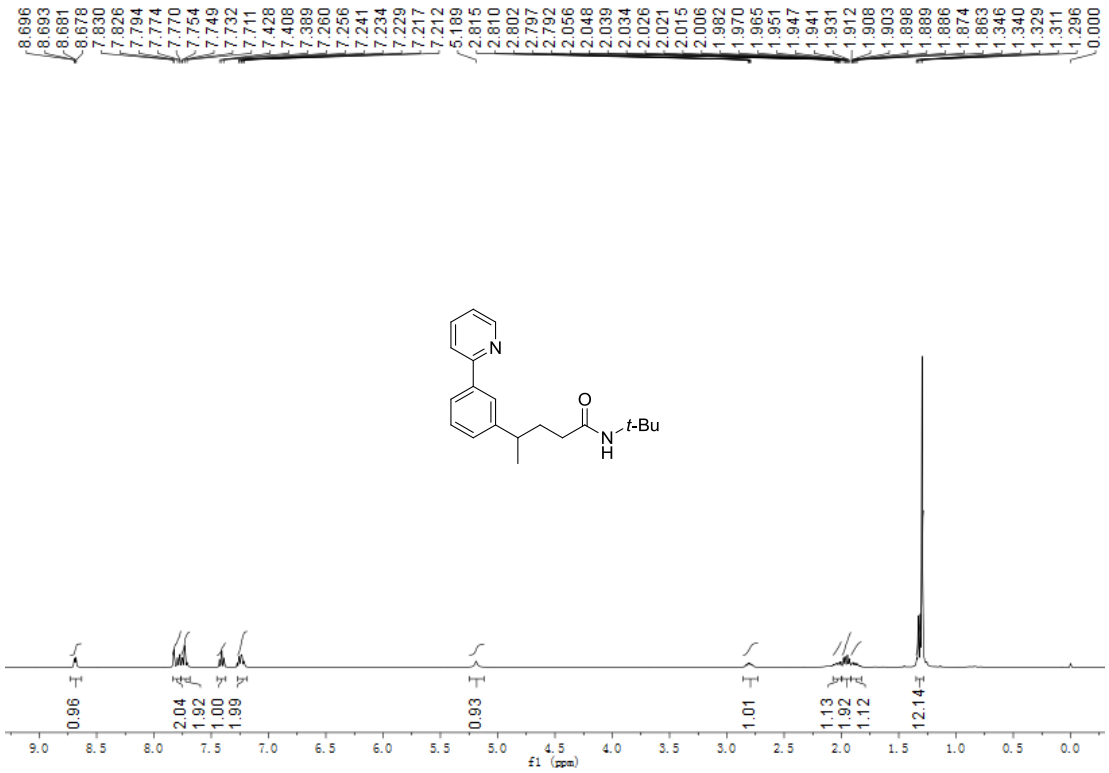
## Compound 3al $^{1}$H NMR (400 MHz, $CDCl_3$)



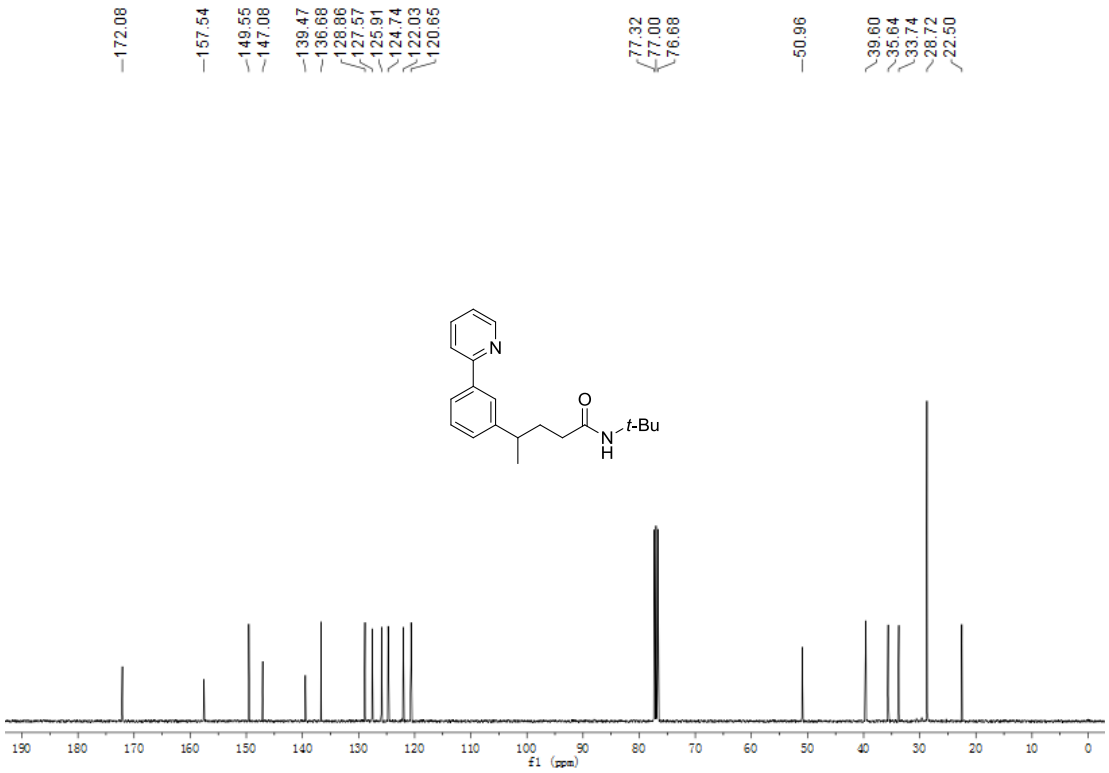

## Compound 3al $^{13}$C NMR (101 MHz, $CDCl_3$)



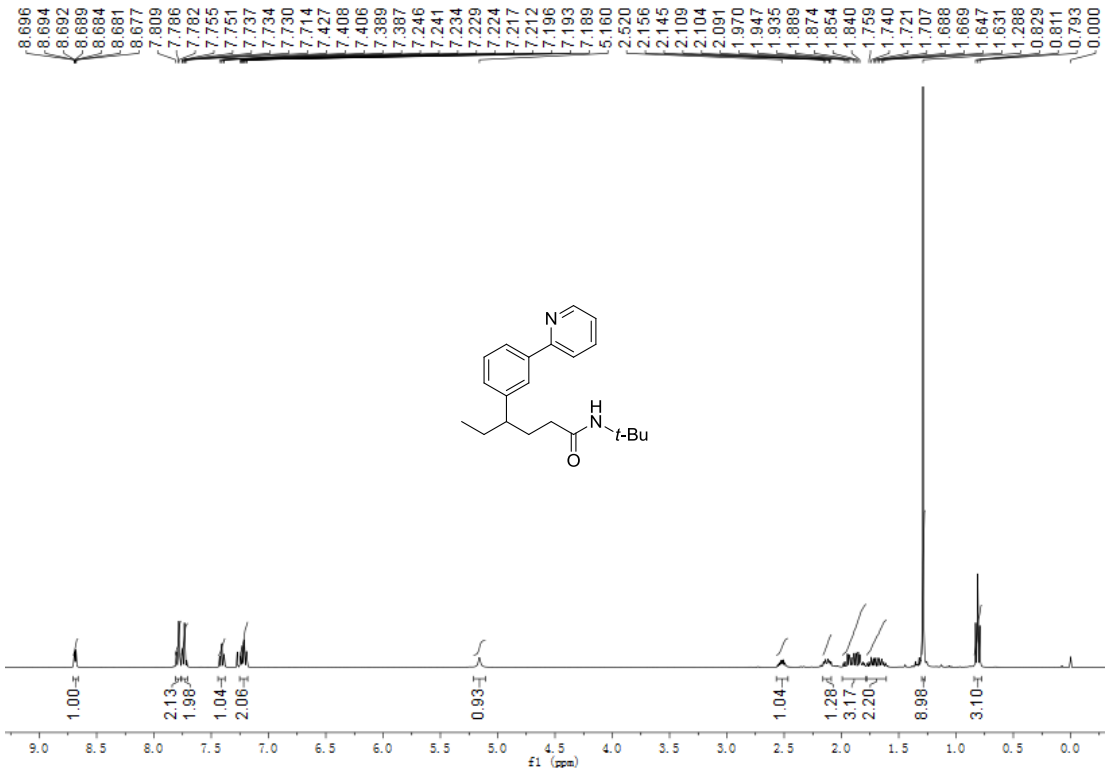
**Compound 3am $^{1}$H NMR (400 MHz, $CDCl_3$)**



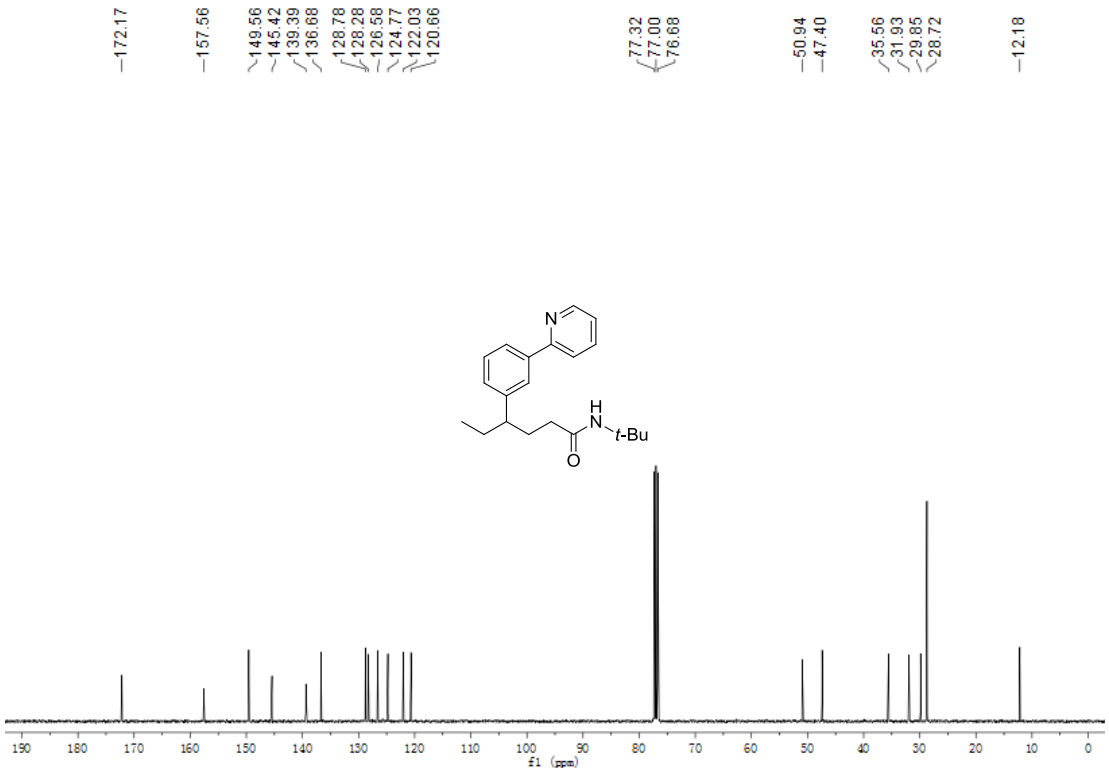

**Compound 3am $^{13}$C NMR (101 MHz, $CDCl_3$)**



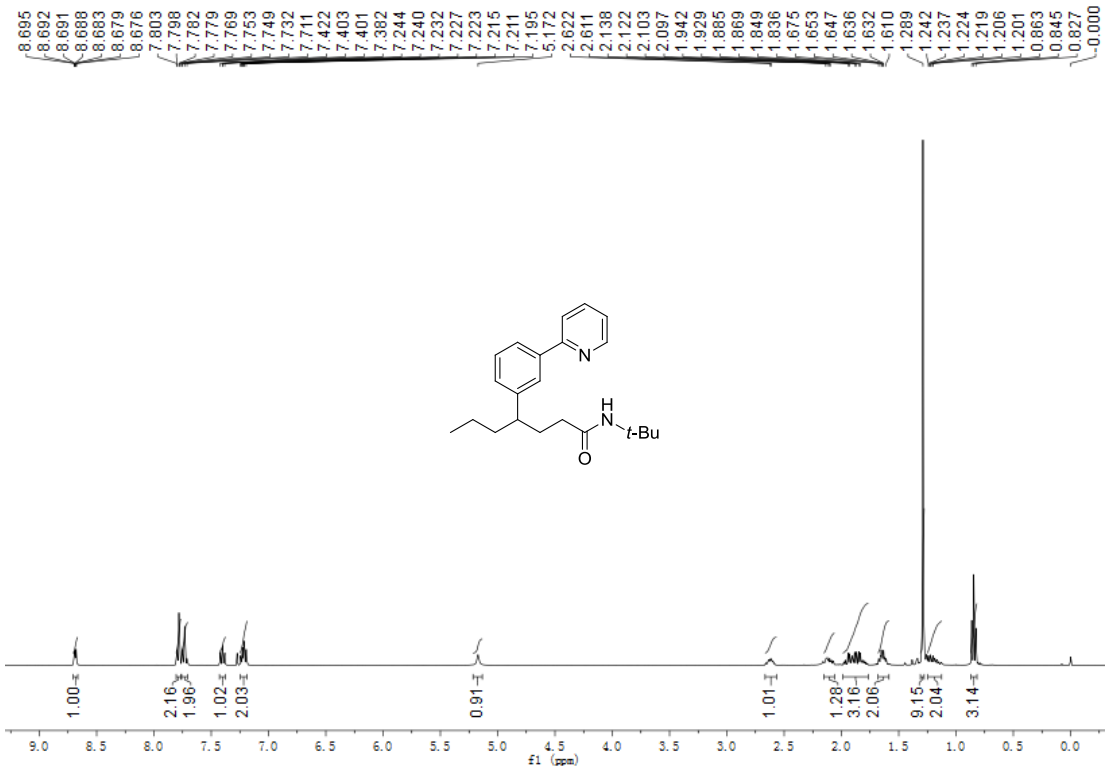
**Compound 3an $^{1}$H NMR (400 MHz, $CDCl_3$)**



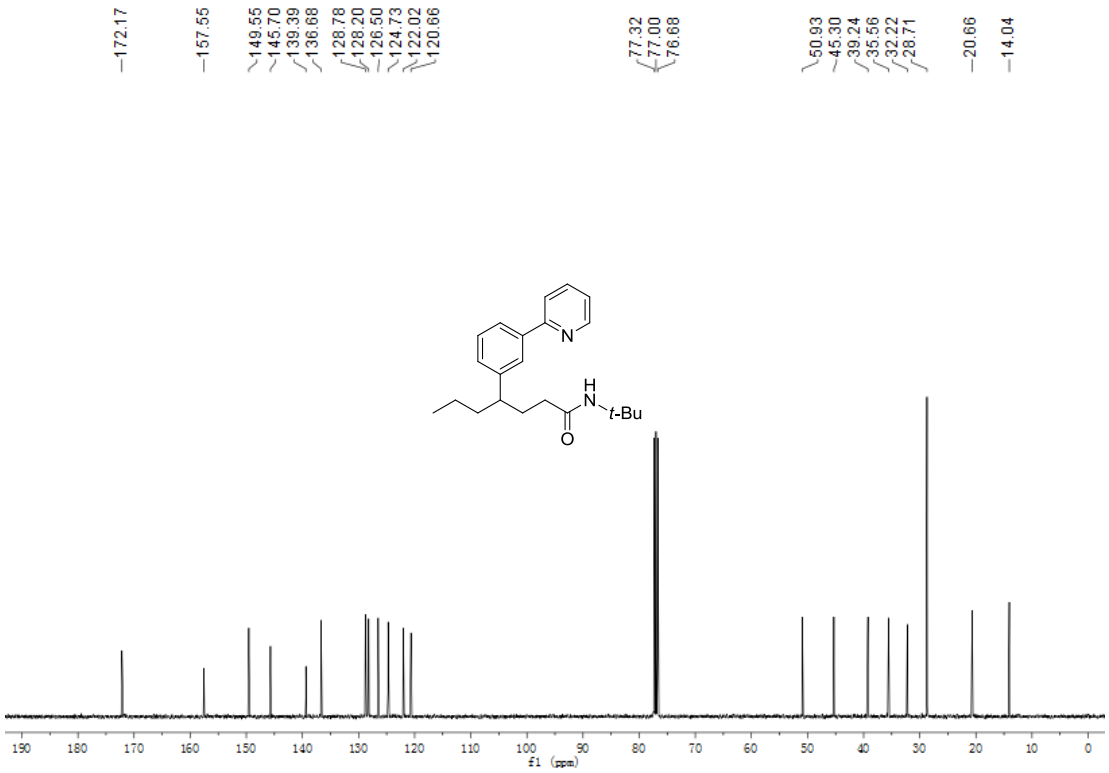

**Compound 3an $^{13}$C NMR (101 MHz, $CDCl_3$)**



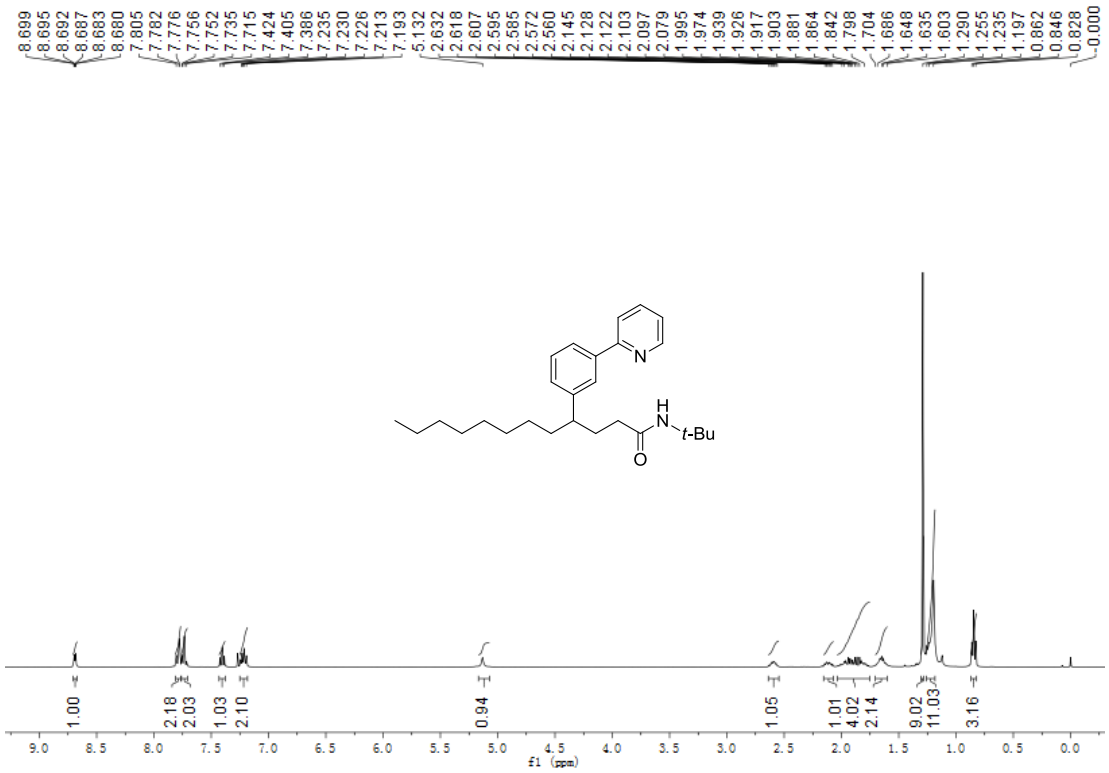
## Compound 3ao $^{1}$H NMR (400 MHz, $CDCl_3$)



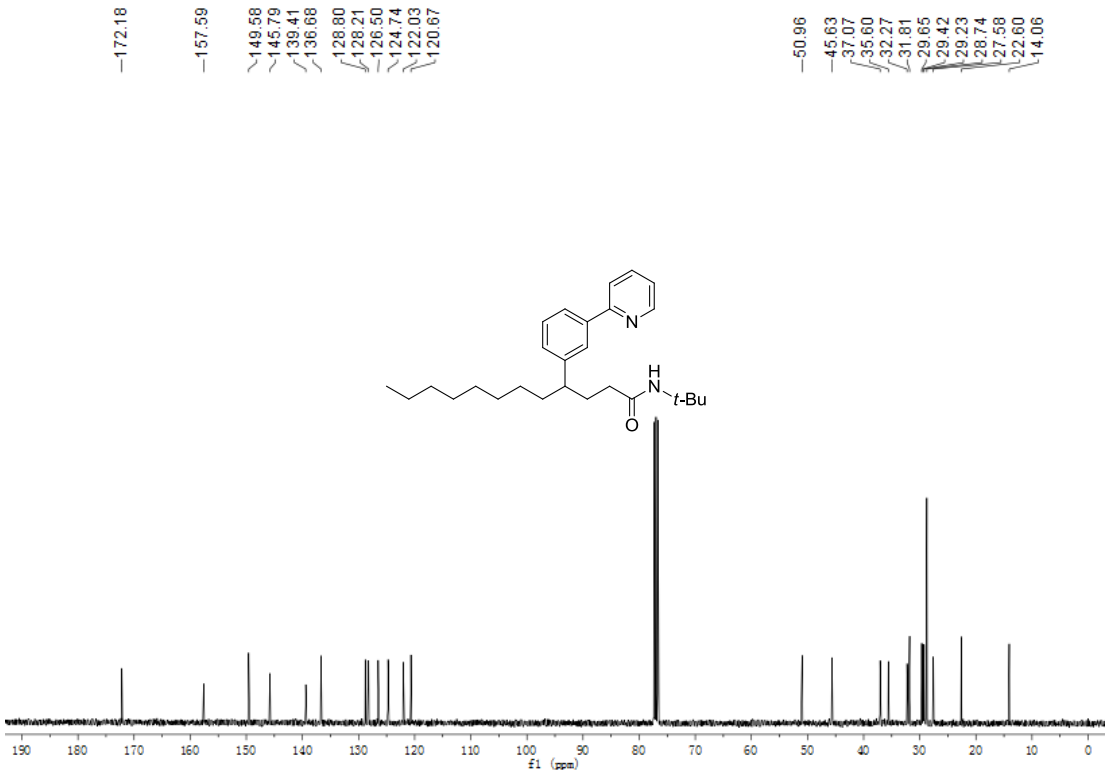

## Compound 3ao $^{13}$C NMR (101 MHz, $CDCl_3$)



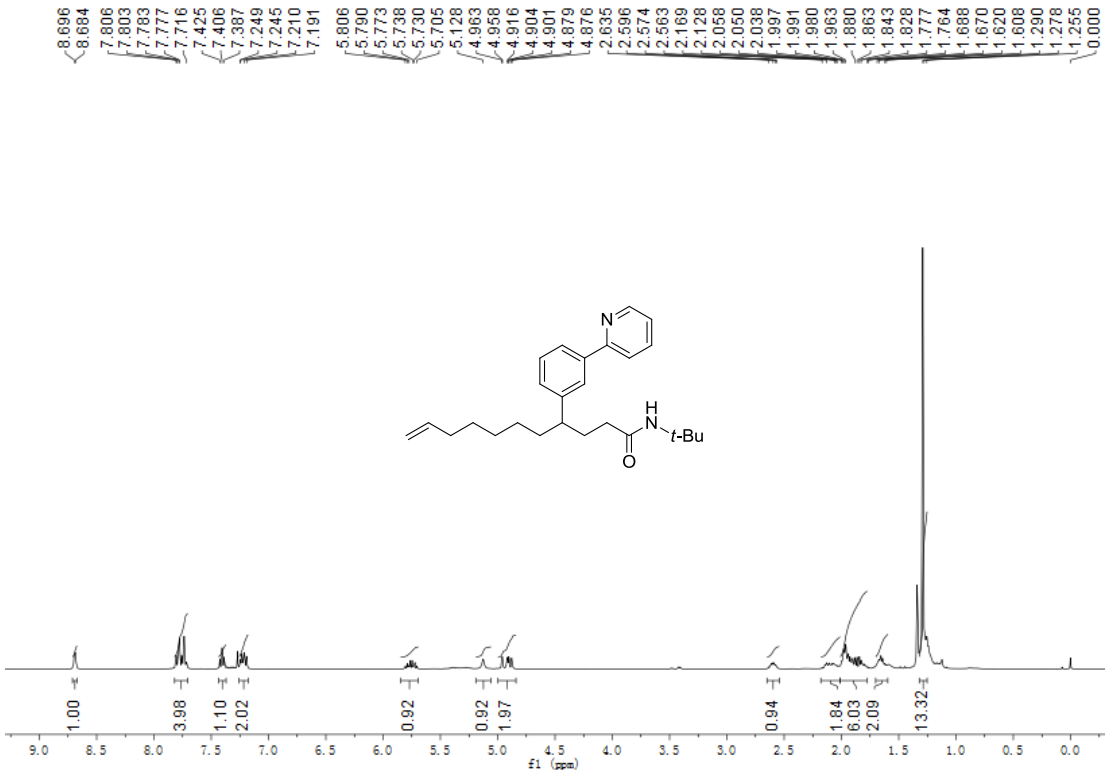
**Compound 3ap $^{1}$H NMR (400 MHz, $CDCl_3$)**



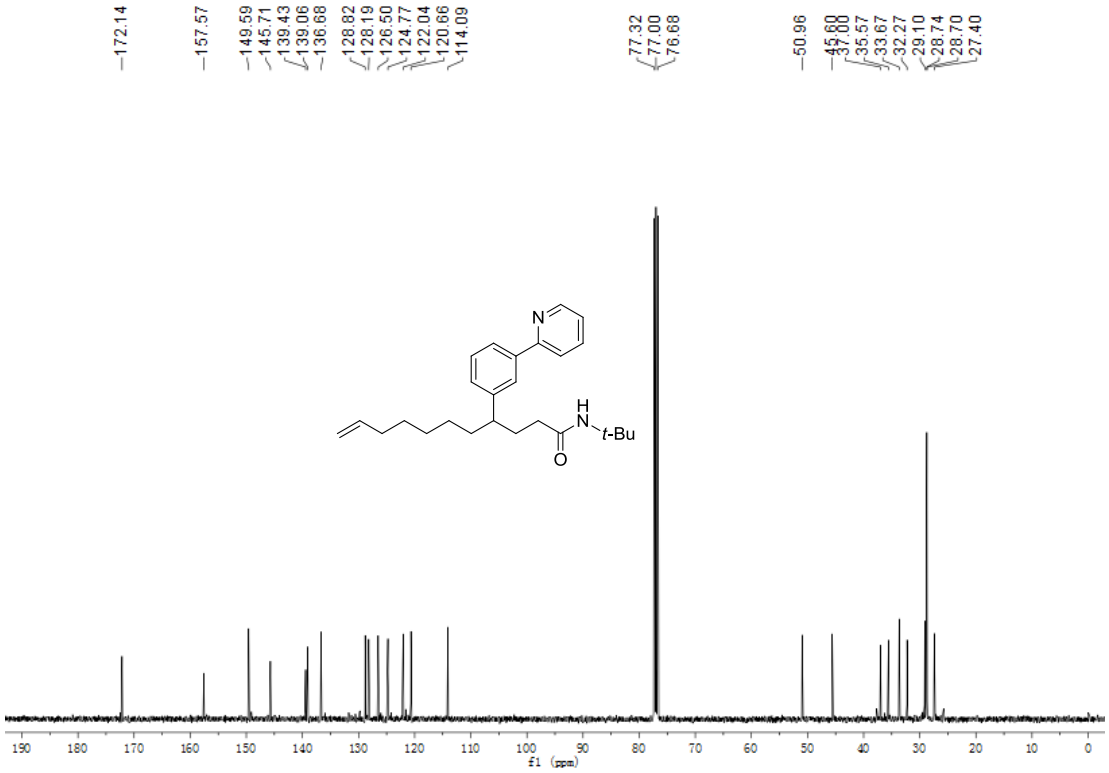

**Compound 3ap $^{13}$C NMR (101 MHz, $CDCl_3$)**



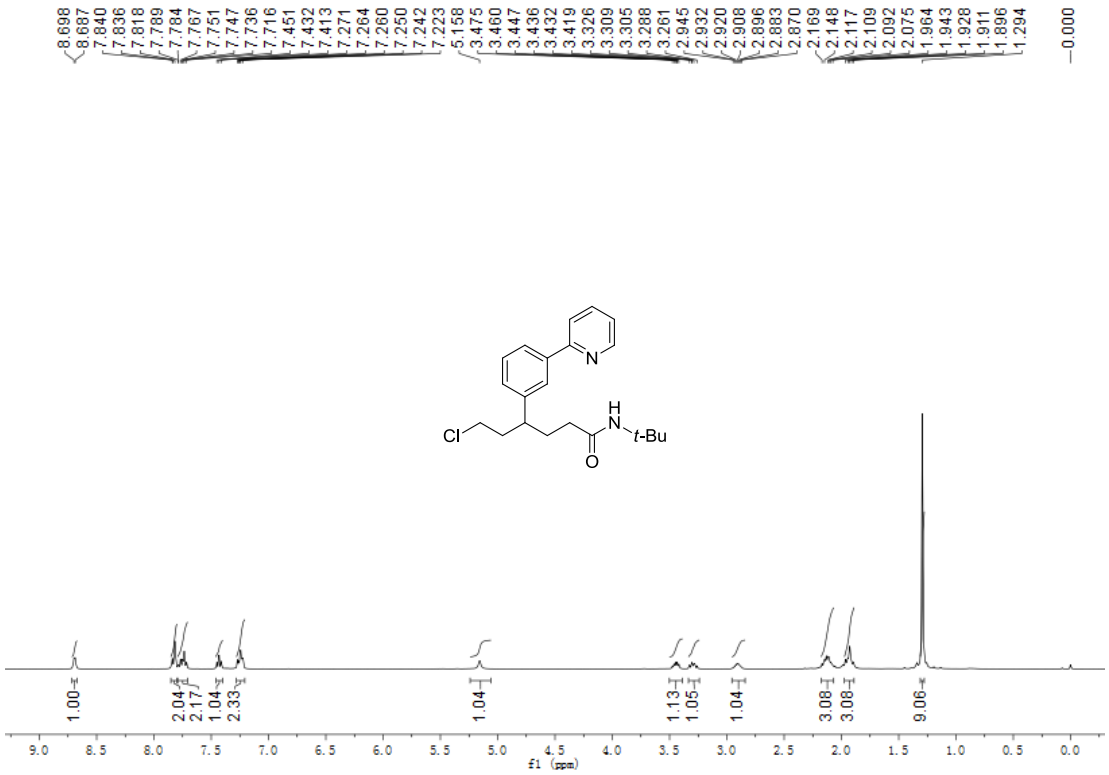
## Compound 3aq $^{1}$H NMR (400 MHz, $CDCl_3$)



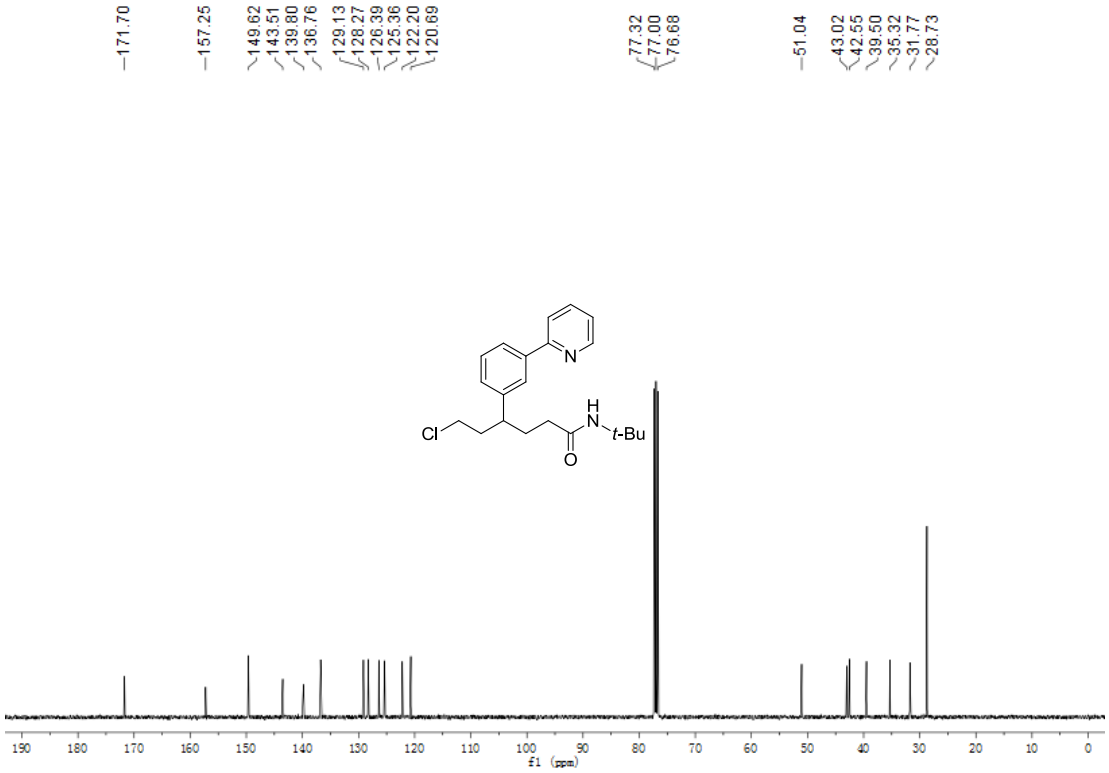

## Compound 3aq $^{13}$C NMR (101 MHz, $CDCl_3$)



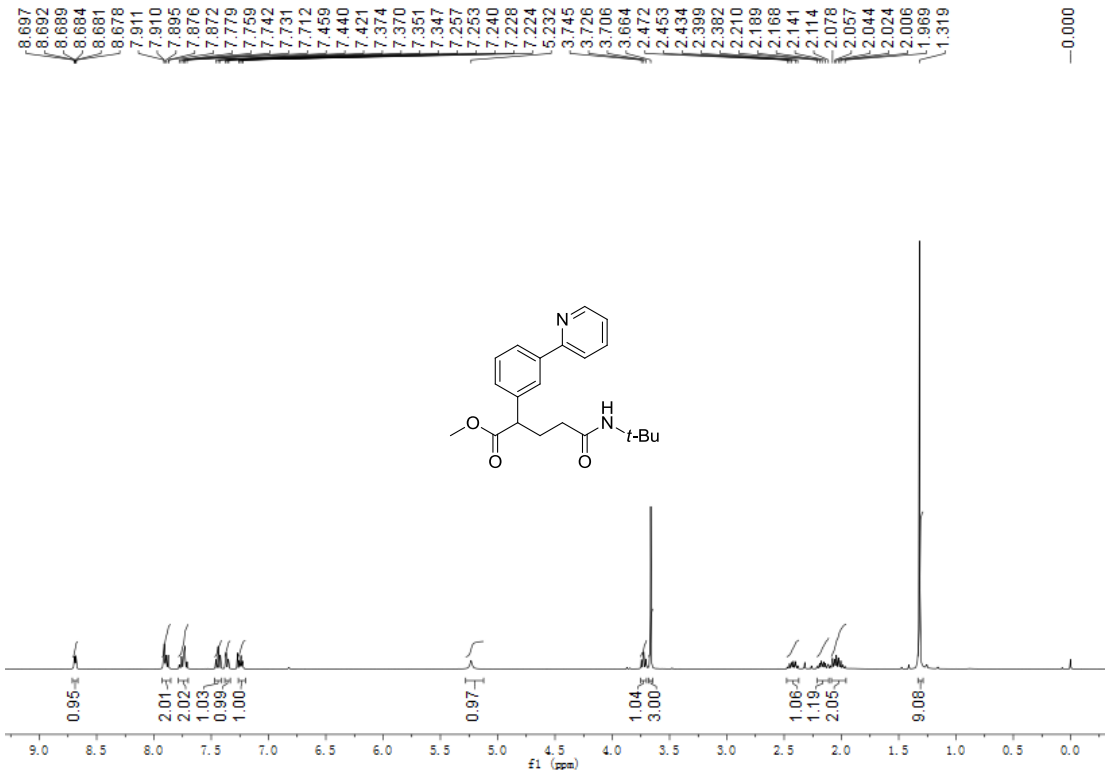
## Compound 3ar $^{1}$H NMR (400 MHz, $CDCl_3$)



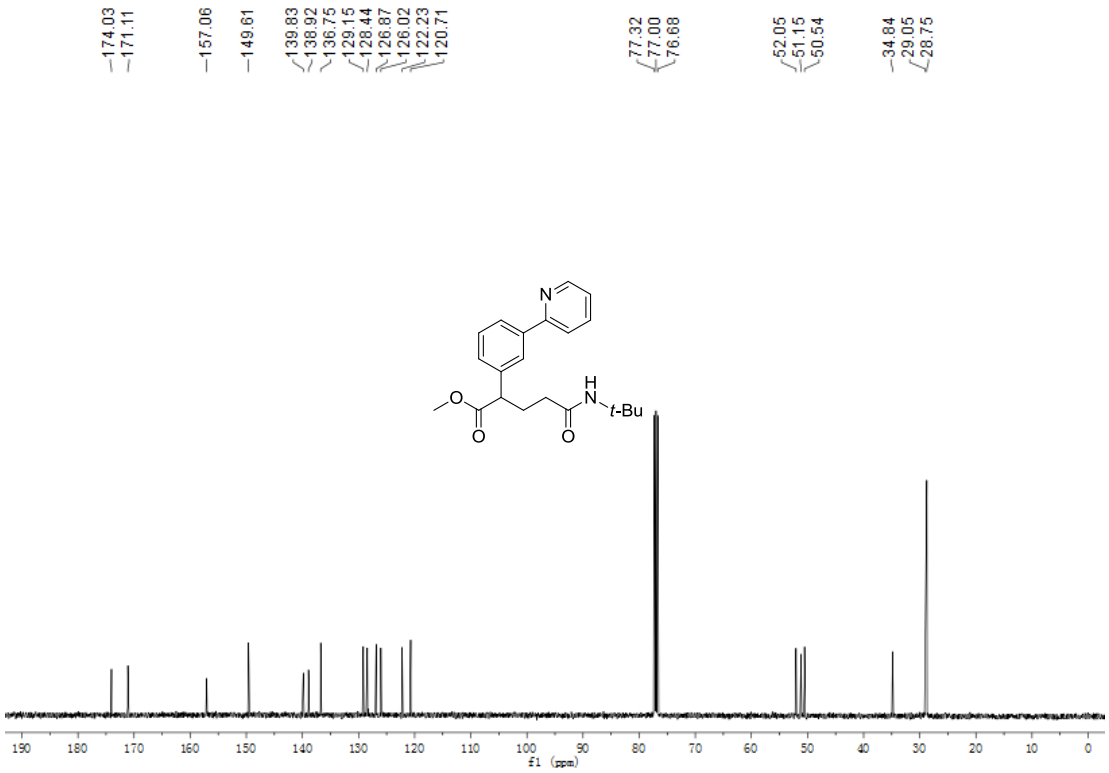

## Compound 3ar $^{13}$C NMR (101 MHz, $CDCl_3$)



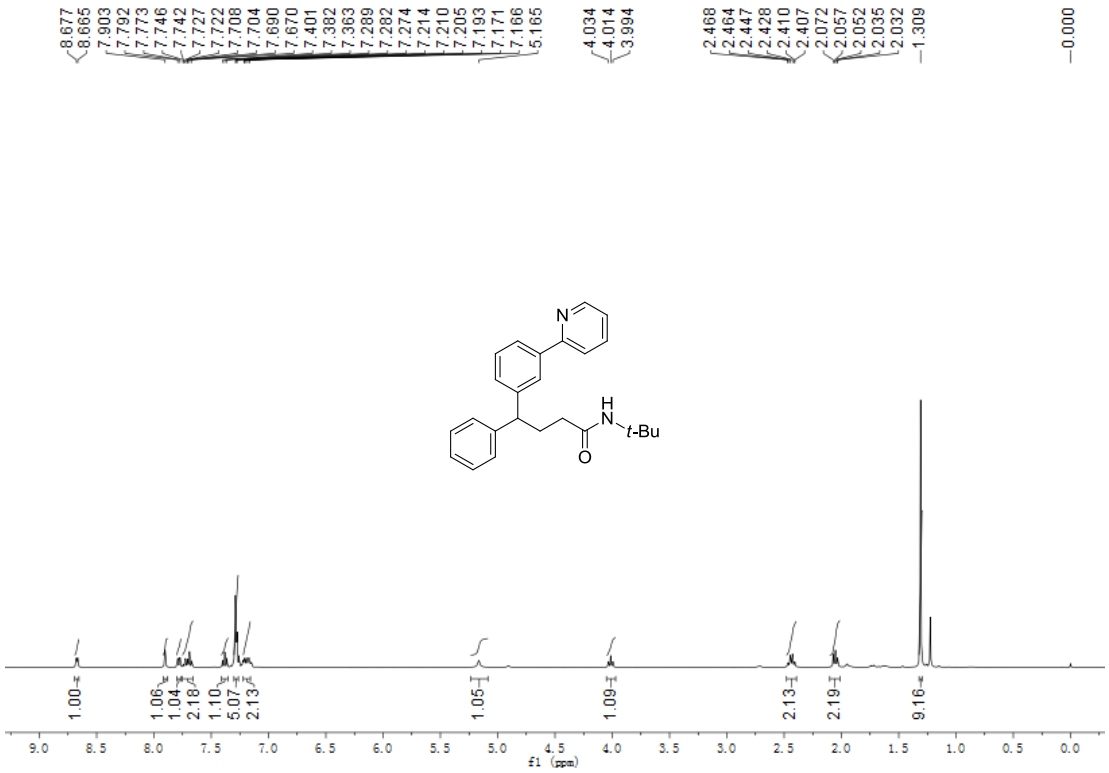
## Compound 3as $^{1}$H NMR (400 MHz, $CDCl_3$)



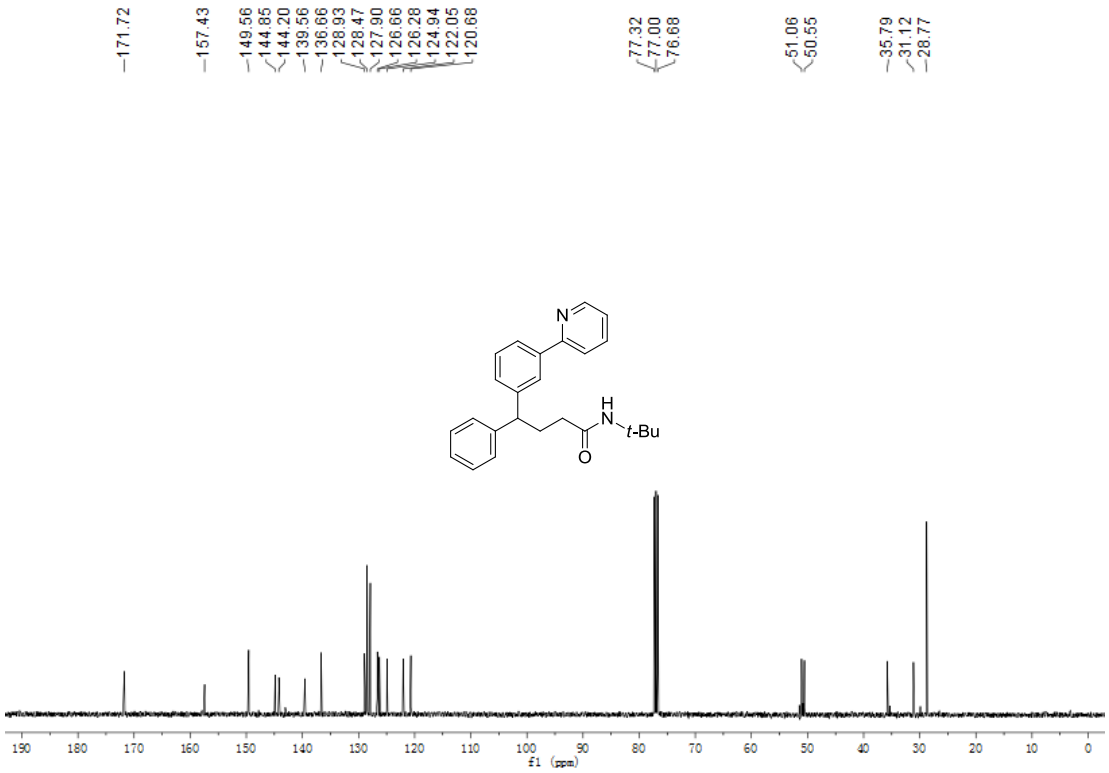

## Compound 3as $^{13}$C NMR (101 MHz, $CDCl_3$)



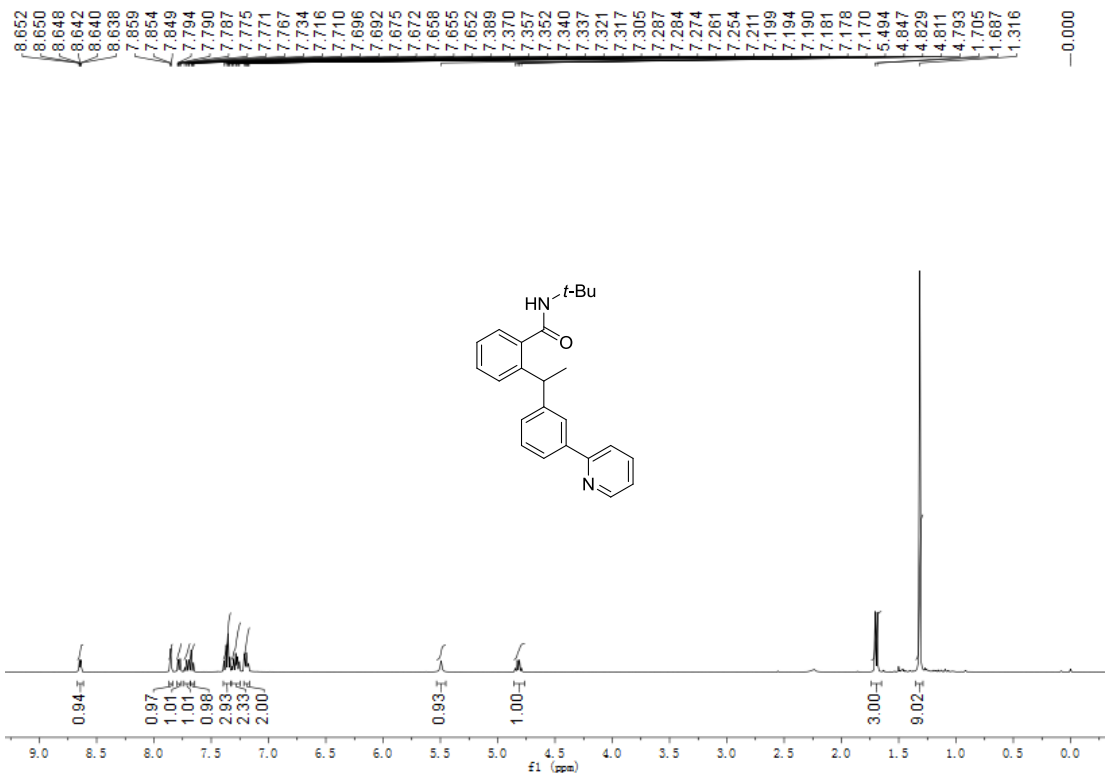
## Compound 3at $^{1}$H NMR (400 MHz, $CDCl_3$)



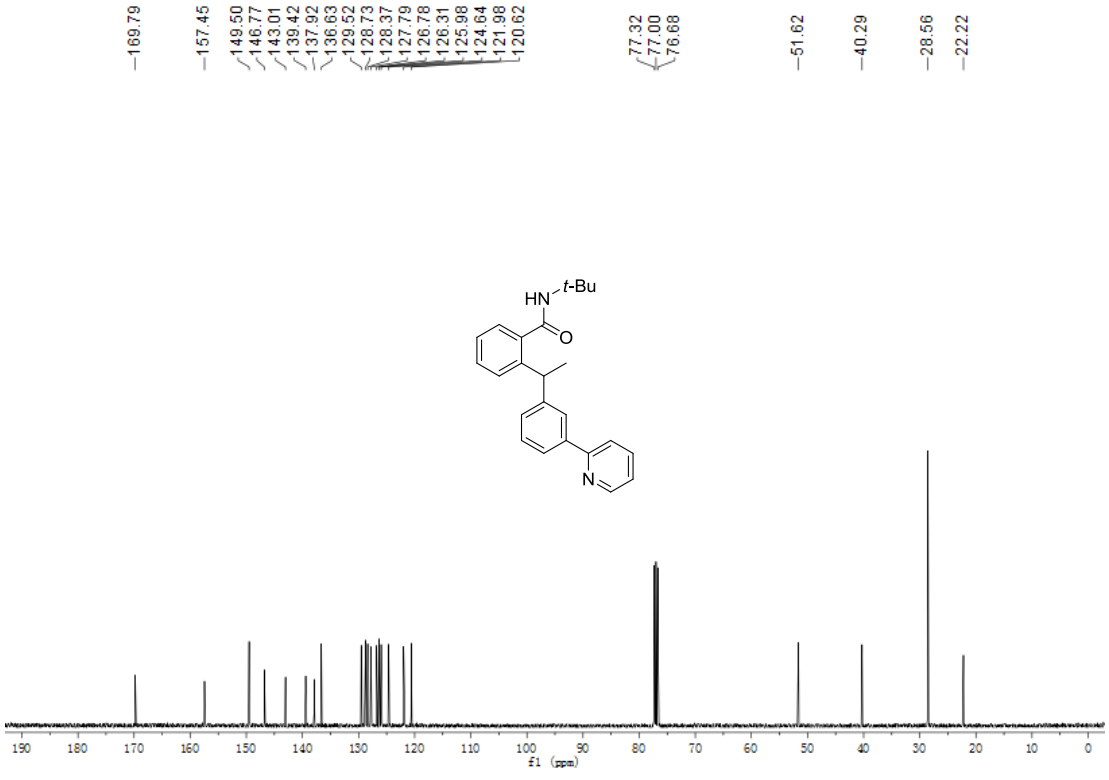

## Compound 3at $^{13}$C NMR (101 MHz, $CDCl_3$)



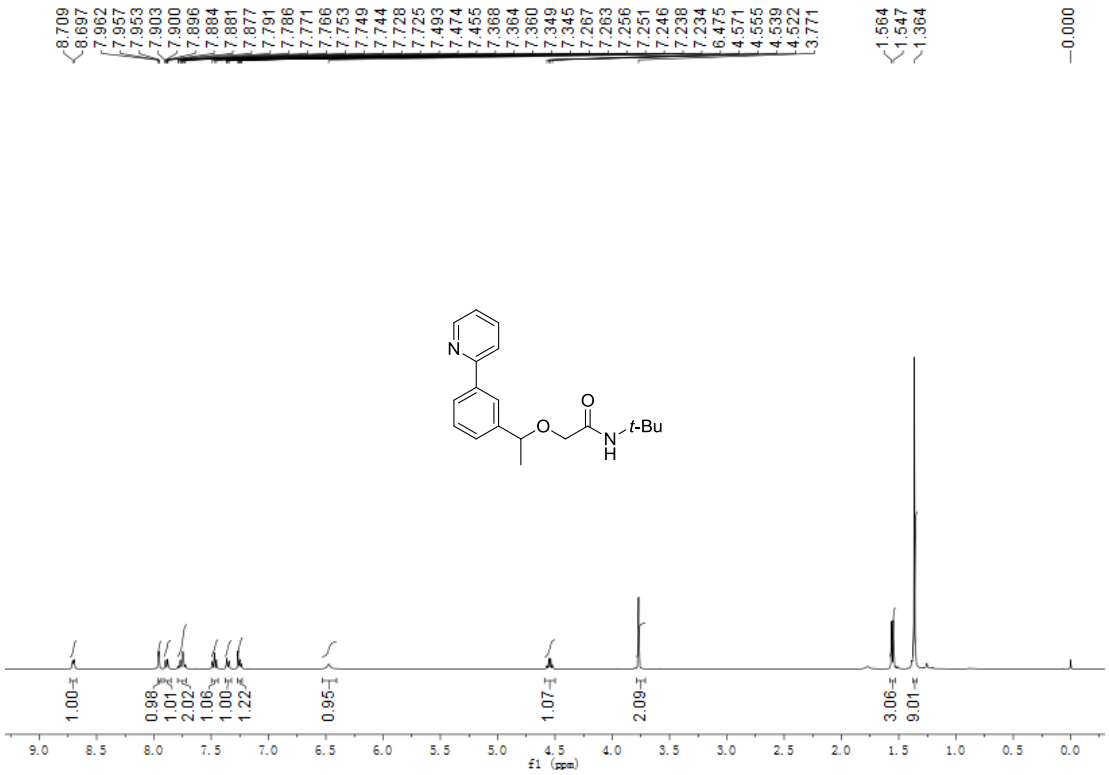
**Compound 3au $^{1}$H NMR (400 MHz, $CDCl_3$)**



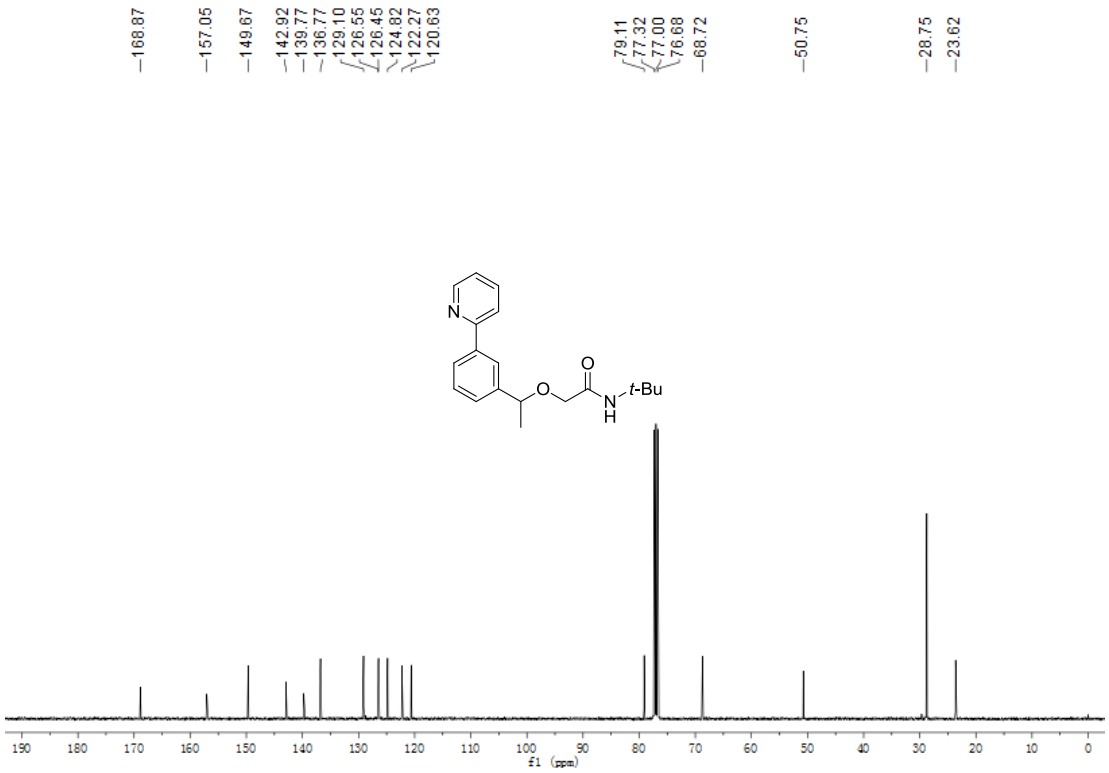

**Compound 3au $^{13}$C NMR (101 MHz, $CDCl_3$)**



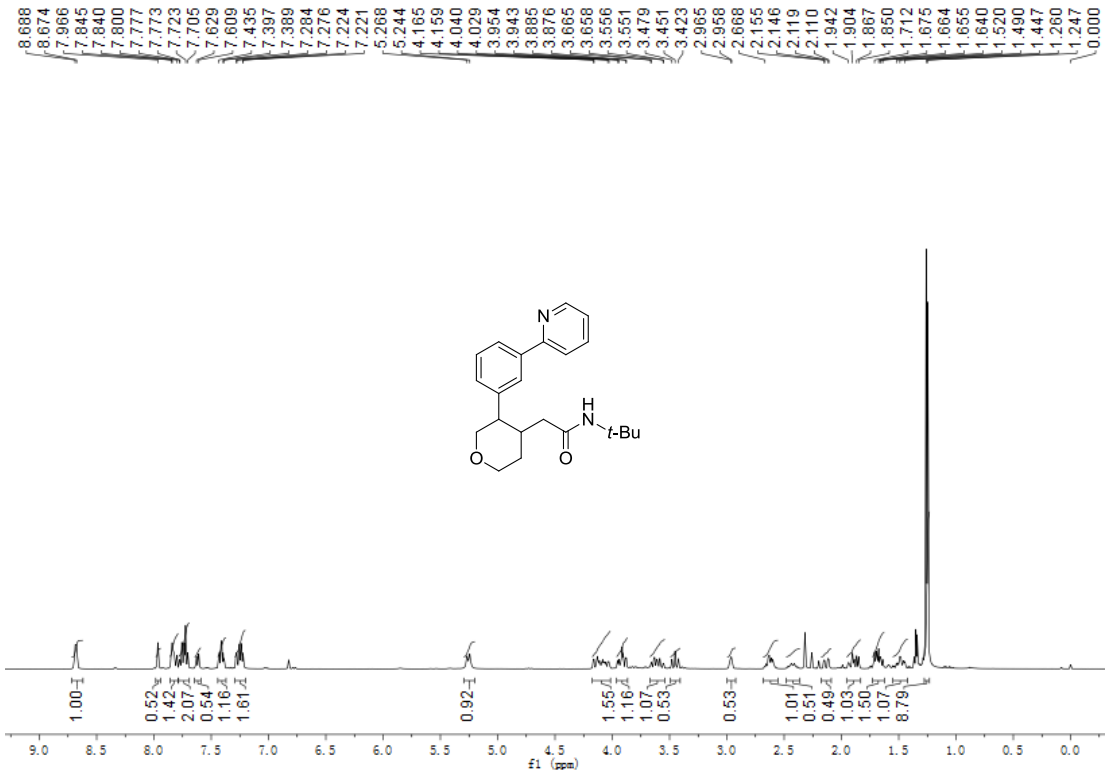
**Compound 3av $^{1}$H NMR (400 MHz, $CDCl_3$)**



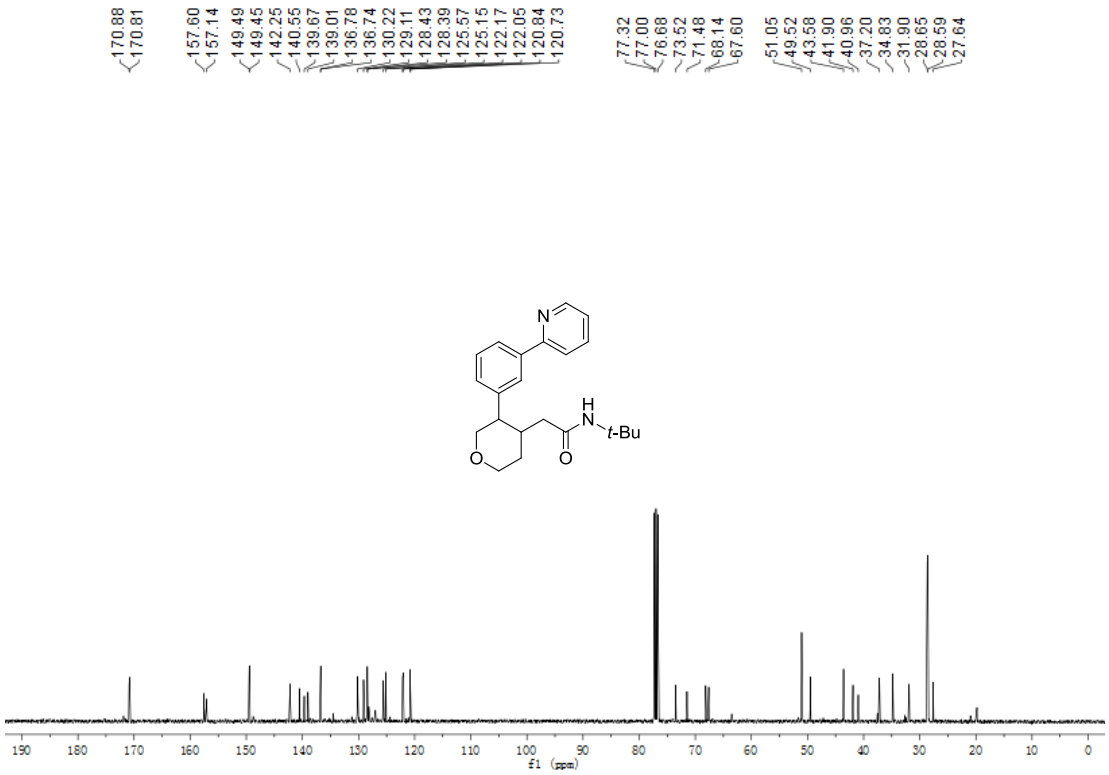

**Compound 3av $^{13}$C NMR (101 MHz, $CDCl_3$)**



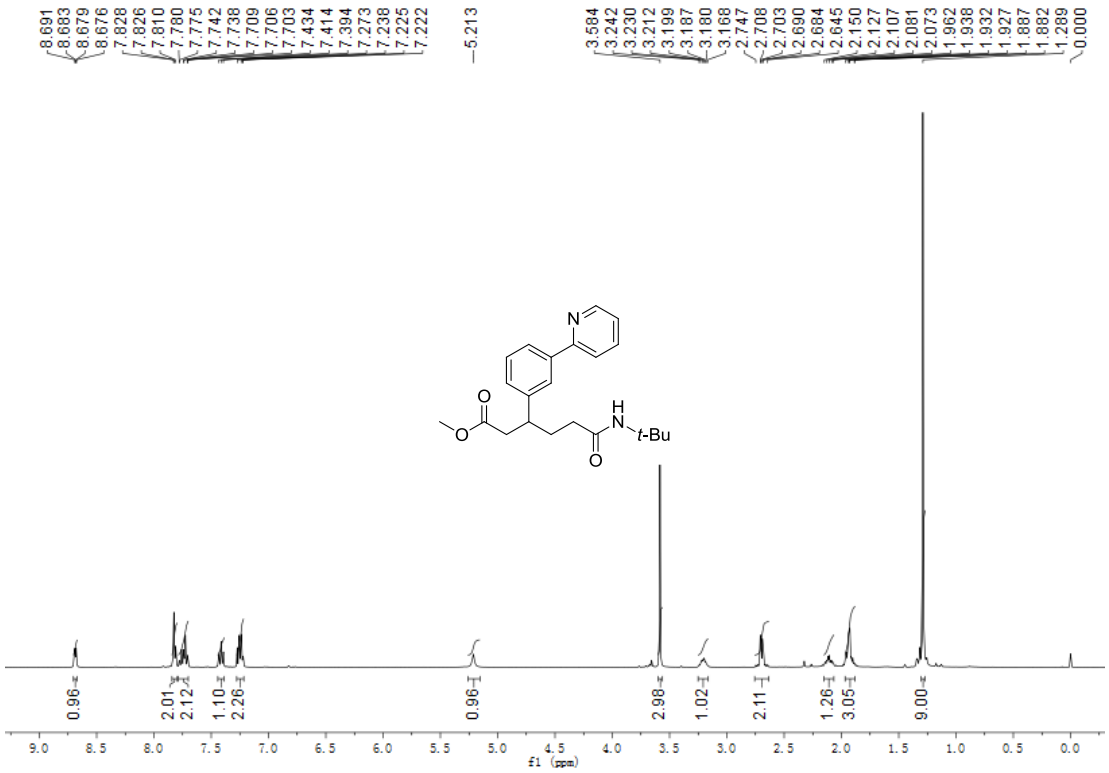
## Compound 3aw $^{1}$H NMR (400 MHz, $CDCl_3$)



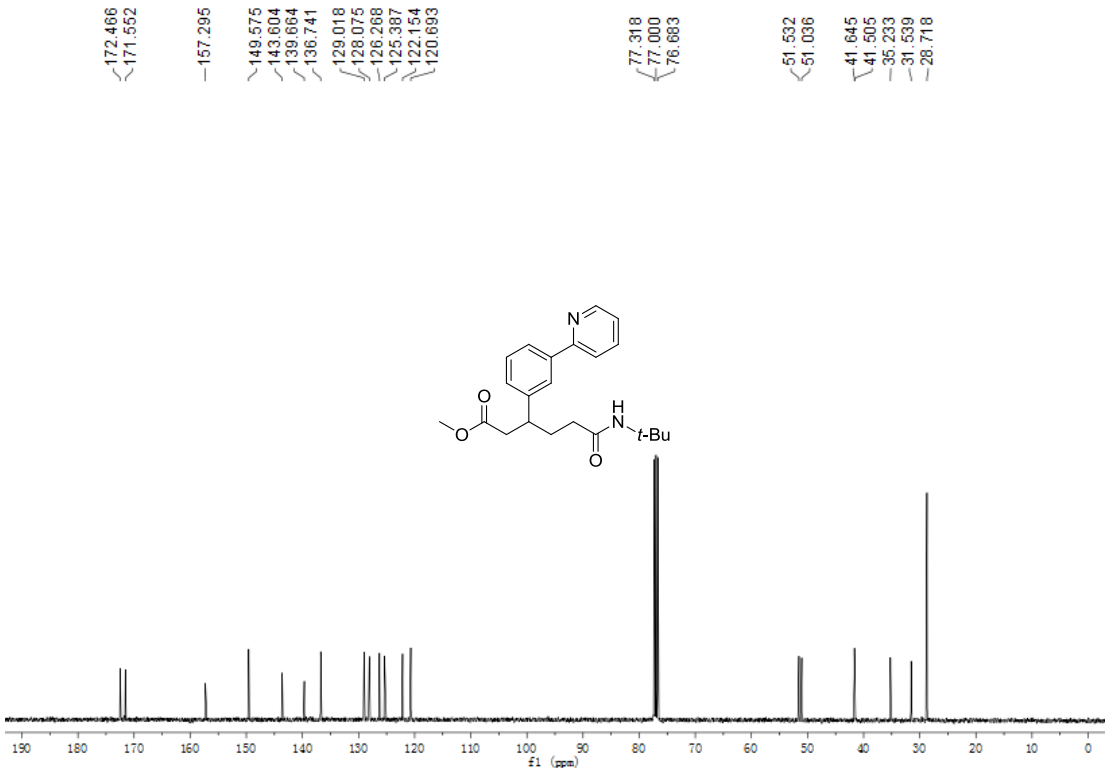

## Compound 3aw $^{13}$C NMR (101 MHz, $CDCl_3$)



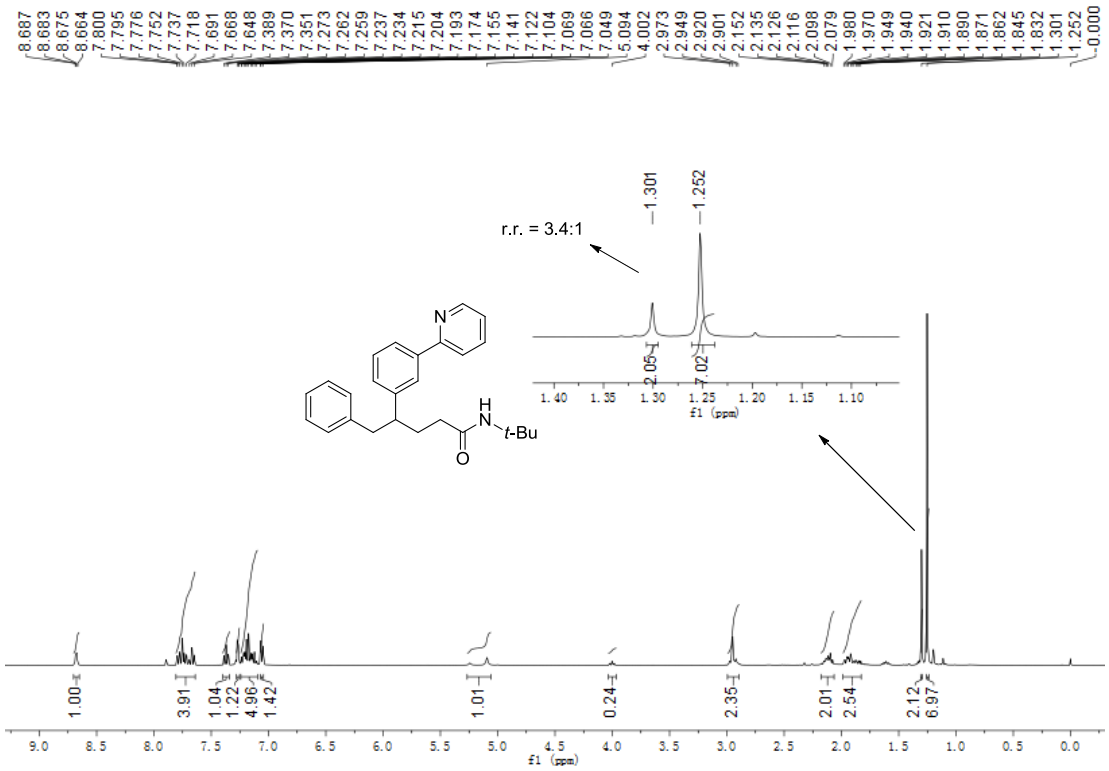
**Compound 3ax $^{1}$H NMR (400 MHz, $CDCl_3$)**



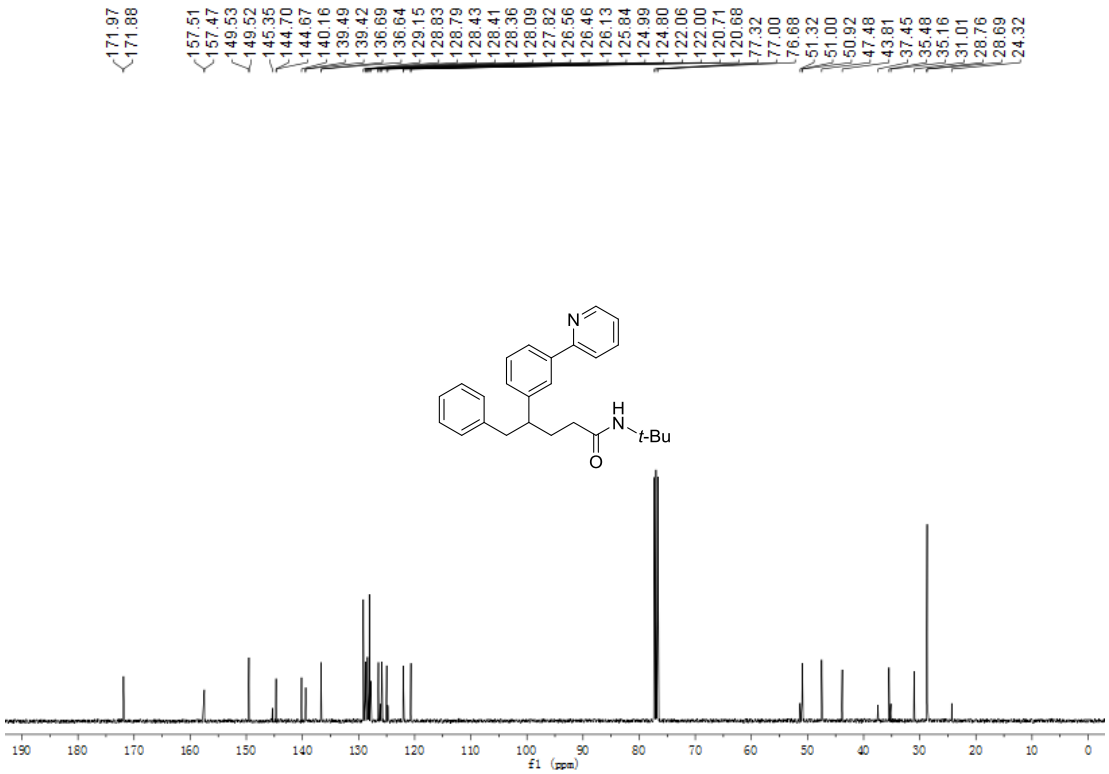

**Compound 3ax $^{13}$C NMR (101 MHz, $CDCl_3$)**



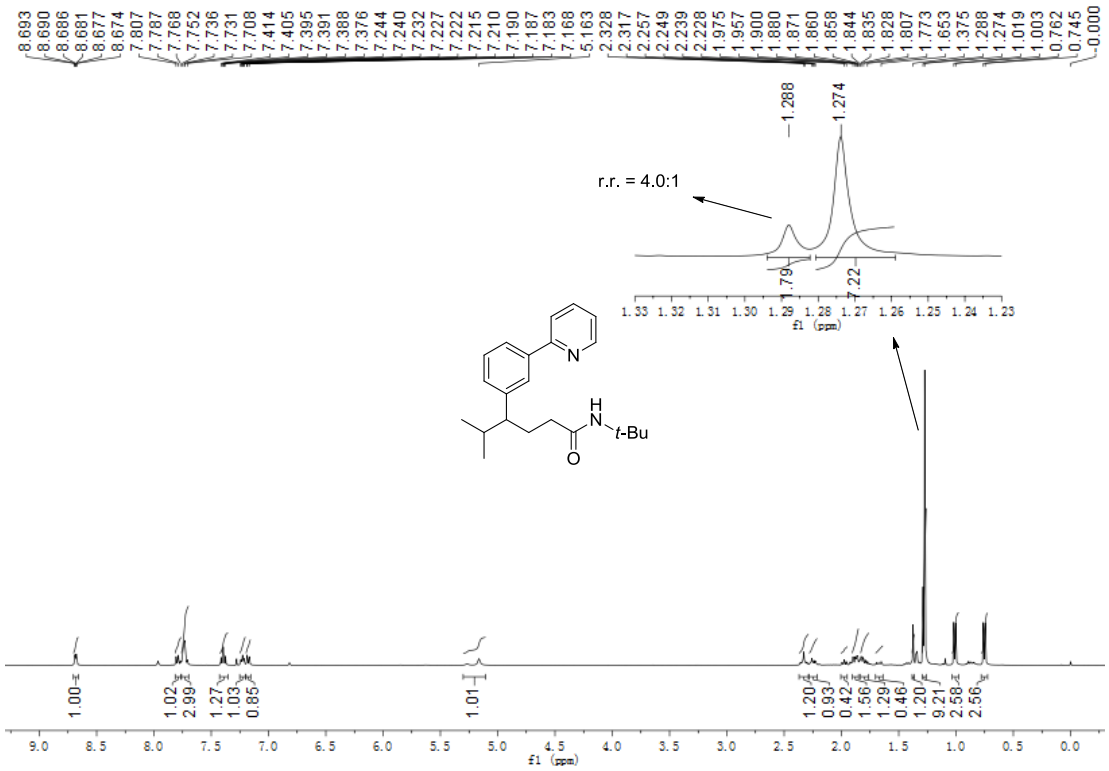
## Compound 3ay $^{1}$H NMR (400 MHz, $CDCl_3$)



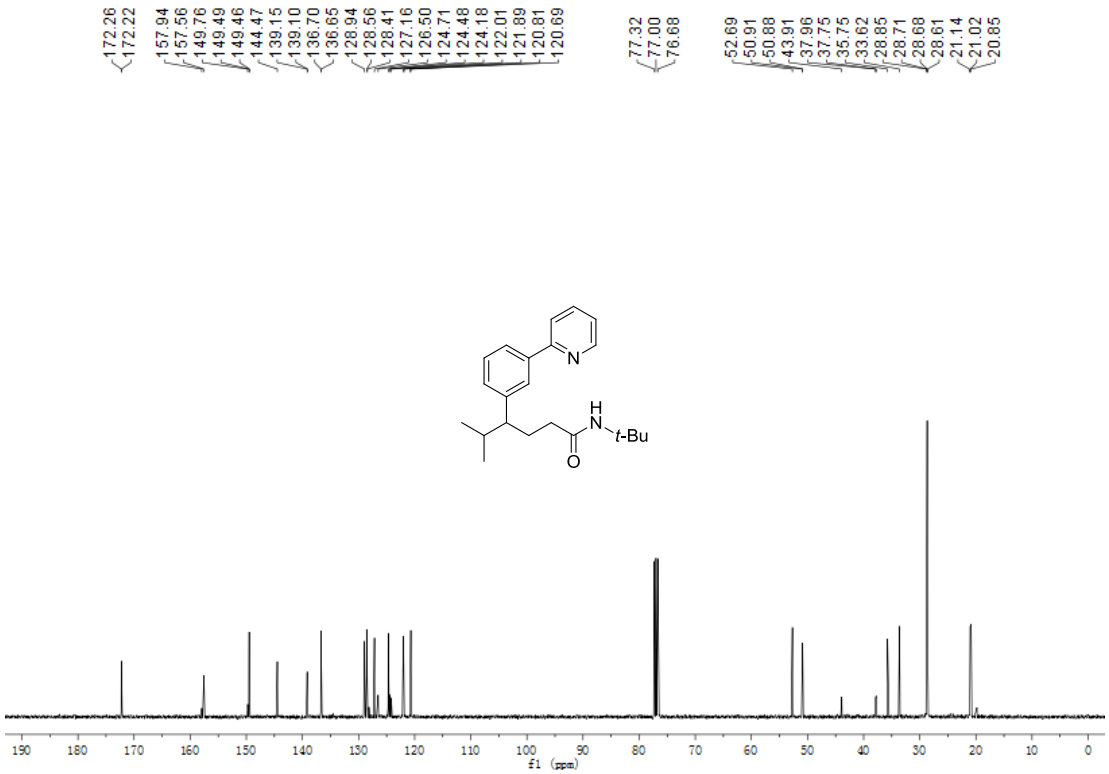

## Compound 3ay $^{13}$C NMR (101 MHz, $CDCl_3$)



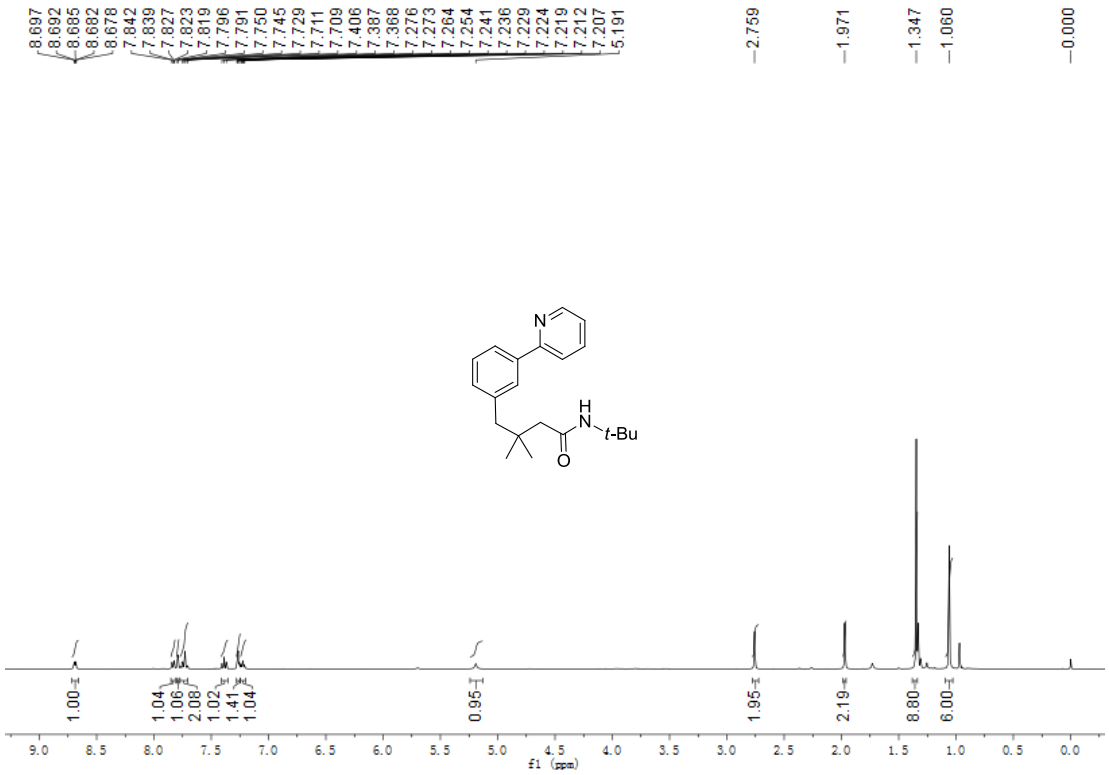
## Compound 3az $^{1}$H NMR (400 MHz, $CDCl_3$)



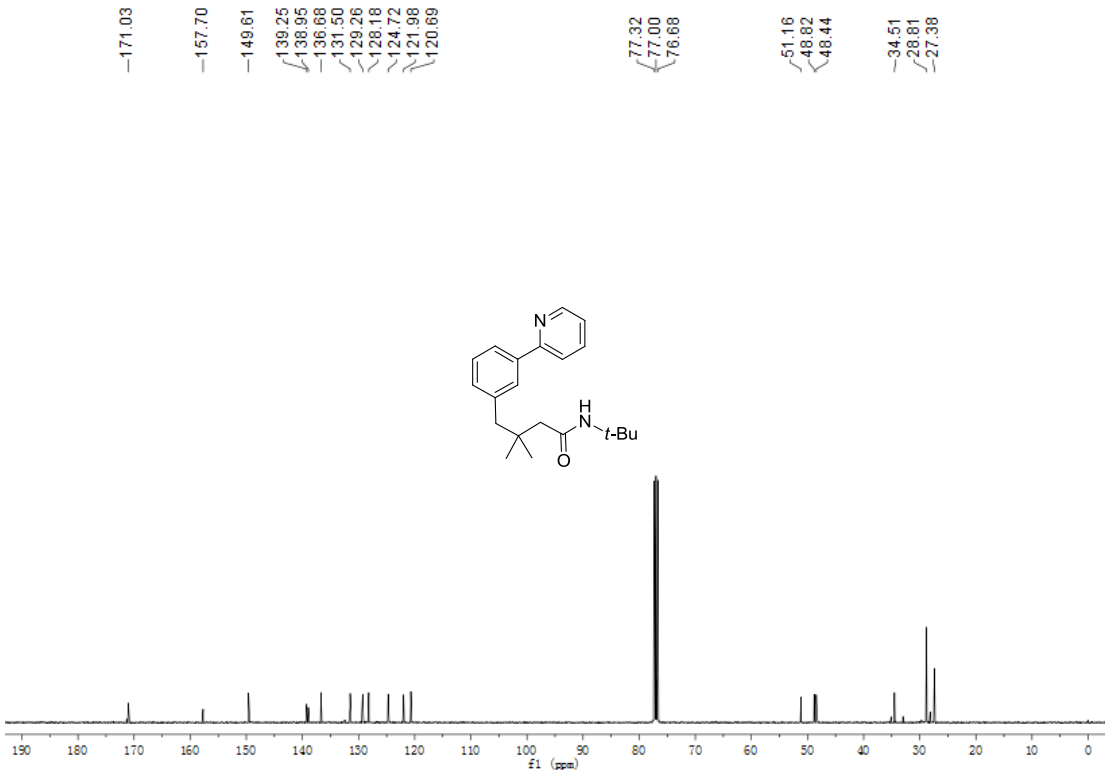

## Compound 3az $^{13}$C NMR (101 MHz, $CDCl_3$)



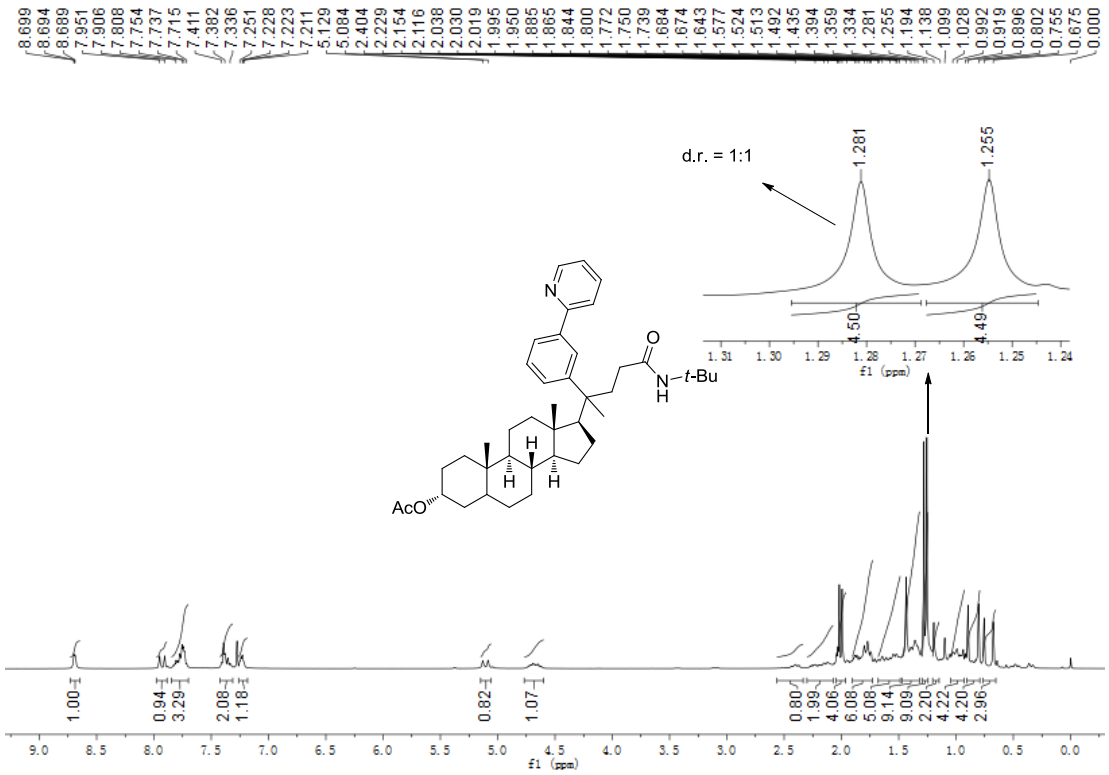
## Compound 3ba $^{1}$H NMR (400 MHz, $CDCl_3$)



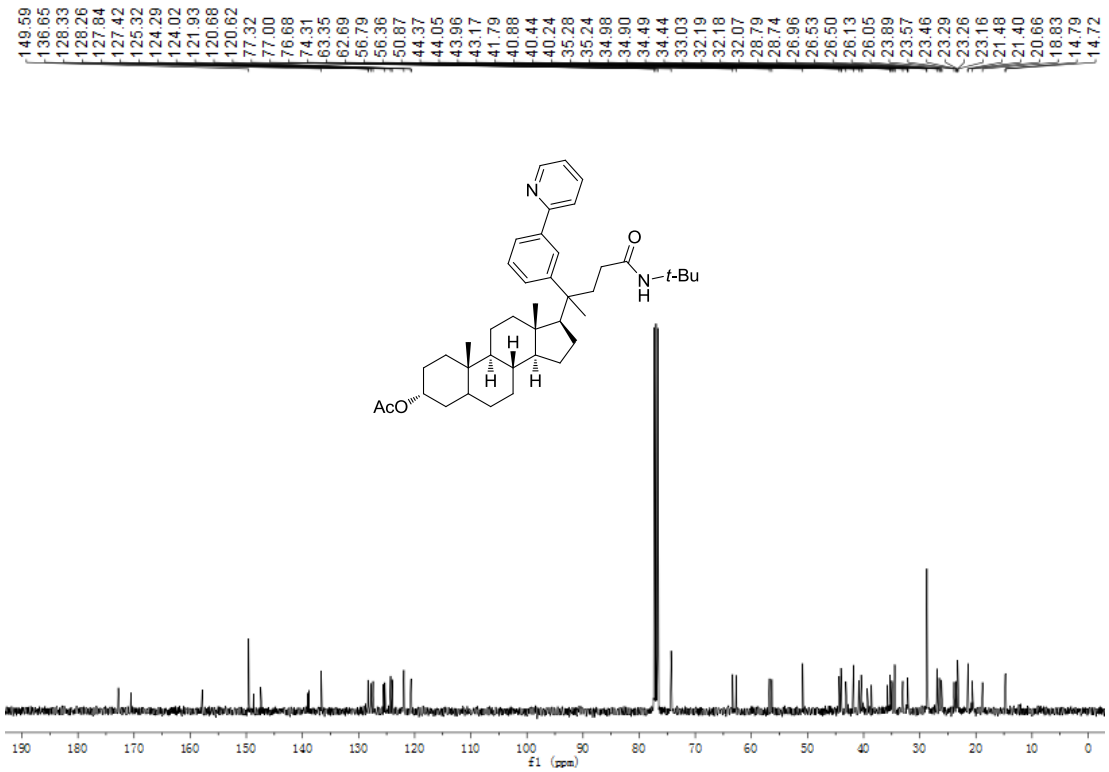

## Compound 3ba $^{13}$C NMR (101 MHz, $CDCl_3$)



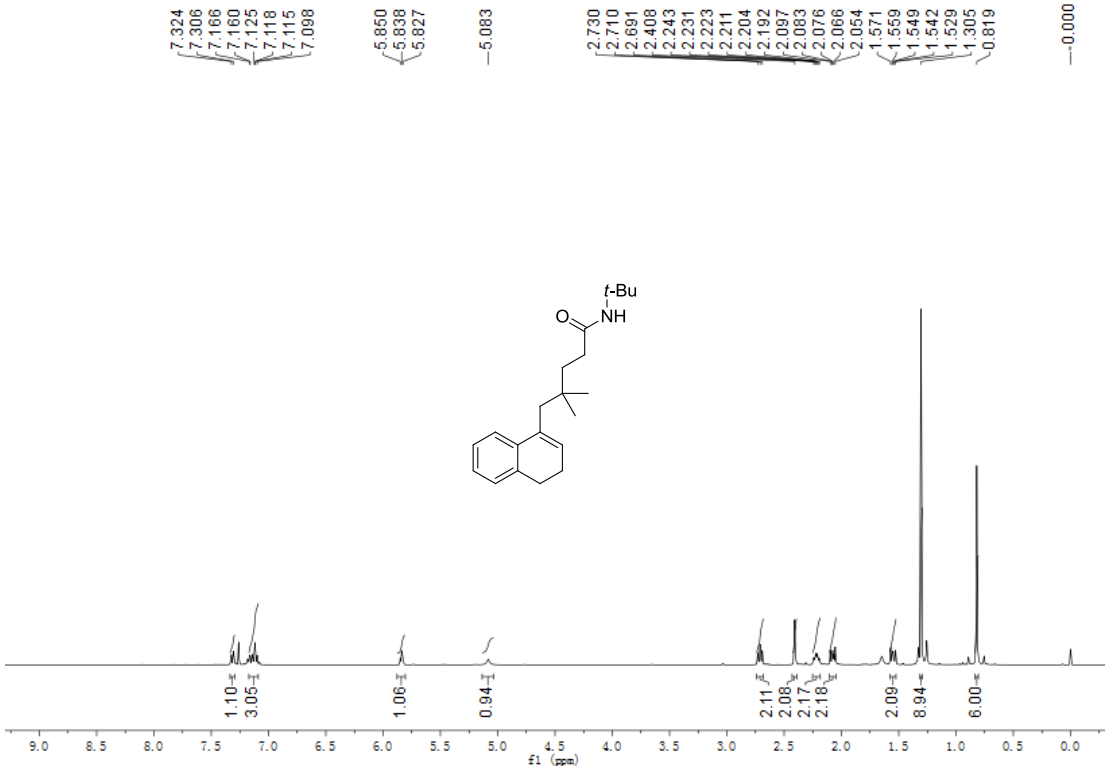
## Compound 3bb $^{1}$H NMR (400 MHz, $CDCl_3$)




## Compound 3bb $^{13}$C NMR (101 MHz, $CDCl_3$)



## Compound 5 $^{1}$H NMR (400 MHz, $CDCl_3$)




## Compound 5 $^{13}$C NMR (101 MHz, $CDCl_3$)