# Supplementary Information

# Electrochemical C−O Bond Cleavage of Diaryl Ethers: Upcycling of Lignin 4-O-5 Models and Polyphenylene Oxide

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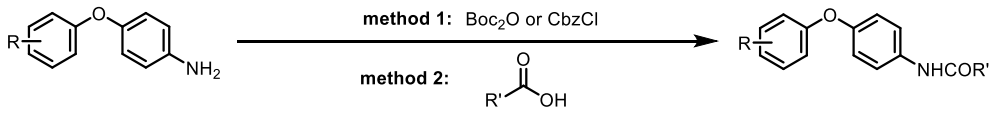
## 1. General considerations

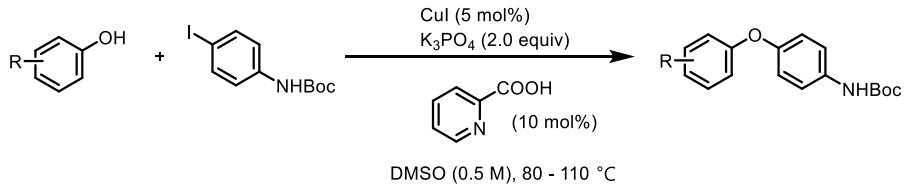
Unless otherwise noted, all reagents were used as received from the commercial suppliers and used without further purification. Electrode material including carbon rod and Platinum plate are commercial available and directly used in this work. Flash chromatography was performed using 200-300 mesh SiliaFlash 60® silica gel (Silicycle Inc.). TLC plates were visualized with UV light (254 nm). $^{1}H$, $^{13}C$ and $^{19}F$ NMR spectra were recorded on a Bruker Avance III HD NMR 400 MHz instrument, and are internally referenced to the residual proto-solvent signals (note: $CDCl_3$ referenced at 7.26 ppm and 77.0 ppm, respectively). Data for $^{1}H$ are reported as: chemical shift (δ ppm), integration, multiplicity (s: singlet, d: doublet, t: triplet, m: multiplet, br: broad peak), coupling constant (Hz) and assignment. GC-MS (EI) was recorded on Agilent 8860A GC systems and 5977 Series MSD. High resolution exact mass measurements (HRMS) were performed on Thermo ScientificTM Orbitrap. All measurements were carried out at room temperature unless otherwise stated.

## 2. Preparation of diaryl ethers




***Method 1****:* According to a reported literature[1], to a solution of commercially available substituted 4-aryloxyaniline (5 mmol, 1.0 equiv) in DMF (3 mL, 0.6 M) was added $Boc_2O$ or CbzCl (1.1 equiv) and $NEt_3$ (1.1 equiv). The reaction was stirred at r.t. overnight. TLC was taken to confirm the complete consumption of starting material. The mixture was dissolved in EtOAc and washed with water twice. The organics were combined, dried over $Na_2SO_4$, filtered, concentrated and purified by silican gel flash chromatography to afford desired diaryl ether products generally in quantitive yields.

***Method 2****:* According to a reported literature[2], to a flask containing a stirred mixture of $Ph_3P$ (1.2 equiv) and DDQ (1.2 equiv) in DCM (20 mL) was added 4-(4-methoxyphenoxy)aniline (1.2 equiv) at room temperature. Carboxylic acid (5 mmol) was then added to the reaction mixture. TLC was taken to confirm the complete consumption of starting material. The solvent was evaporated and residue was chromatographed on a silica gel column to afford desired products.




***Method 3****:* According to a reported literature[3], to a dry, clean round-bottomed flask equipped with a stir bas was added CuI (5 mol%), picolinic acid (10 mool%), tert-butyl N-(4-iodophenyl)carbamate (10 mmol), substituted phenol (1.2 equiv) and $K_3PO_4$ (2.0 equiv). Dry DMSO (0.5 M) was then added to the mixture under $N_2$. The reaction was stirred for 24 h at 80-110℃. TLC was taken to confirm the complete consumption of starting material. The mixture was extracted, washed, dried and concentrated under reduced pressure. The crude product was purified via column chromatography to give the desired diaryl ethers.

## 3. Reaction optimizations

**Table 1:** Reactivity of different leaving groups on diaryl ethers.

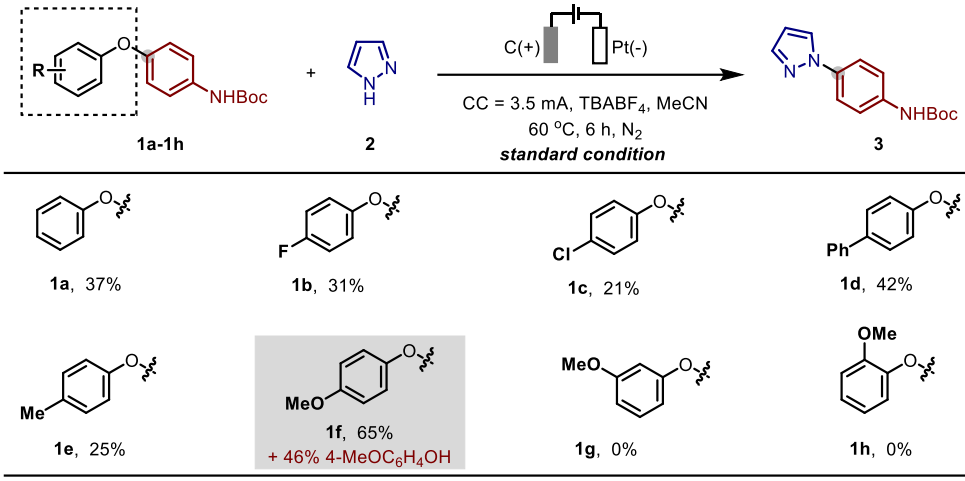
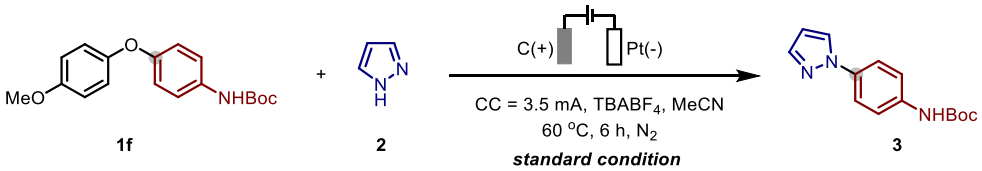


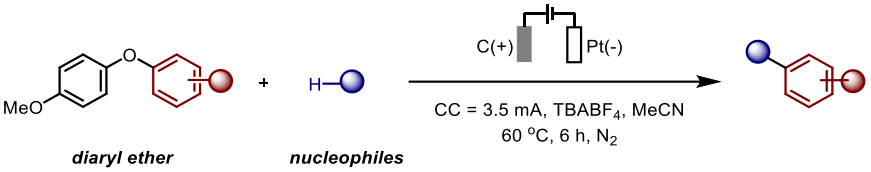

**Table 2:** Influence of other reaction parameters.




| Entry | Variation from "standard conditions" | Yield of **3**[a] |
|---|---|---|
| **1** | **none** | **65%** |
| 2 | Pt (+) instead of C (+) | 31% |
| 3 | C (-) instead of Pt (+) | 35% |
| 4 | DCE instead of MeCN | 28% |
| 5 | DMF instead of MeCN | trace |
| 6 | 80°C instead of 60°C | 43% |
| 7 | 50°C instead of 60°C | 27% |
| 8 | 5 mA instead of 3.5 mA | 43% |
| 9 | 2 mA instead of 3.5 mA, reaction time 10 h | 57% |
| 10 | Raction time 8 h | 56% |
| 11 | 4 equiv of **2** | 61% |
| 12 | $nBu_4OAc$ instead of $TBABF_4$ | 0 |
| 13 | LiOTf instead of $TBABF_4$ | 37% |
| 14 | No electricity | 0 |

Reaction conditions: 1 (0.2 mmol), 2 (1.0 mmol), $TBABF_4$ (0.2 mmol), MeCN (3.0 mL), $N_2$, carbon rod (Φ = 6 mm) anode, Pt cathode (20 mm × 10 mm × 0.2 mm). Reactions performed under constand current conditions for 6 h at 60°C. [a] Isolated yields.

## 4. Reaction procedures for electrochemical SNAr of diaryl ethers



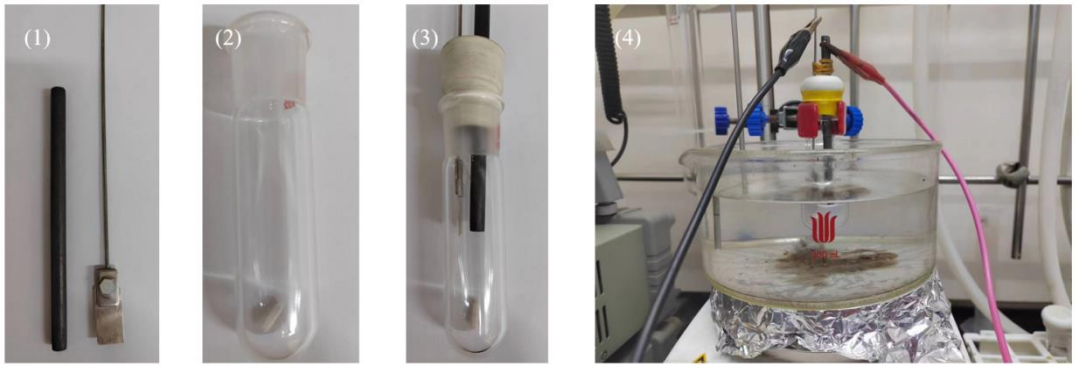



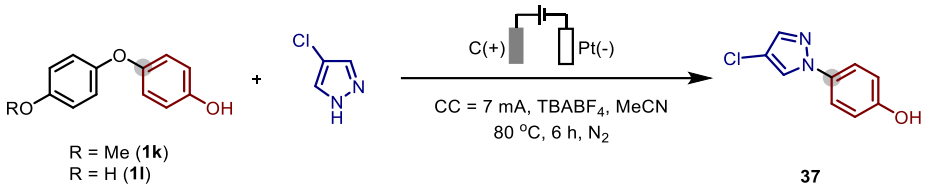

**Fig. 1:** Reaction set-up in batch.
(1) An electrode holder, carbon rod (Φ = 6 mm)and Pt plate (20 mm × 10 mm × 0.2 mm).
(2) A dried 10 mL glass tube.
(3) The carbon rod and Pt electrode were fitted into the tube.
(4) Conducted constant current electrolysis using a potentiostat.

**Condition A:** A dried 10 mL glass tube equipped with a magnetic stirring bar was added diaryl ether (0.2 mmol, 1.0 equiv), N-nucleophile (1.0 mmol, 5.0 equiv), $TBABF_4$ (0.2 mmol, 1.0 equiv), MeCN (3.0 mL). The reactor was equipped with carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) as the cathode. The reaction was bubbled with $N_2$ for three minutes. Then the mixture was electrolyzed under a constant current of 3.5 mA for 6 h at 60℃. After reaction was completed, the reaction solvent was concentrated in vacuo. The resulting residue was purified by silican gel flash chromatography to give the products.

**Condition B:** A dried 10 mL glass tube equipped with a magnetic stirring bar was added diaryl ether (0.2 mmol, 1.0 equiv), N-nucleophile (1.0 mmol, 5.0 equiv), **TBAF** (0.2 mmol, 1.0 equiv), MeCN (3.0 mL). The reactor was equipped with carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) as the cathode. The reaction was bubbled with $N_2$ for three minutes. Then the mixture was electrolyzed under a constant current of 3.5 mA for 6 h at room temperature. After reaction was completed, the reaction solvent was concentrated in vacuo. The resulting residue was purified by silican gel flash chromatography to give the products.

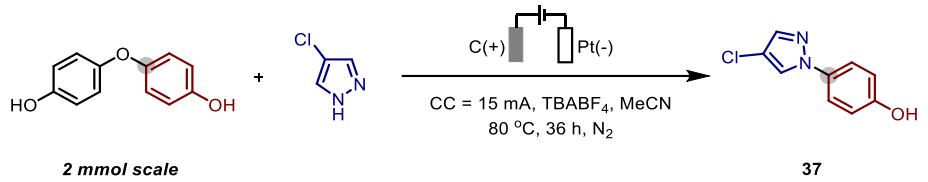
## 5. Reaction procedures for electrochemical SNAr of lignin 4-O-5 models

### 5.1 Reaction procedure in 0.2 mmol scale (in batch)




**Condition C:** A dried 10 mL glass tube equipped with a magnetic stirring bar was added diaryl ether **1k** or **1l** (0.2 mmol, 1.0 equiv), 4-chloropyrazole (1.0 mmol, 5.0 equiv), $TBABF_4$ (0.2 mmol, 1.0 equiv), MeCN (3.0 mL). The reactor was equipped with carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) as the cathode. The reaction was bubbled with $N_2$ for three minutes. Then the mixture was electrolyzed under a constant current of 7 mA for 6 h at 80℃. After reaction was completed, the reaction solvent was concentrated in vacuo. The resulting residue was purified by silican gel flash chromatography to give the desired product **37** in 60% (from **1k**) and 77% (from **1l**) respectively.

### 5.2 Reaction procedure in 2 mmol scale (in batch)




**Condition D:** A dried 100 mL three-necked flash equipped with a magnetic stirring bar was add 4,4'-oxydiphenol **1l** (2 mmol, 1.0 equiv), 4-chloropyrazole (10 mmol, 5.0 equiv), $TBABF_4$ (2mmol, 1.0 equiv) and MeCN (30.0 mL). The reactor was equipped with carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) as the cathode. Then the mixture was electrolyzed under a constant current of 15.0 mA for 36 h at 80℃. After reaction was completed, the reaction solvent was concentrated in vacuo. The resulting residue was purified by silica gel flash chromatography to give the desired product **37** in 60% yield.

### 5.3 Reaction procedure in 20 mmol scale (in flow)

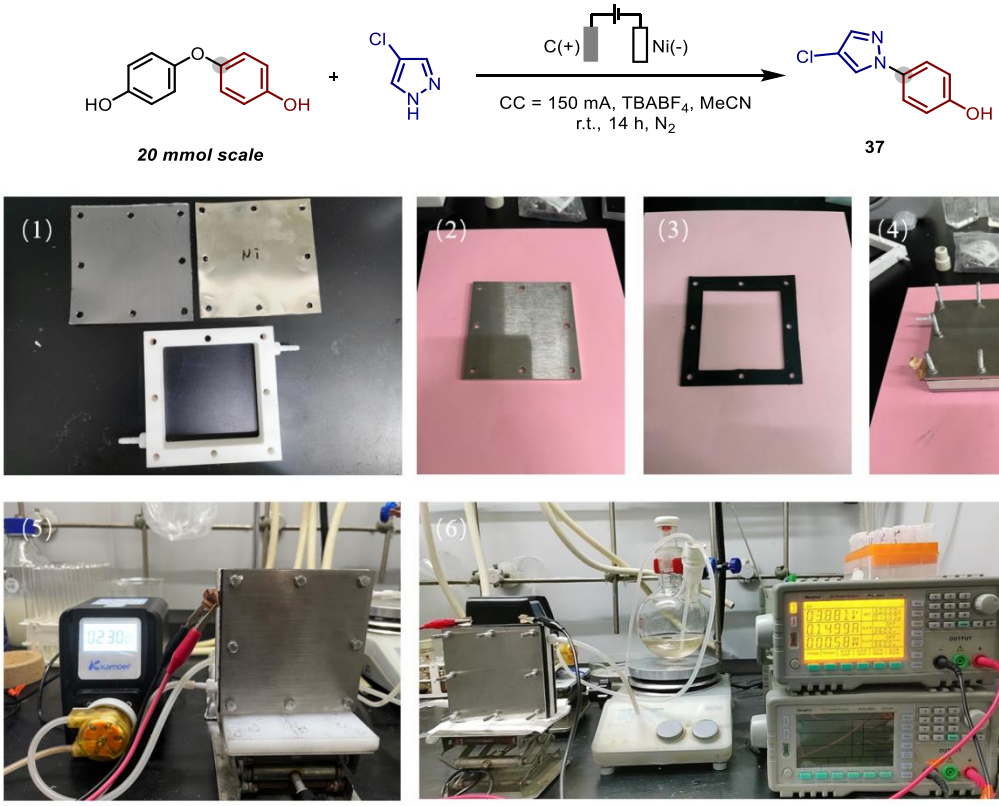



**Fig. 2:** Reaction set-up in flow.
(1) A carbon paper electrode, a nickel electrode and a PTFE frame.
(2) A stainless steel pressure plate.
(3) A fluororubber gasket.
(4) Disassembled flow cell.
(5) A peristaltic pump and silicon tube.
(6) The recycle flow reaction was conducted for 14 h.

*Flow cell setup*

The flow cell was assembled using the following components: 8 hex socket cap screws with nuts (stainless steel, length: 70 mm, thread diameter/outer diameter: 5 mm), 8 stainless steel rings (inner diameter: 5 mm), 2 stainless steel pressure plates (100 mm × 100 mm × 5 mm), 4 fluororubber gaskets (with a space of 100 mm × 100 mm × 2 mm), 1 polytetrafluoroethylene (PTFE) frame (with a inside channel size of 75 mm × 75 mm × 15 mm), 1 carbon paper electrode as cathode (100 mm × 100 mm × 0.5 mm), 1 nickel electrode as anode (100 mm × 100 mm × 0.2 mm).

The cell was assembeled from bottom to top: all the 8 cap screws were wrapped with TPAE tape and inserted through a stainless steel pressure plate (back plate), and then inserted the fluororubber gasket, PTFE frame, carbon paper electrode, nickel electrode and stainless steel

pressure plate (front plate) in sequence, with gaskets inserted between each layer. In addition, copper plates were attached to the two electrodes for conductivity. Finally stainless steel rings and hex nuts were added to each cap screw.

*Preparation for the flow experiment*

A 500-mL two-neck round-bottom flask (reservoir) was charged with 4,4'-oxydiphenol **1l** (20 mmol, 1.0 equiv), 4-chloropyrazole (50 mmol, 2.5 equiv), $TBABF_4$ (20 mmol, 1.0 equiv) and MeCN (200 mL). Then connected a peristalic pump and flow reactor with silicon tube (inner diameter: 2 mm).

*Electrolysis in flow*

With the peristaltic pump turned on (ca 0.07 mL/s) and the reaction mixture flowing through the system, the electrodes were connected to a direct current power source via Alligator clips: red to the carbon paper anode (+) and black to the Ni cathode (-). Then the mixture was electrolyzed under a constant current of 0.15 A for 14 h at room temperature. TLC was taken to confirm the complete consumption of starting material before disconnecting from the power source. The reaction mixture was collected by reversing the direction of the flow. The reaction solvent was concentrated in vacuo. The resulting residue was purified by silica gel flash chromatography to give the desired product **37** in 49% yield (1.9 g).

## 6. Reaction procedures for electrochemical SNAr of polyphenylene oxide (PPO)

*Reaction of pure PPO*

4-Chloropyrazole as a nucleophile: a dried 10 mL glass tube equipped with a magnetic stirring bar was added polyphenylene oxide (PPO) (25.0 mg, 0.2 mmol, 1.0 equiv), 4-chloropyrazole (102.5 mg, 1.0 mmol, 5.0 equiv), $TBABF_4$ (65.9 mg, 0.2 mmol, 1.0 equiv), toluene (2.0 mL) and MeCN (1.0 mL). The reactor was equipped with carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) as the cathode. Then the mixture was electrolyzed under a constant current of 5 mA for 14 h at 80℃. After reaction was completed, the crude product

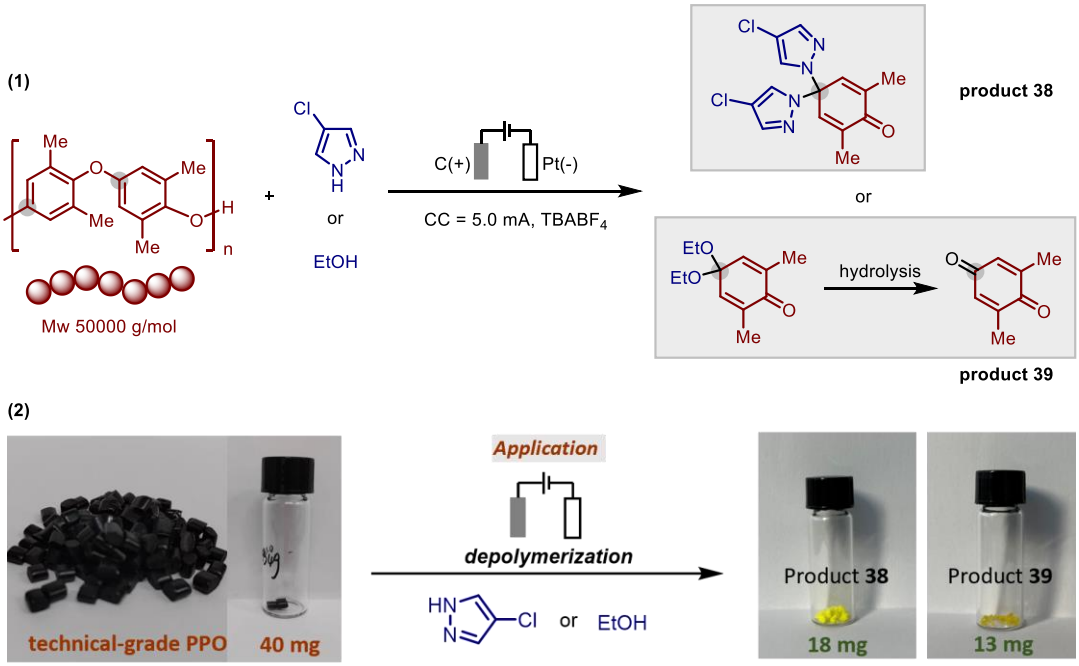



**Fig. 3:** Electrochemical depolymerization of PPO.

yield was obtained by $^1H$ NMR analysis with dibromomethane as the internal standard. The pure product was obtained by silica gel flash chromatography.

EtOH as a nucleophile: a dried 10 mL glass tube equipped with a magnetic stirring bar was added polyphenylene oxide (PPO) (25.0 mg, 0.2 mmol, 1.0 equiv), EtOH (1.0 mL), $TBABF_4$ (65.9 mg, 0.2 mmol, 1.0 equiv), toluene (2.0 mL). The reactor was equipped with carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) as the cathode. Then the mixture was electrolyzed under a constant current of 5 mA for 20 h at 80℃. After reaction was

completed, the crude product yield was obtained by $^1$H NMR analysis with dibromomethane as the internal standard. The pure product was obtained by silica gel flash chromatography.

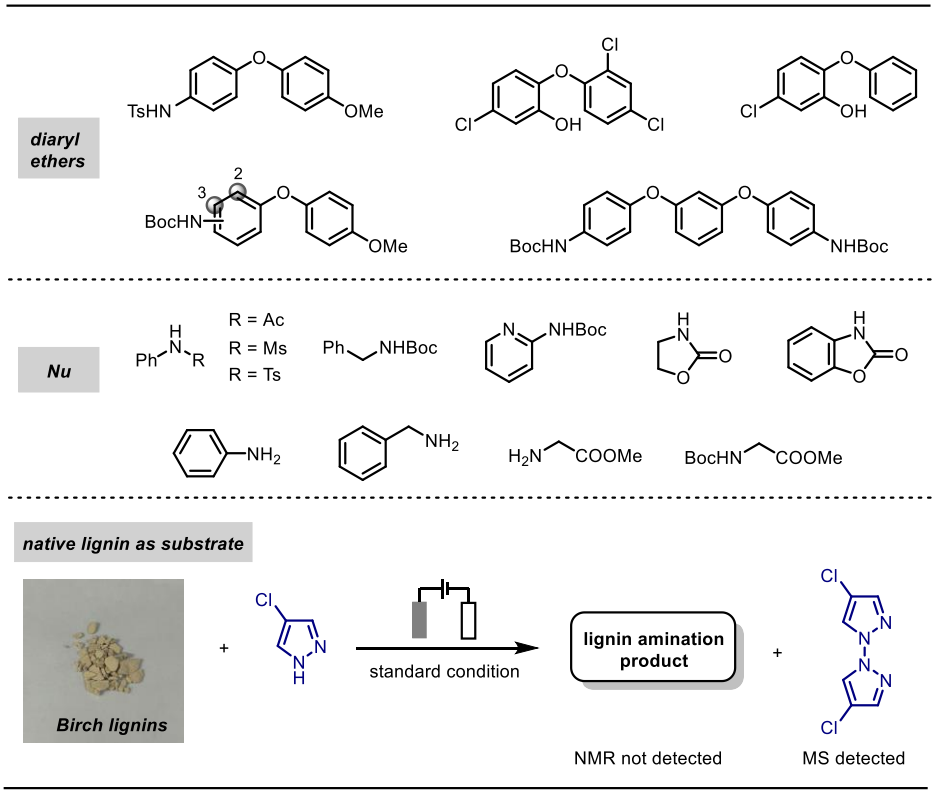
*Reaction of plastic PPO particle*

4-Chloropyrazole as a nucleophile: A dried 10 mL glass tube equipped with a magnetic stirring bar was added PPO plastic particles (40 mg), 4-chloropyrazole (102.5 mg), $TBABF_4$ (65.9 mg), toluene (2.0 mL) and MeCN (1.0 mL). The reactor was equipped with carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) as the cathode. Then the mixture was electrolyzed under a constant current of 5.0 mA for 14 h at 80℃. After reaction was stopted, the reaction solvent was concentrated in vacuo. The resulting residue was purified by silica gel flash chromatography to give the product.

EtOH as a nucleophile: a dried 10 mL glass tube equipped with a magnetic stirring bar was added PPO plastic particles (40 mg), EtOH (1.0 mL), $TBABF_4$ (65.9 mg), toluene (2.0 mL). The reactor was equipped with carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) as the cathode. Then the mixture was electrolyzed under a constant current of 5 mA for 20 h at 80℃. After reaction was completed, the crude product yield was obtained by $^1$H NMR analysis with dibromomethane as the internal standard. The pure product was obtained by silica gel flash chromatography.

## 7. Substrates limitation

**Table 3:** Unsuccessful substrates.



## 8. Mechanistic experiments

### 8.1 Control experiments and radical inhibiting experiments

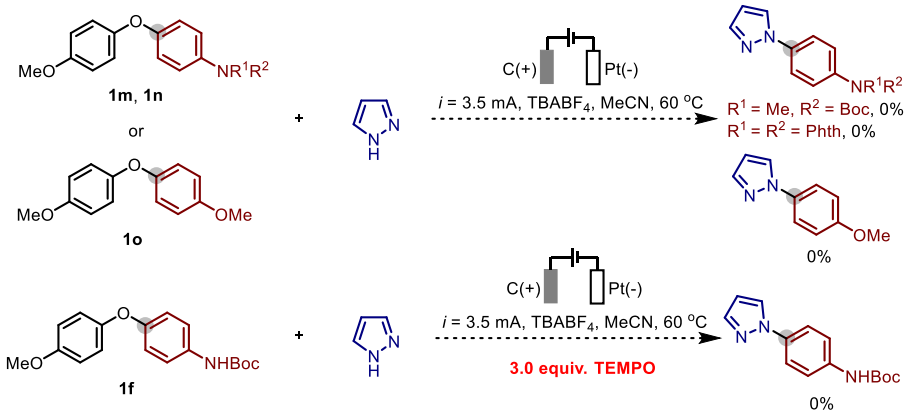
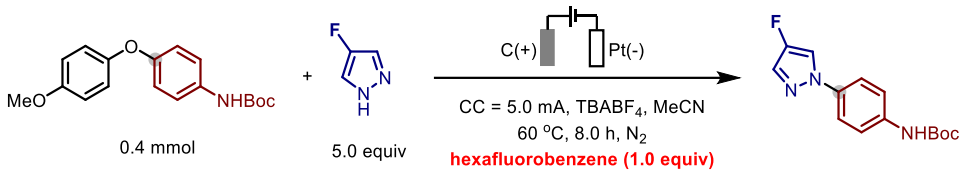



**Fig. 4:** Control experiments and radical inhibiting experiments

A dried 10 mL glass tube equipped with a magnetic stirring bar was added diaryl ether **1m**, **1n** or **1o** (0.2 mmol, 1.0 equiv), pyrazole (1.0 mmol, 5.0 euqiv), $TBABF_4$ (0.2 mmol, 1.0 equiv), MeCN (3.0 mL). The reactor was equipped with carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) as the cathode. The reaction was bubbled with $N_2$ for three minutes. Then the mixture was electrolyzed under a constant current of 3.5 mA for 6 h at 60℃. The reaction was analized by TLC or GC-MS.

A dried 10 mL glass tube equipped with a magnetic stirring bar was added diaryl ether **1f** (0.2 mmol, 1.0 equiv), pyrazole (1.0 mmol, 5.0 euqiv), $TBABF_4$ (0.2 mmol, 1.0 equiv), TEMPO (0.6 mmol, 3.0 equiv), MeCN (3.0 mL). The reactor was equipped with carbon rod(Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) as the cathode. The reaction was bubbled with $N_2$ for three minutes. Then the mixture was electrolyzed under a constant current of 3.5 mA for 6 h at 60℃. The reaction was analized by TLC or GC-MS.

## 8.2 Electrolysis on/off interval experiments




| On/Off | 1 h | 2 h | 3 h | 4 h | 5 h | 6 h | 7 h | 8 h |
|---|---|---|---|---|---|---|---|---|
| Yield | 12% | 12% | 30% | 30% | 42% | 42% | 54% | 54% |

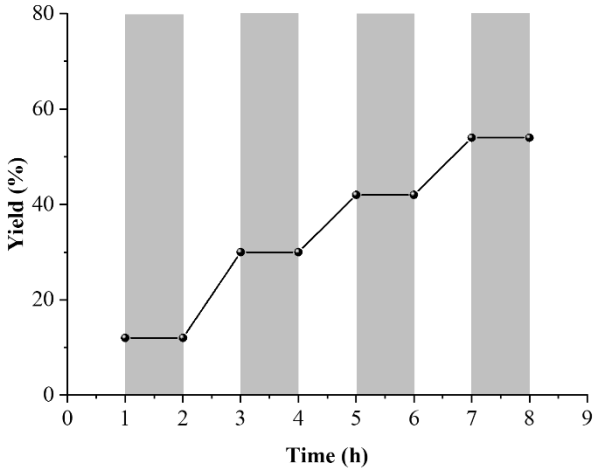



**Fig. 5:** Electrolysis on/off interval experiments.

A dried three-necked undivided cell (10 mL) euipped with a magnetic stirring bar was added $TBABF_4$ (131.6 mg, 0.4 mmol), diaryl ether **1f** (126.0 mg, 0.4 mmol), 4-fluoropyrazole (172.1 mg, 2.0 mmol) and MeCN (5.0 mL). The undivided cell was equipped with carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) and charged with $N_2$ to replace air atmosphere. Added hexafluorobenzene (74.4 mg) as internal standard before reaction. Pre-stirring the resulting mixture until it is completely dissolved, and then the reaction mixture was electrolyed at a constant current of 5.0 mA at 60°C. After the reaction started, aliquots of 0.1 mL were collected from the cell every 1 h. The yield of product was determined by $^{19}F$ NMR.

## 8.3 Reaction kinetic studies

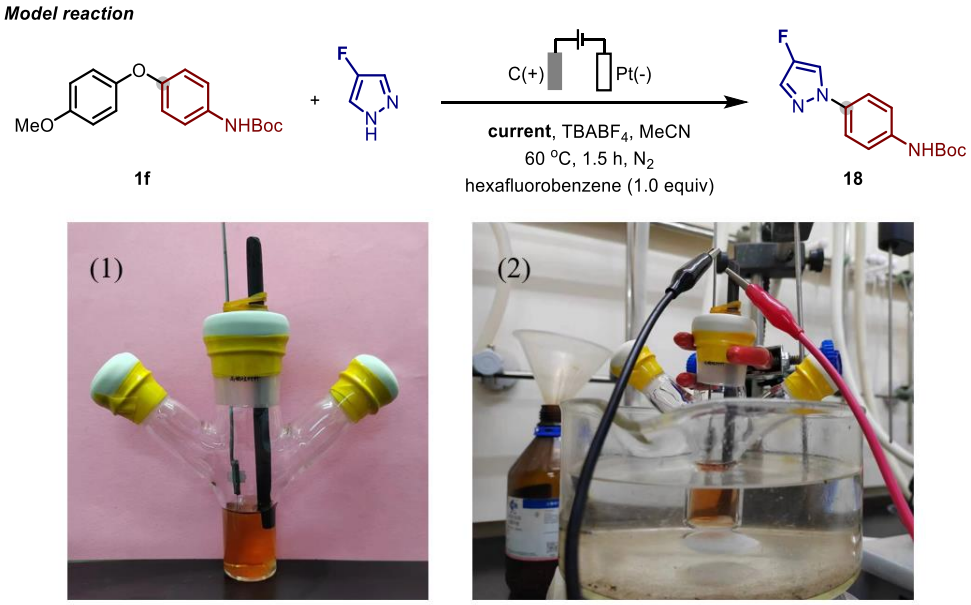



**Fig. 6:** Reaction set-up for kinetics studies.
(1) A three-port reactor with carbon rod electrode and Pt electrode.
(2) Conducted constant current electrolysis (I = 5.0 mA) using a potentiostat.

A dried three-necked undivided cell (10 mL) euipped with a magnetic stirring bar was added $TBABF_4$ (131.6 mg), diaryl ether **1f**, 4-fluoropyrazole and MeCN (5.0 mL). The undivided cell was equipped with carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) and charged with $N_2$ to replace air atmosphere. Added hexafluorobenzene as internal standard before reaction. Pre-stirring the resulting mixture until it is completely dissolved, and then the reaction mixture was electrolyed at a constant current of 5.0 mA at 60℃. After the reaction started, aliquots of 0.1 mL were collected from the cell at 15, 30, 45, 60, 75 and 90 minutes. The yield of product was determined by $^{19}F$ NMR analysis.

8.3.1 Determination of the reaction order in current.

The reaction was performed with the diaryl ether **1f** (126.0 mg, 0.4 mmol, 1.0 equiv), 4-fluoropyrazole (172.1 mg, 2 mmol, 5.0 equiv) and $TBABF_4$ (131.6 mg) in MeCN (5.0 mL). Then the reaction mixture was stirred and reacted at a constant current of 2.0, 3.0, 3.5 or 5.0 mA. The relationship between the initial rate and current was linear, showing the reaction exhibits first-order rate dependence on the current.

**Table 4:** The yield of **18** at different time in various current.

| Time / Yield / *I* (mA) | 15 min | 30 min | 45 min | 60 min | 75 min | 90 min |
|---|---|---|---|---|---|---|
| 2.0 | 0% | 2.1% | 3.0% | 3.9% | 6.0% | 8.1% |
| 3.0 | 0% | 3.0% | 4.5% | 7.2% | 9.0% | 10.8% |
| 3.5 | 1.5% | 3.9% | 6.6% | 8.7% | 11.4% | 15.0% |
| 5.0 | 2.7% | 6.6% | 11.4% | 15.6% | 20.7% | 23.7% |

Note: Yield = the yield of **18**.

**Table 5:** The initial rates with various current.

| *I* (mA) | 2.0 | 3.0 | 3.5 | 5.0 |
|---|---|---|---|---|
| Initial Rate($10^{-3}$ M/min) | 1.0 | 1.4 | 1.8 | 2.9 |

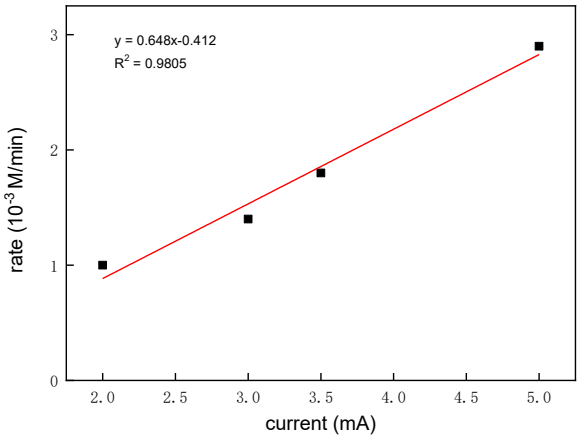



**Fig. 7:** Kinetic plots with different constant current from 2.0-5.0 mA.

8.3.2 Determination of the reaction order in diaryl ether **1f**.

The reaction was performed with the 4-fluoropyrazole (258.2 mg, 3 mmol), $TBABF_4$ (131.6 mg) in MeCN (5.0 mL) in the presence of 0.08, 0.10, 0.12, 0.14, 0.16, 0.18 M diary ether **1f**. The relationship between the initial rates and diary ether **1f** was linear, showing the reaction exhibits first-order rate dependence on the concentration of **1f**.

**Table 6:** The yield of **18** at different time in various **[1f]**.

| Time / Yield / **[1f]** (M) | 15 min | 30 min | 45 min | 60 min | 75 min | 90 min |
|---|---|---|---|---|---|---|
| 0.08 | 1.2% | 2.9% | 4.8% | 6.5% | 8.6% | 10.5% |
| 0.10 | 1.5% | 2.8% | 4.7% | 6.2% | 8.3% | 11.4% |
| 0.12 | 1.3% | 3.2% | 5.0% | 7.0% | 9.6% | 11.2% |
| 0.14 | 1.2% | 3.0% | 5.1% | 6.6% | 8.4% | 10.5% |
| 0.16 | 1.2% | 2.7% | 4.2% | 6.3% | 8.4% | 10.8% |
| 0.18 | 1.4% | 2.7% | 4.1% | 5.9% | 7.7% | 9.9% |

Note: **[1f]** = the initial concentration of diaryl ether **1f**; Yield = the yield of **18**.

**Table 7:** The initial rates with various **[1f]**.

| [**1f**] | 0.08 | 0.10 | 0.12 | 0.14 | 0.16 | 0.18 |
|---|---|---|---|---|---|---|
| Initial Rate($10^{-3}$ M/min) | 1.2 | 1.3 | 1.3 | 1.2 | 1.3 | 1.1 |

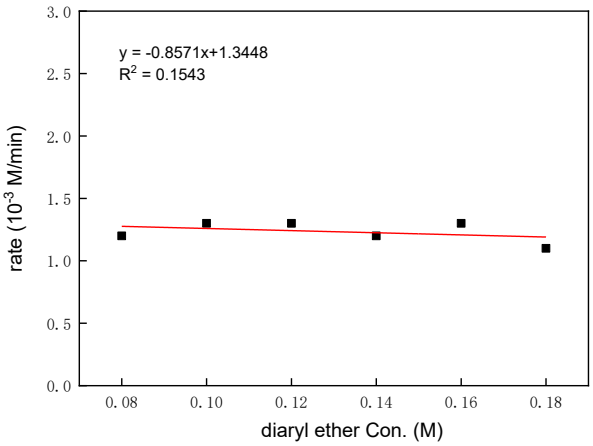



**Fig. 8:** Kinetic plots with different concentrations of diaryl ether **1f** from 0.08-0.18 M.

8.3.3 Determination of the reaction order in 4-fluoropyrazole.

The reaction was performed with the diaryl ether **1f** (126.0 mg, 0.4 mmol),$TBABF_4$ (131.6 mg) in MeCN (5.0 mL) in the presence of 0.08, 0.16, 0.24, 0.32 M 4-fluoropyrazole **18'**. The relationship between the initial rates and [**18'**]$^2$ was linear, showing the reaction exhibits first-order rate dependence on the two molecules of 4-fluoropyrazole.

**Table 8:** The yield of **18** at different time in various 4-fluoro-1H-pyrazole.

| Yield / Time **[18']** (M) | 15 min | 30 min | 45 min | 60 min | 75 min | 90 min |
|---|---|---|---|---|---|---|
| 0.08 | 0% | 4.5% | 6.6% | 8.4% | 10.2% | 12.6% |
| 0.16 | 3.6% | 5.7% | 8.4% | 10.5% | 15.3% | 16.8% |
| 0.24 | 3.6% | 7.2% | 10.2% | 14.4% | 20.0% | 23.0% |
| 0.32 | 3.3% | 6.9% | 11.7% | 16.5% | 21.0% | 25.5% |

Note: [**18'**] = the initial concentration of 4-fluoropyrazole; Yield = the yield of **18**.

**Table 9:** The initial rates with $[\mathbf{18'}]^2$.

| $[\mathbf{18'}]^2$ | $0.08^2$ | $0.16^2$ | $0.24^2$ | $0.32^2$ |
|---|---|---|---|---|
| Initial Rate($10^{-3}$ M/min) | 1.6 | 2.0 | 2.7 | 3.0 |

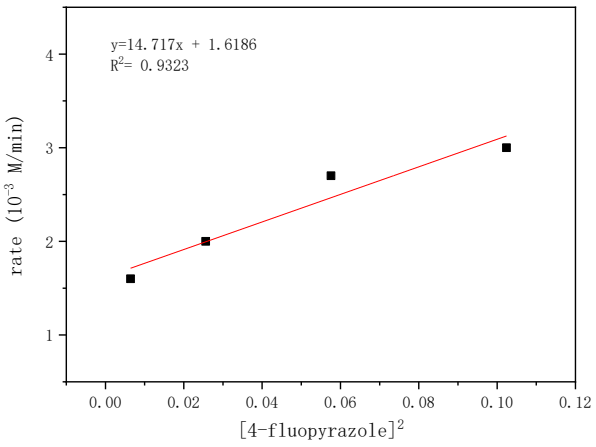



**Fig. 9:** Kinetic plots of different concentrations of 4-fluoropyrazole from 0.08-0.32 M.

### 8.4 Cyclic voltammetry experiments

Cyclic voltammetry was recorded using a CHI660E potentiostat at room temperature. A glassy carbon electrode (3 mm diameter, Ledonlab), Pt wire (0.5 mm diameter, Ledonlab), and Ag/AgCl (in saturated potassium chloride) were used as the working, counter, and reference electrodes, respectively. Prior to the experiment, glassy carbon electrode was polished using 0.5 µm α-$Al_2O_3$ polishing powder. MeCN (6 mL) was used as the solvent in the presence of 100 mM $TBABF_4$ as supporting electrolyte. Unless otherwise noted, scan rate = 100 mV/s.

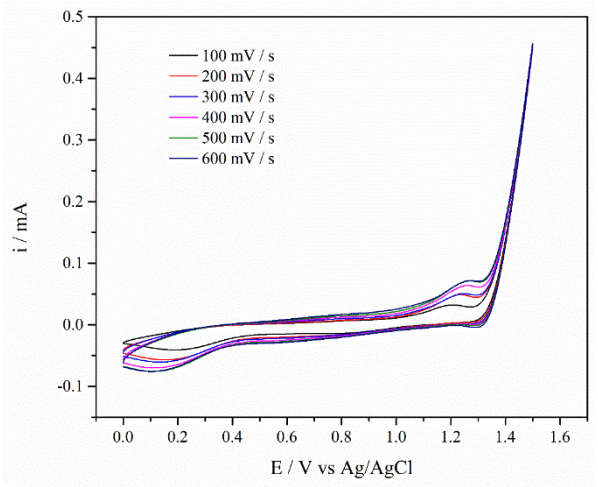



**Fig. 10:** Cyclic voltammetry of tert-butyl (4-(4-methoxyphenoxy) phenyl) carbamate (0.4 mmol) in MeCN (6.0 mL) with 0.1 M $TBABF_4$ at varied sweep rates.

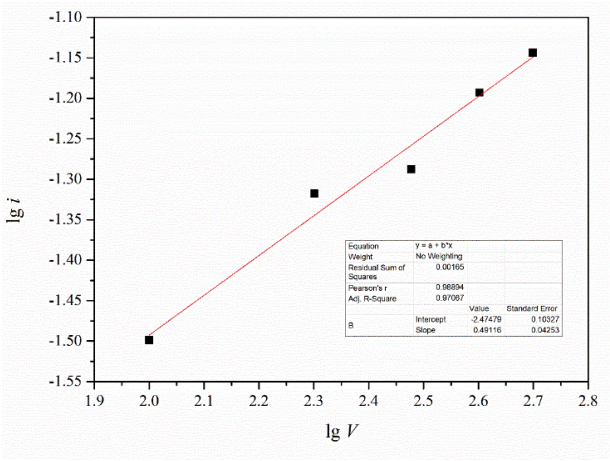



**Fig. 11:** Linear relation between logarithm of oxidation peak current and logarithm of scan rate.

A straight line with a slope of 0.49 close to the theoretical value of 0.5 for a purely diffusion-controlled process.

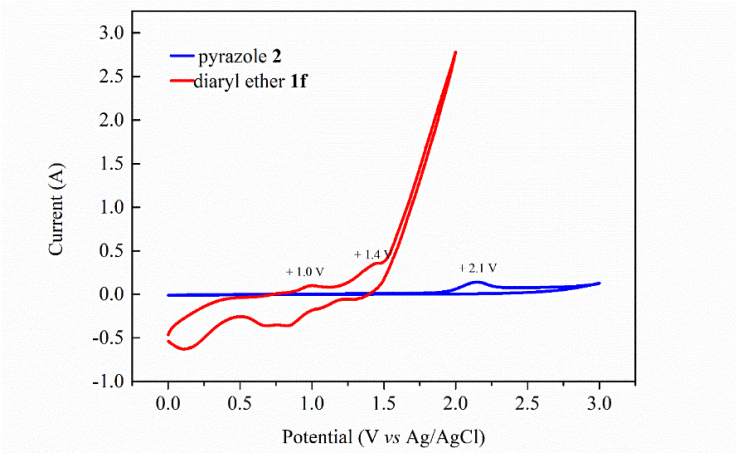



**Fig. 12:** Cyclic voltammetry of ter-butyl (4-(4-methoxyphenoxy) phenyl) carbamate (0.8 mmol) in MeCN (6.0 mL) with 0.1 M $TBABF_4$ and cyclic voltammetry of pyrazole in MeCN with 0.1 M $TBABF_4$, acquired at a scan rate of 100 mV/s.

### 8.5 Controlled potential electrolysis experiments

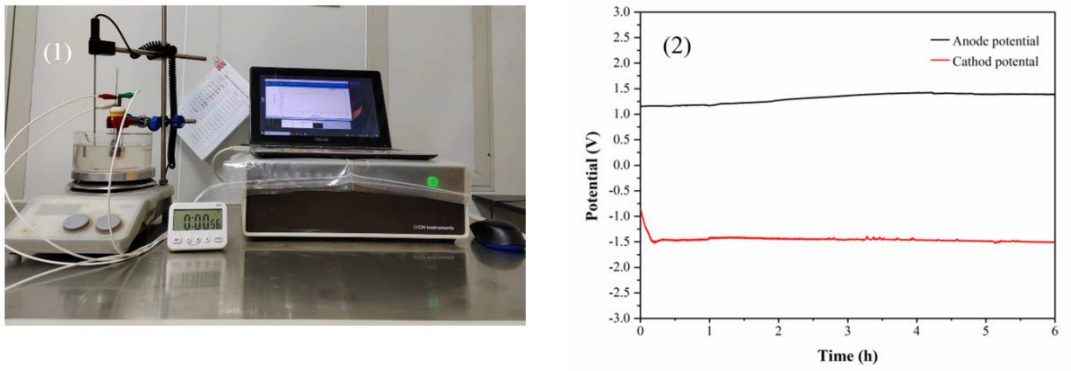
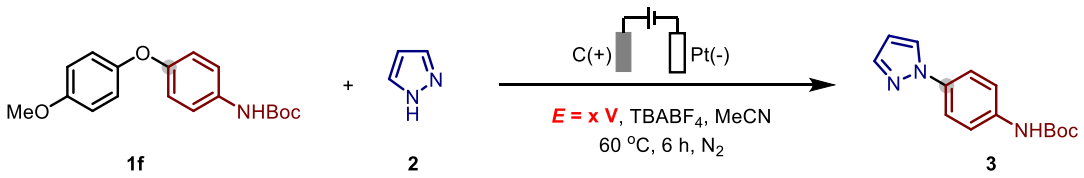



**Fig. 13:** Controlled potential electrolysis and electrode voltage over the course of electrolysis.

**Table 10:** Controlled potential electrolysis




| Entry | *E (vs Ag/AgCl)* | Isolated yield |
|---|---|---|
| 1 | *+ 1.0 v* | N.R. |
| 2 | *+1.4 v* | 42% |

Controlled potential electrolysis was proceeded using a HI660E potentiostat. A dried 10 mL glass tube equipped with a magnetic stirring bar was added sequentially $TBABF_4$ (65.8 mg, 0.2 mmol), diaryl ether **1f** (63.0 mg, 0.2 mmol), pyrazole **2** (68.0 mg, 10 mmol) and MeCN (3.0

mL). A carbon rod (Φ = 6 mm) as the anode and Pt plate (20 mm × 10 mm × 0.2 mm) and Ag/AgCl (in saturated potassium chloride) were used as the working, counter and reference electrodes, respecttively. The reaction was bubbled with $N_2$ for three minutes. Then the mixture was respectively electrolyzed under a constant voltage (vs Ag/AgCl) + 1.0 V, + 1.4 V. After reaction was completed, the reaction solvent was concentrated in vacuo. The resulting residue was purified by silica gel flash chromatography to give the product.

## 9. Density functional theory (DFT) calculations

### 9.1 Calculation details

All density functional theory (DFT) calculations[4] were carried out using the Gaussian 16 software package[5]. All geometries were optimized using M06-2X[6,7] functional with the 6-31G(d,p)[8-10] basis set for all atoms under the SMD continuum solvation model[15] of acetonitrile due to the apparent charge in the structure. Frequency calculations were performed on stationary points at the same level of theory as for geometry optimization to confirm if each optimized structure is a local minimum or a transition state structure with only one imaginary frequency. IRC calculations were performed to ensure that the saddle points found were true TSs connecting the reactants and the products. Single-point energy calculations were conducted on the M06-2X functional and 6-311G++(d,p)[11-14] basis set for all atoms. Solvation energy correction was calculated in toluene solvent with the SMD[15] continuum solvation model based on the optimized geometries. Grimme correction[16] for entropy was performed using Shermo 2.6[17].

### 9.2 Electrostatic potential analysis and charge distribution

Electrostatic potential analysis was conducted utilizing the Multifwn procedure[18-20], with the quantitative molecular surface analysis (main function 12) being predomi-nantly employed. The yellow spheres represent the points of maximum electrostatic potential on the molecular surface, while the blue spheres indicate the points of minimum electrostatic potential. Molecular structure visualizations were obtained using VMD[21].

**Table 11:** Summary charges and ESP of optimized structures

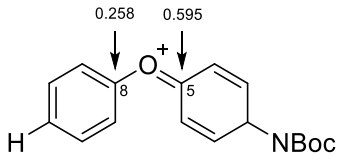
| Structures | C8 position | C5 position | FG | ESP above C5 |
|---|---|---|---|---|
| **ESP-1** | 0.258 | 0.595 | 4-H | 120.39 |
| **ESP-2** | 0.247 | 0.593 | 4-F | 126.02 |
| **ESP-3** | 0.259 | 0.595 | 4-Cl | 126.04 |
| **ESP-4** | 0.259 | 0.592 | 4-Ph | 120.89 |
| **ESP-5** | 0.250 | 0.591 | 4-Me | 119.23 |

| | | | | |
|---|---|---|---|---|
| **ESP-6** | 0.227 | 0.587 | 4-OMe | 119.02 |
| **ESP-7** | 0.216 | 0.598 | 2-OMe | 111.29 |
| **ESP-8** | 0.278 | 0.595 | 3-OMe | 117.38 |

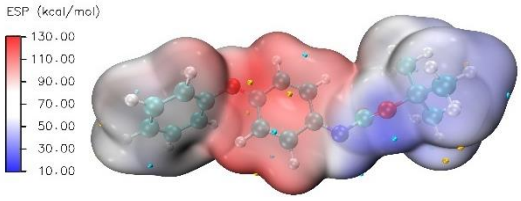
## Details of separated structures

**Table 12:** ESP-1

**a) Structure and NPA charge**




**b) Electrostatic potential analysis**




| Atom | No | NPA Charge | Atom | No | NPA Charge |
|---|---|---|---|---|---|
| **C** | 1 | -0.02509 | C | 21 | -0.62808 |
| **C** | 2 | 0.21033 | H | 22 | 0.26559 |
| **C** | 3 | -0.09603 | H | 23 | 0.26345 |
| **C** | 4 | -0.24002 | H | 24 | 0.27494 |
| **C** | **5** | **0.59482** | H | 25 | 0.28149 |
| **C** | 6 | -0.29882 | H | 26 | 0.25665 |
| **O** | 7 | -0.44437 | H | 27 | 0.23972 |
| **C** | **8** | **0.25821** | H | 28 | 0.23934 |
| **C** | 9 | -0.24709 | H | 29 | 0.2558 |
| **C** | 10 | -0.19396 | H | 30 | 0.2245 |
| **C** | 11 | -0.20995 | H | 31 | 0.21811 |
| **C** | 12 | -0.19293 | H | 32 | 0.2188 |
| **C** | 13 | -0.24014 | H | 33 | 0.22902 |
| **N** | 14 | -0.36022 | H | 34 | 0.2202 |
| **C** | 15 | 0.94285 | H | 35 | 0.22596 |
| **O** | 16 | -0.58293 | H | 36 | 0.22941 |
| **O** | 17 | -0.62194 | H | 37 | 0.22562 |
| **C** | 18 | 0.2824 | H | 38 | 0.21921 |

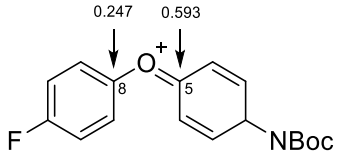
| | | | | | |
|---|---|---|---|---|---|
| **C** | 19 | -0.60397 | H | 39 | 0.23691 |
| **C** | 20 | -0.62778 | | | |

| Electrostatic potential analysis | | | | | | |
|---|---|---|---|---|---|---|
| **Number of surface minima: 12** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.072241 | 1.97 | 45.33 | -6.889721 | 1.725084 | -2.822517 |
| **2** | 0.064141 | 1.75 | 40.25 | -6.411901 | -2.731512 | -0.095498 |
| **3** | 0.075070 | 2.04 | 47.11 | -6.125662 | 0.183092 | 2.526303 |
| **4** | 0.028909 | 0.79 | 18.14 | -3.686801 | -2.707480 | 2.129420 |
| **5** | 0.057673 | 1.57 | 36.19 | -3.512696 | -0.123102 | -2.502146 |
| **6** | 0.061074 | 1.66 | 38.32 | -2.493609 | -2.172500 | -2.165047 |
| **7** | 0.144997 | 3.95 | 90.99 | -0.350252 | 2.316108 | 0.339147 |
| **8** | 0.145592 | 3.96 | 91.36 | 1.104288 | 0.407868 | -2.379245 |
| **9** | 0.145309 | 3.95 | 91.18 | 1.266741 | -2.718596 | -0.119583 |
| **10** | 0.110419 | 3.00 | 69.29 | 3.457665 | 1.715621 | 2.342197 |
| **11** | 0.089956 | 2.45 | 56.45 | 6.190865 | -0.729811 | -2.574478 |
| **12** | 0.074276 | 2.02 | 46.61 | 7.397608 | 0.873814 | 0.938771 |
| **Number of surface maxima: 11** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.101450 | 2.76 | 63.66 | -7.231897 | 1.348301 | 0.279724 |
| **2** | 0.071596 | 1.95 | 44.93 | -6.022898 | -2.123048 | 1.761976 |
| **3** | 0.087984 | 2.39 | 55.21 | -5.773890 | -1.439872 | -2.494193 |
| **4** | 0.088504 | 2.41 | 55.54 | -5.547910 | -0.017008 | -3.322678 |
| **5** | 0.101223 | 2.75 | 63.52 | -3.752951 | -2.062658 | -1.024621 |
| **6** | 0.175000 | 4.76 | 109.81 | -0.747135 | 1.538981 | 2.472494 |
| **7** | 0.169231 | 4.61 | 106.19 | 0.572489 | 2.222836 | 3.037752 |
| **8** | 0.177138 | 4.82 | 111.16 | 1.923574 | -1.803480 | -2.192911 |
| **9** | 0.188500 | 5.13 | 118.29 | 1.917022 | 1.718110 | -0.616841 |

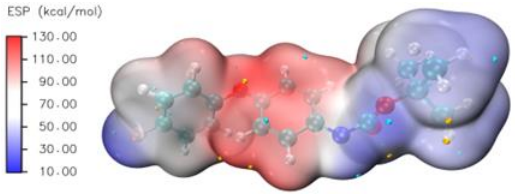
| | | | | | | |
|---|---|---|---|---|---|---|
| **10** | **0.191850** | **5.22** | **120.39** | **2.406732** | **-1.185390** | **1.555164** |
| **11** | 0.113472 | 3.09 | 71.20 | 8.735955 | -0.798963 | -1.599567 |
| **12** | 0.112683 | 3.07 | 70.71 | 7.786093 | 1.063613 | -2.011147 |
| **13** | 0.113471 | 3.09 | 71.20 | 8.727614 | -0.745132 | -1.654197 |

**Table 13:** ESP-2

**b) Structure and NPA charge**




**b) Electrostatic potential analysis**




| Atom | No | NPA Charge | Atom | No | NPA Charge |
|---|---|---|---|---|---|
| **C** | 1 | -0.024200 | C | 21 | -0.628020 |
| **C** | 2 | 0.207110 | H | 22 | 0.266080 |
| **C** | 3 | -0.096170 | H | 23 | 0.262760 |
| **C** | 4 | -0.239310 | H | 24 | 0.275690 |
| **C** | **5** | **0.593020** | H | 25 | 0.281520 |
| **C** | 6 | -0.298880 | H | 26 | 0.262220 |
| **O** | 7 | -0.443470 | H | 27 | 0.259240 |
| **C** | **8** | **0.246700** | H | 28 | 0.258600 |
| **C** | 9 | -0.224860 | H | 29 | 0.261340 |
| **C** | 10 | -0.253940 | H | 30 | 0.224820 |
| **C** | 11 | 0.418290 | H | 31 | 0.218200 |
| **C** | 12 | -0.253040 | H | 32 | 0.218900 |
| **C** | 13 | -0.214740 | H | 33 | 0.229350 |
| **N** | 14 | -0.355980 | H | 34 | 0.220420 |
| **C** | 15 | 0.942250 | H | 35 | 0.226180 |
| **O** | 16 | -0.584920 | H | 36 | 0.229810 |
| **O** | 17 | -0.619500 | H | 37 | 0.225680 |
| **C** | 18 | 0.282550 | H | 38 | 0.219040 |

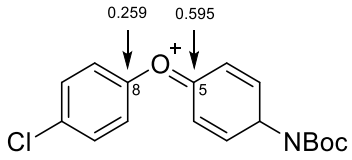
| | | | | | |
|---|---|---|---|---|---|
| **C** | 19 | -0.604160 | F | 39 | -0.360320 |
| **C** | 20 | -0.628250 | | | |

| Electrostatic potential analysis | | | | | | |
|---|---|---|---|---|---|---|
| **Number of surface minima: 13** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.041168 | 1.12 | 25.83 | -9.075461 | -0.503439 | 0.590931 |
| **2** | 0.085431 | 2.32 | 53.61 | -6.988272 | 1.495668 | -0.784342 |
| **3** | 0.086527 | 2.35 | 54.30 | -6.854961 | 0.305019 | -1.577092 |
| **4** | 0.118303 | 3.22 | 74.24 | -2.892429 | 2.157139 | -2.112566 |
| **5** | 0.150977 | 4.11 | 94.74 | -0.785249 | -2.701128 | -0.283132 |
| **6** | 0.149775 | 4.08 | 93.99 | -0.582703 | 0.030373 | 2.425994 |
| **7** | 0.148410 | 4.04 | 93.13 | 0.928619 | 2.299246 | 0.119310 |
| **8** | 0.063169 | 1.72 | 39.64 | 2.750650 | -2.732322 | 1.684672 |
| **9** | 0.063061 | 1.72 | 39.57 | 3.829456 | -0.352288 | 2.475942 |
| **10** | 0.028417 | 0.77 | 17.83 | 4.184899 | -2.643845 | -2.289989 |
| **11** | 0.076728 | 2.09 | 48.15 | 6.536026 | 0.305019 | -2.415205 |
| **12** | 0.065330 | 1.78 | 40.99 | 6.741874 | -2.746737 | -0.025846 |
| **13** | 0.074807 | 2.04 | 46.94 | 7.144108 | 1.506972 | 3.017603 |
| **Number of surface maxima: 10** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.179398 | 4.88 | 112.57 | -3.082928 | -1.587322 | 1.679837 |
| **2** | **0.200819** | **5.46** | **126.02** | **-1.993416** | **-0.873059** | **-1.750305** |
| **3** | 0.194253 | 5.29 | 121.90 | -1.739831 | 1.559293 | 0.955777 |
| **4** | 0.182188 | 4.96 | 114.32 | -1.612192 | -2.087907 | 1.832694 |
| **5** | 0.173990 | 4.73 | 109.18 | -0.001802 | 2.680302 | -2.651587 |
| **6** | 0.179980 | 4.90 | 112.94 | 1.217602 | 1.939509 | -2.150617 |
| **7** | 0.103468 | 2.82 | 64.93 | 4.213412 | -2.140416 | 0.892152 |
| **8** | 0.091364 | 2.49 | 57.33 | 5.804132 | -0.217923 | 3.403828 |

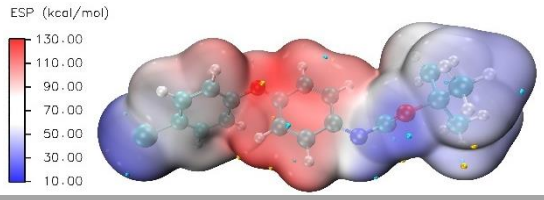
| | | | | | | |
|---|---|---|---|---|---|---|
| **9** | 0.072676 | 1.98 | 45.60 | 6.563940 | -1.687827 | -1.930208 |
| **10** | 0.103853 | 2.83 | 65.17 | 7.530132 | 1.502469 | -0.160338 |

**Table 14:** ESP-3

**c) Structure and NPA charge**




**b) Electrostatic potential analysis**



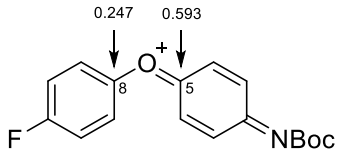

| Atom | No | Charge | Atom | No | Charge |
|---|---|---|---|---|---|
| **C** | 1 | -0.021 | C | 21 | -0.6281 |
| **C** | 2 | 0.208510 | H | 22 | 0.26618 |
| **C** | 3 | -0.093260 | H | 23 | 0.26368 |
| **C** | 4 | -0.240470 | H | 24 | 0.2759 |
| **C** | **5** | **0.594690** | H | 25 | 0.28182 |
| **C** | 6 | -0.300180 | H | 26 | 0.26358 |
| **O** | 7 | -0.445950 | H | 27 | 0.25657 |
| **C** | **8** | **0.259150** | H | 28 | 0.25645 |
| **C** | 9 | -0.223360 | H | 29 | 0.26288 |
| **C** | 10 | -0.210930 | H | 30 | 0.22464 |
| **C** | 11 | -0.049420 | H | 31 | 0.21824 |
| **C** | 12 | -0.210020 | H | 32 | 0.21886 |
| **C** | 13 | -0.217140 | H | 33 | 0.2292 |
| **N** | 14 | -0.356490 | H | 34 | 0.22042 |
| **C** | 15 | 0.942390 | H | 35 | 0.22602 |
| **O** | 16 | -0.582580 | H | 36 | 0.22956 |
| **O** | 17 | -0.620970 | H | 37 | 0.22563 |
| **C** | 18 | 0.282570 | H | 38 | 0.21921 |
| **C** | 19 | -0.604130 | Cl | 39 | 0.00584 |
| **C** | 20 | -0.628010 | | | |

| Electrostatic potential analysis | | | | | | |
|---|---|---|---|---|---|---|
| **Number of surface minima: 12** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.048624 | 1.32 | 30.51 | -9.025042 | 0.385984 | -0.324213 |
| **2** | 0.054008 | 1.47 | 33.89 | -7.649490 | -2.279659 | 2.010234 |
| **3** | 0.118266 | 3.22 | 74.21 | -2.481146 | 2.829575 | -1.453386 |
| **4** | 0.150839 | 4.10 | 94.65 | -0.476373 | -2.349529 | -1.146129 |
| **5** | 0.151423 | 4.12 | 95.02 | -0.356193 | -0.533529 | 2.261899 |
| **6** | 0.149830 | 4.08 | 94.02 | 1.289915 | 2.304924 | 0.663323 |
| **7** | 0.064367 | 1.75 | 40.39 | 3.138331 | -2.921374 | 0.991028 |
| **8** | 0.060644 | 1.65 | 38.05 | 4.277596 | -1.212206 | 2.273895 |
| **9** | 0.031405 | 0.85 | 19.71 | 4.530452 | -1.674655 | -2.984847 |
| **10** | 0.076908 | 2.09 | 48.26 | 7.033884 | 1.056014 | -2.091886 |
| **11** | 0.065915 | 1.79 | 41.36 | 7.180350 | -2.649077 | -1.051814 |
| **12** | 0.073769 | 2.01 | 46.29 | 7.645703 | 0.090335 | 3.381691 |
| **Number of surface maxima: 12** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.073675 | 2.00 | 46.23 | -9.189979 | -1.440250 | 0.953003 |
| **2** | 0.179363 | 4.88 | 112.55 | -2.748357 | -1.863487 | 1.060924 |
| **3** | **0.200850** | **5.47** | **126.04** | **-1.592404** | **-0.154727** | **-2.042023** |
| **4** | 0.197340 | 5.37 | 123.83 | -1.435414 | 1.287729 | 1.266208 |
| **5** | 0.182605 | 4.97 | 114.59 | -1.253051 | -2.354750 | 1.192500 |
| **6** | 0.174076 | 4.74 | 109.23 | 0.176042 | 3.456068 | -1.837909 |
| **7** | 0.179593 | 4.89 | 112.70 | 1.642141 | 2.547400 | -1.564970 |
| **8** | 0.104028 | 2.83 | 65.28 | 4.414484 | -2.359290 | 0.152691 |
| **9** | 0.090395 | 2.46 | 56.72 | 6.254158 | -1.607711 | 3.059681 |
| **10** | 0.090017 | 2.45 | 56.49 | 6.387291 | -2.521756 | 1.719252 |
| **11** | 0.073412 | 2.00 | 46.07 | 6.750722 | -1.343412 | -2.422666 |

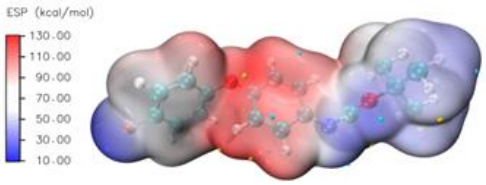
| | | | | | | |
|---|---|---|---|---|---|---|
| **12** | 0.103055 | 2.80 | 64.67 | 8.061002 | 1.170209 | 0.372605 |

**Table 15:** ESP-4

**d) Structure and NPA charge**




**b) Electrostatic potential analysis**



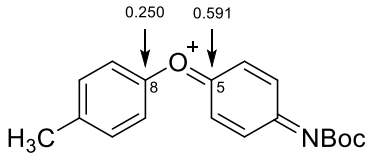

| Atom | No | Charge | Atom | No | Charge |
|---|---|---|---|---|---|
| **C** | 1 | -0.024200 | C | 21 | -0.628010 |
| **C** | 2 | 0.207110 | H | 22 | 0.266080 |
| **C** | 3 | -0.096170 | H | 23 | 0.262760 |
| **C** | 4 | -0.239310 | H | 24 | 0.275690 |
| **C** | **5** | **0.593020** | H | 25 | 0.281520 |
| **C** | 6 | -0.298880 | H | 26 | 0.262220 |
| **O** | 7 | -0.443470 | H | 27 | 0.259240 |
| **C** | **8** | **0.246700** | H | 28 | 0.258600 |
| **C** | 9 | -0.224860 | H | 29 | 0.261340 |
| **C** | 10 | -0.253940 | H | 30 | 0.224820 |
| **C** | 11 | 0.418290 | H | 31 | 0.218200 |
| **C** | 12 | -0.253040 | H | 32 | 0.218900 |
| **C** | 13 | -0.214740 | H | 33 | 0.229350 |
| **N** | 14 | -0.355980 | H | 34 | 0.220420 |
| **C** | 15 | 0.942250 | H | 35 | 0.226180 |
| **O** | 16 | -0.584920 | H | 36 | 0.229810 |
| **O** | 17 | -0.619500 | H | 37 | 0.225680 |
| **C** | 18 | 0.282550 | H | 38 | 0.219040 |
| **C** | 19 | -0.604160 | F | 39 | -0.360320 |
| **C** | 20 | -0.628250 | | | |

| Electrostatic potential analysis | | | | | | |
|---|---|---|---|---|---|---|
| **Number of surface minima: 12** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.032700 | 0.89 | 20.52 | -8.915483 | 0.938603 | 0.578139 |
| **2** | 0.036267 | 0.99 | 22.76 | -7.647705 | -2.853091 | -0.339141 |
| **3** | 0.111459 | 3.03 | 69.94 | -1.080049 | 3.438840 | -0.237574 |
| **4** | 0.145547 | 3.96 | 91.33 | 0.563226 | -1.606698 | -1.870929 |
| **5** | 0.145236 | 3.95 | 91.14 | 0.804882 | -1.133265 | 1.975748 |
| **6** | 0.144419 | 3.93 | 90.62 | 2.596031 | 1.846439 | 1.582208 |
| **7** | 0.060680 | 1.65 | 38.08 | 4.079428 | -3.189767 | -0.308904 |
| **8** | 0.058684 | 1.60 | 36.82 | 5.381718 | -2.105332 | 1.645274 |
| **9** | 0.027741 | 0.75 | 17.41 | 5.637427 | -0.613607 | -3.425031 |
| **10** | 0.063726 | 1.73 | 39.99 | 8.049831 | -2.456523 | -1.927260 |
| **11** | 0.075151 | 2.04 | 47.16 | 8.206293 | 1.392730 | -1.670668 |
| **12** | 0.072503 | 1.97 | 45.50 | 8.775041 | -1.397853 | 3.165823 |
| **Number of surface maxima: 14** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.079829 | 2.17 | 50.09 | -10.998617 | -1.924129 | 0.192869 |
| **2** | 0.085811 | 2.34 | 53.85 | -9.212181 | -0.371973 | -3.179501 |
| **3** | 0.087547 | 2.38 | 54.94 | -8.378018 | -2.059325 | 3.455350 |
| **4** | 0.176750 | 4.81 | 110.91 | -0.260232 | -2.417990 | 0.214341 |
| **5** | **0.192643** | **5.24** | **120.89** | **-0.286778** | **0.850990** | **-1.918570** |
| **6** | 0.187087 | 5.09 | 117.40 | 0.075815 | 1.103358 | 1.723291 |
| **7** | 0.173406 | 4.72 | 108.81 | 1.669186 | 0.321973 | 1.581837 |
| **8** | 0.169631 | 4.62 | 106.45 | 1.803082 | 3.965409 | -0.339141 |
| **9** | 0.175431 | 4.77 | 110.08 | 3.094585 | 2.909075 | -0.501934 |
| **10** | 0.100933 | 2.75 | 63.34 | 5.534666 | -2.381652 | -0.763066 |
| **11** | 0.088783 | 2.42 | 55.71 | 7.281602 | -2.816092 | 2.197541 |
| **12** | 0.088140 | 2.40 | 55.31 | 7.386786 | -3.117679 | 0.782177 |

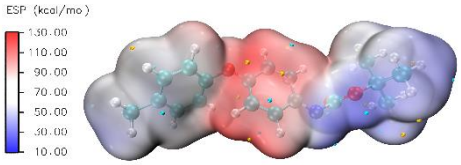
| | | | | | | |
|---|---|---|---|---|---|---|
| **13** | 0.071241 | 1.94 | 44.70 | 7.983105 | -0.536945 | -2.720438 |
| **14** | 0.10173 | 2.77 | 63.84 | 9.275574 | 0.613208 | 0.74194 |

**Table 16:** ESP-5

**a) Structure and NPA charge**




**b) Electrostatic potential analysis**




| Atom | No | Charge | Atom | No | Charge |
|---|---|---|---|---|---|
| **C** | 1 | -0.02975 | H | 22 | 0.265100 |
| **C** | 2 | 0.211610 | H | 23 | 0.263220 |
| **C** | 3 | -0.098530 | H | 24 | 0.275170 |
| **C** | 4 | -0.238620 | H | 25 | 0.281100 |
| **C** | **5** | **0.590980** | H | 26 | 0.255880 |
| **C** | 6 | -0.297120 | H | 27 | 0.236580 |
| **O** | 7 | -0.441020 | H | 28 | 0.236170 |
| **C** | **8** | **0.249600** | H | 29 | 0.254520 |
| **C** | 9 | -0.242460 | H | 30 | 0.224390 |
| **C** | 10 | -0.194210 | H | 31 | 0.218040 |
| **C** | 11 | -0.021250 | H | 32 | 0.218770 |
| **C** | 12 | -0.197560 | H | 33 | 0.228760 |
| **C** | 13 | -0.229760 | H | 34 | 0.220230 |
| **N** | 14 | -0.363770 | H | 35 | 0.226170 |
| **C** | 15 | 0.942980 | H | 36 | 0.229480 |
| **O** | 16 | -0.582980 | H | 37 | 0.225230 |
| **O** | 17 | -0.622640 | H | 38 | 0.219080 |
| **C** | 18 | 0.282220 | C | 39 | -0.615170 |
| **C** | 19 | -0.603900 | H | 40 | 0.229410 |
| **C** | 20 | -0.627800 | H | 41 | 0.22802 |

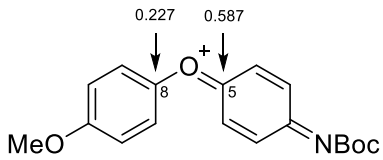
| | | | | | |
|---|---|---|---|---|---|
| **C** | 21 | -0.627970 | H | 42 | 0.22181 |

| Electrostatic potential analysis | | | | | | |
|---|---|---|---|---|---|---|
| **Number of surface minima: 13** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.078445 | 2.13 | 49.225 | -9.641477 | -0.525614 | 0.614303 |
| **2** | 0.075328 | 2.05 | 47.27 | -6.725220 | 1.464556 | -1.000904 |
| **3** | 0.089994 | 2.45 | 56.47 | -5.758012 | -0.519859 | 2.398591 |
| **4** | 0.109321 | 2.97 | 68.60 | -2.938486 | 2.522910 | -1.686919 |
| **5** | 0.144512 | 3.93 | 90.68 | -0.789125 | -2.560914 | -0.571550 |
| **6** | 0.142993 | 3.89 | 89.73 | -0.649192 | -0.131513 | 2.438621 |
| **7** | 0.142416 | 3.88 | 89.37 | 0.856456 | 2.395045 | 0.499079 |
| **8** | 0.059467 | 1.62 | 37.32 | 2.808585 | -2.750074 | 1.400516 |
| **9** | 0.055658 | 1.51 | 34.93 | 3.983094 | -0.974068 | 2.348684 |
| **10** | 0.027982 | 0.76 | 17.56 | 4.021720 | -1.979193 | -2.814746 |
| **11** | 0.074486 | 2.03 | 46.74 | 6.521183 | 0.865822 | -2.351174 |
| **12** | 0.063068 | 1.72 | 39.58 | 6.678125 | -2.737834 | -0.941429 |
| **13** | 0.071207 | 1.94 | 44.68 | 7.454958 | 0.543346 | 3.145807 |
| **Number of surface maxima: 12** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.118861 | 3.23 | 74.59 | -6.840542 | 2.342025 | 2.432387 |
| **2** | **0.190002** | **5.17** | **119.23** | **-1.917028** | **-0.499619** | **-1.846992** |
| **3** | 0.175698 | 4.78 | 110.25 | -1.548769 | -2.239685 | 1.605310 |
| **4** | 0.183313 | 4.99 | 115.03 | -1.548265 | 1.597760 | 1.158329 |
| **5** | 0.167627 | 4.56 | 105.19 | -0.088383 | 3.173206 | -2.136384 |
| **6** | 0.170751 | 4.65 | 107.15 | 0.060929 | 0.983179 | 1.338130 |
| **7** | 0.173155 | 4.71 | 108.66 | 1.229411 | 2.390616 | -1.685331 |
| **8** | 0.099443 | 2.71 | 62.40 | 4.139886 | -2.294387 | 0.364269 |
| **9** | 0.087253 | 2.37 | 54.75 | 6.124300 | -1.245967 | 3.077812 |

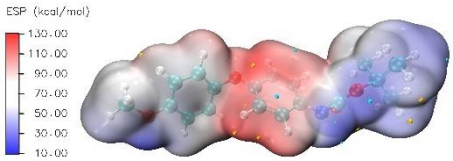
| | | | | | | |
|---|---|---|---|---|---|---|
| **10** | 0.086864 | 2.36 | 54.51 | 6.192214 | -2.304066 | 1.819506 |
| **11** | 0.070725 | 1.92 | 44.38 | 6.360759 | -1.323275 | -2.456266 |
| **12** | 0.100558 | 2.74 | 63.10 | 7.713371 | 1.201155 | 0.100372 |

**Table 17:** ESP-6

**a) Structure and NPA charge**




**b) Electrostatic potential analysis**




| Atom | No | Charge | Atom | No | Charge |
|---|---|---|---|---|---|
| **C** | 1 | -0.03242 | C | 23 | -0.222280 |
| **C** | 2 | 0.210640 | H | 24 | 0.264930 |
| **C** | 3 | -0.101650 | H | 25 | 0.262210 |
| **C** | 4 | -0.237240 | H | 26 | 0.274900 |
| **C** | **5** | **0.587330** | H | 27 | 0.280590 |
| **C** | 6 | -0.295950 | H | 28 | 0.258110 |
| **O** | 7 | -0.437080 | H | 29 | 0.248280 |
| **C** | **8** | **0.227440** | H | 30 | 0.251650 |
| **C** | 9 | -0.232510 | H | 31 | 0.255730 |
| **C** | 10 | -0.238010 | H | 32 | 0.224460 |
| **C** | 11 | 0.341500 | H | 33 | 0.218040 |
| **C** | 12 | -0.283610 | H | 34 | 0.218830 |
| **C** | 13 | -0.209660 | H | 35 | 0.228970 |
| **N** | 14 | -0.364180 | H | 36 | 0.220160 |
| **C** | 15 | 0.942820 | H | 37 | 0.226280 |
| **O** | 16 | -0.584680 | H | 38 | 0.229440 |
| **O** | 17 | -0.621890 | H | 39 | 0.225520 |
| **C** | 18 | 0.282190 | H | 40 | 0.218920 |
| **C** | 19 | -0.603950 | H | 41 | 0.205040 |

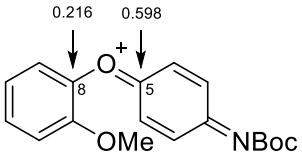
| | | | | | |
|---|---|---|---|---|---|
| **C** | 20 | -0.628070 | H | 42 | 0.186480 |
| **C** | 21 | -0.627870 | H | 43 | 0.186720 |
| **O** | 22 | -0.556140 | | | |

| Electrostatic potential analysis | | | | | | |
|---|---|---|---|---|---|---|
| **Number of surface minima: 11** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.037685 | 1.03 | 23.65 | -7.912484 | -2.226194 | -0.363881 |
| **2** | 0.110954 | 3.02 | 69.62 | -2.473341 | 2.246734 | -2.056333 |
| **3** | 0.143296 | 3.90 | 89.92 | -0.303891 | -2.698754 | -0.394501 |
| **4** | 0.142207 | 3.87 | 89.24 | -0.283764 | -0.011166 | 2.387049 |
| **5** | 0.141678 | 3.86 | 88.90 | 1.284722 | 2.327448 | 0.266983 |
| **6** | 0.058161 | 1.58 | 36.50 | 3.214070 | -2.780450 | 1.514369 |
| **7** | 0.056953 | 1.55 | 35.74 | 4.326084 | -0.663741 | 2.467460 |
| **8** | 0.025407 | 0.69 | 15.94 | 4.501155 | -2.386296 | -2.505725 |
| **9** | 0.073812 | 2.01 | 46.32 | 7.003008 | 0.584664 | -2.312006 |
| **10** | 0.062325 | 1.70 | 39.11 | 7.023654 | -2.786736 | -0.254484 |
| **11** | 0.071710 | 1.95 | 45.00 | 7.661706 | 1.053134 | 3.185289 |
| **Number of surface maxima: 13** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.094091 | 2.56 | 59.04 | -10.198436 | -0.797157 | 1.474808 |
| **2** | 0.134375 | 3.66 | 84.32 | -6.887894 | 2.427103 | 1.779436 |
| **3** | **0.189662** | **5.16** | **119.01** | **-1.457924** | **-0.788664** | **-1.838831** |
| **4** | 0.174469 | 4.75 | 109.48 | -1.205262 | -2.123935 | 1.744618 |
| **5** | 0.182843 | 4.98 | 114.74 | -1.183810 | 1.605458 | 0.947104 |
| **6** | 0.167885 | 4.57 | 105.35 | 0.273614 | 2.902119 | -2.472980 |
| **7** | 0.173188 | 4.71 | 108.68 | 1.700325 | 2.110358 | -1.961961 |
| **8** | 0.098526 | 2.68 | 61.83 | 4.563242 | -2.251273 | 0.673007 |
| **9** | 0.087690 | 2.39 | 55.03 | 6.339629 | -0.671281 | 3.319648 |

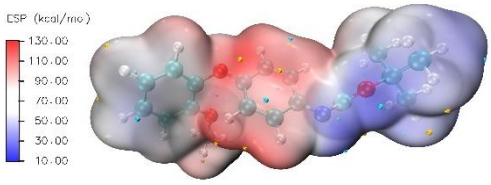
| | | | | | | |
|---|---|---|---|---|---|---|
| **10** | 0.086813 | 2.36 | 54.48 | 6.492142 | -1.843492 | 2.297037 |
| **11** | 0.069722 | 1.90 | 43.75 | 6.970860 | -1.730491 | -2.018954 |
| **12** | 0.069700 | 1.90 | 43.74 | 6.931430 | -1.396791 | -2.105174 |
| **13** | 0.100686 | 2.74 | 63.18 | 8.020520 | 1.444463 | 0.115129 |

**Table 18:** ESP-7

**a) Structure and NPA charge**




**b) Electrostatic potential analysis**




| Atom | No | Charge | Atom | No | Charge |
|---|---|---|---|---|---|
| **C** | 1 | -0.035100 | H | 23 | 0.262530 |
| **C** | 2 | 0.212180 | H | 24 | 0.275000 |
| **C** | 3 | -0.096040 | H | 25 | 0.278660 |
| **C** | 4 | -0.240690 | H | 26 | 0.252270 |
| **C** | **5** | **0.597750** | H | 27 | 0.239360 |
| **C** | 6 | -0.291520 | H | 28 | 0.256230 |
| **O** | 7 | -0.439300 | H | 29 | 0.224440 |
| **C** | **8** | **0.215620** | H | 30 | 0.217980 |
| **C** | 9 | 0.305070 | H | 31 | 0.218840 |
| **C** | 10 | -0.282380 | H | 32 | 0.228930 |
| **C** | 11 | -0.183250 | H | 33 | 0.220210 |
| **C** | 12 | -0.233070 | H | 34 | 0.226040 |
| **C** | 13 | -0.214990 | H | 35 | 0.229430 |
| **N** | 14 | -0.362660 | H | 36 | 0.225410 |
| **C** | 15 | 0.942800 | H | 37 | 0.219080 |
| **O** | 16 | -0.583810 | H | 38 | 0.236850 |
| **O** | 17 | -0.622210 | O | 39 | -0.560270 |
| **C** | 18 | 0.282290 | C | 40 | -0.218080 |

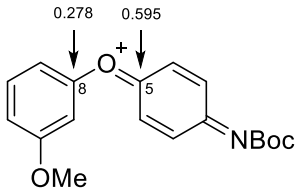
| | | | | | |
|---|---|---|---|---|---|
| **C** | 19 | -0.603920 | H | 41 | 0.208190 |
| **C** | 20 | -0.627840 | H | 42 | 0.190850 |
| **C** | 21 | -0.627920 | H | 43 | 0.192010 |
| **H** | 22 | 0.265030 | | | |

| Electrostatic potential analysis | | | | | | |
|---|---|---|---|---|---|---|
| **Number of surface minima: 15** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.071526 | 1.95 | 44.88 | -6.900625 | -1.305269 | 1.253197 |
| **2** | 0.084811 | 2.31 | 53.22 | -5.813277 | -1.382399 | -2.614310 |
| **3** | 0.107252 | 2.92 | 67.30 | -3.831938 | 3.509340 | 2.277730 |
| **4** | 0.087787 | 2.39 | 55.09 | -3.187350 | 1.380323 | 2.386590 |
| **5** | 0.103221 | 2.81 | 64.77 | -3.064090 | -1.405549 | 2.578730 |
| **6** | 0.118295 | 3.22 | 74.23 | -2.871513 | 4.343389 | -0.536172 |
| **7** | 0.138455 | 3.77 | 86.88 | -0.576340 | -1.455788 | -2.306237 |
| **8** | 0.125874 | 3.43 | 78.99 | 0.486402 | 1.231466 | 2.091242 |
| **9** | 0.138533 | 3.77 | 86.93 | 0.909367 | -2.449423 | 0.794355 |
| **10** | 0.058052 | 1.58 | 36.43 | 2.756860 | 1.504926 | -2.701248 |
| **11** | 0.026371 | 0.72 | 16.55 | 3.783200 | 3.171610 | 1.305692 |
| **12** | 0.055308 | 1.51 | 34.71 | 4.051833 | -0.621593 | -2.433815 |
| **13** | 0.073470 | 2.00 | 46.10 | 6.353129 | 0.728338 | 2.520753 |
| **14** | 0.062661 | 1.71 | 39.32 | 6.455833 | 2.818460 | -0.778400 |
| **15** | 0.070904 | 1.93 | 44.49 | 7.523007 | -2.188950 | -2.107041 |
| **Number of surface maxima: 20** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.115405 | 3.14 | 72.42 | -8.287842 | 0.314277 | -1.620405 |
| **2** | 0.108773 | 2.96 | 68.26 | -7.689651 | -1.799590 | -1.328480 |
| **3** | 0.115119 | 3.13 | 72.24 | -6.707004 | -3.857814 | -1.037080 |
| **4** | 0.142083 | 3.87 | 89.16 | -5.954236 | 2.996495 | -0.659605 |

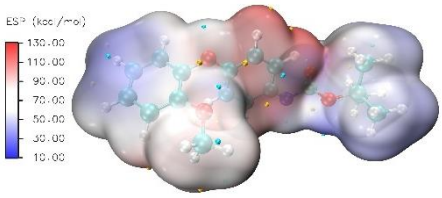
| | | | | | | |
|---|---|---|---|---|---|---|
| **5** | 0.125724 | 3.42 | 78.89 | -4.277984 | 4.514136 | 0.116497 |
| **6** | 0.114570 | 3.12 | 71.89 | -3.566542 | -0.031242 | 2.161077 |
| **7** | 0.169671 | 4.62 | 106.47 | -2.842286 | 0.440116 | -2.539377 |
| **8** | 0.145574 | 3.96 | 91.35 | -1.608852 | 0.241700 | 2.301725 |
| **9** | 0.172485 | 4.69 | 108.24 | -1.593671 | 0.593655 | -2.763707 |
| **10** | 0.128785 | 3.50 | 80.81 | -1.608852 | 3.158853 | 0.588578 |
| **11** | **0.177351** | **4.83** | **111.29** | **-1.377019** | **-2.264721** | **-0.336990** |
| **12** | 0.155153 | 4.22 | 97.36 | -0.277591 | 1.518549 | 0.531275 |
| **13** | 0.163288 | 4.44 | 102.47 | -0.080279 | -1.729095 | 3.373699 |
| **14** | 0.165347 | 4.50 | 103.76 | 0.243268 | -1.733267 | -0.731596 |
| **15** | 0.169373 | 4.61 | 106.28 | 1.169328 | -1.210195 | 2.638891 |
| **16** | 0.098472 | 2.68 | 61.79 | 4.079803 | 1.695498 | -1.536249 |
| **17** | 0.086925 | 2.37 | 54.55 | 6.091682 | -0.744077 | -3.127076 |
| **18** | 0.086486 | 2.35 | 54.27 | 6.162288 | 0.830395 | -2.709510 |
| **19** | 0.069953 | 1.90 | 43.90 | 6.187900 | 2.694926 | 1.181785 |
| **20** | 0.100085 | 2.72 | 62.80 | 7.653586 | -1.007271 | 0.788220 |

**Table 19:** ESP-8

**a) Structure and NPA charge**




**b) Electrostatic potential analysis**




| Atom | No | Charge | Atom | No | Charge |
|---|---|---|---|---|---|
| **C** | 1 | -0.02642 | H | 23 | 0.263990 |
| **C** | 2 | 0.212600 | H | 24 | 0.275200 |
| **C** | 3 | -0.094390 | H | 25 | 0.281590 |
| **C** | 4 | -0.241050 | H | 26 | 0.239990 |
| **C** | **5** | **0.594910** | H | 27 | 0.224340 |

| | | | | | |
|---|---|---|---|---|---|
| **C** | 6 | -0.298720 | H | 28 | 0.218120 |
| **O** | 7 | -0.443890 | H | 29 | 0.218770 |
| **C** | **8** | **0.278440** | H | 30 | 0.228800 |
| **C** | 9 | -0.287540 | H | 31 | 0.220120 |
| **C** | 10 | -0.169230 | H | 32 | 0.226450 |
| **C** | 11 | -0.299220 | H | 33 | 0.229250 |
| **C** | 12 | 0.354150 | H | 34 | 0.225240 |
| **C** | 13 | -0.285970 | H | 35 | 0.219190 |
| **N** | 14 | -0.363400 | H | 36 | 0.248980 |
| **C** | 15 | 0.943010 | H | 37 | 0.256930 |
| **O** | 16 | -0.581520 | H | 38 | 0.263580 |
| **O** | 17 | -0.623100 | O | 39 | -0.554980 |
| **C** | 18 | 0.282230 | C | 40 | -0.221690 |
| **C** | 19 | -0.603980 | H | 41 | 0.187090 |
| **C** | 20 | -0.627990 | H | 42 | 0.205160 |
| **C** | 21 | -0.627850 | H | 43 | 0.187320 |
| **H** | 22 | 0.265500 | | | |

| **Electrostatic potential analysis** | | | | | | |
|---|---|---|---|---|---|---|
| **Number of surface minima: 14** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.115405 | 3.14 | 72.42 | -8.287842 | 0.314277 | -1.620405 |
| **2** | 0.108773 | 2.96 | 68.26 | -7.689651 | -1.799590 | -1.328480 |
| **3** | 0.115119 | 3.13 | 72.24 | -6.707004 | -3.857814 | -1.037080 |
| **4** | 0.142083 | 3.87 | 89.16 | -5.954236 | 2.996495 | -0.659605 |
| **5** | 0.125724 | 3.42 | 78.89 | -4.277984 | 4.514136 | 0.116497 |
| **6** | 0.114570 | 3.12 | 71.89 | -3.566542 | -0.031242 | 2.161077 |
| **7** | 0.169671 | 4.62 | 106.47 | -2.842286 | 0.440116 | -2.539377 |
| **8** | 0.145574 | 3.96 | 91.35 | -1.608852 | 0.241700 | 2.301725 |

| | | | | | | |
|---|---|---|---|---|---|---|
| **9** | 0.172485 | 4.69 | 108.24 | -1.593671 | 0.593655 | -2.763707 |
| **10** | 0.128785 | 3.50 | 80.81 | -1.608852 | 3.158853 | 0.588578 |
| **11** | 0.177351 | 4.83 | 111.29 | -1.377019 | -2.264721 | -0.336990 |
| **12** | 0.155153 | 4.22 | 97.36 | -0.277591 | 1.518549 | 0.531275 |
| **13** | 0.163288 | 4.44 | 102.47 | -0.080279 | -1.729095 | 3.373699 |
| **14** | 0.165347 | 4.50 | 103.76 | 0.243268 | -1.733267 | -0.731596 |
| **15** | 0.169373 | 4.61 | 106.28 | 1.169328 | -1.210195 | 2.638891 |
| **16** | 0.098472 | 2.68 | 61.79 | 4.079803 | 1.695498 | -1.536249 |
| **17** | 0.086925 | 2.37 | 54.55 | 6.091682 | -0.744077 | -3.127076 |
| **18** | 0.086486 | 2.35 | 54.27 | 6.162288 | 0.830395 | -2.709510 |
| **19** | 0.069953 | 1.90 | 43.90 | 6.187900 | 2.694926 | 1.181785 |
| **20** | 0.100085 | 2.72 | 62.80 | 7.653586 | -1.007271 | 0.788220 |
| **Number of surface maxima: 20** | | | | | | |
| # | a.u. | eV | kcal/mol | X/Y/Z coordinate(Angstrom) | | |
| **1** | 0.099690 | 2.71 | 62.56 | -7.977182 | 1.077478 | 0.988069 |
| **2** | 0.071031 | 1.93 | 44.57 | -6.802237 | -2.555702 | 0.044189 |
| **3** | 0.086508 | 2.35 | 54.28 | -6.486573 | 0.537990 | -2.947339 |
| **4** | 0.086446 | 2.35 | 54.25 | -6.282439 | 2.059875 | -2.667343 |
| **5** | 0.100204 | 2.73 | 62.88 | -4.428985 | -0.797808 | -2.129028 |
| **6** | 0.171516 | 4.67 | 107.63 | -1.483049 | -0.516699 | 2.944163 |
| **7** | 0.170756 | 4.65 | 107.15 | -0.267500 | 1.370067 | 0.199711 |
| **8** | 0.165909 | 4.51 | 104.11 | -0.053961 | -0.667379 | 3.824927 |
| **9** | 0.182034 | 4.95 | 114.23 | 1.321582 | 1.374186 | 0.862931 |
| **10** | **0.187060** | **5.09** | **117.38** | **1.405312** | **-2.268855** | **0.433863** |
| **11** | 0.174069 | 4.74 | 109.23 | 1.296443 | 0.011147 | -2.721072 |
| **12** | 0.120472 | 3.28 | 75.60 | 6.858160 | -1.984954 | -1.681492 |
| **13** | 0.128537 | 3.50 | 80.66 | 8.002777 | -0.395660 | -1.703925 |
| **14** | 0.097391 | 2.65 | 61.11 | 8.448152 | 3.981887 | -0.344837 |
| **15** | 0.105000 | 2.86 | 65.89 | 9.008706 | 1.618502 | -1.411048 |

## 9.3 Free energy profile of SNAr reaction

### 9.3.1 Possible reaction pathway for the $SN_{Ar}$ reaction of **B** with **Pyrazole**

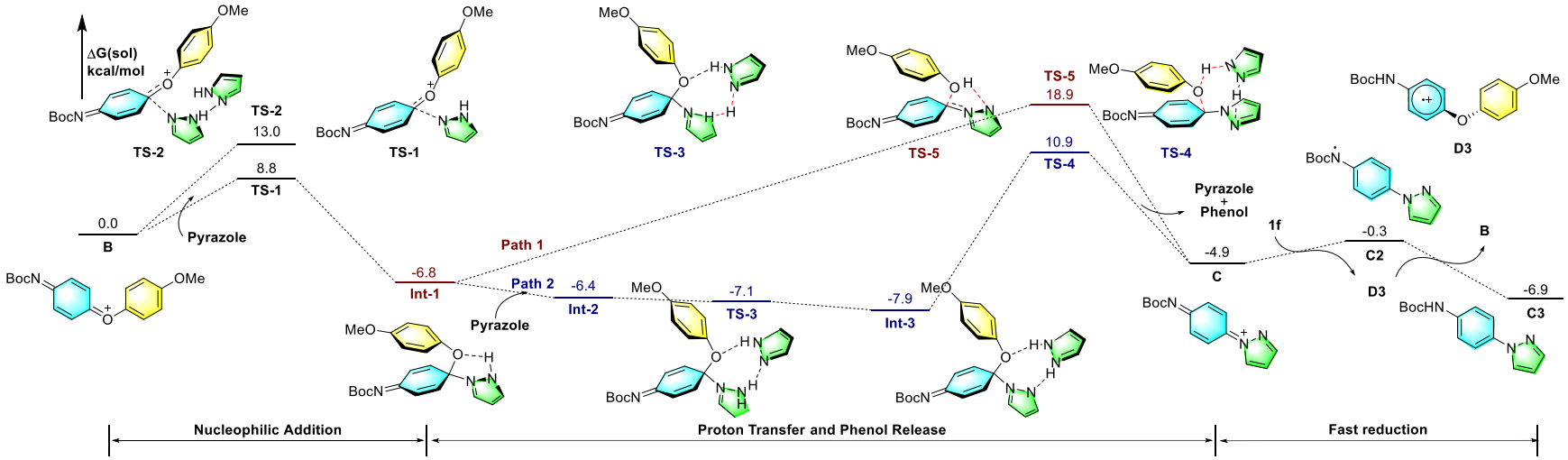



**Fig. 14**: Possible reaction pathway for the SNAr reaction of **B** with **Pyrazole** in acetonitrile via 5-member transition(**TS-5**) or 8-member transition(**TS-4**). The addition of proton shuttle (a second pyra-zole moiety) significantly decreased the barrier of the rate-determining step. **Path 2** was recognized as a more favorable reaction pathway ($\Delta\Delta G^{\neq}$ = 6.9 kcal/mol). All Gibbs energies (sol) were conducted at M06-2X/6-31G(d,p)/SMD(acetonitrile)//M06-2X/6-311++G(d,p)/SMD(acetonitrile) theoretical level. The SMD continuum solvation model was incorporated during structure optimization to account for the apparent charges present in the structures.

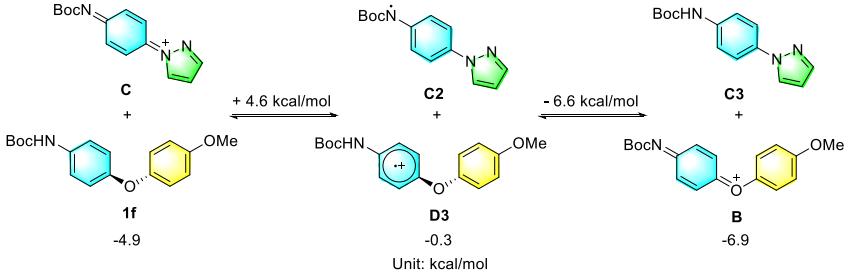



**Fig. 15**: Possible coordinate for the sequential reduction and protonation of product **C.** As shown above, **C** undergoes a swift reductive protonation process immediately to afford the target molecule **C3**. All Gibbs energies (sol) were conducted at M06-2X/6-31G(d,p)/SMD(acetonitrile)//M06-2X/6-311++G(d,p)/SMD(acetonitrile) theoretical level.

The SMD continuum solvation model was incorporated during structure optimization to account for the apparent charges present in the structures.

## **9.3.2** Possible reaction pathway for the $S_NAr$ reaction of **B** with **Imidazole**

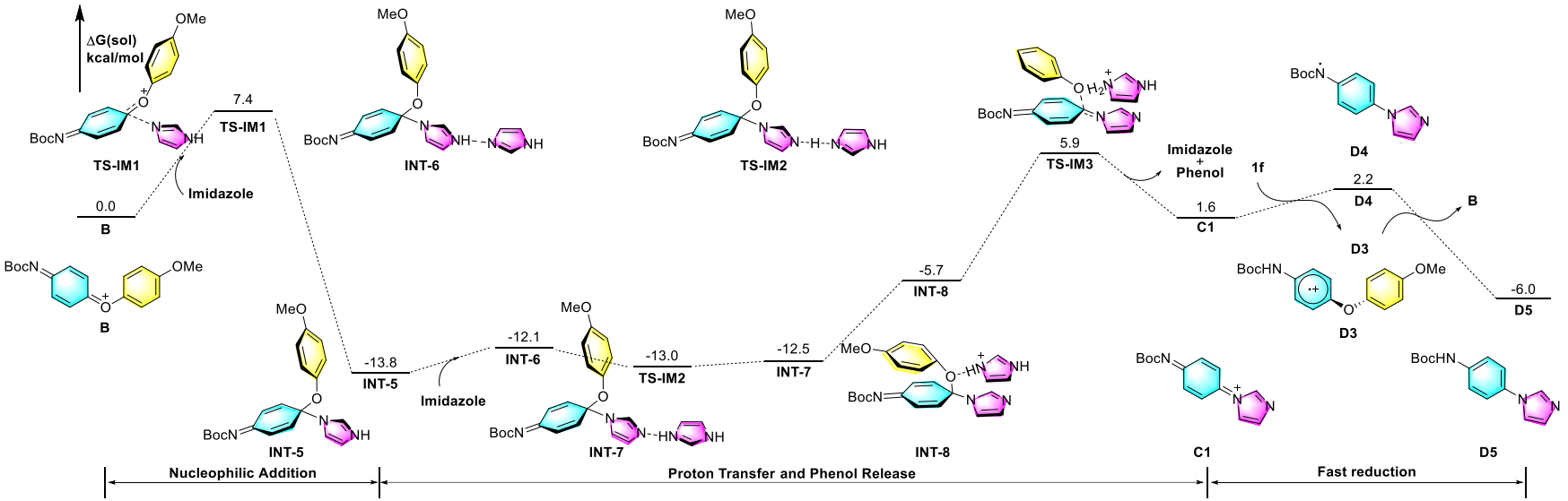



**Fig. 16**: Possible reaction pathway for the $S_NAr$ reaction of **B** with **Imidazole** in acetonitrile. The reaction involved sequential nucleophilic addition and proton transfer, where the C-O cleavage and phenol removal constituted the rate-determining step (**TS-IM3** 18.4 kcal/mol). The **C1** undergoes a swift reductive protonation process immediately to afford the target molecule **D5**. The possible sequential reduction and protonation process were shown above. All Gibbs energies (sol) were conducted at M06-2X/6-31G(d,p)/SMD(acetonitrile)//M06-2X/6-311++G(d,p)/SMD(acetonitrile) theoretical level. The SMD continuum solvation model was incorporated during structure optimization to account for the apparent charges present in the structures.

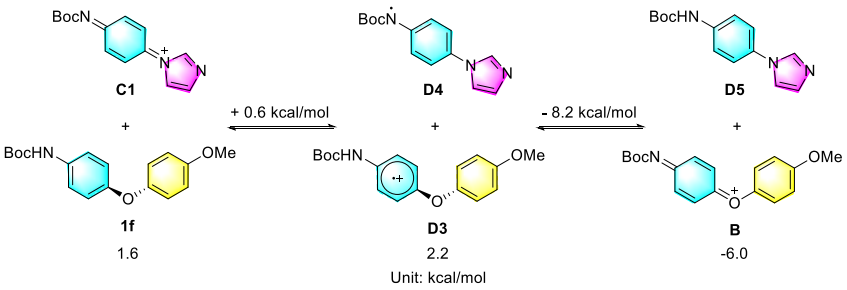



**Fig. 17**: Possible coordinate for the sequential reduction and protonation of product **C1.** As shown above, **C1** undergoes a swift reductive protonation process immediately to afford the target molecule **D5**. All Gibbs energies (sol) were conducted at M06-2X/6-31G(d,p)/SMD(acetonitrile)//M06-2X/6-311++G(d,p)/SMD(acetonitrile) theoretical level. The SMD continuum solvation model was incorporated during structure optimization to account for the apparent charges present in the structures.

### **9.3.3** Unfavored reaction pathway for the $S_NAr$ reaction of **B** with **Imidazole**

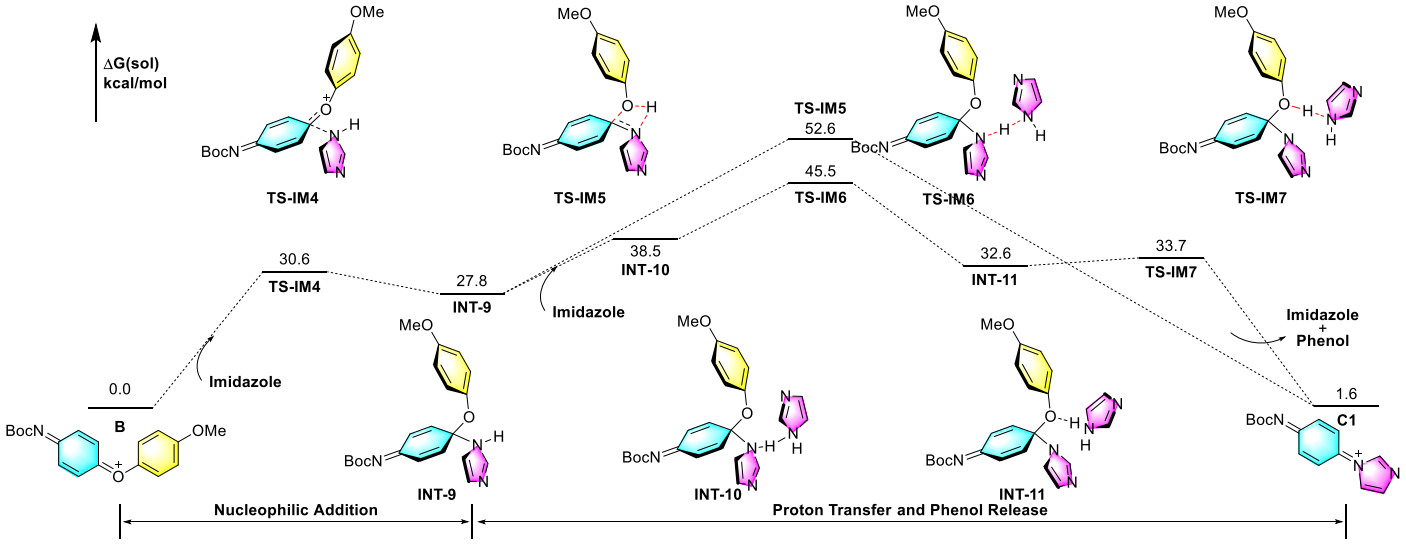


**Fig. 18**: Unfavored reaction pathway for the $S_NAr$ reaction of **B** with **Imidazole** in acetonitrile via 5-member transition(**TS-IM5**) and 6-member transition(**TS-IM4**). Certain pathways were recognized irrational due to their unreachable Gibbs barriers. All Gibbs energies (sol) were conducted at M06-2X/6-31G(d,p)/SMD(acetonitrile)//M06-2X/6-311++G(d,p)/SMD(acetonitrile) theoretical level. The SMD continuum solvation model was incorporated during structure optimization to account for the apparent charges present in the structures.

### **9.3.4** Possible reaction profile for the $S_NAr$ reaction of radical species **A** with **Pyrazole**

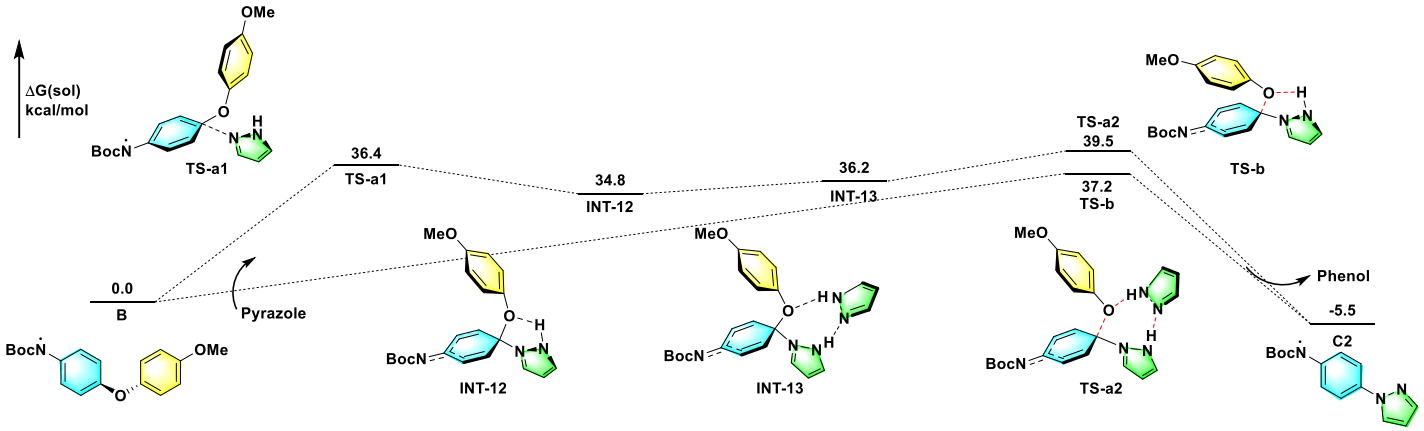
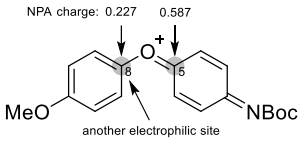



**Fig. 19**: Possible reaction profile for the $S_NAr$ reaction of **A** with **Pyrazole** in acetonitrile via 5-member transition(**TS-b**) and 8-member transition(**TS-a2**). Certain pathways were predicted to be unfavorable because of high activation barriers. All Gibbs energies (sol) were conducted at M06-2X/6-31G(d,p)/SMD(acetonitrile)//M06-2X/6-311++G(d,p)/SMD(acetonitrile) theoretical level.

### **9.3.5** Possible reaction pathway for the regioselective $S_NAr$ reaction of **B** with **Pyrazole** on C8 position.



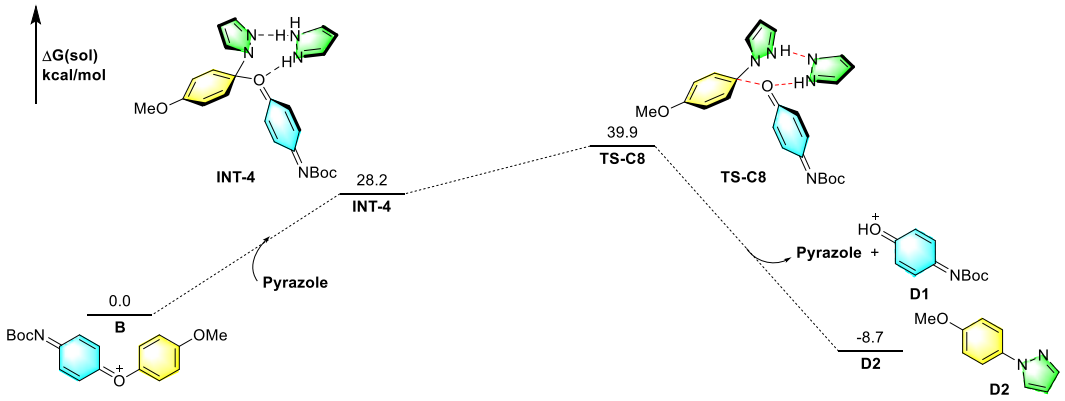



**Fig. 20**: Possible reaction pathway for the regioselective $S_NAr$ reaction of **B** with **Pyrazole** on C8 position. Certain pathway was predicted to be unfavorable because of extremely high activation barriers. The variation in electrophilicity probably accounts for the reactivity difference between the C5 and C8 positions, as the C5 position has a higher electrostatic potential(119.02 kcal/mol) and more positive charge. All Gibbs energies (sol) were conducted at M06-2X/6-31G(d,p)/SMD(acetonitrile)//M06-2X/6-311++G(d,p)/SMD (acetonitrile) theoretical level.

### **9.3.6** Raction profile for general $S_NAr$ reaction of **1f** with **Pyrazole**.

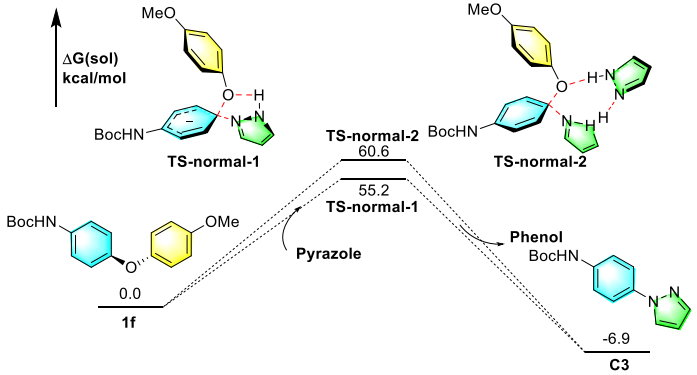



**Fig. 21**: Raction profile for general $S_NAr$ reaction of **1f** with **Pyrazole**. Certain approach was predicted to be unfavorable because of extremely high activation barriers. All Gibbs energies (sol) were conducted at M06-2X/6-31G(d,p)/SMD(acetonitrile)//M06-2X/6-311++G(d,p)/SMD (acetonitrile) theoretical level.

## 9.4 Table of the energies of the calculated structures

Shown in **Table 20** are the zero-point correction (*ZPE*), thermal correction to enthalpy (*TCH*), thermal correction to Gibbs free energy (*TCG*), quasi-harmonic corrected thermal correction to Gibbs free energy (*qh_TCG*), energies (*E*), enthalpies (*H*), Gibbs free energies (*G*) and quasi-harmonic corrected Gibbs free energy (*qh_G*) (in Hartree) of the structures.

**Table 20:** Energies for All Calculated Species

| Structures | *ZPE* | *TCH* | *TCG* | *qh_TCG* | *E* | *H* | *G* | *qh_G* | *freq* |
|---|---|---|---|---|---|---|---|---|---|
| at M06-2X/6-31G(d,p)/ SMD (acetonitrile) //M06-2X/6-311++G(d,p)/ SMD (acetonitrile) level of theory | | | | | | | | | |
| **ESP-1** | 0.319832 | 0.340299 | 0.268934 | 0.263972 | -938.735628 | -938.395329 | -938.466694 | -938.471656 | |
| **ESP-2** | 0.311727 | 0.332935 | 0.260337 | 0.255525 | -1037.975397 | -1037.642462 | -1037.715060 | -1037.719872 | |
| **ESP-3** | 0.310018 | 0.330844 | 0.259091 | 0.253991 | -1398.334913 | -1398.004069 | -1398.075822 | -1398.080922 | |
| **ESP-4** | 0.401493 | 0.426613 | 0.344163 | 0.338233 | -1169.759393 | -1169.332780 | -1169.415230 | -1169.421160 | |
| **ESP-5** | 0.347482 | 0.369749 | 0.294579 | 0.289188 | -978.043397 | -977.673648 | -977.748818 | -977.754209 | |
| **ESP-6** | 0.353196 | 0.376072 | 0.299971 | 0.294157 | -1053.250464 | -1052.874392 | -1052.950493 | -1052.956307 | |
| **ESP-7** | 0.353380 | 0.376255 | 0.300712 | 0.294576 | -1053.250183 | -1052.873928 | -1052.949471 | -1052.955607 | |
| **ESP-8** | 0.352892 | 0.375897 | 0.298720 | 0.293384 | -1053.250161 | -1052.874264 | -1052.951441 | -1052.956777 | |
| **1f** | 0.365129 | 0.388169 | 0.310934 | 0.305347 | -1054.107125 | -1053.718956 | -1053.796191 | -1053.801778 | |
| **Pyrazole** | 0.072462 | 0.077048 | 0.046245 | 0.044071 | -226.182047 | -226.104999 | -226.135802 | -226.137976 | |
| **Imidazole** | 0.072531 | 0.077123 | 0.046317 | 0.044140 | -226.207546 | -226.130423 | -226.161229 | -226.163406 | |
| **A** | 0.351889 | 0.374680 | 0.297269 | 0.292027 | -1053.447863 | -1053.073183 | -1053.150594 | -1053.155836 | |
| **B** | 0.353179 | 0.376082 | 0.299580 | 0.293991 | -1053.250325 | -1052.874243 | -1052.950745 | -1052.956334 | |
| **C** | 0.286354 | 0.304927 | 0.237592 | 0.233140 | -857.489081 | -857.184154 | -857.251489 | -857.255941 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **C1** | 0.286744 | 0.305243 | 0.238836 | 0.233881 | -857.504870 | -857.199627 | -857.266034 | -857.270989 | |
| **C2** | 0.285457 | 0.303774 | 0.237843 | 0.232616 | -857.689087 | -857.385313 | -857.451244 | -857.456471 | |
| **C3** | 0.298891 | 0.316639 | 0.252989 | 0.247006 | -858.351574 | -858.034935 | -858.098585 | -858.104568 | |
| **D1** | 0.238972 | 0.253874 | 0.198195 | 0.192465 | -707.735549 | -707.481675 | -707.537354 | -707.543084 | |
| **D2** | 0.186901 | 0.198306 | 0.149999 | 0.145407 | -571.710448 | -571.512142 | -571.560449 | -571.565041 | |
| **D3** | 0.366358 | 0.389192 | 0.313418 | 0.306657 | -1053.900612 | -1053.511420 | -1053.587194 | -1053.593955 | |
| **D4** | 0.285232 | 0.303614 | 0.237365 | 0.232264 | -857.710072 | -857.406458 | -857.472707 | -857.477808 | |
| **D5** | 0.299212 | 0.317726 | 0.252087 | 0.246455 | -858.374968 | -858.057242 | -858.122881 | -858.128513 | |
| **TS-1** | 0.426679 | 0.454042 | 0.367181 | 0.360691 | -1279.440951 | -1278.986909 | -1279.073770 | -1279.080260 | 173.0*i* |
| **TS-2** | 0.499807 | 0.532657 | 0.431271 | 0.425269 | -1505.636843 | -1505.104186 | -1505.205572 | -1505.211574 | 125.8*i* |
| **TS-3** | 0.498555 | 0.530231 | 0.432666 | 0.425798 | -1505.669368 | -1505.139137 | -1505.236702 | -1505.243570 | 535.1*i* |
| **TS-4** | 0.499706 | 0.531476 | 0.434387 | 0.426908 | -1505.641799 | -1505.110323 | -1505.207412 | -1505.214891 | 230.9*i* |
| **TS-5** | 0.426717 | 0.452882 | 0.371351 | 0.363115 | -1279.427287 | -1278.974405 | -1279.055936 | -1279.064172 | 71.0*i* |
| **TS-IM1** | 0.426767 | 0.454335 | 0.365837 | 0.360055 | -1279.468058 | -1279.013723 | -1279.102221 | -1279.108003 | 41.0*i* |
| **TS-IM2** | 0.498331 | 0.530463 | 0.428353 | 0.423681 | -1505.727569 | -1505.197106 | -1505.299216 | -1505.303888 | 678.7*i* |
| **TS-IM3** | 0.501618 | 0.533023 | 0.439442 | 0.430298 | -1505.704092 | -1505.171069 | -1505.264650 | -1505.273794 | 273.1*i* |
| **TS-IM4** | 0.426778 | 0.453562 | 0.368704 | 0.361624 | -1279.432661 | -1278.979099 | -1279.063957 | -1279.071037 | 253.3*i* |
| **TS-IM5** | 0.422937 | 0.449852 | 0.363722 | 0.357460 | -1279.393349 | -1278.943497 | -1279.029627 | -1279.035889 | 1597.6*i* |
| **TS-IM6** | 0.497039 | 0.528715 | 0.431649 | 0.424572 | -1505.635131 | -1505.106416 | -1505.203482 | -1505.210559 | 1172.9*i* |
| **TS-IM7** | 0.497305 | 0.528914 | 0.432595 | 0.425052 | -1505.654422 | -1505.125508 | -1505.221827 | -1505.229370 | 842.9*i* |
| **TS-a1** | 0.425224 | 0.452237 | 0.364788 | 0.358666 | -1279.594393 | -1279.142156 | -1279.229605 | -1279.235727 | 297.2*i* |
| **TS-a2** | 0.497865 | 0.529740 | 0.430794 | 0.423958 | -1505.792721 | -1505.262981 | -1505.361927 | -1505.368763 | 331.1*i* |
| **TS-b** | 0.425368 | 0.452145 | 0.367054 | 0.359877 | -1279.594397 | -1279.142252 | -1279.227343 | -1279.234520 | 363.5*i* |
| **TS-C8** | 0.498699 | 0.530582 | 0.432622 | 0.425544 | -1505.594298 | -1505.063716 | -1505.161676 | -1505.168754 | 844.3*i* |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **TS-normal-1** | 0.436931 | 0.464212 | 0.377546 | 0.371014 | -1280.222874 | -1279.758662 | -1279.845328 | -1279.851860 | 302.9*i* |
| **TS-normal-2** | 0.511608 | 0.543797 | 0.444622 | 0.437616 | -1506.418727 | -1505.874930 | -1505.974105 | -1505.981111 | 163.8*i* |
| **INT-1** | 0.429278 | 0.456038 | 0.372563 | 0.364918 | -1279.470067 | -1279.014029 | -1279.097504 | -1279.105149 | |
| **INT-2** | 0.501182 | 0.533319 | 0.434014 | 0.427498 | -1505.670057 | -1505.136738 | -1505.236043 | -1505.242559 | |
| **INT-3** | 0.502578 | 0.534596 | 0.436099 | 0.429231 | -1505.674069 | -1505.139473 | -1505.237970 | -1505.244838 | |
| **INT-4** | 0.501751 | 0.533839 | 0.435511 | 0.428406 | -1505.615679 | -1505.081840 | -1505.180168 | -1505.187273 | |
| **INT-5** | 0.429505 | 0.456489 | 0.369866 | 0.363619 | -1279.505341 | -1279.048852 | -1279.135475 | -1279.141722 | |
| **INT-6** | 0.501683 | 0.534130 | 0.431430 | 0.426671 | -1505.729040 | -1505.194910 | -1505.297610 | -1505.302369 | |
| **INT-7** | 0.502189 | 0.534592 | 0.432256 | 0.427297 | -1505.730293 | -1505.195701 | -1505.298037 | -1505.302996 | |
| **INT-8** | 0.503912 | 0.535707 | 0.440418 | 0.431901 | -1505.724053 | -1505.188346 | -1505.283635 | -1505.292152 | |
| **INT-9** | 0.427859 | 0.454934 | 0.368648 | 0.362098 | -1279.437471 | -1278.982537 | -1279.068823 | -1279.075373 | |
| **INT-10** | 0.501454 | 0.533912 | 0.433930 | 0.427585 | -1505.649344 | -1505.115432 | -1505.215414 | -1505.221759 | |
| **INT-11** | 0.501508 | 0.533587 | 0.435739 | 0.428406 | -1505.659652 | -1505.126065 | -1505.223913 | -1505.231246 | |
| **INT-12** | 0.426590 | 0.453622 | 0.367118 | 0.360356 | -1279.598737 | -1279.145115 | -1279.231619 | -1279.238381 | |
| **INT-13** | 0.499412 | 0.531519 | 0.430836 | 0.424704 | -1505.798729 | -1505.267210 | -1505.367893 | -1505.374025 | |

## 9.5 Cartesian coordinates of all calculated structures

**ESP-1**

| | | | |
|---|---|---|---|
| C | -0.48721800 | -1.04559400 | 0.96433900 |
| C | 0.72272000 | -0.64789500 | 0.22971200 |
| C | 0.57680700 | 0.25363600 | -0.92420000 |
| C | -0.63979100 | 0.70166700 | -1.27760600 |
| C | -1.79853500 | 0.27997900 | -0.52587300 |
| C | -1.70809800 | -0.59926700 | 0.60612400 |
| O | -2.91587000 | 0.77074300 | -0.95322500 |
| C | -4.15946100 | 0.42282000 | -0.36741200 |
| C | -4.71634200 | -0.80800400 | -0.67447200 |
| C | -5.96701300 | -1.10028800 | -0.13484100 |
| C | -6.61774600 | -0.17188000 | 0.67625100 |
| C | -6.02556400 | 1.05877800 | 0.95562900 |
| C | -4.77571900 | 1.37395700 | 0.42689200 |
| N | 1.83585200 | -1.10722600 | 0.66448100 |
| C | 3.04581000 | -0.81544600 | -0.02442000 |
| O | 3.75691400 | 0.02417800 | 0.69501100 |
| O | 3.32764700 | -1.36435600 | -1.06130100 |
| C | 5.10200300 | 0.44949500 | 0.24768300 |
| C | 5.52780600 | 1.40946500 | 1.34719000 |
| C | 6.02093200 | -0.76253900 | 0.19192400 |
| C | 4.98568100 | 1.16669200 | -1.09007800 |
| H | -0.34817600 | -1.70558800 | 1.81440900 |
| H | 1.46107000 | 0.54704600 | -1.48158300 |
| H | -0.79833400 | 1.37026700 | -2.11604800 |
| H | -2.60214600 | -0.87864900 | 1.14945300 |
| H | -4.18891100 | -1.50796500 | -1.31442400 |
| H | -6.43083800 | -2.05586500 | -0.35429400 |

| | | | |
|---|---|---|---|
| H | -6.53386900 | 1.78041300 | 1.58593200 |
| H | -4.28987300 | 2.32354300 | 0.62292800 |
| H | 6.52559500 | 1.79516100 | 1.12413300 |
| H | 4.83321700 | 2.25129900 | 1.41240900 |
| H | 5.55775300 | 0.89803800 | 2.31300100 |
| H | 7.04167600 | -0.41876500 | 0.00307100 |
| H | 6.00803100 | -1.29161600 | 1.14912900 |
| H | 5.73224600 | -1.44981800 | -0.60436800 |
| H | 5.95484900 | 1.60971300 | -1.33525000 |
| H | 4.70427800 | 0.48158600 | -1.89107100 |
| H | 4.24738700 | 1.97152300 | -1.02444200 |
| H | -7.59208200 | -0.40771700 | 1.09072100 |

**ESP-2**

| | | | |
|---|---|---|---|
| C | -0.11528800 | -1.17069300 | 0.79450200 |
| C | 1.12022100 | -0.69907900 | 0.15330700 |
| C | 1.02905200 | 0.39627600 | -0.82505800 |
| C | -0.16451400 | 0.94331200 | -1.11273700 |
| C | -1.35267800 | 0.42959400 | -0.47296000 |
| C | -1.31376500 | -0.62828200 | 0.49726900 |
| O | -2.44719700 | 1.01435300 | -0.84097600 |
| C | -3.71809100 | 0.57689600 | -0.40133800 |
| C | -4.21891000 | -0.62400800 | -0.88236400 |
| C | -5.49720100 | -1.00430200 | -0.48867500 |
| C | -6.20981100 | -0.16448800 | 0.35537100 |
| C | -5.70556900 | 1.04047500 | 0.82373800 |
| C | -4.42771800 | 1.42547900 | 0.43231800 |
| N | 2.21091900 | -1.26570200 | 0.51142800 |
| C | 3.43562200 | -0.89030500 | -0.10719000 |
| O | 4.08865800 | -0.07015100 | 0.68575800 |

| | | | |
|---|---|---|---|
| O | 3.76883900 | -1.36442600 | -1.16459300 |
| C | 5.43922000 | 0.41636100 | 0.32182700 |
| C | 5.79850100 | 1.30829500 | 1.49954500 |
| C | 6.39208200 | -0.76595700 | 0.21892600 |
| C | 5.35187500 | 1.22055300 | -0.96766900 |
| H | -0.01433100 | -1.96566800 | 1.52632000 |
| H | 1.93435200 | 0.75093600 | -1.30967600 |
| H | -0.28426100 | 1.75162500 | -1.82519800 |
| H | -2.22628700 | -0.96089700 | 0.97604600 |
| H | -3.62833700 | -1.24364900 | -1.54962200 |
| H | -5.94097700 | -1.93183400 | -0.83131900 |
| H | -6.30642000 | 1.66044300 | 1.47892300 |
| H | -3.99009100 | 2.35892600 | 0.76832200 |
| H | 6.79018000 | 1.73789300 | 1.33785000 |
| H | 5.07590100 | 2.12274100 | 1.59904300 |
| H | 5.81375300 | 0.73147100 | 2.42814700 |
| H | 7.40993600 | -0.38414100 | 0.10104900 |
| H | 6.35335100 | -1.36392300 | 1.13397400 |
| H | 6.15679300 | -1.39975200 | -0.63701400 |
| H | 6.32293000 | 1.68674900 | -1.15605200 |
| H | 5.09956400 | 0.58797800 | -1.82001800 |
| H | 4.60464100 | 2.01373000 | -0.86960800 |
| F | -7.44307800 | -0.53241100 | 0.73271600 |

**ESP-3**

| | | | |
|---|---|---|---|
| C | 0.23973800 | -1.23872000 | 0.37765300 |
| C | 1.48752300 | -0.61136300 | -0.08143800 |
| C | 1.41122300 | 0.70707900 | -0.73044400 |
| C | 0.22027200 | 1.30961700 | -0.89155800 |
| C | -0.97756700 | 0.64426900 | -0.43844700 |

| | | | |
|---|---|---|---|
| C | -0.95531600 | -0.63701000 | 0.20733900 |
| O | -2.06829200 | 1.30816800 | -0.65644600 |
| C | -3.33940700 | 0.77787200 | -0.33642100 |
| C | -3.90064500 | -0.15810500 | -1.18972700 |
| C | -5.17809800 | -0.62523000 | -0.89861300 |
| C | -5.83941400 | -0.13447200 | 0.22329100 |
| C | -5.26201300 | 0.81163500 | 1.06488700 |
| C | -3.98416300 | 1.28259300 | 0.77925200 |
| N | 2.56901500 | -1.26220400 | 0.13238900 |
| C | 3.81282200 | -0.75801700 | -0.33988200 |
| O | 4.52257800 | -0.33916000 | 0.68381300 |
| O | 4.11440700 | -0.82514300 | -1.50614800 |
| C | 5.90031500 | 0.16658400 | 0.48996200 |
| C | 6.31794500 | 0.53638700 | 1.90429000 |
| C | 6.77373900 | -0.94943000 | -0.06524600 |
| C | 5.86388900 | 1.39370800 | -0.41015200 |
| H | 0.32778800 | -2.20431700 | 0.86469900 |
| H | 2.32394200 | 1.18131000 | -1.07764400 |
| H | 0.11212200 | 2.28095100 | -1.36042900 |
| H | -1.87756900 | -1.09001100 | 0.54916500 |
| H | -3.35665000 | -0.51165000 | -2.05927200 |
| H | -5.65125500 | -1.35894300 | -1.54097700 |
| H | -5.79871400 | 1.18003800 | 1.93168400 |
| H | -3.50246900 | 2.02168900 | 1.40961800 |
| H | 7.33694600 | 0.93068700 | 1.88905700 |
| H | 5.65219700 | 1.30067700 | 2.31412100 |
| H | 6.29218200 | -0.34252700 | 2.55407100 |
| H | 7.81359300 | -0.61125700 | -0.06587700 |
| H | 6.70152200 | -1.83752200 | 0.56908500 |
| H | 6.49231500 | -1.21088900 | -1.08611000 |

| | | | |
|---|---|---|---|
| H | 6.85891900 | 1.84684100 | -0.42523100 |
| H | 5.58503800 | 1.13425000 | -1.43255600 |
| H | 5.15706300 | 2.13047400 | -0.01684200 |
| Cl | -7.44380400 | -0.72115700 | 0.58226400 |

**ESP-4**

| | | | |
|---|---|---|---|
| C | -1.35599900 | 1.18723600 | -0.05769100 |
| C | -2.64979000 | 0.52135800 | -0.26341500 |
| C | -2.67652300 | -0.94762800 | -0.34898800 |
| C | -1.53255900 | -1.64733200 | -0.25708200 |
| C | -0.28186500 | -0.94400600 | -0.09638300 |
| C | -0.20754900 | 0.48539000 | 0.02215800 |
| O | 0.75754400 | -1.71296400 | -0.05172000 |
| C | 2.07363200 | -1.19507900 | -0.01692200 |
| C | 2.58265400 | -0.57433300 | -1.14665700 |
| C | 3.89754200 | -0.12527300 | -1.10243200 |
| C | 4.68456100 | -0.30213500 | 0.04387000 |
| C | 4.12537000 | -0.94879900 | 1.15477800 |
| C | 2.81232100 | -1.40620100 | 1.13393600 |
| N | -3.68053000 | 1.27651600 | -0.34307800 |
| C | -4.95723100 | 0.70820300 | -0.60764300 |
| O | -5.66503400 | 0.70393600 | 0.49987400 |
| O | -5.27872400 | 0.38333000 | -1.72397000 |
| C | -7.06769400 | 0.23016700 | 0.49612000 |
| C | -7.47989200 | 0.40628200 | 1.94889900 |
| C | -7.89996000 | 1.11540900 | -0.42061700 |
| C | -7.09975500 | -1.23682600 | 0.09076100 |
| H | -1.37105000 | 2.26832800 | 0.03346600 |
| H | -3.62704500 | -1.45318500 | -0.49170100 |
| H | -1.49850800 | -2.72917500 | -0.31725300 |

| | | | |
|---|---|---|---|
| H | 0.74759500 | 0.96948500 | 0.18387500 |
| H | 1.96669900 | -0.44166400 | -2.03052200 |
| H | 4.30858000 | 0.38442800 | -1.96772500 |
| H | 4.72674100 | -1.11638300 | 2.04237000 |
| H | 2.37219400 | -1.91504700 | 1.98441300 |
| H | -8.51470100 | 0.07804400 | 2.07357300 |
| H | -6.84113100 | -0.19181200 | 2.60435900 |
| H | -7.40733800 | 1.45656700 | 2.24377000 |
| H | -8.95403700 | 0.85247000 | -0.29585600 |
| H | -7.77387500 | 2.16725700 | -0.14837400 |
| H | -7.62852500 | 0.97859700 | -1.46804500 |
| H | -8.11811400 | -1.61399300 | 0.21869800 |
| H | -6.80824100 | -1.37185100 | -0.95201600 |
| H | -6.43448500 | -1.82195400 | 0.73267900 |
| C | 6.08660000 | 0.18671200 | 0.07985600 |
| C | 6.89451300 | 0.12282000 | -1.06280000 |
| C | 6.62398600 | 0.72349900 | 1.25698800 |
| C | 8.20716100 | 0.58419000 | -1.02831200 |
| H | 6.49994100 | -0.31041300 | -1.97733500 |
| C | 7.93661200 | 1.18514000 | 1.28969200 |
| H | 6.00367800 | 0.79997400 | 2.14535700 |
| C | 8.73239200 | 1.11722100 | 0.14749200 |
| H | 8.82246300 | 0.52086100 | -1.92033800 |
| H | 8.33553300 | 1.60579000 | 2.20741900 |
| H | 9.75588800 | 1.47756300 | 0.17361700 |

**ESP-5**

| | | | |
|---|---|---|---|
| C | -0.09524300 | -1.16641100 | 0.67550000 |
| C | 1.12824700 | -0.59874700 | 0.09060100 |
| C | 1.01600400 | 0.63243900 | -0.70856100 |

| | | | |
|---|---|---|---|
| C | -0.18790500 | 1.19555700 | -0.90789300 |
| C | -1.36658800 | 0.57123700 | -0.35396100 |
| C | -1.30414200 | -0.60993700 | 0.46124900 |
| O | -2.47072900 | 1.18026600 | -0.63840200 |
| C | -3.73849000 | 0.65007400 | -0.30001100 |
| C | -4.16111200 | -0.52899900 | -0.89728900 |
| C | -5.43766500 | -0.98563400 | -0.59277600 |
| C | -6.27371000 | -0.27815900 | 0.28054600 |
| C | -5.80262400 | 0.90979500 | 0.84644200 |
| C | -4.52834700 | 1.39313700 | 0.55729100 |
| N | 2.22140300 | -1.21887700 | 0.33498800 |
| C | 3.43859300 | -0.77672300 | -0.25199000 |
| O | 4.19950400 | -0.25053700 | 0.68233300 |
| O | 3.68260100 | -0.97240500 | -1.41744300 |
| C | 5.55424000 | 0.24888100 | 0.35914100 |
| C | 6.04600400 | 0.76492900 | 1.70223500 |
| C | 6.41613800 | -0.90543500 | -0.13219400 |
| C | 5.44415200 | 1.37938500 | -0.65448900 |
| H | 0.02342800 | -2.05180500 | 1.29142700 |
| H | 1.91171400 | 1.07321700 | -1.13565100 |
| H | -0.32407500 | 2.09983700 | -1.49010400 |
| H | -2.20720900 | -1.01932100 | 0.89616600 |
| H | -3.51187000 | -1.06511100 | -1.58283800 |
| H | -5.79310900 | -1.90633200 | -1.04633300 |
| H | -6.44015200 | 1.46998700 | 1.52368300 |
| H | -4.15468100 | 2.31556900 | 0.98806000 |
| H | 7.05501400 | 1.16838300 | 1.58734200 |
| H | 5.39122600 | 1.55847900 | 2.07226000 |
| H | 6.07382500 | -0.04396200 | 2.43721200 |
| H | 7.44860000 | -0.55650500 | -0.22196700 |

| | | | |
|---|---|---|---|
| H | 6.39274100 | -1.72807100 | 0.58830100 |
| H | 6.08511000 | -1.26876100 | -1.10579400 |
| H | 6.42957100 | 1.83668800 | -0.77884100 |
| H | 5.10503200 | 1.01706800 | -1.62620900 |
| H | 4.75319900 | 2.14636200 | -0.29191600 |
| C | -7.65478200 | -0.79229000 | 0.58619200 |
| H | -8.27063200 | -0.80575000 | -0.31839300 |
| H | -7.61217100 | -1.81715300 | 0.96630700 |
| H | -8.15301900 | -0.16786500 | 1.33027700 |

**ESP-6**

| | | | |
|---|---|---|---|
| C | 0.30839800 | -1.18255400 | 0.72222600 |
| C | 1.54415200 | -0.66960800 | 0.11371300 |
| C | 1.44866500 | 0.48005400 | -0.79980500 |
| C | 0.25182000 | 1.02940300 | -1.06729400 |
| C | -0.93879400 | 0.46493600 | -0.47587900 |
| C | -0.89371700 | -0.64147600 | 0.44026500 |
| O | -2.03324900 | 1.05605900 | -0.82749300 |
| C | -3.31410500 | 0.57056300 | -0.48312400 |
| C | -3.71999300 | -0.68573200 | -0.92174600 |
| C | -5.00955900 | -1.09359500 | -0.62862600 |
| C | -5.87681500 | -0.25060400 | 0.08354000 |
| C | -5.44498000 | 1.01450800 | 0.49833400 |
| C | -4.14955600 | 1.43144700 | 0.20256400 |
| N | 2.63622400 | -1.25017600 | 0.44503100 |
| C | 3.86350000 | -0.83892300 | -0.14332800 |
| O | 4.54309000 | -0.12722000 | 0.72926100 |
| O | 4.18128700 | -1.20156700 | -1.24913700 |
| C | 5.89734100 | 0.37312600 | 0.40419300 |
| C | 6.28776700 | 1.11836300 | 1.67075100 |

| | | | |
|---|---|---|---|
| C | 6.82737400 | -0.80538700 | 0.15392000 |
| C | 5.81006300 | 1.32082300 | -0.78397900 |
| O | -7.11030400 | -0.74364200 | 0.31578100 |
| C | -8.02928500 | 0.07836800 | 1.02411700 |
| H | 0.41247500 | -2.00744400 | 1.41951300 |
| H | 2.35332300 | 0.87279200 | -1.25412400 |
| H | 0.13066500 | 1.87598300 | -1.73349700 |
| H | -1.80512700 | -1.00491100 | 0.89802600 |
| H | -3.04465800 | -1.32207900 | -1.48597900 |
| H | -5.37137200 | -2.06339300 | -0.95186900 |
| H | -6.10183600 | 1.68059200 | 1.04346000 |
| H | -3.79386300 | 2.40943000 | 0.50812700 |
| H | 7.28680900 | 1.54342000 | 1.54679700 |
| H | 5.58373700 | 1.93046200 | 1.87128400 |
| H | 6.29970100 | 0.43920600 | 2.52746500 |
| H | 7.85031800 | -0.42951100 | 0.06431200 |
| H | 6.79011900 | -1.50251900 | 0.99597000 |
| H | 6.56881100 | -1.33430600 | -0.76418100 |
| H | 6.78592600 | 1.79227400 | -0.92939800 |
| H | 5.53981300 | 0.79304700 | -1.69986700 |
| H | 5.07529800 | 2.10738800 | -0.58776200 |
| H | -8.94901700 | -0.50008100 | 1.10297900 |
| H | -7.65739200 | 0.31182700 | 2.02720800 |
| H | -8.22756400 | 1.00774800 | 0.47996300 |

**ESP-7**

| | | | |
|---|---|---|---|
| C | -0.11678500 | 0.37922100 | -1.33748400 |
| C | 1.08506200 | 0.29297400 | -0.49528900 |
| C | 0.96012200 | -0.30098300 | 0.84552300 |
| C | -0.23504300 | -0.73660900 | 1.27996700 |

| | | | |
|---|---|---|---|
| C | -1.39264800 | -0.59399600 | 0.42998800 |
| C | -1.31684100 | -0.04373100 | -0.89458400 |
| O | -2.49270900 | -1.03104900 | 0.95353500 |
| C | -3.74480200 | -0.83636500 | 0.33851300 |
| C | -4.20427400 | 0.47823800 | 0.18192300 |
| C | -5.48136000 | 0.65746500 | -0.34960500 |
| C | -6.25047500 | -0.45562800 | -0.69036400 |
| C | -5.77373900 | -1.75076700 | -0.50954100 |
| C | -4.50040100 | -1.94710400 | 0.02208500 |
| N | 2.17680300 | 0.73125300 | -1.00028700 |
| C | 3.36689500 | 0.73559800 | -0.22199200 |
| O | 4.16516100 | -0.21627600 | -0.65252600 |
| O | 3.56026000 | 1.57130300 | 0.62639400 |
| C | 5.50944100 | -0.39918800 | -0.06144200 |
| C | 6.05472200 | -1.58555500 | -0.84063400 |
| C | 6.34522900 | 0.84866400 | -0.30815100 |
| C | 5.36746800 | -0.73371900 | 1.41691400 |
| H | 0.01106100 | 0.79212300 | -2.33270700 |
| H | 1.84179500 | -0.37687900 | 1.47474600 |
| H | -0.37773100 | -1.17985300 | 2.25901200 |
| H | -2.20550400 | -0.00025300 | -1.51285300 |
| H | -5.87519600 | 1.65654500 | -0.49332800 |
| H | -6.38395100 | -2.60601200 | -0.77545100 |
| H | -4.08996200 | -2.93749500 | 0.18748500 |
| H | 7.06128600 | -1.81962700 | -0.48550400 |
| H | 5.41961000 | -2.46390500 | -0.69753700 |
| H | 6.10473700 | -1.35369300 | -1.90787500 |
| H | 7.37450500 | 0.64590100 | 0.00043800 |
| H | 6.34853400 | 1.09752200 | -1.37324800 |
| H | 5.97275300 | 1.70144100 | 0.26067800 |

| | | | |
|---|---|---|---|
| H | 6.34960900 | -1.01060400 | 1.80982800 |
| H | 4.99263500 | 0.11729700 | 1.98757900 |
| H | 4.69272700 | -1.58483900 | 1.54902500 |
| H | -7.24192200 | -0.29850200 | -1.10206000 |
| O | -3.35222400 | 1.45169900 | 0.55884900 |
| C | -3.78230400 | 2.80154900 | 0.39234100 |
| H | -2.96047900 | 3.42026700 | 0.74928400 |
| H | -3.97850300 | 3.01819500 | -0.66193900 |
| H | -4.67914700 | 2.99780000 | 0.98740600 |

**ESP-8**

| | | | |
|---|---|---|---|
| C | -0.22393700 | -0.23660900 | -1.34300400 |
| C | -1.45196200 | -0.35065900 | -0.54163300 |
| C | -1.32553000 | -0.48702600 | 0.91893300 |
| C | -0.10818600 | -0.51938500 | 1.48763000 |
| C | 1.06791900 | -0.43314500 | 0.65394600 |
| C | 0.99706400 | -0.28121800 | -0.77271700 |
| O | 2.18504600 | -0.48578500 | 1.30309700 |
| C | 3.43177900 | -0.50558900 | 0.62956000 |
| C | 3.83738400 | -1.68773700 | 0.02753000 |
| C | 5.09257600 | -1.68102700 | -0.57176300 |
| C | 5.89810600 | -0.54321200 | -0.56306400 |
| C | 5.44561100 | 0.62473800 | 0.06139400 |
| C | 4.18538400 | 0.64685000 | 0.67553400 |
| N | -2.55906200 | -0.31522500 | -1.18393600 |
| C | -3.79076400 | -0.50177400 | -0.49677700 |
| O | -4.48218400 | 0.61522300 | -0.54682800 |
| O | -4.10637800 | -1.57551600 | -0.04462300 |
| C | -5.84014000 | 0.68613700 | 0.03606000 |
| C | -6.24536900 | 2.12434500 | -0.24564900 |

| | | | |
|---|---|---|---|
| C | -6.75459900 | -0.29151700 | -0.68891800 |
| C | -5.75859300 | 0.42166700 | 1.53298600 |
| H | -0.34967200 | -0.11385800 | -2.41381700 |
| H | -2.22461100 | -0.56220600 | 1.52239800 |
| H | 0.03763900 | -0.61763400 | 2.55753100 |
| H | 1.90559600 | -0.19326600 | -1.35552000 |
| H | 5.45498500 | -2.58148800 | -1.05591300 |
| H | -7.24934400 | 2.30131300 | 0.14775000 |
| H | -5.55250700 | 2.82019400 | 0.23503200 |
| H | -6.25185800 | 2.31674100 | -1.32190800 |
| H | -7.78184400 | -0.12162600 | -0.35474300 |
| H | -6.71178000 | -0.12030200 | -1.76840900 |
| H | -6.48610200 | -1.32707100 | -0.47676600 |
| H | -6.73710800 | 0.62020600 | 1.97875000 |
| H | -5.48471500 | -0.61326500 | 1.74386300 |
| H | -5.02782700 | 1.09162500 | 1.99579900 |
| H | 6.86999300 | -0.57545000 | -1.03927700 |
| H | 3.20072700 | -2.56541700 | 0.03647400 |
| H | 3.82308000 | 1.54338400 | 1.16562800 |
| O | 6.14224000 | 1.77702300 | 0.12595300 |
| C | 7.42682300 | 1.80731800 | -0.48456400 |
| H | 7.35686100 | 1.60854400 | -1.55890400 |
| H | 7.80949600 | 2.81461700 | -0.32471400 |
| H | 8.10122200 | 1.08103900 | -0.01940200 |

**1f**

| | | | |
|---|---|---|---|
| C | -0.29443300 | 0.32580400 | -1.03188600 |
| C | -1.37048300 | -0.24536900 | -0.34038200 |
| C | -1.12941500 | -1.31830500 | 0.52554100 |
| C | 0.16878100 | -1.79136800 | 0.69420600 |

| | | | |
|---|---|---|---|
| C | 1.22968700 | -1.21772900 | 0.00214600 |
| C | 0.99761400 | -0.15532800 | -0.87108200 |
| O | 2.46992700 | -1.79052700 | 0.17233200 |
| C | 3.59233900 | -0.99123600 | 0.07717000 |
| C | 4.65336900 | -1.45567300 | -0.69798500 |
| C | 5.83069400 | -0.72503100 | -0.76206400 |
| C | 5.95381100 | 0.48077500 | -0.06168200 |
| C | 4.88598800 | 0.94398600 | 0.71186200 |
| C | 3.70793600 | 0.20062100 | 0.78293500 |
| N | -2.64200300 | 0.30327900 | -0.57799200 |
| C | -3.82039500 | -0.01686400 | 0.03575400 |
| O | -4.79256800 | 0.75414100 | -0.47704000 |
| O | -3.96003900 | -0.86094000 | 0.90123100 |
| C | -6.16953200 | 0.62854400 | -0.00516300 |
| C | -6.90684900 | 1.66555400 | -0.84264700 |
| C | -6.70073000 | -0.76991500 | -0.29922600 |
| C | -6.25153300 | 0.98264300 | 1.47540400 |
| O | 7.14152300 | 1.12654200 | -0.19392800 |
| C | 7.30192200 | 2.34573300 | 0.51169500 |
| H | -0.47774900 | 1.15493000 | -1.70965700 |
| H | -1.94647500 | -1.77349300 | 1.06646800 |
| H | 0.36645600 | -2.62001600 | 1.36646000 |
| H | 1.81768600 | 0.29437100 | -1.42094900 |
| H | 4.54623200 | -2.38983100 | -1.23959600 |
| H | 6.66942800 | -1.07079500 | -1.35737200 |
| H | 4.95841100 | 1.87094800 | 1.26791400 |
| H | 2.87906500 | 0.55400300 | 1.38886200 |
| H | -2.69254600 | 1.04452600 | -1.26572400 |
| H | -7.96691700 | 1.66855700 | -0.57655200 |
| H | -6.49784700 | 2.66379900 | -0.66297100 |

| | | | |
|---|---|---|---|
| H | -6.81399100 | 1.43416900 | -1.90748300 |
| H | -7.77232200 | -0.79786000 | -0.08158600 |
| H | -6.55926800 | -1.01054000 | -1.35728400 |
| H | -6.19845500 | -1.52249000 | 0.30913800 |
| H | -7.30293500 | 1.03306500 | 1.77289700 |
| H | -5.74718300 | 0.23751900 | 2.09122600 |
| H | -5.79750000 | 1.96231900 | 1.65283800 |
| H | 8.30708200 | 2.69915600 | 0.28180600 |
| H | 6.57091200 | 3.09432800 | 0.18597600 |
| H | 7.20859000 | 2.19559700 | 1.59320000 |

**Pyrazole**

| | | | |
|---|---|---|---|
| C | -1.09783400 | -0.37772100 | -0.00007500 |
| C | -0.69752200 | 0.97456300 | -0.00001500 |
| C | 0.68198500 | 0.92211100 | 0.00006100 |
| N | 1.01225200 | -0.38599400 | 0.00005000 |
| H | 1.94384200 | -0.78027900 | 0.00009200 |
| H | -2.10071900 | -0.78336900 | -0.00014200 |
| H | -1.32033600 | 1.85584400 | -0.00002800 |
| H | 1.43764500 | 1.69366100 | 0.00012400 |
| N | -0.05228200 | -1.19966000 | -0.00003100 |

**Imidazole**

| | | | |
|---|---|---|---|
| C | -0.59315200 | 0.99003000 | 0.00007600 |
| C | -1.14067200 | -0.26580400 | 0.00008200 |
| C | 0.98084000 | -0.54867700 | -0.00003400 |
| N | 0.76252300 | 0.78810300 | -0.00004600 |
| H | 1.47360200 | 1.50766800 | -0.00012800 |
| H | -1.02778700 | 1.97714100 | 0.00015000 |
| H | -2.18822300 | -0.53259800 | 0.00015600 |

| | | | |
|---|---|---|---|
| H | 1.97601100 | -0.96936700 | -0.00009000 |
| N | -0.15048000 | -1.22183600 | -0.00007300 |

**A**

| | | | |
|---|---|---|---|
| C | -0.23745900 | -0.95111600 | 0.47724500 |
| C | -1.44782700 | -0.21533000 | 0.26150000 |
| C | -1.32301800 | 1.12785500 | -0.23619000 |
| C | -0.08904900 | 1.67118600 | -0.47432300 |
| C | 1.08131700 | 0.91836000 | -0.23450900 |
| C | 1.00048700 | -0.40376000 | 0.24204000 |
| O | 2.24176700 | 1.55016000 | -0.50617700 |
| C | 3.44538100 | 0.89825300 | -0.24431700 |
| C | 3.98056900 | 0.93756000 | 1.04096900 |
| C | 5.20447400 | 0.33361900 | 1.28078800 |
| C | 5.89365100 | -0.30634300 | 0.24077700 |
| C | 5.34626200 | -0.33674400 | -1.04451800 |
| C | 4.11211300 | 0.26987100 | -1.28213400 |
| N | -2.59174600 | -0.85852200 | 0.49440800 |
| C | -3.79192800 | -0.15510500 | 0.47828700 |
| O | -4.72543700 | -0.89333900 | -0.12980800 |
| O | -3.98435700 | 0.92337300 | 1.01029200 |
| C | -6.10517900 | -0.42255400 | -0.22964000 |
| C | -6.78924500 | -1.54651200 | -0.99746100 |
| C | -6.71302200 | -0.28061800 | 1.16153400 |
| C | -6.16401600 | 0.87732100 | -1.02481100 |
| O | 7.08172400 | -0.86387800 | 0.57757600 |
| C | 7.80951300 | -1.52317600 | -0.44699800 |
| H | -0.32999900 | -1.96926500 | 0.84095300 |
| H | -2.21680700 | 1.71122800 | -0.42115800 |
| H | 0.01867200 | 2.68217300 | -0.85307900 |

| | | | |
|---|---|---|---|
| H | 1.90114300 | -0.98056700 | 0.41672900 |
| H | 3.43845600 | 1.43825400 | 1.83704800 |
| H | 5.64939400 | 0.34734400 | 2.27014100 |
| H | 5.86278000 | -0.82382600 | -1.86236500 |
| H | 3.67158400 | 0.25605700 | -2.27384900 |
| H | -7.84722100 | -1.30972100 | -1.13643600 |
| H | -6.32700100 | -1.67490100 | -1.98030600 |
| H | -6.71047900 | -2.48834500 | -0.44716100 |
| H | -7.78321600 | -0.07581800 | 1.06446700 |
| H | -6.59171300 | -1.21304500 | 1.72125300 |
| H | -6.24822600 | 0.53389500 | 1.71766700 |
| H | -7.20998000 | 1.12309300 | -1.22983400 |
| H | -5.71070100 | 1.70281500 | -0.47536000 |
| H | -5.64675300 | 0.75578200 | -1.98155300 |
| H | 8.71948200 | -1.89714500 | 0.02169000 |
| H | 7.24093600 | -2.36374400 | -0.85965900 |
| H | 8.07414700 | -0.83174000 | -1.25455000 |

**B**

| | | | |
|---|---|---|---|
| C | 0.29632100 | -1.16733900 | 0.64398800 |
| C | 1.52948200 | -0.60434100 | 0.07511000 |
| C | 1.42933600 | 0.61597800 | -0.74208600 |
| C | 0.22814000 | 1.17363900 | -0.97089400 |
| C | -0.96008900 | 0.55289400 | -0.43303500 |
| C | -0.90966500 | -0.61786500 | 0.39822200 |
| O | -2.05921200 | 1.15667200 | -0.74672900 |
| C | -3.33371700 | 0.62652900 | -0.44386300 |
| C | -3.72683200 | -0.58353700 | -1.00565600 |
| C | -5.00786200 | -1.03816600 | -0.74579400 |
| C | -5.87877100 | -0.28630100 | 0.05796400 |

| | | | |
|---|---|---|---|
| C | -5.45942700 | 0.93482200 | 0.59811100 |
| C | -4.17265100 | 1.39927500 | 0.33570400 |
| N | 2.61947300 | -1.21702400 | 0.35086500 |
| C | 3.84772100 | -0.77902100 | -0.21485100 |
| O | 4.58410100 | -0.23282600 | 0.72799600 |
| O | 4.12079200 | -0.99358700 | -1.37053800 |
| C | 5.94329900 | 0.26854900 | 0.42825100 |
| C | 6.39997000 | 0.81122800 | 1.77330000 |
| C | 6.82285000 | -0.88923600 | -0.02202200 |
| C | 5.85171000 | 1.38025500 | -0.60774100 |
| O | -7.10290600 | -0.81913100 | 0.24908700 |
| C | -8.02588800 | -0.08919000 | 1.04734700 |
| H | 0.40558300 | -2.04213100 | 1.27653300 |
| H | 2.33189500 | 1.05265400 | -1.15895800 |
| H | 0.10143900 | 2.07012500 | -1.56711900 |
| H | -1.81952400 | -1.02266000 | 0.82314500 |
| H | -3.04775400 | -1.14807800 | -1.63747400 |
| H | -5.35939300 | -1.97485100 | -1.16398600 |
| H | -6.11859200 | 1.53046700 | 1.21697700 |
| H | -3.82722300 | 2.34503400 | 0.73871500 |
| H | 7.40966500 | 1.21751900 | 1.67568100 |
| H | 5.73284900 | 1.60808700 | 2.11285300 |
| H | 6.41343200 | 0.01584300 | 2.52327600 |
| H | 7.85521300 | -0.53597600 | -0.09421200 |
| H | 6.78714800 | -1.69902100 | 0.71236300 |
| H | 6.51633600 | -1.27171100 | -0.99633700 |
| H | 6.83745200 | 1.84075900 | -0.71684700 |
| H | 5.53765400 | 0.99891300 | -1.58058000 |
| H | 5.14846500 | 2.14977100 | -0.27543000 |
| H | -8.93607000 | -0.68713500 | 1.07477400 |

| | | | |
|---|---|---|---|
| H | -7.64657100 | 0.04545200 | 2.06565900 |
| H | -8.24407100 | 0.88805400 | 0.60406900 |

**C**

| | | | |
|---|---|---|---|
| C | -0.93316200 | 2.00006000 | 0.31125500 |
| C | 0.13637400 | 1.08126900 | -0.09315900 |
| C | -0.23588600 | -0.29556100 | -0.44586800 |
| C | -1.51827400 | -0.69654100 | -0.38869500 |
| C | -2.54323900 | 0.24048600 | 0.02002000 |
| C | -2.21713200 | 1.59937400 | 0.37175500 |
| N | 1.33221300 | 1.54050400 | -0.09933200 |
| C | 2.40708600 | 0.71896900 | -0.53066800 |
| O | 3.02065800 | 0.21619000 | 0.52017700 |
| C | 4.24371800 | -0.60045600 | 0.36082000 |
| C | 4.60459700 | -0.94086100 | 1.79826700 |
| C | 3.90936600 | -1.85657700 | -0.43153600 |
| C | 5.33324800 | 0.23843100 | -0.29209900 |
| O | 2.69031800 | 0.62014500 | -1.69920000 |
| N | -3.81159700 | -0.17803400 | 0.06430900 |
| N | -4.12316200 | -1.48207700 | -0.28148000 |
| C | -5.41208300 | -1.56176700 | -0.13783400 |
| C | -5.99783300 | -0.31815500 | 0.30743000 |
| C | -4.96454100 | 0.53768700 | 0.42645100 |
| H | -0.64256500 | 3.01418400 | 0.56419300 |
| H | 0.53936000 | -0.98958200 | -0.75674900 |
| H | -1.81111500 | -1.70598000 | -0.64220800 |
| H | -2.99262400 | 2.28785700 | 0.67787800 |
| H | 5.50522700 | -1.55971600 | 1.80861500 |
| H | 4.79859600 | -0.03028500 | 2.37143800 |
| H | 3.79316100 | -1.49553100 | 2.27714400 |

| | | | |
|---|---|---|---|
| H | 4.78242900 | -2.51506100 | -0.43134600 |
| H | 3.07773100 | -2.39001500 | 0.03843500 |
| H | 3.65148800 | -1.62177400 | -1.46528200 |
| H | 6.27103200 | -0.32321400 | -0.26303600 |
| H | 5.09642700 | 0.46739100 | -1.33179400 |
| H | 5.47439000 | 1.17167000 | 0.26079200 |
| H | -5.92217500 | -2.49286900 | -0.34867900 |
| H | -7.04066100 | -0.12016600 | 0.50218300 |
| H | -4.92411600 | 1.57150900 | 0.72930200 |

**C1**

| | | | |
|---|---|---|---|
| C | -0.92813700 | -1.99360000 | 0.36975500 |
| C | 0.15654000 | -1.12552700 | -0.09550900 |
| C | -0.19953900 | 0.21235900 | -0.58324800 |
| C | -1.47699100 | 0.63466100 | -0.55711300 |
| C | -2.51567300 | -0.22829700 | -0.03856500 |
| C | -2.20544000 | -1.56590400 | 0.40082600 |
| N | 1.35055600 | -1.58438800 | -0.02652300 |
| C | 2.44128000 | -0.79565700 | -0.48314500 |
| O | 2.97157600 | -0.15759200 | 0.53814400 |
| O | 2.79937500 | -0.83068400 | -1.63398300 |
| C | 4.18996000 | 0.66532900 | 0.36671300 |
| C | 4.44029500 | 1.18344900 | 1.77413800 |
| C | 5.33629300 | -0.21851400 | -0.10349500 |
| C | 3.89185600 | 1.80904300 | -0.59252700 |
| H | -0.65614200 | -2.98892900 | 0.70480100 |
| H | 0.57994500 | 0.86008200 | -0.97425500 |
| H | -1.72550900 | 1.62004100 | -0.92648700 |
| H | -2.98283700 | -2.22163200 | 0.76731800 |
| H | 5.32814900 | 1.82055900 | 1.77253300 |

| | | | |
|---|---|---|---|
| H | 3.58784500 | 1.77197900 | 2.12399100 |
| H | 4.60593600 | 0.35296500 | 2.46559900 |
| H | 6.25966100 | 0.36686700 | -0.08230900 |
| H | 5.45566600 | -1.07279800 | 0.56907000 |
| H | 5.17613600 | -0.57915300 | -1.12036700 |
| H | 4.75051500 | 2.48598400 | -0.60884800 |
| H | 3.71544600 | 1.44703600 | -1.60650700 |
| H | 3.01836700 | 2.37220100 | -0.25044500 |
| C | -5.57632100 | 1.48381300 | -0.07775400 |
| C | -4.25213800 | 1.51253000 | -0.31503700 |
| C | -4.91915300 | -0.49177400 | 0.46525900 |
| N | -5.97734400 | 0.22721400 | 0.40528300 |
| H | -6.29075700 | 2.28174500 | -0.21574400 |
| H | -3.61269700 | 2.30034800 | -0.67366800 |
| H | -4.85632500 | -1.51764500 | 0.79176000 |
| N | -3.77578200 | 0.23076000 | 0.02816500 |

**C2**

| | | | |
|---|---|---|---|
| C | -0.92482200 | 1.88124700 | 0.07240400 |
| C | 0.08125200 | 0.87530700 | -0.09889600 |
| C | -0.36025000 | -0.48770700 | -0.18911600 |
| C | -1.69361600 | -0.80195400 | -0.12914200 |
| C | -2.65803100 | 0.21685600 | 0.02305600 |
| C | -2.25783800 | 1.56464300 | 0.12885200 |
| N | 1.34843100 | 1.28119300 | -0.11630800 |
| C | 2.35119400 | 0.37129200 | -0.45017600 |
| O | 3.35078900 | 0.47154200 | 0.42709600 |
| C | 4.56257600 | -0.33496800 | 0.27647400 |
| C | 5.39069300 | 0.07322000 | 1.48778300 |
| C | 4.21799900 | -1.81891100 | 0.34106100 |

| | | | |
|---|---|---|---|
| C | 5.28132600 | 0.03994400 | -1.01449800 |
| O | 2.34310500 | -0.33517600 | -1.44040500 |
| N | -4.01334900 | -0.12661000 | 0.07278900 |
| N | -4.38217300 | -1.43076800 | 0.09977800 |
| C | -5.70024300 | -1.41420400 | 0.14062000 |
| C | -6.21156000 | -0.09161900 | 0.13811900 |
| C | -5.10068700 | 0.70646800 | 0.09400900 |
| H | -0.59712400 | 2.91201400 | 0.15603600 |
| H | 0.37272200 | -1.27687400 | -0.30977300 |
| H | -2.02210300 | -1.83100100 | -0.19756900 |
| H | -2.98921100 | 2.35218700 | 0.26399500 |
| H | 6.34029900 | -0.46796900 | 1.48534800 |
| H | 5.59909900 | 1.14653700 | 1.46461900 |
| H | 4.85660500 | -0.16099200 | 2.41296900 |
| H | 5.14439600 | -2.39762200 | 0.39840500 |
| H | 3.62675800 | -2.02842100 | 1.23785100 |
| H | 3.65898400 | -2.13842700 | -0.53898000 |
| H | 6.25240400 | -0.46294800 | -1.04099300 |
| H | 4.70648700 | -0.25987100 | -1.89122900 |
| H | 5.45306400 | 1.12000700 | -1.04926900 |
| H | -6.24839600 | -2.34623500 | 0.17163500 |
| H | -7.24295700 | 0.22438800 | 0.16144200 |
| H | -5.00049400 | 1.77990400 | 0.06487900 |

**C3**

| | | | |
|---|---|---|---|
| C | 0.89549200 | 1.64220800 | -0.00002400 |
| C | 0.02358100 | 0.54586000 | 0.00000600 |
| C | 0.56321700 | -0.74556700 | 0.00003400 |
| C | 1.94238100 | -0.92272000 | 0.00003100 |
| C | 2.80239200 | 0.17353300 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | 2.27012200 | 1.46386400 | -0.00002700 |
| N | -1.34938300 | 0.82590300 | 0.00000500 |
| C | -2.38802300 | -0.06547900 | 0.00003300 |
| O | -3.53953200 | 0.62235300 | 0.00000100 |
| C | -4.82351700 | -0.07640900 | -0.00001700 |
| C | -5.82797800 | 1.06862000 | 0.00002700 |
| C | -4.96640600 | -0.91193300 | -1.26714600 |
| C | -4.96638100 | -0.91201200 | 1.26706300 |
| O | -2.27760500 | -1.27670800 | 0.00005500 |
| N | 4.20905700 | -0.03322100 | -0.00000300 |
| N | 4.70529700 | -1.28624600 | 0.00000300 |
| C | 6.02220800 | -1.13897300 | -0.00000100 |
| C | 6.39314400 | 0.22202900 | -0.00001000 |
| C | 5.19706200 | 0.90190400 | -0.00001200 |
| H | 0.48738600 | 2.64887300 | -0.00004600 |
| H | -0.08901100 | -1.60671900 | 0.00005800 |
| H | 2.35489900 | -1.92387700 | 0.00005300 |
| H | 2.91083000 | 2.33798300 | -0.00005300 |
| H | -1.61034900 | 1.80418800 | -0.00002000 |
| H | -6.84446100 | 0.66699500 | 0.00002300 |
| H | -5.69787100 | 1.69210700 | 0.88902200 |
| H | -5.69788500 | 1.69216200 | -0.88893100 |
| H | -5.98759300 | -1.29955100 | -1.32532100 |
| H | -4.78459800 | -0.29064300 | -2.14936200 |
| H | -4.27109500 | -1.75182100 | -1.27122700 |
| H | -5.98756200 | -1.29964600 | 1.32522600 |
| H | -4.27105900 | -1.75189200 | 1.27108200 |
| H | -4.78456800 | -0.29077600 | 2.14931400 |
| H | 6.65961800 | -2.01300600 | 0.00000200 |
| H | 7.38543800 | 0.64607200 | -0.00001500 |

| | | | |
|---|---|---|---|
| H | 4.98640700 | 1.95980100 | -0.00001600 |

**D1**

| | | | |
|---|---|---|---|
| C | -2.40550200 | -1.48191200 | 0.42512800 |
| C | -1.23154900 | -0.71522500 | -0.01944300 |
| C | -1.41453200 | 0.69535500 | -0.40138900 |
| C | -2.63236100 | 1.26113500 | -0.33668500 |
| C | -3.75039700 | 0.46659200 | 0.10692700 |
| C | -3.62411700 | -0.91145900 | 0.48851900 |
| O | -4.88721100 | 1.07472900 | 0.14067800 |
| N | -0.11102900 | -1.33357400 | -0.03379300 |
| C | 1.05805800 | -0.67728200 | -0.51077200 |
| O | 1.81059800 | -0.33976500 | 0.51260500 |
| O | 1.27466700 | -0.56649900 | -1.69204400 |
| C | 3.12432700 | 0.30971600 | 0.30066300 |
| C | 3.62267200 | 0.51975100 | 1.72153000 |
| C | 4.03823600 | -0.63455300 | -0.46698800 |
| C | 2.91667800 | 1.64039100 | -0.40918000 |
| H | -2.24077400 | -2.51909000 | 0.69785700 |
| H | -0.55494600 | 1.26846200 | -0.73583300 |
| H | -2.81566300 | 2.29540800 | -0.60424800 |
| H | -4.50654400 | -1.45409100 | 0.81357400 |
| H | 4.60078600 | 1.00614000 | 1.69302300 |
| H | 2.93135100 | 1.15568700 | 2.28098600 |
| H | 3.72261600 | -0.43797300 | 2.23924000 |
| H | 5.04429900 | -0.20649800 | -0.48663400 |
| H | 4.08763500 | -1.60510900 | 0.03493500 |
| H | 3.69974000 | -0.77592500 | -1.49412500 |
| H | 3.86953200 | 2.17610000 | -0.43610200 |
| H | 2.56884600 | 1.49980700 | -1.43375300 |

| | | | |
|---|---|---|---|
| H | 2.19444700 | 2.25293600 | 0.13882100 |
| H | -5.61762400 | 0.49639000 | 0.44905000 |

**D2**

| | | | |
|---|---|---|---|
| C | -0.14233100 | 1.33241800 | -0.21878400 |
| C | -1.52483500 | 1.41597400 | -0.21776200 |
| C | -2.30562600 | 0.26773500 | -0.03378500 |
| C | -1.68239400 | -0.96863500 | 0.15443300 |
| C | -0.29138600 | -1.04648500 | 0.17086000 |
| O | -3.64767100 | 0.45343300 | -0.05743300 |
| C | -4.46937000 | -0.69199700 | 0.10565000 |
| H | 0.45239300 | 2.22295400 | -0.39324400 |
| H | -2.02310400 | 2.36663900 | -0.37572000 |
| H | -2.26214800 | -1.87211800 | 0.29934600 |
| H | 0.19943300 | -2.00006100 | 0.32901700 |
| H | -5.49808100 | -0.33653300 | 0.05020500 |
| H | -4.29362800 | -1.42318200 | -0.69106100 |
| H | -4.30095000 | -1.16706100 | 1.07838400 |
| C | 2.78306200 | 0.96129700 | 0.37954600 |
| C | 4.04028500 | 0.41649200 | 0.23949400 |
| C | 3.80366600 | -0.89256500 | -0.22864600 |
| N | 2.50665300 | -1.13601800 | -0.37019900 |
| H | 2.45322900 | 1.92770500 | 0.73107100 |
| H | 4.98610700 | 0.89057500 | 0.45226400 |
| H | 4.52323500 | -1.66278100 | -0.47189900 |
| N | 1.89539800 | 0.00439000 | 0.00314300 |
| C | 0.47735100 | 0.09706600 | -0.01425700 |

**D3**

| | | | |
|---|---|---|---|
| C | -0.25886400 | 0.65698600 | -0.63483700 |

| | | | |
|---|---|---|---|
| C | -1.38279200 | -0.10149700 | -0.17346800 |
| C | -1.17486400 | -1.39530900 | 0.39902500 |
| C | 0.09631900 | -1.87663900 | 0.51095800 |
| C | 1.20592500 | -1.09887100 | 0.08022200 |
| C | 1.01110500 | 0.17780100 | -0.51161400 |
| O | 2.39112700 | -1.66577300 | 0.24195700 |
| C | 3.57244800 | -0.93060800 | 0.09163200 |
| C | 4.51677800 | -1.40967600 | -0.80958400 |
| C | 5.72314200 | -0.74018500 | -0.92793200 |
| C | 5.98484100 | 0.39370800 | -0.14439200 |
| C | 5.02735200 | 0.85164700 | 0.76658000 |
| C | 3.81313500 | 0.17939100 | 0.88671000 |
| N | -2.59643900 | 0.47160700 | -0.32153300 |
| C | -3.85974500 | -0.05577800 | 0.02427500 |
| O | -4.76425000 | 0.85414800 | -0.28101100 |
| O | -4.02373500 | -1.14802200 | 0.50836700 |
| C | -6.20028000 | 0.60129300 | -0.03964100 |
| C | -6.84627500 | 1.89224700 | -0.51806300 |
| C | -6.65321200 | -0.58258500 | -0.88251500 |
| C | -6.43610600 | 0.39192400 | 1.44969700 |
| O | 7.18983800 | 0.97425400 | -0.33470300 |
| C | 7.49752500 | 2.12230000 | 0.44389100 |
| H | -0.43828000 | 1.62162200 | -1.09932300 |
| H | -2.01730700 | -1.97781400 | 0.74085800 |
| H | 0.29068700 | -2.85117400 | 0.94497200 |
| H | 1.85562100 | 0.74949100 | -0.87665300 |
| H | 4.29966100 | -2.28888700 | -1.40652000 |
| H | 6.48214900 | -1.08006900 | -1.62412800 |
| H | 5.21556600 | 1.71676800 | 1.38995200 |
| H | 3.06723900 | 0.51492300 | 1.60104300 |

| | | | |
|---|---|---|---|
| H | -2.61996600 | 1.40269700 | -0.73304300 |
| H | -7.92919000 | 1.82259400 | -0.39051700 |
| H | -6.47920600 | 2.74331800 | 0.06188700 |
| H | -6.62814300 | 2.06214800 | -1.57580900 |
| H | -7.74064600 | -0.66809900 | -0.80689600 |
| H | -6.39303900 | -0.42166400 | -1.93262200 |
| H | -6.20715100 | -1.51661000 | -0.53843600 |
| H | -7.51418600 | 0.36236800 | 1.62983000 |
| H | -5.99953700 | -0.54400600 | 1.80027000 |
| H | -6.01508400 | 1.22465600 | 2.02039700 |
| H | 8.49794900 | 2.43093100 | 0.14222300 |
| H | 6.78998900 | 2.93483200 | 0.24717900 |
| H | 7.49550900 | 1.88698100 | 1.51351700 |

**D4**

| | | | |
|---|---|---|---|
| C | -0.92727500 | -1.85988200 | 0.28659500 |
| C | 0.09017200 | -0.90010300 | -0.02118000 |
| C | -0.32690100 | 0.44652400 | -0.28643200 |
| C | -1.65628900 | 0.78837100 | -0.25497500 |
| C | -2.63166000 | -0.18241400 | 0.04552700 |
| C | -2.25407800 | -1.51101300 | 0.32101000 |
| N | 1.35244600 | -1.32385100 | 0.00305500 |
| C | 2.36644000 | -0.47064900 | -0.43730900 |
| O | 3.32032700 | -0.39800500 | 0.48965600 |
| O | 2.39618900 | 0.04561900 | -1.53718500 |
| C | 4.53218500 | 0.39128000 | 0.25703800 |
| C | 5.29505000 | 0.22880800 | 1.56497800 |
| C | 5.32290900 | -0.20196000 | -0.90293700 |
| C | 4.17045300 | 1.85471700 | 0.02836900 |
| H | -0.61384300 | -2.87526100 | 0.50453700 |

| | | | |
|---|---|---|---|
| H | 0.41660700 | 1.19799800 | -0.52656000 |
| H | -1.95840100 | 1.80496300 | -0.48013000 |
| H | -3.00418000 | -2.24886200 | 0.58184600 |
| H | 6.23982600 | 0.77572900 | 1.51110800 |
| H | 4.70982100 | 0.62220800 | 2.40092300 |
| H | 5.51149000 | -0.82644400 | 1.75327500 |
| H | 6.28744500 | 0.30893400 | -0.97487600 |
| H | 5.50997400 | -1.26540100 | -0.72617600 |
| H | 4.79215600 | -0.08335200 | -1.84807800 |
| H | 5.08630500 | 2.45261000 | 0.03423300 |
| H | 3.66456000 | 1.99806400 | -0.92689200 |
| H | 3.52290200 | 2.21185900 | 0.83520400 |
| C | -5.85801000 | 1.30763100 | 0.19849400 |
| C | -4.50510400 | 1.44837400 | 0.27856100 |
| C | -5.06191700 | -0.65214800 | -0.12911700 |
| N | -6.19541100 | -0.00605300 | -0.06355100 |
| H | -6.61060400 | 2.07359300 | 0.31937800 |
| H | -3.87535300 | 2.29734600 | 0.49169200 |
| H | -4.93394500 | -1.70288700 | -0.34536500 |
| N | -3.98742500 | 0.18029800 | 0.07255200 |

**D5**

| | | | |
|---|---|---|---|
| C | -0.89951400 | 1.60080800 | -0.25620900 |
| C | -0.02356900 | 0.52070400 | -0.07884500 |
| C | -0.55252700 | -0.76022800 | 0.12464200 |
| C | -1.93132500 | -0.94098900 | 0.15606300 |
| C | -2.79342800 | 0.13587200 | -0.03076900 |
| C | -2.27249100 | 1.41219800 | -0.24306900 |
| N | 1.34689600 | 0.80521900 | -0.11959600 |
| C | 2.39138100 | -0.07084300 | 0.01399200 |

| | | | |
|---|---|---|---|
| O | 3.53783100 | 0.61572200 | -0.09210000 |
| O | 2.28744900 | -1.26843000 | 0.19769100 |
| C | 4.82745000 | -0.06550700 | 0.01403400 |
| C | 5.82306100 | 1.07316300 | -0.16464900 |
| C | 4.97583200 | -0.69334100 | 1.39514200 |
| C | 4.97574000 | -1.08577900 | -1.10885700 |
| H | -0.49446200 | 2.59501700 | -0.42072900 |
| H | 0.10668000 | -1.60357500 | 0.26906800 |
| H | -2.33595400 | -1.93132700 | 0.33953000 |
| H | -2.93703800 | 2.25326600 | -0.41140000 |
| H | 6.84257900 | 0.68420100 | -0.10269700 |
| H | 5.68862600 | 1.54959100 | -1.13980400 |
| H | 5.68761000 | 1.82632700 | 0.61662500 |
| H | 5.99751600 | -1.06692400 | 1.50895500 |
| H | 4.79681700 | 0.05760100 | 2.17060100 |
| H | 4.28132700 | -1.52260700 | 1.53246400 |
| H | 5.99903900 | -1.47207400 | -1.10640200 |
| H | 4.28500300 | -1.91993900 | -0.98315000 |
| H | 4.79140000 | -0.60915900 | -2.07641900 |
| C | -6.20513300 | -0.90610600 | -0.23302700 |
| C | -4.88583300 | -1.15649500 | -0.49189000 |
| C | -5.13144900 | 0.78108600 | 0.52505700 |
| N | -6.34945100 | 0.30562500 | 0.40409200 |
| H | -7.05632400 | -1.52723800 | -0.47399100 |
| H | -4.37798800 | -1.97074800 | -0.98538800 |
| H | -4.84594900 | 1.71222100 | 0.99489800 |
| N | -4.20078700 | -0.06421500 | -0.00399800 |
| H | 1.60309500 | 1.77337700 | -0.27006600 |

**TS-1**

| | | | |
|---|---|---|---|
| C | 0.66100400 | -0.63805200 | -1.30599100 |
| C | 1.89203100 | -0.23543200 | -0.60567000 |
| C | 1.77647800 | 0.23576100 | 0.78671600 |
| C | 0.57810300 | 0.31543700 | 1.37741000 |
| C | -0.62129900 | -0.08189300 | 0.64854400 |
| C | -0.54263400 | -0.57289900 | -0.71816300 |
| O | -1.65871000 | -0.26272500 | 1.40973600 |
| C | -2.88421700 | -0.71898600 | 0.87089600 |
| C | -3.06020800 | -2.08074800 | 0.65760900 |
| C | -4.28360000 | -2.51882200 | 0.17898400 |
| C | -5.31447000 | -1.60173200 | -0.07480300 |
| C | -5.11399200 | -0.23749900 | 0.15861900 |
| C | -3.88341100 | 0.20798900 | 0.64040900 |
| N | 2.98920300 | -0.33065500 | -1.25856700 |
| C | 4.19923400 | 0.11409000 | -0.67152900 |
| O | 4.98415700 | -0.92553600 | -0.46007600 |
| O | 4.44109700 | 1.28512700 | -0.49560500 |
| C | 6.33323300 | -0.74584400 | 0.10832700 |
| C | 6.85174500 | -2.17360600 | 0.19074300 |
| C | 7.18256100 | 0.08719900 | -0.84215600 |
| C | 6.22199300 | -0.12680700 | 1.49540000 |
| O | -6.46697100 | -2.13114200 | -0.53938300 |
| C | -7.54054300 | -1.24025500 | -0.80911300 |
| H | 0.77582600 | -0.99250600 | -2.32504200 |
| H | 2.67850700 | 0.51067500 | 1.32433400 |
| H | 0.44657000 | 0.64489400 | 2.40259900 |
| H | -1.45186400 | -0.86078700 | -1.23176800 |
| H | -2.25384500 | -2.77752800 | 0.86290500 |
| H | -4.46442800 | -3.57250500 | -0.00309800 |
| H | -5.89972100 | 0.48469800 | -0.02495800 |

| | | | |
|---|---|---|---|
| H | -3.71567300 | 1.26215500 | 0.83819700 |
| H | 7.86274200 | -2.17024700 | 0.60560800 |
| H | 6.20970100 | -2.77871700 | 0.83665500 |
| H | 6.88257400 | -2.62799400 | -0.80329800 |
| H | 8.21504400 | 0.08677700 | -0.48172700 |
| H | 7.16846800 | -0.35100300 | -1.84437700 |
| H | 6.83129000 | 1.11829800 | -0.89495200 |
| H | 7.20808800 | -0.14102500 | 1.96781300 |
| H | 5.87433300 | 0.90610100 | 1.44764100 |
| H | 5.53592900 | -0.71162800 | 2.11565500 |
| H | -8.36111000 | -1.85931800 | -1.17036200 |
| H | -7.85370100 | -0.71227900 | 0.09784500 |
| H | -7.26599400 | -0.51243000 | -1.57993900 |
| C | -1.77328800 | 2.39295300 | -1.16272400 |
| C | -2.58041200 | 3.52867000 | -0.97331900 |
| C | -2.49229100 | 3.80038600 | 0.37957300 |
| N | -1.68210600 | 2.86369400 | 0.91075400 |
| H | -1.38033900 | 2.78249000 | 1.87523900 |
| H | -1.56958900 | 1.83838600 | -2.06906100 |
| H | -3.14475800 | 4.07208900 | -1.71498700 |
| H | -2.92739200 | 4.57621100 | 0.99203300 |
| N | -1.22614300 | 2.00981000 | -0.01203300 |

**TS-2**

| | | | |
|---|---|---|---|
| C | -1.48449000 | 1.13502400 | -1.64778400 |
| C | -2.59466800 | 0.58674300 | -0.85176800 |
| C | -2.27297500 | -0.07077400 | 0.42551800 |
| C | -0.99976100 | -0.18309200 | 0.82446400 |
| C | 0.07606300 | 0.34563200 | -0.00537200 |
| C | -0.20561700 | 1.03082400 | -1.25227700 |

| | | | |
|---|---|---|---|
| O | 1.21792100 | 0.39629300 | 0.60133700 |
| C | 2.41434900 | 0.84949800 | 0.01156100 |
| C | 2.85202100 | 0.36998700 | -1.22032400 |
| C | 4.08880400 | 0.78791900 | -1.68207600 |
| C | 4.87913500 | 1.66140800 | -0.92003800 |
| C | 4.42019800 | 2.12011700 | 0.31880600 |
| C | 3.17784200 | 1.70049300 | 0.78896500 |
| N | -3.77794200 | 0.74164000 | -1.31567400 |
| C | -4.88142300 | 0.19678300 | -0.61431800 |
| O | -5.51436200 | 1.16453500 | 0.02166600 |
| O | -5.17942100 | -0.97068700 | -0.69655100 |
| C | -6.75276200 | 0.88664500 | 0.77445400 |
| C | -7.12084500 | 2.25591600 | 1.32523500 |
| C | -7.82612700 | 0.37656700 | -0.17748900 |
| C | -6.45223000 | -0.09090400 | 1.90283600 |
| O | 6.06853100 | 1.99983000 | -1.46254100 |
| C | 6.91230200 | 2.86437000 | -0.71428300 |
| H | -1.75268300 | 1.65332800 | -2.56262900 |
| H | -3.08201100 | -0.46469700 | 1.03337100 |
| H | -0.71397800 | -0.65966600 | 1.75609300 |
| H | 0.60526600 | 1.46271400 | -1.82458400 |
| H | 2.24930600 | -0.32588200 | -1.79357000 |
| H | 4.46948500 | 0.43717000 | -2.63512300 |
| H | 5.01606200 | 2.78895000 | 0.92707500 |
| H | 2.80737800 | 2.02933400 | 1.75418400 |
| H | -8.03848700 | 2.17674700 | 1.91335200 |
| H | -6.32368600 | 2.63747800 | 1.96907900 |
| H | -7.28722400 | 2.96508800 | 0.50984300 |
| H | -8.77512500 | 0.31820300 | 0.36277400 |
| H | -7.94940500 | 1.07019800 | -1.01431400 |

| | | | |
|---|---|---|---|
| H | -7.58276000 | -0.61398800 | -0.56338100 |
| H | -7.33806300 | -0.17846700 | 2.53806300 |
| H | -6.19924300 | -1.08060300 | 1.51996100 |
| H | -5.62664900 | 0.28268500 | 2.51617700 |
| H | 7.80922400 | 3.00440200 | -1.31676300 |
| H | 6.43292900 | 3.83400000 | -0.54277100 |
| H | 7.18453700 | 2.41520900 | 0.24684700 |
| C | -0.38560100 | -2.38854700 | -1.86392100 |
| C | -0.11960700 | -3.76851000 | -1.85334100 |
| C | 0.90426700 | -3.91691600 | -0.93266400 |
| N | 1.19057800 | -2.69096700 | -0.45796100 |
| H | -1.11962800 | -1.83256900 | -2.43413500 |
| H | -0.60006900 | -4.54287700 | -2.43105900 |
| H | 1.44210200 | -4.78850900 | -0.58913800 |
| N | 0.42124100 | -1.75153800 | -1.02038200 |
| C | 4.52149200 | -1.66670500 | 1.17691400 |
| C | 5.13036100 | -0.97213200 | 2.23854100 |
| C | 4.09527400 | -0.70298300 | 3.11402700 |
| N | 2.98107200 | -1.22131200 | 2.56256700 |
| H | 2.04368500 | -1.20922500 | 2.94398600 |
| H | 4.96964300 | -2.05981900 | 0.27447900 |
| H | 6.16945900 | -0.70289600 | 2.34862700 |
| H | 4.06516100 | -0.19405400 | 4.06590000 |
| N | 3.21590500 | -1.81563200 | 1.38654100 |
| H | 1.91142400 | -2.42155300 | 0.23673300 |

**TS-3**

| | | | |
|---|---|---|---|
| C | -1.16359500 | -1.73121500 | 1.18654200 |
| C | -2.30672500 | -0.89348400 | 0.78724600 |
| C | -2.00890100 | 0.45688700 | 0.27732200 |

| | | | |
|---|---|---|---|
| C | -0.75780000 | 0.90976200 | 0.21885700 |
| C | 0.43005400 | 0.10070900 | 0.67540700 |
| C | 0.09178600 | -1.28682700 | 1.14837700 |
| O | 1.33052800 | 0.11903200 | -0.41983000 |
| C | 2.43575600 | -0.73960400 | -0.38332600 |
| C | 3.60976900 | -0.35435700 | 0.26192500 |
| C | 4.70681000 | -1.20234600 | 0.23140900 |
| C | 4.63848800 | -2.42883000 | -0.44250600 |
| C | 3.45877100 | -2.80129500 | -1.09431000 |
| C | 2.35731100 | -1.94785000 | -1.05971400 |
| N | -3.47830600 | -1.40070300 | 0.89140800 |
| C | -4.60916300 | -0.61219400 | 0.60342300 |
| O | -5.22500600 | -1.10013400 | -0.46485600 |
| O | -4.97150300 | 0.30896400 | 1.30084700 |
| C | -6.47081300 | -0.49395500 | -0.95444900 |
| C | -6.79707500 | -1.34043300 | -2.17664900 |
| C | -7.56083100 | -0.62858500 | 0.10128500 |
| C | -6.21682000 | 0.95451800 | -1.35406400 |
| O | 5.76331400 | -3.18155200 | -0.41233000 |
| C | 5.73720200 | -4.42813800 | -1.09118800 |
| H | -1.39563600 | -2.73541900 | 1.52638200 |
| H | -2.83264500 | 1.07815300 | -0.06007800 |
| H | -0.53117600 | 1.90068500 | -0.16853500 |
| H | 0.92273500 | -1.90922500 | 1.46650500 |
| H | 3.67304100 | 0.60205700 | 0.77108400 |
| H | 5.63458500 | -0.92860700 | 0.72256200 |
| H | 3.38469100 | -3.74112900 | -1.62747300 |
| H | 1.43304200 | -2.21993100 | -1.55989900 |
| H | -7.72154000 | -0.98066000 | -2.63525500 |
| H | -5.99211100 | -1.27585600 | -2.91398200 |

| | | | |
|---|---|---|---|
| H | -6.93167800 | -2.38768400 | -1.89229500 |
| H | -8.51321900 | -0.30833400 | -0.33069400 |
| H | -7.65838800 | -1.67335200 | 0.41095900 |
| H | -7.34847200 | -0.01292500 | 0.97589500 |
| H | -7.10315300 | 1.34272500 | -1.86376600 |
| H | -6.01204400 | 1.58023800 | -0.48448200 |
| H | -5.37090300 | 1.01078200 | -2.04619700 |
| H | 6.72383200 | -4.86880400 | -0.95062100 |
| H | 4.97744800 | -5.09440900 | -0.66834000 |
| H | 5.54807000 | -4.29300200 | -2.16161200 |
| C | 1.07531200 | 0.58218600 | 3.11576200 |
| C | 1.73084300 | 1.62864800 | 3.74055400 |
| C | 2.11177400 | 2.49029500 | 2.70853100 |
| N | 1.70300400 | 1.99372700 | 1.54339100 |
| H | 0.60250300 | -0.30305800 | 3.51503200 |
| H | 1.91175300 | 1.74505700 | 4.79713700 |
| H | 2.65807000 | 3.42241800 | 2.73762100 |
| N | 1.08830100 | 0.82541300 | 1.79136400 |
| C | 2.89707300 | 4.09994900 | -1.01737400 |
| C | 3.02534900 | 4.29600900 | -2.39866700 |
| C | 2.43798100 | 3.18023800 | -2.97074500 |
| N | 2.00638400 | 2.40306100 | -1.96598400 |
| H | 1.53293400 | 1.50674100 | -2.00970500 |
| H | 3.21698100 | 4.72589300 | -0.19625500 |
| H | 3.48151600 | 5.12973600 | -2.90831500 |
| H | 2.29966200 | 2.88570900 | -4.00024600 |
| N | 2.27797500 | 2.94641000 | -0.77366900 |
| H | 1.93459900 | 2.39582700 | 0.43646000 |

**TS-4**

| | | | |
|---|---|---|---|
| C | -0.93131900 | -2.43998200 | 0.63255900 |
| C | -2.11096700 | -1.56556600 | 0.67738100 |
| C | -1.89656300 | -0.15722200 | 1.04580500 |
| C | -0.66910300 | 0.31528000 | 1.29526200 |
| C | 0.50513100 | -0.55557100 | 1.16205700 |
| C | 0.30058000 | -1.97669000 | 0.87640400 |
| O | 1.02327400 | -0.00443800 | -0.67356200 |
| C | 2.35004800 | -0.25004900 | -0.91056000 |
| C | 3.33125800 | 0.71667000 | -0.65460600 |
| C | 4.66505100 | 0.40490900 | -0.85123000 |
| C | 5.03971000 | -0.87289200 | -1.29245800 |
| C | 4.05788800 | -1.83552500 | -1.55237800 |
| C | 2.71675300 | -1.51741300 | -1.36035700 |
| N | -3.24655200 | -2.08612800 | 0.39217700 |
| C | -4.42016300 | -1.30509800 | 0.48488800 |
| O | -4.88993500 | -1.07483200 | -0.72943200 |
| O | -4.91478100 | -0.99665000 | 1.54458700 |
| C | -6.13869300 | -0.31764400 | -0.92105700 |
| C | -6.27440200 | -0.27702800 | -2.43606100 |
| C | -7.30060000 | -1.07539600 | -0.29244200 |
| C | -5.97713900 | 1.08705900 | -0.35398100 |
| O | 6.36711800 | -1.07945100 | -1.44119200 |
| C | 6.78989200 | -2.36346600 | -1.87752000 |
| H | -1.10381300 | -3.48390900 | 0.39327200 |
| H | -2.76021700 | 0.49247100 | 1.14731600 |
| H | -0.51672500 | 1.33944200 | 1.60966500 |
| H | 1.15888600 | -2.63480600 | 0.82197500 |
| H | 3.05281600 | 1.70406800 | -0.29942800 |
| H | 5.44151300 | 1.13871200 | -0.66248900 |
| H | 4.32290000 | -2.82504900 | -1.90394100 |

| | | | |
|---|---|---|---|
| H | 1.94302600 | -2.25021600 | -1.56645800 |
| H | -7.18179800 | 0.26860500 | -2.70669200 |
| H | -5.41484100 | 0.22809000 | -2.88515900 |
| H | -6.34070000 | -1.29006300 | -2.84221200 |
| H | -8.23497200 | -0.57757400 | -0.56673400 |
| H | -7.33300700 | -2.10053000 | -0.67290900 |
| H | -7.22245700 | -1.09730700 | 0.79507100 |
| H | -6.84516300 | 1.68636900 | -0.64255900 |
| H | -5.90867900 | 1.07543800 | 0.73462300 |
| H | -5.08103500 | 1.55978300 | -0.76760200 |
| H | 7.87777200 | -2.32267200 | -1.92349100 |
| H | 6.48360700 | -3.14223200 | -1.17087200 |
| H | 6.39176700 | -2.59519000 | -2.87116200 |
| C | 2.71735000 | -0.97968700 | 2.21269600 |
| C | 3.61174700 | -0.15646000 | 2.82253500 |
| C | 3.01790700 | 1.13742100 | 2.76605600 |
| N | 1.84525900 | 1.11662400 | 2.17681200 |
| H | 2.73702800 | -2.04358800 | 2.03704900 |
| H | 4.56209000 | -0.42861700 | 3.25445600 |
| H | 3.41855200 | 2.07425700 | 3.12994500 |
| N | 1.63872000 | -0.19457000 | 1.84314300 |
| C | 0.48026900 | 4.56045800 | 0.09358900 |
| C | -0.04914800 | 4.59868800 | -1.18449700 |
| C | 0.00272000 | 3.27068300 | -1.63325900 |
| N | 0.52523700 | 2.48496800 | -0.69467000 |
| H | 0.81499900 | 1.04945700 | -0.69014900 |
| H | 0.64284800 | 5.33278300 | 0.83038900 |
| H | -0.41887900 | 5.46226700 | -1.71442000 |
| H | -0.30816300 | 2.84965600 | -2.57890700 |
| N | 0.81047600 | 3.28322500 | 0.34405100 |

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|---|---|---|---|
| H | 1.21601600 | 2.87160400 | 1.18466700 |

**TS-5**

| | | | |
|---|---|---|---|
| C | -1.20073600 | -1.29371900 | 1.99589200 |
| C | -0.17973400 | -1.61605800 | 0.98202800 |
| C | -0.56207700 | -1.47665000 | -0.43713900 |
| C | -1.71042200 | -0.89156200 | -0.78010000 |
| C | -2.61548900 | -0.32335700 | 0.25706600 |
| C | -2.35383300 | -0.70804200 | 1.66483700 |
| O | -2.43372500 | 1.26502000 | 0.19876700 |
| C | -1.12089300 | 1.79513100 | 0.08427100 |
| C | -0.56869200 | 2.00024600 | -1.17502300 |
| C | 0.72750700 | 2.47748500 | -1.24635400 |
| C | 1.45783800 | 2.72018000 | -0.07134200 |
| C | 0.87382300 | 2.50785600 | 1.18173600 |
| C | -0.43676000 | 2.04079200 | 1.25923300 |
| N | 0.97867700 | -1.96819400 | 1.39266300 |
| C | 1.98477600 | -2.25197600 | 0.44049400 |
| O | 2.76920900 | -1.19367700 | 0.31153400 |
| O | 2.09829100 | -3.33282500 | -0.08773400 |
| C | 3.91521400 | -1.21421600 | -0.61379400 |
| C | 4.52173800 | 0.16926500 | -0.42898400 |
| C | 4.90288100 | -2.29645000 | -0.19778700 |
| C | 3.40332000 | -1.39587300 | -2.03673600 |
| O | 2.72119400 | 3.15749200 | -0.25134500 |
| C | 3.52261900 | 3.35571700 | 0.90746100 |
| H | -0.95812300 | -1.52823500 | 3.02718500 |
| H | 0.10365700 | -1.87468700 | -1.19737200 |
| H | -2.02152200 | -0.77662300 | -1.81440500 |
| H | -3.10381400 | -0.42929000 | 2.39795200 |

| | | | |
|---|---|---|---|
| H | -1.13841500 | 1.78887900 | -2.07530400 |
| H | 1.20162400 | 2.65846100 | -2.20471000 |
| H | 1.41892300 | 2.70599100 | 2.09582100 |
| H | -0.91424400 | 1.87671000 | 2.21906700 |
| H | 5.38972200 | 0.27572900 | -1.08489200 |
| H | 3.79585200 | 0.94780300 | -0.68174400 |
| H | 4.84811700 | 0.30873500 | 0.60565300 |
| H | 5.81463800 | -2.18648700 | -0.79163100 |
| H | 5.16578900 | -2.18112300 | 0.85792500 |
| H | 4.49764900 | -3.29543600 | -0.36001700 |
| H | 4.23660200 | -1.27167700 | -2.73392700 |
| H | 2.97245600 | -2.38771800 | -2.18324900 |
| H | 2.64895800 | -0.63562000 | -2.26314700 |
| H | 4.51133200 | 3.63415500 | 0.54409400 |
| H | 3.11887600 | 4.16191700 | 1.52889400 |
| H | 3.59381200 | 2.43690800 | 1.49873100 |
| C | -4.99679000 | -1.20137700 | 0.27785100 |
| C | -6.10031800 | -0.85684100 | -0.47067600 |
| C | -5.67371900 | 0.20921800 | -1.29000700 |
| N | -4.39561700 | 0.49002600 | -1.07961700 |
| H | -3.07828700 | 1.51964200 | -0.54575900 |
| H | -4.83423800 | -1.95841400 | 1.03163900 |
| H | -7.08040800 | -1.30525000 | -0.42678600 |
| H | -6.24108000 | 0.78346300 | -2.00897600 |
| N | -4.00151200 | -0.36962400 | -0.11624100 |

**TS-IM1**

| | | | |
|---|---|---|---|
| C | 0.49456500 | -0.62017000 | -1.47328000 |
| C | 1.72251100 | -0.35345600 | -0.70666900 |
| C | 1.59190600 | -0.04953200 | 0.72764900 |

| | | | |
|---|---|---|---|
| C | 0.38058300 | 0.00110000 | 1.29821200 |
| C | -0.81090400 | -0.23953300 | 0.49974300 |
| C | -0.72329200 | -0.56386500 | -0.90739500 |
| O | -1.89211100 | -0.35428600 | 1.19736400 |
| C | -3.16904100 | -0.56370400 | 0.63575800 |
| C | -3.68071800 | 0.29987700 | -0.32770000 |
| C | -4.96997400 | 0.07988200 | -0.78359300 |
| C | -5.73474000 | -0.98163400 | -0.27794200 |
| C | -5.20071400 | -1.82482900 | 0.70267400 |
| C | -3.90622600 | -1.60607500 | 1.16703200 |
| N | 2.83117900 | -0.42513000 | -1.34296200 |
| C | 4.04620300 | -0.12570200 | -0.67794600 |
| O | 4.68724300 | -1.24839800 | -0.41630600 |
| O | 4.40661500 | 1.01120700 | -0.48862400 |
| C | 6.02553900 | -1.22438700 | 0.20623300 |
| C | 6.36843100 | -2.70242900 | 0.31348000 |
| C | 7.00307100 | -0.50378200 | -0.71205000 |
| C | 5.93087400 | -0.58553800 | 1.58529200 |
| O | -6.97549900 | -1.10874800 | -0.79409000 |
| C | -7.78236500 | -2.17793200 | -0.31831200 |
| H | 0.62137400 | -0.88181100 | -2.51873500 |
| H | 2.48820600 | 0.13197700 | 1.31290900 |
| H | 0.23478300 | 0.21687900 | 2.35069800 |
| H | -1.62210100 | -0.78424400 | -1.46924400 |
| H | -3.08294800 | 1.12399600 | -0.70199500 |
| H | -5.40826800 | 0.72763900 | -1.53485800 |
| H | -5.77609200 | -2.64554300 | 1.11210700 |
| H | -3.47381300 | -2.24391000 | 1.93036500 |
| H | 7.35390200 | -2.81482200 | 0.77216400 |
| H | 5.63261500 | -3.22325700 | 0.93219700 |

| | | | |
|---|---|---|---|
| H | 6.38843200 | -3.16446400 | -0.67729000 |
| H | 8.01389900 | -0.62565500 | -0.31296900 |
| H | 6.97401600 | -0.94234800 | -1.71378200 |
| H | 6.78038700 | 0.56173500 | -0.77885800 |
| H | 6.89184900 | -0.70162500 | 2.09410600 |
| H | 5.69809000 | 0.47825000 | 1.51956900 |
| H | 5.16401900 | -1.08826200 | 2.18237300 |
| H | -8.72381900 | -2.10829400 | -0.86213200 |
| H | -7.31360400 | -3.14664100 | -0.52156900 |
| H | -7.97333300 | -2.08142300 | 0.75571900 |
| C | -0.06593700 | 4.17001100 | -0.43551100 |
| C | -0.12036600 | 2.83602800 | -0.73643100 |
| C | -1.47796700 | 3.14219300 | 0.90732800 |
| N | -0.93655900 | 4.34235800 | 0.61042900 |
| H | -1.13706600 | 5.21586700 | 1.08160100 |
| H | 0.49183300 | 4.98997400 | -0.85914800 |
| H | 0.41755800 | 2.29645600 | -1.50504900 |
| H | -2.19677600 | 2.99764400 | 1.70074200 |
| N | -1.00629800 | 2.20770800 | 0.10466000 |

**TS-IM2**

| | | | |
|---|---|---|---|
| C | -0.80592200 | -0.57164200 | -2.01037100 |
| C | -1.69511500 | -1.19679400 | -1.01743000 |
| C | -1.24195800 | -1.21476200 | 0.38670800 |
| C | -0.07325400 | -0.68027300 | 0.74086800 |
| C | 0.85722600 | -0.01501800 | -0.24172700 |
| C | 0.36131900 | -0.02982700 | -1.66466100 |
| O | 1.18370700 | 1.29865000 | 0.18777100 |
| C | 0.17346400 | 2.25006700 | 0.07670500 |
| C | 0.14300900 | 3.08023200 | -1.04373900 |

| | | | |
|---|---|---|---|
| C | -0.82256400 | 4.06960700 | -1.13680300 |
| C | -1.76489000 | 4.23527500 | -0.11244600 |
| C | -1.72499200 | 3.40540000 | 1.01087300 |
| C | -0.74771500 | 2.41328000 | 1.10112600 |
| N | -2.80950400 | -1.67531100 | -1.43083800 |
| C | -3.65787800 | -2.34825900 | -0.53194500 |
| O | -4.73900900 | -1.61268900 | -0.30640800 |
| O | -3.43289100 | -3.46390700 | -0.11846000 |
| C | -5.81667800 | -2.11005800 | 0.55941500 |
| C | -6.81589600 | -0.96193700 | 0.54293800 |
| C | -6.42965500 | -3.36684600 | -0.04538900 |
| C | -5.28149400 | -2.33826500 | 1.96787100 |
| O | -2.66824800 | 5.22832700 | -0.29686700 |
| C | -3.63292500 | 5.43363800 | 0.72344400 |
| H | -1.14973900 | -0.57622900 | -3.03965600 |
| H | -1.88464400 | -1.67500300 | 1.13144000 |
| H | 0.27101100 | -0.68459400 | 1.77178400 |
| H | 1.02440500 | 0.42652500 | -2.39481500 |
| H | 0.88166300 | 2.94996300 | -1.82816800 |
| H | -0.86455900 | 4.73055600 | -1.99616400 |
| H | -2.43654300 | 3.52169500 | 1.81912600 |
| H | -0.69916200 | 1.77494900 | 1.97736300 |
| H | -7.67807200 | -1.21697600 | 1.16428400 |
| H | -6.35835000 | -0.04984000 | 0.93598900 |
| H | -7.16298700 | -0.77119400 | -0.47631300 |
| H | -7.32263100 | -3.63538500 | 0.52621500 |
| H | -6.72872200 | -3.17919100 | -1.08089700 |
| H | -5.73193400 | -4.20439200 | -0.01922300 |
| H | -6.11990400 | -2.55763900 | 2.63502000 |
| H | -4.58195200 | -3.17451400 | 1.99966900 |

| | | | |
|---|---|---|---|
| H | -4.78147900 | -1.43511800 | 2.33122500 |
| H | -4.25485400 | 6.26360600 | 0.38883500 |
| H | -4.25745500 | 4.54463800 | 0.86403500 |
| H | -3.15572000 | 5.69655700 | 1.67396100 |
| C | 3.67020000 | -2.29326000 | -0.30336200 |
| C | 2.33178700 | -2.06485200 | -0.41224100 |
| C | 3.36170600 | -0.15991400 | 0.03464500 |
| N | 4.29046100 | -1.09856200 | -0.02531400 |
| H | 5.51426600 | -0.92457600 | 0.14293700 |
| H | 4.22291400 | -3.21455900 | -0.40197100 |
| H | 1.49862500 | -2.71855400 | -0.62129700 |
| H | 3.51955500 | 0.88699800 | 0.23552800 |
| N | 2.15794100 | -0.71388400 | -0.19306500 |
| C | 8.96248800 | -0.44115000 | -0.13931000 |
| C | 7.73072500 | -0.60103600 | -0.70450000 |
| C | 7.45194200 | -0.68378200 | 1.45146600 |
| N | 8.75864100 | -0.49711800 | 1.21754900 |
| H | 9.47400600 | -0.41090200 | 1.93014300 |
| H | 9.94148200 | -0.29647700 | -0.56659100 |
| H | 7.44794600 | -0.61929400 | -1.74563500 |
| H | 7.01638100 | -0.76414600 | 2.43527100 |
| N | 6.80394800 | -0.75068000 | 0.30121400 |

**TS-IM3**

| | | | |
|---|---|---|---|
| C | -0.09700600 | -1.58634700 | -1.87430200 |
| C | -0.86987700 | -1.36824100 | -0.64823000 |
| C | -0.10843100 | -1.30610900 | 0.60717700 |
| C | 1.24205400 | -1.32526800 | 0.59661900 |
| C | 1.94612300 | -1.24057300 | -0.65800300 |
| C | 1.25081300 | -1.60851500 | -1.86799300 |

| | | | |
|---|---|---|---|
| O | 1.83535200 | 0.70022700 | -0.88926100 |
| C | 0.60821200 | 1.15254900 | -0.94995100 |
| C | -0.06857700 | 1.24469500 | -2.20091900 |
| C | -1.37061000 | 1.68082400 | -2.26377300 |
| C | -2.06000100 | 2.02567400 | -1.08286500 |
| C | -1.41028700 | 1.96252100 | 0.16287100 |
| C | -0.10125300 | 1.51976700 | 0.22395200 |
| N | -2.15309300 | -1.23655300 | -0.78757800 |
| C | -3.00431000 | -1.27147400 | 0.32748100 |
| O | -4.09996800 | -0.55269300 | 0.07788300 |
| O | -2.82571400 | -1.95064300 | 1.32045200 |
| C | -5.28959400 | -0.71578400 | 0.92055600 |
| C | -6.33391900 | 0.13790200 | 0.21305100 |
| C | -5.73153000 | -2.17666400 | 0.91979800 |
| C | -5.02633800 | -0.19691400 | 2.32930800 |
| O | -3.31622200 | 2.46283300 | -1.25057100 |
| C | -3.98963700 | 2.99271300 | -0.11546500 |
| H | -0.66499200 | -1.76635700 | -2.78128200 |
| H | -0.65053400 | -1.25402200 | 1.54184600 |
| H | 1.80146400 | -1.23428600 | 1.52169700 |
| H | 1.82040400 | -1.78842800 | -2.77305500 |
| H | 0.47848100 | 0.98804900 | -3.10208200 |
| H | -1.89241200 | 1.77230800 | -3.21044900 |
| H | -1.92154300 | 2.25311400 | 1.07246400 |
| H | 0.41544500 | 1.47216800 | 1.17797900 |
| H | -7.28647900 | 0.06295900 | 0.74390100 |
| H | -6.03297700 | 1.18754000 | 0.18956900 |
| H | -6.47759100 | -0.20974100 | -0.81373500 |
| H | -6.71078600 | -2.24812800 | 1.40148300 |
| H | -5.82872600 | -2.53891900 | -0.10826900 |

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|---|---|---|---|
| H | -5.03076800 | -2.81331800 | 1.45984100 |
| H | -5.96622600 | -0.19858600 | 2.88914300 |
| H | -4.30422700 | -0.82309600 | 2.85363000 |
| H | -4.65214400 | 0.83075800 | 2.29767100 |
| H | -4.96921500 | 3.31288400 | -0.46894300 |
| H | -4.10680400 | 2.23204700 | 0.66068800 |
| H | -3.44655900 | 3.85281800 | 0.29033100 |
| C | 5.43908400 | -1.60334600 | -0.05352200 |
| C | 4.16244900 | -1.79235000 | 0.38595400 |
| C | 4.18338200 | -0.89562500 | -1.63840600 |
| N | 5.44184900 | -1.03480700 | -1.31362300 |
| H | 2.93799100 | 1.18323600 | 0.32876500 |
| H | 6.35720200 | -1.85026700 | 0.46035300 |
| H | 3.76467400 | -2.22754000 | 1.28893900 |
| H | 3.79144400 | -0.45728400 | -2.54542600 |
| N | 3.34995900 | -1.33930800 | -0.64150900 |
| C | 5.00775100 | 1.11263800 | 2.77172500 |
| C | 3.73028700 | 0.97096300 | 2.32462600 |
| C | 4.97890600 | 1.57846500 | 0.60736500 |
| N | 5.75783900 | 1.48957600 | 1.68229100 |
| H | 6.75500300 | 1.67945400 | 1.68701800 |
| H | 5.44138600 | 0.98424700 | 3.74976200 |
| H | 2.82625400 | 0.69134100 | 2.84136100 |
| H | 5.29856900 | 1.83485800 | -0.39022200 |
| N | 3.74343500 | 1.27043200 | 0.98137300 |

**TS-IM4**

| | | | |
|---|---|---|---|
| C | 0.48036200 | 0.01962500 | -1.31633100 |
| C | 1.72345800 | 0.05556100 | -0.52536300 |
| C | 1.59464500 | 0.18982800 | 0.93876500 |

| | | | |
|---|---|---|---|
| C | 0.40442700 | 0.40007500 | 1.50190400 |
| C | -0.84014500 | 0.49535000 | 0.68770700 |
| C | -0.72296600 | 0.18791800 | -0.76314200 |
| O | -1.86431100 | -0.02064100 | 1.40578400 |
| C | -3.02819200 | -0.52337000 | 0.80566100 |
| C | -2.98098200 | -1.69007600 | 0.04523500 |
| C | -4.16011200 | -2.20118300 | -0.47042100 |
| C | -5.38406800 | -1.56691200 | -0.21046000 |
| C | -5.41917200 | -0.41818700 | 0.58478600 |
| C | -4.23016100 | 0.09881700 | 1.09893900 |
| N | 2.82891000 | -0.05488400 | -1.16127400 |
| C | 4.04851700 | 0.06206600 | -0.45931500 |
| O | 4.72829800 | -1.06707400 | -0.57819300 |
| O | 4.40356000 | 1.08494400 | 0.08175800 |
| C | 6.05824900 | -1.21131300 | 0.03364200 |
| C | 6.43778000 | -2.64013100 | -0.32738300 |
| C | 7.02610900 | -0.21849700 | -0.59691000 |
| C | 5.94853700 | -1.04655800 | 1.54427500 |
| O | -6.47407800 | -2.14501900 | -0.76280200 |
| C | -7.73486500 | -1.53787700 | -0.51856300 |
| H | 0.58901600 | -0.16297800 | -2.38046600 |
| H | 2.48607000 | 0.10764000 | 1.55206700 |
| H | 0.27450900 | 0.49361300 | 2.57590300 |
| H | -1.62920000 | 0.15103000 | -1.35754400 |
| H | -2.03433400 | -2.18961000 | -0.13525200 |
| H | -4.15734000 | -3.10318700 | -1.07272400 |
| H | -6.35358200 | 0.07841000 | 0.81508300 |
| H | -4.24198300 | 0.98208300 | 1.73066900 |
| H | 7.42698700 | -2.86897100 | 0.07680100 |
| H | 5.71589500 | -3.34637800 | 0.09193500 |

| | | | |
|---|---|---|---|
| H | 6.46510600 | -2.76631200 | -1.41318600 |
| H | 8.03665700 | -0.43584300 | -0.23956400 |
| H | 7.01726000 | -0.32275900 | -1.68586600 |
| H | 6.77469400 | 0.80903500 | -0.33195100 |
| H | 6.90519300 | -1.31643700 | 2.00020300 |
| H | 5.70893500 | -0.01875000 | 1.81988400 |
| H | 5.17876200 | -1.71564500 | 1.94098600 |
| H | -8.46887000 | -2.14431300 | -1.04830100 |
| H | -7.97027000 | -1.53174200 | 0.55105400 |
| H | -7.76161700 | -0.51300900 | -0.90427000 |
| C | -0.06152400 | 3.03537500 | 0.21267900 |
| C | -0.48461600 | 3.64133400 | -0.90282500 |
| C | -2.23800600 | 2.58509500 | -0.22126800 |
| N | -1.16231500 | 2.24730200 | 0.69616200 |
| H | -1.40412500 | 2.41384200 | 1.68510400 |
| H | 0.88608300 | 3.03109700 | 0.72753700 |
| H | 0.07161900 | 4.29115000 | -1.56257900 |
| H | -3.22470700 | 2.16515600 | -0.07589000 |
| N | -1.84690500 | 3.34952000 | -1.16084600 |

**TS-IM5**

| | | | |
|---|---|---|---|
| C | -0.08815100 | -1.57655800 | 1.95839700 |
| C | 0.94969700 | -1.38566500 | 0.93350800 |
| C | 0.50239000 | -1.00459100 | -0.41993000 |
| C | -0.79229000 | -0.90048200 | -0.71897400 |
| C | -1.85274500 | -1.18855000 | 0.28968600 |
| C | -1.38763200 | -1.48382600 | 1.67401600 |
| O | -2.87635900 | -0.09793500 | 0.31396600 |
| C | -2.51375800 | 1.24637600 | 0.09536400 |
| C | -2.69901100 | 1.80275000 | -1.16504300 |

| | | | |
|---|---|---|---|
| C | -2.35729800 | 3.13076000 | -1.35603400 |
| C | -1.82349600 | 3.88403200 | -0.29927200 |
| C | -1.64143600 | 3.29991800 | 0.95901600 |
| C | -1.99905500 | 1.96760600 | 1.15756700 |
| N | 2.17150400 | -1.52583900 | 1.28424600 |
| C | 3.19456900 | -1.40526500 | 0.31880500 |
| O | 3.85418900 | -0.27507500 | 0.51770100 |
| O | 3.43477900 | -2.27052400 | -0.49131400 |
| C | 5.01833800 | 0.07190400 | -0.31342900 |
| C | 5.43986200 | 1.42127900 | 0.24967500 |
| C | 6.11818200 | -0.96344100 | -0.11777300 |
| C | 4.58736100 | 0.20365100 | -1.76864800 |
| O | -1.51852200 | 5.16620900 | -0.59217400 |
| C | -0.98015200 | 5.97166500 | 0.44764600 |
| H | 0.25364700 | -1.78850300 | 2.96598000 |
| H | 1.25234000 | -0.79556000 | -1.17664500 |
| H | -1.12196400 | -0.59070300 | -1.70642400 |
| H | -2.14681300 | -1.59807400 | 2.44065000 |
| H | -3.11216600 | 1.20801900 | -1.97373100 |
| H | -2.49284500 | 3.60738600 | -2.32068200 |
| H | -1.23435000 | 3.86628500 | 1.78735200 |
| H | -1.87736500 | 1.49905900 | 2.12885400 |
| H | 6.31093400 | 1.78951200 | -0.29800100 |
| H | 4.62971200 | 2.14881900 | 0.14958500 |
| H | 5.70375500 | 1.32984700 | 1.30685000 |
| H | 7.02461100 | -0.61392200 | -0.62004800 |
| H | 6.33972200 | -1.08194100 | 0.94697100 |
| H | 5.83742000 | -1.93044100 | -0.53633600 |
| H | 5.42255400 | 0.60391400 | -2.35023400 |
| H | 4.29931400 | -0.76038400 | -2.19003000 |

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|---|---|---|---|
| H | 3.74743600 | 0.90030600 | -1.85117000 |
| H | -0.80737000 | 6.95341600 | 0.00800100 |
| H | -1.68474900 | 6.06356700 | 1.28091600 |
| H | -0.03198900 | 5.56334500 | 0.81297600 |
| C | -2.70985400 | -2.93413700 | -1.43941400 |
| C | -3.43900400 | -4.04672000 | -1.26125400 |
| C | -3.68936200 | -2.98689400 | 0.59748700 |
| N | -2.88299100 | -2.15698900 | -0.25355500 |
| H | -3.48161900 | -1.00068200 | -0.33780500 |
| H | -2.12784100 | -2.57454400 | -2.27267100 |
| H | -3.59228700 | -4.85724900 | -1.95843700 |
| H | -3.97823900 | -2.64865200 | 1.58379300 |
| N | -4.04672400 | -4.06247300 | 0.00737800 |

**TS-IM6**

| | | | |
|---|---|---|---|
| C | -0.56507100 | 0.15929100 | -2.25435900 |
| C | -1.50990000 | 0.24887600 | -1.13028000 |
| C | -1.03482200 | -0.20459400 | 0.19091900 |
| C | 0.19378500 | -0.69581700 | 0.35402200 |
| C | 1.18445200 | -0.81147700 | -0.77412600 |
| C | 0.66985200 | -0.31651000 | -2.09860100 |
| O | 2.43579700 | -0.23100800 | -0.43999700 |
| C | 2.42953200 | 1.14017400 | -0.18284700 |
| C | 2.25582000 | 1.58919300 | 1.12580100 |
| C | 2.30588400 | 2.94814700 | 1.39195200 |
| C | 2.53017900 | 3.86378700 | 0.35462500 |
| C | 2.71309000 | 3.40510700 | -0.95278900 |
| C | 2.66207000 | 2.03597000 | -1.21574200 |
| N | -2.68340400 | 0.70217500 | -1.37168400 |
| C | -3.59775700 | 0.88490300 | -0.31593300 |

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|---|---|---|---|
| O | -4.61923000 | 0.05345500 | -0.47044400 |
| O | -3.47031700 | 1.73919300 | 0.53267700 |
| C | -5.75097800 | 0.07382600 | 0.46664900 |
| C | -6.65304100 | -1.02610000 | -0.07487100 |
| C | -5.26377600 | -0.26922400 | 1.86905900 |
| C | -6.45135700 | 1.42527100 | 0.40324800 |
| O | 2.56004000 | 5.16852400 | 0.71700400 |
| C | 2.78799300 | 6.12759000 | -0.30418200 |
| H | -0.92109700 | 0.51072800 | -3.21737200 |
| H | -1.70952100 | -0.12561300 | 1.03766700 |
| H | 0.53888100 | -1.02485200 | 1.33213900 |
| H | 1.36787800 | -0.36620200 | -2.93027700 |
| H | 2.09496300 | 0.87135800 | 1.92422600 |
| H | 2.17702100 | 3.32465500 | 2.40118900 |
| H | 2.89828100 | 4.09424500 | -1.76760500 |
| H | 2.81498200 | 1.66694400 | -2.22494000 |
| H | -7.54652700 | -1.10752700 | 0.54916900 |
| H | -6.96077800 | -0.79883800 | -1.09926600 |
| H | -6.13214200 | -1.98754200 | -0.06821600 |
| H | -6.13014000 | -0.41000900 | 2.52145400 |
| H | -4.69266600 | -1.20262900 | 1.85100500 |
| H | -4.64113000 | 0.52525200 | 2.28221700 |
| H | -7.37326100 | 1.37358300 | 0.98944000 |
| H | -5.82374500 | 2.22031900 | 0.80698300 |
| H | -6.71539200 | 1.66456700 | -0.63114400 |
| H | 2.77151500 | 7.10063000 | 0.18617500 |
| H | 3.76303700 | 5.97646800 | -0.78021400 |
| H | 2.00183700 | 6.09055300 | -1.06629000 |
| C | 0.56699200 | -3.24617400 | -1.14749700 |
| C | 1.05034700 | -4.07896000 | -2.08315600 |

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|---|---|---|---|
| C | 2.58847300 | -2.58148400 | -1.89668200 |
| N | 1.58297400 | -2.26338200 | -0.91750100 |
| H | 2.16093300 | -2.61026500 | 0.19396900 |
| H | -0.34605600 | -3.24044000 | -0.57132300 |
| H | 0.59212200 | -4.97276800 | -2.48063000 |
| H | 3.47274800 | -1.96329700 | -1.97784500 |
| N | 2.31319400 | -3.65242400 | -2.54005300 |
| C | 3.33417500 | -1.94036500 | 1.99689400 |
| C | 2.62049200 | -1.86093800 | 3.13442100 |
| C | 1.84765600 | -3.62011200 | 2.16146800 |
| N | 2.80971700 | -3.05410900 | 1.27718900 |
| H | 3.48256200 | -3.70508800 | 0.85315400 |
| H | 4.11990100 | -1.33156000 | 1.57800700 |
| H | 2.69341400 | -1.12105300 | 3.91845000 |
| H | 1.31221700 | -4.51730900 | 1.88013600 |
| N | 1.69113400 | -2.91481400 | 3.22174600 |

**TS-IM7**

| | | | |
|---|---|---|---|
| C | -0.64771100 | 0.29674600 | -2.18305200 |
| C | -1.62121000 | 0.23092500 | -1.08148200 |
| C | -1.20388100 | -0.45960200 | 0.15520800 |
| C | -0.00079100 | -1.02292700 | 0.26054900 |
| C | 1.00576800 | -0.97428000 | -0.85048100 |
| C | 0.56989400 | -0.23409900 | -2.08005600 |
| O | 2.24412600 | -0.30963100 | -0.34061700 |
| C | 2.23236400 | 1.09665500 | -0.14752900 |
| C | 1.64690400 | 1.64095200 | 0.99113100 |
| C | 1.68647100 | 3.01551200 | 1.15839700 |
| C | 2.30021400 | 3.83055400 | 0.19569500 |
| C | 2.88455600 | 3.25922300 | -0.94068100 |

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|---|---|---|---|
| C | 2.84803200 | 1.87750500 | -1.10938900 |
| N | -2.76948700 | 0.76549500 | -1.26636500 |
| C | -3.70779100 | 0.79282800 | -0.21456100 |
| O | -4.72978000 | 0.00610100 | -0.51819300 |
| O | -3.59037800 | 1.50424400 | 0.75759200 |
| C | -5.87435400 | -0.12278000 | 0.39580800 |
| C | -6.76988400 | -1.11733400 | -0.32889600 |
| C | -5.40388000 | -0.69110900 | 1.72896700 |
| C | -6.57170300 | 1.22321900 | 0.54545700 |
| O | 2.28201900 | 5.15436100 | 0.45329900 |
| C | 2.89181700 | 6.02129100 | -0.49427700 |
| H | -0.96985600 | 0.80261100 | -3.08724300 |
| H | -1.90011300 | -0.50192000 | 0.98712600 |
| H | 0.31293300 | -1.53939300 | 1.16626300 |
| H | 1.29047200 | -0.18719700 | -2.89222200 |
| H | 1.17743100 | 1.00691500 | 1.73587600 |
| H | 1.24545200 | 3.48109500 | 2.03280700 |
| H | 3.36668700 | 3.87148000 | -1.69234900 |
| H | 3.29874300 | 1.41199200 | -1.97978600 |
| H | -7.67065500 | -1.29789000 | 0.26300300 |
| H | -7.06556700 | -0.72526700 | -1.30590800 |
| H | -6.24920100 | -2.06801400 | -0.47325800 |
| H | -6.27822200 | -0.92968300 | 2.34103700 |
| H | -4.83754600 | -1.61324800 | 1.56590800 |
| H | -4.78210100 | 0.02214100 | 2.27179200 |
| H | -7.50186000 | 1.07860700 | 1.10230500 |
| H | -5.94894700 | 1.93868600 | 1.08334500 |
| H | -6.82092500 | 1.63039300 | -0.43889900 |
| H | 2.76639100 | 7.02982300 | -0.10180000 |
| H | 3.95918100 | 5.80104100 | -0.60118800 |

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|---|---|---|---|
| H | 2.40189700 | 5.94555800 | -1.47063800 |
| C | 0.85808200 | -3.50314400 | -0.87353500 |
| C | 1.64470200 | -4.46510400 | -1.43820700 |
| C | 2.59273300 | -2.60334100 | -1.91882400 |
| N | 1.47872500 | -2.30531400 | -1.17552700 |
| H | 2.82733600 | -0.91801000 | 0.50049000 |
| H | -0.05623000 | -3.55118700 | -0.30312700 |
| H | 1.49600900 | -5.53495500 | -1.41648200 |
| H | 3.25679600 | -1.83297300 | -2.28705300 |
| N | 2.72635800 | -3.89562000 | -2.07692600 |
| C | 3.08034100 | -1.00033500 | 2.69133900 |
| C | 2.34200600 | -1.96167400 | 3.27444800 |
| C | 3.06528900 | -2.88914900 | 1.46940100 |
| N | 3.51572500 | -1.53788900 | 1.44327400 |
| H | 4.49253900 | -1.37944500 | 1.16672200 |
| H | 3.32585700 | 0.01254700 | 2.97110200 |
| H | 1.80063100 | -1.91493100 | 4.20795200 |
| H | 3.29734900 | -3.55947800 | 0.65009000 |
| N | 2.33865400 | -3.13568500 | 2.49767500 |

**TS-a1**

| | | | |
|---|---|---|---|
| C | -0.37956100 | 0.41795200 | 1.45792700 |
| C | -1.37660800 | 0.16296700 | 0.45037000 |
| C | -0.96469500 | 0.38567800 | -0.91230700 |
| C | 0.28067700 | 0.85425600 | -1.22036700 |
| C | 1.23094300 | 1.22329500 | -0.19061600 |
| C | 0.86869500 | 0.87309700 | 1.17047600 |
| O | 2.59493700 | 1.11666000 | -0.52150000 |
| C | 3.22650000 | -0.09519400 | -0.31251100 |
| C | 4.61292300 | -0.03008500 | -0.15459200 |

| | | | |
|---|---|---|---|
| C | 5.34775600 | -1.19173300 | 0.00982800 |
| C | 4.70671800 | -2.43737900 | 0.02887900 |
| C | 3.32240200 | -2.49866600 | -0.12520600 |
| C | 2.58123100 | -1.32640000 | -0.30156500 |
| N | -2.57822100 | -0.23372700 | 0.90253300 |
| C | -3.55161700 | -0.65174500 | 0.03890100 |
| O | -4.72858100 | -0.71016300 | 0.71219600 |
| O | -3.45145200 | -0.97782500 | -1.14050300 |
| C | -5.94175300 | -1.15041100 | 0.05326600 |
| C | -6.98647800 | -1.04940500 | 1.16021700 |
| C | -6.30577900 | -0.21146600 | -1.09445600 |
| C | -5.81144500 | -2.59937400 | -0.41005500 |
| O | 5.51168800 | -3.51833300 | 0.20192700 |
| C | 4.89127700 | -4.79290600 | 0.21430600 |
| H | -0.65755100 | 0.20463300 | 2.48622700 |
| H | -1.65597500 | 0.14564600 | -1.70860000 |
| H | 0.58969900 | 0.99995400 | -2.25113600 |
| H | 1.61219500 | 1.03619600 | 1.94543100 |
| H | 5.10112900 | 0.93939700 | -0.16555400 |
| H | 6.42532000 | -1.15586900 | 0.13217000 |
| H | 2.80040000 | -3.44792200 | -0.11582100 |
| H | 1.50709800 | -1.39390400 | -0.42984700 |
| H | -7.96472900 | -1.36032700 | 0.78371200 |
| H | -6.71451800 | -1.69386500 | 2.00125500 |
| H | -7.06173400 | -0.01949900 | 1.52118900 |
| H | -7.30120800 | -0.46665400 | -1.47046400 |
| H | -6.33012200 | 0.82280800 | -0.73671600 |
| H | -5.58814800 | -0.28843600 | -1.91127700 |
| H | -6.78543800 | -2.95854100 | -0.75628000 |
| H | -5.09067200 | -2.69149300 | -1.22245400 |

| | | | |
|---|---|---|---|
| H | -5.49136300 | -3.23075300 | 0.42490500 |
| H | 5.69159800 | -5.51913700 | 0.35638700 |
| H | 4.17300500 | -4.87887900 | 1.03751100 |
| H | 4.38045300 | -4.99664200 | -0.73361900 |
| C | 0.24794600 | 3.84305800 | -0.27858400 |
| C | 0.68097400 | 5.12362700 | 0.08780900 |
| C | 2.02933900 | 4.98354100 | 0.37646300 |
| N | 2.34395700 | 3.69261100 | 0.18314400 |
| H | 3.24166700 | 3.22503500 | 0.25821400 |
| H | -0.73042800 | 3.48160600 | -0.56430000 |
| H | 0.09382200 | 6.02701700 | 0.13490900 |
| H | 2.77681900 | 5.69604900 | 0.69218000 |
| N | 1.27844500 | 3.00463200 | -0.23054600 |

**TS-a2**

| | | | |
|---|---|---|---|
| C | -0.83932500 | -1.47733000 | 1.33240800 |
| C | -1.93649200 | -0.67431500 | 0.87009200 |
| C | -1.66533600 | 0.73215100 | 0.70706500 |
| C | -0.41758100 | 1.24395400 | 0.89539800 |
| C | 0.71030500 | 0.37569000 | 1.14321600 |
| C | 0.41719700 | -0.98060100 | 1.51844800 |
| O | 1.51437000 | 0.32118200 | -0.48605400 |
| C | 2.44110800 | -0.64828100 | -0.59781600 |
| C | 3.77047200 | -0.43931400 | -0.18402600 |
| C | 4.71462500 | -1.44787700 | -0.29834300 |
| C | 4.35752600 | -2.69869800 | -0.81862800 |
| C | 3.04043000 | -2.92623800 | -1.22562200 |
| C | 2.09597200 | -1.90685900 | -1.10528900 |
| N | -3.11704600 | -1.29370200 | 0.73067300 |
| C | -4.15227800 | -0.66009900 | 0.09661900 |

| | | | |
|---|---|---|---|
| O | -5.30866500 | -1.29141700 | 0.41126300 |
| O | -4.10244200 | 0.28479900 | -0.68383000 |
| C | -6.56949400 | -0.86613400 | -0.16588900 |
| C | -7.57274200 | -1.82927100 | 0.46026800 |
| C | -6.89575200 | 0.56774400 | 0.24419900 |
| C | -6.55385900 | -1.04034600 | -1.68241300 |
| O | 5.35624500 | -3.62048300 | -0.89023800 |
| C | 5.02579200 | -4.89577100 | -1.41087800 |
| H | -1.04691000 | -2.52232000 | 1.54285500 |
| H | -2.48470700 | 1.39725800 | 0.46799000 |
| H | -0.24382000 | 2.31360600 | 0.81875800 |
| H | 1.22454800 | -1.62248600 | 1.85467500 |
| H | 4.05740200 | 0.53286800 | 0.20851900 |
| H | 5.74369900 | -1.28900300 | 0.00911700 |
| H | 2.73911600 | -3.88509000 | -1.63134200 |
| H | 1.06888300 | -2.07462300 | -1.41591700 |
| H | -8.58063100 | -1.60961100 | 0.09798200 |
| H | -7.32443000 | -2.86205300 | 0.19895400 |
| H | -7.56425600 | -1.73409100 | 1.54997700 |
| H | -7.91673700 | 0.80997400 | -0.06594100 |
| H | -6.83636300 | 0.66744500 | 1.33267700 |
| H | -6.20790600 | 1.27709900 | -0.21605900 |
| H | -7.55907200 | -0.86529500 | -2.07777200 |
| H | -5.86156900 | -0.34242000 | -2.15331100 |
| H | -6.25920600 | -2.06315100 | -1.93778100 |
| H | 5.94394200 | -5.48297600 | -1.38425800 |
| H | 4.26153300 | -5.39087500 | -0.80089300 |
| H | 4.67068600 | -4.82537100 | -2.44542400 |
| C | 2.44747400 | 0.59417500 | 2.96928800 |
| C | 3.42964800 | 1.52887900 | 3.26233200 |

| | | | |
|---|---|---|---|
| C | 3.34086300 | 2.48500400 | 2.25306600 |
| N | 2.36669900 | 2.13108300 | 1.41518300 |
| H | 2.06590900 | 2.59814100 | 0.47452500 |
| H | 2.13861000 | -0.29914800 | 3.49063000 |
| H | 4.10907700 | 1.51701800 | 4.09927000 |
| H | 3.90917100 | 3.38646300 | 2.07524400 |
| N | 1.82407300 | 0.98254300 | 1.84294700 |
| C | 1.59283500 | 4.61656900 | -1.25512200 |
| C | 1.03897300 | 4.71288300 | -2.54167900 |
| C | 0.74147600 | 3.40641500 | -2.89214400 |
| N | 1.11111500 | 2.63092600 | -1.86087200 |
| H | 1.05346800 | 1.61806300 | -1.72769400 |
| H | 1.96169800 | 5.39937600 | -0.60704200 |
| H | 0.87780200 | 5.60269400 | -3.13000300 |
| H | 0.30270100 | 2.98151300 | -3.78259400 |
| N | 1.63091300 | 3.34634800 | -0.85672900 |

**TS-b**

| | | | |
|---|---|---|---|
| C | -0.84446900 | -0.87940000 | 1.67429600 |
| C | 0.12999400 | -1.14526100 | 0.64930000 |
| C | -0.39357700 | -1.39257200 | -0.66776900 |
| C | -1.72411800 | -1.25230600 | -0.94811400 |
| C | -2.61698600 | -0.70508200 | 0.03361500 |
| C | -2.16929700 | -0.72191800 | 1.40413600 |
| O | -2.87934200 | 1.00654600 | -0.39627800 |
| C | -1.76826500 | 1.74170300 | -0.23508400 |
| C | -1.50577800 | 2.40349700 | 0.97931100 |
| C | -0.34520600 | 3.14061000 | 1.14857800 |
| C | 0.59625500 | 3.22494900 | 0.11368700 |
| C | 0.34802400 | 2.58321300 | -1.10242700 |

| | | | |
|---|---|---|---|
| C | -0.82721300 | 1.85161900 | -1.26730800 |
| N | 1.41113400 | -1.21122800 | 1.04796600 |
| C | 2.41733200 | -1.22047300 | 0.12473700 |
| O | 3.57578000 | -1.55705000 | 0.74828100 |
| O | 2.37141700 | -0.93345600 | -1.06863700 |
| C | 4.82891800 | -1.58877900 | 0.02276700 |
| C | 5.83439700 | -1.99203900 | 1.09687600 |
| C | 4.78933700 | -2.64520000 | -1.07874100 |
| C | 5.17601900 | -0.20511600 | -0.52233700 |
| O | 1.71123500 | 3.95682400 | 0.38160200 |
| C | 2.71016700 | 4.00576500 | -0.62174000 |
| H | -0.48147200 | -0.81153400 | 2.69584100 |
| H | 0.28609000 | -1.70896600 | -1.44774600 |
| H | -2.11206500 | -1.44651600 | -1.94355900 |
| H | -2.89344800 | -0.52589100 | 2.18930900 |
| H | -2.23210100 | 2.32704000 | 1.78317300 |
| H | -0.13744000 | 3.65476000 | 2.08187800 |
| H | 1.05690200 | 2.64243800 | -1.92010800 |
| H | -1.02788100 | 1.34973900 | -2.20859100 |
| H | 6.83806700 | -2.05709700 | 0.66810600 |
| H | 5.84621100 | -1.25419000 | 1.90442000 |
| H | 5.57091000 | -2.96598100 | 1.51957400 |
| H | 5.78869900 | -2.75991600 | -1.50949500 |
| H | 4.48468300 | -3.60960200 | -0.65989700 |
| H | 4.09255300 | -2.36440200 | -1.86861700 |
| H | 6.19878900 | -0.21403400 | -0.91148400 |
| H | 4.49478900 | 0.08684700 | -1.32159400 |
| H | 5.12225500 | 0.53655400 | 0.28121100 |
| H | 3.52484400 | 4.60324700 | -0.21202400 |
| H | 3.08080200 | 3.00262400 | -0.86317500 |

| | | | |
|---|---|---|---|
| H | 2.33735500 | 4.48176300 | -1.53586500 |
| C | -4.55834600 | -2.23676900 | -0.49819100 |
| C | -5.94170000 | -2.12414000 | -0.40808800 |
| C | -6.18592500 | -0.82179600 | 0.01174000 |
| N | -5.00736100 | -0.21412200 | 0.16209500 |
| H | -4.75747800 | 0.75765400 | 0.34379600 |
| H | -3.92244900 | -3.07034300 | -0.75861500 |
| H | -6.67049500 | -2.88996100 | -0.61819000 |
| H | -7.10586700 | -0.28913400 | 0.20148200 |
| N | -4.01982100 | -1.05765500 | -0.16220900 |

**TS-C8**

| | | | |
|---|---|---|---|
| C | -1.40435900 | -1.95200800 | -1.02801600 |
| C | -2.33632400 | -0.92033100 | -0.66109300 |
| C | -1.76815400 | 0.35279700 | -0.31800200 |
| C | -0.40573700 | 0.54522700 | -0.31758100 |
| C | 0.48229900 | -0.48956300 | -0.68065600 |
| C | -0.04898100 | -1.75339000 | -1.02683800 |
| O | 1.81225300 | -0.26438800 | -0.73617700 |
| C | 2.77636400 | -2.18073100 | 0.44925600 |
| C | 3.87838300 | -2.72953400 | -0.10087400 |
| C | 5.00043100 | -1.90285300 | -0.43290100 |
| C | 5.00900100 | -0.51084400 | -0.10197100 |
| C | 3.91249900 | 0.03624800 | 0.47066100 |
| N | -3.63425800 | -1.25918300 | -0.72845700 |
| C | -4.59616000 | -0.41106900 | -0.26601800 |
| O | -5.81075400 | -0.88367300 | -0.65327800 |
| O | -4.47998000 | 0.60304900 | 0.41824800 |
| C | -7.02907900 | -0.18972200 | -0.29219500 |
| C | -8.11405000 | -1.04887800 | -0.93440900 |

| | | | |
|---|---|---|---|
| C | -7.21304600 | -0.16613500 | 1.22351700 |
| C | -7.05316600 | 1.21371900 | -0.89361000 |
| O | 5.98748100 | -2.51047000 | -1.01425700 |
| C | 7.17238400 | -1.78164400 | -1.40489000 |
| H | -1.82034900 | -2.91367300 | -1.31188300 |
| H | -2.42736200 | 1.17138000 | -0.06883300 |
| H | -0.00511800 | 1.52800100 | -0.08432500 |
| H | 0.62837200 | -2.55162000 | -1.31722100 |
| H | 1.91119700 | -2.79649200 | 0.67151200 |
| H | 3.94254700 | -3.79022300 | -0.31381600 |
| H | 5.89810300 | 0.08619000 | -0.25976500 |
| H | 3.92971400 | 1.07594300 | 0.78230800 |
| H | -9.10064200 | -0.62299800 | -0.73249300 |
| H | -7.96964400 | -1.09852300 | -2.01764500 |
| H | -8.08314500 | -2.06588800 | -0.53257400 |
| H | -8.21059000 | 0.21498300 | 1.46281900 |
| H | -7.12965100 | -1.18103200 | 1.62522000 |
| H | -6.46667000 | 0.46799500 | 1.70167700 |
| H | -8.04291500 | 1.65620400 | -0.74495600 |
| H | -6.30435400 | 1.85514000 | -0.42897800 |
| H | -6.86029000 | 1.16156900 | -1.96994100 |
| H | 7.80377600 | -2.51500500 | -1.89995700 |
| H | 6.90092600 | -0.98035700 | -2.09400700 |
| H | 7.66860300 | -1.38672600 | -0.51701800 |
| C | 1.20903700 | -1.03892700 | 2.65456300 |
| C | 0.53808300 | -0.15962900 | 3.48300400 |
| C | 0.81149400 | 1.11277300 | 2.97916100 |
| N | 1.60718200 | 0.99564500 | 1.92111000 |
| H | 1.90276400 | 1.76549400 | 1.18094200 |
| H | 1.29328100 | -2.11433800 | 2.68988300 |

| | | | |
|---|---|---|---|
| H | -0.06637800 | -0.41007800 | 4.33976100 |
| H | 0.48148900 | 2.08949500 | 3.30292200 |
| N | 1.85593900 | -0.31253800 | 1.71592500 |
| C | 2.47026600 | 4.12967600 | 0.23152200 |
| C | 2.74534300 | 4.70430600 | -1.01830100 |
| C | 2.68246200 | 3.64945400 | -1.91169900 |
| N | 2.38787500 | 2.54993900 | -1.19946300 |
| H | 2.26544800 | 1.59408900 | -1.52248100 |
| H | 2.41794700 | 4.59487000 | 1.20581600 |
| H | 2.95840800 | 5.73821100 | -1.23958600 |
| H | 2.82230000 | 3.59979800 | -2.98123500 |
| N | 2.25544900 | 2.82112100 | 0.10721200 |
| C | 2.66183000 | -0.72451600 | 0.60458300 |

**TS-normal-1**

| | | | |
|---|---|---|---|
| C | -0.40637000 | -2.09320200 | 0.92600400 |
| C | 0.25541300 | -1.86736700 | -0.28542200 |
| C | -0.46789300 | -1.27948300 | -1.32844700 |
| C | -1.77742100 | -0.87101500 | -1.16338900 |
| C | -2.40451500 | -0.91765600 | 0.12971700 |
| C | -1.71210500 | -1.68906000 | 1.12654700 |
| N | 1.62932100 | -2.21246500 | -0.44301700 |
| C | 2.62393800 | -1.38325100 | -0.02752900 |
| O | 3.82002400 | -1.91574200 | -0.35054600 |
| O | 2.45535100 | -0.32559200 | 0.55682200 |
| C | 5.05541800 | -1.21967200 | -0.01802400 |
| C | 6.12845900 | -2.15891400 | -0.55542700 |
| C | 5.11680600 | 0.12307300 | -0.73907500 |
| C | 5.19077000 | -1.07040900 | 1.49382900 |
| O | -2.77033700 | 0.63697000 | 0.70280100 |

| | | | |
|---|---|---|---|
| C | -1.86816300 | 1.60820000 | 0.45440300 |
| C | -2.33749400 | 2.88220600 | 0.09032200 |
| C | -1.46131000 | 3.93352100 | -0.13980500 |
| C | -0.07973600 | 3.73603800 | -0.04272100 |
| C | 0.40346200 | 2.47321000 | 0.29992100 |
| C | -0.48371100 | 1.42495900 | 0.55333500 |
| O | 0.70500300 | 4.82325100 | -0.30180800 |
| C | 2.10480100 | 4.63793600 | -0.21272700 |
| H | 0.12241100 | -2.60378500 | 1.72765200 |
| H | 0.00824600 | -1.15766100 | -2.29894300 |
| H | -2.34018100 | -0.44647400 | -1.98978300 |
| H | -2.21792400 | -1.87705800 | 2.06830500 |
| H | 1.90442300 | -3.04015800 | -0.95552700 |
| H | 7.11943700 | -1.73848400 | -0.36528700 |
| H | 6.06223300 | -3.13461900 | -0.06561800 |
| H | 6.00881300 | -2.29928200 | -1.63351100 |
| H | 6.10811500 | 0.56342500 | -0.59697600 |
| H | 4.95566700 | -0.01996900 | -1.81205200 |
| H | 4.36524800 | 0.81324000 | -0.35428200 |
| H | 6.18778700 | -0.68687700 | 1.72989200 |
| H | 4.44389000 | -0.38290100 | 1.89118700 |
| H | 5.07480100 | -2.04474900 | 1.97852500 |
| H | -3.40953900 | 3.03704200 | 0.00105500 |
| H | -1.83054900 | 4.91826600 | -0.41035700 |
| H | 1.46671900 | 2.27435200 | 0.37492800 |
| H | -0.07090100 | 0.45702800 | 0.81570900 |
| H | 2.55742000 | 5.60088700 | -0.45165300 |
| H | 2.40668400 | 4.33764900 | 0.79765200 |
| H | 2.45722600 | 3.88578000 | -0.92873100 |
| C | -6.01469000 | -1.05241800 | -0.31064900 |

| | | | |
|---|---|---|---|
| C | -5.75281300 | -2.41482400 | -0.24243900 |
| C | -4.38258900 | -2.51987900 | -0.01375400 |
| N | -3.87011800 | -1.28840600 | 0.06283300 |
| H | -4.62402800 | 0.57643500 | -0.02447500 |
| H | -6.93217800 | -0.50317900 | -0.46059100 |
| H | -6.45999300 | -3.22205600 | -0.34532200 |
| H | -3.73807400 | -3.38071100 | 0.08521500 |
| N | -4.85743400 | -0.40901400 | -0.13455600 |

**Ts-normal-2**

| | | | |
|---|---|---|---|
| C | 1.13942700 | 1.26110300 | 1.29109500 |
| C | 2.11553800 | 0.32615200 | 0.96859900 |
| C | 1.69399700 | -0.96428000 | 0.62007800 |
| C | 0.36162000 | -1.29749800 | 0.56130300 |
| C | -0.67559900 | -0.32821700 | 0.83083500 |
| C | -0.21387300 | 0.95473600 | 1.28515500 |
| O | -1.65895800 | -0.31021400 | -0.39575000 |
| C | -2.51161100 | 0.75885400 | -0.47769400 |
| C | -3.81189400 | 0.68244700 | 0.03359900 |
| C | -4.66719900 | 1.76828800 | -0.06682600 |
| C | -4.23353100 | 2.95369400 | -0.66890600 |
| C | -2.93582300 | 3.03982700 | -1.17418500 |
| C | -2.08225800 | 1.94160000 | -1.07380500 |
| N | 3.49522800 | 0.66513700 | 1.04418900 |
| C | 4.41328600 | 0.35691200 | 0.09128700 |
| O | 5.62055400 | 0.85148400 | 0.46920000 |
| O | 4.19779900 | -0.27308500 | -0.92473400 |
| C | 6.78390700 | 0.62689300 | -0.36516400 |
| C | 7.89741900 | 1.32376200 | 0.41008900 |
| C | 7.07357300 | -0.86779900 | -0.48409200 |

| | | | |
|---|---|---|---|
| C | 6.59471300 | 1.28349200 | -1.73079900 |
| O | -5.14911800 | 3.96237000 | -0.71675800 |
| C | -4.74731400 | 5.16975200 | -1.32102800 |
| H | 1.44173400 | 2.26732100 | 1.57409400 |
| H | 2.44032400 | -1.71354200 | 0.37711000 |
| H | 0.05656300 | -2.30459000 | 0.28881900 |
| H | -0.94922400 | 1.71178000 | 1.53706100 |
| H | -4.15044800 | -0.24148500 | 0.49256000 |
| H | -5.68298900 | 1.72605400 | 0.31102200 |
| H | -2.57784800 | 3.94741200 | -1.64496100 |
| H | -1.06740900 | 1.98966100 | -1.45366200 |
| H | 8.84558700 | 1.22619700 | -0.12515600 |
| H | 7.66883500 | 2.38603200 | 0.52948200 |
| H | 8.00609600 | 0.87745400 | 1.40205200 |
| H | 8.02898500 | -1.01375300 | -0.99681200 |
| H | 7.14749700 | -1.31203900 | 0.51292000 |
| H | 6.28607300 | -1.37211200 | -1.04325200 |
| H | 7.52959800 | 1.22377300 | -2.29608300 |
| H | 5.80298700 | 0.78840500 | -2.29225100 |
| H | 6.33742500 | 2.33897300 | -1.60244600 |
| H | -5.60414500 | 5.84059600 | -1.26390200 |
| H | -3.89827800 | 5.62035400 | -0.79241800 |
| H | -4.47322300 | 5.02052400 | -2.37265100 |
| C | -1.91691800 | -0.60780300 | 3.12832600 |
| C | -2.85150800 | -1.48794900 | 3.67977200 |
| C | -3.19389900 | -2.34234700 | 2.64237500 |
| N | -2.51132100 | -1.96970900 | 1.55062600 |
| H | -2.50585800 | -2.39767800 | 0.57342900 |
| H | -1.34856300 | 0.20611900 | 3.55187700 |
| H | -3.21936500 | -1.50373900 | 4.69232300 |

| | | | |
|---|---|---|---|
| H | -3.86952500 | -3.18355900 | 2.60670200 |
| N | -1.74777500 | -0.91670800 | 1.84599700 |
| C | -2.72338200 | -4.40921500 | -1.39384300 |
| C | -2.28280000 | -4.53141000 | -2.72088400 |
| C | -1.69555300 | -3.31093000 | -3.00063500 |
| N | -1.80836900 | -2.55804100 | -1.89480200 |
| H | -1.50183500 | -1.60290000 | -1.69287700 |
| H | -3.23456900 | -5.13485500 | -0.77775800 |
| H | -2.37580500 | -5.38106900 | -3.37742400 |
| H | -1.21398100 | -2.93307700 | -3.88912500 |
| N | -2.43081700 | -3.20655000 | -0.90493500 |
| H | 3.83861500 | 1.18002100 | 1.84022900 |

**INT-1**

| | | | |
|---|---|---|---|
| C | -1.21209400 | -1.15614700 | 2.03332100 |
| C | -0.21839900 | -1.57844400 | 1.03094300 |
| C | -0.59986000 | -1.46161600 | -0.39032300 |
| C | -1.68486400 | -0.77890900 | -0.75139300 |
| C | -2.52881900 | -0.04584800 | 0.25898500 |
| C | -2.29584500 | -0.46357000 | 1.68413500 |
| O | -2.39387600 | 1.37278500 | 0.11982900 |
| C | -1.08221600 | 1.84451700 | 0.05279300 |
| C | -0.49741800 | 2.04730600 | -1.19690800 |
| C | 0.80942100 | 2.49872100 | -1.27397200 |
| C | 1.53900900 | 2.74634200 | -0.10237100 |
| C | 0.93851600 | 2.56706600 | 1.14566900 |
| C | -0.38047300 | 2.11526400 | 1.21747800 |
| N | 0.92209600 | -1.98398300 | 1.44659200 |
| C | 1.90901800 | -2.31384100 | 0.49430500 |
| O | 2.70676700 | -1.26745600 | 0.32274400 |

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|---|---|---|---|
| O | 2.00963200 | -3.40916500 | -0.00798700 |
| C | 3.82631200 | -1.31758200 | -0.62838300 |
| C | 4.45653200 | 0.06044900 | -0.47975500 |
| C | 4.81282400 | -2.40624000 | -0.22524300 |
| C | 3.27519300 | -1.51231900 | -2.03512700 |
| O | 2.81881000 | 3.15629900 | -0.28194700 |
| C | 3.61719400 | 3.33247400 | 0.87889800 |
| H | -0.98850900 | -1.38041300 | 3.07132300 |
| H | 0.02502000 | -1.94529600 | -1.13558200 |
| H | -1.97623400 | -0.66799700 | -1.79292400 |
| H | -3.00572000 | -0.08711700 | 2.41518600 |
| H | -1.06715100 | 1.83911800 | -2.09730900 |
| H | 1.29056200 | 2.65880500 | -2.23320900 |
| H | 1.47883600 | 2.77185000 | 2.06178400 |
| H | -0.85726400 | 1.97310700 | 2.18146800 |
| H | 5.30381700 | 0.14938700 | -1.16484200 |
| H | 3.73297700 | 0.84677800 | -0.71519600 |
| H | 4.81885100 | 0.20623300 | 0.54210000 |
| H | 5.71177100 | -2.31221300 | -0.84107400 |
| H | 5.10155500 | -2.28330200 | 0.82291900 |
| H | 4.39286500 | -3.40214900 | -0.36703700 |
| H | 4.09163600 | -1.41655200 | -2.75640300 |
| H | 2.82151900 | -2.49803800 | -2.15254500 |
| H | 2.52938600 | -0.74150400 | -2.25437400 |
| H | 4.61699600 | 3.58145800 | 0.52340600 |
| H | 3.23641200 | 4.15092300 | 1.49981800 |
| H | 3.65867000 | 2.41374100 | 1.47423000 |
| C | -4.79955600 | -1.21864300 | 0.30350300 |
| C | -5.97273900 | -1.07895800 | -0.42627600 |
| C | -5.77126900 | 0.01638800 | -1.25867400 |

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|---|---|---|---|
| N | -4.54269000 | 0.48384100 | -1.03133300 |
| H | -4.07205900 | 1.30347100 | -1.40987300 |
| H | -4.50527200 | -1.93944600 | 1.05326700 |
| H | -6.85775400 | -1.69009800 | -0.35494900 |
| H | -6.41502700 | 0.49815700 | -1.97976100 |
| N | -3.95645500 | -0.24658000 | -0.07256700 |

**INT-2**

| | | | |
|---|---|---|---|
| C | -1.12766900 | -1.82763900 | 1.17405700 |
| C | -2.28149600 | -0.98136900 | 0.82799300 |
| C | -2.00278700 | 0.40600400 | 0.41639400 |
| C | -0.75670500 | 0.87278400 | 0.36482700 |
| C | 0.44556600 | 0.03861300 | 0.72951700 |
| C | 0.12384300 | -1.37190200 | 1.14245000 |
| O | 1.30354300 | 0.12005800 | -0.39475900 |
| C | 2.43678800 | -0.70232500 | -0.42684200 |
| C | 3.65196500 | -0.23077000 | 0.06596900 |
| C | 4.77919100 | -1.03257600 | -0.03251200 |
| C | 4.69834600 | -2.30026800 | -0.62351400 |
| C | 3.47624100 | -2.75960800 | -1.12450000 |
| C | 2.34608300 | -1.95002000 | -1.02623800 |
| N | -3.44602600 | -1.51057300 | 0.88624700 |
| C | -4.58471100 | -0.72178700 | 0.62960700 |
| O | -5.13586700 | -1.10374000 | -0.51426100 |
| O | -5.00247200 | 0.10932800 | 1.40415900 |
| C | -6.37904000 | -0.48204300 | -0.99234000 |
| C | -6.62388700 | -1.19680000 | -2.31361000 |
| C | -7.50791200 | -0.76353800 | -0.00893700 |
| C | -6.15639400 | 1.00827800 | -1.21884900 |
| O | 5.85348400 | -3.00420400 | -0.67108900 |

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|---|---|---|---|
| C | 5.81408200 | -4.28904400 | -1.27401100 |
| H | -1.34701500 | -2.85066100 | 1.46217900 |
| H | -2.83778400 | 1.04379400 | 0.14281900 |
| H | -0.54594000 | 1.89014200 | 0.04233700 |
| H | 0.96364600 | -2.00419700 | 1.41382800 |
| H | 3.72214600 | 0.75943400 | 0.50488300 |
| H | 5.73940700 | -0.69007300 | 0.33830200 |
| H | 3.39247200 | -3.73247900 | -1.59289400 |
| H | 1.39084000 | -2.28870300 | -1.41519100 |
| H | -7.53829300 | -0.81354700 | -2.77336300 |
| H | -5.78978400 | -1.02926300 | -3.00064100 |
| H | -6.73733600 | -2.27233700 | -2.15216100 |
| H | -8.45142800 | -0.42645800 | -0.44746800 |
| H | -7.58237500 | -1.83829800 | 0.18150000 |
| H | -7.35482900 | -0.24106400 | 0.93590900 |
| H | -7.03471600 | 1.42600700 | -1.71900800 |
| H | -6.00543900 | 1.53829900 | -0.27761400 |
| H | -5.28723700 | 1.16514100 | -1.86513200 |
| H | 6.82907000 | -4.68099100 | -1.21454900 |
| H | 5.13328100 | -4.95841800 | -0.73707000 |
| H | 5.50951300 | -4.22517100 | -2.32426400 |
| C | 1.23133800 | 0.36108400 | 3.16113400 |
| C | 1.90105800 | 1.37730900 | 3.82359800 |
| C | 2.19488300 | 2.32672900 | 2.84545300 |
| N | 1.72012800 | 1.89997700 | 1.67707100 |
| H | 0.80809300 | -0.56543300 | 3.52048400 |
| H | 2.14597100 | 1.41801900 | 4.87268800 |
| H | 2.71741300 | 3.27048800 | 2.90715000 |
| N | 1.14797300 | 0.69965100 | 1.86254900 |
| C | 2.53039000 | 4.27151400 | -0.93813000 |

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|---|---|---|---|
| C | 2.61503800 | 4.50278900 | -2.31996400 |
| C | 2.15008500 | 3.33562000 | -2.89909000 |
| N | 1.82835400 | 2.50313700 | -1.89499100 |
| H | 1.44797600 | 1.56491900 | -1.94697100 |
| H | 2.79260400 | 4.92219800 | -0.11549700 |
| H | 2.96441100 | 5.39017200 | -2.82387300 |
| H | 2.02730100 | 3.03986600 | -3.93026200 |
| N | 2.05064200 | 3.05366800 | -0.69481000 |
| H | 1.82524400 | 2.34984400 | 0.67423400 |

**INT-3**

| | | | |
|---|---|---|---|
| C | -1.16078500 | -1.84913300 | 1.04368800 |
| C | -2.30950500 | -0.97841300 | 0.74522300 |
| C | -2.02164400 | 0.42804900 | 0.41356200 |
| C | -0.77246900 | 0.89078000 | 0.40008200 |
| C | 0.42490300 | 0.04011600 | 0.74187500 |
| C | 0.09106900 | -1.39324500 | 1.05833300 |
| O | 1.28648800 | 0.15281300 | -0.39238800 |
| C | 2.42915000 | -0.65357300 | -0.42400100 |
| C | 3.59021200 | -0.26569300 | 0.24453000 |
| C | 4.72112800 | -1.06325300 | 0.15418800 |
| C | 4.70102700 | -2.24204200 | -0.60286200 |
| C | 3.53588200 | -2.61621400 | -1.27903600 |
| C | 2.39982100 | -1.81397900 | -1.18339700 |
| N | -3.47732600 | -1.50580900 | 0.77119100 |
| C | -4.61286700 | -0.69826500 | 0.57255800 |
| O | -5.22106700 | -1.06126600 | -0.54956900 |
| O | -4.98788400 | 0.13195700 | 1.37065000 |
| C | -6.47137100 | -0.41319300 | -0.96669500 |
| C | -6.78842000 | -1.11262100 | -2.28101300 |

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|---|---|---|---|
| C | -7.56209900 | -0.68119000 | 0.06281000 |
| C | -6.23165500 | 1.07472600 | -1.19259300 |
| O | 5.85557600 | -2.94937000 | -0.62403100 |
| C | 5.87312000 | -4.15349800 | -1.37559100 |
| H | -1.38546300 | -2.88855800 | 1.26033400 |
| H | -2.85239000 | 1.08362000 | 0.17218200 |
| H | -0.55616900 | 1.92595100 | 0.14673100 |
| H | 0.92594400 | -2.04696100 | 1.29269400 |
| H | 3.61131000 | 0.65381000 | 0.82121500 |
| H | 5.63842300 | -0.78697000 | 0.66342000 |
| H | 3.49919900 | -3.51889900 | -1.87645700 |
| H | 1.48543900 | -2.09012800 | -1.69933400 |
| H | -7.71518300 | -0.70945700 | -2.69691300 |
| H | -5.98272900 | -0.95536600 | -3.00347600 |
| H | -6.91444500 | -2.18718200 | -2.12214900 |
| H | -8.51731800 | -0.32376800 | -0.33222200 |
| H | -7.64828100 | -1.75582900 | 0.24916100 |
| H | -7.35837800 | -0.16883200 | 1.00356400 |
| H | -7.12143700 | 1.51154500 | -1.65477800 |
| H | -6.03359800 | 1.59555700 | -0.25501600 |
| H | -5.38594800 | 1.22063900 | -1.87177800 |
| H | 6.87486800 | -4.56654600 | -1.26007900 |
| H | 5.13752300 | -4.87006500 | -0.99416500 |
| H | 5.67883300 | -3.96223700 | -2.43648600 |
| C | 1.27107300 | 0.17407300 | 3.15167600 |
| C | 1.93517900 | 1.14966200 | 3.86520100 |
| C | 2.13959700 | 2.19039100 | 2.94198300 |
| N | 1.63255200 | 1.87798400 | 1.75486400 |
| H | 0.89796700 | -0.79672200 | 3.44227100 |
| H | 2.23127100 | 1.11218700 | 4.90177300 |

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|---|---|---|---|
| H | 2.63291700 | 3.14246400 | 3.08299200 |
| N | 1.11598200 | 0.64350400 | 1.89191100 |
| C | 2.82473100 | 4.15833300 | -0.92873500 |
| C | 2.87158600 | 4.35054000 | -2.30786600 |
| C | 2.22190900 | 3.25233100 | -2.85717700 |
| N | 1.82300300 | 2.47141400 | -1.84930500 |
| H | 1.33613100 | 1.57733600 | -1.85564400 |
| H | 3.20017900 | 4.75836200 | -0.11294300 |
| H | 3.31873000 | 5.17581800 | -2.83780700 |
| H | 2.02207300 | 2.97442600 | -3.88109800 |
| N | 2.18797300 | 3.01274100 | -0.68447300 |
| H | 1.94290400 | 2.55576200 | 0.24692200 |

**INT-4**

| | | | |
|---|---|---|---|
| C | -1.37491800 | -1.18722200 | -1.73440100 |
| C | -2.30707900 | -0.64210600 | -0.80911600 |
| C | -1.76281800 | 0.20043400 | 0.19786400 |
| C | -0.39776300 | 0.47070500 | 0.26252200 |
| C | 0.46747000 | -0.08935200 | -0.66824600 |
| C | -0.01818600 | -0.92222400 | -1.67319900 |
| O | 1.84214000 | 0.22591800 | -0.66150000 |
| C | 2.45664000 | -1.97171500 | 0.14603700 |
| C | 3.43711700 | -2.80927600 | -0.20470900 |
| C | 4.76174400 | -2.29491000 | -0.49184600 |
| C | 5.05964700 | -0.88586500 | -0.43808600 |
| C | 4.07268700 | -0.03725500 | -0.11508000 |
| N | -3.61893800 | -0.99620400 | -1.01301300 |
| C | -4.57809000 | -0.53665700 | -0.19983100 |
| O | -5.79449400 | -1.02465500 | -0.62841500 |
| O | -4.51606900 | 0.20057800 | 0.79352500 |

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|---|---|---|---|
| C | -7.01328300 | -0.68448300 | 0.05770400 |
| C | -8.07999100 | -1.42455900 | -0.74648000 |
| C | -7.00290500 | -1.20322100 | 1.49530600 |
| C | -7.27923000 | 0.81961200 | -0.00000800 |
| O | 5.62260700 | -3.18549400 | -0.80443900 |
| C | 6.99905700 | -2.84532800 | -1.13205500 |
| H | -1.76564600 | -1.83186500 | -2.51626600 |
| H | -2.42881600 | 0.64304100 | 0.92379600 |
| H | -0.01254700 | 1.12926400 | 1.03704300 |
| H | 0.67195200 | -1.34972800 | -2.39558600 |
| H | 1.45674800 | -2.33676600 | 0.36232000 |
| H | 3.28566200 | -3.87926900 | -0.29246400 |
| H | 6.05452100 | -0.52598900 | -0.66842400 |
| H | 4.24628200 | 1.03552600 | -0.07633000 |
| H | -9.07152200 | -1.24515100 | -0.32108100 |
| H | -8.07868300 | -1.08241900 | -1.78575500 |
| H | -7.88542700 | -2.50124900 | -0.73684400 |
| H | -7.99415100 | -1.07489400 | 1.94188900 |
| H | -6.76110300 | -2.27121100 | 1.50242000 |
| H | -6.26716300 | -0.66971200 | 2.09652800 |
| H | -8.28070000 | 1.03325500 | 0.38714400 |
| H | -6.54328800 | 1.36801800 | 0.58751700 |
| H | -7.23427000 | 1.16498900 | -1.03819700 |
| H | 7.47516400 | -3.79963800 | -1.33878800 |
| H | 7.00659800 | -2.20470300 | -2.01406900 |
| H | 7.45968600 | -2.35650500 | -0.27349500 |
| C | 2.18011100 | -0.75635400 | 2.73360200 |
| C | 2.02897200 | 0.15307000 | 3.75573600 |
| C | 2.18392700 | 1.41248100 | 3.14366400 |
| N | 2.42158000 | 1.28675200 | 1.84529400 |

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|---|---|---|---|
| H | 2.15271000 | 2.41448100 | 0.55525400 |
| H | 2.14790600 | -1.83636700 | 2.72517800 |
| H | 1.82804300 | -0.06063600 | 4.79377800 |
| H | 2.12567400 | 2.39731200 | 3.58666500 |
| N | 2.40652400 | -0.03938800 | 1.60412200 |
| C | 1.69378300 | 4.45958000 | 0.03482900 |
| C | 1.46995400 | 5.05311100 | -1.20491600 |
| C | 1.59459500 | 4.02823300 | -2.13446700 |
| N | 1.87501400 | 2.90565500 | -1.46688000 |
| H | 2.02093400 | 1.95862400 | -1.80791100 |
| H | 1.69700400 | 4.87195400 | 1.03297300 |
| H | 1.24530500 | 6.08862600 | -1.40258300 |
| H | 1.50047300 | 4.01829700 | -3.20990900 |
| N | 1.93344800 | 3.16193100 | -0.15758600 |
| C | 2.67385600 | -0.48324600 | 0.23655900 |

**INT-5**

| | | | |
|---|---|---|---|
| C | 0.22758100 | 0.18504200 | -1.57324200 |
| C | 1.50441000 | 0.29527300 | -0.84760300 |
| C | 1.47365400 | 0.91462500 | 0.48984500 |
| C | 0.33390600 | 1.36391900 | 1.01298100 |
| C | -0.99114700 | 1.26887200 | 0.30025700 |
| C | -0.92175100 | 0.61768200 | -1.05604900 |
| O | -1.88936900 | 0.66577200 | 1.20313100 |
| C | -2.73931400 | -0.34125800 | 0.74556100 |
| C | -4.04621800 | -0.03189900 | 0.37610400 |
| C | -4.89779500 | -1.05090200 | -0.02332800 |
| C | -4.44791900 | -2.37776400 | -0.05633900 |
| C | -3.13498900 | -2.67831200 | 0.31832000 |
| C | -2.28345400 | -1.65071400 | 0.72186400 |

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|---|---|---|---|
| N | 2.55541500 | -0.16248100 | -1.41756400 |
| C | 3.80727000 | -0.02282300 | -0.78781700 |
| O | 4.16704300 | -1.18083600 | -0.24998200 |
| O | 4.45325600 | 0.99945700 | -0.83007000 |
| C | 5.47351400 | -1.32958200 | 0.40704500 |
| C | 5.45430900 | -2.78088300 | 0.86517000 |
| C | 6.58995900 | -1.09748100 | -0.60313300 |
| C | 5.55855100 | -0.38822200 | 1.60222000 |
| O | -5.35534200 | -3.29835900 | -0.46135300 |
| C | -4.93852300 | -4.65450300 | -0.50453600 |
| H | 0.26823900 | -0.26625400 | -2.55933000 |
| H | 2.40165900 | 0.99215900 | 1.04904500 |
| H | 0.29127200 | 1.81216500 | 2.00192000 |
| H | -1.85636200 | 0.54895400 | -1.60458100 |
| H | -4.39132400 | 0.99669900 | 0.40441700 |
| H | -5.92145600 | -0.84020400 | -0.31452300 |
| H | -2.76690600 | -3.69681900 | 0.30409700 |
| H | -1.26153600 | -1.86568000 | 1.01897900 |
| H | 6.38878100 | -3.01445000 | 1.38159800 |
| H | 4.62159600 | -2.95469400 | 1.55230700 |
| H | 5.35048500 | -3.45207200 | 0.00817600 |
| H | 7.54551700 | -1.36033000 | -0.14056000 |
| H | 6.44454300 | -1.73760200 | -1.47836900 |
| H | 6.63059900 | -0.05575900 | -0.92281600 |
| H | 6.47106100 | -0.60917000 | 2.16320600 |
| H | 5.58577200 | 0.65590600 | 1.28803900 |
| H | 4.70277900 | -0.54418100 | 2.26628300 |
| H | -5.80059100 | -5.22446600 | -0.85027900 |
| H | -4.10699900 | -4.79245300 | -1.20430900 |
| H | -4.64138100 | -5.01021900 | 0.48801700 |

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|---|---|---|---|
| C | -1.65893800 | 4.73965900 | -0.62216900 |
| C | -0.97524700 | 3.57924800 | -0.80219500 |
| C | -2.45442400 | 3.25275100 | 0.81392900 |
| N | -2.56648500 | 4.50434300 | 0.38288300 |
| H | -3.23272800 | 5.17759000 | 0.74945900 |
| H | -1.58224500 | 5.69420700 | -1.11640500 |
| H | -0.17733300 | 3.31943500 | -1.48048100 |
| H | -3.03145600 | 2.78856600 | 1.59719400 |
| N | -1.49425700 | 2.66871200 | 0.09808200 |

**INT-6**

| | | | |
|---|---|---|---|
| C | -0.83178100 | -0.57513800 | -2.01898100 |
| C | -1.71792700 | -1.19911600 | -1.02237300 |
| C | -1.25814600 | -1.21983800 | 0.37967000 |
| C | -0.08703000 | -0.68814200 | 0.72954900 |
| C | 0.83762000 | -0.02198700 | -0.25746100 |
| C | 0.33839900 | -0.03637600 | -1.67884100 |
| O | 1.17381300 | 1.28775900 | 0.17134200 |
| C | 0.16755200 | 2.24541100 | 0.06635600 |
| C | 0.13690600 | 3.07679200 | -1.05291700 |
| C | -0.82427300 | 4.07089000 | -1.14018300 |
| C | -1.76138000 | 4.23938900 | -0.11144500 |
| C | -1.72067900 | 3.40772400 | 1.01059800 |
| C | -0.74789600 | 2.41080000 | 1.09528700 |
| N | -2.83516400 | -1.67433600 | -1.43094900 |
| C | -3.68164900 | -2.34537800 | -0.52818900 |
| O | -4.75670900 | -1.60438000 | -0.29354200 |
| O | -3.45934800 | -3.46331200 | -0.11983400 |
| C | -5.83174400 | -2.09801700 | 0.57813000 |
| C | -6.82474900 | -0.94448500 | 0.57055200 |

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|---|---|---|---|
| C | -6.45513300 | -3.35010900 | -0.02567600 |
| C | -5.28848700 | -2.33224600 | 1.98245000 |
| O | -2.66074800 | 5.23673500 | -0.29051200 |
| C | -3.62056100 | 5.44477100 | 0.73396000 |
| H | -1.18052200 | -0.57728100 | -3.04659200 |
| H | -1.89806800 | -1.67955200 | 1.12707300 |
| H | 0.26237000 | -0.69379200 | 1.75869300 |
| H | 0.99929400 | 0.41970100 | -2.41106000 |
| H | 0.87156700 | 2.94405600 | -1.84064000 |
| H | -0.86684800 | 4.73330700 | -1.99836000 |
| H | -2.42821000 | 3.52626800 | 1.82201400 |
| H | -0.69848000 | 1.77085100 | 1.97029000 |
| H | -7.68421500 | -1.19633600 | 1.19692400 |
| H | -6.35978500 | -0.03574500 | 0.96266600 |
| H | -7.17742900 | -0.74966400 | -0.44600000 |
| H | -7.34580000 | -3.61521800 | 0.55109100 |
| H | -6.75989100 | -3.15845000 | -1.05878200 |
| H | -5.76174800 | -4.19143300 | -0.00590800 |
| H | -6.12361800 | -2.54919000 | 2.65447400 |
| H | -4.59289600 | -3.17202400 | 2.00769400 |
| H | -4.78175600 | -1.43243000 | 2.34474000 |
| H | -4.23997900 | 6.27808000 | 0.40307600 |
| H | -4.24849000 | 4.55833500 | 0.87548200 |
| H | -3.13837200 | 5.70398900 | 1.68294400 |
| C | 3.64217900 | -2.31965900 | -0.33857300 |
| C | 2.30872200 | -2.07624900 | -0.45073300 |
| C | 3.33436200 | -0.17335600 | 0.02841400 |
| N | 4.25261600 | -1.12518600 | -0.04143500 |
| H | 5.32290000 | -0.97193800 | 0.11609400 |
| H | 4.19907800 | -3.23679700 | -0.44443100 |

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|---|---|---|---|
| H | 1.47357600 | -2.72280900 | -0.67292200 |
| H | 3.50549600 | 0.86811200 | 0.24482100 |
| N | 2.13995000 | -0.72611700 | -0.21508500 |
| C | 9.04698800 | -0.41520200 | -0.12028800 |
| C | 7.81004000 | -0.57901800 | -0.67821800 |
| C | 7.53731000 | -0.69477700 | 1.46105900 |
| N | 8.84894300 | -0.49228100 | 1.23511900 |
| H | 9.56417200 | -0.41024000 | 1.94729200 |
| H | 10.02301300 | -0.25563400 | -0.54970700 |
| H | 7.53309400 | -0.58346900 | -1.72183300 |
| H | 7.11406300 | -0.79227300 | 2.44926000 |
| N | 6.87787800 | -0.75250100 | 0.31936500 |

**INT-7**

| | | | |
|---|---|---|---|
| C | -0.82792400 | -0.58186200 | -2.01446500 |
| C | -1.71814600 | -1.20544500 | -1.02175400 |
| C | -1.26411200 | -1.22633700 | 0.38183600 |
| C | -0.09448300 | -0.69328000 | 0.73563200 |
| C | 0.83897400 | -0.02862600 | -0.24512400 |
| C | 0.33941500 | -0.04072400 | -1.66734400 |
| O | 1.15684400 | 1.28894300 | 0.18596300 |
| C | 0.14273000 | 2.23417200 | 0.07300300 |
| C | 0.10936800 | 3.06471600 | -1.04743600 |
| C | -0.86042800 | 4.04984000 | -1.14241000 |
| C | -1.80502000 | 4.21172300 | -0.11962600 |
| C | -1.76301400 | 3.38224900 | 1.00380600 |
| C | -0.78137000 | 2.39445800 | 1.09561500 |
| N | -2.83484600 | -1.68046900 | -1.43397600 |
| C | -3.68435500 | -2.34877200 | -0.53346700 |
| O | -4.75453300 | -1.60110900 | -0.29326700 |

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|---|---|---|---|
| O | -3.47117000 | -3.47028200 | -0.12949000 |
| C | -5.83182300 | -2.09184900 | 0.57631800 |
| C | -6.81773300 | -0.93211000 | 0.57474900 |
| C | -6.46409000 | -3.33721400 | -0.03238600 |
| C | -5.28978300 | -2.33597300 | 1.97949700 |
| O | -2.71258900 | 5.20104600 | -0.30562900 |
| C | -3.67939600 | 5.40220300 | 0.71331000 |
| H | -1.17125300 | -0.58688500 | -3.04395400 |
| H | -1.90665700 | -1.68837900 | 1.12566000 |
| H | 0.25001800 | -0.70062600 | 1.76651100 |
| H | 1.00277300 | 0.41476600 | -2.39791900 |
| H | 0.84972500 | 2.93763200 | -1.83082300 |
| H | -0.90402400 | 4.71038700 | -2.00203400 |
| H | -2.47626800 | 3.49556300 | 1.81102800 |
| H | -0.73148600 | 1.75664900 | 1.97216600 |
| H | -7.67829300 | -1.18111700 | 1.20078200 |
| H | -6.34667400 | -0.02799500 | 0.97031200 |
| H | -7.17002600 | -0.73058000 | -0.44064300 |
| H | -7.35645600 | -3.59869500 | 0.54343800 |
| H | -6.76776900 | -3.13914800 | -1.06462400 |
| H | -5.77639100 | -4.18325200 | -0.01646600 |
| H | -6.12583200 | -2.55193500 | 2.65072900 |
| H | -4.59849000 | -3.17940800 | 2.00022800 |
| H | -4.77822800 | -1.44066800 | 2.34617000 |
| H | -4.30457900 | 6.22943100 | 0.37791500 |
| H | -4.30030900 | 4.51054400 | 0.85327500 |
| H | -3.20471300 | 5.66727000 | 1.66452900 |
| C | 3.65887200 | -2.28574900 | -0.30459500 |
| C | 2.31402000 | -2.07344600 | -0.40279000 |
| C | 3.35513100 | -0.17068200 | 0.01008000 |

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|---|---|---|---|
| N | 4.29457500 | -1.09375500 | -0.04659800 |
| H | 5.88730100 | -0.86421900 | 0.16175100 |
| H | 4.20294200 | -3.21351000 | -0.40112800 |
| H | 1.48191000 | -2.73379800 | -0.59568300 |
| H | 3.49739800 | 0.88143000 | 0.19701400 |
| N | 2.13662400 | -0.72273500 | -0.19650200 |
| C | 9.09468400 | -0.44316000 | -0.12255100 |
| C | 7.88128100 | -0.62576200 | -0.71279900 |
| C | 7.56002900 | -0.59632100 | 1.46363800 |
| N | 8.86183000 | -0.42909900 | 1.23258900 |
| H | 9.56613000 | -0.31098200 | 1.95336300 |
| H | 10.08311600 | -0.32455300 | -0.53499100 |
| H | 7.60666300 | -0.69732200 | -1.75276800 |
| H | 7.09225300 | -0.62590300 | 2.43465700 |
| N | 6.94922300 | -0.71762600 | 0.29398000 |

**INT-8**

| | | | |
|---|---|---|---|
| C | -0.11801900 | -2.32144500 | -1.80206500 |
| C | -0.96784200 | -2.15866700 | -0.61301100 |
| C | -0.33846000 | -1.57670500 | 0.58983800 |
| C | 0.88376200 | -1.04793900 | 0.53901300 |
| C | 1.64011400 | -0.90639900 | -0.75280600 |
| C | 1.07271800 | -1.72816500 | -1.88124800 |
| O | 1.66527000 | 0.50147000 | -1.13808400 |
| C | 0.43864900 | 1.16305600 | -1.13964100 |
| C | -0.39982800 | 1.10304300 | -2.25203800 |
| C | -1.61908400 | 1.76465600 | -2.22271800 |
| C | -2.00183100 | 2.49584300 | -1.09080700 |
| C | -1.14364700 | 2.57812000 | 0.00995600 |
| C | 0.07498600 | 1.90247800 | -0.02202600 |

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|---|---|---|---|
| N | -2.20523200 | -2.47734600 | -0.71251100 |
| C | -3.06739400 | -2.20741000 | 0.36805100 |
| O | -3.83136900 | -1.17288000 | 0.03589300 |
| O | -3.12167900 | -2.86378300 | 1.38323700 |
| C | -4.74057200 | -0.55300900 | 1.00558900 |
| C | -5.36676600 | 0.57414600 | 0.19565800 |
| C | -5.80298900 | -1.54653200 | 1.45776800 |
| C | -3.91896700 | -0.00031200 | 2.16354000 |
| O | -3.21850900 | 3.09268800 | -1.15466000 |
| C | -3.64616700 | 3.83347400 | -0.02156200 |
| H | -0.53797800 | -2.87697800 | -2.63437400 |
| H | -0.89727300 | -1.58869400 | 1.52029200 |
| H | 1.33752700 | -0.59317000 | 1.41582000 |
| H | 1.67309300 | -1.78056300 | -2.78498600 |
| H | -0.09693500 | 0.54157000 | -3.12933200 |
| H | -2.29249500 | 1.72963800 | -3.07265700 |
| H | -1.41050800 | 3.15123400 | 0.88961500 |
| H | 0.74369900 | 1.94302400 | 0.83394400 |
| H | -6.01953900 | 1.17246800 | 0.83695100 |
| H | -4.59110400 | 1.22180200 | -0.22370100 |
| H | -5.96199000 | 0.16784200 | -0.62724400 |
| H | -6.56681000 | -1.01001200 | 2.02826500 |
| H | -6.28408500 | -2.00368200 | 0.58795500 |
| H | -5.37949600 | -2.33021200 | 2.08589300 |
| H | -4.56624600 | 0.59136600 | 2.81699700 |
| H | -3.47195100 | -0.80360400 | 2.75286900 |
| H | -3.12462500 | 0.64941900 | 1.78018500 |
| H | -4.64222800 | 4.20475800 | -0.26250900 |
| H | -3.70116000 | 3.20014600 | 0.87167300 |
| H | -2.97778500 | 4.67949400 | 0.17275100 |

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|---|---|---|---|
| C | 5.00441500 | -1.78840800 | 0.22276000 |
| C | 3.67560800 | -1.74439400 | 0.54199000 |
| C | 4.02252100 | -0.98815700 | -1.50286400 |
| N | 5.21166000 | -1.31076000 | -1.05319900 |
| H | 3.14257100 | 1.43628900 | -0.10553200 |
| H | 5.81966000 | -2.14080500 | 0.83865700 |
| H | 3.13522800 | -2.03853300 | 1.42790300 |
| H | 3.79151600 | -0.56517400 | -2.47098100 |
| N | 3.05026400 | -1.22493000 | -0.57199700 |
| C | 4.69869800 | 1.32838800 | 2.66469900 |
| C | 3.51472500 | 1.35244000 | 1.99601900 |
| C | 5.14032100 | 1.48492600 | 0.49905000 |
| N | 5.68489300 | 1.41240700 | 1.70923000 |
| H | 6.68396600 | 1.41920900 | 1.89043500 |
| H | 4.92348100 | 1.26233900 | 3.71641800 |
| H | 2.49686500 | 1.31062600 | 2.34925600 |
| H | 5.67071600 | 1.54057700 | -0.43787000 |
| N | 3.82191400 | 1.45369900 | 0.65752600 |

**INT-9**

| | | | |
|---|---|---|---|
| C | 0.29683400 | -1.15860400 | -1.59357900 |
| C | -0.86660400 | -1.06882000 | -0.69577100 |
| C | -0.60538400 | -1.04560400 | 0.75712400 |
| C | 0.63501800 | -1.14420500 | 1.23604100 |
| C | 1.83710200 | -1.26295900 | 0.34216300 |
| C | 1.54164100 | -1.25565700 | -1.12878500 |
| O | 2.85554800 | -0.35711800 | 0.70229400 |
| C | 2.55723000 | 0.99696700 | 0.52111800 |
| C | 1.99995900 | 1.72100500 | 1.57345700 |
| C | 1.75816200 | 3.07580000 | 1.41195700 |

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|---|---|---|---|
| C | 2.07346400 | 3.71120100 | 0.20290800 |
| C | 2.63956000 | 2.97807600 | -0.84383800 |
| C | 2.88138500 | 1.61456200 | -0.67714900 |
| N | -2.02520200 | -1.00366200 | -1.23593100 |
| C | -3.18131700 | -0.99814000 | -0.42917100 |
| O | -3.81282600 | 0.15630500 | -0.58083100 |
| O | -3.54295700 | -1.95586800 | 0.21712600 |
| C | -5.09210200 | 0.40798600 | 0.09831500 |
| C | -5.42441300 | 1.82939100 | -0.33238500 |
| C | -6.14369100 | -0.57055700 | -0.40874100 |
| C | -4.89892000 | 0.33261700 | 1.60779700 |
| O | 1.80125800 | 5.03607700 | 0.14587300 |
| C | 2.11953600 | 5.72004200 | -1.05668900 |
| H | 0.09003700 | -1.14030400 | -2.65866700 |
| H | -1.44836400 | -0.94388000 | 1.43341600 |
| H | 0.84156100 | -1.12695600 | 2.30366300 |
| H | 2.39673100 | -1.31231800 | -1.79737600 |
| H | 1.77222100 | 1.22522300 | 2.51155100 |
| H | 1.32918100 | 3.66591900 | 2.21478300 |
| H | 2.89987000 | 3.45097300 | -1.78277400 |
| H | 3.33441700 | 1.03744600 | -1.47696500 |
| H | -6.37508100 | 2.13388500 | 0.11240600 |
| H | -4.64526200 | 2.52201400 | -0.00230100 |
| H | -5.51161400 | 1.88910900 | -1.42072700 |
| H | -7.11880400 | -0.28188500 | -0.00632500 |
| H | -6.19813700 | -0.53311900 | -1.50074600 |
| H | -5.92414700 | -1.59162900 | -0.09483100 |
| H | -5.81013400 | 0.68468100 | 2.09944400 |
| H | -4.69682300 | -0.68771700 | 1.93577500 |
| H | -4.07166200 | 0.98043500 | 1.91380600 |

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|---|---|---|---|
| H | 1.82954800 | 6.75855200 | -0.89889300 |
| H | 3.19304200 | 5.66995700 | -1.26926400 |
| H | 1.56087600 | 5.31096200 | -1.90544100 |
| C | 1.77350800 | -3.80790600 | 0.38498800 |
| C | 2.54587800 | -4.55726500 | -0.40103800 |
| C | 3.80580800 | -2.82915900 | -0.04473900 |
| N | 2.53743700 | -2.60200500 | 0.69068700 |
| H | 2.75795500 | -2.55517600 | 1.70469000 |
| H | 0.78211600 | -3.93438000 | 0.79297100 |
| H | 2.31985300 | -5.52332500 | -0.82844100 |
| H | 4.57840500 | -2.07322300 | 0.00680900 |
| N | 3.80063800 | -3.93619500 | -0.65563600 |

**INT-10**

| | | | |
|---|---|---|---|
| C | -0.49900600 | 0.30823800 | -2.23860100 |
| C | -1.44226400 | 0.44168000 | -1.11571300 |
| C | -1.03515400 | -0.12132500 | 0.18638600 |
| C | 0.13141400 | -0.75036200 | 0.33147600 |
| C | 1.10588300 | -0.91086400 | -0.80073100 |
| C | 0.67090900 | -0.31600900 | -2.10786300 |
| O | 2.41594700 | -0.53595000 | -0.43444100 |
| C | 2.60612700 | 0.82417300 | -0.17151000 |
| C | 2.42870200 | 1.30318900 | 1.12492100 |
| C | 2.66801200 | 2.64178200 | 1.39178400 |
| C | 3.08568600 | 3.50359900 | 0.36803100 |
| C | 3.26991100 | 3.01093100 | -0.92712400 |
| C | 3.02716000 | 1.66323900 | -1.19162000 |
| N | -2.56001000 | 1.02027300 | -1.34833400 |
| C | -3.47602300 | 1.23448300 | -0.29840000 |
| O | -4.55198100 | 0.48727300 | -0.49798200 |

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|---|---|---|---|
| O | -3.29698800 | 2.04758700 | 0.57993300 |
| C | -5.69939600 | 0.56404600 | 0.41836300 |
| C | -6.66477500 | -0.45527400 | -0.16925000 |
| C | -5.26782000 | 0.15281700 | 1.82058200 |
| C | -6.29878500 | 1.96374900 | 0.37534500 |
| O | 3.29154600 | 4.79179500 | 0.73030400 |
| C | 3.71561100 | 5.69756100 | -0.27714000 |
| H | -0.80303000 | 0.74980600 | -3.18209800 |
| H | -1.70650500 | -0.00985200 | 1.03230600 |
| H | 0.44052400 | -1.17579000 | 1.28502400 |
| H | 1.36764100 | -0.40085900 | -2.93775900 |
| H | 2.11776500 | 0.62334200 | 1.91185800 |
| H | 2.54066500 | 3.04275800 | 2.39173100 |
| H | 3.60128300 | 3.65630700 | -1.73130800 |
| H | 3.17617000 | 1.26556000 | -2.19049600 |
| H | -7.57597500 | -0.48605000 | 0.43335200 |
| H | -6.93172200 | -0.18355600 | -1.19424700 |
| H | -6.21427600 | -1.45171900 | -0.17419800 |
| H | -6.15649000 | 0.05590600 | 2.45056300 |
| H | -4.76210500 | -0.81719600 | 1.78930400 |
| H | -4.60156600 | 0.89141900 | 2.26787800 |
| H | -7.23062400 | 1.96704100 | 0.94789500 |
| H | -5.62137900 | 2.70213100 | 0.80568600 |
| H | -6.52887200 | 2.24356100 | -0.65695600 |
| H | 3.82027700 | 6.66561900 | 0.21221400 |
| H | 4.68047600 | 5.39745700 | -0.70023500 |
| H | 2.97391800 | 5.77361200 | -1.07969000 |
| C | 0.14405400 | -3.18678000 | -1.42897900 |
| C | 0.50475600 | -3.84968400 | -2.52783100 |
| C | 2.32354600 | -2.78308900 | -2.02347000 |

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|---|---|---|---|
| N | 1.31486400 | -2.43176400 | -0.99707900 |
| H | 1.65553000 | -2.78582300 | -0.07536000 |
| H | -0.77110100 | -3.13091900 | -0.85936800 |
| H | -0.09482800 | -4.51920300 | -3.12703500 |
| H | 3.31206500 | -2.34951000 | -1.95177400 |
| N | 1.85793800 | -3.58824800 | -2.88086100 |
| C | 2.93236000 | -2.27435300 | 2.37392700 |
| C | 1.96203600 | -1.88365100 | 3.25638300 |
| C | 1.27505500 | -3.73512500 | 2.42262800 |
| N | 2.47285000 | -3.45442800 | 1.83474100 |
| H | 3.00641200 | -4.08770900 | 1.24817500 |
| H | 3.87411300 | -1.83748200 | 2.08098200 |
| H | 1.94579900 | -0.99673000 | 3.87440500 |
| H | 0.71203300 | -4.62513400 | 2.18014000 |
| N | 0.92830100 | -2.79732800 | 3.27395200 |

**INT-11**

| | | | |
|---|---|---|---|
| C | -0.64838200 | 0.38361700 | -2.22427100 |
| C | -1.60225000 | 0.28520700 | -1.10822400 |
| C | -1.14527900 | -0.39379400 | 0.12077100 |
| C | 0.07934400 | -0.91295800 | 0.20641200 |
| C | 1.08510600 | -0.81918400 | -0.90951100 |
| C | 0.58814700 | -0.10457400 | -2.13642000 |
| O | 2.29582500 | -0.19436300 | -0.41993400 |
| C | 2.24534000 | 1.18405700 | -0.17369000 |
| C | 1.77249300 | 1.65772700 | 1.04848700 |
| C | 1.78004200 | 3.02206500 | 1.29312600 |
| C | 2.25832000 | 3.91256500 | 0.32204300 |
| C | 2.73810800 | 3.42472200 | -0.89746700 |
| C | 2.72899100 | 2.05212700 | -1.14002800 |

| | | | |
|---|---|---|---|
| N | -2.77183600 | 0.77976700 | -1.27717000 |
| C | -3.69722600 | 0.77597700 | -0.21662200 |
| O | -4.69033800 | -0.05623300 | -0.50176400 |
| O | -3.60302200 | 1.49965800 | 0.74957700 |
| C | -5.82509900 | -0.21258900 | 0.41819400 |
| C | -6.68468300 | -1.25347900 | -0.28500300 |
| C | -5.33131300 | -0.73914700 | 1.76022700 |
| C | -6.57349800 | 1.10817700 | 0.54638600 |
| O | 2.22211600 | 5.22307500 | 0.65636200 |
| C | 2.69145100 | 6.15926200 | -0.30277900 |
| H | -1.00288900 | 0.87792400 | -3.12289400 |
| H | -1.83079700 | -0.46345300 | 0.96000200 |
| H | 0.42201700 | -1.42233400 | 1.10637700 |
| H | 1.29567400 | -0.03351600 | -2.95842800 |
| H | 1.40855500 | 0.96414000 | 1.80025100 |
| H | 1.41971700 | 3.42113300 | 2.23521400 |
| H | 3.12033300 | 4.09434700 | -1.65793200 |
| H | 3.10465700 | 1.65651900 | -2.07826100 |
| H | -7.57545200 | -1.45885600 | 0.31397100 |
| H | -6.99923900 | -0.89032200 | -1.26731900 |
| H | -6.12789100 | -2.18556800 | -0.41549400 |
| H | -6.19487700 | -0.99843900 | 2.37920100 |
| H | -4.73202600 | -1.64281500 | 1.61204600 |
| H | -4.73436100 | 0.00591200 | 2.28777500 |
| H | -7.49523600 | 0.93900700 | 1.11032900 |
| H | -5.97636900 | 1.85714300 | 1.06753000 |
| H | -6.84206300 | 1.48683200 | -0.44428900 |
| H | 2.56880600 | 7.14236400 | 0.15089200 |
| H | 3.74949900 | 5.99454600 | -0.53357700 |
| H | 2.10430300 | 6.10872800 | -1.22601000 |

| | | | |
|---|---|---|---|
| C | 0.81870600 | -3.32967100 | -1.17830500 |
| C | 1.62709500 | -4.29671900 | -1.70874000 |
| C | 2.73684700 | -2.46879900 | -1.86439900 |
| N | 1.54501500 | -2.16113800 | -1.26701500 |
| H | 3.07625100 | -1.17105900 | 0.73257900 |
| H | -0.17444900 | -3.35724400 | -0.75699600 |
| H | 1.41758600 | -5.35230700 | -1.80589900 |
| H | 3.48979800 | -1.71746100 | -2.05532200 |
| N | 2.82204500 | -3.75283000 | -2.12489600 |
| C | 3.00904900 | -1.35527100 | 2.81219300 |
| C | 2.27958400 | -2.35492900 | 3.31213000 |
| C | 2.91145200 | -3.15478100 | 1.39953000 |
| N | 3.46219600 | -1.79615400 | 1.50184600 |
| H | 4.49156500 | -1.78548700 | 1.39669800 |
| H | 3.28027700 | -0.37524500 | 3.17257600 |
| H | 1.76615000 | -2.39495100 | 4.26149400 |
| H | 3.11107700 | -3.74103000 | 0.50941100 |
| N | 2.22953300 | -3.46296600 | 2.42265000 |

**INT-12**

| | | | |
|---|---|---|---|
| C | 0.22905900 | -0.68982600 | 1.48876600 |
| C | 1.22374000 | -0.51835700 | 0.45816300 |
| C | 0.78164900 | -0.80291400 | -0.88218000 |
| C | -0.48372500 | -1.22588600 | -1.16048900 |
| C | -1.50789100 | -1.43336300 | -0.11257900 |
| C | -1.04160500 | -1.09492900 | 1.25388500 |
| O | -2.79383200 | -0.87526100 | -0.44011100 |
| C | -3.02042700 | 0.47456800 | -0.27884900 |
| C | -4.36849300 | 0.84115400 | -0.21197400 |
| C | -4.72605900 | 2.17296100 | -0.09345900 |

| | | | |
|---|---|---|---|
| C | -3.73990900 | 3.16580900 | -0.02945300 |
| C | -2.39686100 | 2.79971300 | -0.09375600 |
| C | -2.03518800 | 1.45458600 | -0.22337400 |
| N | 2.43938800 | -0.10791100 | 0.88531700 |
| C | 3.46687900 | 0.06677200 | 0.01553200 |
| O | 4.55767400 | 0.49709600 | 0.71455500 |
| O | 3.50946900 | -0.10903900 | -1.20307100 |
| C | 5.80952400 | 0.76633300 | 0.04427000 |
| C | 6.72014700 | 1.21079100 | 1.18541900 |
| C | 6.36773100 | -0.50102200 | -0.60039200 |
| C | 5.65423400 | 1.90060500 | -0.96693700 |
| O | -4.18713300 | 4.44375600 | 0.09421700 |
| C | -3.20956800 | 5.46800500 | 0.15910200 |
| H | 0.54044700 | -0.46634400 | 2.50596400 |
| H | 1.48106400 | -0.66176400 | -1.69475600 |
| H | -0.80261700 | -1.42088000 | -2.18047200 |
| H | -1.76627300 | -1.20951000 | 2.05571000 |
| H | -5.12732100 | 0.06618500 | -0.25800700 |
| H | -5.76951600 | 2.46651000 | -0.04228900 |
| H | -1.61170300 | 3.54491200 | -0.04751300 |
| H | -0.98454800 | 1.19839400 | -0.27966700 |
| H | 7.71679400 | 1.44829100 | 0.80333000 |
| H | 6.31194200 | 2.10024900 | 1.67436000 |
| H | 6.81200800 | 0.41580600 | 1.93134100 |
| H | 7.38313100 | -0.31034800 | -0.96152300 |
| H | 6.41417200 | -1.30611500 | 0.14004100 |
| H | 5.74747800 | -0.82321800 | -1.43664300 |
| H | 6.63985400 | 2.19378200 | -1.34160400 |
| H | 5.03047100 | 1.59593300 | -1.80714400 |
| H | 5.19999300 | 2.77122500 | -0.48291600 |

| | | | |
|---|---|---|---|
| H | -3.75717400 | 6.40536000 | 0.25766800 |
| H | -2.55305500 | 5.33833100 | 1.02706800 |
| H | -2.60120100 | 5.49733500 | -0.75206500 |
| C | -1.15431600 | -3.98978600 | -0.30506100 |
| C | -1.90857800 | -5.12398800 | -0.01142800 |
| C | -3.16192300 | -4.65403700 | 0.35635600 |
| N | -3.13172800 | -3.31909200 | 0.28276600 |
| H | -3.87290300 | -2.63654300 | 0.41536300 |
| H | -0.12448300 | -3.87452600 | -0.61107200 |
| H | -1.58586900 | -6.15126100 | -0.06282300 |
| H | -4.06500700 | -5.16812000 | 0.65054200 |
| N | -1.92703300 | -2.91431600 | -0.13622400 |

**INT-13**

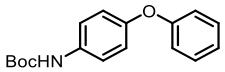
| | | | |
|---|---|---|---|
| C | -1.21964100 | -1.54374000 | 0.84926300 |
| C | -2.25178800 | -0.63368100 | 0.43286800 |
| C | -1.81434200 | 0.71573100 | 0.17651400 |
| C | -0.51522300 | 1.09435700 | 0.29064000 |
| C | 0.57517500 | 0.15150300 | 0.65229000 |
| C | 0.08954200 | -1.20983600 | 0.98095000 |
| O | 1.55030700 | 0.20717100 | -0.42812900 |
| C | 2.57148900 | -0.73619000 | -0.43243000 |
| C | 3.79755700 | -0.44897500 | 0.16903300 |
| C | 4.82513800 | -1.37902500 | 0.11093000 |
| C | 4.63701300 | -2.60230300 | -0.54461900 |
| C | 3.41064400 | -2.88318400 | -1.15381600 |
| C | 2.38259400 | -1.94287000 | -1.09479900 |
| N | -3.50139800 | -1.14929500 | 0.36766900 |
| C | -4.54067500 | -0.40516300 | -0.08479800 |
| O | -5.68604600 | -1.14092400 | 0.03162700 |

| | | | |
|---|---|---|---|
| O | -4.55219200 | 0.73522200 | -0.55253000 |
| C | -6.95946300 | -0.60318500 | -0.38816300 |
| C | -7.93008600 | -1.73946200 | -0.07804800 |
| C | -7.32932600 | 0.63138200 | 0.43186500 |
| C | -6.96286800 | -0.31429700 | -1.88816600 |
| O | 5.69987800 | -3.44462000 | -0.54237600 |
| C | 5.54451600 | -4.69430800 | -1.19561400 |
| H | -1.53158400 | -2.56096600 | 1.07265500 |
| H | -2.55348700 | 1.45034300 | -0.11275300 |
| H | -0.21623400 | 2.12247000 | 0.09736700 |
| H | 0.82451100 | -1.93865300 | 1.30728800 |
| H | 3.95279700 | 0.50538700 | 0.66240200 |
| H | 5.78862000 | -1.17450000 | 0.56619900 |
| H | 3.24470300 | -3.81844300 | -1.67467600 |
| H | 1.42637700 | -2.14412600 | -1.56707200 |
| H | -8.94868400 | -1.45317300 | -0.35422400 |
| H | -7.65579400 | -2.63858300 | -0.63769300 |
| H | -7.91081700 | -1.97611900 | 0.98990000 |
| H | -8.36074200 | 0.92232500 | 0.20964900 |
| H | -7.26158700 | 0.40236800 | 1.50032200 |
| H | -6.66727600 | 1.46692900 | 0.20538200 |
| H | -7.97807600 | -0.06170400 | -2.20976400 |
| H | -6.29648300 | 0.51328900 | -2.13074900 |
| H | -6.64134100 | -1.20407000 | -2.43909500 |
| H | 6.49359100 | -5.21711000 | -1.07840700 |
| H | 4.74466100 | -5.28610200 | -0.73687400 |
| H | 5.33200500 | -4.56219800 | -2.26223000 |
| C | 1.36521800 | 0.30272200 | 3.11433000 |
| C | 2.12623900 | 1.21139900 | 3.84140500 |
| C | 2.53993600 | 2.16634300 | 2.91791900 |

| | | | |
|---|---|---|---|
| N | 2.05115400 | 1.83519500 | 1.72072400 |
| H | 2.19126900 | 2.32088800 | 0.76393600 |
| H | 0.83171600 | -0.58553700 | 3.41818100 |
| H | 2.34631200 | 1.17924600 | 4.89632300 |
| H | 3.14934200 | 3.05109300 | 3.03237600 |
| N | 1.34990700 | 0.69967200 | 1.83563800 |
| C | 2.92488800 | 4.31614800 | -0.89792300 |
| C | 2.87673400 | 4.57994100 | -2.27669500 |
| C | 2.30787600 | 3.44592800 | -2.82879200 |
| N | 2.05761700 | 2.60251900 | -1.81335000 |
| H | 1.64442200 | 1.67483600 | -1.83208900 |
| H | 3.29530800 | 4.93742300 | -0.09428700 |
| H | 3.20753900 | 5.46612800 | -2.79531500 |
| H | 2.06839100 | 3.18106000 | -3.84781000 |
| N | 2.42530800 | 3.11152200 | -0.63104500 |

## 10. Characterization of diaryl ethers and products

### 10.1 Characterization of diaryl ethers

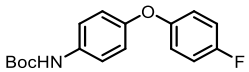



***tert*-butyl (4-phenoxyphenyl)carbamate (1a)**

Following the representative **Method 1**[1]**,** 10 mmol scale, white solid, yield: 35% (0.98 g). Flash silica gel chromatography (petroleum ether/ether acetate = 50:1, *v/v*).

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.30 (m, 4H), 7.11 – 7.06 (m, 1H), 7.02 – 6.96 (m, 4H), 6.49 (s, 1H), 1.55 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 157.9, 152.9, 152.3, 134.0, 129.6, 122.8, 120.0, 118.0, 80.5, 28.3.



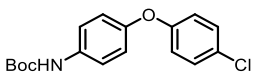

***tert*-butyl (4-(4-fluorophenoxy)phenyl)carbamate (1b)**

Following the representative **Method 1**[1]**,** 1 mmol scale, white solid, yield: 56% (0.174g), Flash silica gel chromatography (petroleum ether/ether acetate = 50:1, *v/v*).

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.31 (m, 2H), 7.06 – 6.98 (m, 2H), 6.98 – 6.92 (m, 4H), 6.45 (s, 1H), 1.54 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 158.5 (J $_{C\text{-}F}$ = 242.4 Hz), 153.6, 152.8 (J $_{C\text{-}F}$ = 10.1 Hz), 146.7, 133.9, 120.3, 119.5 (J $_{C\text{-}F}$ = 20.2Hz), 119.3, 116.2 (J $_{C\text{-}F}$ = 30.3Hz), 80.5, 28.3.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -120.8.

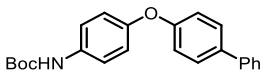



***tert*-butyl (4-(4-chlorophenoxy)phenyl)carbamate (1c)**

Following the representative **Method 1**[1]**,** 5 mmol scale, white solid, yield: 52% (0.83 g). Flash silica gel chromatography (petroleum ether/ether acetate = 50:1, *v/v*).

$^{1}$H NMR (400 MHz, Chloroform-d) δ 7.40 – 7.33 (m, 2H), 7.30 – 7.25 (m, 2H), 7.02 – 6.94 (m, 2H), 6.94 – 6.89 (m, 2H), 6.48 (s, 1H), 1.54 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 156.6, 152.9, 151.9, 134.4, 129.6, 127.7, 120.0, 119.2, 80.6, 28.3.

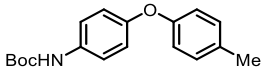



***tert*-butyl (4-([1,1'-biphenyl]-4-yloxy)phenyl)carbamate (1d)**

Following the representative **Method 1**[1]**,** 5 mmol scale, white solid, yield: 23% (0.42 g). Flash silica gel chromatography (petroleum ether/ether acetate = 50:1, *v/v*).

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.52 (m, 4H), 7.49 – 7.41 (m, 2H), 7.41 – 7.32 (m, 3H), 7.07 – 7.02 (m, 4H), 6.49 (s, 1H), 1.55 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 157.5, 153.0, 140.6, 135.9, 134.2, 128.8, 128.4, 127.0, 126.9, 120.1, 118.2, 28.4.

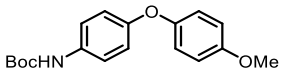



***tert*-butyl (4-(p-tolyloxy)phenyl)carbamate (1e)**

Following the representative **Method 1**[1]**,** 5 mmol scale, white solid, yield: 34% (0.51 g). Flash silica gel chromatography (petroleum ether/ether acetate = 45:1, *v/v*).

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.29 (m, 2H), 7.16 – 7.10 (m, 2H), 6.99 – 6.93 (m, 2H), 6.91 – 6.86 (m, 2H), 6.44 (s, 1H), 2.34 (s, 3H), 1.54 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.4, 153.0, 133.6, 132.4, 130.1, 120.4, 119.4, 118.3, 77.0, 28.3, 20.6.

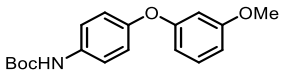



***tert*-butyl (4-(4-methoxyphenoxy)phenyl)carbamate (1f)**

Following the representative **Method 1**[1]**,** 5 mmol scale, white solid, yield: 73% (0.69 g). Flash silica gel chromatography (petroleum ether/ether acetate = 30:1, *v/v*).

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.29 (m, 2H), 6.99 – 6.85 (m, 6H), 6.45 (s, 1H), 3.81 (s, 3H), 1.53 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.6, 153.8, 150.8, 133.2, 120.0, 118.6, 114.8, 55.6, 28.3.

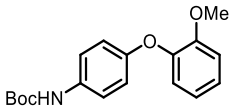



***tert*-butyl (4-(3-methoxyphenoxy)phenyl)carbamate (1g)**

Following the representative **Method 3**[3]**,** 5 mmol scale, white solid, yield: 36% (0.60 g). Flash silica gel chromatography (petroleum ether/ether acetate = 30:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.5 Hz, 2H), 7.24 – 7.14 (m, 1H), 7.03 – 6.94 (m, 2H), 6.67 – 6.58 (m, 1H), 6.58 – 6.52 (m, 2H), 6.50 (s, 1H), 3.79 (s, 3H), 1.54 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 160.9, 159.1, 152.9, 152.1, 134.1, 130.0, 120.1, 110.1, 108.5, 104.0, 80.5, 55.3, 28.3

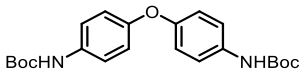



***tert*-butyl (4-(2-methoxyphenoxy)phenyl)carbamate (1h)**

Following the representative **Method 3**[3]**,** 5 mmol scale, white solid, yield:58% (0.94 g). Flash silica gel chromatography (petroleum ether/ether acetate = 30:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.29 (m, 2H), 7.15 – 7.08 (m, 1H), 7.03 – 6.99 (m, 1H), 6.96 – 6.89 (m, 4H), 6.44 (s, 1H), 3.87 (s, 3H), 1.53 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 153.2, 153.0, 151.0, 145.8, 133.3, 124.2, 121.0, 120.0, 118.3, 112.6, 55.9, 28.3.

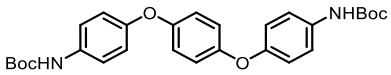



**di-*tert*-butyl (oxybis(4,1-phenylene))dicarbamate (1i)**

Following the representative **Method 1**[1]**,** 5 mmol scale, tetrahydrofuran as solvent, sodium bicarbonate as base, white solid, yield: 99% (1.9 g). Flash silica gel chromatography (petroleum ether/ether acetate = 20:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.29 (m, 4H), 6.96 – 6.89 (m, 4H), 6.51 (s, 2H), 1.53 (s, 18H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 153.1, 153.0, 146.7, 133.6, 119.1, 85.2, 80.4, 28.3.

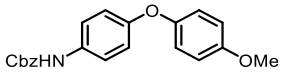



**di-*tert*-butyl ((1,4-phenylenebis(oxy))bis(4,1-phenylene))dicarbamate (1j)**

Following the representative **Method 1**[1]**,** 3 mmol scale, tetrahydrofuran as solvent, sodium bicarbonate as base, white solid, yield: 37% (0.55 g). Flash silica gel chromatography (petroleum ether/ether acetate = 20:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 8.5 Hz, 4H), 7.00 – 6.93 (m, 8H), 6.45 (s, 2H), 1.54 (s, 18H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 153.0, 133.7, 120.4, 119.6, 119.3, 80.7, 28.3.

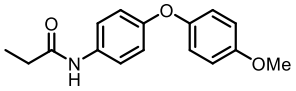



**benzyl (4-(4-methoxyphenoxy)phenyl)carbamate (1m)**

Following the representative **Method 1**[1]**,** 2 mmol scale, white solid, yield: 34% (0.23 g). Flash silica gel chromatography (petroleum ether/ether acetate = 10:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.36 (m, 5H), 7.35 – 7.30 (m, 2H), 7.01 – 6.85 (m, 6H), 6.65 (s, 1H), 5.22 (s, 2H), 3.82 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.7, 150.6, 136.0, 128.6, 128.3, 128.3, 120.2, 118.5, 114.8, 67.0, 55.6.

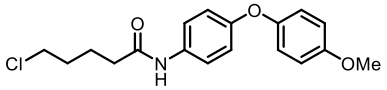



***N*-(4-(4-methoxyphenoxy)phenyl)propionamide (1n)**

Following the representative **Method 2**[2]**,** 2 mmol scale, white solid, yield: 89% (0.48 g). Flash silica gel chromatography (petroleum ether/ether acetate = 4:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.42 (m, 2H), 7.00 – 6.85 (m, 6H), 6.41 (s, 1H), 3.82 (s, 3H), 2.44 – 2.36 (m, 2H), 1.29 – 1.24 (m, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.0, 133.7, 121.6, 120.3, 118.2, 114.8, 105.3, 55.6, 30.6, 9.7.

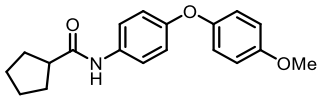


**5-chloro-*N*-(4-(4-methoxyphenoxy)phenyl)pentanamide (1o)**

Following the representative **Method 2**[2]**,** 2 mmol scale, white solid, yield: 40% (0.27 g). Flash silica gel chromatography (petroleum ether/ether acetate = 4:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.42 (m, 2H), 7.22 (s, 1H), 7.00 – 6.87 (m, 6H), 3.82 (s, 3H), 3.62 – 3.57 (m, 2H), 2.45 – 2.37 (m, 2H), 1.95 – 1.84 (m, 4H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.5, 132.5, 121.6, 120.4, 118.2, 114.8, 55.6, 44.6, 36.5, 31.9, 22.8.

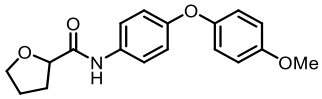



***N*-(4-(4-methoxyphenoxy)phenyl)cyclopentanecarboxamide (1p)**

Following the representative **Method 2**[2]**,** 2 mmol scale, white solid, yield: 53% (0.33 g). Flash silica gel chromatography (petroleum ether/ether acetate = 8:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.44 (m, 2H), 7.20 (s, 1H), 7.02 – 6.80 (m, 6H), 3.82 (s, 3H), 2.74 – 2.62 (m, 1H), 2.00 – 1.87 (m, 4H), 1.85 – 1.74 (m, 2H), 1.70 – 1.60 (m, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 174.5, 155.7, 154.6, 133.0, 121.4, 120.3, 118.3, 114.8, 55.6, 46.7, 30.5, 26.0.

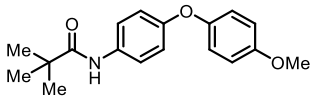



***N*-(4-(4-methoxyphenoxy)phenyl)tetrahydrofuran-2-carboxamide (1q)**

Following the representative **Method 2**[2]**,** 3 mmol scale, white solid, yield: 43% (0.41 g). Flash silica gel chromatography (petroleum ether/ether acetate = 8:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 7.56 – 7.45 (m, 2H), 7.00 – 6.91 (m, 4H), 6.91 – 6.86 (m, 2H), 4.52 – 4.44 (m, 1H), 4.11 – 4.02 (m, 1H), 4.01 – 3.93 (m, 1H), 3.82 (s, 3H), 2.44 – 2.32 (m, 1H), 2.27 – 2.13 (m, 1H), 2.07 – 1.89 (m, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.1, 155.7, 154.9, 150.5, 132.1, 121.3, 120.3, 118.3, 114.8, 78.6, 69.7, 30.2, 25.6.

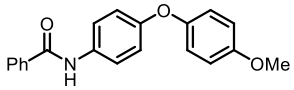


***N*-(4-(4-methoxyphenoxy)phenyl)pivalamide (1r)**

Following the representative **Method 2**[2]**,** 3 mmol scale, white solid, yield: 54% (0.33 g). Flash silica gel chromatography (petroleum ether/ether acetate = 5:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 9.0 Hz, 2H), 7.30 (s, 1H), 7.00 – 6.92 (m, 4H), 6.89 (d, *J* = 9.0 Hz, 2H), 3.82 (s, 3H), 1.33 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 176.5, 155.7, 154.7, 150.6, 132.8, 121.8, 120.3, 118.3, 114.8, 55.6, 39.5, 27.6.

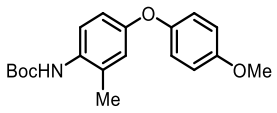


***N*-(4-(4-methoxyphenoxy)phenyl)benzamide (1s)**

Following the representative **Method 2**[2]**,** 5 mmol scale, white solid, yield: 33% (0.32 g). Flash silica gel chromatography (petroleum ether/ether acetate = 10:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.86 (m, 2H), 7.82 (s, 1H), 7.62 – 7.53 (m, 3H), 7.55 – 7.46 (m, 2H), 7.05 – 6.95 (m, 4H), 6.94 – 6.87 (m, 2H), 3.83 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.8, 155.1, 150.4, 134.9, 132.6, 131.8, 128.8, 127.0, 122.0, 120.5, 118.3, 114.8, 55.7.

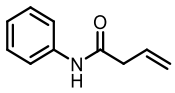


***tert*-butyl (4-(4-methoxyphenoxy)-2-methylphenyl)carbamate (1t)**

Following the representative **Method 3**[3]**,** 5 mmol scale, white solid, yield: 27% (0.46 g). Flash silica gel chromatography (petroleum ether/ether acetate = 30:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 6.98 – 6.94 (m, 2H), 6.92 – 6.85 (m, 2H), 6.83 – 6.77 (m, 2H), 6.14 (s, 1H), 3.82 (s, 3H), 2.23 (s, 3H), 1.54 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 157.9, 152.9, 152.3, 131.0, 120.2, 119.7, 116.1, 114.7, 55.6, 28.3, 17.9.

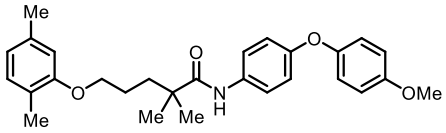


***N*-phenylbut-3-enamide (1u)**

Following the representative **Method 1**[1]**,** 5 mmol scale, white solid, yield: 97% (0.86 g). Flash silica gel chromatography (petroleum ether/ether acetate = 30:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.1 Hz, 2H), 7.37 – 7.30 (m, 2H), 7.13 – 7.06 (m, 1H), 6.66 (s, 1H), 6.07 – 5.92 (m, 1H), 5.45 – 5.35 (m, 1H), 5.32 – 5.25 (m, 1H), 4.74 – 4.66 (m, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 173.6, 136.4, 135.0, 130.4, 129.8, 119.2, 116.8, 37.2.

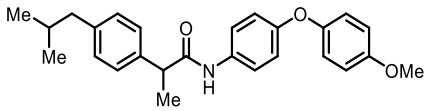


**5-(2,5-dimethylphenoxy)-*N*-(4-(4-methoxyphenoxy)phenyl)-2,2-dimethylpentanamide (1v)**

Following the representative **Method 2**[2]**,** 5 mmol scale, white solid, yield: 37% (0.82 g). Flash silica gel chromatography (petroleum ether/ether acetate = 10:1, *v/v*).

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.42 (m, 2H), 7.33 (s, 1H), 7.02 (d, *J* = 7.5 Hz, 1H), 7.00 – 6.87 (m, 6H), 6.68 (d, *J* = 7.5 Hz, 1H), 6.63 (s, 1H), 4.00 – 3.94 (m, 2H), 3.83 (s, 3H), 2.32 (s, 3H), 2.19 (s, 3H), 1.89 – 1.74 (m, 4H), 1.36 (s, 6H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 175.6, 156.8, 155.7, 154.8, 150.5, 136.5, 132.6, 130.3, 123.5, 121.9, 120.8, 120.3, 118.3, 114.8, 112.1, 67.8, 55.6, 42.7, 37.7, 25.6, 25.1, 21.4, 15.8.



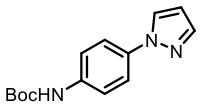
**2-(4-isobutylphenyl)-*N*-(4-(4-methoxyphenoxy)phenyl)propenamide (1w)**

Following the representative **Method 2**[2]**,** 5 mmol scale, white solid, yield: 64% (1.3 g). Flash silica gel chromatography (petroleum ether/ether acetate = 10:1, *v/v*).

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.33 (m, 2H), 7.31 – 7.28 (m, 1H), 7.20 – 7.15 (m, 2H), 7.07 (s, 1H), 6.97 – 6.91 (m, 2H), 6.91 – 6.84 (m, 4H), 3.81 (s, 3H), 3.74 – 3.67 (m, 1H), 2.49 (d, *J* = 7.2 Hz, 2H), 1.94 – 1.82 (m, 1H), 1.61 (d, *J* = 7.2 Hz, 3H), 0.97 – 0.89 (m, 6H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.5, 155.7, 154.7, 150.5, 141.1, 138.0, 132.7, 129.8, 127.4, 121.4, 120.2, 118.2, 114.8, 55.6, 47.6, 45.0, 30.2, 22.4, 18.5.

## 10.2 Characterization of products

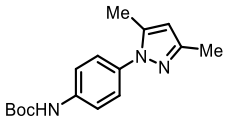



***tert*-butyl (4-(1*H*-pyrazol-1-yl)phenyl)carbamate (3)**

Following the representative **Condition A**, white solid, yield: 65% (33.6 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 15:1, *v/v*), reported compound[22].

**$^{1}$H NMR** (400 MHz,$CDCl_3$) δ 7.87 (d, *J* = 1.9 Hz, 1H), 7.72 (d, *J* = 1.9 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.4 Hz, 2H), 6.75 (s, 1H), 6.46 (t, *J* = 1.9 Hz, 1H), 1.54 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.7, 140.7, 136.9, 135.4, 126.8, 120.0, 119.2, 107.3, 80.7, 28.3.



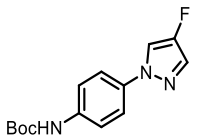

***tert*-butyl (4-(3,5-dimethyl-1*H*-pyrazol-1-yl)phenyl)carbamate (4)**

Following the representative **Condition A**, white oil: 50% (28.5 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 8:1, *v/v*).

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.3 Hz, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 6.73 (s, 1H), 6.00 (s, 1H), 2.32 (s, 3H), 2.27 (s, 3H), 1.54 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.7, 148.6, 139.7, 137.8, 134.5, 125.6, 118.8, 106.6, 80.8, 28.3, 13.4, 12.2.

**ESI HRMS** for [$C_{16}H_{21}N_3O_2$+$H^+$] calculated: 288.1707, found: 288.1711.




***tert*-butyl (4-(4-fluoro-1*H*-pyrazol-1-yl)phenyl)carbamate (5)**

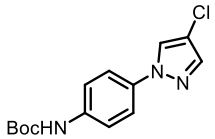
Following the representative **Condition A** with the following change: N-nucleophile (1.6 mmol), 5.0 mA, 8 h. White solid: 82% (45.5 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 25:1, *v/v*).

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 7.76 (d, $J$ = 4.7 Hz, 1H), 7.57 – 7.52 (m, 3H), 7.47 (d, $J$ = 8.7 Hz, 2H), 6.63 (s, 1H), 1.55 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.6, 151.0 (d, $J_{C\text{-}F}$ = 249.5 Hz), 137.2, 135.5, 128.1 (d, $J_{C\text{-}F}$ = 14.1 Hz), 119.6, 119.2, 113.0 (d, $J_{C\text{-}F}$ = 28.3 Hz), 80.9, 28.3.

**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -175.3.

**ESI HRMS** for [$C_{14}H_{16}FN_3O_2$+$H^+$] calculated: 278.1299, found: 278.1306.



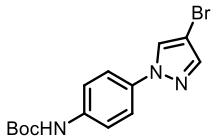

***tert*-butyl (4-(4-chloro-1*H*-pyrazol-1-yl)phenyl)carbamate (6)**

Following the representative **Condition A** with the following change: N-nucleophile (1.6 mmol), 5.0 mA, 8h. White solid: 78% (45.9 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 25:1, *v/v*).

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.63 (s, 1H), 7.56 (d, $J$ = 9.0 Hz, 2H), 7.48 (d, $J$ = 8.9 Hz, 2H), 6.62 (s, 1H), 1.55 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.6, 139.1, 137.4, 135.1, 124.8, 119.8, 119.2, 112.1, 80.9, 28.3.

**ESI HRMS** for [$C_{14}H_{16}ClN_3O_2$+$H^+$] calculated: 294.1004, found: 294.0996.



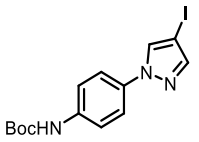

***tert*-butyl (4-(4-bromo-1*H*-pyrazol-1-yl)phenyl)carbamate (7)**

Following the representative **Condition A** with the following change: N-nucleophile (1.6 mmol), 5.0 mA, 4 h. White solid: 66% (44.9 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 25:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.66 (s, 1H), 7.57 (d, *J* = 9.0 Hz, 2H), 7.48 (d, *J* = 9.0 Hz, 2H), 6.62 (s, 1H), 1.55 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.6, 141.2, 137.4, 135.0, 126.9, 119.9, 119.2, 95.3, 80.9, 28.3.

**ESI HRMS** for [$C_{14}H_{16}BrN_3O_2$+$H^+$] calculated: 338.0499, found: 338.0490.



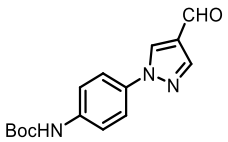

***tert*-butyl (4-(4-iodo-1*H*-pyrazol-1-yl)phenyl)carbamate (8)**

Following the representative **Condition A** with the following change: N-nucleophile (1.6 mmol), 5.0 mA, 8 h. White solid: 66% (50.7 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 25:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.71 (s, 1H), 7.57 (d, *J* = 8.7 Hz, 2H), 7.47 (d, *J* = 8.7 Hz, 2H), 6.62 (s, 1H), 1.55 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.6, 145.6, 137.4, 134.9, 131.2, 119.9, 119.2, 80.9, 58.4, 28.3.

**ESI HRMS** for [$C_{14}H_{16}IN_3O_2$+$H^+$] calculated: 386.0360, found: 386.0351.



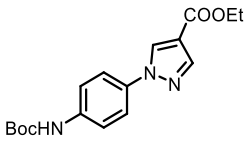

***tert*-butyl (4-(4-formyl-1*H*-pyrazol-1-yl)phenyl)carbamate (9)**

Following the representative **Condition A** with the following change: N-nucleophile (1.6 mmol), 8 h. White solid: 56% (32.4 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 5:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 9.97 (s, 1H), 8.39 (s, 1H), 8.16 (s, 1H), 7.64 (d, *J* = 8.6 Hz, 2H), 7.53 (d, *J* = 8.6 Hz, 2H), 6.74 (s, 1H), 1.55 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 184.0, 152.5, 141.5, 138.3, 134.2, 129.8, 125.5, 120.6, 119.2, 81.1, 28.3.

**ESI HRMS** for [$C_{15}H_{17}N_3O_3$+$H^+$] calculated: 288.1343, found: 288.1338.



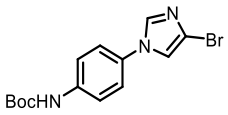

**ethyl 1-(4-((*tert*-butoxycarbonyl)amino)phenyl)-1*H*-pyrazole-4-carboxylate (10)**

Following the representative **Condition A** with the following change: N-nucleophile (1.6 mmol), 8 h. White solid: 61% (40.2 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 10:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.09 (s, 1H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 2H), 6.69 (s, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 1.55 (s, 9H), 1.39 (t, *J* = 7.1 Hz, 3H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 162.9, 152.5, 142.0, 137.9, 134.6, 129.8, 120.4, 119.1, 116.6, 81.0, 60.4, 28.3, 14.4.

**ESI HRMS** for [$C_{17}H_{21}N_3O_4$+$H^+$] calculated: 332.1605, found: 332.1601.



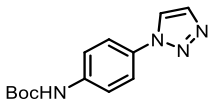

***tert*-butyl (4-(4-bromo-1*H*-imidazol-1-yl)phenyl)carbamate (11)**

Following the representative **Condition A** with the following change: 5.0 mA was instead of 3.5 mA, 8 h. White solid: 52% (35.0 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 2:1, *v/v*).

**$^1$H NMR** (400 MHz, DMSO-$d_6$) δ 9.66 (s, 1H), 7.98 (s, 1H), 7.62 (d, *J* = 8.9 Hz, 2H), 7.34 (d, *J* = 8.8 Hz, 2H), 7.15 (s, 1H), 1.49 (s, 9H).

**$^{13}$C NMR** (101 MHz, DMSO) δ 153.2, 140.7, 139.7, 137.9, 130.1, 129.4, 127.2, 118.9, 104.0, 80.0, 28.5.

**ESI HRMS** for [$C_{14}H_{16}BrN_3O_2$+$H^+$] calculated: 338.0499, found: 338.0501.



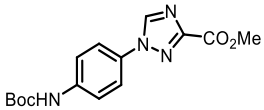

***tert*-butyl (4-(1*H*-1,2,3-triazol-1-yl)phenyl)carbamate (12)**

Following the representative **Condition A** with the following change: N-nucleophile (1.6 mmol), 5.0 mA, 8 h. White solid: 51% (26.6 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 2:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 1.1 Hz, 1H), 7.84 (d, *J* = 1.1 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 2H), 7.57 (d, *J* = 8.8 Hz, 2H), 6.98 (s, 1H), 1.54 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.5, 139.1, 134.2, 132.0, 121.7, 121.4, 119.1, 81.0, 28.3.

**ESI HRMS** for [$C_{13}H_{16}N_4O_2$+$H^+$] calculated: 261.1346, found: 261.1352.



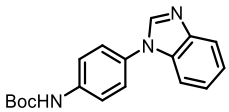

**methyl 1-(4-((*tert*-butoxycarbonyl)amino)phenyl)-1*H*-1,2,4-triazole-3-carboxylate (13)**

Following the representative **Condition A** with the following change: 7.0 mA, 8 h. White solid: 41% (25.9 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 5:4, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 8.5 Hz, 2H), 6.75 (s, 1H), 4.04 (s, 3H), 1.53 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 160.1, 155.1, 152.4, 142.0, 139.3, 131.2, 121.4, 119.1, 81.2, 52.9, 28.3.

**ESI HRMS** for [$C_{15}H_{18}N_4O_4$+$H^+$] calculated: 319.1401, found: 319.1395.



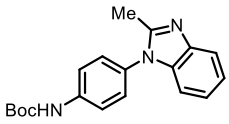

***tert*-butyl (4-(1*H*-benzo[*d*]imidazol-1-yl)phenyl)carbamate (14)**

Following the representative **Condition A** with the following change: N-nucleophile (1.6 mmol), 5.0 mA, 8 h. Light yellow oil: 34% (21.1 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 2:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.91 – 7.87 (m, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.52 – 7.47 (m, 1H), 7.44 (d, *J* = 8.3 Hz, 2H), 7.38 – 7.31 (m, 2H), 6.95 (s, 1H), 1.57 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.6, 143.7, 142.3, 138.4, 133.9, 130.9, 124.9, 123.6, 122.7, 120.5, 119.6, 110.4, 81.1, 28.3.

**ESI HRMS** for [$C_{18}H_{19}N_3O_2$+$H^+$] calculated: 310.1550, found: 310.1547.



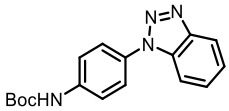

***tert*-butyl (4-(2-methyl-1*H*-benzo[*d*]imidazol-1-yl)phenyl)carbamate (15)**

Following the representative **Condition A** with the following change: N-nucleophile (1.6 mmol), 5.0 mA, 8 h. Light yellow oil: 33% (21.3 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 2:1, *v/v*).

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 8.3 Hz, 2H), 7.32 – 7.27 (m, 3H), 7.23 – 7.18 (m, 1H), 7.12 (d, *J* = 7.9 Hz, 1H), 6.96 (s, 1H), 2.51 (s, 3H), 1.57 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.6, 151.7, 142.3, 139.0, 136.5, 130.4, 127.7, 122.5, 122.3, 119.4, 118.8, 109.9, 81.1, 28.3, 14.3.

**ESI HRMS** for [$C_{19}H_{21}N_3O_2$+$H^+$] calculated: 324.1707, found: 324.1703.



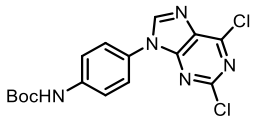

***tert*-butyl (4-(1*H*-benzo[*d*][1,2,3]triazol-1-yl)phenyl)carbamate (16)**

Following the representative **Condition A** with the following change: N-nucleophile (1.6 mmol), 5.0 mA, 8 h. Light yellow oil: 42% (26.3 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 9:1, *v/v*).

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.4 Hz, 1H), 7.71 (d, *J* = 8.7 Hz, 3H), 7.65 (d, *J* = 8.6 Hz, 2H), 7.59 – 7.53 (m, 1H), 7.49 – 7.42 (m, 1H), 6.83 (s, 1H), 1.57 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.5, 146.1, 139.0, 132.4, 131.7, 128.2, 124.4, 123.8, 120.1, 119.3, 110.3, 81.1, 28.3.

**ESI HRMS** for [$C_{17}H_{18}N_4O_2$+$H^+$] calculated: 311.1503, found: 311.1500.



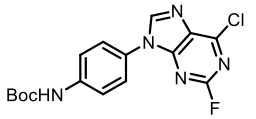
***tert*-butyl (4-(2,6-dichloro-9*H*-purin-9-yl)phenyl)carbamate (17)**

Following the representative **Condition A** with the following change: N-nucleophile (0.2 mmol), 7.0 mA, 4.5 h. White soild: 42% (32.0 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 2:1, *v/v*).

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.65 – 7.55 (m, 4H), 6.80 (s, 1H), 1.56 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 153.6, 152.6, 152.4, 152.3, 144.9, 139.5, 131.1, 127.9, 124.5, 119.4, 81.3, 28.3.

**ESI HRMS** for [$C_{16}H_{15}Cl_2N_5O_2$+$H^+$] calculated: 380.0676, found: 380.0677.



***tert*-butyl (4-(6-chloro-2-fluoro-9*H*-purin-9-yl)phenyl)carbamate (18)**

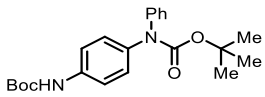
Following the representative **Condition A** with the following change: N-nucleophile (0.2 mmol), 7.0 mA, 4.5 h. Red oil: 33% (24.0 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 2:1, *v/v*).

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.62 (d, $J$ = 8.7 Hz, 2H), 7.57 (d, $J$ = 8.6 Hz, 2H), 6.85 (s, 1H), 1.55 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 157.7 (d, $J_{C\text{-}F}$ = 222.2 Hz), 153.3 (d, $J_{C\text{-}F}$ = 21.2 Hz), 153.1 (d, $J_{C\text{-}F}$ = 17.2), 152.4, 144.9 (d, $J_{C\text{-}F}$ = 3.0 Hz), 139.4, 130.7 (d, $J_{C\text{-}F}$ = 5.1 Hz), 127.8, 124.3, 119.4, 81.3, 28.2.

**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -48.4.

**ESI HRMS** for [$C_{16}H_{15}ClFN_5O_2$+$H^+$] calculated: 364.0971, found: 364.0975.



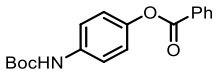
***tert*-butyl (4-((*tert*-butoxycarbonyl)amino)phenyl)(phenyl)carbamate (19)**

Following the representative **Condition B**, light yellow oil: 52% (40.3 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 15:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.36 – 7.29 (m, 3H), 7.24 – 7.11 (m, 4H), 6.97 – 6.90 (m, 2H), 6.57 (s, 1H), 1.53 (s, 9H), 1.46 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 153.9, 152.7, 143.0, 138.0, 136.0, 129.7, 128.6, 128.1, 127.7, 126.6, 125.4, 119.9, 119.0, 118.7, 81.2, 81.1, 28.3, 28.2.

**ESI HRMS** for [$C_{22}H_{28}N_2O_4$+$H^+$] calculated: 385.2122, found: 385.2115.



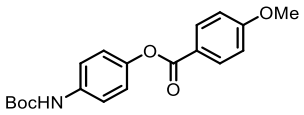

**4-((*tert*-butoxycarbonyl)amino)phenyl benzoate (20)**

Following the representative **Condition A**, white solid, yield: 57% (35.6 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 30:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.26 – 8.18 (m, 2H), 7.69 – 7.63 (m, 1H), 7.56 – 7.50 (m, 2H), 7.44 (d, J = 8.7 Hz, 2H), 7.17 (d, J = 8.7 Hz, 2H), 6.58 (s, 1H), 1.55 (s, 9H).

**$^{13}$C NMR** (101 MHz, CDCl3) δ 165.3, 152.7, 146.2, 136.1, 133.5, 130.1, 129.5, 128.5, 122.1, 80.6, 28.3.

**ESI HRMS** for [$C_{18}H_{19}NO_4$+$H^+$] calculated: 314.1387, found: 314.1383.



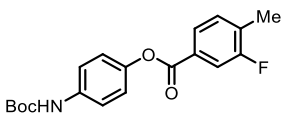

**4-((*tert*-butoxycarbonyl)amino)phenyl 4-methoxybenzoate (21)**

Following the representative **Condition A**, white solid, yield: 45% (30.9 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 15:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.16 (d, J = 8.7 Hz, 2H), 7.42 (d, J = 8.7 Hz, 2H), 7.18 – 7.11 (m, 2H), 7.03 – 6.96 (m, 2H), 6.58 (s, 1H), 3.91 (s, 3H), 1.54 (s, 9H).

**$^{13}$C NMR** (101 MHz, CDCl3) δ 165.1, 163.8, 152.7, 146.3, 135.9, 132.2, 122.1, 121.8, 119.4, 113.8, 80.6, 55.5, 28.3.

**ESI HRMS** for [$C_{19}H_{21}NO_5$+$H^+$] calculated: 344.1492, found: 344.1489.



**4-((*tert*-butoxycarbonyl)amino)phenyl 3-fluoro-4-methylbenzoate (22)**

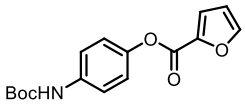
Following the representative **Condition A**, white solid, yield: 40% (27.6 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 30:1, *v/v*).

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 8.9, 1.7 Hz, 1H), 7.82 (dd, *J* = 8.9, 1.7 Hz, 1H), 7.43 (m, 2H), 7.33 (m, 1H), 7.18 – 7.12 (m, 2H), 6.59 (s, 1H), 2.39 (d, *J* = 2.2 Hz, 3H), 1.54 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 164.4 (d, $J_{C-F}$ = 3.03), 160.9 (d, $J_{C-F}$ = 252.5), 152.7, 146.0, 136.2, 131.5 (d, $J_{C-F}$ = 5.05), 131.4 (d, $J_{C-F}$ = 17.17), 129.0 (d, $J_{C-F}$ = 7.07), 125.6 (d, $J_{C-F}$ = 10.10), 122.0, 116.5 (d, $J_{C-F}$ = 24.24), 80.7, 28.3, 14.9 (d, $J_{C-F}$ = 4.04).

**$^{19}$F NMR** (376 MHz, $CDCl_3$) δ -116.3.

**ESI HRMS** for [$C_{19}H_{20}FNO_4$+$H^+$] calculated: 346.1449, found: 346.1448.



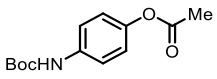

**4-((*tert*-butoxycarbonyl)amino)phenyl furan-2-carboxylate (23)**

Following the representative **Condition A**, white solid, yield: 29% (17.6 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 15:1, *v/v*).

**$^{1}$H NMR** (600 MHz, CDCl3) δ 7.70 – 7.67 (m, 1H), 7.42 (d, J = 8.4 Hz, 2H), 7.39 (m, 1H), 7.15 (d, J = 8.4 Hz, 2H), 6.63 – 6.59 (m, 2H), 1.53 (s, 9H).

**$^{13}$C NMR** (101 MHz, CDCl3) δ 157.1, 152.7, 147.1, 145.4, 144.0, 136.3, 122.0, 119.4, 112.1, 80.7, 28.3.

**ESI HRMS** for [$C_{16}H_{17}NO_5$+$H^+$] calculated: 304.1179, found: 304.1177.

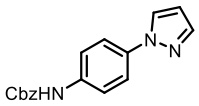



**4-((*tert*-butoxycarbonyl)amino)phenyl acetate (24)**

Following the representative **Condition A**, white solid, yield: 18% (9.1 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 15:1, *v/v*), reported compound[23].

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.38 (d, J = 8.7 Hz, 2H), 7.03 (d, J = 8.7 Hz, 2H), 6.51 (s, 1H), 2.30 (s, 3H), 1.53 (s, 9H).

**$^{13}$C NMR** (101 MHz, CDCl3) δ 169.7, 152.7, 146.0, 136.0, 121.9, 80.7, 28.3, 21.1.



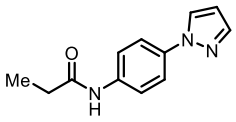

**benzyl (4-(1*H*-pyrazol-1-yl)phenyl)carbamate (25)**

Following the representative **Condition A**, white solid, yield: 74% (43.4 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 6:1, *v/v*).

**$^1$H NMR** (400 MHz,$CDCl_3$) δ 7.88 (d, *J* = 2.4 Hz, 1H), 7.73 (d, *J* = 2.4 Hz, 1H), 7.63 (d, *J* = 8.6 Hz, 2H), 7.49 (d, *J* = 8.6 Hz, 2H), 7.45 – 7.36 (m, 4H), 6.96 (s, 1H), 6.47 (t, *J* = 2.2 Hz, 1H), 5.23 (s, 2H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 186.7, 153.3, 140.9, 136.2, 135.9, 135.9, 128.6, 128.4, 128.3, 126.7, 120.0, 107.4, 67.1.

**ESI HRMS** for [$C_{17}H_{15}N_3O_2$+$H^+$] calculated: 294.1237, found: 294.1245.



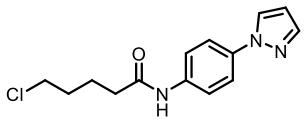

***N*-(4-(1*H*-pyrazol-1-yl)phenyl)butyramide (26)**

Following the representative **Condition A**, white solid: 89% (38.3 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 3:1, *v/v*).

**$^1$H NMR** (400 MHz,$CDCl_3$) δ 7.90 (s, 1H), 7.75 (s, 1H), 7.69 – 7.55 (m, 4H), 6.49 (s, 1H), 2.43 (q, *J* = 7.4 Hz, 2H), 1.27 (t, *J* = 7.4 Hz, 3H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 172.2, 140.6, 136.7, 135.9, 127.1, 120.6, 120.0, 107.6, 30.6, 9.6.

**ESI HRMS** for [$C_{12}H_{13}N_3O$+$H^+$] calculated: 216.1131, found: 216.1132.



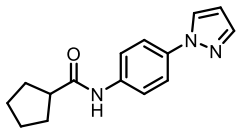
***N*-(4-(1*H*-pyrazol-1-yl)phenyl)-5-chloropentanamide (27)**

Following the representative **Condition A** with the following change: 5.0 mA was instead of 3.5 mA. White solid: 36% (20.0 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 3:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.75 (s, 1H), 7.72 (s, 1H), 7.66 – 7.61 (m, 4H), 6.50 (s, 1H), 3.64 – 3.55 (m, 2H), 2.49 – 2.36 (m, 2H), 1.98 – 1.81 (m, 4H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 170.9, 140.9, 136.5, 136.3, 127.1, 120.8, 120.0, 107.6, 44.6, 36.6, 31.9, 22.8.

**ESI HRMS** for [$C_{14}H_{16}ClN_3O+H^+$] calculated: 278.1055, found: 278.1051.



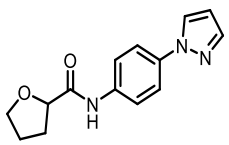
***N*-(4-(1*H*-pyrazol-1-yl)phenyl)cyclopentanecarboxamide (28)**

Following the representative **Condition A**, white solid: 48% (24.5 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 5:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.75 (s, 1H), 7.69 – 7.60 (m, 4H), 6.49 (s, 1H), 2.94 (s, 1H), 2.79 – 2.68 (m, 1H), 2.02 – 1.86 (m, 4H), 1.85 – 1.75 (m, 2H), 1.69 – 1.58 (m, 2H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 174.9, 140.5, 137.0, 135.7, 127.2, 120.6, 120.0, 107.6, 46.7, 30.5, 26.0.

**ESI HRMS** for [$C_{15}H_{17}N_3O+H^+$] calculated: 256.1444, found: 256.1445.



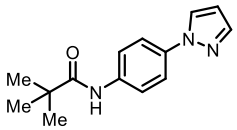
***N*-(4-(1*H*-pyrazol-1-yl)phenyl)tetrahydrofuran-2-carboxamide (29)**

Following the representative **Condition A**, white solid: 34% (17.5 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 3:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 7.91 (d, *J* = 2.1 Hz, 1H), 7.73 (d, *J* = 2.1 Hz, 1H), 7.73 – 7.65 (m, 4H), 6.48 (t, *J* = 2.1 Hz, 1H), 4.52 – 4.47 (m, 1H), 4.11 – 4.04 (m, 1H), 4.02 – 3.95 (m, 1H), 2.45 – 2.34 (m, 1H), 2.26 – 2.16 (m, 1H), 2.06 – 1.90 (m, 2H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 171.3, 140.8, 136.4, 135.7, 126.7, 120.4, 119.8, 107.5, 78.6, 69.7, 30.2, 25.6.

**ESI HRMS** for [$C_{14}H_{15}N_3O_2$+$H^+$] calculated: 258.1237, found: 258.1235.



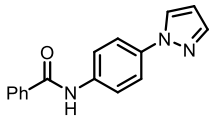

***N*-(4-(1*H*-pyrazol-1-yl)phenyl)pivalamide (30)**

Following the representative **Condition A**, white solid: 76% (36.9 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 8:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.92 (s,, 1H), 7.76 (s, 1H), 7.70 – 7.64 (m, 4H), 7.45 (s, 1H), 6.50 (s, 1H), 1.36 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 176.7, 140.6, 136.7, 136.0, 127.0, 120.8, 119.9, 107.6, 39.6, 27.6.

**ESI HRMS** for [$C_{14}H_{17}N_3O$+$H^+$] calculated: 244.1444, found: 244.1447.



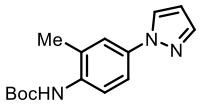

***N*-(4-(1*H*-pyrazol-1-yl)phenyl)benzamide (31)**

Following the representative **Condition A**, white solid: 40% (21.0 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 5:1, *v/v*).

**$^1$H NMR** (400 MHz, DMSO-$d_6$) δ 10.39 (s, 1H), 8.46 (d, *J* = 2.1 Hz, 1H), 8.02 – 7.95 (m, 2H), 7.95 – 7.89 (m, 2H), 7.87 – 7.80 (m, 2H), 7.74 (d, *J* = 2.1 Hz, 1H), 7.64 – 7.52 (m, 3H), 6.54 (t, *J* = 2.1 Hz, 1H).

**$^{13}$C NMR** (101 MHz, DMSO-$d_6$) δ 166.0, 141.1, 137.8, 136.0, 135.3, 132.1, 128.9, 128.1, 127.9, 121.5, 119.1, 108.1.

**ESI HRMS** for [$C_{16}H_{13}N_3O$+$H^+$] calculated: 264.1131, found: 264.1128.



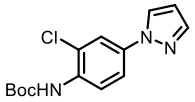

***tert*-butyl (2-methyl-4-(1*H*-pyrazol-1-yl)phenyl)carbamate (32)**

Following the representative **Condition A** with the following change: 5.0 mA was instead of 3.5 mA.White solid: 48% (26.2 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 15:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.6 Hz, 1H), 7.88 (d, *J* = 2.1 Hz, 1H), 7.72 (d, *J* = 2.1 Hz, 1H), 7.57 (d, *J* = 2.6 Hz, 1H), 7.46 (dd, *J* = 8.6, 2.7 Hz, 1H), 6.46 (t, *J* = 2.1 Hz, 1H), 6.34 (s, 1H), 2.33 (s, 3H), 1.56 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.9, 140.7, 135.8, 134.9, 126.8, 121.4, 117.4, 107.3, 80.7, 28.3, 17.8.

**ESI HRMS** for [$C_{15}H_{19}N_3O_2$+$H^+$] calculated: 274.1550, found: 274.1548.



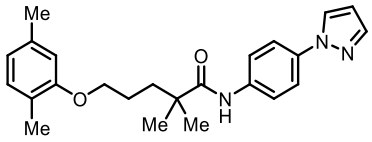

***tert*-butyl (2-chloro-4-(1*H*-pyrazol-1-yl)phenyl)carbamate (33)**

Following the representative **Condition A**, white solid: 30% (17.5 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 15:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 9.0 Hz, 1H), 7.87 (d, *J* = 2.5 Hz, 1H), 7.78 (d, *J* = 2.5 Hz, 1H), 7.71 (d, *J* = 2.1 Hz, 1H), 7.53 (dd, *J* = 9.0, 2.1 Hz, 1H), 7.02 (s, 1H), 6.47 (t, *J* = 2.1 Hz, 1H), 1.55 (s, 9H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 152.2, 141.1, 135.3, 133.6, 126.7, 122.4, 120.1, 118.1, 107.8, 81.4, 28.3.

**ESI HRMS** for [$C_{14}H_{16}N_3O_2$+$H^+$] calculated: 294.1004, found: 294.0995.



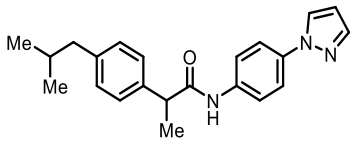
***N*-(4-(1*H*-pyrazol-1-yl)phenyl)-5-(2,5-dimethylphenoxy)-2,2-dimethylpentanamide (34)**

Following the representative **Condition A** with the following change: 5.0 mA was instead of 3.5 mA. White soild: 45% (30.5 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 7:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 2.1 Hz, 1H), 7.75 (d, *J* = 2.1 Hz, 1H), 7.68 – 7.61 (m, 4H), 7.50 (s, 1H), 7.02 (d, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 7.5 Hz, 1H), 6.64 (s, 1H), 6.51 – 6.46 (m, 1H), 4.00 – 3.96 (m, 2H), 2.31 (s, 3H), 2.20 (s, 3H), 1.90 – 1.82 (m, 4H), 1.38 (s, 6H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 175.8, 156.8, 140.8, 136.5, 136.4, 136.3, 130.3, 126.8, 123.5, 121.0, 120.9, 119.8, 112.2, 107.5, 67.8, 42.8, 37.6, 25.6, 25.1, 21.3, 15.8.

**ESI HRMS** for [$C_{24}H_{29}N_3O_2$+$H^+$] calculated: 392.2333, found: 392.2335.



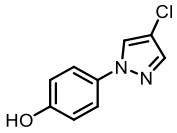
***N*-(4-(1*H*-pyrazol-1-yl)phenyl)-2-(4-isobutylphenyl)propanamide (35)**

Following the representative **Condition A** with the following change: 5.0 mA was instead of 3.5 mA. White soild: 50% (38.7 mg). Flash silica gel chromatography (petroleum ether/ether acetate = 8:1, *v/v*).

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 2.0 Hz, 1H), 7.71 (d, *J* = 2.0 Hz, 1H), 7.62 – 7.50 (m, 4H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.18 (d, *J* = 7.8 Hz, 2H), 6.46 (t, *J* = 2.1 Hz, 1H), 3.73 (q, *J* = 7.1 Hz, 1H), 2.50 (d, *J* = 7.1 Hz, 2H), 1.95 – 1.83 (m, 1H), 1.61 (d, *J* = 7.1 Hz, 3H), 0.93 (d, *J* = 7.1 Hz, 6H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 172.7, 141.1, 140.8, 137.9, 136.4, 136.2, 129.9, 127.4, 126.8, 120.5, 119.7, 107.5, 47.6, 45.0, 30.1, 22.3, 18.5.

**ESI HRMS** for [$C_{22}H_{25}N_3O$+$H^+$] calculated: 348.2070, found: 348.2069.



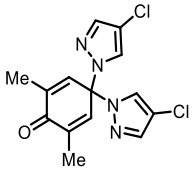
**4-(4-chloro-1*H*-pyrazol-1-yl)phenol (37)**

Following the methods in section 5. White solid, flash silica gel chromatography (petroleum ether/ethyl acetate = 15/1, v/v).

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.64 (s, 1H), 7.47 (d, *J* = 8.8 Hz, 2H), 6.89 (d, *J* = 8.9 Hz, 2H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 155.1, 138.9, 133.3, 125.3, 121.3, 116.2, 111.9.

**ESI HRMS** for [$C_9H_7ClN_2O+H^+$] calculated: 195.0320, found: 195.0316.



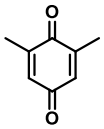
**4,4-bis(4-chloro-1*H*-pyrazol-1-yl)-2,6-dimethylcyclohexa-2,5-dien-1-one (38)**

Following the method in section 6. White solid, flash silica gel chromatography (petroleum ether/ether acetate = 30:1, *v/v*).

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 7.58 (s, 2H), 7.56 (s, 2H), 7.29 (s, 2H), 2.06 (s, 6H).

**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 184.7, 139.6, 137.8, 134.9, 126.0, 111.7, 72.8, 16.1.

**ESI HRMS** for [$C_{14}H_{12}Cl_2N_4O+H^+$] calculated: 323.0461, found: 323.0464.



**2,6-dimethylcyclohexa-2,5-diene-1,4-dione (39)**[1]

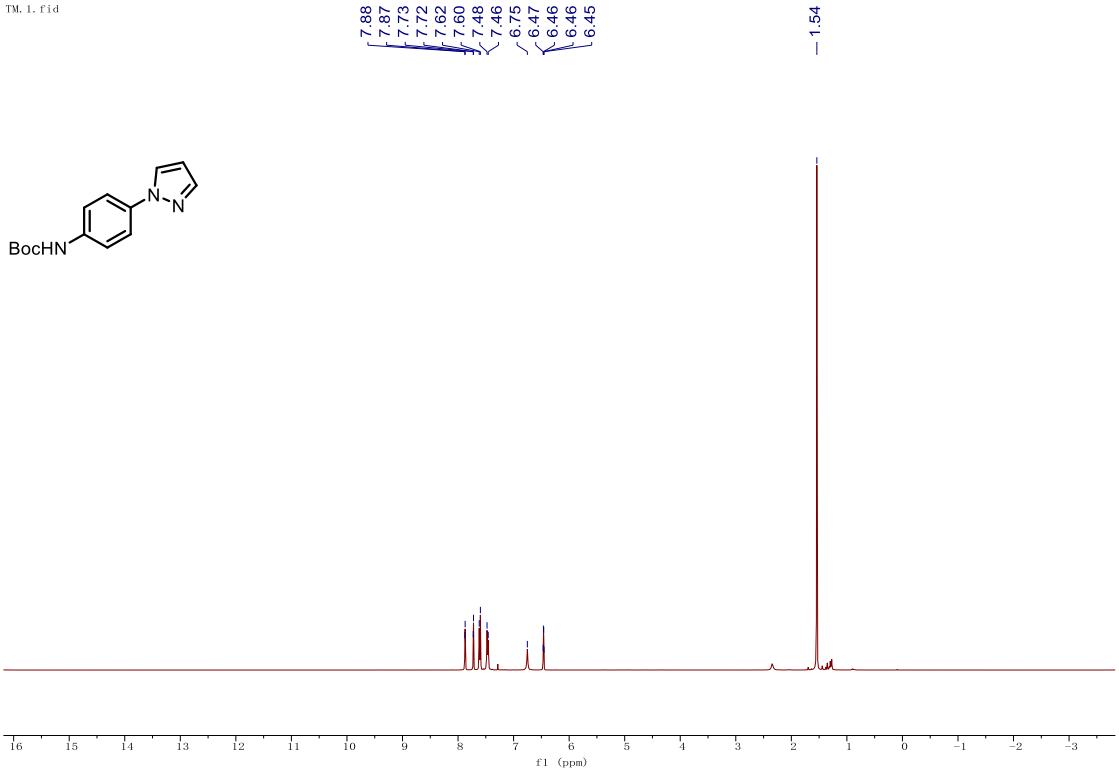
Following the method in section 6. 20 h was instead of 14 h. Pale yellow crystal, flash silica gel chromatography (petroleum ether/ether acetate = 40:1, *v/v*).

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 6.57 (s, 2H), 2.08 (s, 6H).

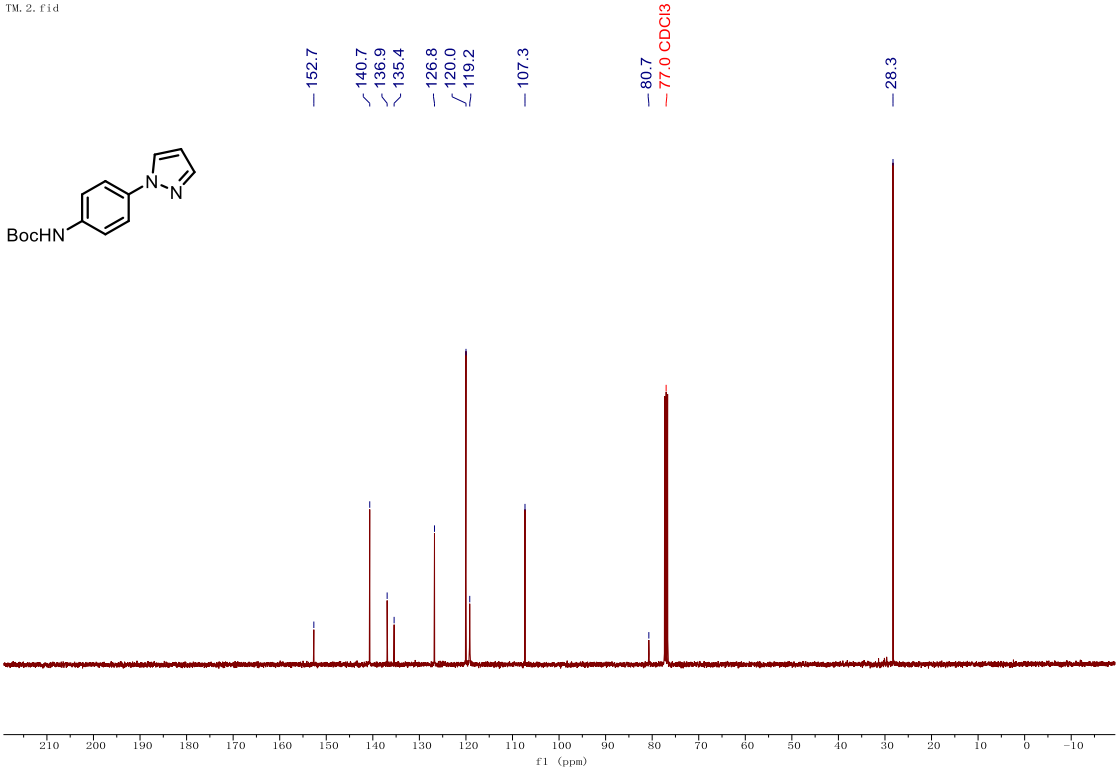
**$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 188.2, 187.7, 145.8, 133.3, 16.0.

## 11. NMR spectra of products

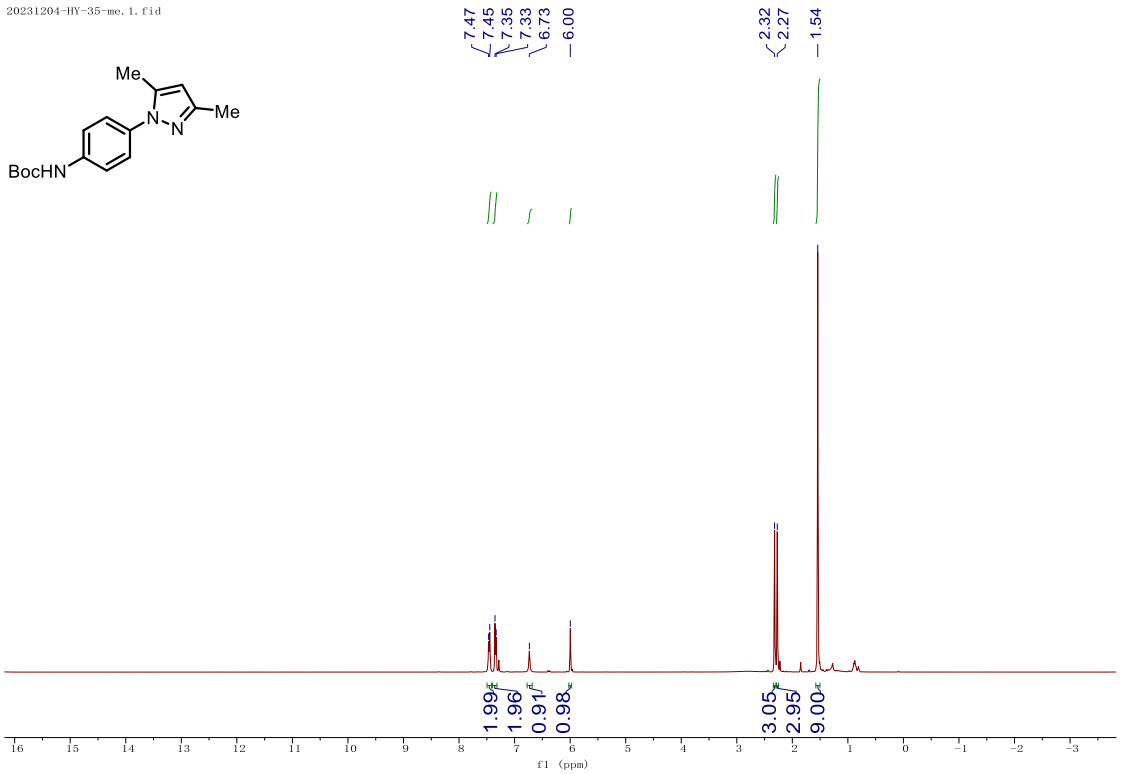
### $^{1}$H NMR of Compound 3 (400 MHz, $CDCl_3$)



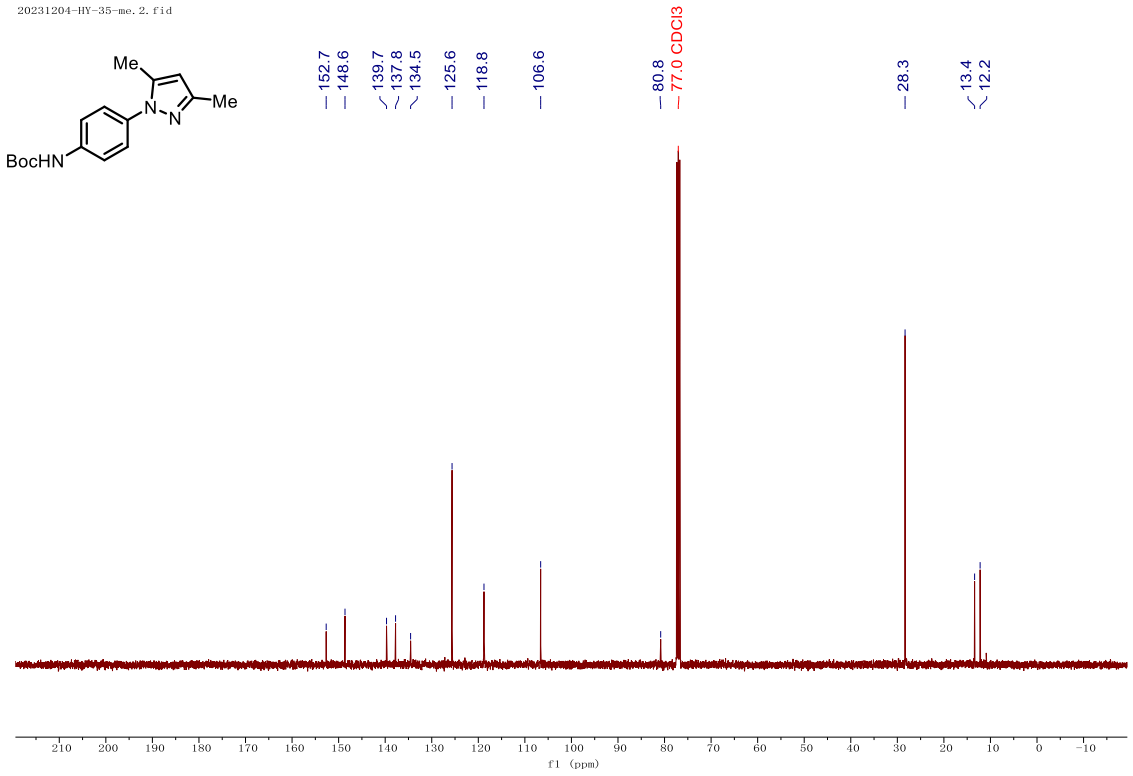

### $^{13}$C NMR of Compound 3 (101 MHz, $CDCl_3$)



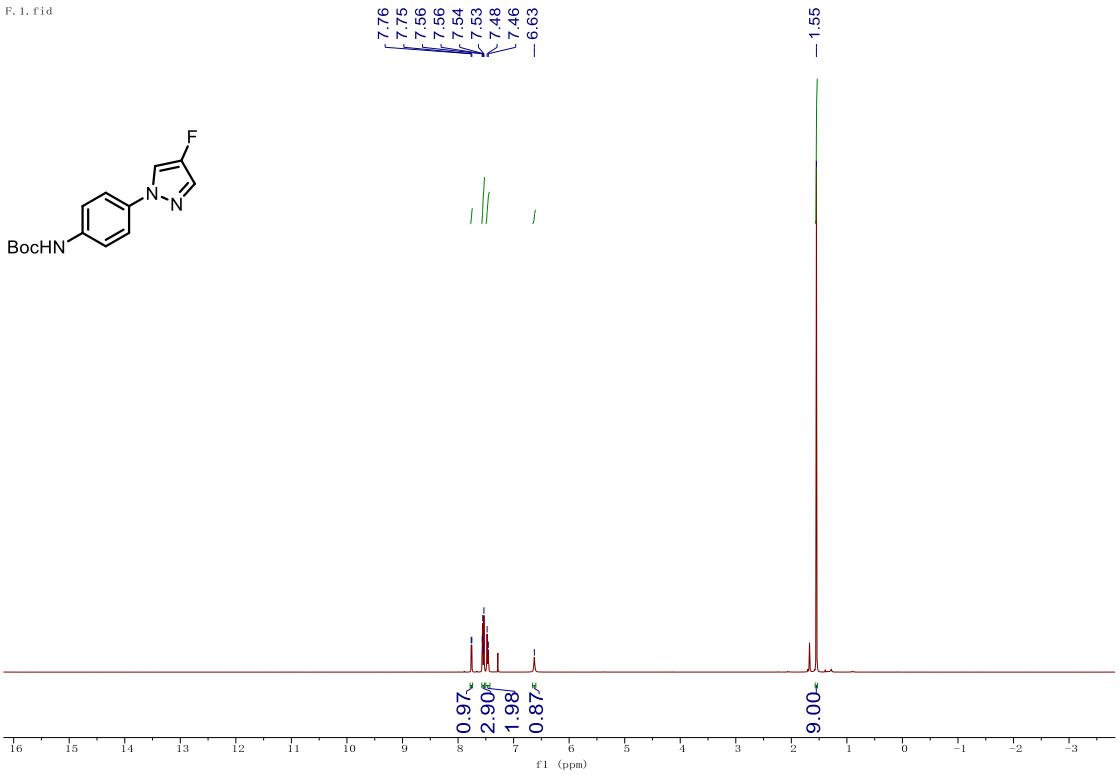
## $^{1}$H NMR of Compound 4 (400 MHz, $CDCl_3$)



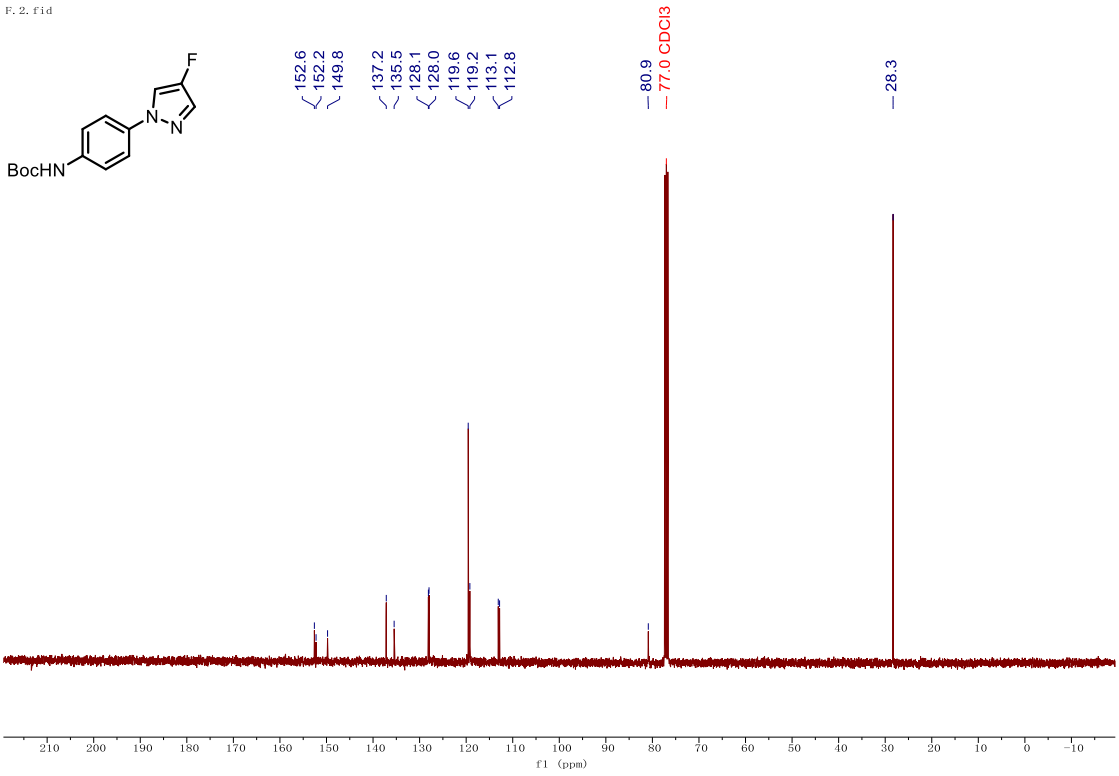

## $^{13}$C NMR of Compound 4 (101 MHz, $CDCl_3$)



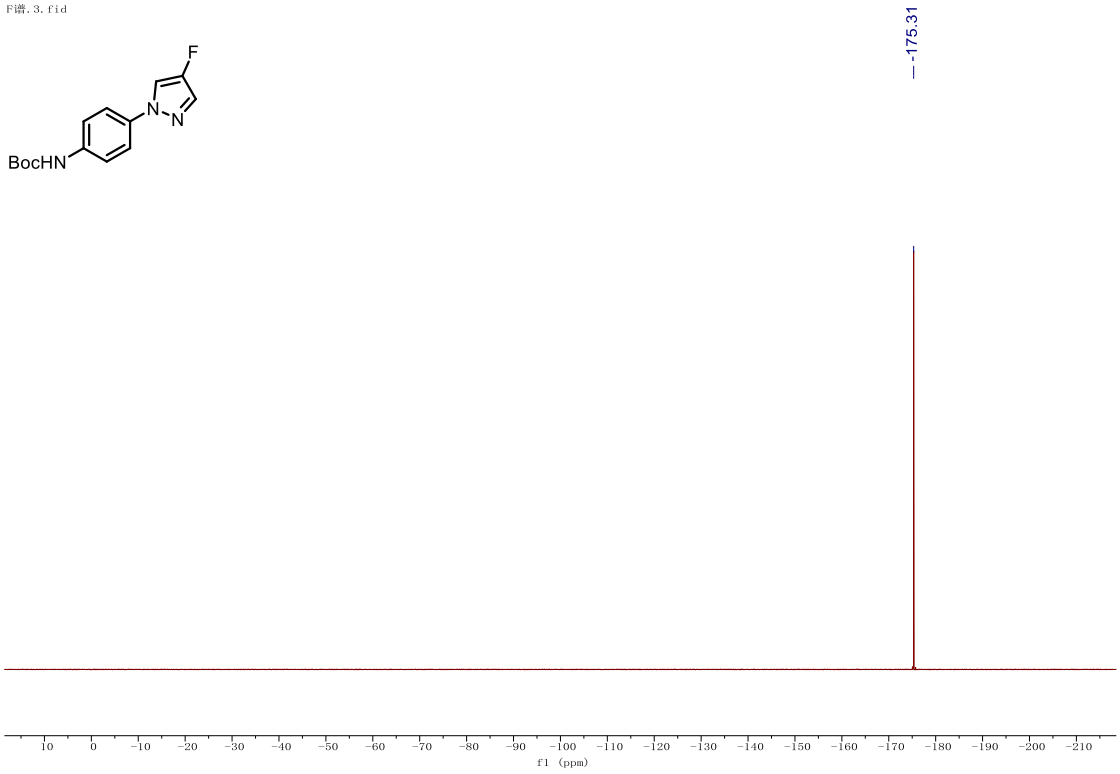
## $^{1}$H NMR of Compound 5 (400 MHz, $CDCl_3$)



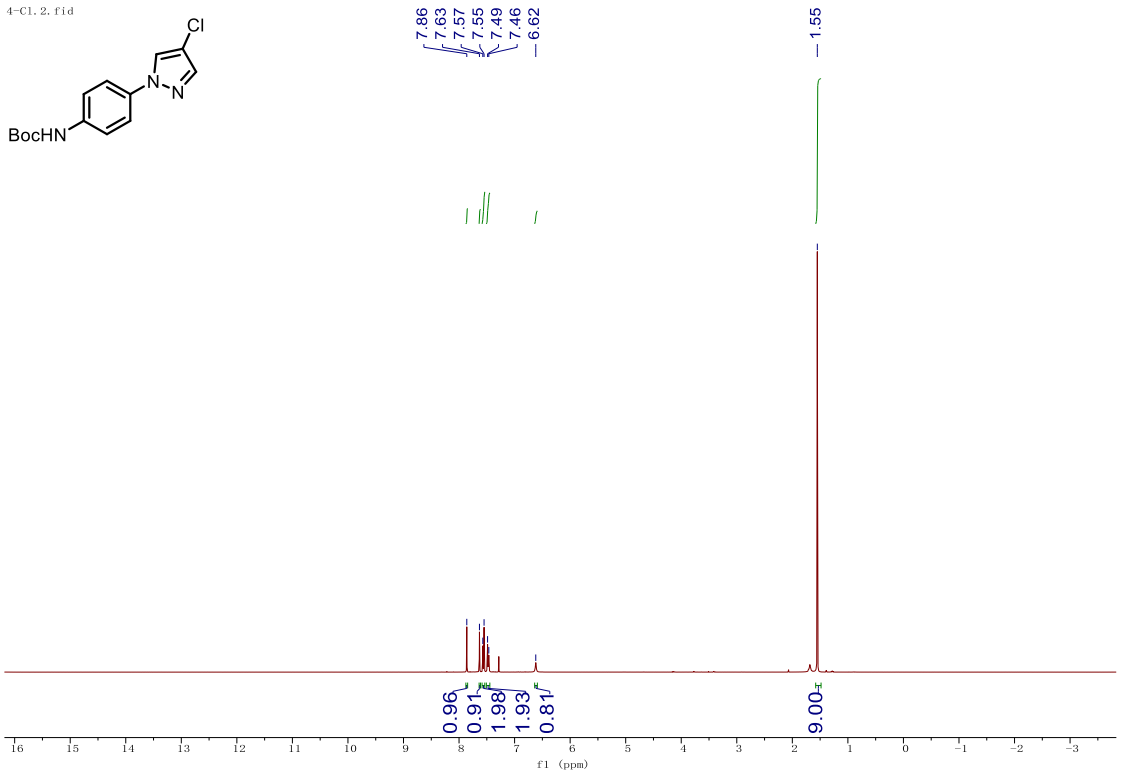

## $^{13}$C NMR of Compound 5 (101 MHz, $CDCl_3$)



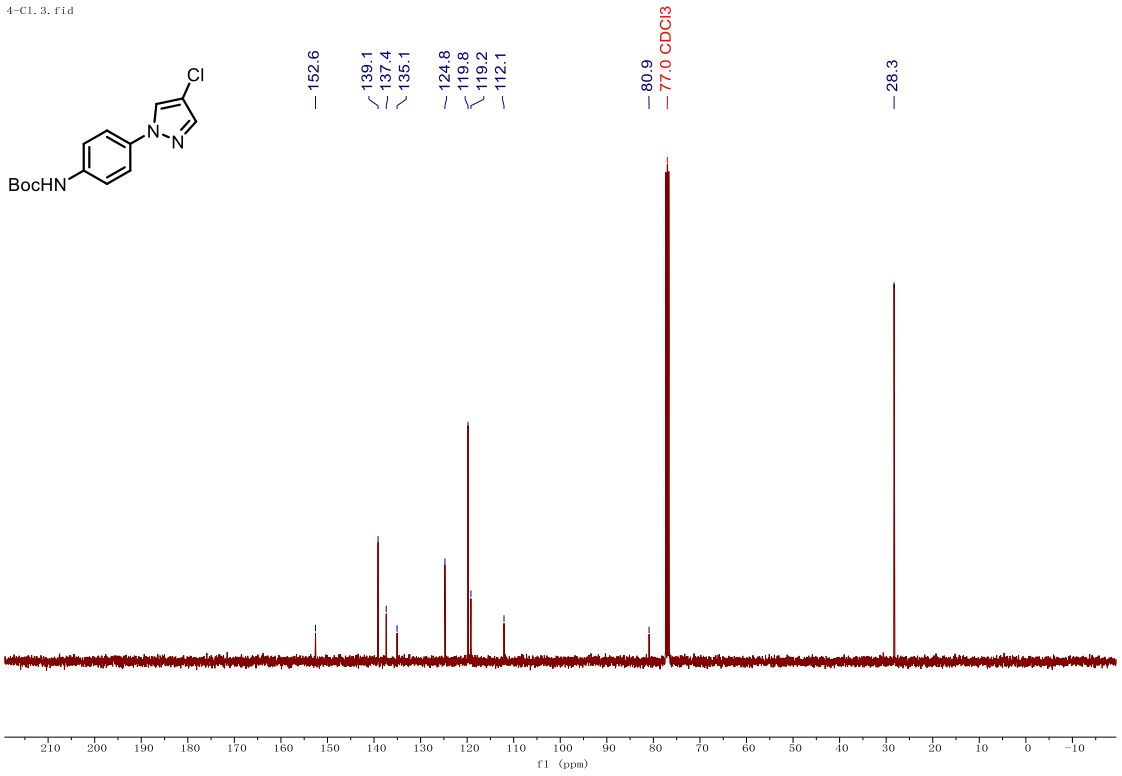
## $^{19}$F NMR of Compound 5 (376 MHz, $CDCl_3$)



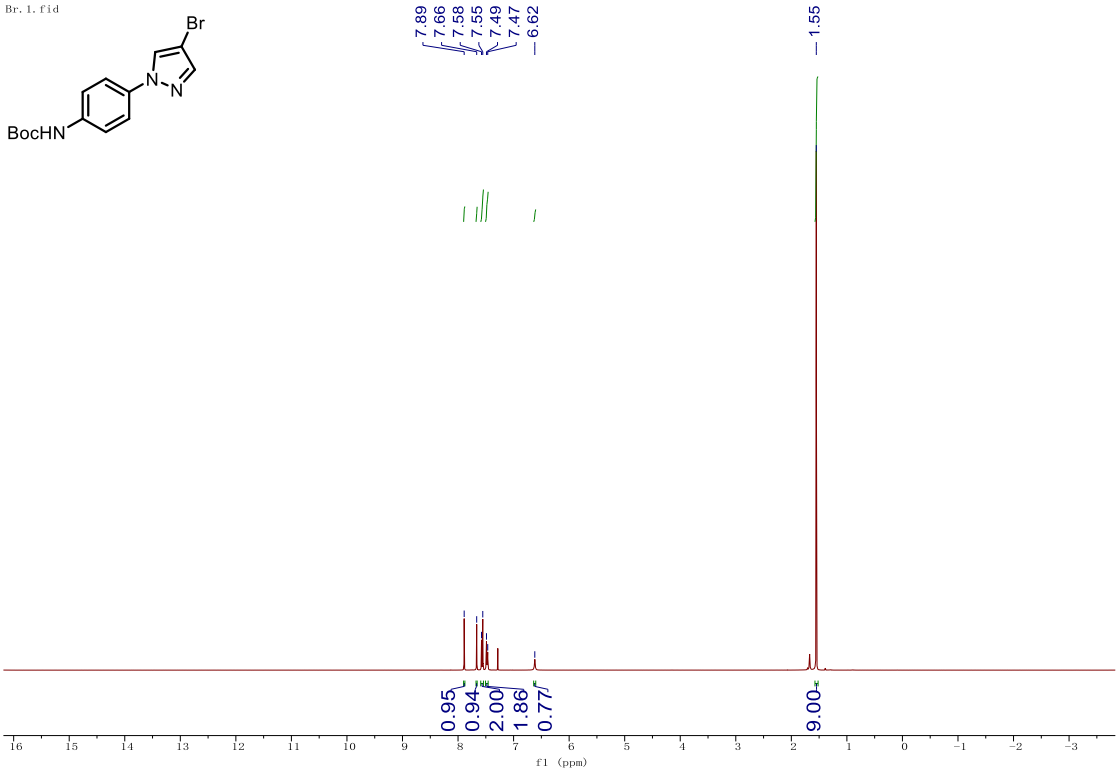
## $^{1}$H NMR of Compound 6 (400 MHz, $CDCl_3$)



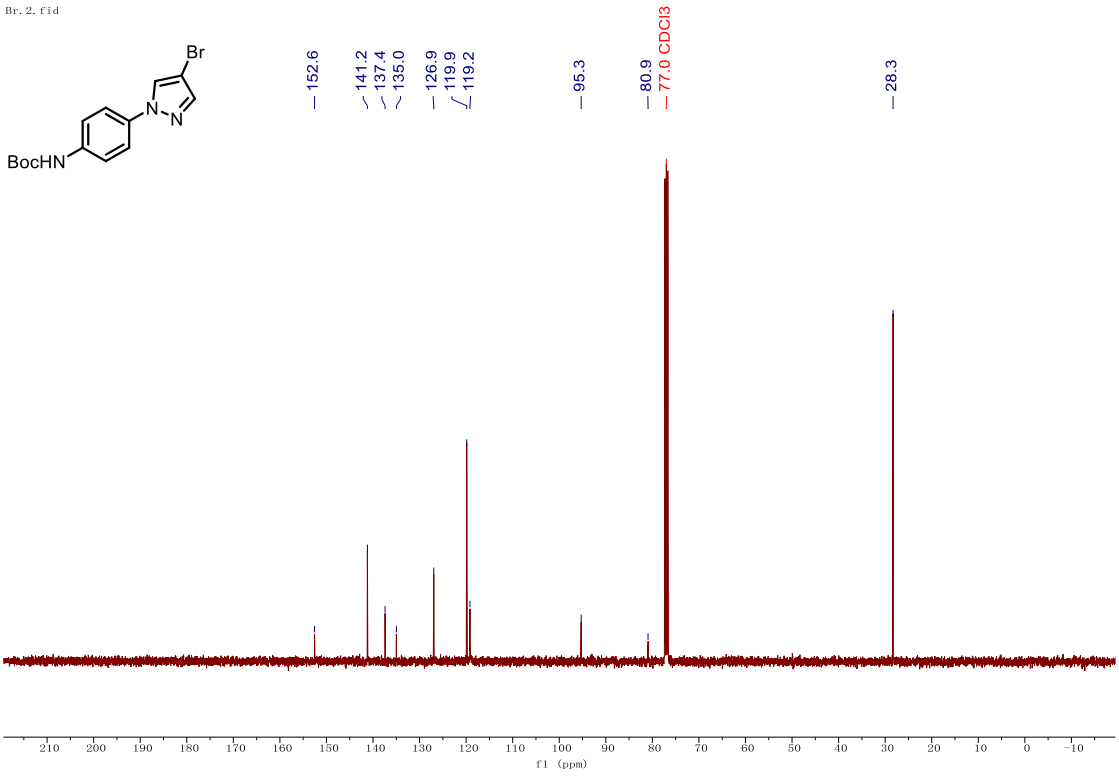

## $^{13}$C NMR of Compound 6 (101 MHz, $CDCl_3$)



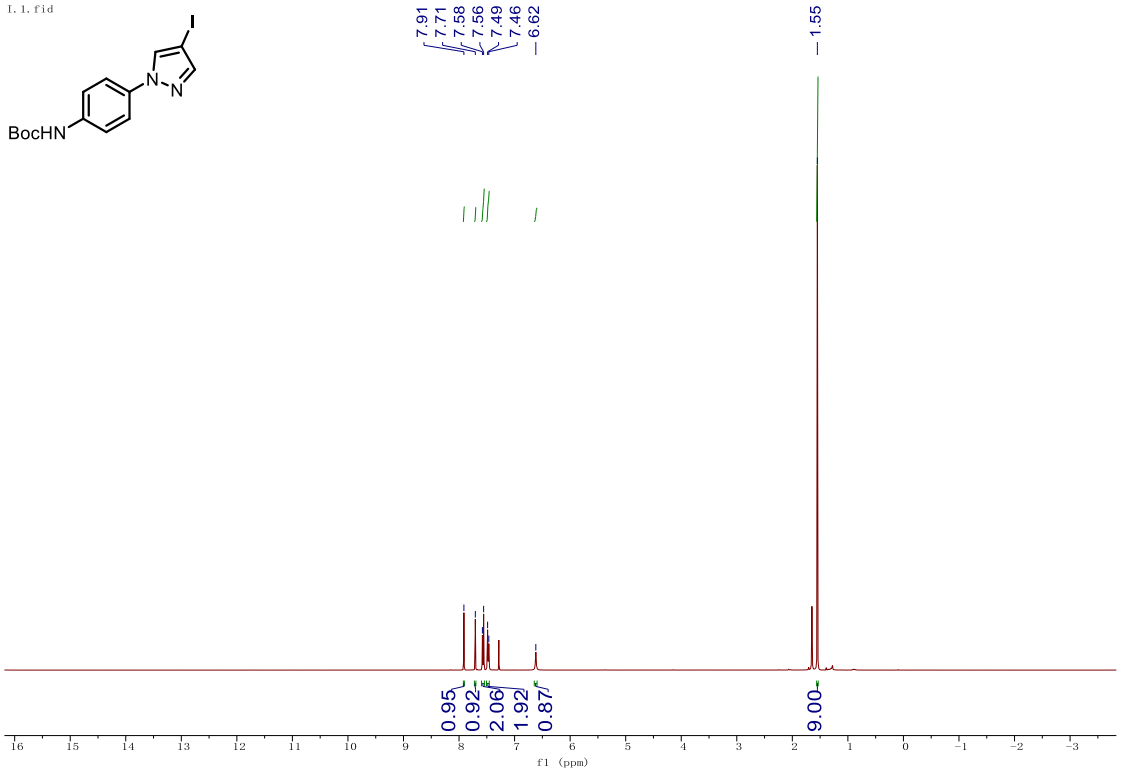
## $^{1}$H NMR of Compound 7 (400 MHz, $CDCl_3$)



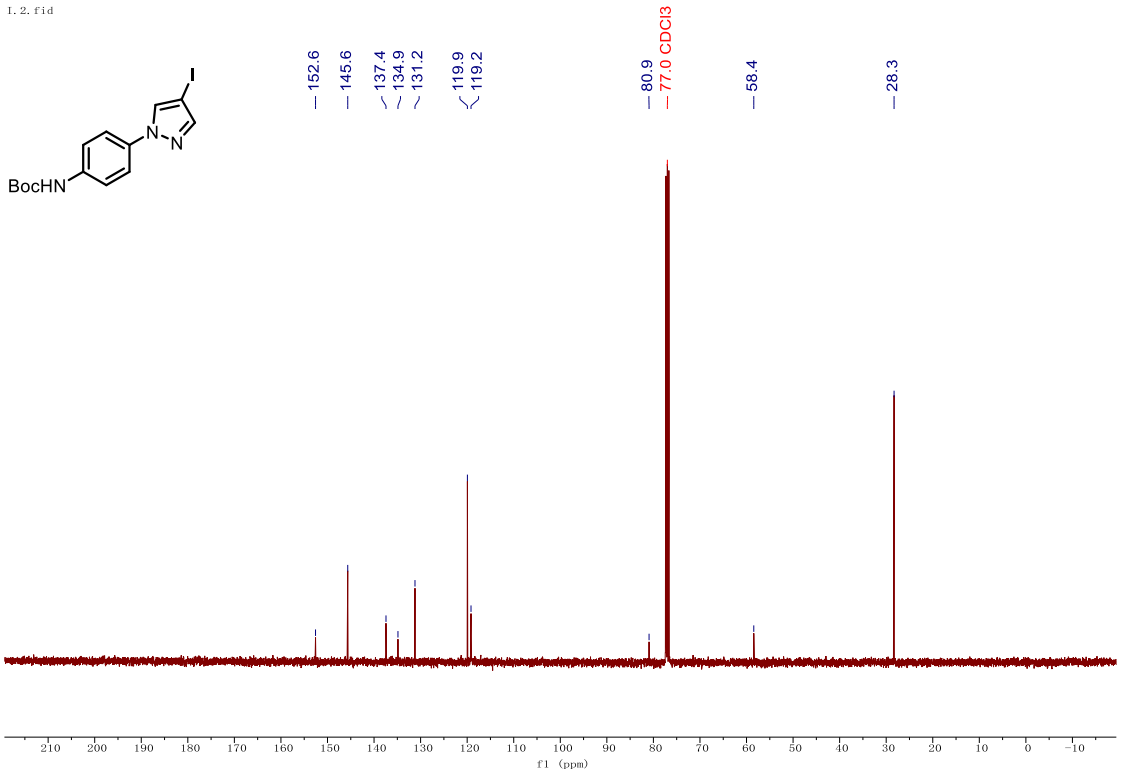

## $^{13}$C NMR of Compound 7 (101 MHz, $CDCl_3$)



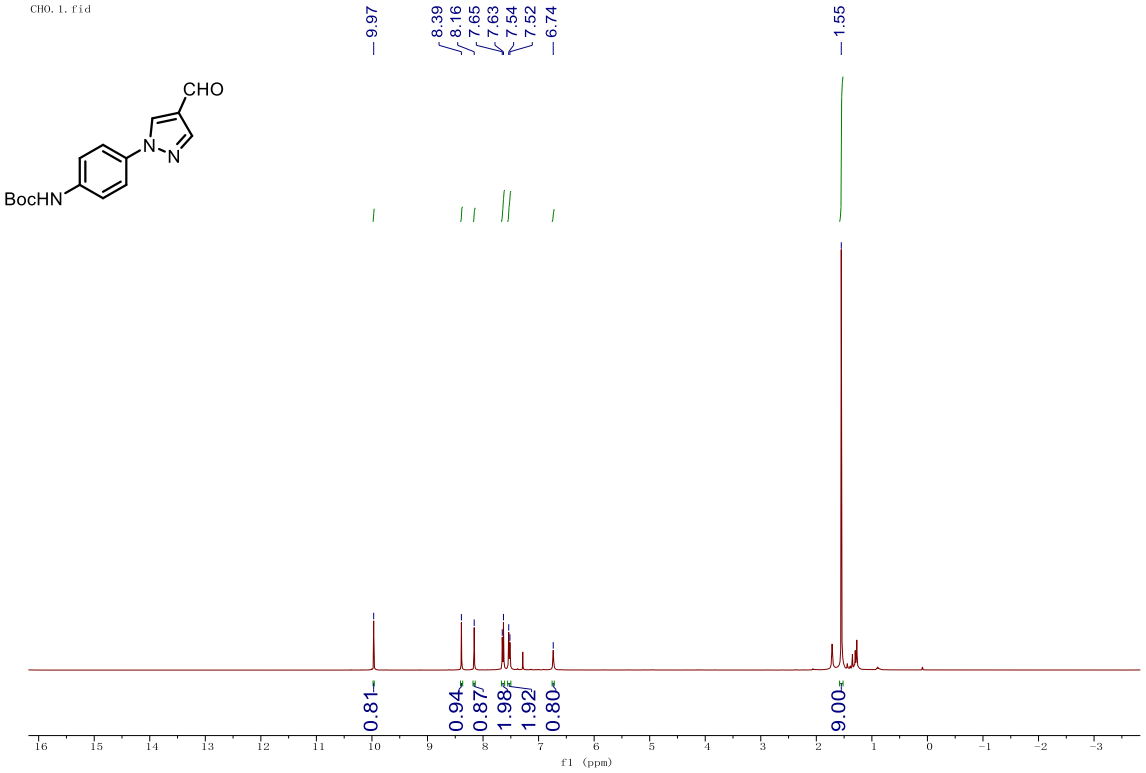
## $^{1}$H NMR of Compound 8 (400 MHz, $CDCl_3$)



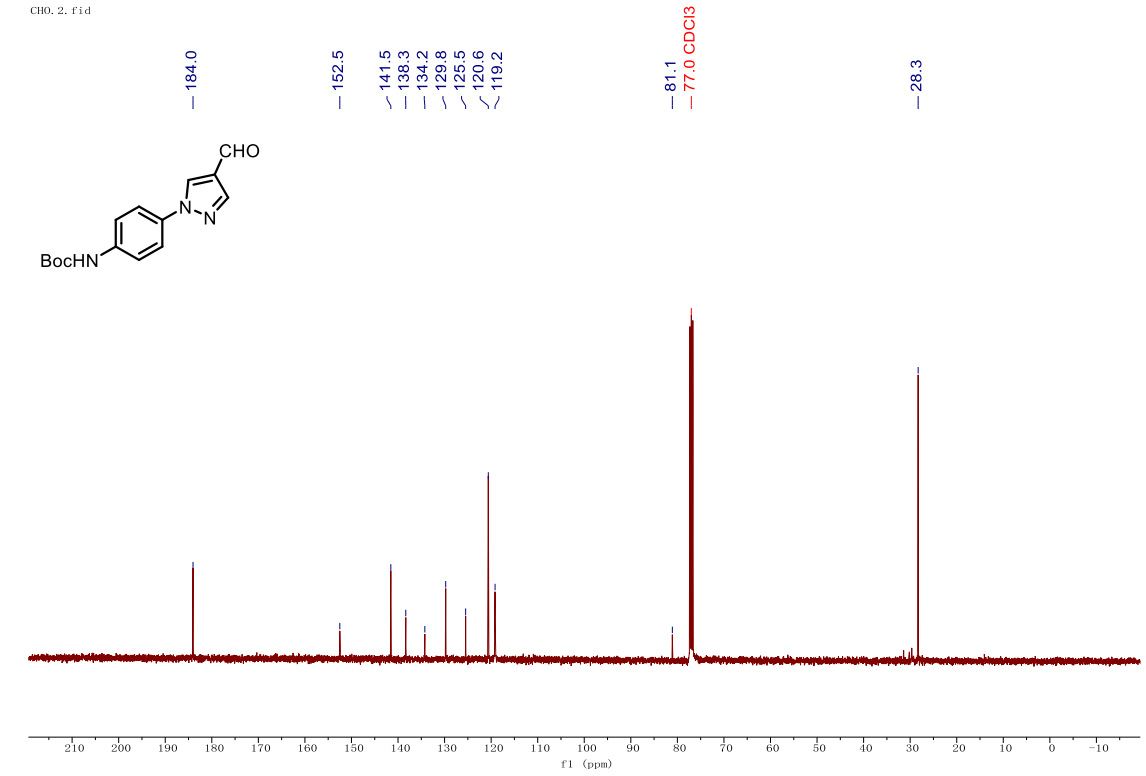

## $^{13}$C NMR of Compound 8 (101 MHz, $CDCl_3$)



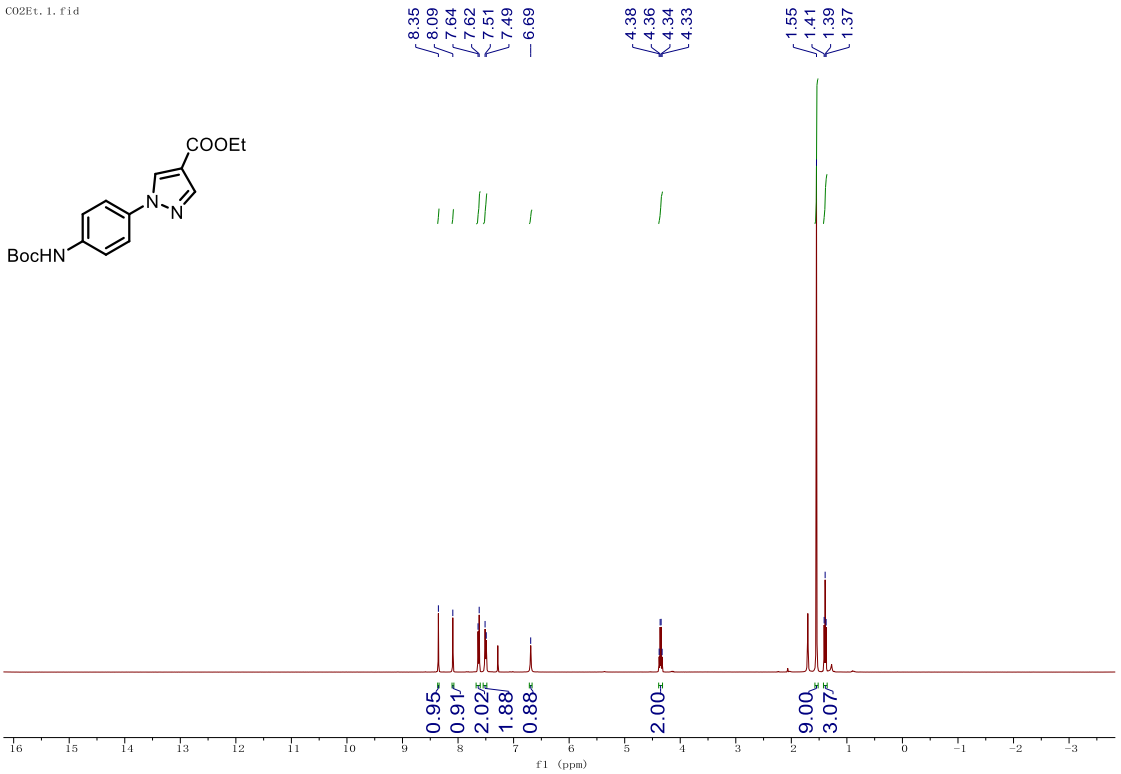
## $^{1}$H NMR of Compound 9 (400 MHz, $CDCl_3$)



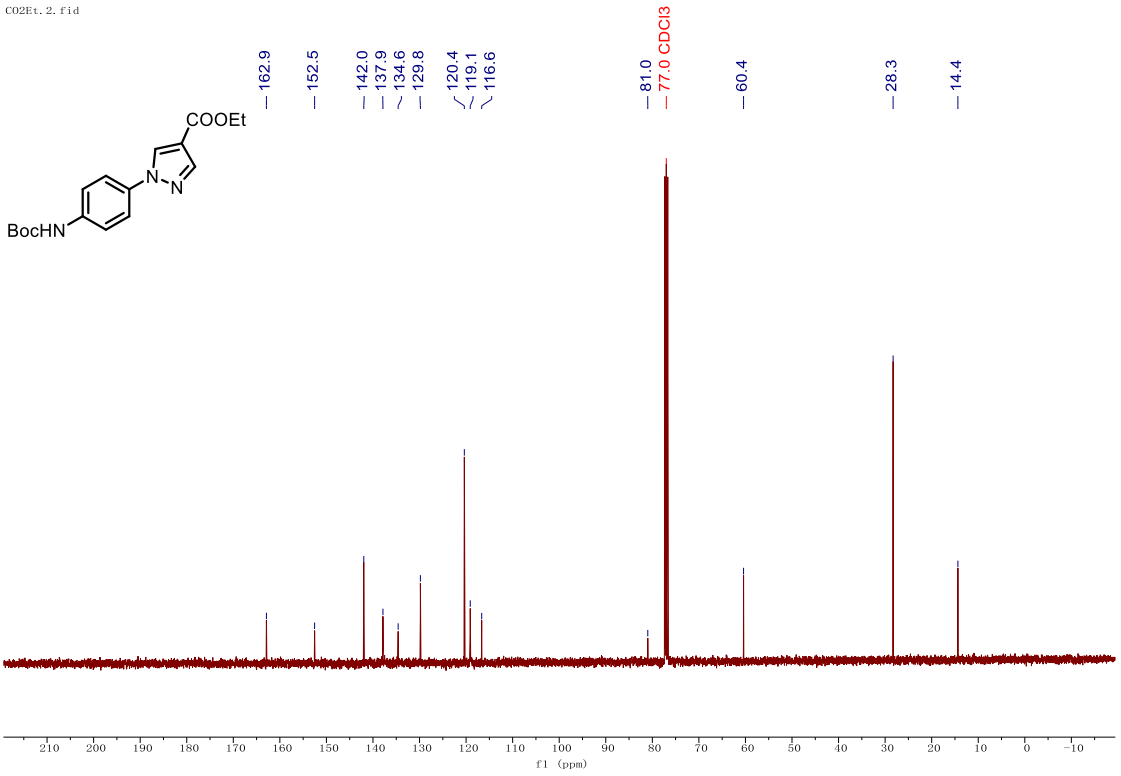

## $^{13}$C NMR of Compound 9 (101 MHz, $CDCl_3$)



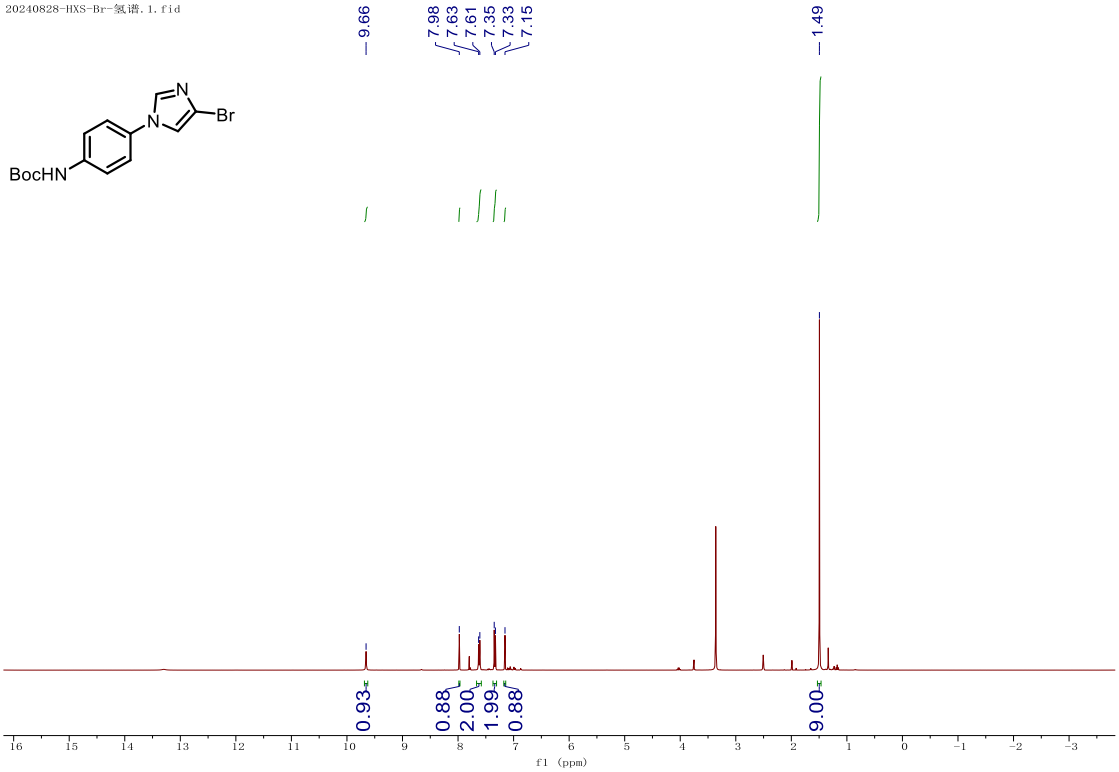
## $^{1}$H NMR of Compound 10 (400 MHz, $CDCl_3$)



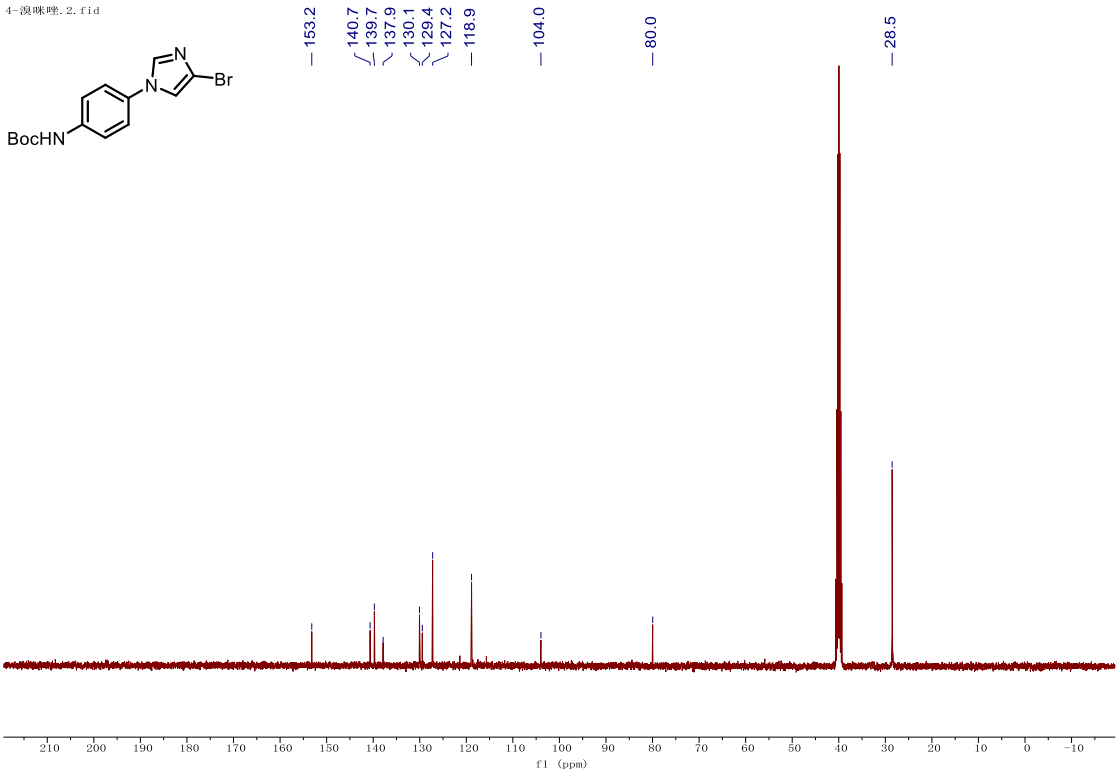

## $^{13}$C NMR of Compound 10 (101 MHz, $CDCl_3$)



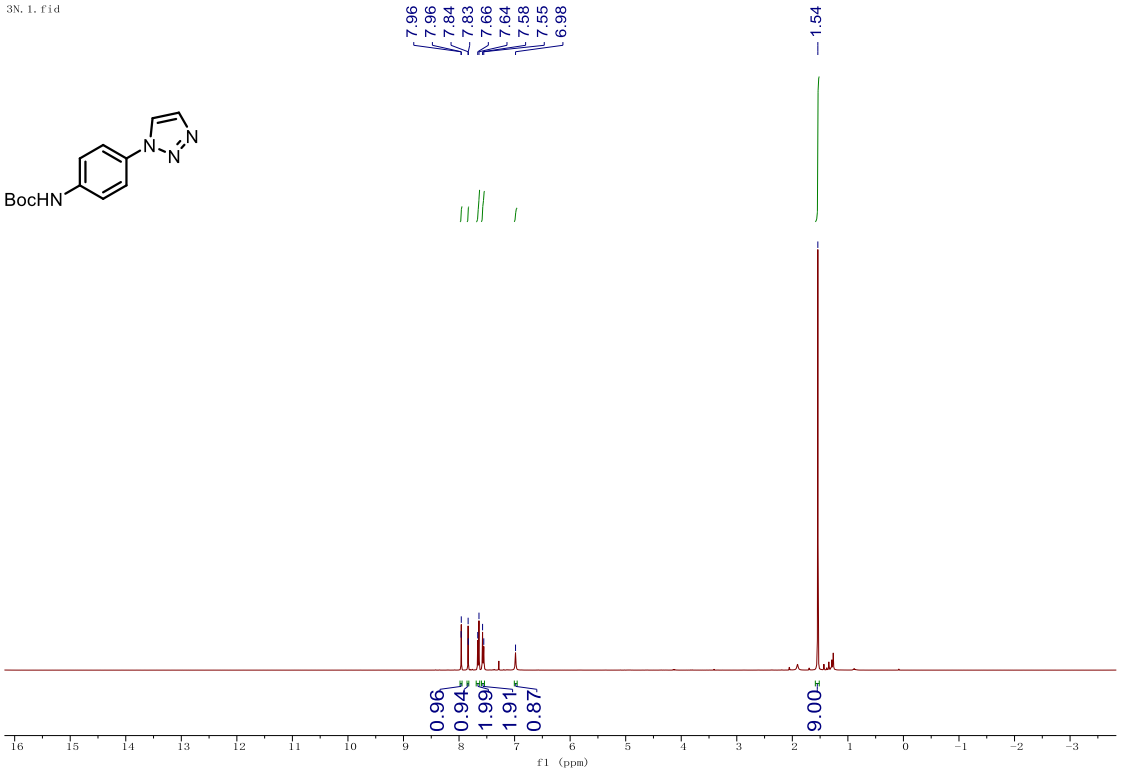
## $^{1}$H NMR of Compound 11 (400 MHz, DMSO-$d_6$)



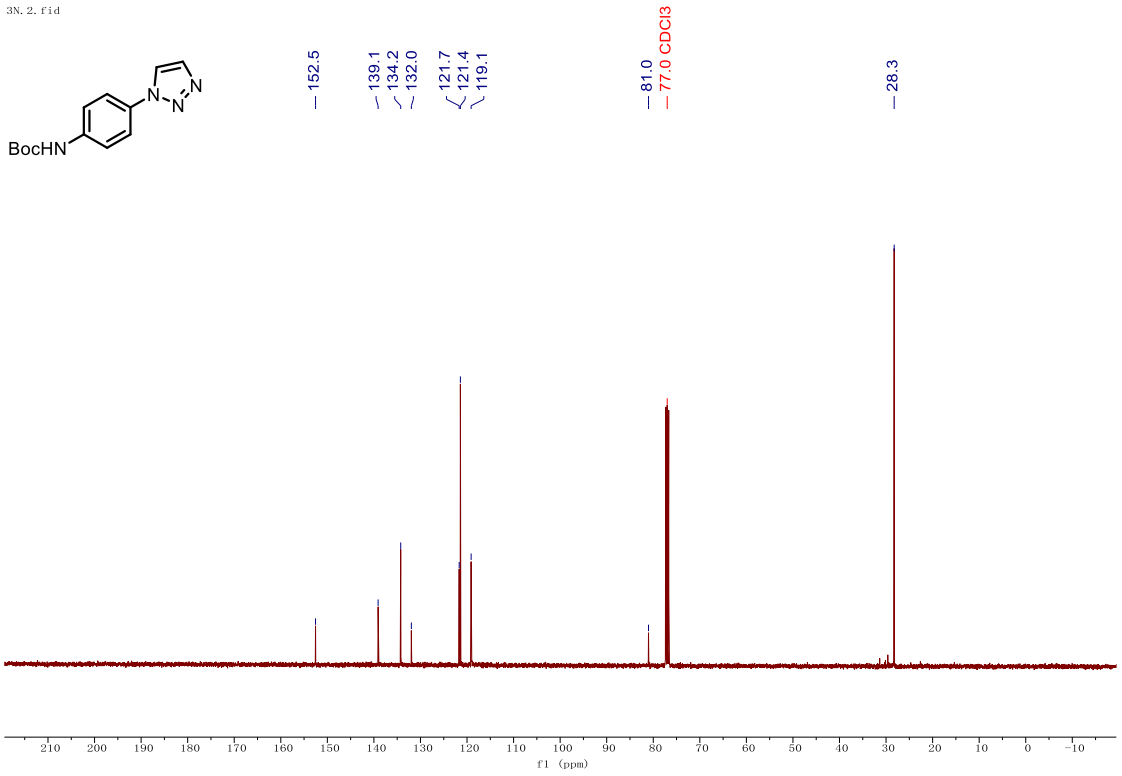

## $^{13}$C NMR of Compound 11 (101 MHz, DMSO-$d_6$)



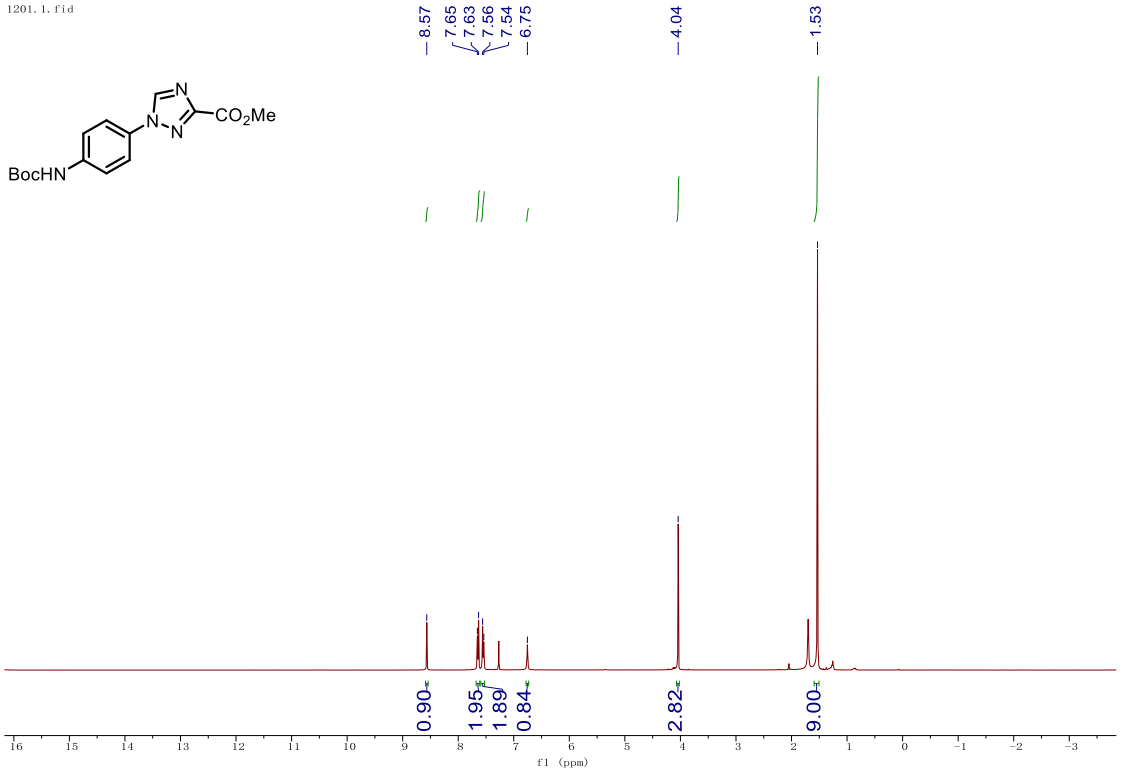
## $^{1}$H NMR of Compound 12 (400 MHz, $CDCl_3$)



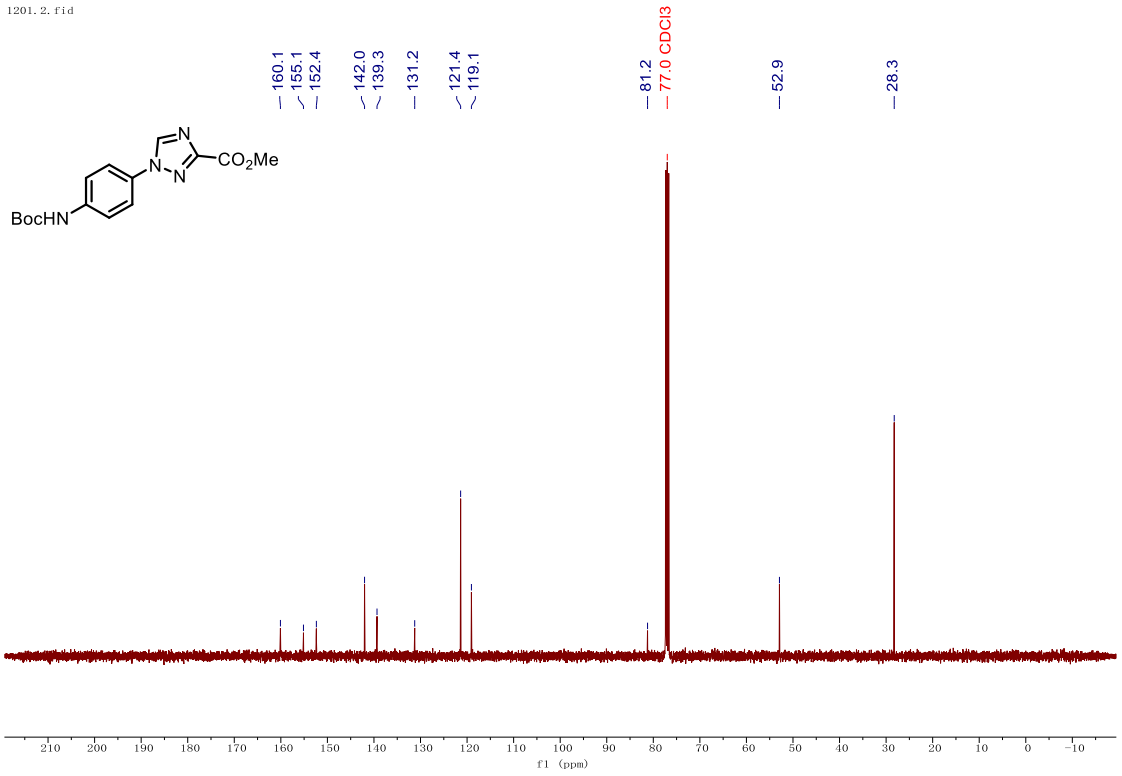

## $^{13}$C NMR of Compound 12 (101 MHz, $CDCl_3$)



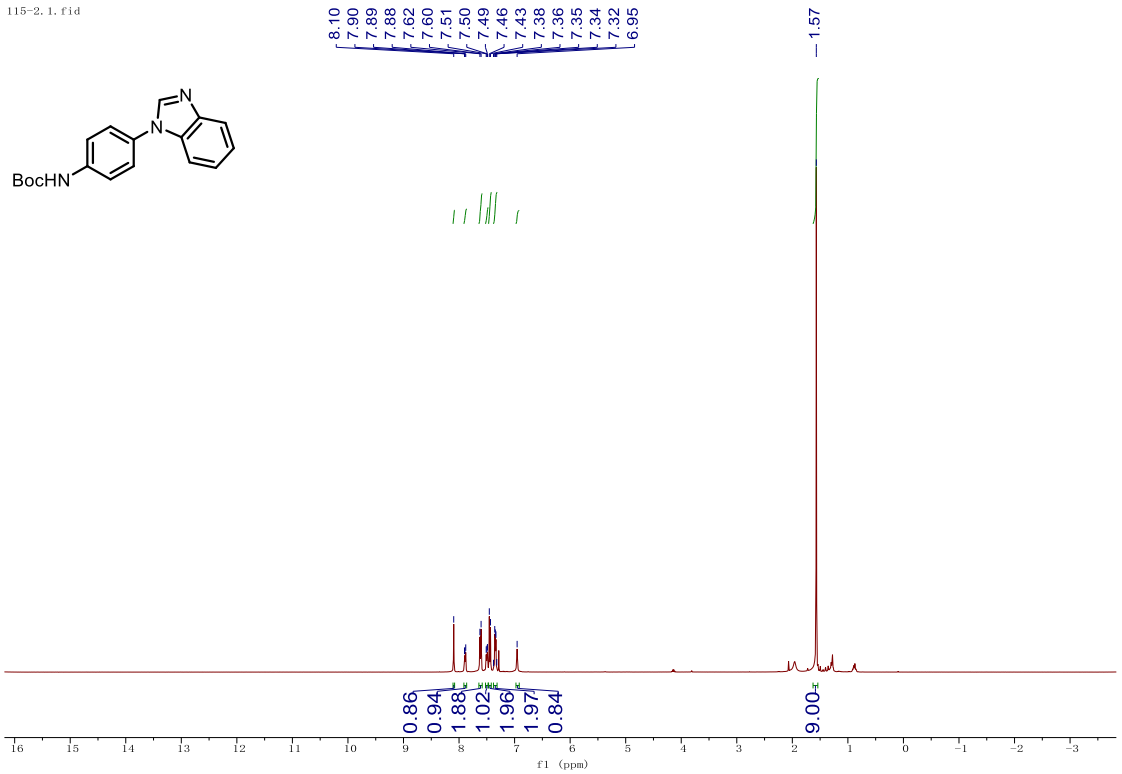
## $^{1}$H NMR of Compound 13 (400 MHz, $CDCl_3$)



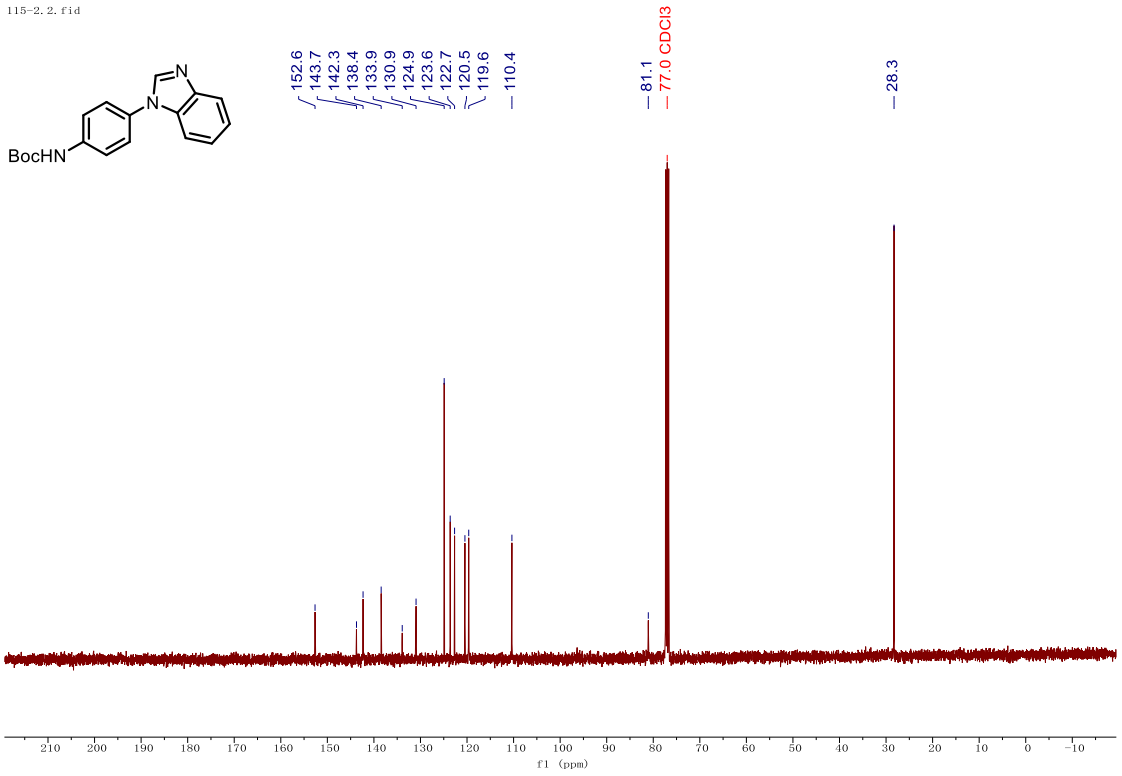

## $^{13}$C NMR of Compound 13 (101 MHz, $CDCl_3$)



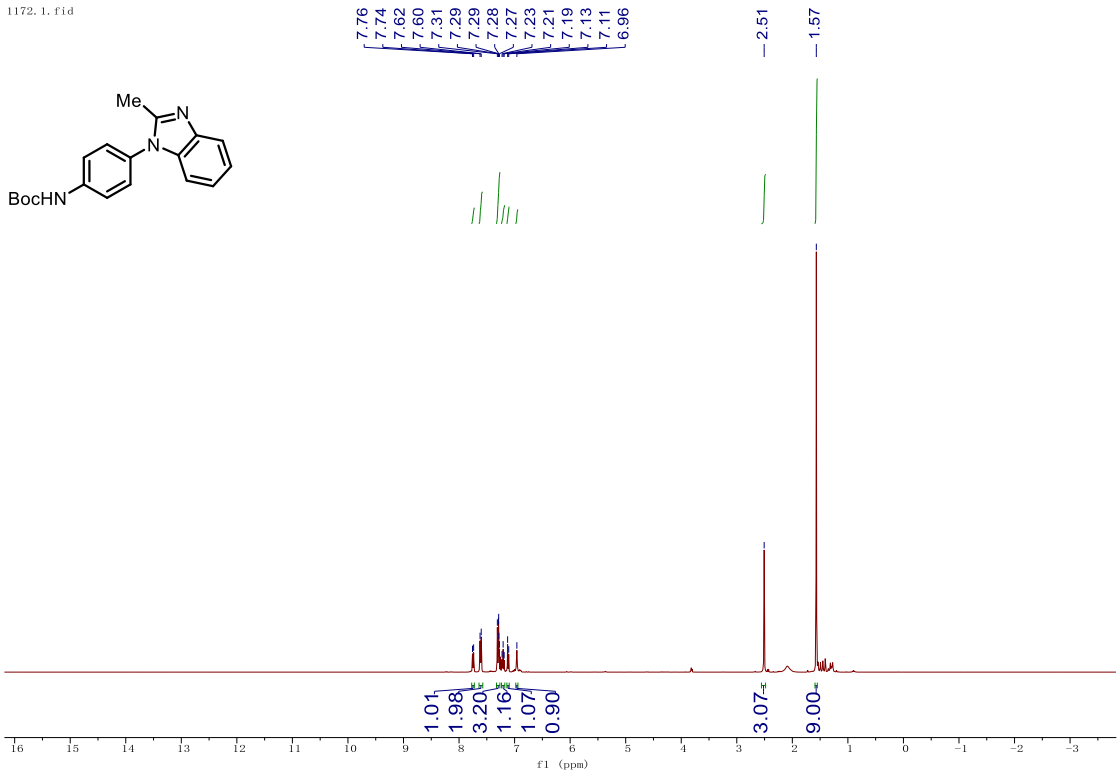
## $^{1}$H NMR of Compound 14 (400 MHz, $CDCl_3$)



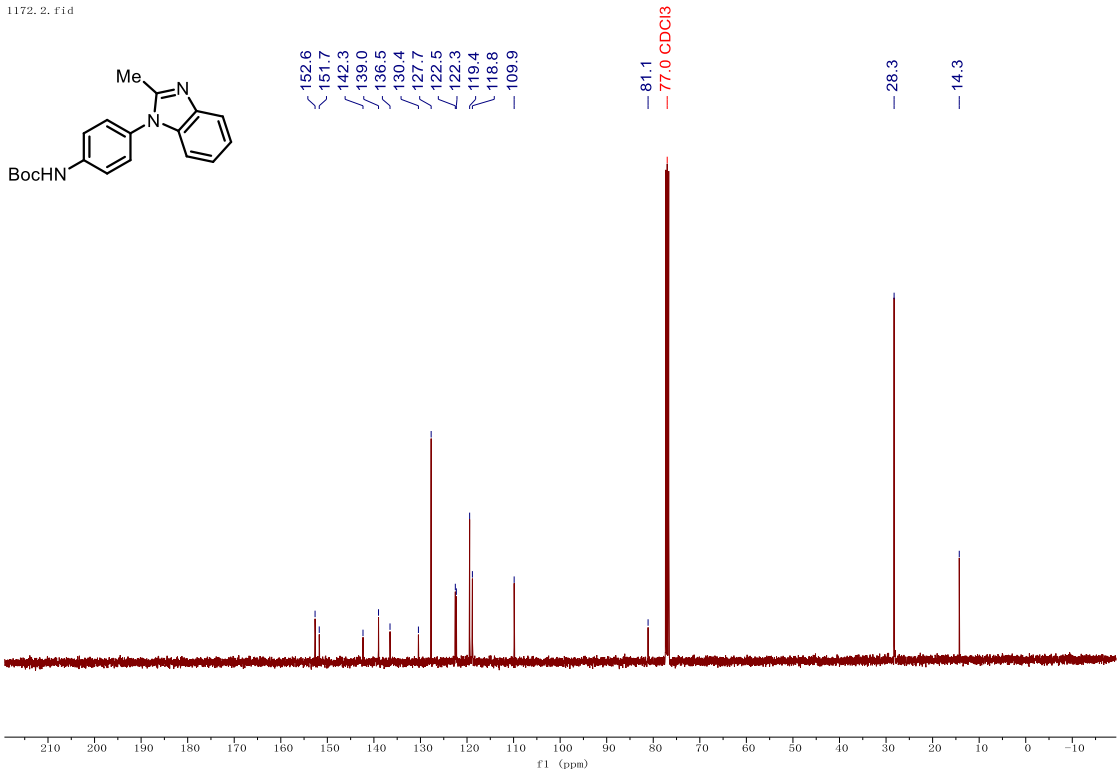

## $^{13}$C NMR of Compound 14 (101 MHz, $CDCl_3$)



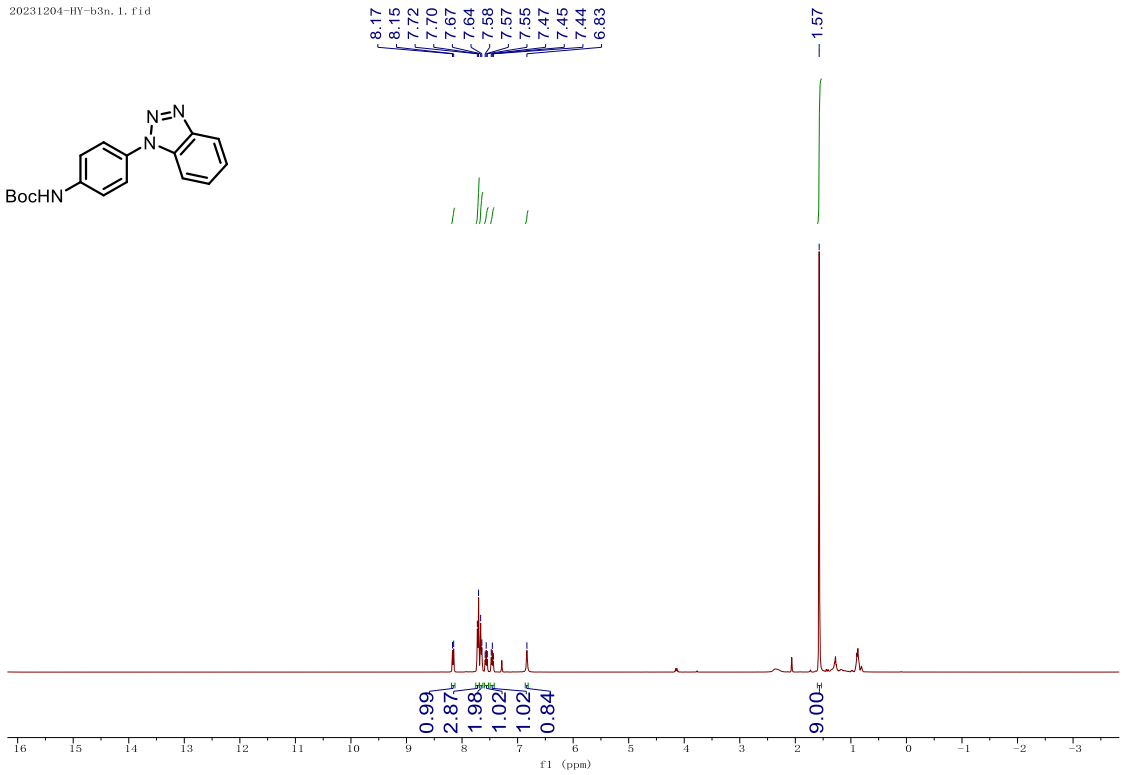
## $^{1}$H NMR of Compound 15 (400 MHz, $CDCl_3$)



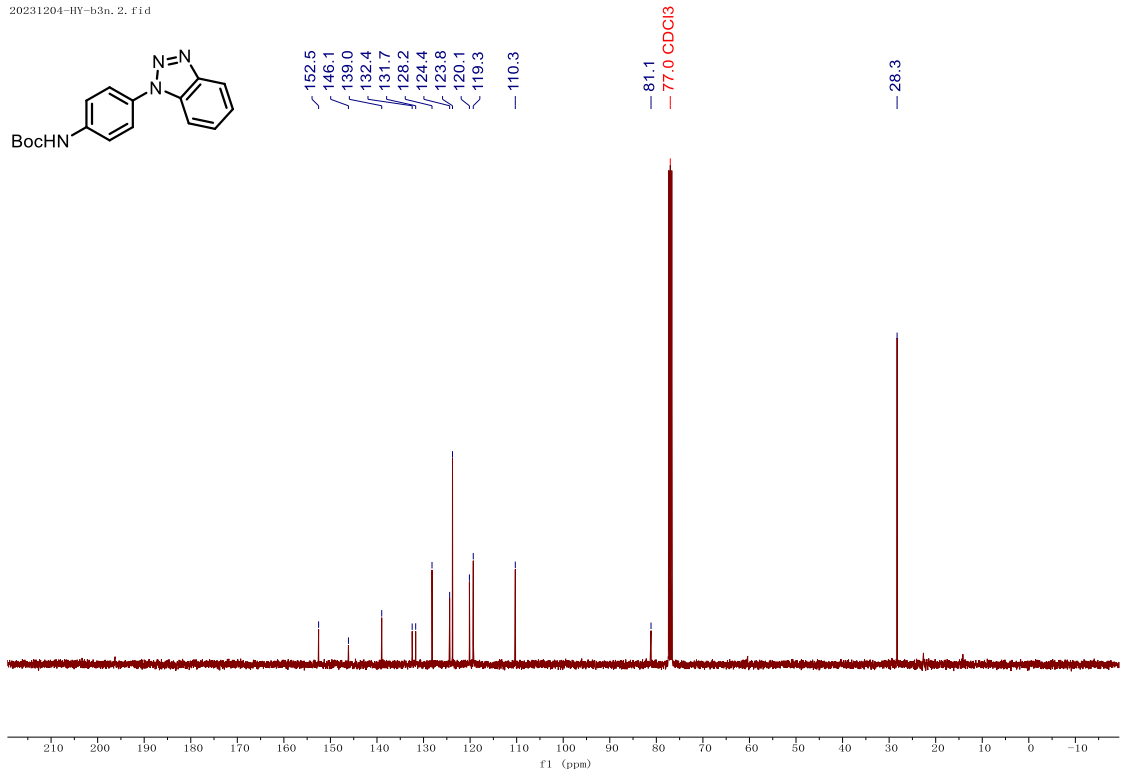

## $^{13}$C NMR of Compound 15 (101 MHz, $CDCl_3$)



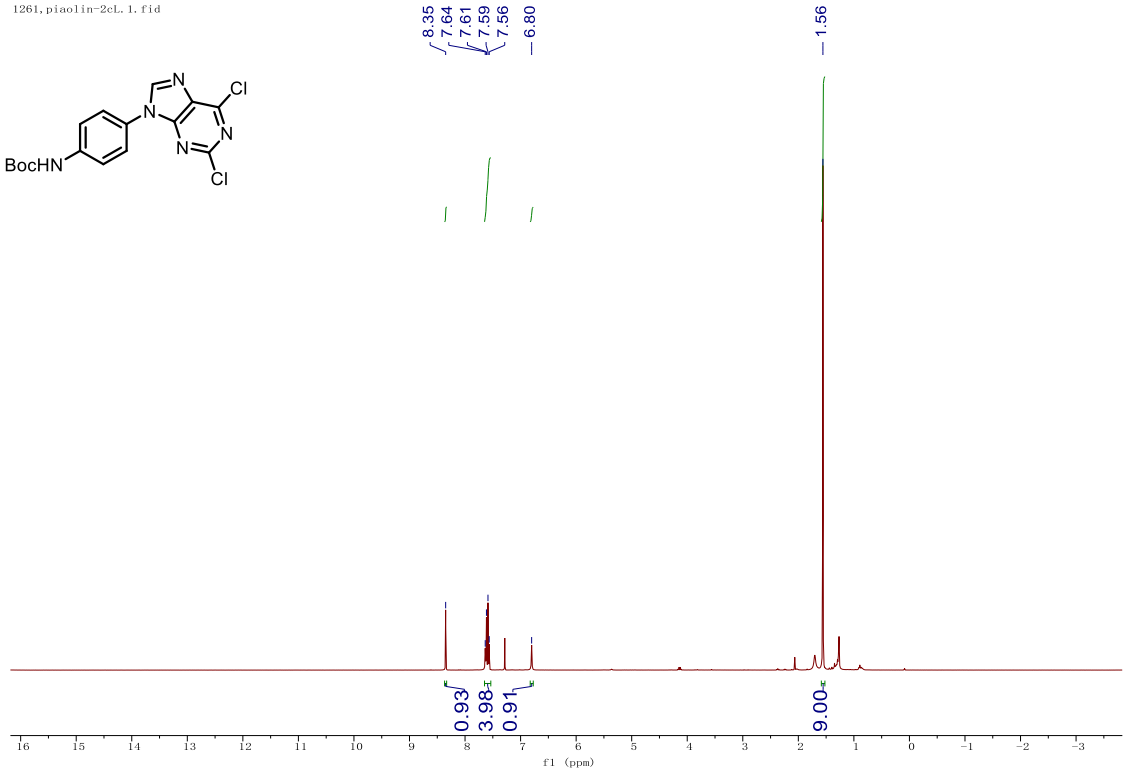
## $^{1}$H NMR of Compound 16 (400 MHz, $CDCl_3$)



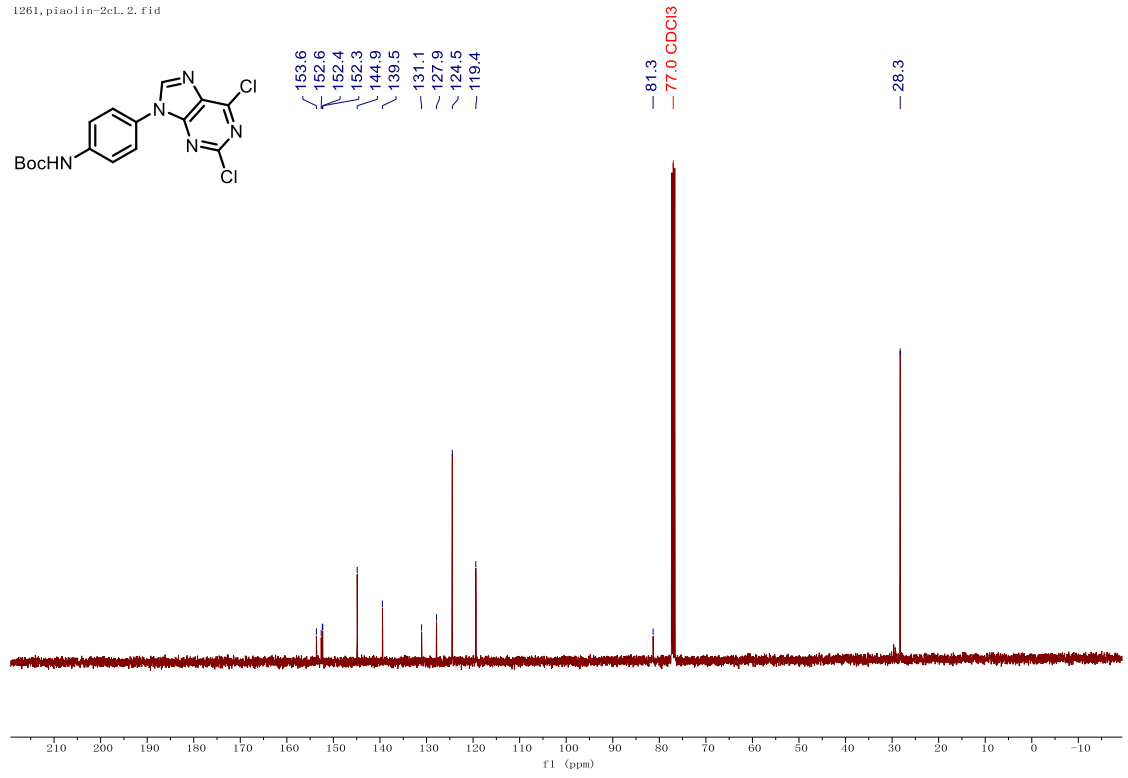

## $^{13}$C NMR of Compound 16 (101 MHz, $CDCl_3$)



## $^{1}$H NMR of Compound 17 (400 MHz, $CDCl_3$)




## $^{13}$C NMR of Compound 17 (101 MHz, $CDCl_3$)



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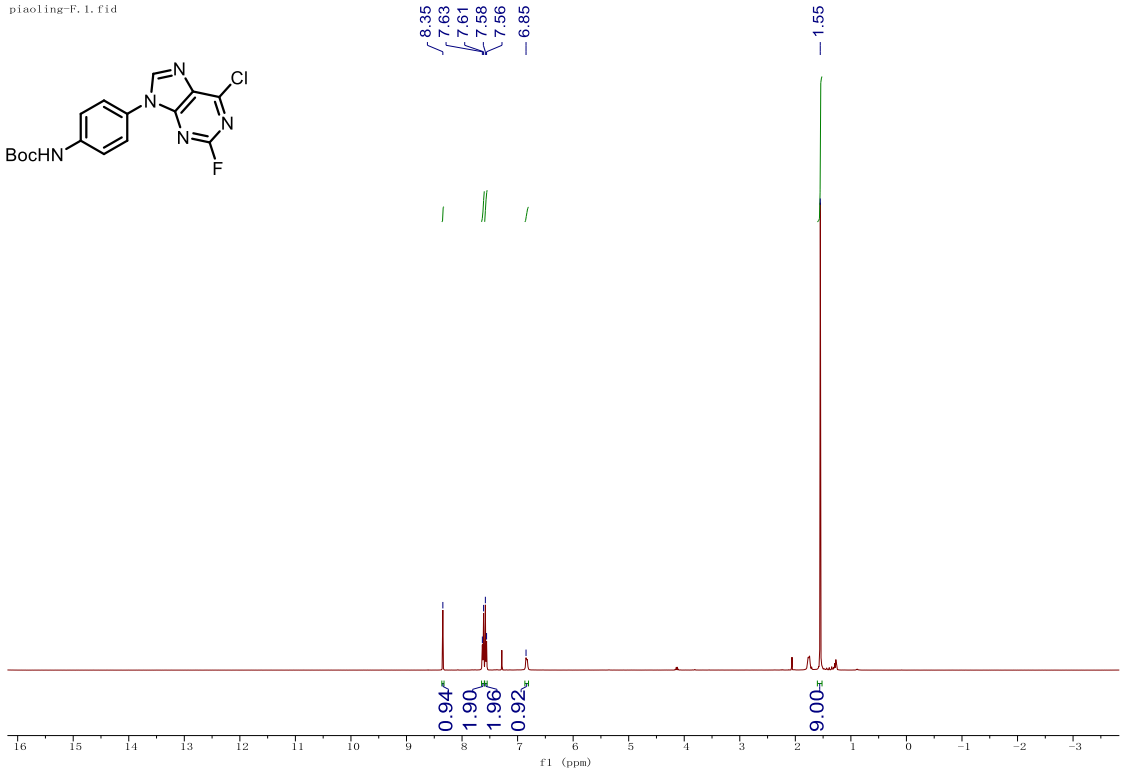
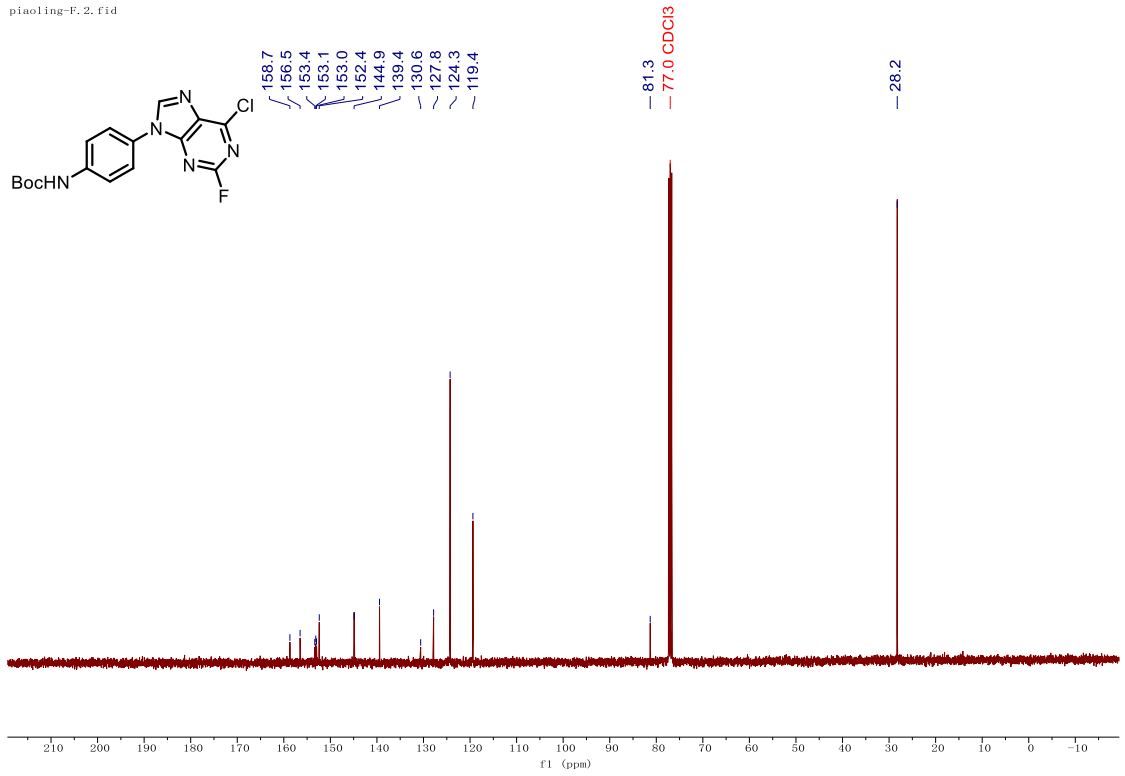
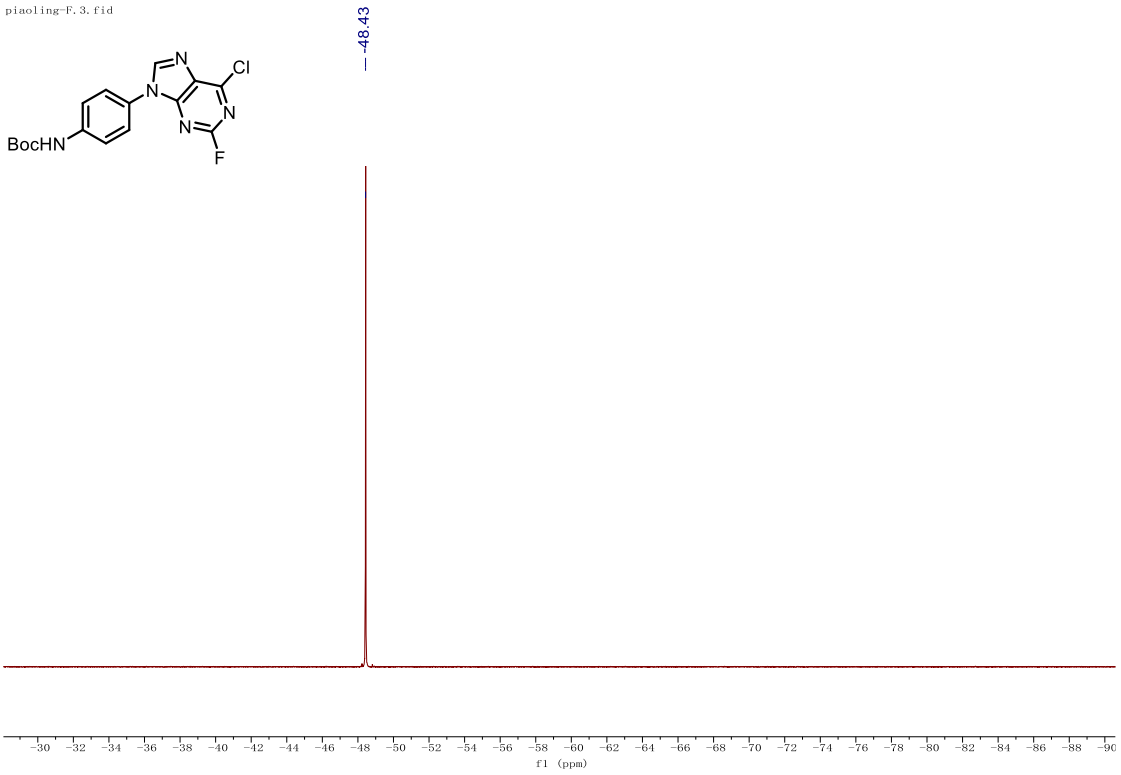



## $^{13}$C NMR of Compound 18 (101 MHz, $CDCl_3$)



## $^{19}$F NMR of Compound 18 (376 MHz, $CDCl_3$)



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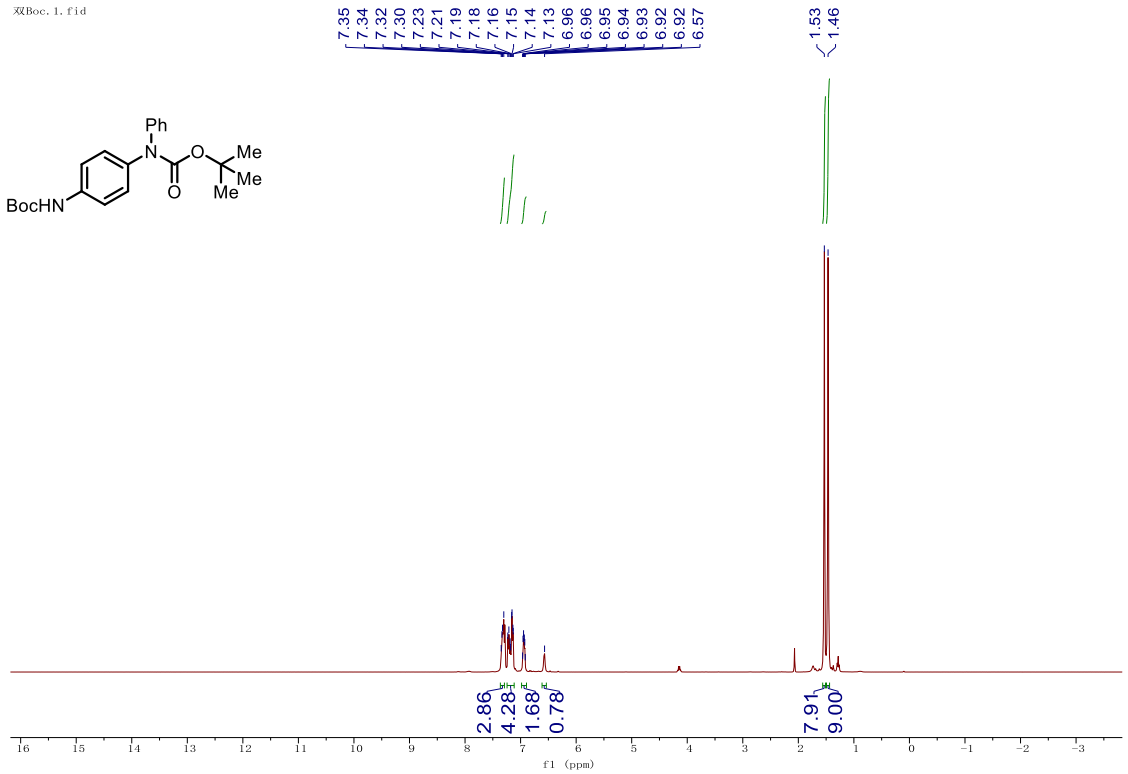


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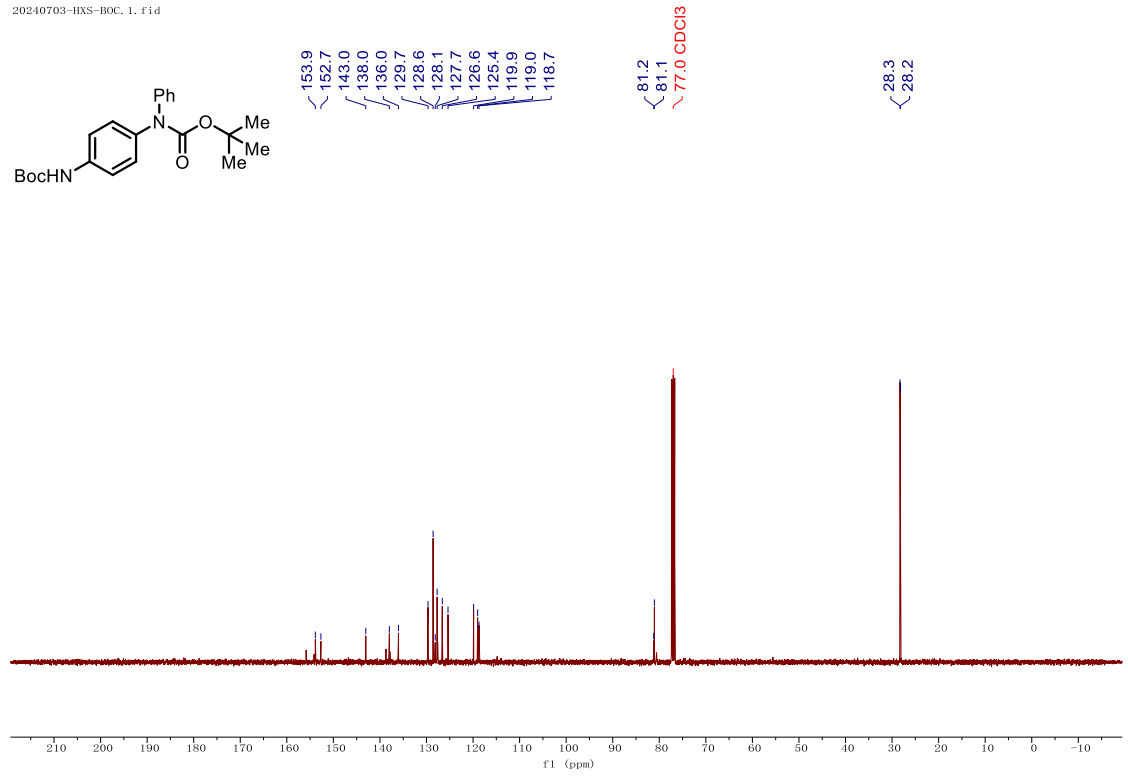

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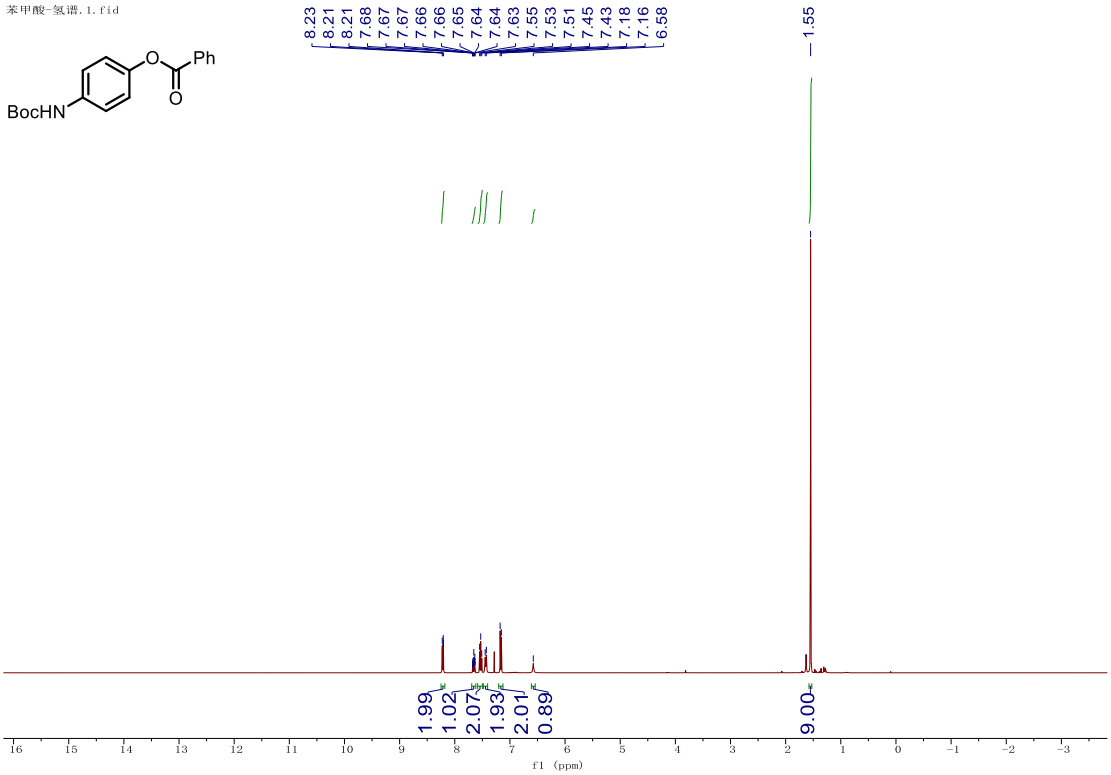
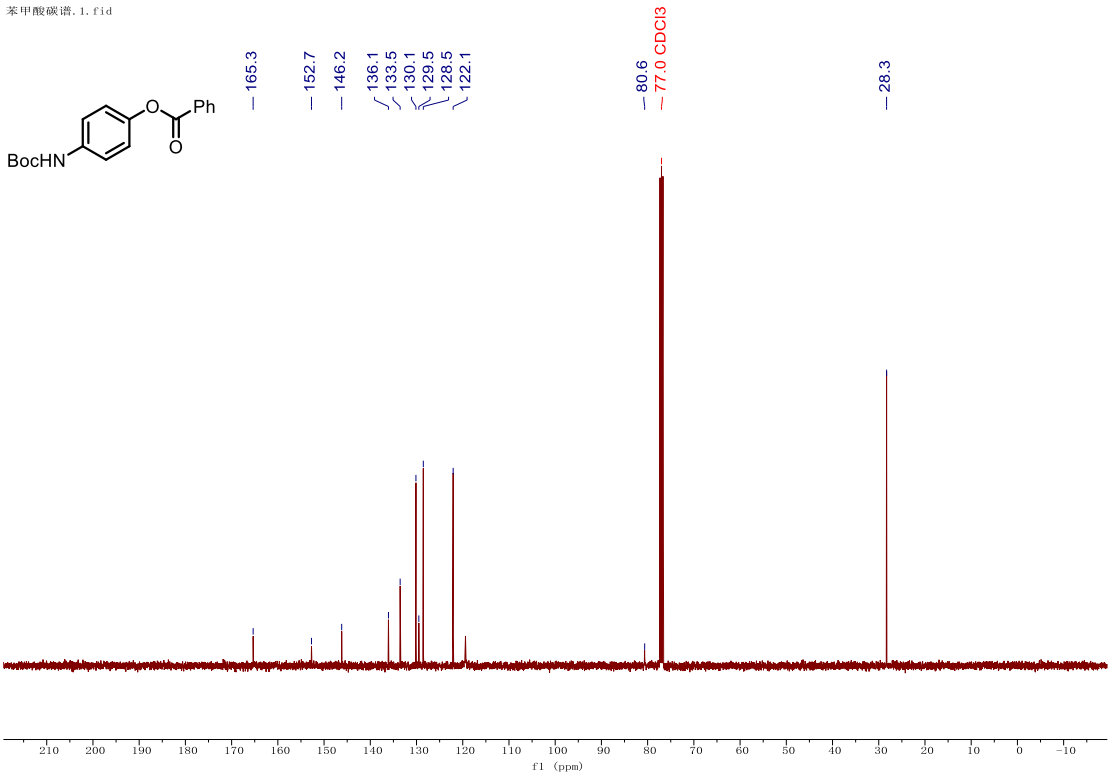



## $^{13}$C NMR of Compound 20 (101 MHz, $CDCl_3$)



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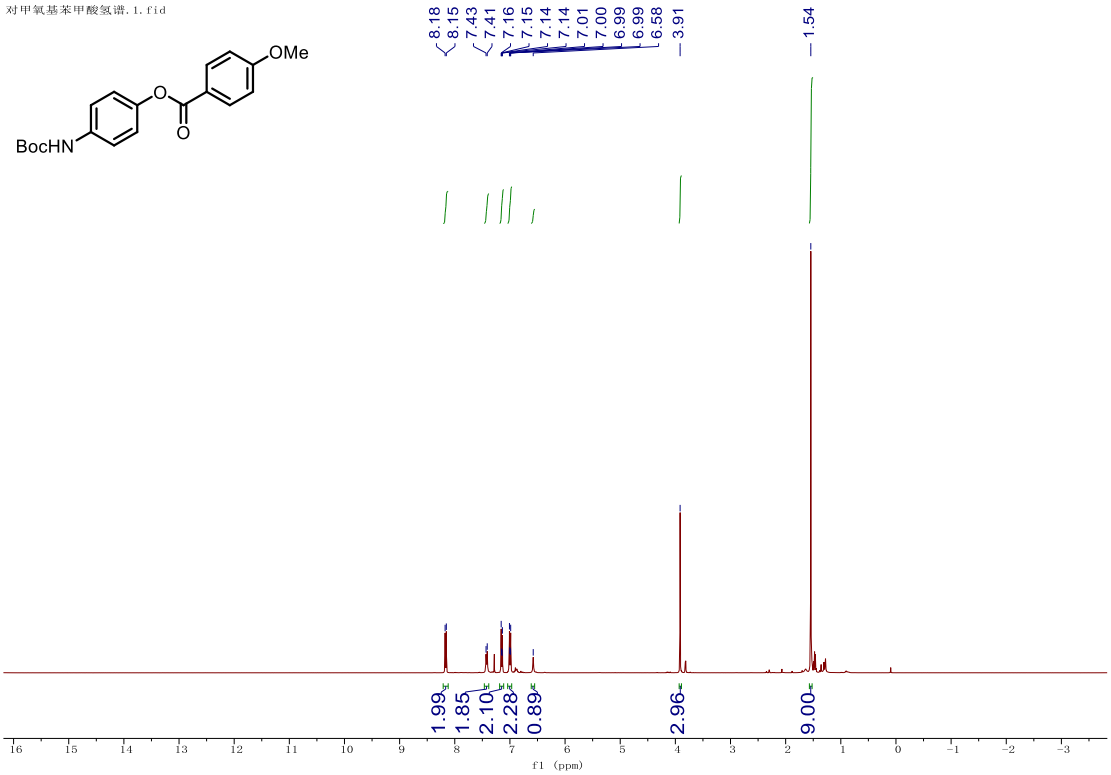
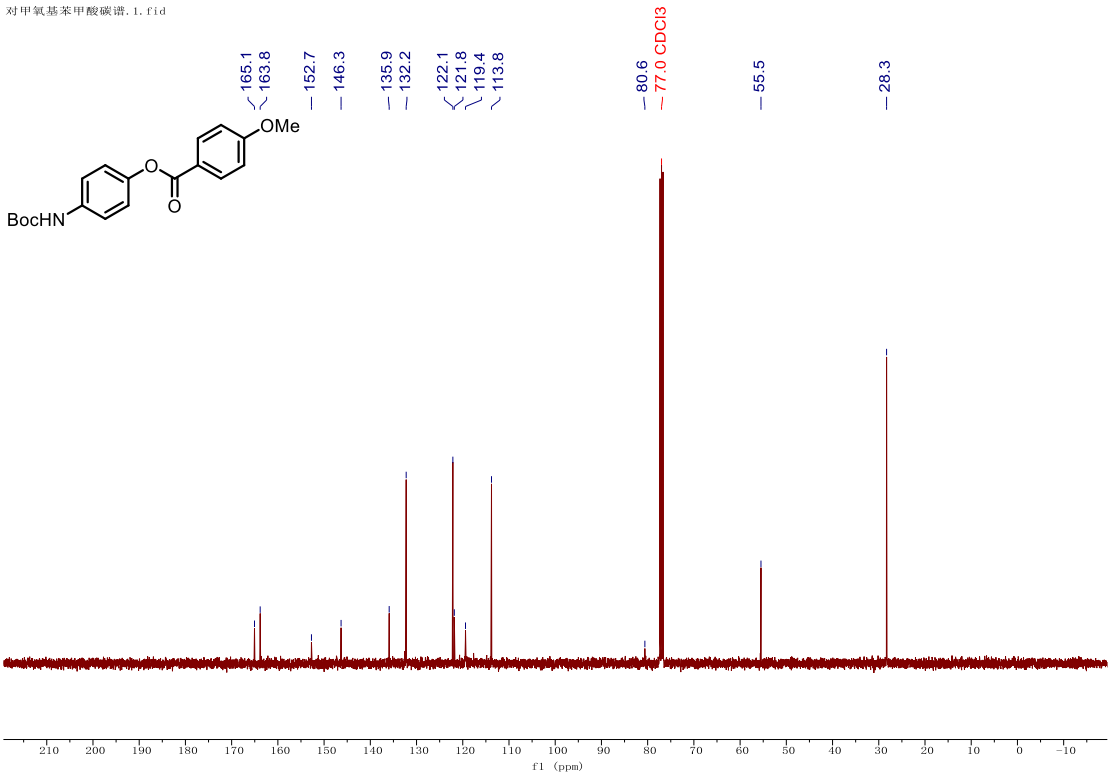



## $^{13}$C NMR of Compound 21 (101 MHz, $CDCl_3$)



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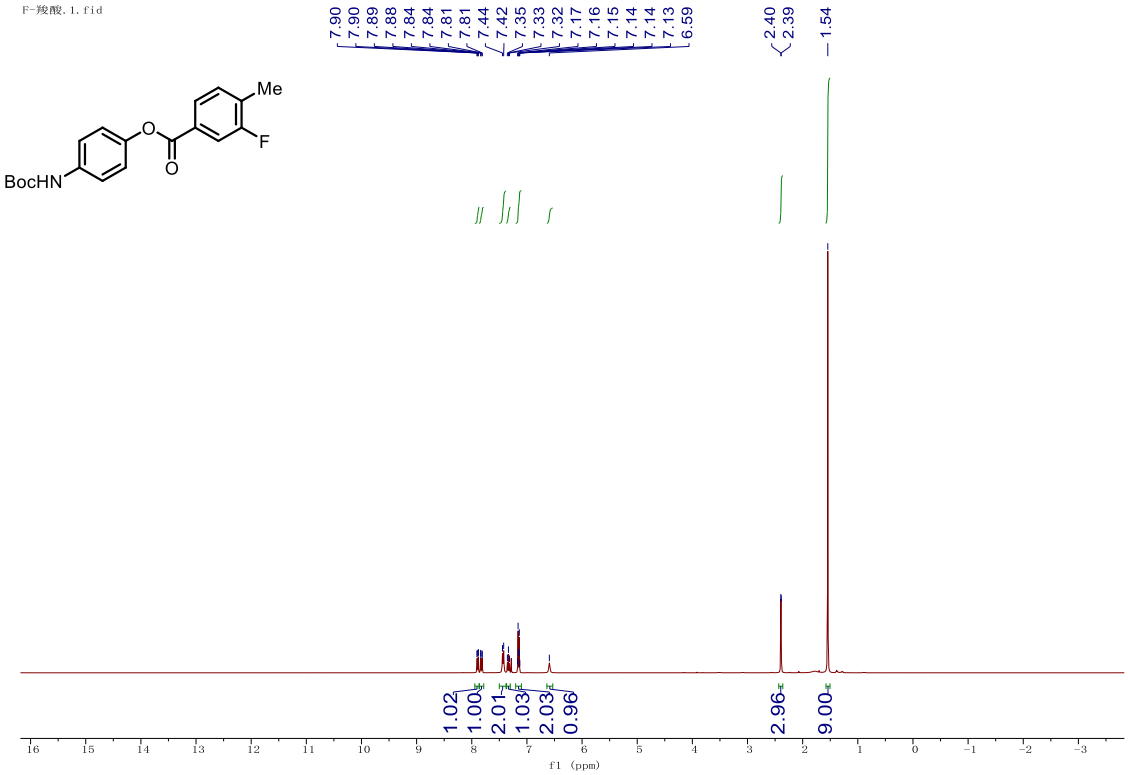


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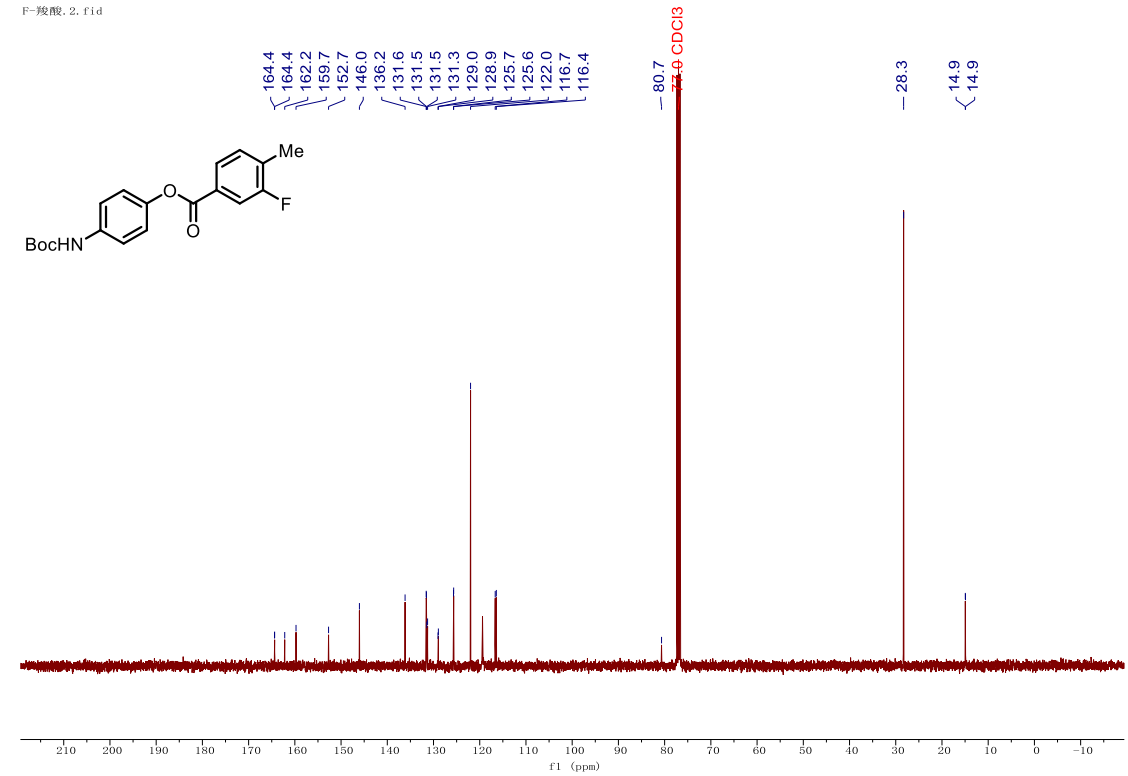
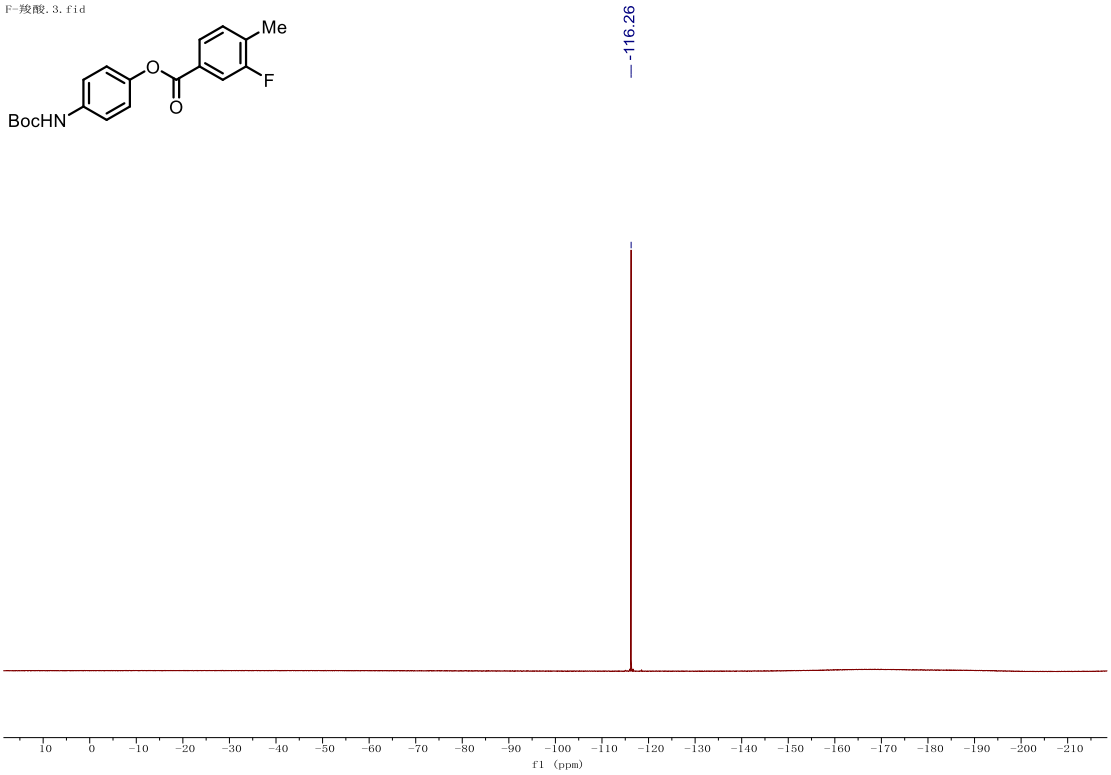


## $^{19}$F NMR of Compound 22 (376 MHz, $CDCl_3$)



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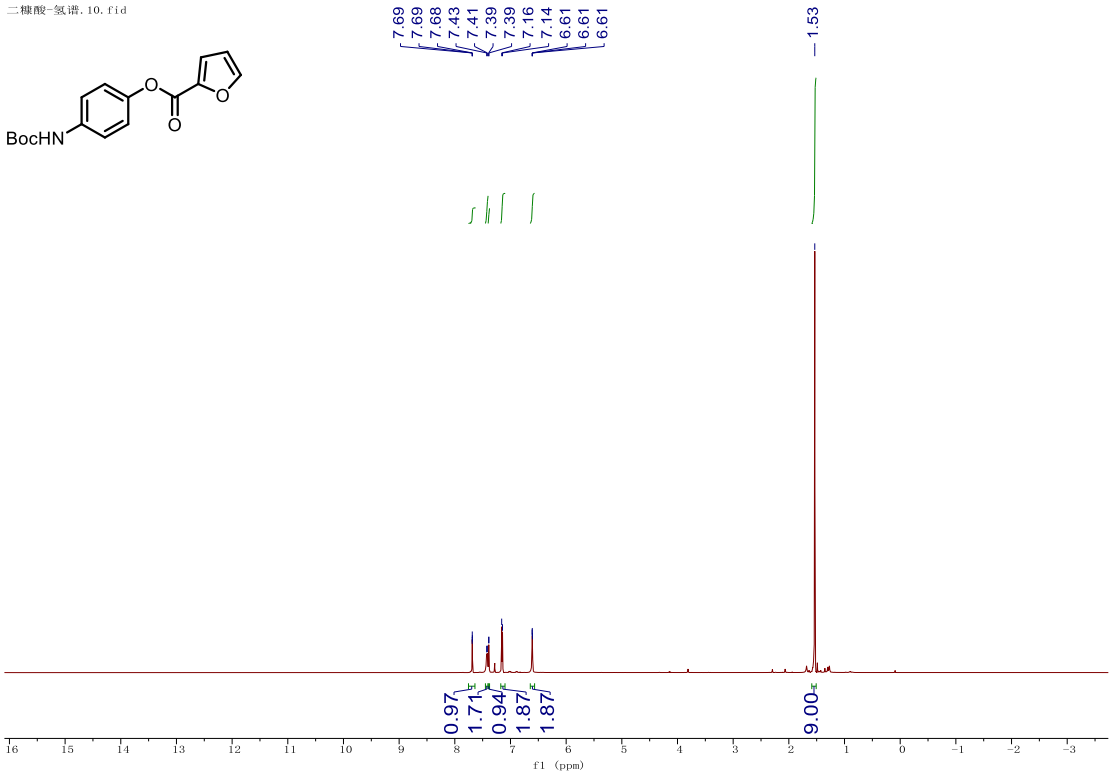


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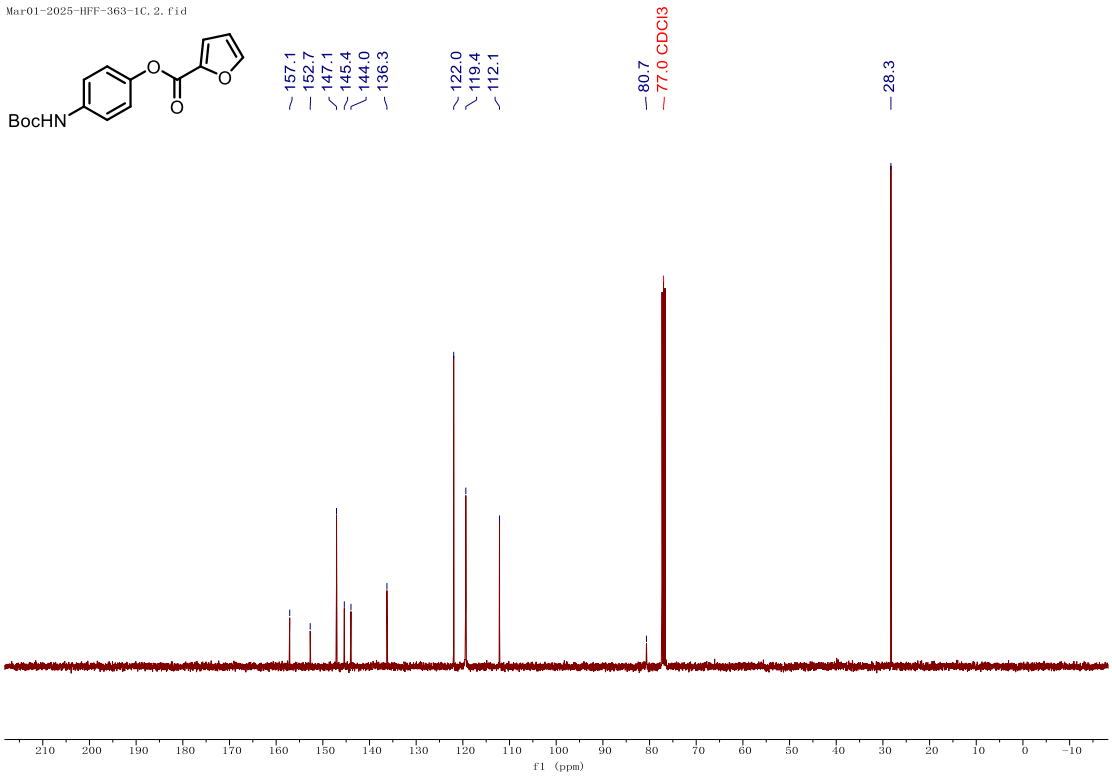

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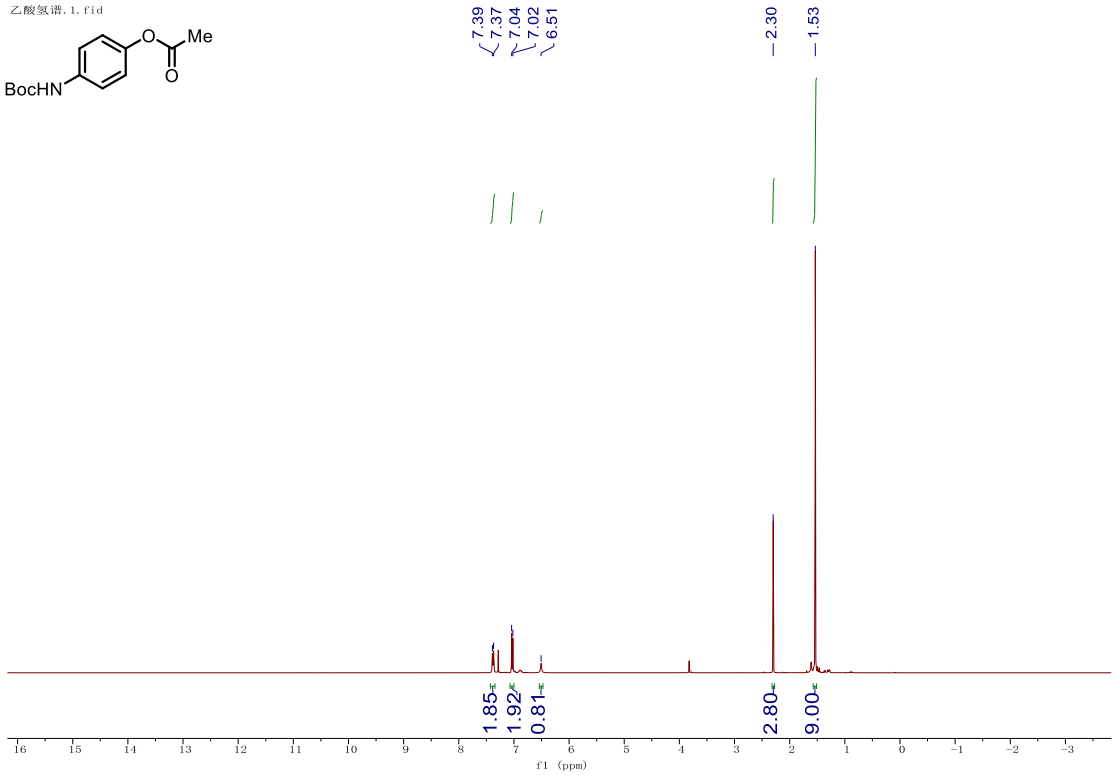


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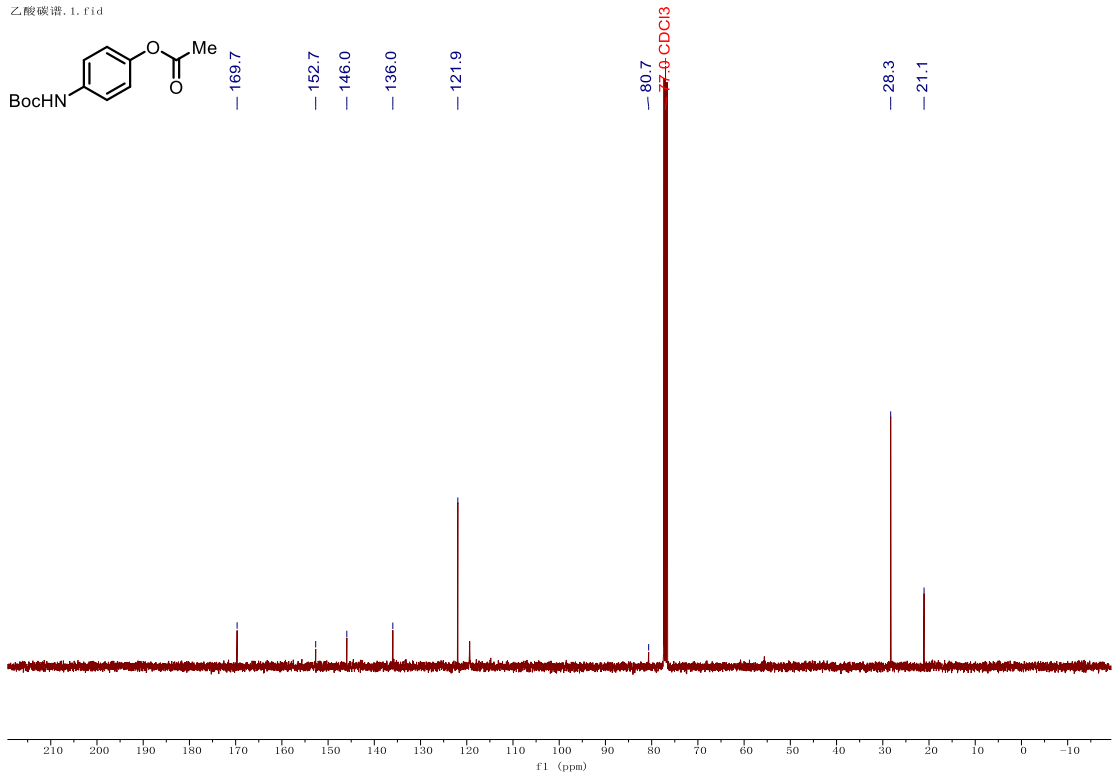
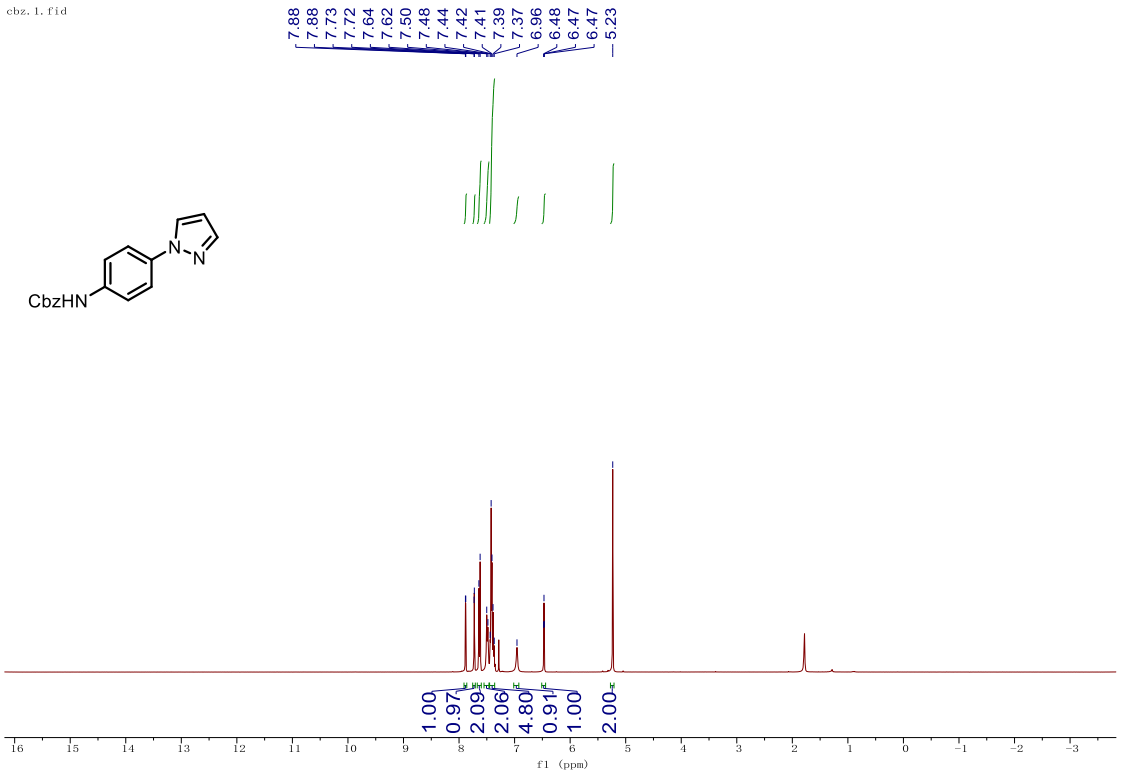


## $^{1}$H NMR of Compound 25 (400 MHz, $CDCl_3$)

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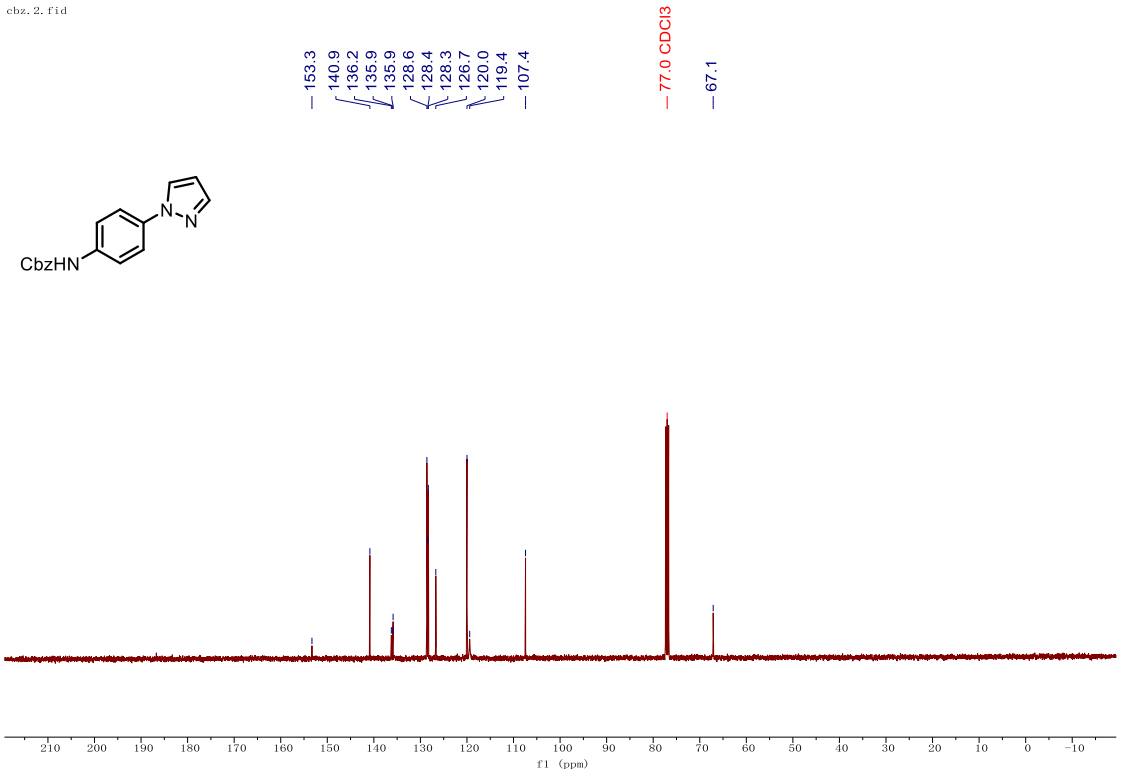
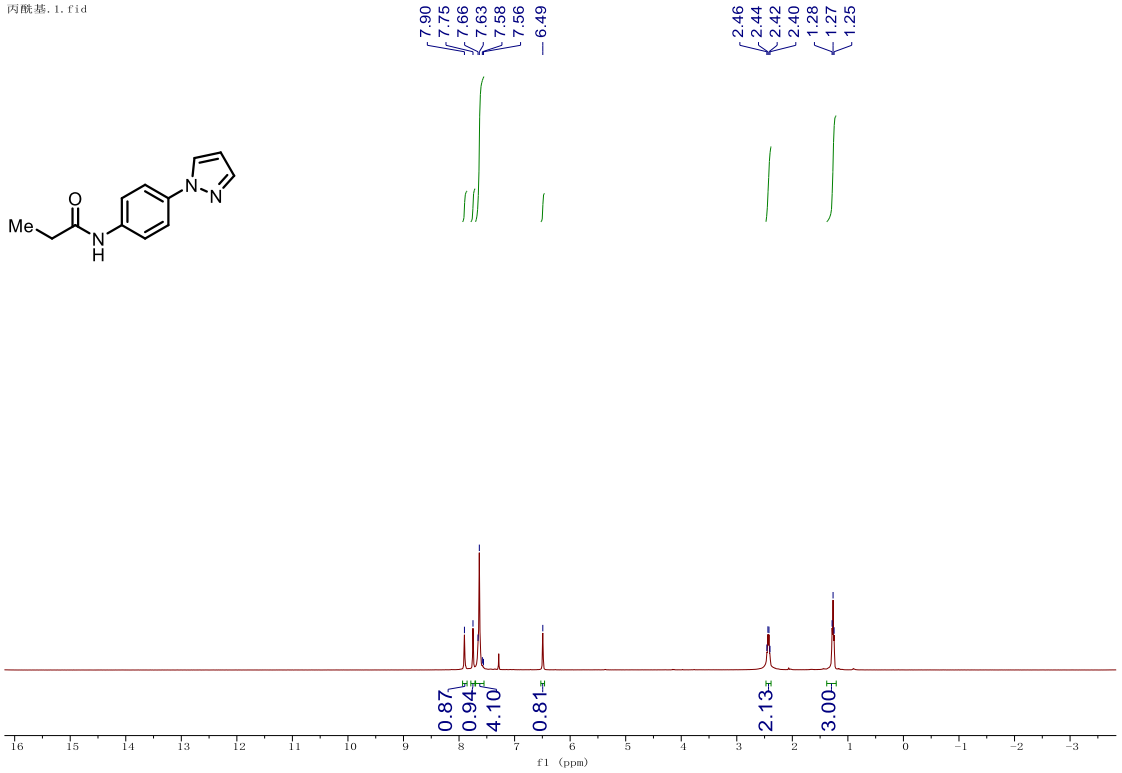


## $^{1}$H NMR of Compound 26 (400 MHz, $CDCl_3$)

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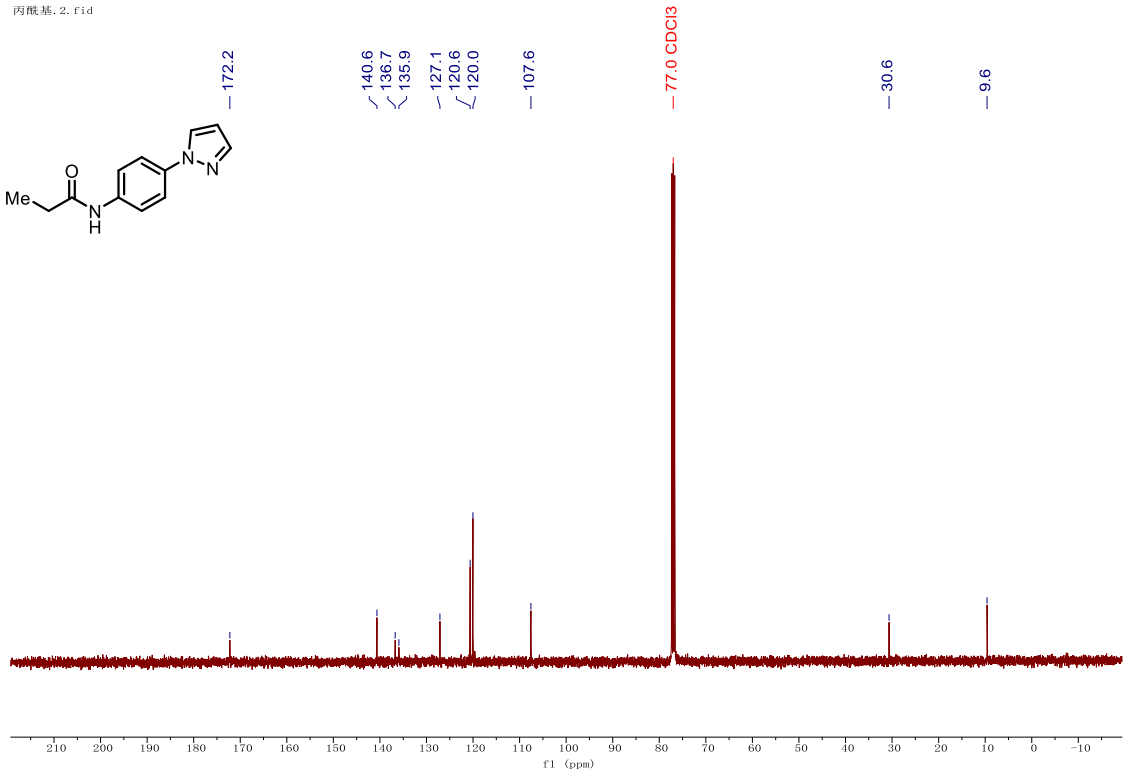

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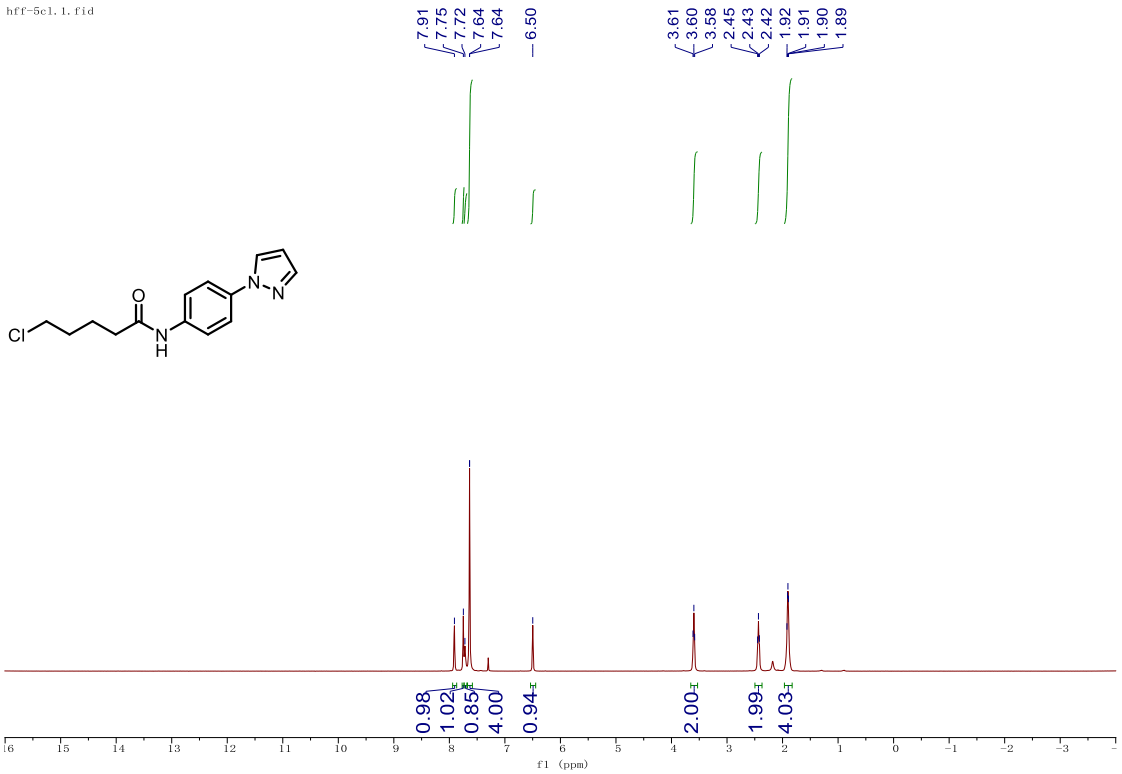
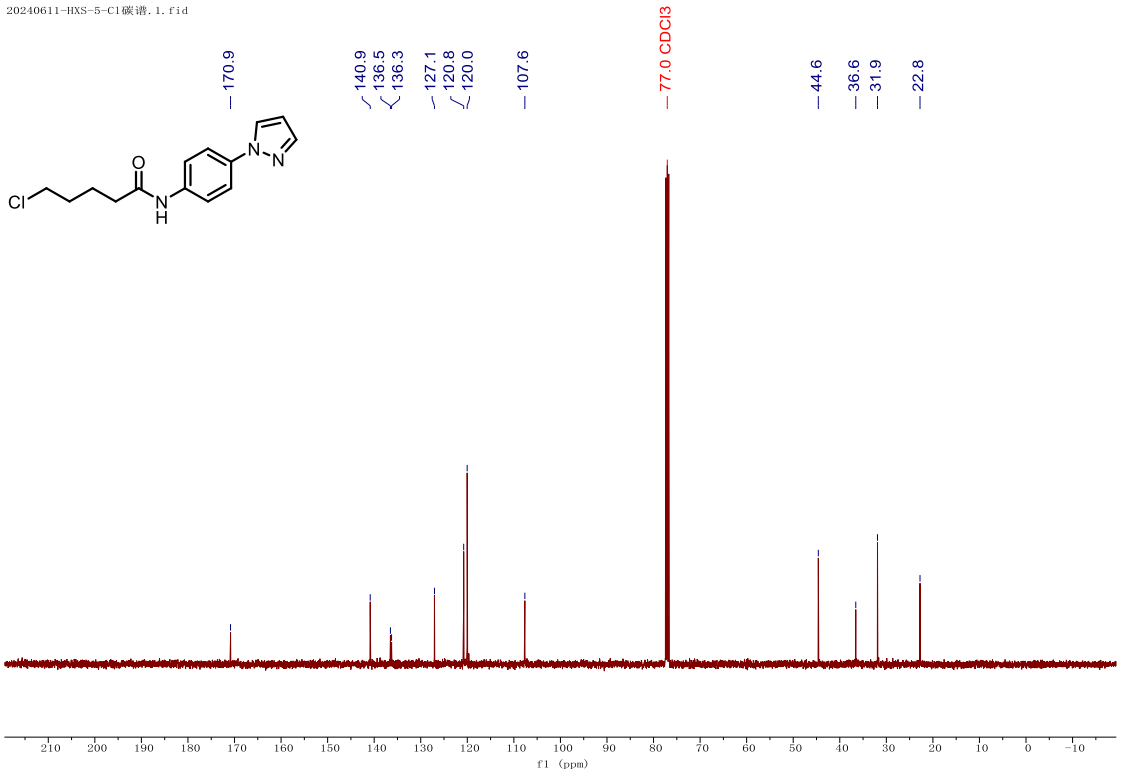



## $^{13}$C NMR of Compound 27 (101 MHz, $CDCl_3$)



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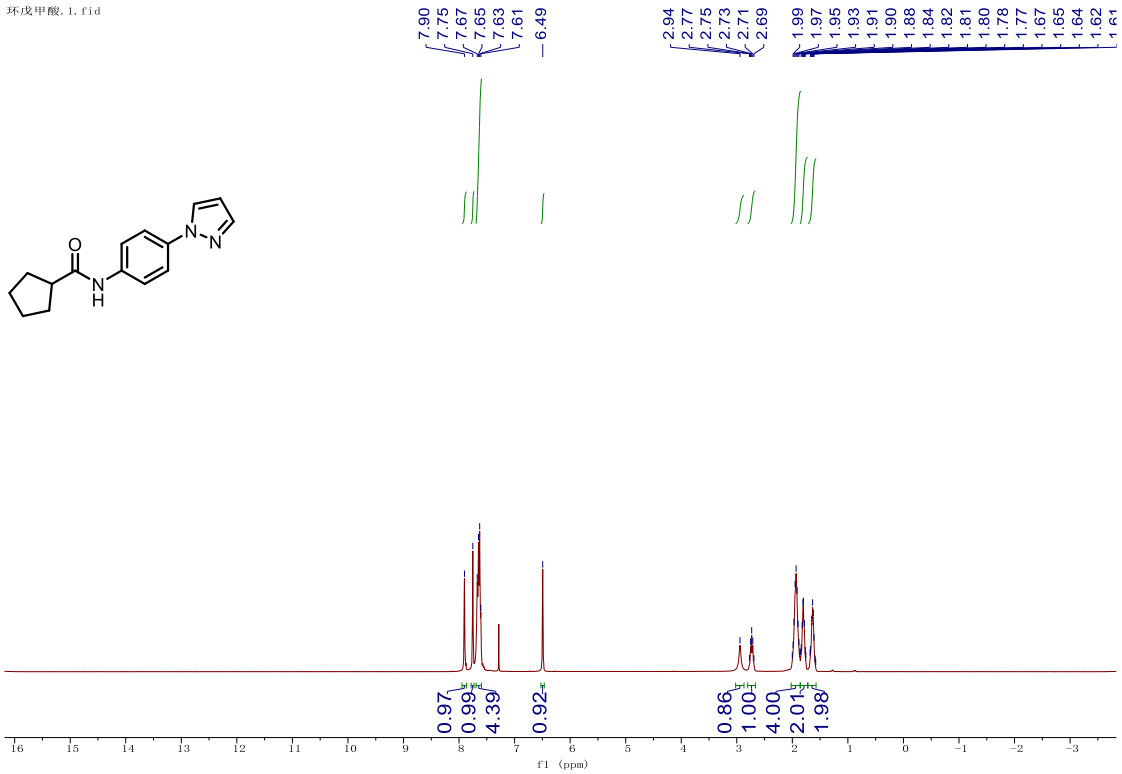


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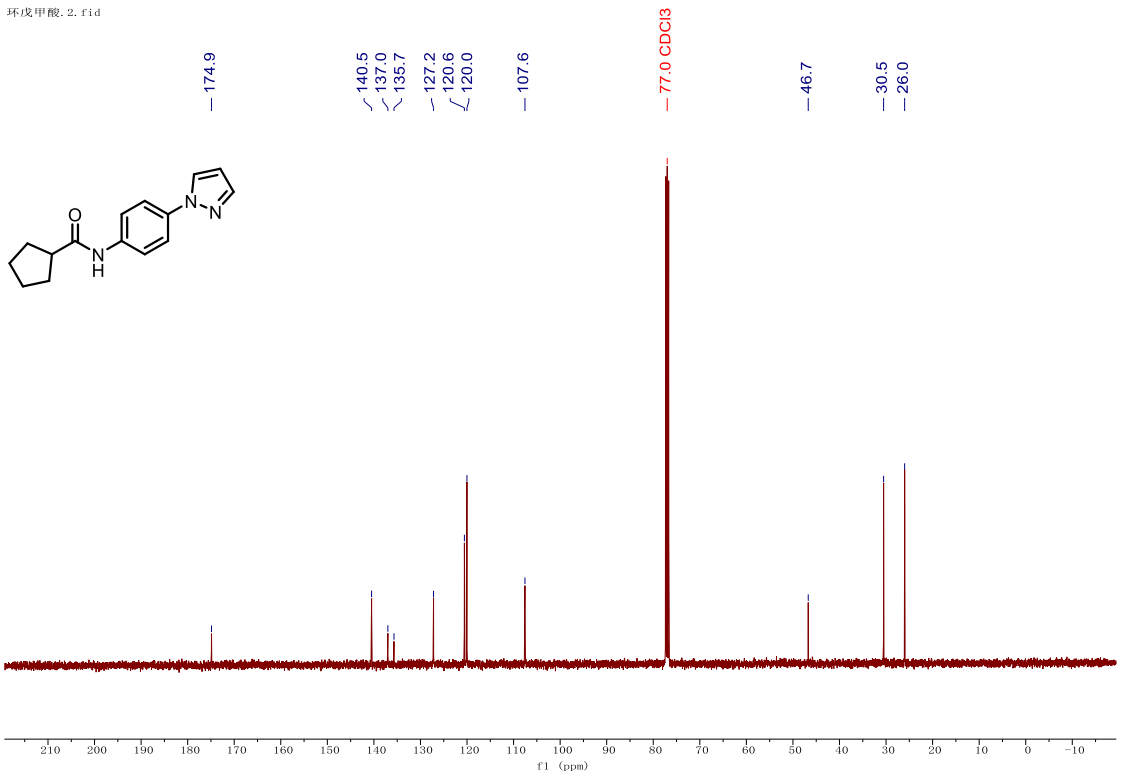

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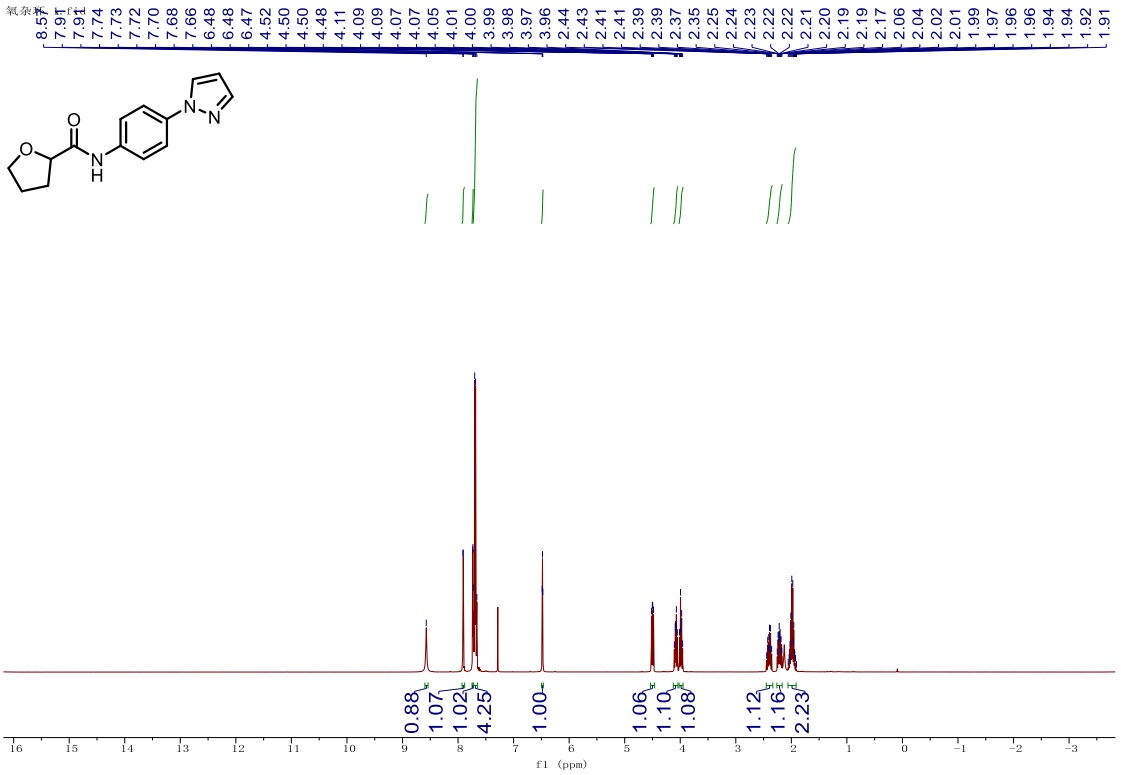


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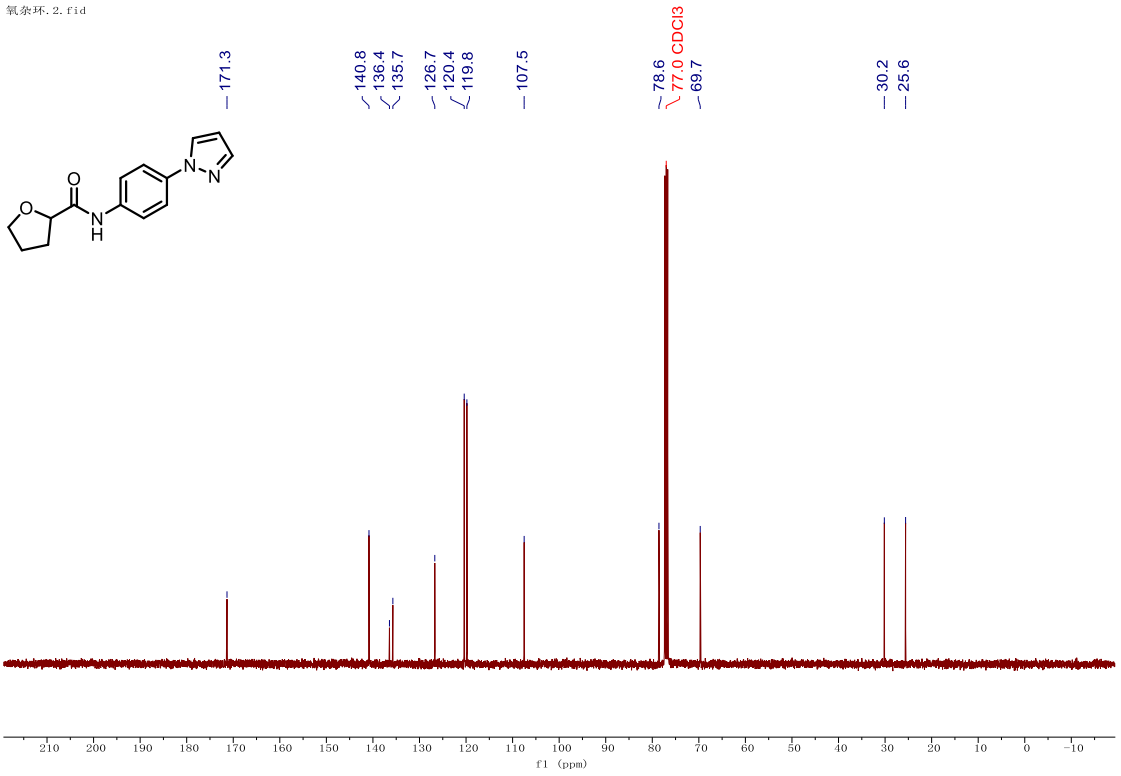

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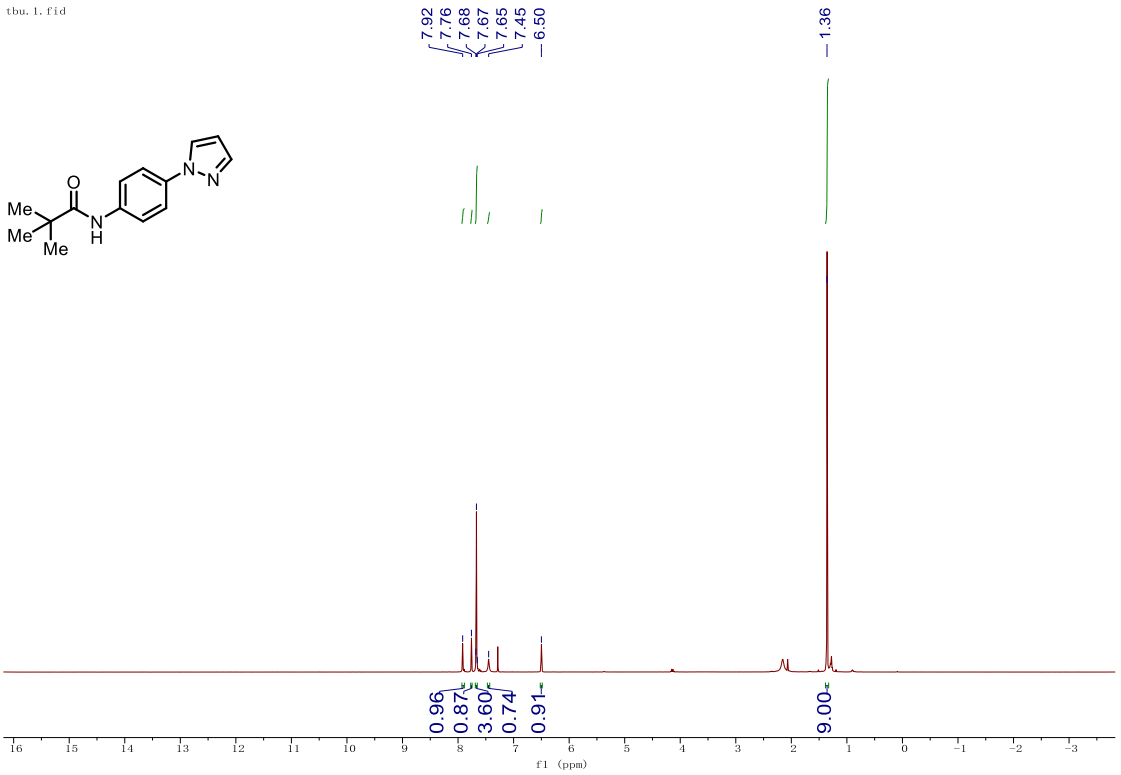


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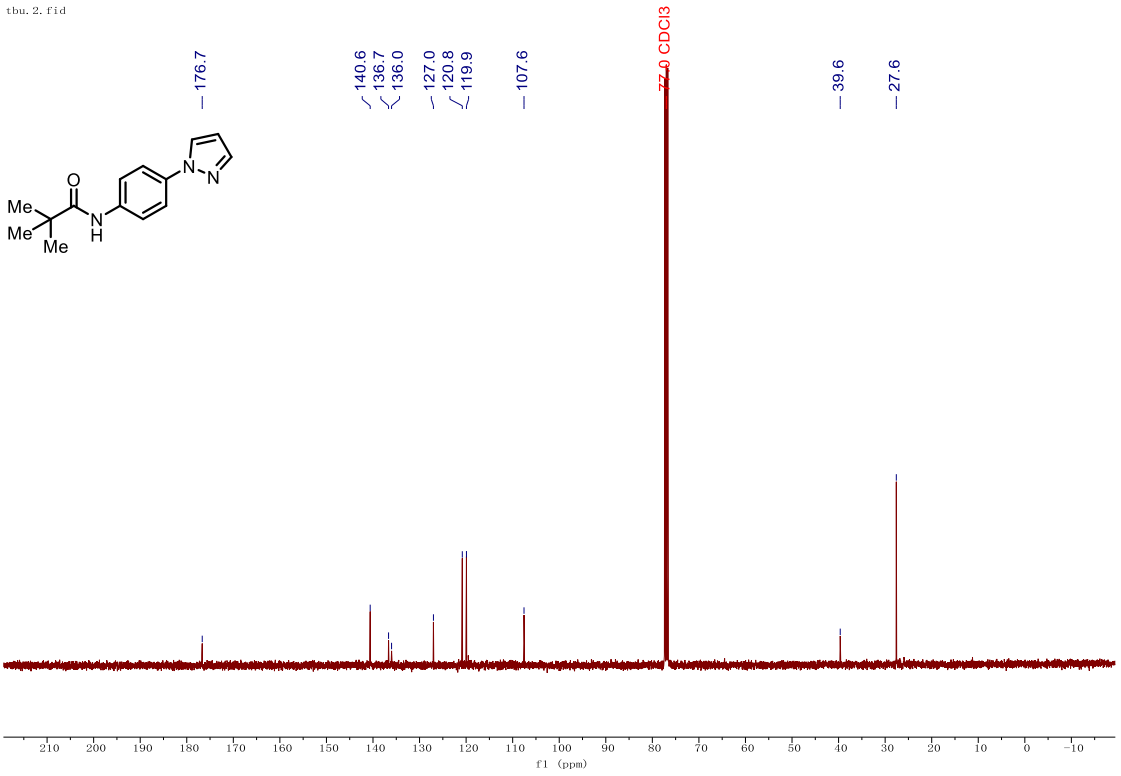

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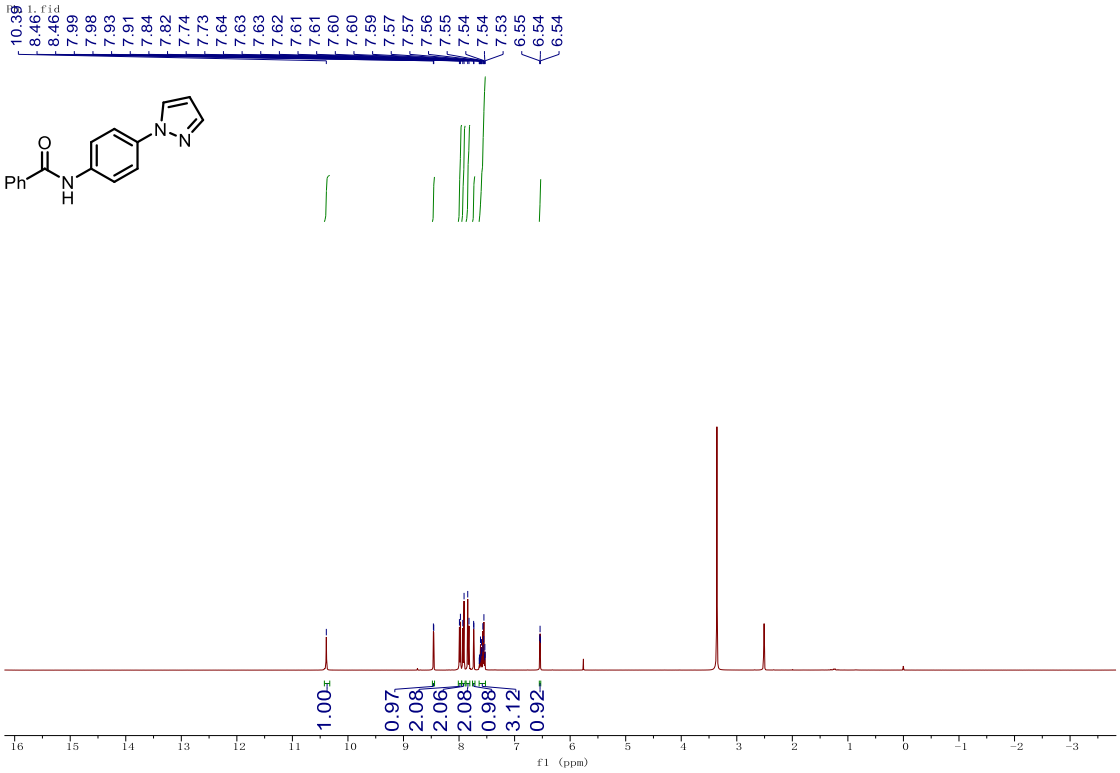
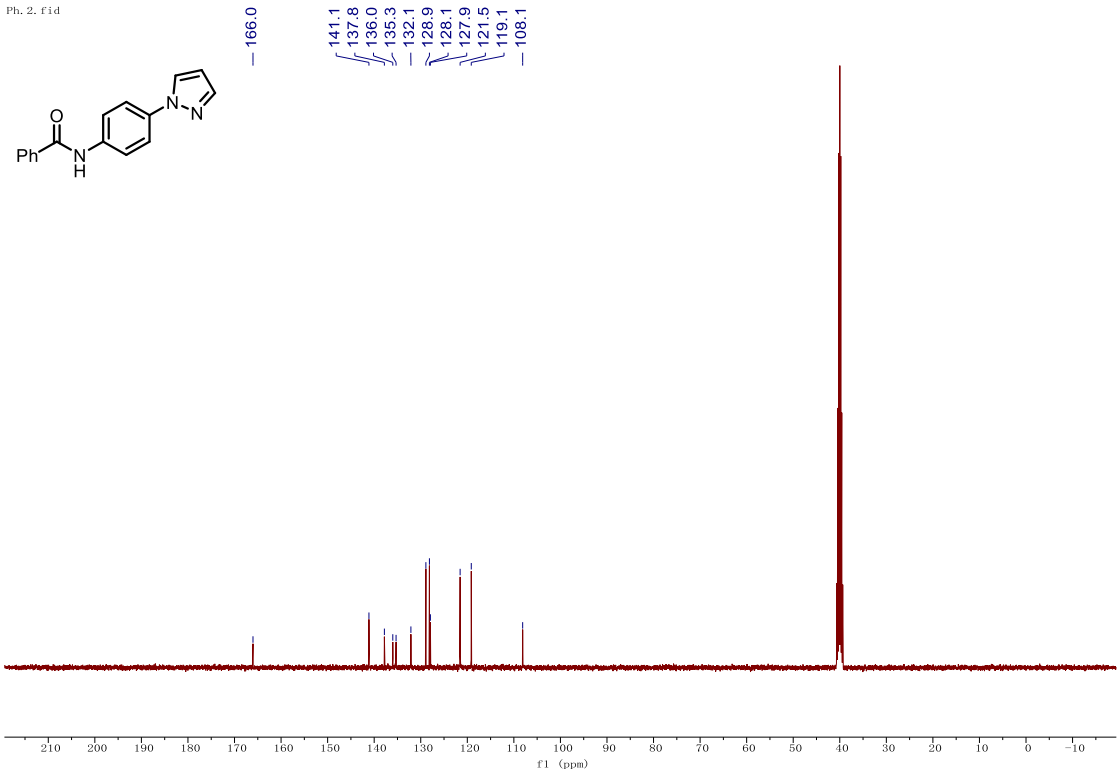



## $^{13}$C NMR of Compound 31 (101 MHz, DMSO-$d_6$)



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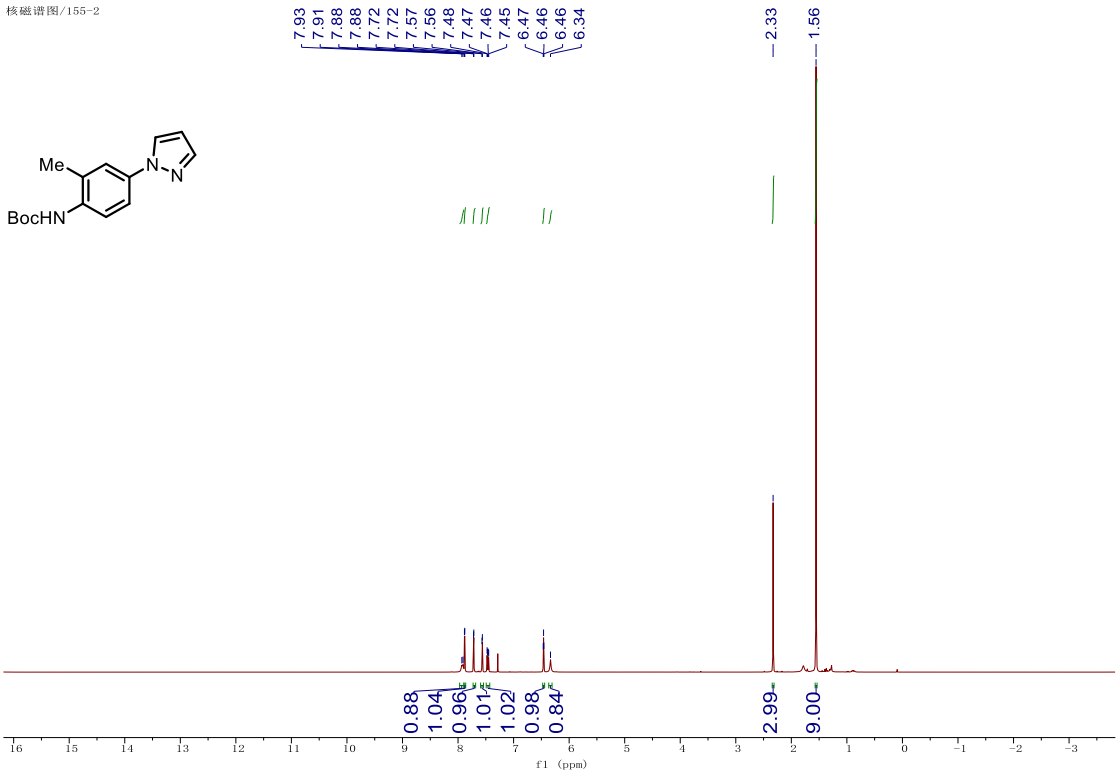


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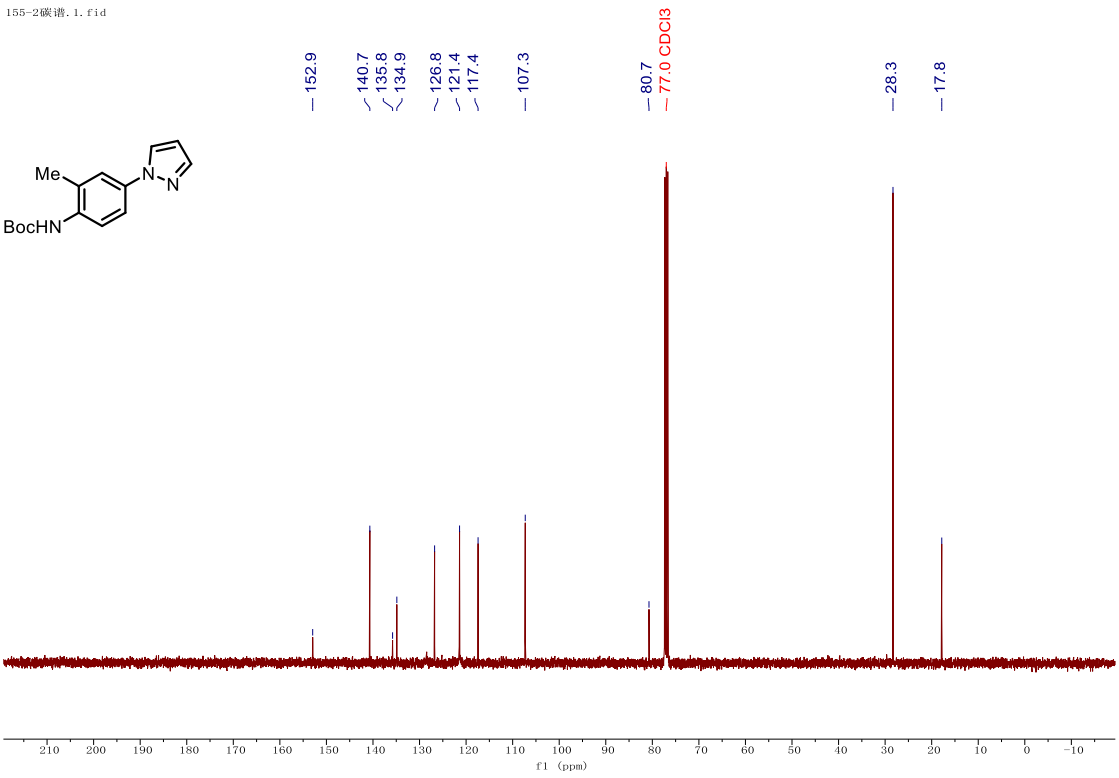

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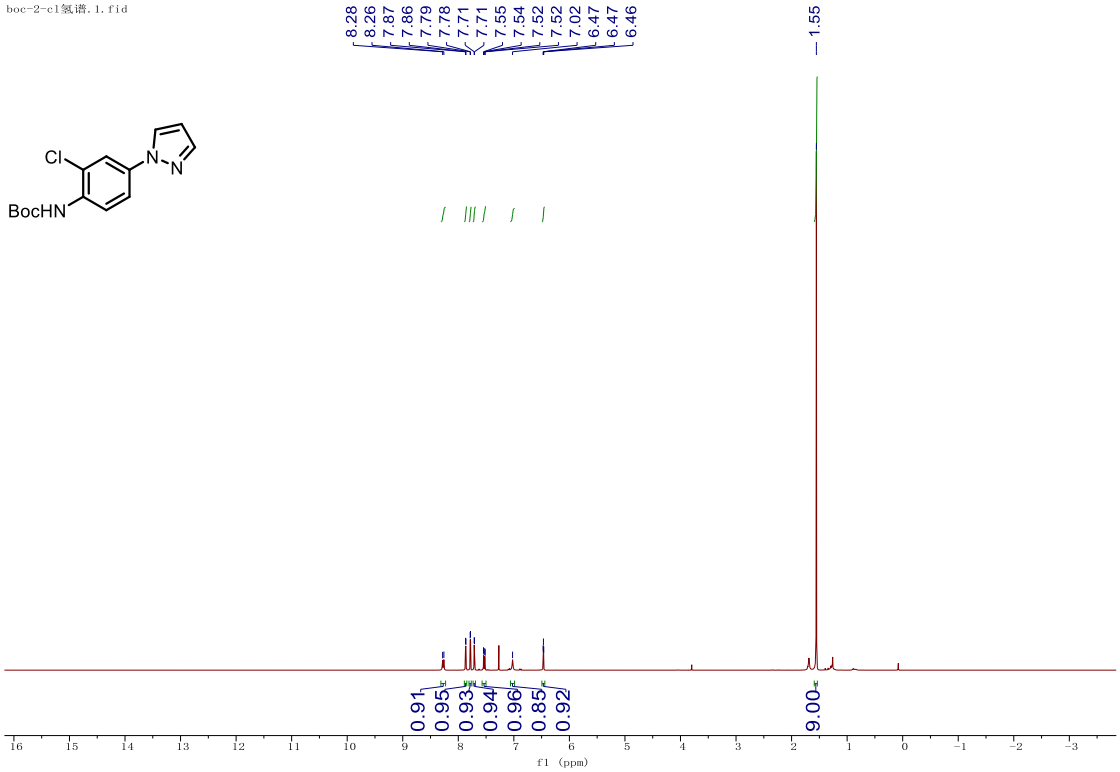


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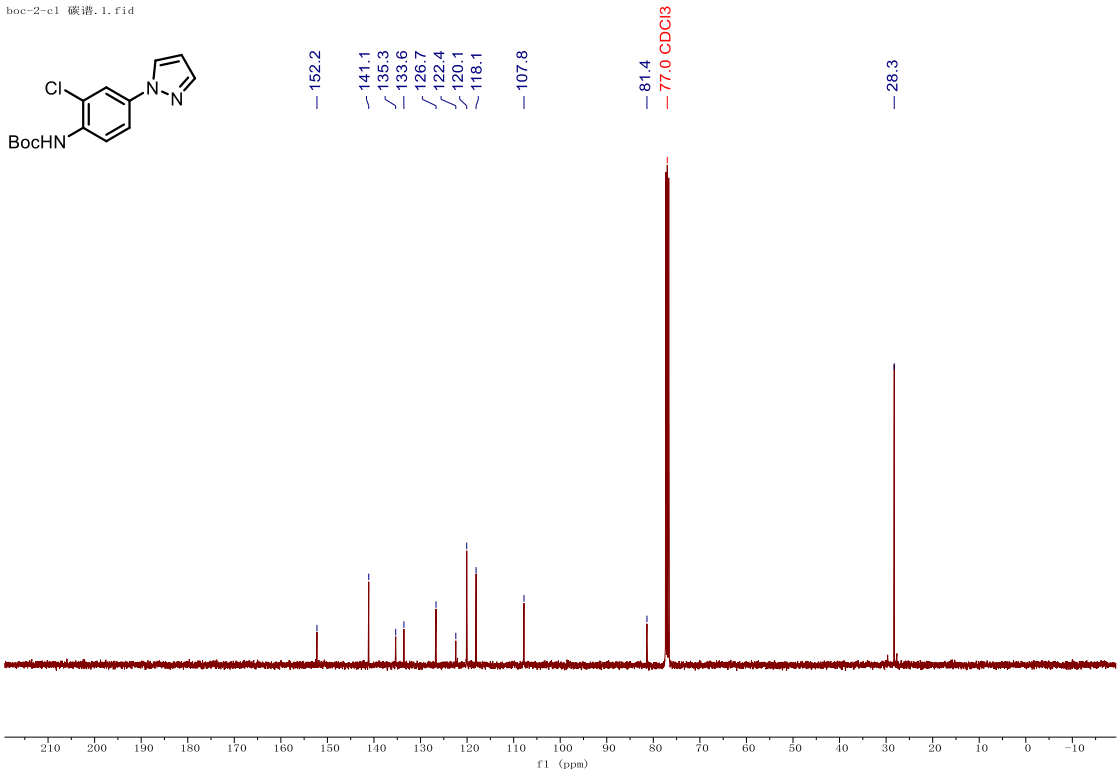

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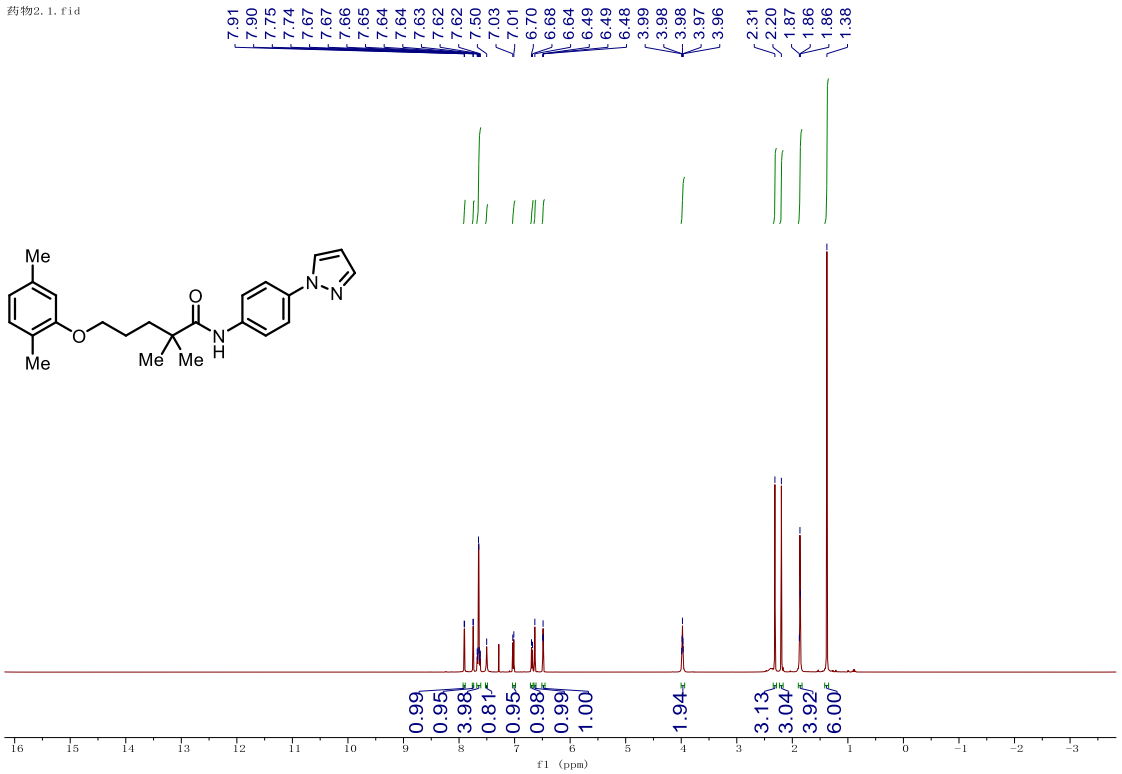


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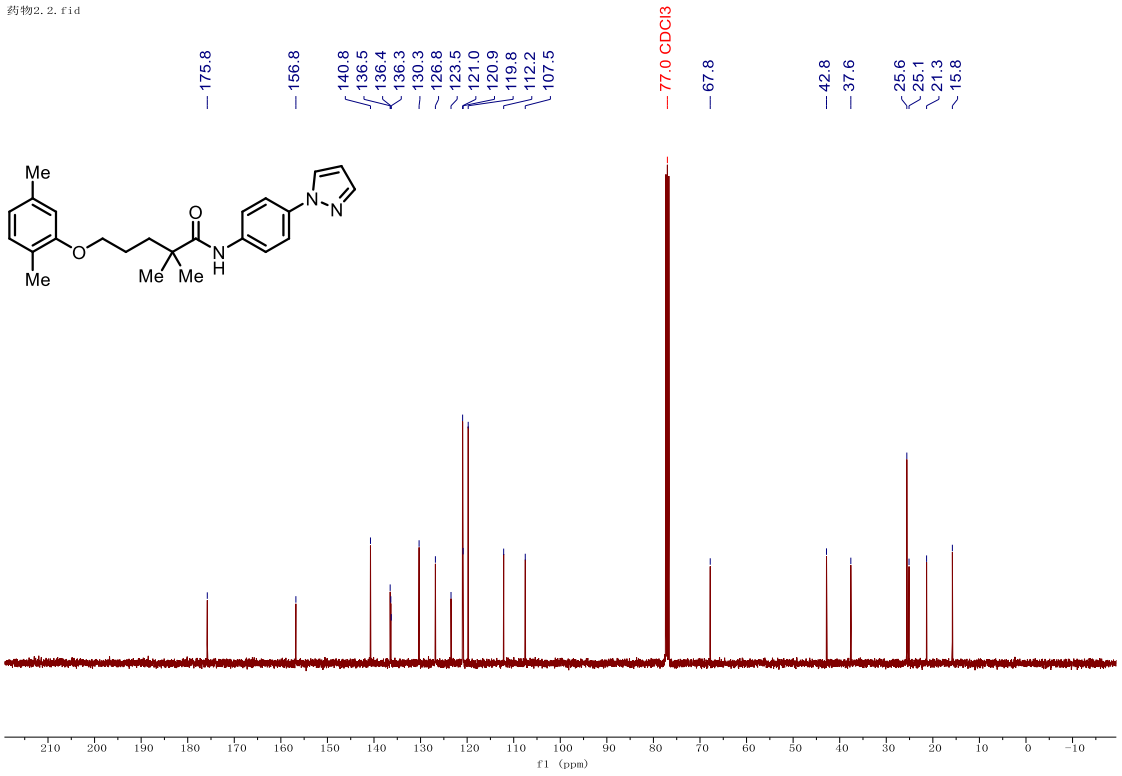

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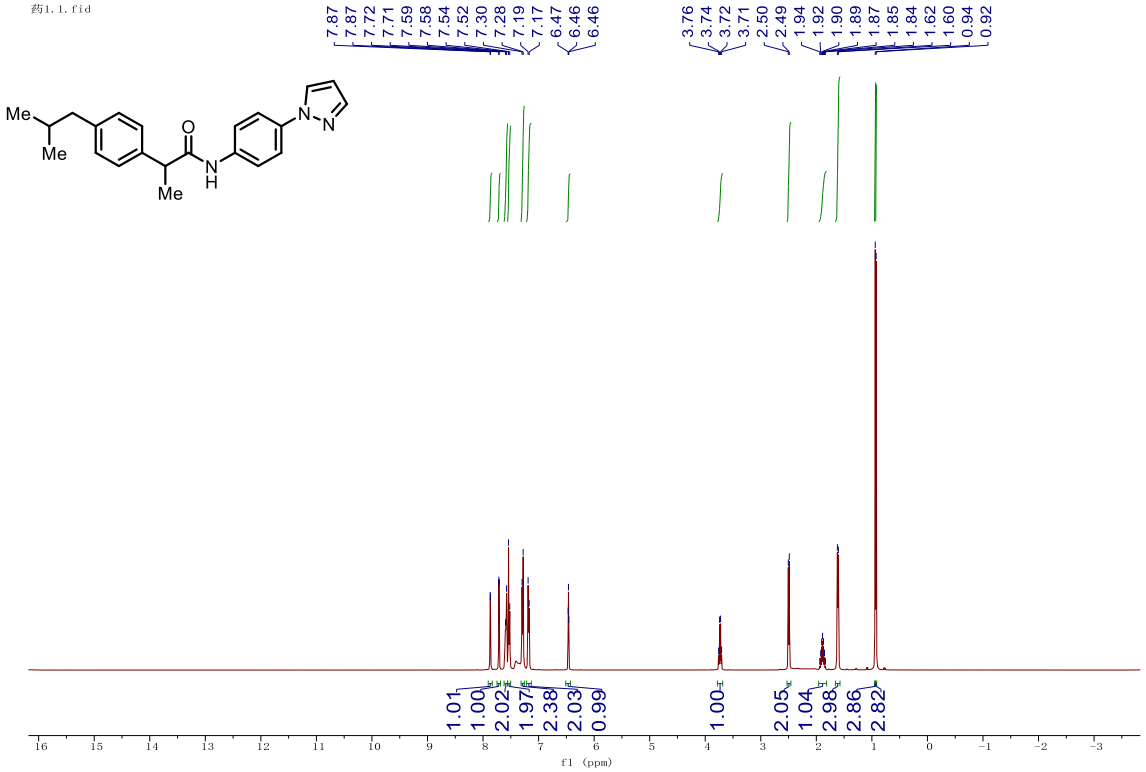


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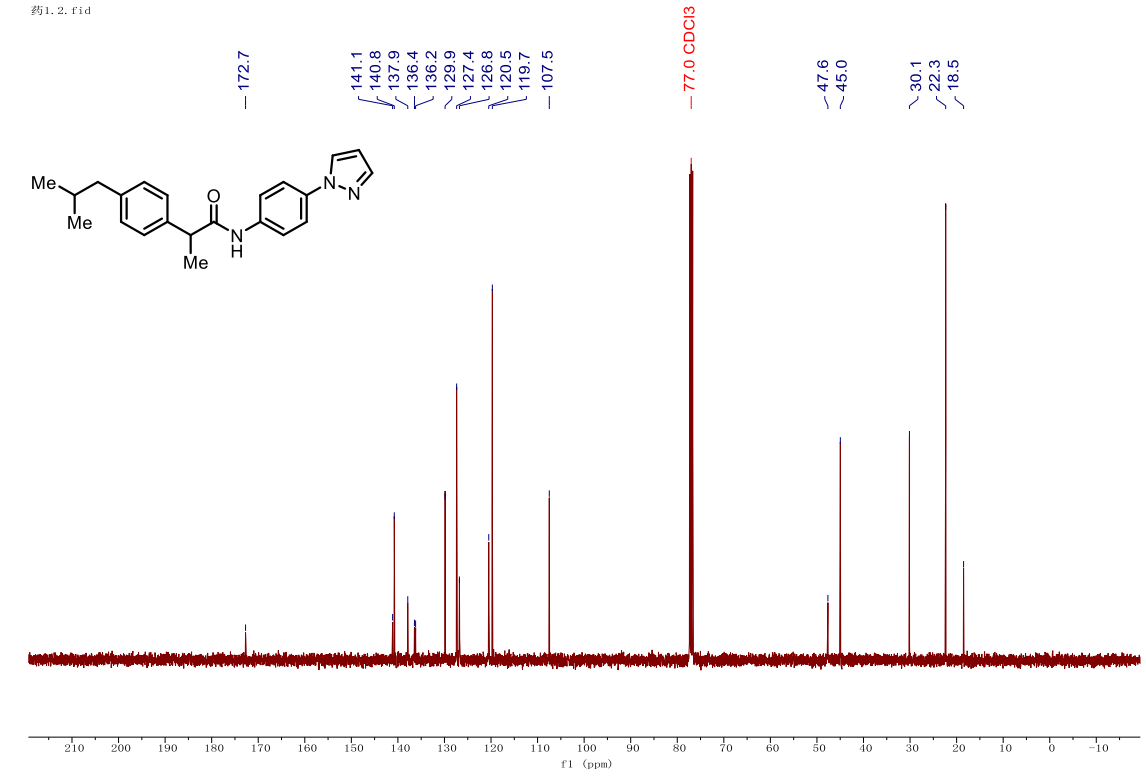

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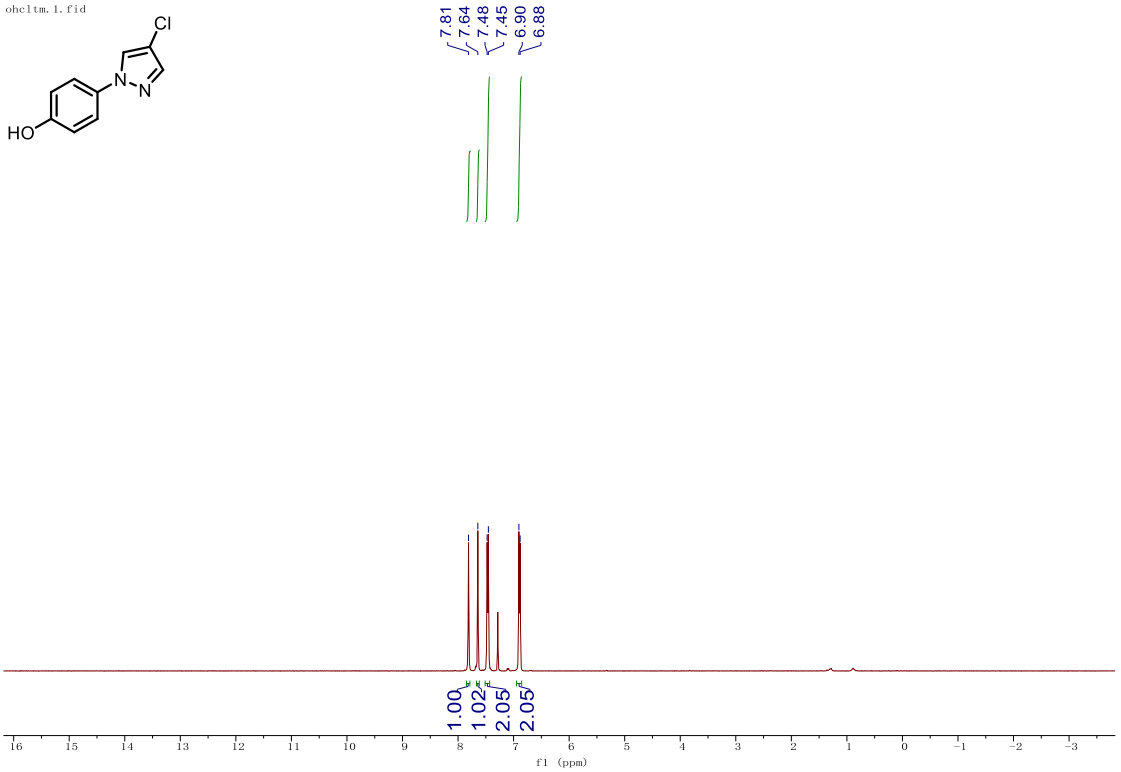


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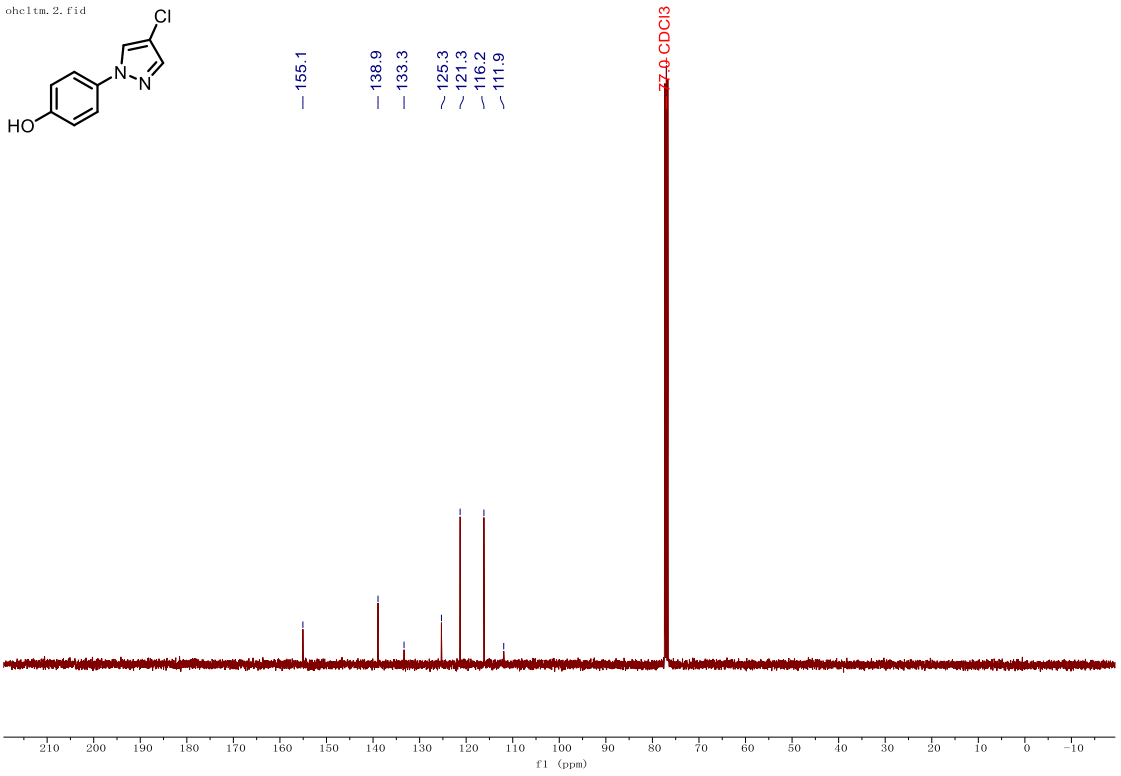

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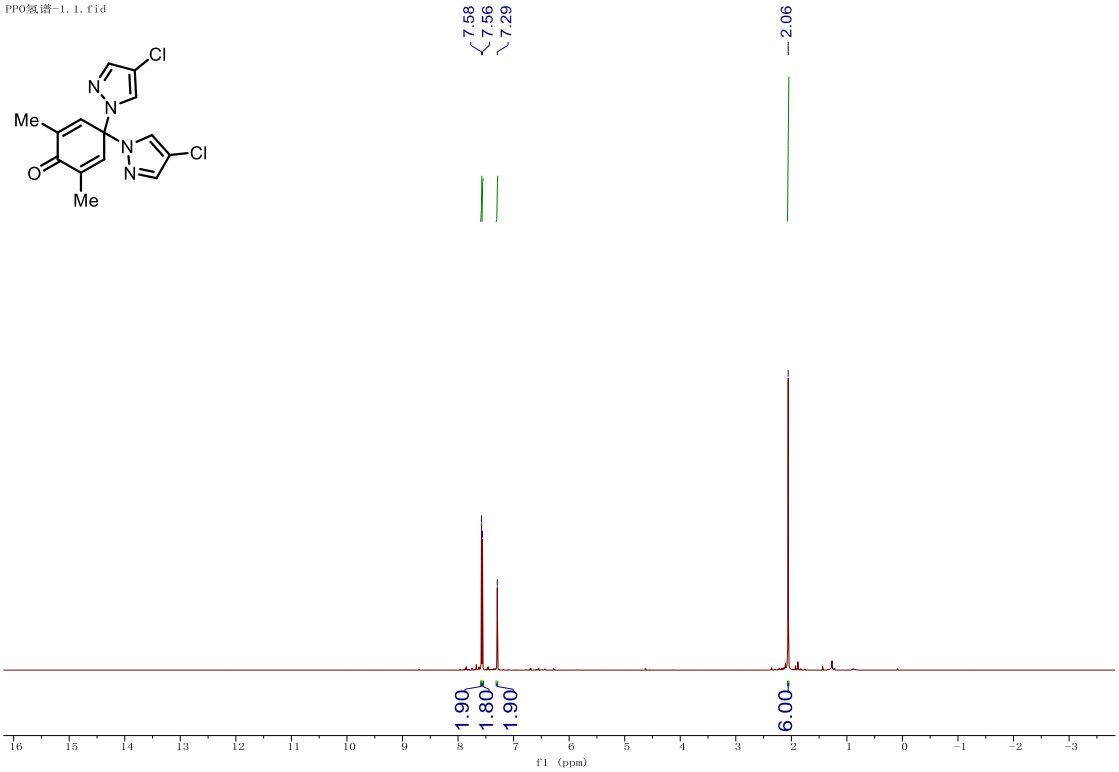


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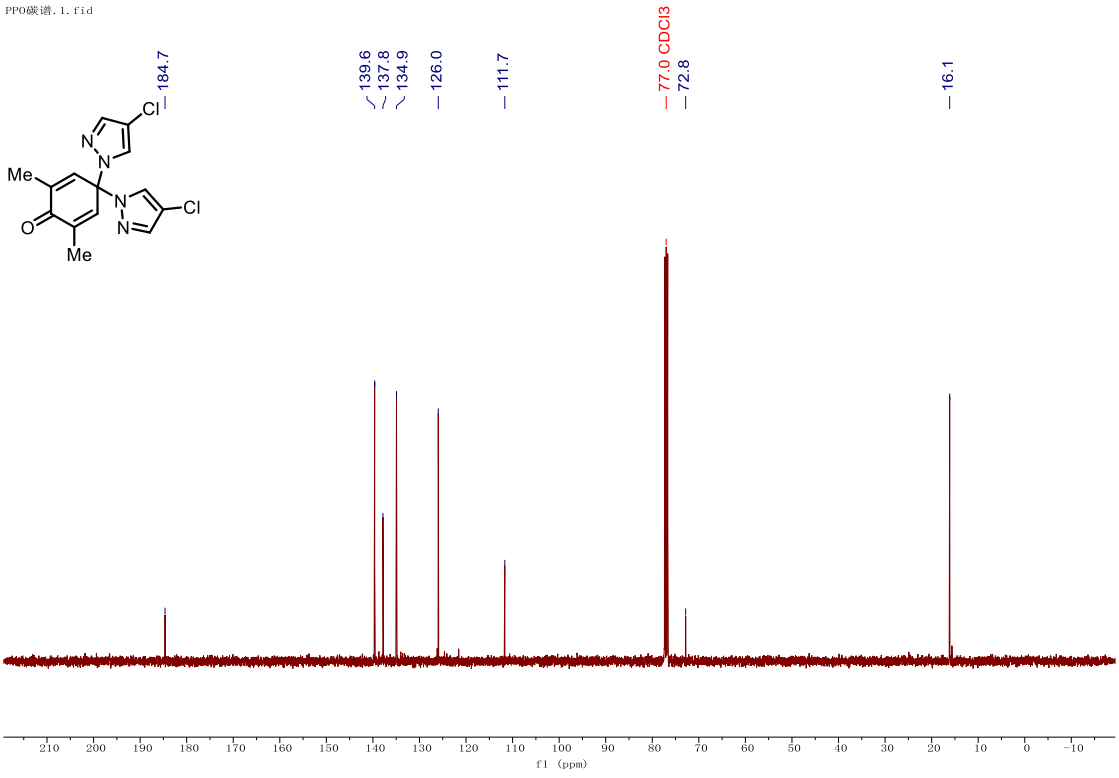

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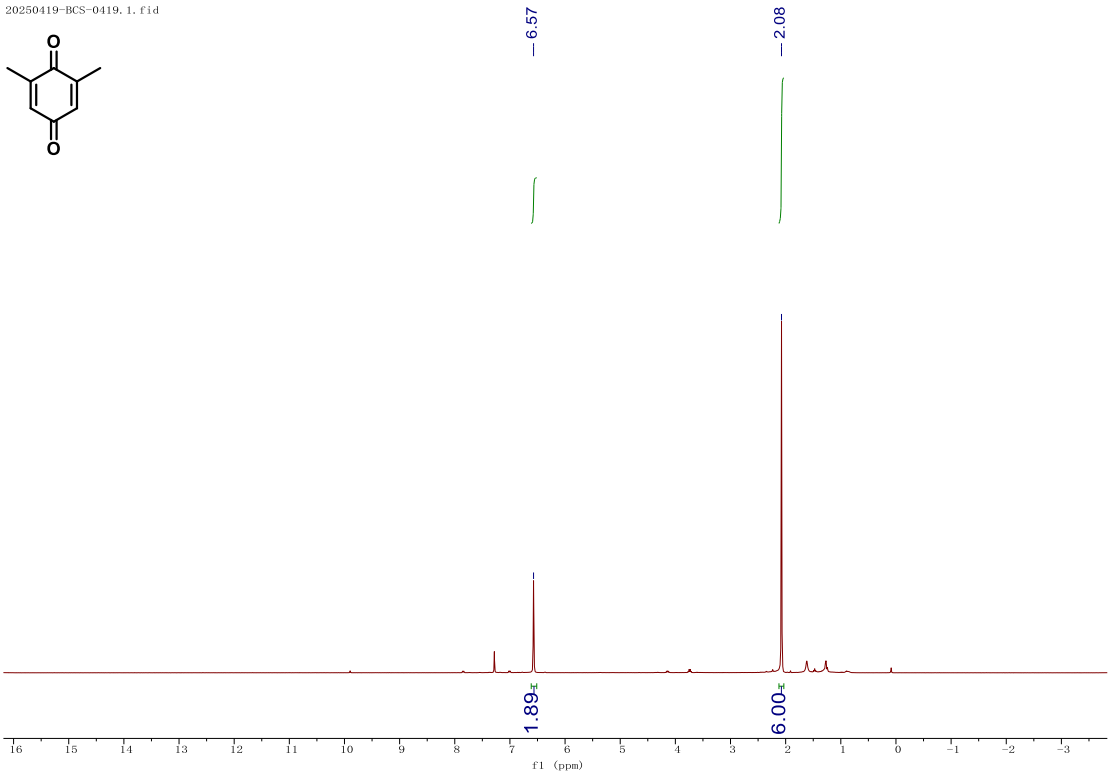


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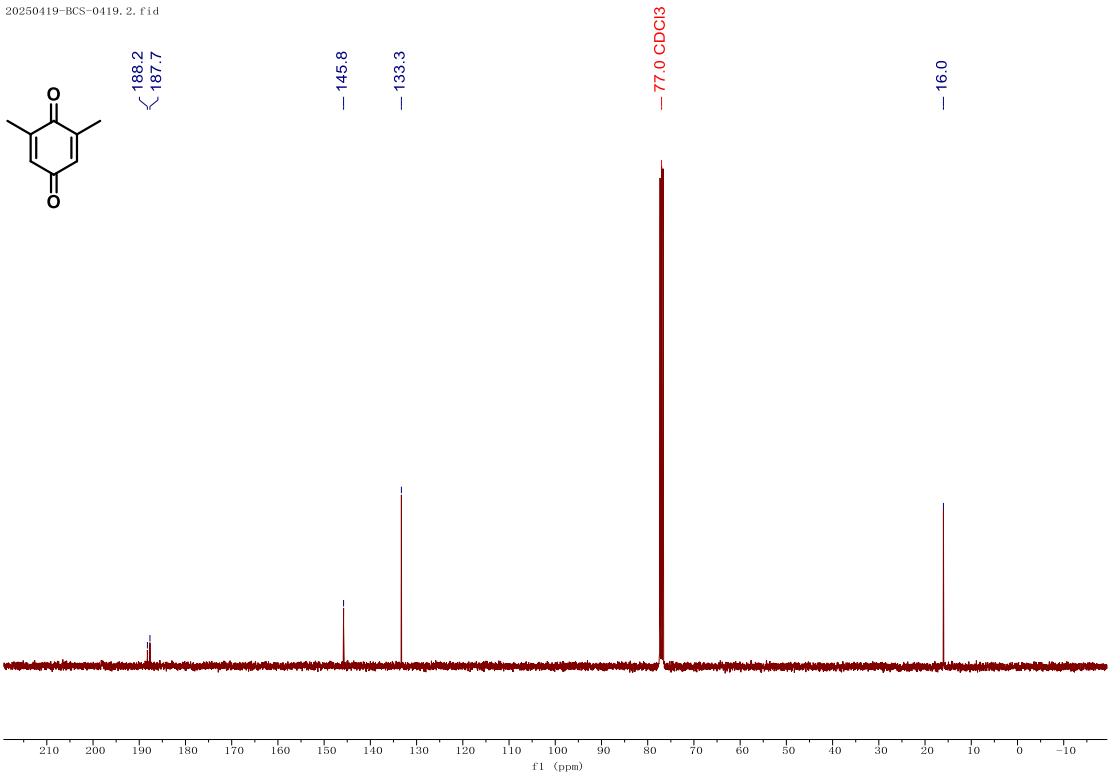

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