Supporting Information

Electrochemical Oxidative C(sp^3)-H Azolation of Lactams Under Mild Conditions

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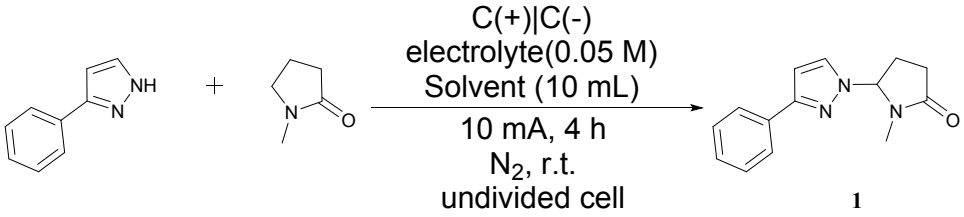
1. General information

All glassware was oven dried at 110 °C for hours and cooled down under vacuum. **1-ethynyl-4-fluorobenzene, 1-ethynyl-4-methylbenzene, 1-(tert-butyl)-4-ethynylbenzene** were prepared according to reported procedures[1]. Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. The instrument for electrolysis is dual display potentiostat (DJS-292B) (made in China). The anode electrode is carbon cloth (15 mm×15 mm×0.36 mm) and the cathode electrode is platinum plate (15 mm×15 mm×0.3 mm). Cyclic voltammograms were obtained on a CHI 605E potentiostat. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (bp. 60-90 °C). GC-MS spectra were recorded on Varian GC MS 3900-2100T or SHIMADZU GC MS-2010. All new compounds were characterized by ^{1}H NMR, ^{13}C NMR and HRMS. The ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a Bruker 400 MHz NMR spectrometer. For ^{1}H NMR, chemical shifts (δ) were given in ppm relatives to internal standard (TMS at 0 ppm, DMSO-d_6 at 2.50 ppm). For ^{13}C NMR, chemical shifts (δ) were reported in ppm using solvent as internal standard ($CDCl_3$ at 77.00 ppm, DMSO-d_6 at 39.52 ppm). High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument and Thermo Fisher Scientific LTQ FT Ultra.

2. Optimization of the reaction conditions

Table 1. Preliminary optimization of electrolysis conditions.

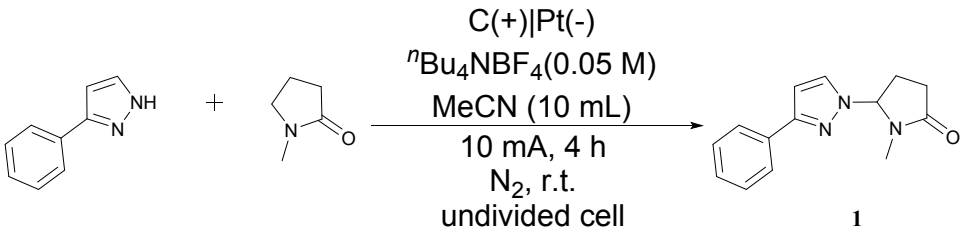


1

Entry	Solvent	Electrolyte	Yield (%)[b]
1	MeCN	$^{n}Bu_4NBF_4$	28
2	MeOH	$^{n}Bu_4NBF_4$	N.D.
3	DMF	$^{n}Bu_4NBF_4$	N.D.
4	MeCN	$^{n}Bu_4OAc$	20
5	MeCN	$^{n}Bu_4NPF_4$	trace
6[c]	MeCN	$^{n}Bu_4NBF_4$	50
7[d]	MeCN	$^{n}Bu_4NBF_4$	72
8[e]	MeCN	$^{n}Bu_4NBF_4$	60
9[f]	MeCN	$^{n}Bu_4NBF_4$	87(88[g])

[a]Reaction conditions: 3-phenyl-1*H*-pyrazole (0.3 mmol), 1-methyl-2-pyrrolidinone (0.3 mmol), carbon cloth anode (15 mm*15 mm*0.36 mm), carbon cloth cathode (15 mm*15 mm*0.36 mm), constant current=10 mA, $^{n}Bu_4NBF_4$ (0.5 mmol), MeCN (10 mL), r.t., 4 h, undivided cell (4.97 F). [b]GC Yield. [c]1-methyl-2-pyrrolidinone (0.45 mmol). [d]1-methyl-2-pyrrolidinone (0.6 mmol). [e]1-methyl-2-pyrrolidinone (0.2 mL), MeCN (9.8 mL). N.D. = not detected. [f]Pt plate instead of carbon cloth. [g]Isolated yield.

Table 2. Further optimization of electrolysis conditions.



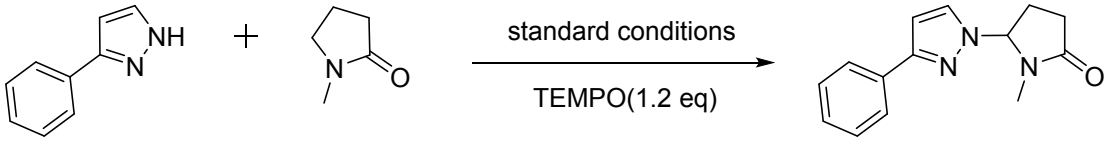
1

Entry	Variation from the "standard conditions"	Yield (%)[b]
1	none	87(88[c])
2	8 mA, 5 h	81
3	12 mA, 3.3 h	67
4	Ni plate cathode[d]	77
5	^{n}Bu$_4$NPF$_4$ instead of ^{n}Bu$_4$NBF$_4$	32
6	^{n}Et$_4$NBF$_4$ instead of ^{n}Bu$_4$NBF$_4$	80
7	LiClO$_4$ instead of ^{n}Bu$_4$NBF$_4$	78
8	MeOH instead of MeCN	N.D.
9	DCE instead of MeCN	29
10	DMF instead of MeCN	N.D.
11	air instead of N$_2$	52
12	no electric current	N.R.

[a]Reaction conditions: 3-phenyl-1*H*-pyrazole (0.3 mmol), 1-methyl-2-pyrrolidinone (0.6 mmol), carbon cloth anode (15 mm*15 mm*0.36 mm), Pt plate cathode (15 mm*15 mm*0.3 mm), constant current=10 mA, ^{n}Bu$_4$NBF$_4$ (0.5 mmol), MeCN (10 mL), r.t., 4 h, undivided cell (4.97 F). [b]GC Yield. [c]Isolated yield. [d]Ni plate cathode (15 mm*15 mm*0.5 mm). N.D. = not detected. N.R.= not reaction.

3. Additional experiments

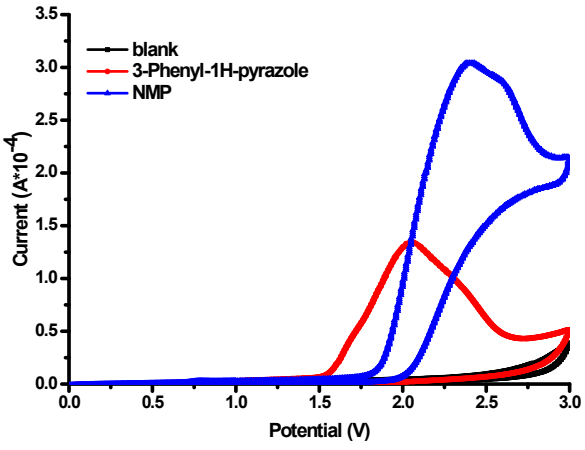
3.1 Radical trapping experiments



0.3 mmol **0.6 mmol** **trace**

Procedure for radical trapping experiments: In an oven-dried undivided three-necked bottle (100 mL) equipped with a stir bar, Phenyl-1*H*-pyrazole (43.3 mg, 0.3 mmol), TEMPO (56.2 mg, 0.36 mmol) and $^{n}Bu_4NBF_4$ (164.6 mg, 0.5 mmol) were combined and added. The bottle was equipped with carbon cloth (1.5×1.5 cm^2) and platinum electrode (1.5×1.5 cm^2) and was then charged with nitrogen. Under the protection of N_2, CH_3CN (10 mL) and *N*-methyl pyrrolidone (59.5 mg, 0.6 mmol) were injected respectively into the tubes via syringes. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA at room temperature for 4 h.

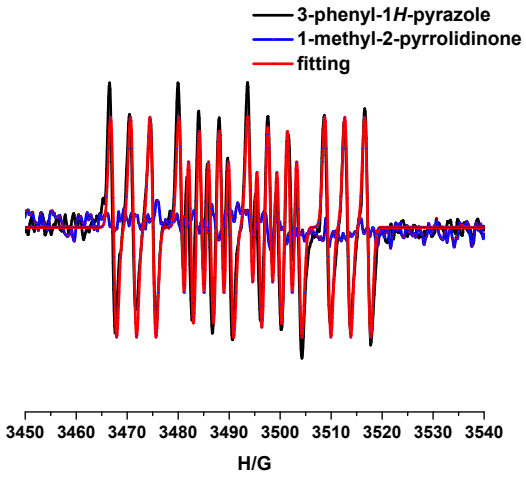
3.2 Cyclic voltammetry of Phenyl-1*H*-pyrazole and NMP.

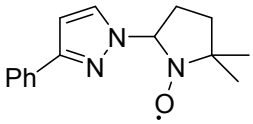


General procedure for cyclic voltammetry (CV): Cyclic voltammetry was performed in a three-electrode cell connected to a schlenk line under nitrogen at room temperature.

The working electrode was a steady glassy carbon disk electrode, the counter electrode a platinum wire. The reference was a Ag/AgCl electrode submerged in saturated aqueous KCl solution, and separated from reaction by a salt bridge. MeCN (10 ml) of acetonitrile acontaining $^{n}Bu_4NBF_4$ (0.2 mmol) were poured into the electrochemical cell in all experiments. The scan rate is 0.1 V/s, ranging from 0 V to 3.0 V.

3.3 Procedures for the electron paramagnetic resonance (EPR) experiment.





Under 10 mA constant current conditions, a dried three-necked flask equipped with a stir bar was loaded with Phenyl-1*H*-pyrazole (43.3 mg, 0.3 mmol) or 1-methyl-2-pyrrolidinone (29.8 mg, 0.6 mmol), $LiClO_4$ (53.2 mg, 0.5 mmol) in CH_3CN (10.0 mL) was stirred under an N_2 atmosphere at 25 ºC. The flask was equipped with carbon cloth (1.5 cm×1.5 cm×0.36 mm) as the anode and platinum plate (1.5 cm×1.5 cm×0.3 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under room temperature for 15 min. DMPO was added to the reaction mixture and continued to react for 1 minute; the solution sample was taken out into a small tube for EPR test. EPR spectra was recorded at room temperature on EPR spectrometer operated at 9.823 GHz. Typical spectrometer parameters were shown as follows, sweep width: 100 G; center field set: 3505 G; time constant: 163.84 ms; sweep time: 30.72 s;

modulation amplitude: 1.0 G; modulation frequency: 100 kHz; receiver gain: 1.00×104; microwave power: 22.10 mW.

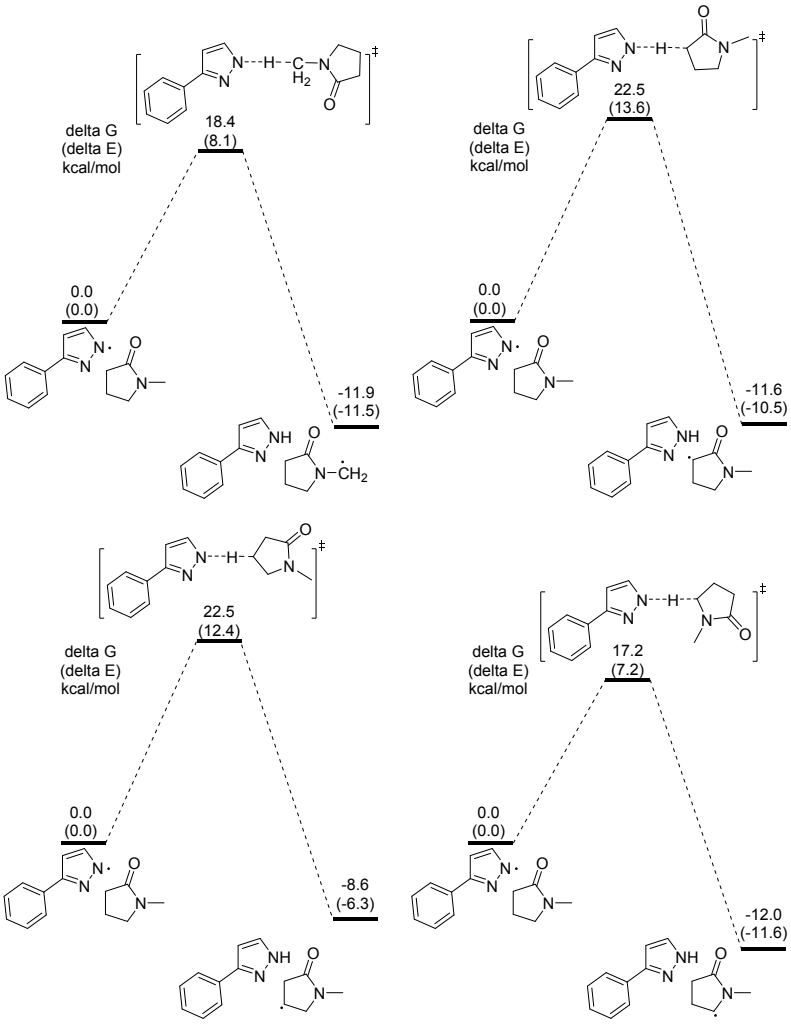
3.4 Procedures for gram scale synthesis in flow cell.

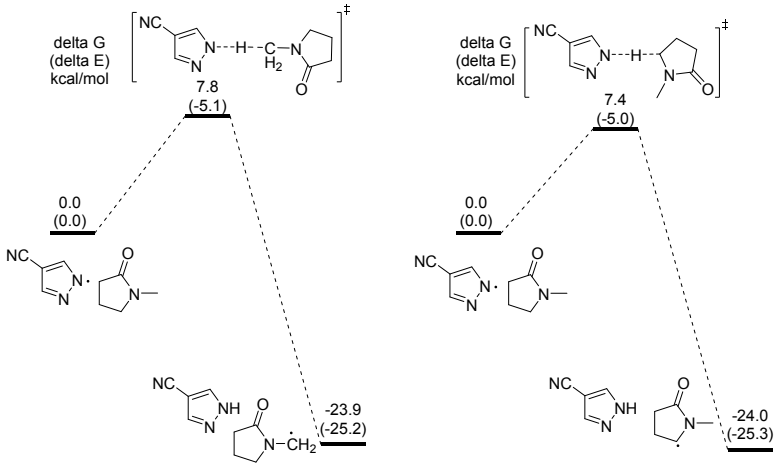
In an oven-dried schlenck tube (100 mL) equipped with a stir bar, 1a (1.44 g, 10 mmol), $^{n}Bu_4NBF_4$ (658.8 mg, 2 mmol) were added. The flow cell was equipped with carbon paper (9.3 cm×9.3 cm×0.2 mm) as the anode (contact area 1.6 cm^2) and carbon paper (9.3 cm×9.3 cm×0.3 mm) as the cathode (contact area 1.6 cm^2). We flushed the whole system with nitrogen before the direct electrolysis. Under the protection of N_2, CH_3CN (50 mL) and *N*-methyl pyrrolidone (991 mg, 10 mmol) were injected respectively into the tubes via syringes. The reaction mixture was pumped into the electrochemical reactor for single-pass in a flow rate of 0.20 mL s^{-1}. A constant current of 20 mA was employed during the electrolysis under room temperature for 33.0 h. When the reaction was finished, the reaction mixture was washed with water and extracted with dichloromethane (200 mL x 3). The organic layers were combined, dried over Na_2SO_4, and concentrated. The pure product was obtained by flash column chromatography on silica gel using petroleum ether and ethyl acetate as the eluent. Isolated yield: 67%, 1.61 g.

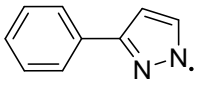
4. DFT calculation

General Computational Calculation Details

DFT calculations were performed using the M06-2x method[2] with the Gaussian09 program[3]. The 6-31G(d) basis set was used for all the elements and acetonitrile was employed as the solvent during the geometry optimization. For the integration grid in the calculations, the parameter int = ultrafine was used. Frequency calculations at the same level of theory have been performed to identify all of the stationary points as minima (zero imaginary frequencies) or transition state (one imaginary frequencies) and to provide free energies at 298.15 K. The transition states were checked through intrinsic reaction coordinate (IRC) calculations. The solvent effects were considered during the geometry optimization with SMD model[4]. For the single point energy calculations, 6-311+G(d,p) basis set was used for all the elements.







Thermal correction to Gibbs Free Energy= 0.106130

Sum of electronic and thermal Free Energies= -456.302817

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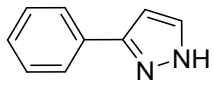
C	1.94243900	1.15460400	-0.00000600
C	3.16435600	0.56063600	-0.00009300
N	3.02093200	-0.84616400	0.00007200
H	1.70342600	2.20759100	-0.00004100
H	4.15434400	0.99656000	-0.00015600
N	1.77058800	-1.13895300	0.00004900
C	-0.39502300	0.03083100	-0.00000200
C	-1.13385200	1.23605800	0.00002500
C	-1.08657900	-1.20318100	-0.00002600
C	-2.51780300	1.20333500	0.00003500
H	-0.61208700	2.18772700	0.00006300
C	-2.47111900	-1.22384100	-0.00004100
H	-0.51704300	-2.12583000	-0.00004000
C	-3.18933000	-0.02405300	-0.00001000
H	-3.08154100	2.13034000	0.00006000
H	-2.99848300	-2.17206800	-0.00006200
H	-4.27473900	-0.04457200	-0.00002500



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Sum of electronic and thermal Free Energies= -456.960854

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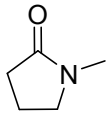
C	3.15497000	0.62371300	0.00041000
N	2.99649900	-0.71644700	-0.00049000
H	3.72475800	-1.42015200	-0.00102200
H	1.62807600	2.21170700	0.00154000
H	4.13577000	1.07598800	0.00072600
N	1.71628300	-1.09579600	-0.00075200
C	-0.45548500	0.02065400	0.00002500
C	-1.18784700	1.21351100	-0.00045500
C	-1.14874500	-1.19723300	0.00048600
C	-2.58024400	1.18956700	-0.00046400
H	-0.66964000	2.16799900	-0.00087900
C	-2.53953800	-1.21913000	0.00045100
H	-0.58786400	-2.12657300	0.00091200
C	-3.26215700	-0.02584100	-0.00001800
H	-3.13263000	2.12444000	-0.00085200
H	-3.06140500	-2.17148500	0.00082300
H	-4.34774700	-0.04380900	-0.00003400

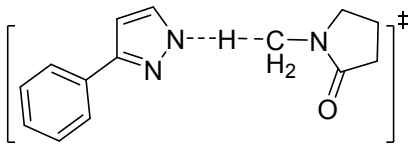


Thermal correction to Gibbs Free Energy= 0.109923

Sum of electronic and thermal Free Energies= -325.694106

C	1.77924400	0.52047600	0.20219800
C	0.54623400	1.37426500	-0.13324900

C	1.33367700	-0.90303700	-0.14476400
H	2.66475700	0.84433100	-0.34671400
H	1.99096000	0.59343200	1.27262600
H	0.56520300	1.73839600	-1.16993000
H	0.43160500	2.23715200	0.52972700
H	1.76510200	-1.68038000	0.48869200
H	1.55316500	-1.15679400	-1.18886400
N	-0.55467200	0.44181600	0.05405500
C	-1.93045500	0.87121100	0.01168900
H	-2.16557400	1.33979100	-0.95179200
H	-2.56530900	-0.00558700	0.14875800
H	-2.13143800	1.59382400	0.80924800
C	-0.18103800	-0.86371600	0.00508600
O	-0.93896700	-1.82400900	0.04801300

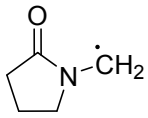


Thermal correction to Gibbs Free Energy= 0.232384

Sum of electronic and thermal Free Energies= -781.967969

C	0.57172300	-1.21889000	0.20041300
C	-0.20741500	-1.48695900	1.37893400
C	-1.32548000	-2.10826700	0.89677700
N	-1.19388900	-2.26965500	-0.46539500
H	0.04276900	-1.26721400	2.40713900
H	-2.20521900	-2.47522300	1.40757900
N	-0.06092300	-1.66082400	-0.88165600
C	1.87805500	-0.55800400	0.10649500
C	2.55765100	-0.14495600	1.26110600
C	2.45213100	-0.30287200	-1.14879800

C	3.77999600	0.51292200	1.16193400
H	2.12845000	-0.33718400	2.24004600
C	3.67332100	0.35418800	-1.24359000
H	1.93223100	-0.62989100	-2.04379700
C	4.34182900	0.76474300	-0.08913700
H	4.29566100	0.82775200	2.06395800
H	4.10707900	0.54585000	-2.22036300
H	5.29607700	1.27689200	-0.16498500
C	-2.84091400	-0.48057300	-1.41873700
H	-2.23627100	-1.51883100	-1.11401100
H	-2.72842700	-0.41244800	-2.50174800
H	-3.86105600	-0.66254900	-1.07626000
C	-1.18315600	1.42965200	-1.29351400
C	-0.62690600	2.14568200	-0.05344500
H	-1.62395900	2.13063600	-2.01252700
H	-0.43732800	0.81724300	-1.80622400
C	-1.80043200	2.15791900	0.93125100
H	0.19925200	1.56253300	0.36314500
H	-0.25867500	3.14340600	-0.29504800
H	-1.50980500	2.08999500	1.98117800
H	-2.42979500	3.04740900	0.80873900
N	-2.23783000	0.57963600	-0.74264600
C	-2.62952300	0.95381900	0.53196100
O	-3.51347100	0.40089000	1.15764500

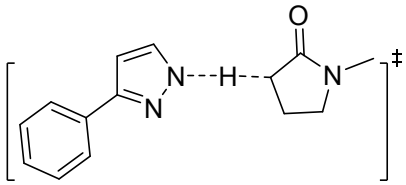


Thermal correction to Gibbs Free Energy= 0.095232

Sum of electronic and thermal Free Energies= -325.049808

C	1.77948000	-0.30234200	-0.23341700

C	0.69153800	-1.31520500	0.14740800
C	1.16331100	1.04792500	0.14382100
H	2.72080000	-0.50681800	0.27859900
H	1.95545900	-0.34299000	-1.31188400
H	0.78826000	-1.65372500	1.18541700
H	0.66623700	-2.19027000	-0.50624500
H	1.48219000	1.88071400	-0.48598900
H	1.37332200	1.31288100	1.18751300
N	-0.54529400	-0.54625900	-0.00131900
C	-1.78729100	-1.11567100	-0.01851300
H	-1.85821000	-2.19048900	-0.09148800
H	-2.63759700	-0.45771000	-0.11626900
C	-0.33003200	0.81531200	0.00909100
O	-1.22192800	1.64901300	-0.05259400



Thermal correction to Gibbs Free Energy= 0.230144

Sum of electronic and thermal Free Energies= -781.961273

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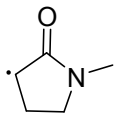
C	0.84567500	1.18598900	-1.35481300
N	0.74552600	-0.14973400	-1.69992700
H	-0.65661200	2.55032900	-0.50671800
H	1.73976600	1.74868900	-1.58782200
N	-0.38855500	-0.67726200	-1.22951300
C	-2.47028500	0.14709800	-0.25110700
C	-3.24930300	1.24689100	0.13421100
C	-3.01051500	-1.14409700	-0.14510000

C	-4.53731800	1.05824500	0.62553300
H	-2.84853800	2.25214200	0.04775200
C	-4.29727100	-1.32778300	0.34478800
H	-2.41113000	-1.99618200	-0.44953300
C	-5.06484700	-0.22775400	0.73261200
H	-5.13100000	1.91749200	0.92160900
H	-4.70490000	-2.33079100	0.42452500
H	-6.07106900	-0.37325200	1.11340200
C	2.72258600	-1.38385500	-0.58276900
H	1.84871500	-0.88664200	-1.33203500
H	3.26424600	-2.07033500	-1.23336500
C	3.47301400	-0.15910300	-0.12815100
O	4.33208800	0.45363500	-0.74985500
C	1.99919600	-1.91210200	0.63314200
H	1.02778500	-2.35477800	0.39749100
H	2.61260600	-2.67634000	1.12447000
C	1.86908600	-0.66813500	1.52829100
H	0.90979500	-0.15422500	1.37467300
H	1.96880000	-0.89773200	2.59317900
N	2.96527600	0.18149800	1.08585800
C	3.26039200	1.43337000	1.73787200
H	3.54029300	1.26496000	2.78242400
H	4.08975100	1.90767200	1.21100300
H	2.38728600	2.09765500	1.71119400

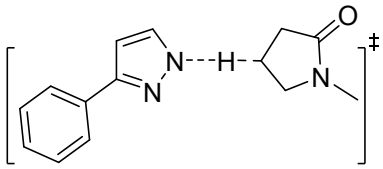


Thermal correction to Gibbs Free Energy= 0.094090

Sum of electronic and thermal Free Energies= -325.050959

C	-1.87475100	-0.31989100	0.02925500

C	-0.68940500	-1.31202200	-0.03633200
C	-1.22162600	1.01407200	-0.02091100
H	-2.57833000	-0.47127900	-0.79715300
H	-2.45041700	-0.44748000	0.95532100
H	-0.68737800	-1.88445900	-0.97210200
H	-0.69659400	-2.02663100	0.79375700
H	-1.72592000	1.97014100	-0.03916800
N	0.48992800	-0.46736300	0.03508300
C	1.81878200	-1.01796300	0.00405800
H	1.98317400	-1.59294200	-0.91567400
H	2.53028400	-0.19128300	0.04328700
H	1.98490500	-1.68083300	0.86095800
C	0.22844600	0.87833400	0.00100500
O	1.08026300	1.76764100	-0.00465600

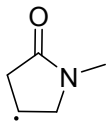


Thermal correction to Gibbs Free Energy= 0.232082

Sum of electronic and thermal Free Energies= -781.961331

C	-0.64116600	1.33140800	-0.25996100
C	-0.39541500	2.58577200	0.40425800
C	0.88521100	2.90630200	0.05096600
N	1.32385900	1.96666800	-0.85531000
H	-1.07372900	3.14615400	1.03195400
H	1.50739600	3.75046100	0.31391800
N	0.42093600	0.96655800	-0.96299600
C	-1.84328800	0.49141700	-0.20569400
C	-3.05248000	0.99947000	0.28454500
C	-1.77787700	-0.84833900	-0.62052600

C	-4.17847300	0.18376300	0.35823200
H	-3.11449200	2.03637100	0.60180100
C	-2.90471200	-1.65837400	-0.54376900
H	-0.83532100	-1.24871800	-0.98639900
C	-4.10818300	-1.14542200	-0.05539200
H	-5.11204700	0.58788400	0.73732800
H	-2.84478200	-2.69505100	-0.86119400
H	-4.98675100	-1.78062000	0.00278100
C	3.20134300	0.45498800	-0.00102000
H	2.49713700	1.35754200	-0.51094600
C	2.49612300	0.03573400	1.28061800
H	3.21051700	-0.19091200	2.08393900
H	1.81126900	0.81099500	1.65728200
C	3.07519900	-0.70574300	-0.96621500
H	2.80388500	-0.41062600	-1.98433400
H	4.00330100	-1.28854000	-1.02531100
N	1.74822300	-1.14629300	0.89747500
C	0.73115500	-1.69919800	1.75665500
H	0.28001500	-2.55235600	1.24721500
H	1.16496500	-2.03004000	2.70654900
H	-0.04272000	-0.95047800	1.96703300
C	1.97706100	-1.57533400	-0.36799800
O	1.41424600	-2.51390400	-0.91750300
H	4.17928400	0.92198200	0.11603100

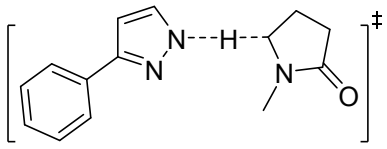


Thermal correction to Gibbs Free Energy= 0.092279

Sum of electronic and thermal Free Energies= -325.045918

C	1.73696000	-0.67089400	-0.00001200

C	0.46020600	-1.44894600	0.00007600
C	1.45466900	0.78934200	-0.00003600
H	2.71641400	-1.12653700	-0.00016100
H	0.34603700	-2.09636900	0.88416600
H	0.34601000	-2.09659200	-0.88383300
H	1.84122200	1.32368200	-0.87946700
H	1.84130900	1.32377900	0.87929400
N	-0.55397300	-0.40717500	-0.00001900
C	-1.96103800	-0.72127200	-0.00005300
H	-2.22832900	-1.30194700	0.88985800
H	-2.51832400	0.21664500	-0.00006000
H	-2.22828300	-1.30194300	-0.88997800
C	-0.06980000	0.86132300	0.00000700
O	-0.74552900	1.88152300	0.00005200

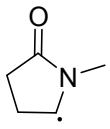


Thermal correction to Gibbs Free Energy= 0.232014

Sum of electronic and thermal Free Energies= -781.971366

C	-0.83379000	1.21883700	-0.30434100
C	-0.67823400	2.55755300	0.17496600
C	0.61993000	2.86758200	-0.13137500
N	1.16033900	1.81882700	-0.85086500
H	-1.40772600	3.16920900	0.68616900
H	1.19838200	3.76273000	0.05244300
N	0.30432800	0.80259800	-0.88229200
C	-2.00907700	0.35128400	-0.22308900
C	-3.25679600	0.86684800	0.15768700
C	-1.89368000	-1.02057400	-0.50138900

C	-4.36178900	0.02870000	0.26492400
H	-3.36242800	1.92754600	0.36603900
C	-3.00097400	-1.85352800	-0.39315100
H	-0.92708100	-1.42472900	-0.78559300
C	-4.23824500	-1.33311100	-0.01019900
H	-5.32226600	0.43927900	0.56090000
H	-2.89967800	-2.91347700	-0.60594900
H	-5.10188400	-1.98585300	0.07212800
C	3.76763800	-0.42307800	-0.79858500
C	2.72247300	-1.50816400	-1.08332700
C	3.10982300	0.41046300	0.29935000
H	4.69229900	-0.86469200	-0.41392800
H	4.01305800	0.18057700	-1.67370800
H	3.14207000	-2.49134200	-1.30371300
H	2.05510800	-1.22506200	-1.90442100
H	2.42771800	1.24570200	-0.24803800
H	3.75647900	0.96338600	0.98580000
N	2.21008100	-0.45976700	0.94543000
C	1.87880600	-1.55946100	0.17669200
O	1.04903200	-2.39224600	0.49066400
C	1.47051700	-0.07640800	2.12733200
H	0.64566300	-0.77830400	2.25818100
H	2.11783700	-0.09833900	3.00940500
H	1.07734600	0.93807600	2.00009000

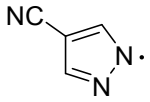


Thermal correction to Gibbs Free Energy= 0.095169

Sum of electronic and thermal Free Energies= -325.051366

C	-1.77641000	-0.64804300	-0.10496200

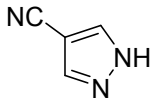
C	-0.48160000	-1.37795100	0.11712500
C	-1.38401700	0.82625500	0.09648100
H	-2.14723400	-0.81199500	-1.12652100
H	-2.56609600	-0.97213800	0.57864700
H	-0.28432900	-2.40718000	-0.15770400
H	-1.65064200	1.18791400	1.09564800
H	-1.82148700	1.51028000	-0.63305600
N	0.55814000	-0.46145000	0.01262100
C	1.95797700	-0.82839500	0.00449300
H	2.16530700	-1.50383000	-0.83042600
H	2.54457600	0.08384300	-0.10737200
H	2.22806700	-1.32539900	0.94101600
C	0.13369400	0.84478600	-0.00608100
O	0.86587500	1.82109300	-0.06136500



Thermal correction to Gibbs Free Energy= 0.025846

Sum of electronic and thermal Free Energies= -317.612279

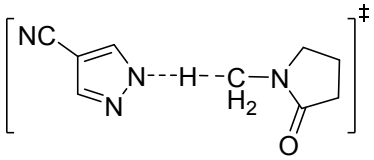
C	0.52407200	-1.09589700	-0.00005100
C	-0.33280900	-0.00017000	0.00000100
C	0.52472100	1.09585100	0.00013600
N	1.85849000	0.63828100	-0.00017100
H	0.29693200	2.15303900	0.00004500
N	1.85845400	-0.63831800	0.00011600
H	0.29643200	-2.15309400	0.00002100
C	-1.75467300	-0.00007000	-0.00002100
N	-2.91140600	0.00029100	-0.00001000



Thermal correction to Gibbs Free Energy= 0.042540

Sum of electronic and thermal Free Energies= -318.288984

C	0.49093800	-1.09639600	0.00000000
C	-0.36266500	-0.00089000	0.00000000
C	0.49459800	1.12918100	0.00000000
N	1.76130200	0.75631300	-0.00000100
H	0.21921500	2.17446700	0.00000100
H	0.29626100	-2.15851700	0.00000000
C	-1.78225800	-0.02007700	0.00000000
N	-2.94056900	-0.02335500	0.00000000
N	1.72804300	-0.58725600	0.00000000
H	2.59941500	-1.10677900	0.00000000

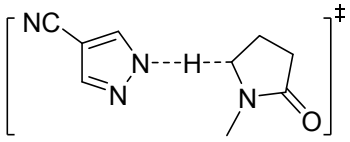


Thermal correction to Gibbs Free Energy= 0.156307

Sum of electronic and thermal Free Energies= -643.295410

C	-1.55044300	-0.81389700	0.10584400
C	-2.70420900	-0.01042500	-0.00470500
C	-2.20126200	1.28535500	-0.22258700
N	-0.87098100	1.20499500	-0.23237900
H	-2.72951900	2.21742200	-0.36589400
N	-0.47641800	-0.03830200	-0.03599500
C	1.78820000	1.98240700	-0.27156300
H	0.62468400	2.04154800	-0.32255400
H	2.18162600	2.47692300	-1.16126600
C	-4.06086000	-0.41321400	0.08047200

N	-5.17057100	-0.74424600	0.14957900
H	-1.47227300	-1.87882600	0.27923300
H	2.08690800	2.45144500	0.66746900
C	2.23065100	-0.19600800	-1.46220700
C	2.04734600	-1.64030700	-0.97022900
H	3.23432500	-0.01401700	-1.86661800
H	1.49396300	0.11456700	-2.20792100
C	2.35460900	-1.58565100	0.53098000
H	2.70441700	-2.32587900	-1.50557700
H	1.01212000	-1.94577700	-1.13023600
H	1.72634200	-2.23716800	1.14123900
H	3.40227600	-1.82606100	0.74663800
N	2.07460700	0.61625200	-0.26725000
C	2.13671600	-0.14593500	0.92655700
O	2.07427300	0.36012300	2.01905200



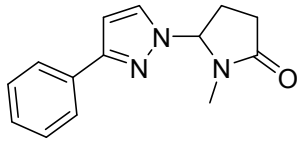
Thermal correction to Gibbs Free Energy= 0.155468

Sum of electronic and thermal Free Energies= -643.296312

C	-1.65752100	-0.86701900	-0.19763600
C	-2.72227000	0.03682900	-0.00487100
C	-2.09779900	1.21417700	0.44949500
N	-0.78600800	0.98271400	0.50611300
H	-2.53333800	2.16453300	0.72437100
N	-0.52167500	-0.24598200	0.11888300
C	2.45061300	1.58840500	-0.80054000
C	2.13369500	0.33083100	-1.62014300
C	2.00089200	1.22887700	0.62229300
H	3.52511300	1.78835400	-0.80623600

H	1.93101900	2.47367400	-1.16797800
H	2.86294500	0.10886400	-2.40058400
H	1.14061700	0.37997200	-2.07910300
H	0.90859100	1.53507900	0.77805200
H	2.57279700	1.66258700	1.44863800
N	2.00096800	-0.18257500	0.67425200
C	2.10149700	-0.78682200	-0.60486900
O	2.16848300	-1.98045900	-0.75655300
C	1.90942900	-0.93935400	1.89711300
H	1.70405900	-1.98014900	1.64825300
H	2.85495900	-0.86144800	2.44464600
H	1.10479500	-0.52523800	2.51067900
C	-4.10612000	-0.18738200	-0.21703600
N	-5.23806900	-0.37167400	-0.39182300
H	-1.68042000	-1.89120000	-0.54313400

5. Procedure and analytical data of compounds

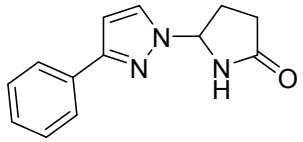


1-methyl-5-(3-phenyl-1*H*-pyrazol-1-yl)pyrrolidin-2-one (1)[5].

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 - 7.79 (m, 2H), 7.49 (d, *J* = 2.4 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 8.0 Hz, 1H), 6.61 (d, *J* = 2.4 Hz, 1H), 5.69 (dd, *J* = 7.7, 2.4 Hz, 1H), 2.89 - 2.81 (m, 1H), 2.70 (s, 3H), 2.61 – 2.43 (m, 2H), 2.40 – 2.32 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.79, 152.34, 132.81, 128.86, 128.43, 127.76, 125.42, 103.34, 76.24, 28.96, 27.10, 25.70.

HRMS (ESI) calcd for $C_{14}H_{15}N_3O$ $[M+Na]^+$: 264.1107; found: 264.1107.

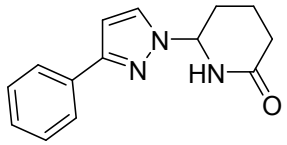


5-(3-phenyl-1*H*-pyrazol-1-yl)pyrrolidin-2-one (2).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 - 7.76 (m, 3H), 7.46 (d, *J* = 2.4 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 6.52 (d, *J* = 2.4 Hz, 1H), 5.82 (d, *J* = 7.5 Hz, 1H), 2.77 - 2.68 (m, 1H), 2.63 - 2.55 (m, 1H), 2.42 - 2.29 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 178.81, 152.24, 132.97, 128.54, 128.29, 127.80, 125.47, 103.27, 70.77, 28.62, 28.33.

HRMS (ESI) calcd for $C_{13}H_{13}N_3O$ $[M+Na]^+$: 250.0951; found: 250.0948.

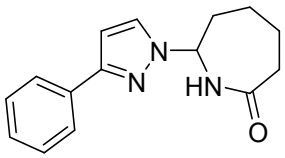


6-(3-phenyl-1*H*-pyrazol-1-yl)piperidin-2-one (3).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.1 Hz, 2H), 7.56 (d, *J* = 2.4 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 7.16 (s, 1H), 6.57 (d, *J* = 2.4 Hz, 1H), 5.79 (q, *J* = 4.8 Hz, 1H), 2.52 - 2.36 (m, 2H), 2.31 - 2.24 (m, 1H), 2.21 - 2.13 (m, 1H), 1.92 - 1.72 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.25, 152.06, 133.05, 128.59, 128.21, 127.83, 125.55, 103.10, 68.90, 31.23, 28.52, 16.77.

HRMS (ESI) calcd for $C_{14}H_{15}N_3O$ $[M+Na]^+$: 264.1107; found: 264.1104.

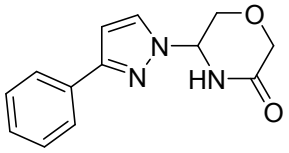


7-(3-phenyl-1*H*-pyrazol-1-yl)azepan-2-one (4).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.1 Hz, 2H), 7.55 (d, *J* = 2.4 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 6.60 (d, *J* = 2.4 Hz, 1H), 6.60 (d, *J* = 3.2 Hz, 1H), 5.65 (q, *J* = 2.4 Hz, 1H), 2.55 - 2.43 (m, 3H), 2.21 - 2.16 (m, 1H), 2.07 - 2.01 (m, 1H), 1.90 - 1.69 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.88, 152.28, 132.89, 128.81, 128.61, 127.96, 125.61, 103.58, 70.10, 37.09, 35.47, 26.79, 22.54.

HRMS (ESI) calcd for $C_{15}H_{17}N_3O$ $[M+Na]^+$: 278.1264; found: 278.1260.

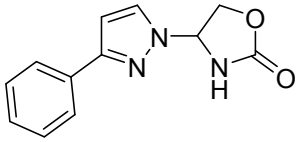


5-(3-phenyl-1*H*-pyrazol-1-yl)morpholin-3-one (5).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.1 Hz, 2H), 7.73 (d, *J* = 2.5 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.29 (s, 1H), 6.63 (d, *J* = 2.5 Hz, 1H), 5.80 (q, *J* = 3.0 Hz, 1H), 4.40 (d, *J* = 16.9 Hz, 1H), 4.23 (d, *J* = 17.0 Hz, 2H), 4.04 (dd, *J* = 12.5, 3.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.25, 152.14, 132.78, 128.83, 128.69, 128.05, 125.63, 104.17, 68.06, 67.08, 66.97.

HRMS (ESI) calcd for $C_{13}H_{13}N_3O_2$ $[M+Na]^+$: 266.0900; found: 266.0898.

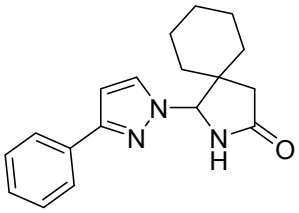


4-(3-phenyl-1*H*-pyrazol-1-yl)oxazolidin-2-one (6).

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.90 (s, 1H), 7.94 (d, *J* = 2.4 Hz, 1H), 7.81 (d, *J* = 7.3 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 6.79 (d, *J* = 2.4 Hz, 1H), 6.18 (d, *J* = 6.4 Hz, 1H), 4.72 (dd, *J* = 9.6, 7.5 Hz, 1H), 4.54 (dd, *J* = 9.7, 2.1 Hz, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 158.09, 151.64, 133.00, 130.97, 128.74, 127.88, 125.30, 103.29, 69.53, 68.00.

HRMS (ESI) calcd for $C_{12}H_{11}N_3O_2$ $[M+Na]^+$: 252.0743; found: 252.0742.

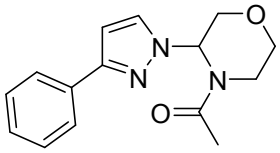


1-(3-phenyl-1*H*-pyrazol-1-yl)-2-azaspiro[4.5]decan-3-one (7).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.1 Hz, 2H), 7.44 (d, *J* = 2.4 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 6.95 (s, 1H), 6.57 (d, *J* = 2.4 Hz, 1H), 5.41 (s, 1H), 2.51 (d, *J* = 17.0 Hz, 1H), 2.33 (d, *J* = 17.0 Hz, 1H), 1.74 - 1.62 (m, 3H), 1.55 - 1.45 (m, 3H), 1.17 - 0.86 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 177.86, 151.69, 133.10, 128.90, 128.59, 127.83, 125.56, 103.19, 44.90, 36.20, 31.18, 25.47, 22.83, 22.29.

HRMS (ESI) calcd for $C_{18}H_{21}N_3O$ $[M+Na]^+$: 318.1577; found: 318.1577.

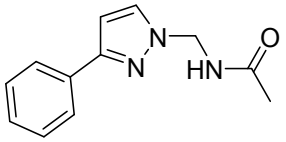


1-(3-(3-phenyl-1*H*-pyrazol-1-yl)morpholino)ethan-1-one (8).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 - 7.66 (m, 3H), 7.41 - 7.29 (m, 3H), 6.59 - 5.96 (2×s, 2H), 4.67 - 409 (m, 1.8H), 4.09 - 3.86 (m, 2H), 3.66 - 3.51 (m, 1.5H), 2.98 - 2.90 (m, 0.7H), 2.47, 2.15 (2×s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.05, 151.53, 132.85, 130.18, 128.54, 127.87, 125.55, 103.25, 68.10, 67.69, 66.83, 37.03, 21.39.

HRMS (ESI) calcd for $C_{15}H_{17}N_3O_2$ $[M+Na]^+$: 294.1213; found: 294.1206.

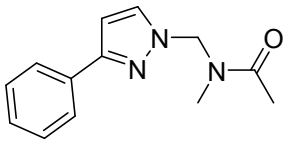


***N*-((3-phenyl-1*H*-pyrazol-1-yl)methyl)acetamide (9).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.1 Hz, 2H), 7.69 (d, *J* = 2.4 Hz, 1H), 7.40 - 7.36 (m, 3H), 7.30 (t, *J* = 7.3 Hz, 1H), 6.53 (d, *J* = 2.4 Hz, 1H), 5.49 (d, *J* = 6.6 Hz, 2H), 1.86 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.88, 152.28, 132.98, 132.14, 128.63, 127.90, 125.64, 103.52, 54.69, 22.81.

HRMS (ESI) calcd for $C_{12}H_{13}N_3O$ [M+Na]$^+$: 238.0951; found: 238.0946.

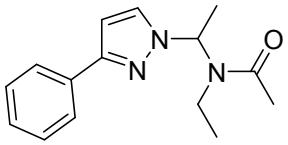


***N*-methyl-*N*-((3-phenyl-1*H*-pyrazol-1-yl)methyl)acetamide (10).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 - 7.78 (m, 2H), 7.65 - 7.46 (2×m, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.31 - 7.28 (2×m, 1H), 6.60 - 6.56 (2×m, 1H), 5.61 & 5.53 (2×s, 2H), 3.15 & 2.98 (2×s, 3H), 2.41 & 2.09 (2×s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.49 & 171.02, 152.40 & 151.42, 133.19 & 132.80, 131.55 & 129.89, 128.53 & 128.50, 127.88 & 127.63, 125.53 & 125.50, 103.71 & 103.54, 65.62 & 61.49, 35.71 & 32.77, 21.69 & 21.61.

HRMS (ESI) calcd for $C_{13}H_{15}N_3O$ [M+Na]$^+$: 252.1107; found: 252.1108.

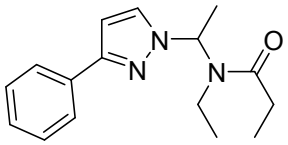


***N*-ethyl-*N*-(1-(3-phenyl-1*H*-pyrazol-1-yl)ethyl)acetamide (11).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.1 Hz, 2H), 7.58 (d, *J* = 2.3 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 6.96 (q, *J* = 6.9 Hz, 1H), 6.55 (d, *J* = 2.3 Hz, 1H), 3.53 - 3.34 (m, 2H), 2.39 & 2.13 (2×s, 3H), 1.84 (d, *J* = 6.9 Hz, 3H), 0.94 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.96, 151.04, 133.55, 131.07, 128.52, 127.60, 125.62, 103.13, 63.48, 37.98, 21.69, 17.52, 15.31.

HRMS (ESI) calcd for $C_{15}H_{19}N_3O$ [M+Na]$^+$: 280.1420; found: 280.1418.

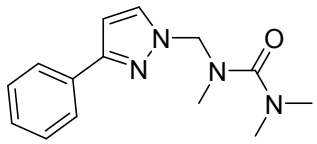


***N*-ethyl-*N*-(1-(3-phenyl-1*H*-pyrazol-1-yl)ethyl)propionamide (12).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.3 Hz, 2H), 7.59 (d, *J* = 2.3 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 6.98 (q, *J* = 6.9 Hz, 1H), 6.54 (d, *J* = 2.3 Hz, 1H), 3.54 - 3.34 (m, 2H), 2.39 - 2.32 (m, 2H), 1.85 (d, *J* = 6.9 Hz, 3H), 1.17 (t, *J* = 7.4 Hz, 3H), 0.94 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.20, 150.94, 133.60, 131.06, 128.52, 127.56, 125.61, 103.06, 63.72, 37.16, 26.50, 17.56, 15.47, 9.38.

HRMS (ESI) calcd for $C_{16}H_{21}N_3O$ $[M+Na]^+$: 294.1577; found: 294.1574.

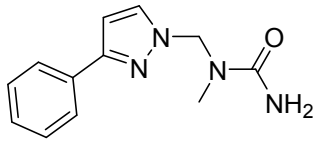


1,1,3-trimethyl-3-((3-phenyl-1*H*-pyrazol-1-yl)methyl)urea (13).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 2.2 Hz, 1H), 7.80 (d, *J* = 7.4 Hz, 2H), 7.39 (t, *J* = 7.7 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 1H), 6.58 (d, *J* = 2.2 Hz, 1H), 5.45 (s, 2H), 2.92 (s, 3H), 2.86 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.35, 151.03, 133.48, 131.78, 128.54, 127.55, 125.61, 103.67, 64.70, 38.48, 35.79.

HRMS (ESI) calcd for $C_{14}H_{18}N_4O$ $[M+Na]^+$: 281.1373; found: 281.1374.

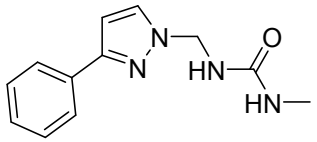


1-methyl-1-((3-phenyl-1*H*-pyrazol-1-yl)methyl)urea (14).

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.79 (d, *J* = 7.1 Hz, 2H), 7.76 (d, *J* = 2.3 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 6.73 (d, *J* = 2.3 Hz, 1H), 6.26 (s, 2H), 5.52 (s, 2H), 2.90, 2.07 (2×s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 158.45, 150.29, 133.30, 131.69, 128.72, 127.61 & 127.50, 125.22 & 125.11, 103.06 & 102.76, 63.34, 34.27.

HRMS (ESI) calcd for $C_{12}H_{14}N_4O$ $[M+Na]^+$: 253.1060; found: 253.1058.

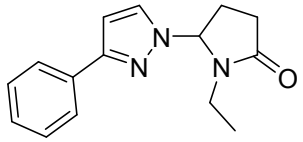


1-methyl-3-((3-phenyl-1*H*-pyrazol-1-yl)methyl)urea (15).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 - 7.72 (2×m, 2H), 7.67 - 7.60 (2×m, 1H) , 7.41 - 7.36 (m, 2H), 7.36 - 7.29 (m, 1H), 6.57 - 6.51 (2×m, 1H), 5.54 (s, 2H), 3.02 (s, 2H), 2.83 - 2.70 (2×m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.88 & 158.43, 151.88 & 151.64, 133.20 & 133.07, 131.64 & 131.04, 128.62 & 128.60, 127.80, 125.61 & 125.55, 103.63 & 103.35, 64.13 & 56.45, 34.25 & 33.54, 27.55 & 26.79.

HRMS (ESI) calcd for $C_{12}H_{14}N_4O$ [M+Na]$^+$: 253.1060; found: 253.1060.

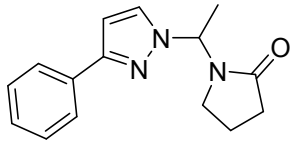


1-ethyl-5-(3-phenyl-1*H*-pyrazol-1-yl)pyrrolidin-2-one (16).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.1 Hz, 2H), 7.47 (d, *J* = 2.4 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 6.61 (d, *J* = 2.4 Hz, 1H), 5.83 (dd, *J* = 7.7, 2.2 Hz, 1H), 3.57 - 3.48 (m, 1H), 2.93 - 2.82 (m, 2H), 2.62 - 2.44 (m, 2H), 2.39 - 2.32 (m, 1H), 0.98 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.61, 152.34, 132.93, 128.56, 127.89, 125.57, 103.68, 74.47, 35.41, 29.32, 26.12, 12.31.

HRMS (ESI) calcd for $C_{15}H_{17}N_3O$ [M+Na]$^+$: 278.1264; found: 278.1264.

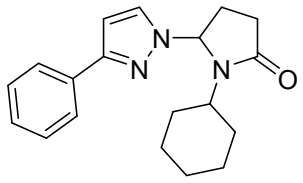


1-(1-(3-phenyl-1*H*-pyrazol-1-yl)ethyl)pyrrolidin-2-one (16').

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.1 Hz, 2H), 7.57 (d, *J* = 2.4 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 6.54 (d, *J* = 2.4 Hz, 1H), 6.41 (q, *J* = 6.8 Hz, 1H), 3.61 - 3.55 (m, 1H), 3.44 - 3.38 (m, 1H), 2.46 - 2.29 (m, 2H), 2.02 - 1.91 (m, 2H), 1.86 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.00, 151.34, 133.50, 130.52, 128.53, 127.63, 125.61, 102.86, 62.31, 42.64, 31.18, 17.76, 17.14.

HRMS (ESI) calcd for $C_{15}H_{17}N_3O$ [M+Na]$^+$: 278.1264; found: 278.1261.

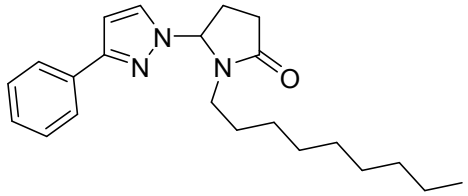


1-cyclohexyl-5-(3-phenyl-1*H*-pyrazol-1-yl)pyrrolidin-2-one (17).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.2 Hz, 2H), 7.47 (d, *J* = 2.4 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 6.60 (d, *J* = 2.4 Hz, 1H), 5.93 (d, *J* = 7.4 Hz, 1H), 3.91 - 3.83 (m, 1H), 2.96 - 2.90 (m, 1H), 2.57 - 2.42 (m, 2H), 2.23 - 2.18 (m, 1H), 1.81 - 1.77 (m, 1H), 1.70 - 1.65 (m, 2H), 1.57 - 1.50 (m, 3H), 1.34 - 1.15 (m, 2H), 1.01 - 0.94 (m, 1H), 0.68 - 0.57 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.05, 151.83, 133.08, 128.58, 128.14, 127.83, 125.57, 103.58, 73.12, 52.21, 29.92, 29.87, 29.56, 27.54, 25.71, 25.63, 25.21.

HRMS (ESI) calcd for $C_{19}H_{23}N_3O$ [M+Na]$^+$: 332.1733; found: 332.1735.

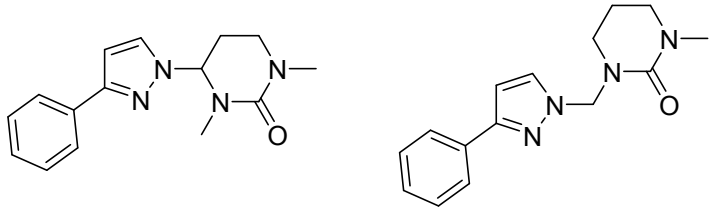


1-nonyl-5-(3-phenyl-1*H*-pyrazol-1-yl)pyrrolidin-2-one (18).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.1 Hz, 2H), 7.47 (d, *J* = 2.4 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 6.61 (d, *J* = 2.4 Hz, 1H), 5.83 (dd, *J* = 7.6, 2.1 Hz, 1H), 3.54 - 3.47 (m, 1H), 3.39 - 3.24 (m, 1H), 2.91 - 2.83 (m, 1H), 2.79 - 2.72 (m, 1H), 2.61 - 2.46 (m, 2H), 2.40 - 2.33 (m, 1H), 2.04 - 1.97 (m, 1H), 1.25 - 1.20 (m, 12H), 0.84 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.88, 152.41, 133.00, 128.77, 128.61, 128.52, 127.93, 125.63, 103.70, 74.81, 40.64, 31.71, 29.31, 29.14, 29.11, 27.08, 26.83, 26.23, 22.58, 14.06.

HRMS (ESI) calcd for $C_{22}H_{31}N_3O$ [M+Na]$^+$: 376.2359; found: 376.2370.

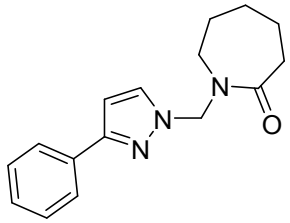


1,3-dimethyl-4-(3-phenyl-1*H*-pyrazol-1-yl)tetrahydropyrimidin-2(1*H*)-one compound with 1-methyl-3-((3-phenyl-1*H*-pyrazol-1-yl)methyl)tetrahydropyrimidin-2(1*H*)-one (1.14:1) (19).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 - 7.79 (m, 2.14H), 7.71 (d, *J* = 2.4 Hz, 0.5H), 7.46 (d, *J* = 2.4 Hz, 0.57H), 7.41 - 7.37 (m, 2.14H), 7.32 - 7.29 (m, 1.07H), 6.60 (d, *J* = 2.4 Hz, 0.57H), 6.57 (d, *J* = 2.4 Hz, 0.5H), 5.66 (t, *J* = 3.1 Hz, 0.57H), 5.62 (s, 1H), 3.51 (t, *J* = 5.6 Hz, 1H), 3.32 - 3.25 (m, 0.57H), 3.23 - 3.17 (m, 1.14H), 3.14 - 3.09 (m, 0.57H), 3.01 - 3.00 (m, 3.42H), 2.93 (s, 1.5H), 2.38 - 2.33 (m, 1H), 1.96 - 1.89 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.54, 155.10, 152.02, 151.01, 133.35, 133.03, 131.27, 128.46, 128.39, 128.11, 127.64, 127.40, 125.42, 125.36, 103.35, 102.69, 73.96, 62.95, 47.57, 45.64, 43.14, 35.74, 35.47, 34.41, 27.80, 21.81.

HRMS (ESI) calcd for $C_{15}H_{18}N_4O$ [M+Na]$^+$: 293.1374; found: 293.1374.

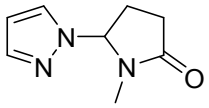


1-((3-phenyl-1*H*-pyrazol-1-yl)methyl)azepan-2-one (20').

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.1 Hz, 2H), 7.65 (d, *J* = 2.4 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 6.58 (d, *J* = 2.4 Hz, 1H), 5.65 (s, 2H), 3.78 – 3.47 (m, 2H), 2.55 – 2.53 (m, 2H), 1.64 – 1.63 (m, 4H), 1.45 (p, *J* = 5.4, 5.0 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 176.62, 151.40, 133.31, 131.41, 128.57, 127.68, 125.61, 104.02, 62.11, 49.24, 36.89, 29.68, 28.13, 23.18.

HRMS (ESI) calcd for $C_{16}H_{19}N_3O$ $[M+Na]^+$: 294.1420; found: 294.1421.

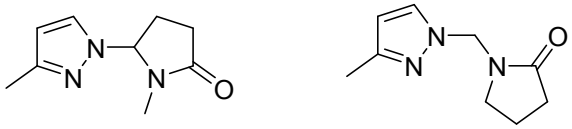


1-methyl-5-(1*H*-pyrazol-1-yl)pyrrolidin-2-one (21).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 1.5 Hz, 1H), 7.45 (d, *J* = 2.3 Hz, 1H), 6.28 (t, *J* = 2.4 Hz, 1H), 5.69 (dd, *J* = 7.9, 2.5 Hz, 1H), 2.79 - 2.71 (m, 1H), 2.61 (s, 3H), 2.57 – 2.50 (m, 1H), 2.46 – 2.39 (m, 1H), 2.32 – 2.24 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.58, 140.50, 127.43, 106.36, 76.11, 28.92, 27.09, 25.64.

HRMS (ESI) calcd for $C_8H_{11}N_3O$ $[M+Na]^+$: 188.0794; found: 188.0791.

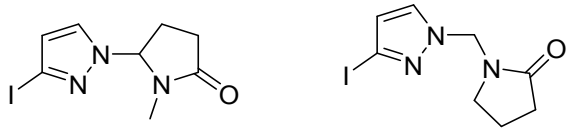


1-((3-methyl-1*H*-pyrazol-1-yl)methyl)pyrrolidin-2-one compound with 1-methyl-5-(3-methyl-1*H*-pyrazol-1-yl)pyrrolidin-2-one (20:1) (22).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 2.3 Hz, 1H), 6.06 (d, *J* = 2.4 Hz, 1H), 5.60 (dd, *J* = 7.8, 2.9 Hz, 1H), 2.84 – 2.70 (m, 1H), 2.63 (s, 3H), 2.57 – 2.49 (m, 1H), 2.48 – 2.38 (m, 1H), 2.33 – 2.27 (m, 1H), 2.24 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.87, 174.58, 149.82, 139.99, 138.30, 128.05, 106.19, 105.98, 75.98, 72.27, 29.26, 29.03, 27.12, 26.84, 25.68, 25.18, 13.60, 10.90.

HRMS (ESI) calcd for $C_9H_{13}N_3O$ $[M+Na]^+$: 202.0951; found: 202.0954.

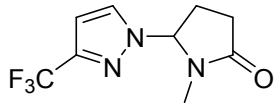


1-((3-iodo-1*H*-pyrazol-1-yl)methyl)pyrrolidin-2-one compound with 5-(3-iodo-1*H*-pyrazol-1-yl)-1-methylpyrrolidin-2-one (2.7:1) (23).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 5.5 Hz, 0.37H), 7.29 (d, *J* = 2.4 Hz, 1H), 6.46 – 6.44 (m, 1H), 6.41 – 6.39 (m, 0.37H), 5.67 (dd, *J* = 7.9, 2.5 Hz, 1H), 5.47 (s, 0.74H), 3.50 – 3.46 (m, 0.74H), 2.79 – 2.65 (m, 4H), 2.60 – 2.50 (m, 1H), 2.46 – 2.32 (m, 1.74H), 2.30 – 2.23 (m, 1H), 2.03 – 2.00 (m, 0.74H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.58, 174.55, 131.90, 129.33, 115.71, 115.54, 95.93, 95.13, 76.68, 57.48, 46.47, 30.39, 28.72, 27.28, 25.81, 17.61.

HRMS (ESI) calcd for $C_8H_{10}IN_3O$ $[M+Na]^+$: 313.9761; found: 313.9755.



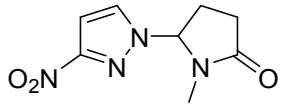
1-methyl-5-(3-(trifluoromethyl)-1*H*-pyrazol-1-yl)pyrrolidin-2-one (24).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 1.5 Hz, 1H), 6.60 (d, *J* = 2.4 Hz, 1H), 5.77 (dd, *J* = 7.8, 2.2 Hz, 1H), 2.83 – 2.74 (m, 1H), 2.72 (s, 3H), 2.68 – 2.58 (m, 1H), 2.53 – 2.46 (m, 1H), 2.34 – 2.27 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.69, 143.39 (q, J = 38.4 Hz), 128.73, 120.82 (q, J = 268.7 Hz), 105.12 (d, J = 2.0 Hz), 77.10, 28.57, 27.30, 25.79.

^{19}F NMR (377 MHz, $CDCl_3$) δ -62.17.

HRMS (ESI) calcd for $C_9H_{10}F_3N_3O$ $[M+Na]^+$: 256.0668; found: 256.0664.

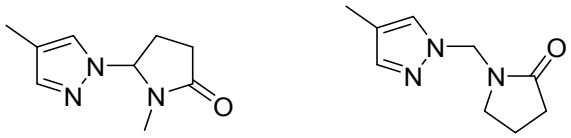


1-methyl-5-(3-nitro-1*H*-pyrazol-1-yl)pyrrolidin-2-one (25).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 2.6 Hz, 1H), 6.98 (d, *J* = 2.6 Hz, 1H), 5.81 (dd, *J* = 7.8, 2.1 Hz, 1H), 2.86 – 2.73 (m, 4H), 2.71 – 2.63 (m, 1H), 2.55 – 2.48 (m, 1H), 2.35 – 2.28 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.52, 156.33, 129.61, 103.76, 78.34, 28.32, 27.63, 25.98.

HRMS (ESI) calcd for $C_8H_{10}N_4O_3$ $[M+Na]^+$: 233.0645; found: 233.0643.

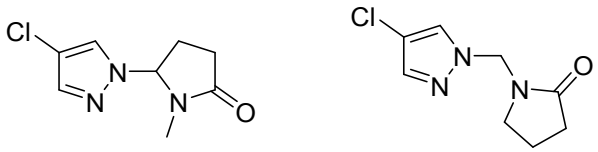


1-((4-methyl-1*H*-pyrazol-1-yl)methyl)pyrrolidin-2-one compound with 1-methyl-5-(4-methyl-1*H*-pyrazol-1-yl)pyrrolidin-2-one (20:1) (26).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (s, 1H), 7.20 (s, 1H), 5.61 (dd, *J* = 7.9, 2.7 Hz, 1H), 2.82 – 2.67 (m, 1H), 2.61 (s, 3H), 2.57 – 2.38 (m, 2H), 2.27 – 2.20 (m, 1H), 2.03 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.41, 174.49, 140.89, 140.23, 128.21, 127.07, 125.81, 117.08, 76.05, 57.17, 52.67, 46.30, 30.52, 28.94, 27.09, 25.60, 17.53, 8.75.

HRMS (ESI) calcd for $C_9H_{13}N_3O$ $[M+Na]^+$: 202.0951; found: 202.0951.

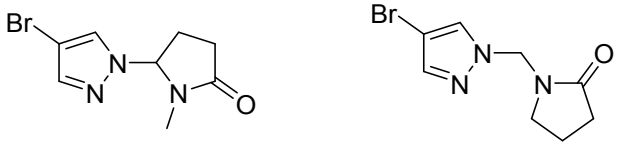


1-((4-chloro-1*H*-pyrazol-1-yl)methyl)pyrrolidin-2-one compound with 5-(4-chloro-1*H*-pyrazol-1-yl)-1-methylpyrrolidin-2-one (12.5:1) (27).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (s, 0.08H), 7.47 (s, 1H), 7.46 (s, 1H), 7.40 (s, 0.08H), 5.63 (dd, *J* = 7.8, 2.3 Hz, 1H), 5.44 (s, 0.16H), 3.45 (t, *J* = 7.2 Hz, 0.16H), 2.79 – 2.67 (m, 4H), 2.62 – 2.52 (m, 1H), 2.49 – 2.41 (m, 1H), 2.38 (t, *J* = 8.2 Hz, 0.16H), 2.29 – 2.22 (m, 1H), 2.05 – 1.99 (m, 0.16H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.55, 139.00, 125.29, 111.11, 77.00, 28.73, 27.30, 25.71.

HRMS (ESI) calcd for $C_8H_{10}ClN_3O$ $[M+Na]^+$: 222.0405; found: 222.0406.

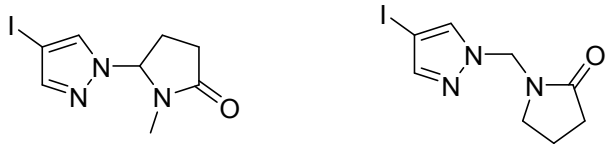


1-((4-bromo-1*H*-pyrazol-1-yl)methyl)pyrrolidin-2-one compound with 5-(4-bromo-1*H*-pyrazol-1-yl)-1-methylpyrrolidin-2-one (5:1) (28).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 0.21H), 7.49 (s, 2H), 7.41 (s, 0.21H), 5.64 (dd, *J* = 7.8, 2.2 Hz, 1H), 5.45 (s, 0.42H), 3.44 (t, *J* = 6.8 Hz, 0.42H), 2.78 – 2.68 (m, 1H), 2.66 (s, 3H), 2.61 – 2.51 (m, 1H), 2.47 – 2.40 (m, 1H), 2.36 (t, *J* = 8.1 Hz, 0.42H), 2.28 – 2.21 (m, 1H), 1.99 (dt, *J* = 15.6, 7.6 Hz, 0.42H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.58, 174.56, 141.04, 140.30, 129.76, 127.53, 94.30, 94.19, 76.85, 57.84, 46.34, 30.37, 28.70, 27.26, 25.68, 17.61.

HRMS (ESI) calcd for $C_8H_{10}BrN_3O$ [M+Na]$^+$: 265.9899; found: 265.9899.

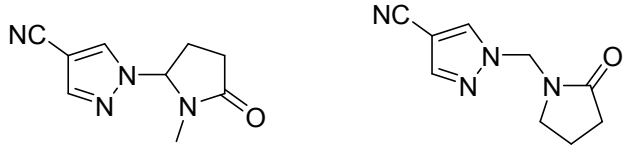


1-((4-iodo-1*H*-pyrazol-1-yl)methyl)pyrrolidin-2-one compound with 5-(4-iodo-1*H*-pyrazol-1-yl)-1-methylpyrrolidin-2-one (10:1) (29).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (s, 0.11H), 7.54 (s, 1H), 7.51 (s, 11H), 7.47 (s, 0.1H), 5.68 (dd, *J* = 7.8, 2.2 Hz, 1H), 5.48 (s, 0.23H), 3.45 (t, *J* = 7.2 Hz, 0.23H), 2.84 – 2.70 (m, 1H), 2.66 (s, 3H), 2.61 – 2.51 (m, 1H), 2.48 – 2.40 (m, 1H), 2.37 (t, *J* = 8.2 Hz, 0.23H), 2.28 – 2.21 (m, 1H), 2.03 – 1.96 (m, 0.23H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.57, 174.58, 145.49, 144.75, 134.07, 131.84, 76.65, 57.55, 57.44, 46.38, 30.39, 28.72, 27.30, 25.74, 17.61.

HRMS (ESI) calcd for $C_8H_{10}IN_3O$ [M+Na]$^+$: 313.9761; found: 313.9756.

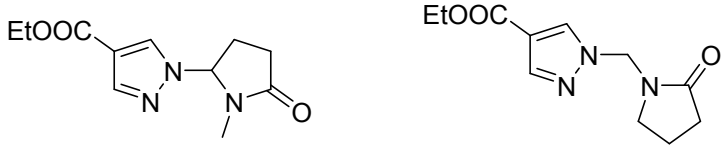


1-((2-oxopyrrolidin-1-yl)methyl)-1*H*-pyrazole-4-carbonitrile compound with 1-(1-methyl-5-oxopyrrolidin-2-yl)-1*H*-pyrazole-4-carbonitrile (2.2:1) (30).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 0.45H), 7.98 (s, 1H), 7.85 (s, 1H), 7.76 (s, 0.45H), 5.71 (dd, *J* = 7.8, 1.8 Hz, 1H), 5.52 (s, 0.9H), 3.51 (t, *J* = 7.2 Hz, 0.9H), 2.84 – 2.74 (m, 1H), 2.67 (s, 3H), 2.63 – 2.56 (m, 1H), 2.50 – 2.42 (m, 1H), 2.38 (t, *J* = 8.1 Hz, 0.9H), 2.32 – 2.25 (m, 1H), 2.04 (p, *J* = 7.5 Hz, 0.9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.84, 174.74, 143.34, 142.41, 135.10, 133.11, 112.92, 112.80, 93.30, 92.96, 77.07, 57.96, 46.58, 30.18, 28.50, 27.31, 25.70, 17.69.

HRMS (ESI) calcd for $C_9H_{10}N_4O$ [M+Na]$^+$: 213.0747; found: 213.0746.

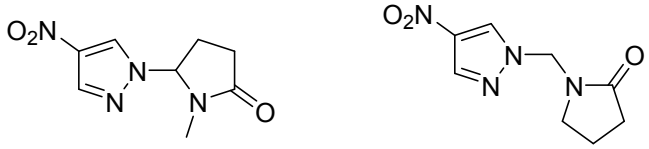


ethyl 1-((2-oxopyrrolidin-1-yl)methyl)-1*H*-pyrazole-4-carboxylate compound with ethyl 1-(1-methyl-5-oxopyrrolidin-2-yl)-1*H*-pyrazole-4-carboxylate (2.6:1) (31).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 0.38H), 7.96 (s, 1H), 7.91 (s, 1H), 7.85 (s, 0.38H), 5.68 (dd, *J* = 7.9, 2.1 Hz, 1H), 5.48 (s, 0.76H), 4.27 – 4.22 (m, 2.76H), 3.46 (t, *J* = 7.1 Hz, 0.76H), 2.81 – 2.72 (m, 1H), 2.65 (s, 3H), 2.62 – 2.52 (m, 1H), 2.47 – 2.40 (m, 1H), 2.36 (t, *J* = 8.1 Hz, 0.76H), 2.31 – 2.24 (m, 1H), 1.99 (p, *J* = 7.5 Hz, 0.76H), 1.32 – 1.26 (m, 4.08H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.58, 174.67, 162.59, 162.51, 141.98, 141.27, 132.98, 130.96, 116.04, 115.73, 76.70, 60.31, 60.18, 57.72, 46.39, 30.29, 28.63, 27.23, 25.64, 17.62, 14.23.

HRMS (ESI) calcd for $C_{11}H_{15}N_3O_3$ $[M+Na]^+$: 260.1006; found: 260.1007.

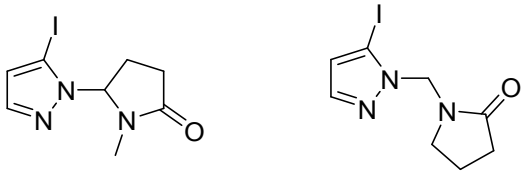


1-((4-nitro-1*H*-pyrazol-1-yl)methyl)pyrrolidin-2-one compound with 1-methyl-5-(4-nitro-1*H*-pyrazol-1-yl)pyrrolidin-2-one (5.6:1) (32).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (s, 0.19H), 8.31 (s, 1H), 8.11 (s, 1H), 8.03 (s, 0.19H), 5.72 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.52 (s, 0.38H), 3.54 (t, *J* = 7.1 Hz, 0.38H), 2.83 – 2.75 (m, 1H), 2.71 (s, 3H), 2.66 – 2.58 (m, 1H), 2.51 – 2.43 (m, 1H), 2.40 (t, *J* = 8.2 Hz, 0.38H), 2.35 – 2.28 (m, 1H), 2.09 – 2.03 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.97, 174.85, 136.79, 135.98, 135.92, 129.13, 127.24, 77.66, 58.66, 46.64, 30.14, 28.41, 27.40, 25.66, 17.72.

HRMS (ESI) calcd for $C_8H_{10}N_4O3$ $[M+Na]^+$: 233.0645; found: 233.0646.

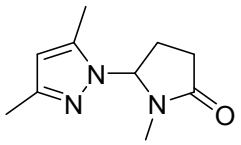


1-((5-iodo-1*H*-pyrazol-1-yl)methyl)pyrrolidin-2-one compound with 5-(5-iodo-1*H*-pyrazol-1-yl)-1-methylpyrrolidin-2-one (4:1) (33).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.38 (m, 0.25H), 7.29 (d, *J* = 2.4 Hz, 1H), 6.44 – 6.43 (m, 1H), 6.40 – 6.39 (m, 0.25H), 5.68 – 5.67 (m, 1H), 5.47 – 5.46 (m, 0.5H), 3.49 – 3.45 (m, 0.5H), 2.77 – 2.64 (m, 4H), 2.59 – 2.49 (m, 1H), 2.42 – 2.32 (m, 1.5H), 2.29 – 2.23 (m, 1H), 2.02 – 1.98 (m, 0.5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.55, 174.52, 131.88, 129.35, 115.68, 115.50, 95.91, 95.11, 76.64, 57.46, 46.44, 30.37, 28.70, 27.25, 25.78, 17.59.

HRMS (ESI) calcd for $C_8H_{10}IN_3O$ $[M+Na]^+$: 313.9761; found: 313.9758.

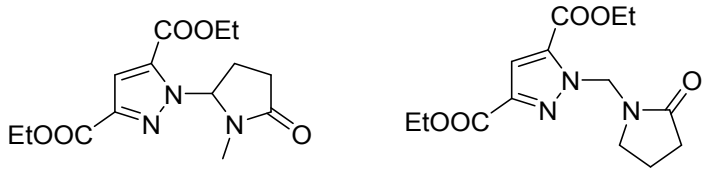


5-(3,5-dimethyl-1*H*-pyrazol-1-yl)-1-methylpyrrolidin-2-one (34)[6].

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.77 (s, 1H), 5.57 (dd, *J* = 8.0, 3.1 Hz, 1H), 2.85 - 2.76 (m, 1H), 2.54 (s, 3H), 2.49 - 2.42 (m, 1H), 2.39 - 2.31 (m, 2H), 2.25 (s, 3H), 2.14 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.68, 148.99, 139.09, 105.95, 72.04, 29.42, 26.70, 25.00, 13.58, 10.84.

HRMS (ESI) calcd for $C_{10}H_{15}N_3O$ $[M+Na]^+$: 216.1107; found: 216.1115.

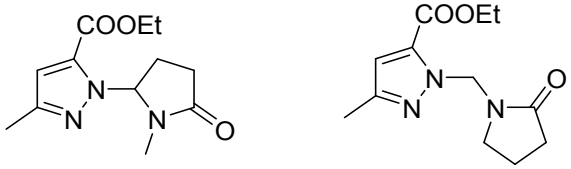


diethyl 1-((2-oxopyrrolidin-1-yl)methyl)-1*H*-pyrazole-3,5-dicarboxylate compound with diethyl 1-(1-methyl-5-oxopyrrolidin-2-yl)-1*H*-pyrazole-3,5-dicarboxylate (3.6:1) (35).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (s, 1H), 7.29 (s, 0.27H), 6.85 (dd, *J* = 7.9, 1.5 Hz, 1H), 6.03 (s, 0.54H), 4.38 – 4.30 (m, 5.1H), 3.38 (t, *J* = 7.2Hz, 0.55H), 2.96 – 2.87 (m, 1H), 2.63 (s, 3H), 2.55 – 2.48 (m, 1H), 2.43 – 2.30 (m, 2.55H), 1.96 (p, *J* = 7.5 Hz, 0.58H), 1.38 – 1.32 (m, 7.65H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.52, 175.13, 161.23, 161.13, 159.11, 158.66, 143.65, 143.20, 134.51, 134.23, 114.12, 114.01, 74.67, 61.78, 61.75, 61.21, 61.17, 57.80, 46.25, 30.44, 29.06, 27.16, 25.69, 17.74, 14.16, 14.12, 14.01.

HRMS (ESI) calcd for $C_{14}H_{19}N_3O_5$ $[M+Na]^+$: 332.1217; found: 332.1217.

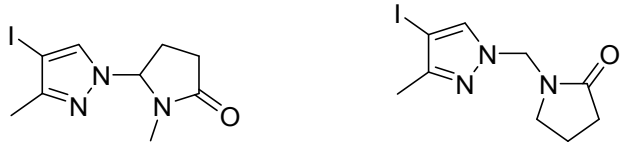


ethyl 3-methyl-1-((2-oxopyrrolidin-1-yl)methyl)-1*H*-pyrazole-5-carboxylate compound with ethyl 3-methyl-1-(1-methyl-5-oxopyrrolidin-2-yl)-1*H*-pyrazole-5-carboxylate (1:1) (36).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.58 (s, 1H), 6.55 (s, 0.5H), 5.85 (dd, *J* = 8.2, 3.2 Hz, 1H), 5.58 (s, 1H), 4.40 – 4.33 (m, 3H), 3.74 (t, *J* = 7.2 Hz, 1H), 2.91 – 2.81 (m, 1H), 2.66 – 2.45 (m, 5H), 2.42 – 2.33 (m, 6.5H), 2.00 (p, *J* = 7.6 Hz, 1H), 1.41 – 1.35 (m, 4.5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.95, 174.55, 162.28, 162.14, 143.61, 143.17, 140.52, 139.58, 109.22, 108.73, 74.29, 60.91, 60.84, 55.76, 46.06, 30.52, 29.15, 26.98, 24.89, 17.61, 14.27, 14.21, 11.02, 10.89.

HRMS (ESI) calcd for $C_{12}H_{17}N_3O_3$ $[M+Na]^+$: 274.1162; found: 274.1163.

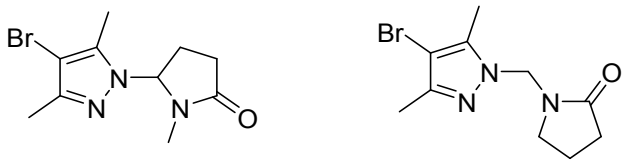


1-((4-iodo-3-methyl-1*H*-pyrazol-1-yl)methyl)pyrrolidin-2-one compound with 5-(4-iodo-3-methyl-1*H*-pyrazol-1-yl)-1-methylpyrrolidin-2-one (10:1) (37).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (s, 0.2H), 7.42 (s, 1H), 5.60 (dd, *J* = 7.7, 2.4 Hz, 1H), 5.42 (s, 0.2H), 3.48 (t, *J* = 7.2 Hz, 0.2H), 2.83 – 2.74 (m, 1H), 2.69 (s, 3H), 2.60 – 2.41 (m, 3H), 2.39 – 2.38 (m, 0.2H), 2.23 – 2.22 (m, 3.3H), 2.05 – 1.99 (m, 0.2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.64, 152.17, 132.40, 76.60, 60.94, 28.88, 27.36, 25.83, 13.67.

HRMS (ESI) calcd for $C_9H_{12}IN_3O$ $[M+Na]^+$: 317.9917; found: 317.9913.

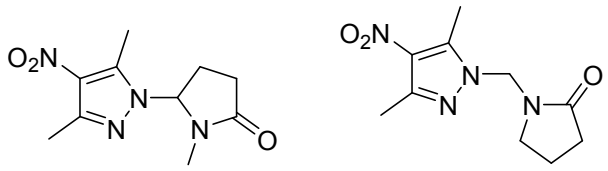


1-((4-bromo-3,5-dimethyl-1*H*-pyrazol-1-yl)methyl)pyrrolidin-2-one compound with 5-(4-bromo-3,5-dimethyl-1*H*-pyrazol-1-yl)-1-methylpyrrolidin-2-one (18.2:1) (38).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.62 (dd, *J* = 7.9, 2.9 Hz, 1H), 5.43 (s, 0.11H), 3.43 (t, *J* = 7.2 Hz, 0.11H), 2.88 – 2.80 (m, 1H), 2.60 (s, 3H), 2.52 – 2.47 (m, 1H), 2.46 – 2.39 (m, 1H), 2.35 – 2.31 (m, 1.11H), 2.29 (s, 3H), 2.17 (s, 3H), 2.01 – 1.99 (m, 0.11H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.89, 147.74, 136.96, 95.35, 73.38, 29.31, 26.98, 25.13, 12.49, 10.16.

HRMS (ESI) calcd for $C_{10}H_{14}BrN_3O$ $[M+Na]^+$: 294.0212; found: 294.0211.

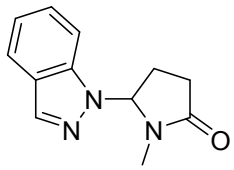


1-((3,5-dimethyl-4-nitro-1*H*-pyrazol-1-yl)methyl)pyrrolidin-2-one compound with 5-(3,5-dimethyl-4-nitro-1*H*-pyrazol-1-yl)-1-methylpyrrolidin-2-one (4.3:1) (39).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.71 (dd, *J* = 7.8, 1.6 Hz, 1H), 5.44 (s, 0.46H), 3.50 (t, *J* = 7.1 Hz, 0.46H), 2.91 – 2.82 (m, 1H), 2.69 – 2.68 (m, 3.69H), 2.62 (s, 3H), 2.56 – 2.48 (m, 1H), 2.45 – 2.44 (m, 3.69H), 2.39 – 2.35 (m, 0.46H), 2.33 – 2.26 (m, 1H), 2.06 – 2.00 (m, 0.46H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.23, 175.11, 147.33, 146.32, 141.08, 140.10, 131.20, 72.65, 55.67, 46.42, 30.29, 28.92, 27.04, 25.12, 17.67, 14.34, 14.05, 11.36, 11.02.

HRMS (ESI) calcd for $C_{10}H_{14}N_4O_3$ $[M+Na]^+$: 261.0958; found: 261.0958.

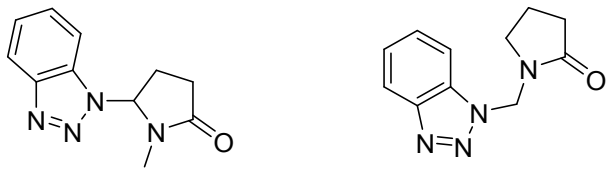


5-(1*H*-indazol-1-yl)-1-methylpyrrolidin-2-one (40).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.47 – 7.39 (m, 2H), 7.19 (t, *J* = 7.0 Hz, 1H), 6.19 (dd, *J* = 8.0, 3.2 Hz, 1H) 2.96 – 2.88 (m, 1H), 2.73 – 2.58 (m, 5H), 2.49 – 2.42 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.45, 139.43, 135.17, 127.15, 124.38, 121.48, 121.39, 108.43, 73.50, 29.69, 27.38, 24.82.

HRMS (ESI) calcd for $C_{12}H_{13}N_3O$ $[M+H]^+$: 216.1131; found: 216.1128.



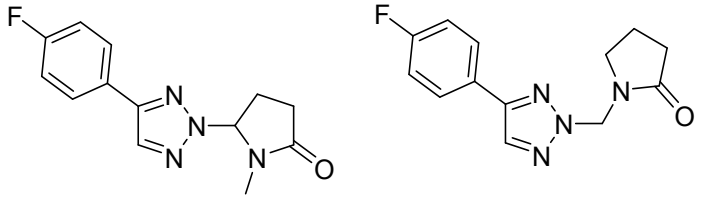
1-((1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)pyrrolidin-2-one compound with 5-(1*H*-benzo[d][1,2,3]triazol-1-yl)-1-methylpyrrolidin-2-one (7.1:1) (41)[7].

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.3 Hz, 1H), 8.02 (d, *J* = 8.4 Hz, 0.14H), 7.83 (d, *J* = 8.4 Hz, 0.14H), 7.53 – 7.49 (m, 1.14H), 7.43 – 7.39 (m, 2.14H), 6.48 (dd,

J = 8.5, 2.8 Hz, 1H), 6.08 (s, 0.28H), 3.43 – 3.34 (m, 0.28H), 2.96 – 2.78 (m, 2H), 2.71 – 2.61 (m, 4H), 2.49 – 2.37 (m, 1.28H), 2.01 – 1.95 (m, 0.28H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.63, 174.32, 146.47, 145.99, 132.08, 131.16, 128.28, 128.03, 124.51, 124.40, 120.56, 119.60, 110.47, 108.87, 74.49, 53.70, 45.83, 30.33, 29.18, 27.53, 24.97, 17.46.

HRMS (ESI) calcd for $C_{11}H_{12}N_4O$ $[M+Na]^+$: 239.0903; found: 239.0905.



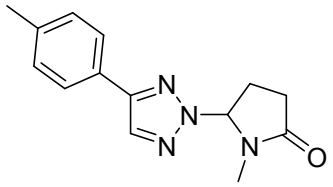
1-((4-(4-fluorophenyl)-2*H*-1,2,3-triazol-2-yl)methyl)pyrrolidin-2-one compound with 5-(4-(4-fluorophenyl)-2*H*-1,2,3-triazol-2-yl)-1-methylpyrrolidin-2-one (6.7:1) (42)[5].

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 - 7.83 (m, 1.15H), 7.77 – 7.74 (m, 2.3H), 7.14 – 7.10 (m, 2.3H), 6.03 (dd, *J* = 7.5, 1.6 Hz, 1H), 5.84 (s, 0.3H), 3.48 (t, *J* = 7.2 Hz, 0.3H), 2.99 - 2.90 (m, 1H), 2.73 (s, 3H), 2.65 – 2.57 (m, 1H), 2.54 – 2.43 (m, 2.3H), 2.04 (p, *J* = 7.5 Hz, 0.3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.47, 175.26, 164.21, 161.74, 147.77, 147.63, 131.69, 131.53, 127.78 (d, *J* = 8.2 Hz), 127.72 (d, *J* = 8.2 Hz), 126.00 (d, *J* = 3.3 Hz), 116.01 (d, *J* = 21.9 Hz), 115.80 (d, *J* = 21.8 Hz), 78.84, 59.97, 46.20, 30.47, 28.85, 27.58, 25.17, 17.70.

^{19}F NMR (377 MHz, $CDCl_3$) δ -112.36, -112.60.

HRMS (ESI) calcd for $C_{13}H_{13}FN_4O$ $[M+Na]^+$: 283.0966; found: 283.0960.

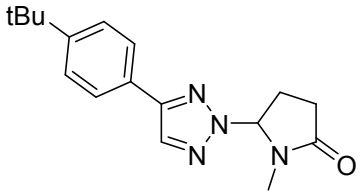


1-methyl-5-(4-(p-tolyl)-2*H*-1,2,3-triazol-2-yl)pyrrolidin-2-one (43).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.67 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 7.9 Hz, 2H), 6.03 (dd, *J* = 7.5, 1.7 Hz, 1H), 3.00 - 2.90 (m, 1H), 2.73 (s, 3H), 2.66 - 2.46 (m, 3H), 2.38 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.29, 148.67, 138.76, 131.62, 129.56, 126.93, 125.81, 78.73, 28.91, 27.56, 25.16, 21.30.

HRMS (ESI) calcd for $C_{14}H_{16}N_4O$ [M+Na]$^+$: 279.1216; found: 279.1213.

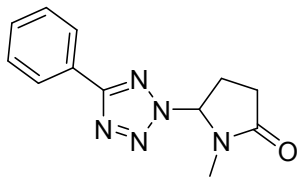


5-(4-(4-(tert-butyl)phenyl)-2*H*-1,2,3-triazol-2-yl)-1-methylpyrrolidin-2-one (44).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.71 (d, *J* = 8.6 Hz, 2H), 7.46 (d, *J* = 8.5 Hz, 2H), 6.03 (dd, *J* = 7.5, 1.7 Hz, 1H), 3.00 - 2.91 (m, 1H), 2.72 (s, 3H), 2.64 - 2.58 (m, 1H), 2.56 - 2.46 (m, 2H), 1.34 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.25, 151.99, 148.60, 131.69, 126.95, 125.81, 125.67, 78.72, 34.68, 31.20, 28.91, 27.53, 25.14.

HRMS (ESI) calcd for $C_{17}H_{22}N_4O$ [M+Na]$^+$: 321.1686; found: 321.1687.

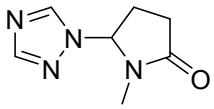


1-methyl-5-(5-phenyl-2*H*-tetrazol-2-yl)pyrrolidin-2-one (45).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 - 8.14 (m, 2H), 7.51 – 7.50 (m, 3H), 6.36 (dd, *J* = 7.8, 1.3 Hz, 1H), 3.06 - 2.97 (m, 1H), 2.80 (s, 3H), 2.77 – 2.69 (m, 1H), 2.62 – 2.53 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.08, 165.87, 130.67, 128.89, 126.86, 126.73, 77.91, 28.47, 27.67, 25.17.

HRMS (ESI) calcd for $C_{12}H_{13}N_5O$ [M+Na]$^+$: 266.1012; found: 266.1012.

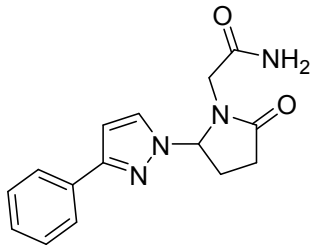


1-methyl-5-(1*H*-1,2,4-triazol-1-yl)pyrrolidin-2-one (46)[5].

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (s, 1H), 7.90 (s, 1H), 5.76 (dd, *J* = 7.9, 1.7 Hz, 1H), 2.80 - 2.71(m, 1H), 2.58 (s, 3H), 2.56 - 2.48 (m, 1H), 2.42 - 2.35 (m, 1H), 2.29 - 2.22 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.68, 152.78, 142.37, 74.06, 28.51, 27.00, 25.33.

HRMS (ESI) calcd for $C_7H_{10}N_4O$ [M+Na]$^+$: 189.0747; found: 189.0749.

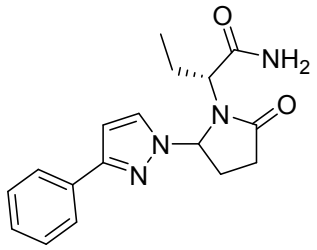


2-(2-oxo-5-(3-phenyl-1*H*-pyrazol-1-yl)pyrrolidin-1-yl)acetamide (47).

^{1}H NMR (101 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 2.4 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.26 (t, *J* = 7.3 Hz, 1H), 6.74 (s, 1H), 6.53 (d, *J* = 2.3 Hz, 1H), 6.23 (s, 1H), 5.88 (dd, *J* = 7.7, 2.4 Hz, 1H), 4.07 (d, *J* = 3.0 Hz, 1H), 3.33 (d, *J* = 16.9 Hz, 1H), 2.89 - 2.81 (m, 1H), 2.59 - 2.53 (m, 1H), 2.50 - 2.34 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.68, 170.13, 153.37, 132.70, 130.83, 128.64, 128.14, 125.55, 103.35, 74.94, 43.71, 29.07, 25.94.

HRMS (ESI) calcd for $C_{15}H_{16}N_4O_2$ $[M+Na]^+$: 307.1165; found: 307.1167.

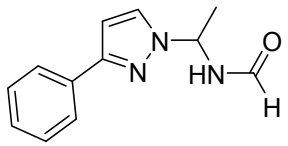


(2R)-2-(2-oxo-5-(3-phenyl-1*H*-pyrazol-1-yl)pyrrolidin-1-yl)butanamide (48).

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.01 - 7.93 (2×m, 1H), 7.80 (d, *J* = 8.3 Hz, 2H), 7.52 (s, 0.7H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 1H), 6.20 - 6.00 (m, 1.3H), 6.73 - 6.72 (m, 1H), 6.31 - 5.94 (2×m, 1H), 4.36 - 4.26 (m, 0.7H), 3.77 (t, *J* = 7.3 Hz, 0.3H), 3.00 - 2.84 (m, 1H), 2.64 - 2.54 (m, 1H), 2.40 - 2.32 (m, 1H), 2.27 - 2.08 (m, 1H), 1.81 (p, *J* = 7.6 Hz, 0.7H), 1.49 (dt, *J* = 13.8, 6.6 Hz, 0.7H), 1.13 - 1.05 (m, 0.6H), 0.75 - 0.51 (m, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 177.71, 175.67, 175.32, 172.10, 171.21, 170.11, 151.33 & 151.21, 133.20, 131.87 & 131.77, 128.76 & 128.74, 127.81, 125.35 & 125.29, 102.94 & 102.71, 74.00 & 73.05, 58.06, 56.30, 54.64, 29.70, 29.18, 28.19, 27.20, 26.37, 22.56, 21.09, 20.43, 10.90 & 10.82.

HRMS (ESI) calcd for $C_{17}H_{20}N_4O_2$ $[M+Na]^+$: 335.1478; found: 335.1472.



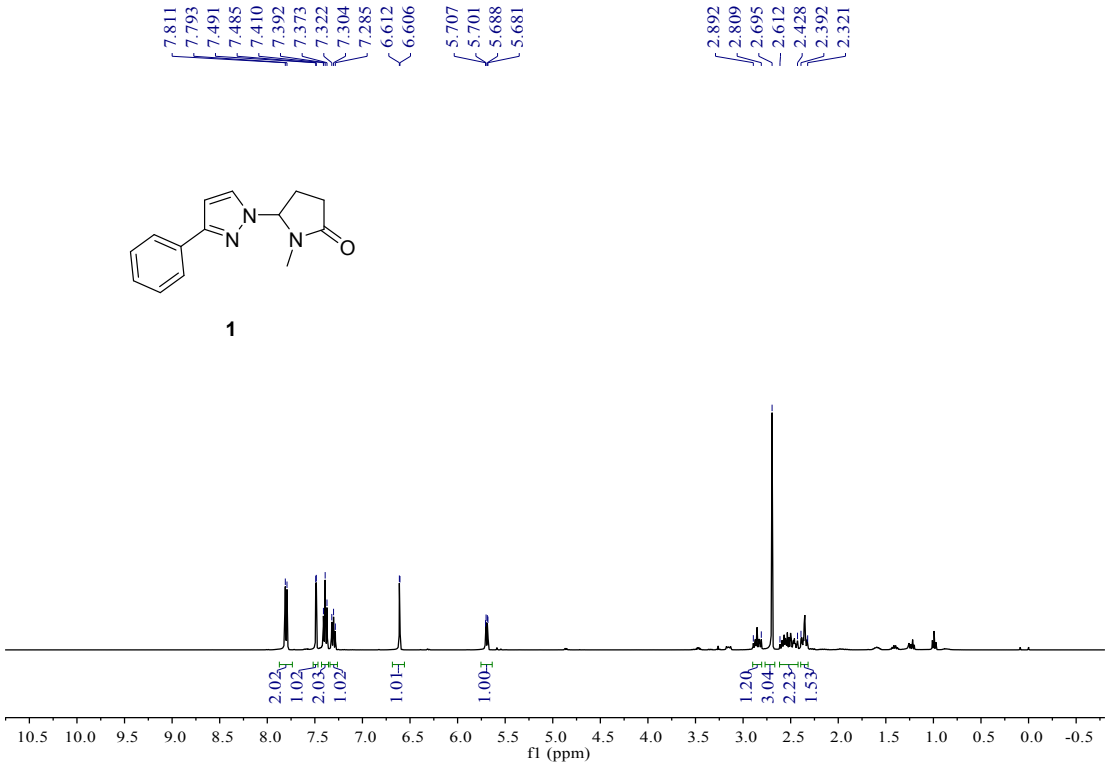
***N*-(1-(3-phenyl-1*H*-pyrazol-1-yl)ethyl)formamide (49).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.77 (d, *J* = 7.1 Hz, 2H), 7.61 (d, *J* = 2.4 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 6.51 (d, *J* = 2.4 Hz, 1H), 6.34 - 6.27 (m, 1H), 1.80 (d, *J* = 6.7 Hz, 3H).

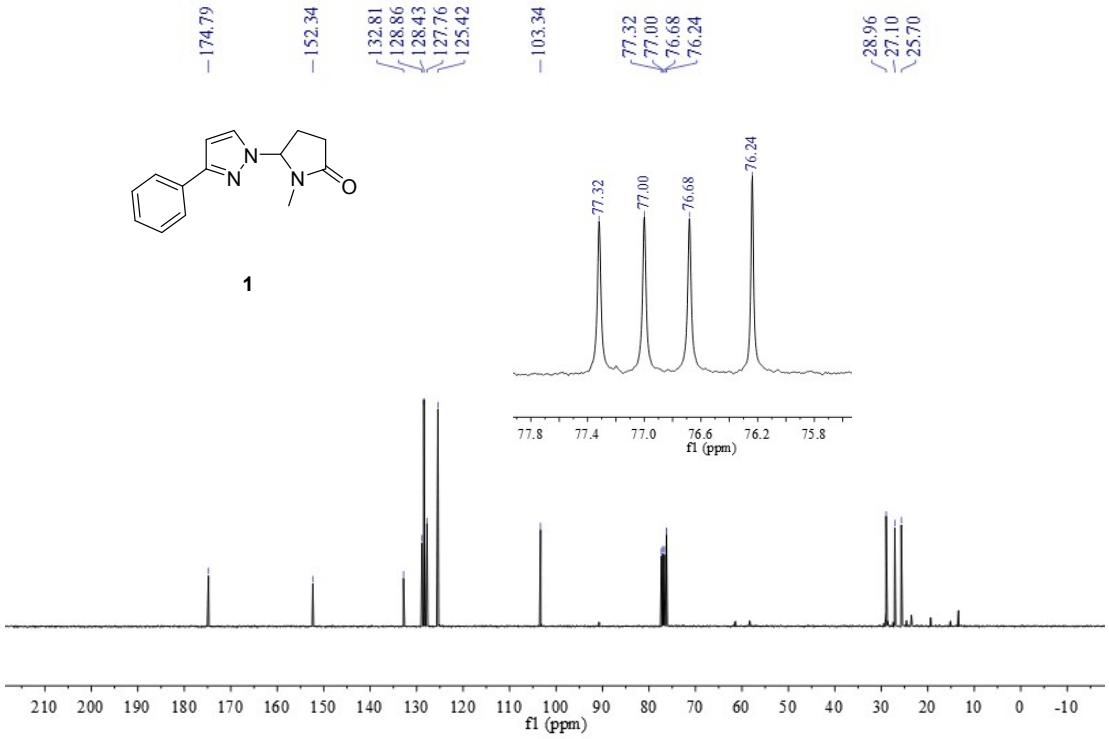
^{13}C NMR (101 MHz, $CDCl_3$) δ 164.19 & 160.48, 152.28, 133.18, 130.94, 128.61 & 127.94, 127.88 & 127.46, 125.73 & 125.65, 103.65 & 102.71, 65.07 & 59.87, 20.86 & 20.52.

HRMS (ESI) calcd for $C_{12}H_{13}N_3O$ $[M+Na]^+$: 238.0951; found: 238.0951.

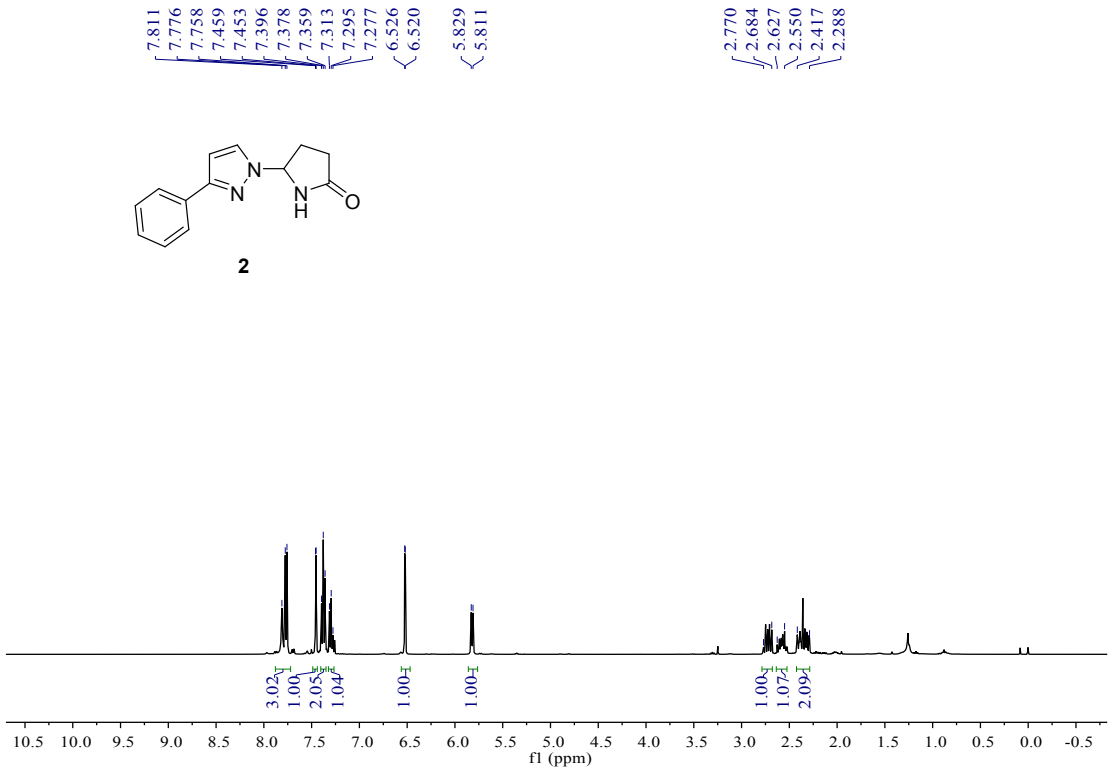
6. NMR Spectra of Products



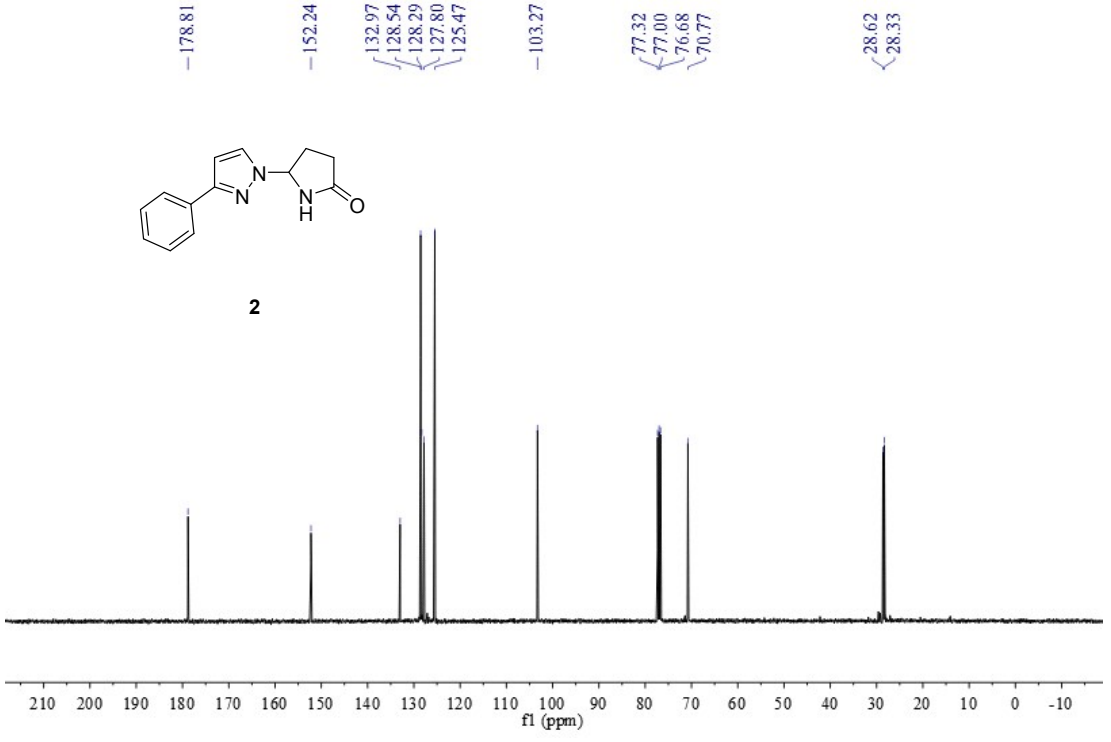
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 1



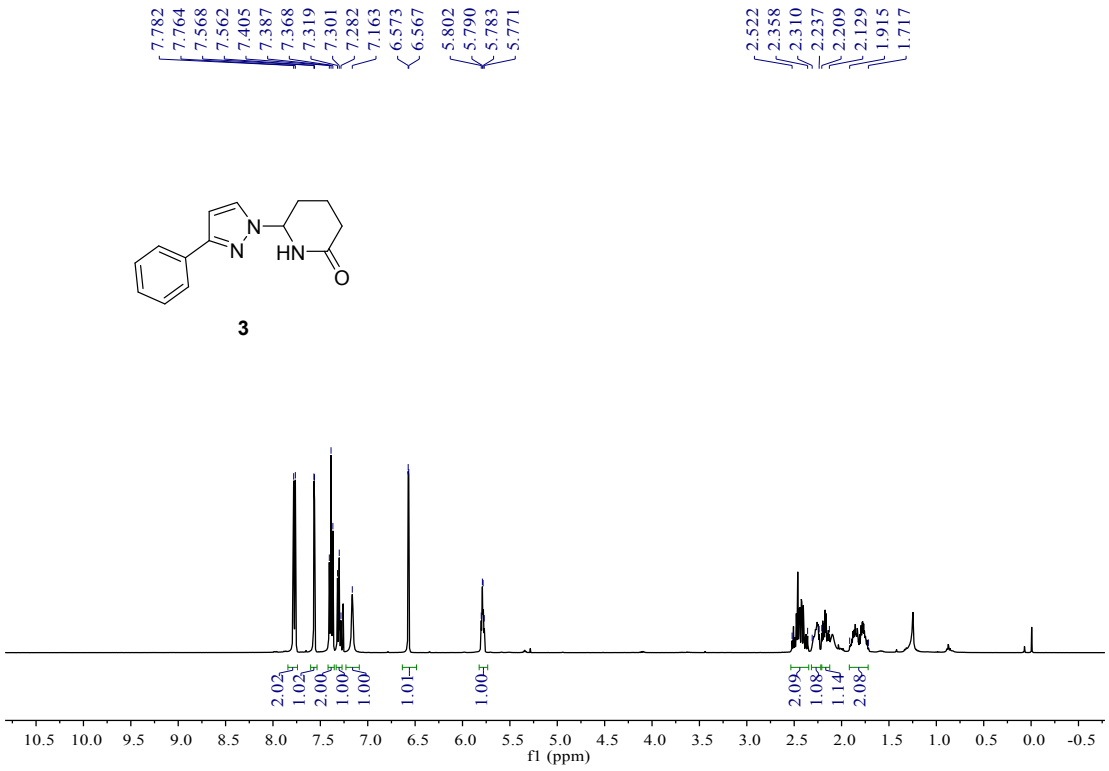
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 1



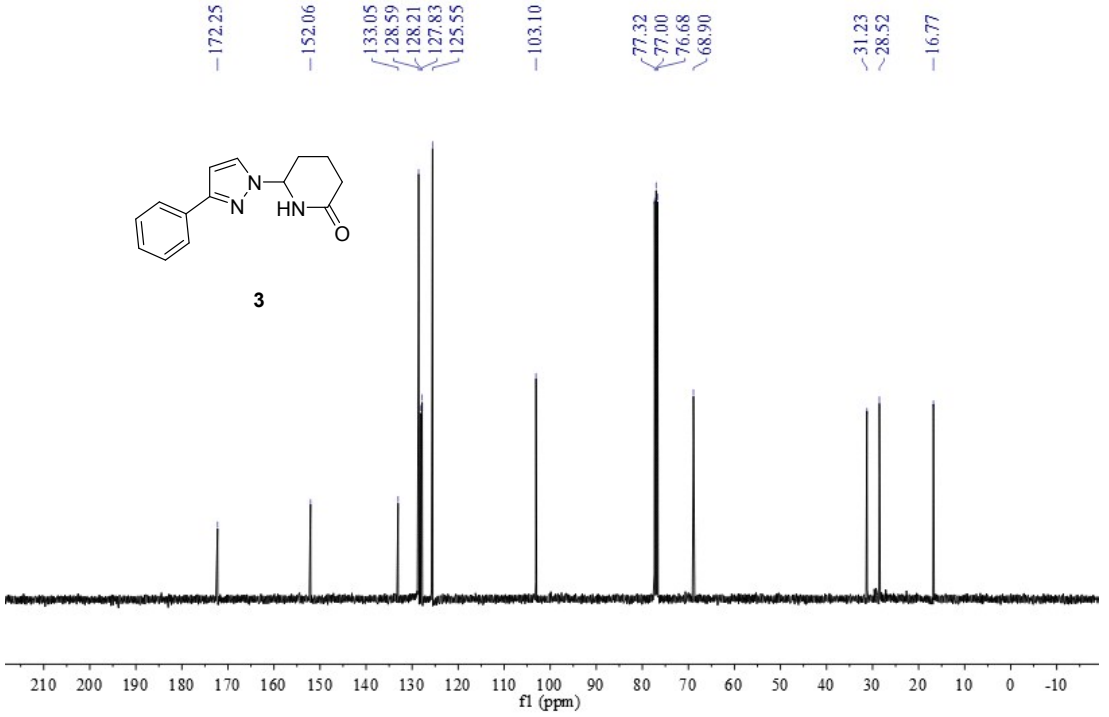
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 2



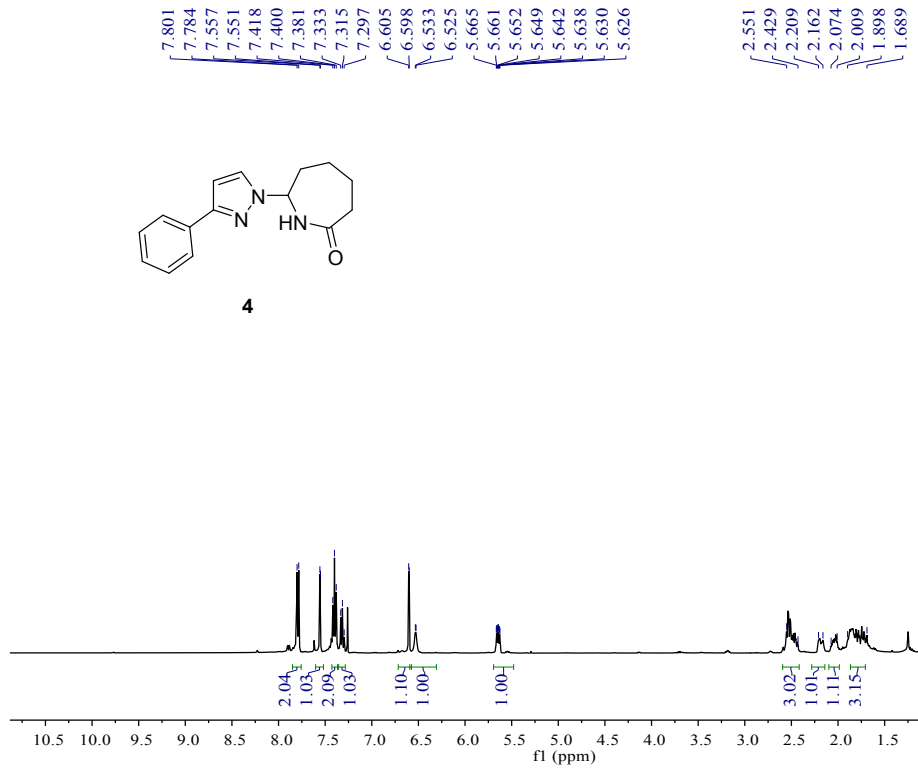
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 2



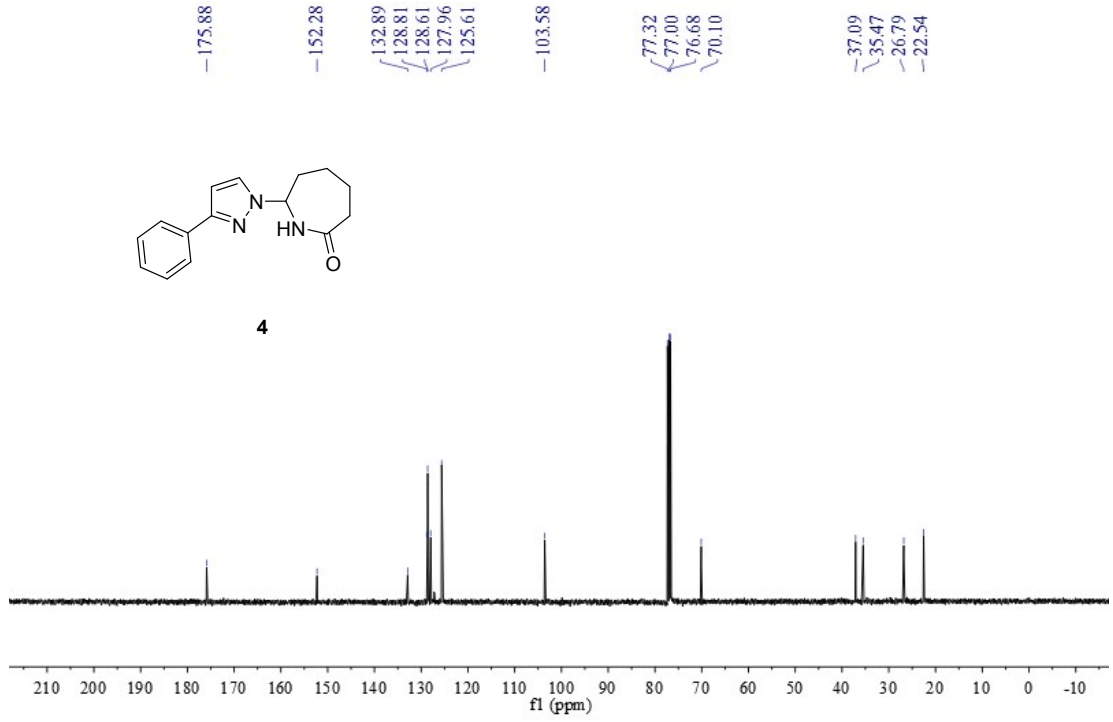
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3



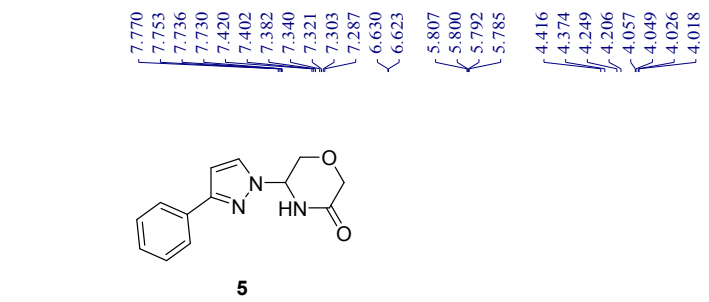
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3



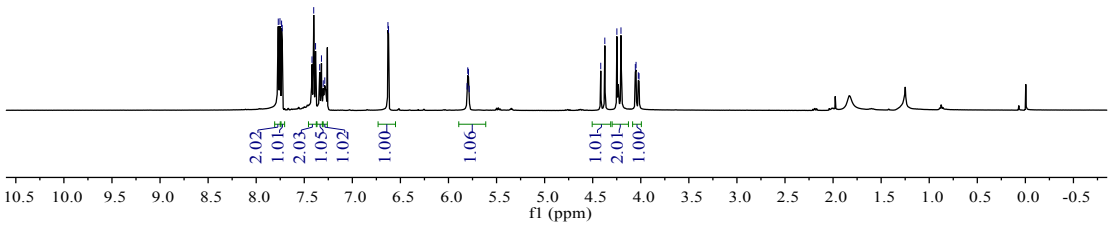
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4



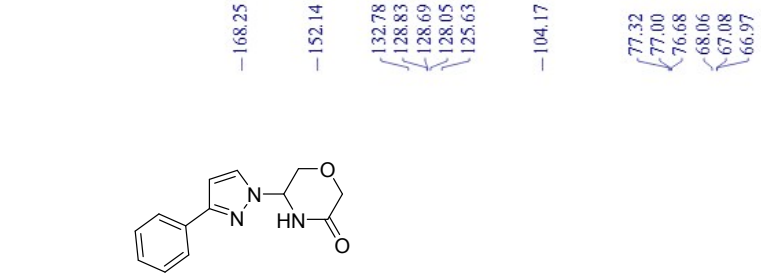
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 4



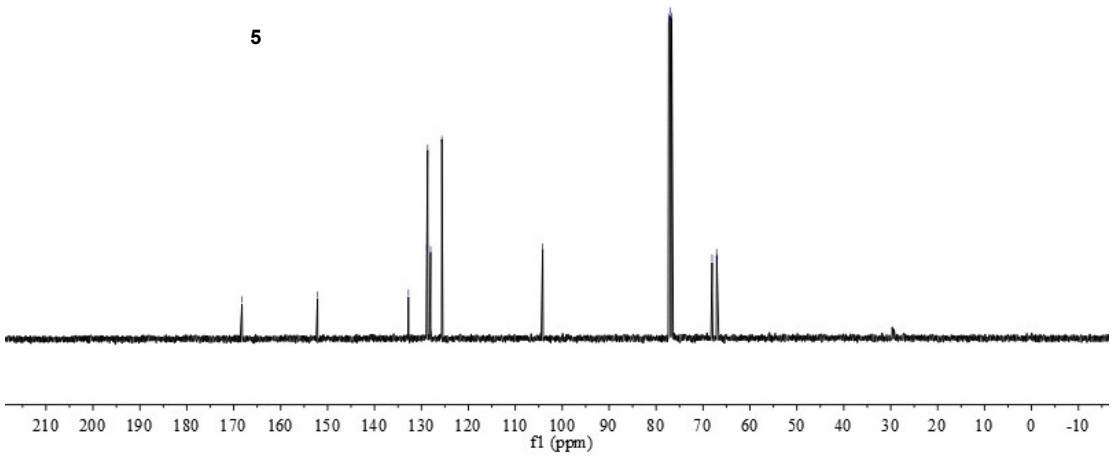
5



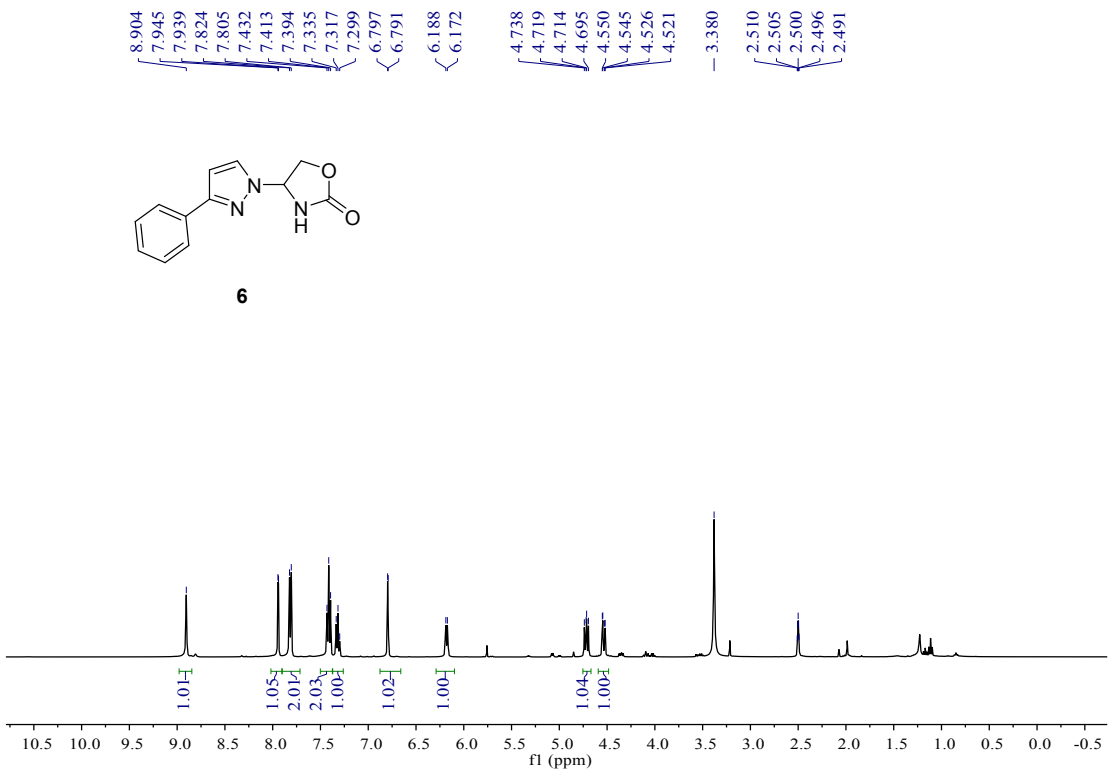
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5



5

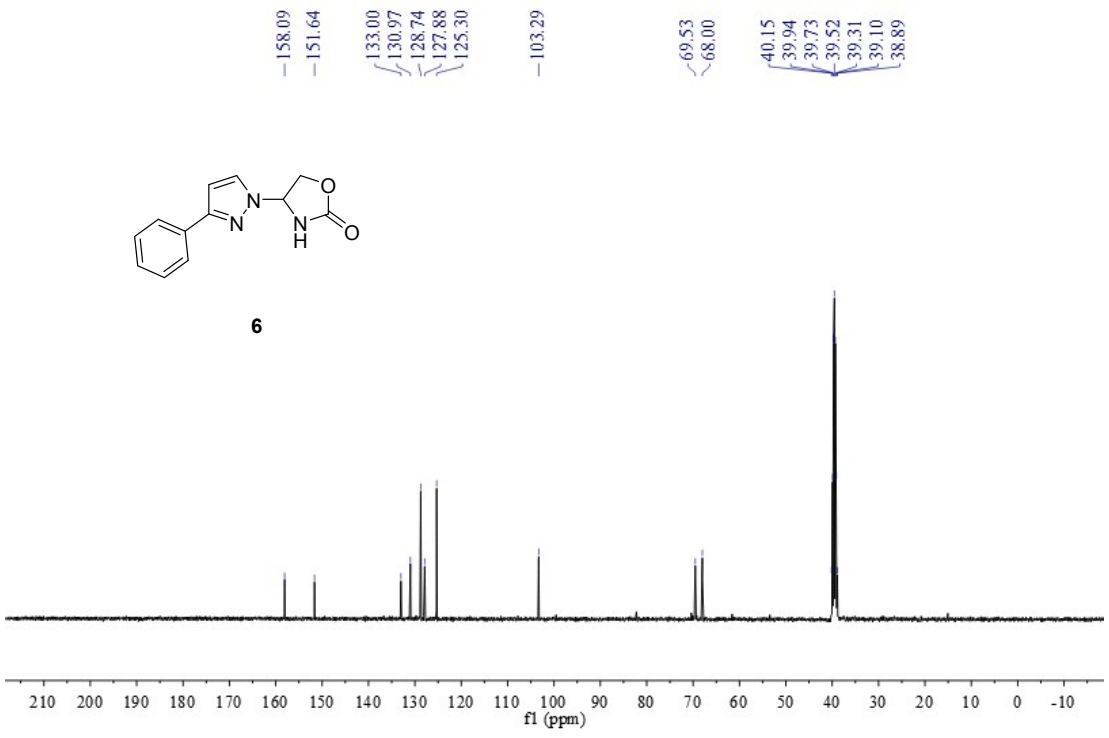


^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 5



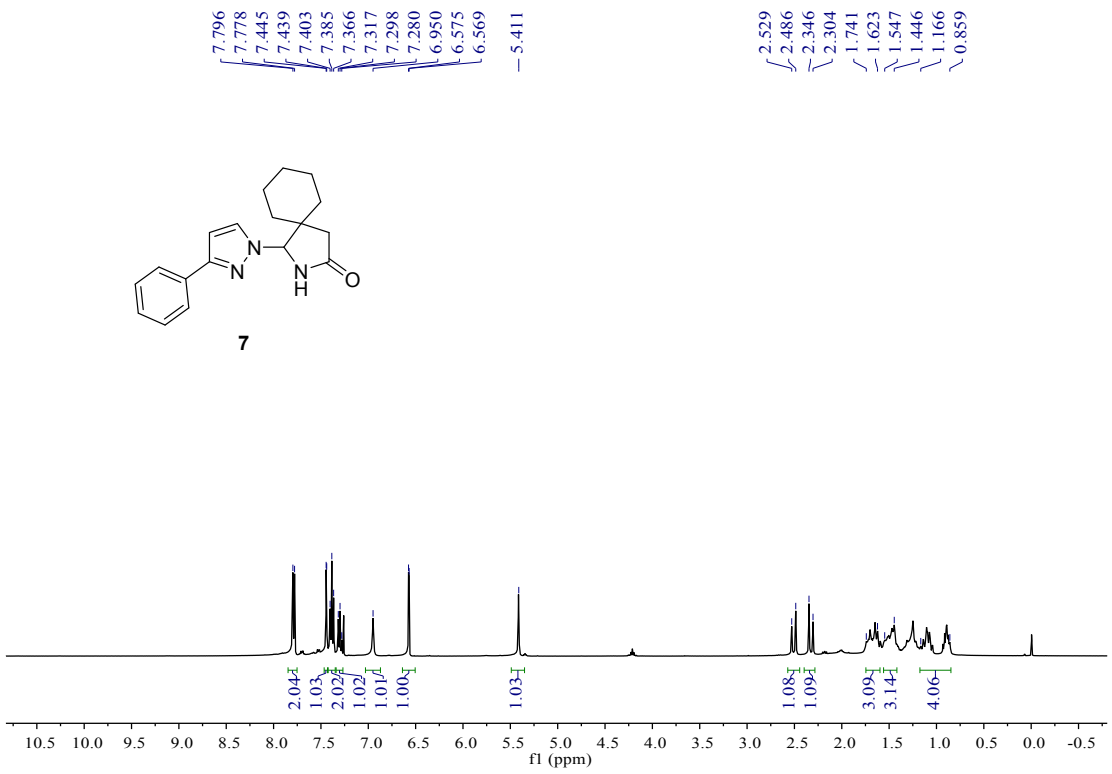
6

^{1}H NMR (400 MHz, DMSO-d$_6$) spectrum of 6

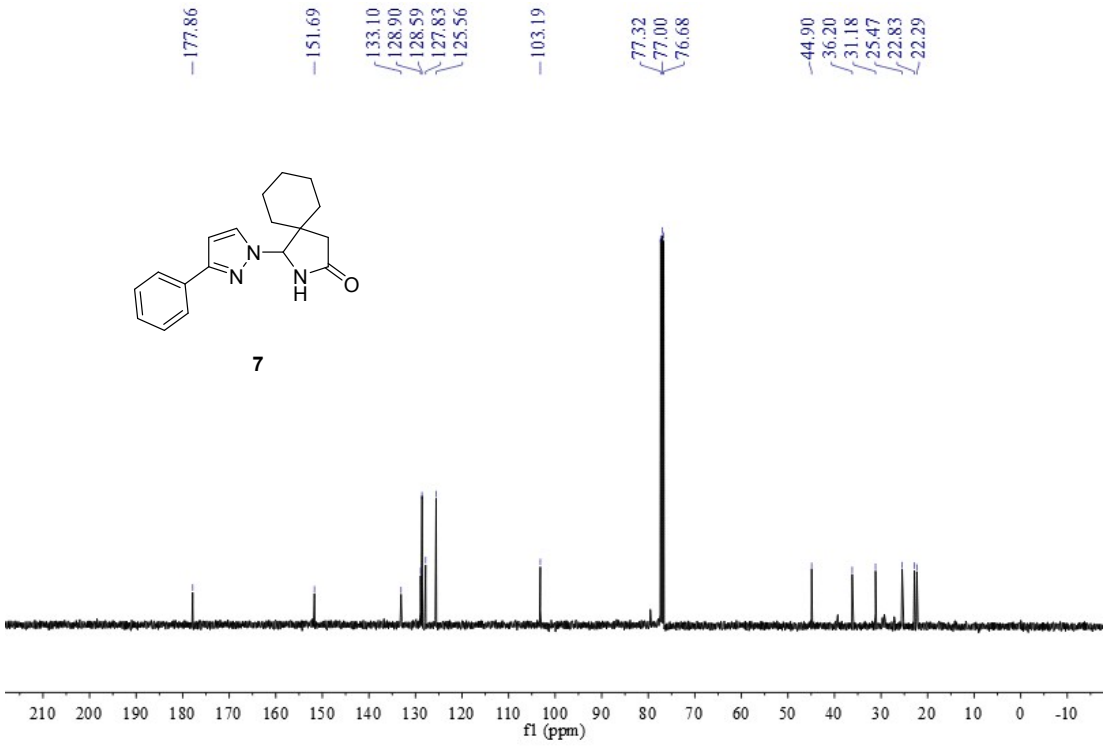


6

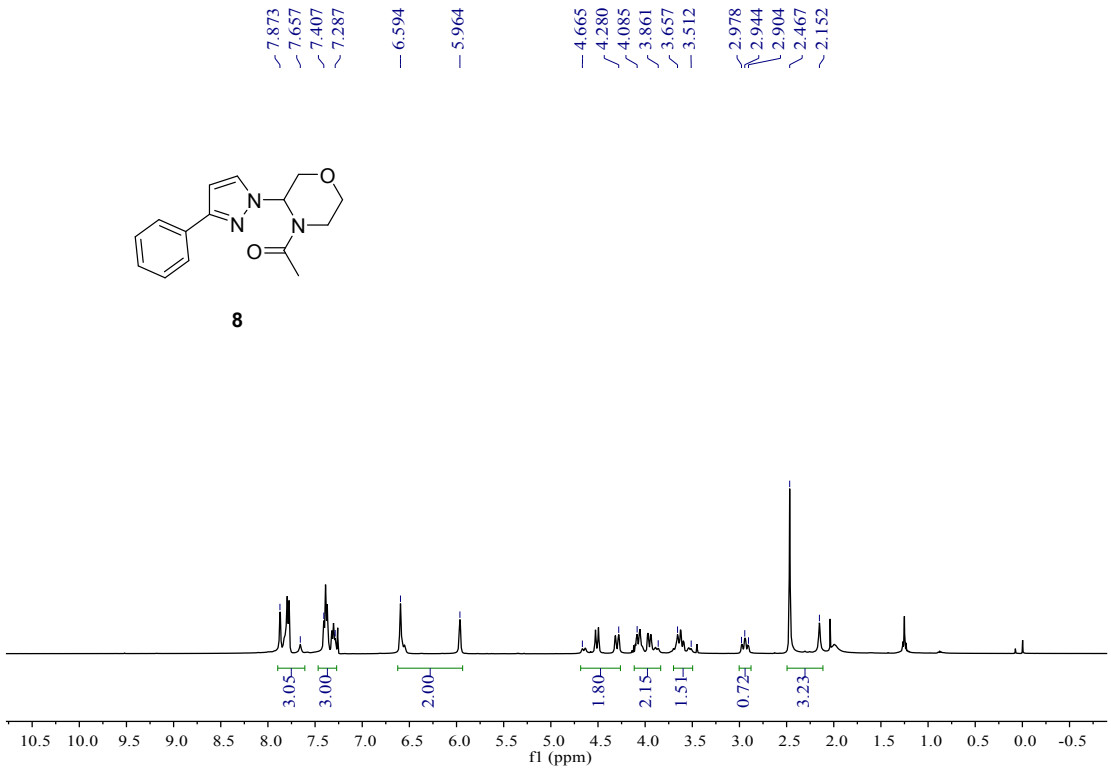
^{13}C NMR (101 MHz, DMSO-d$_6$) spectrum of 6



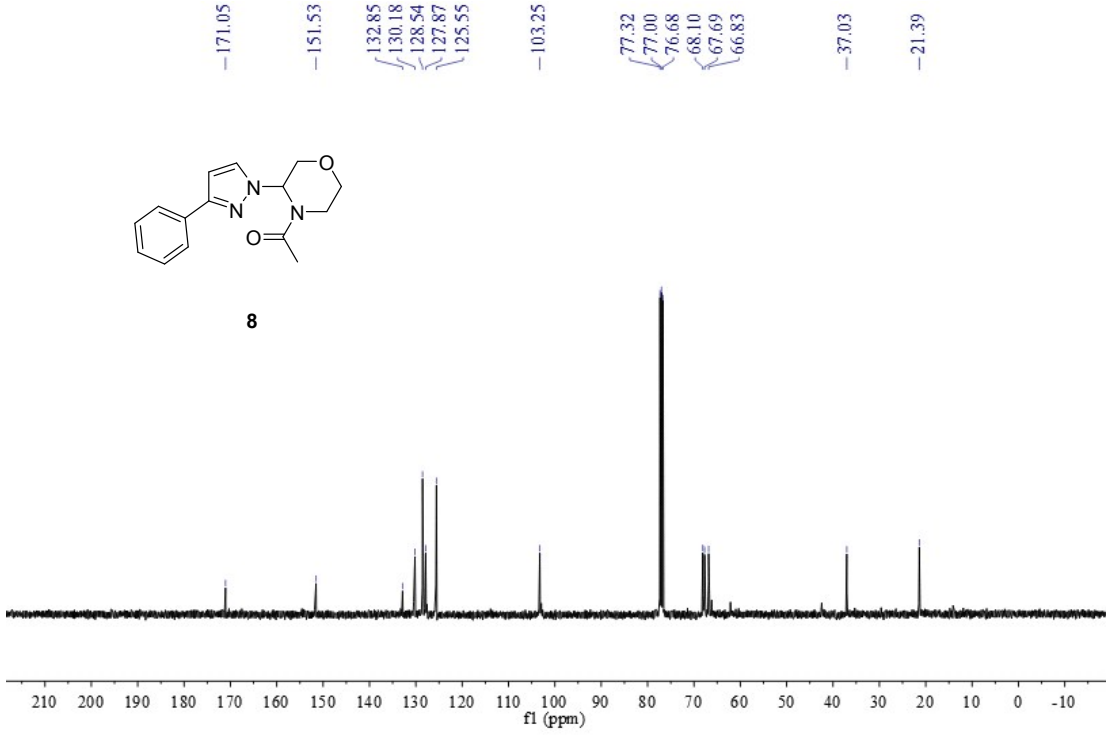
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 7



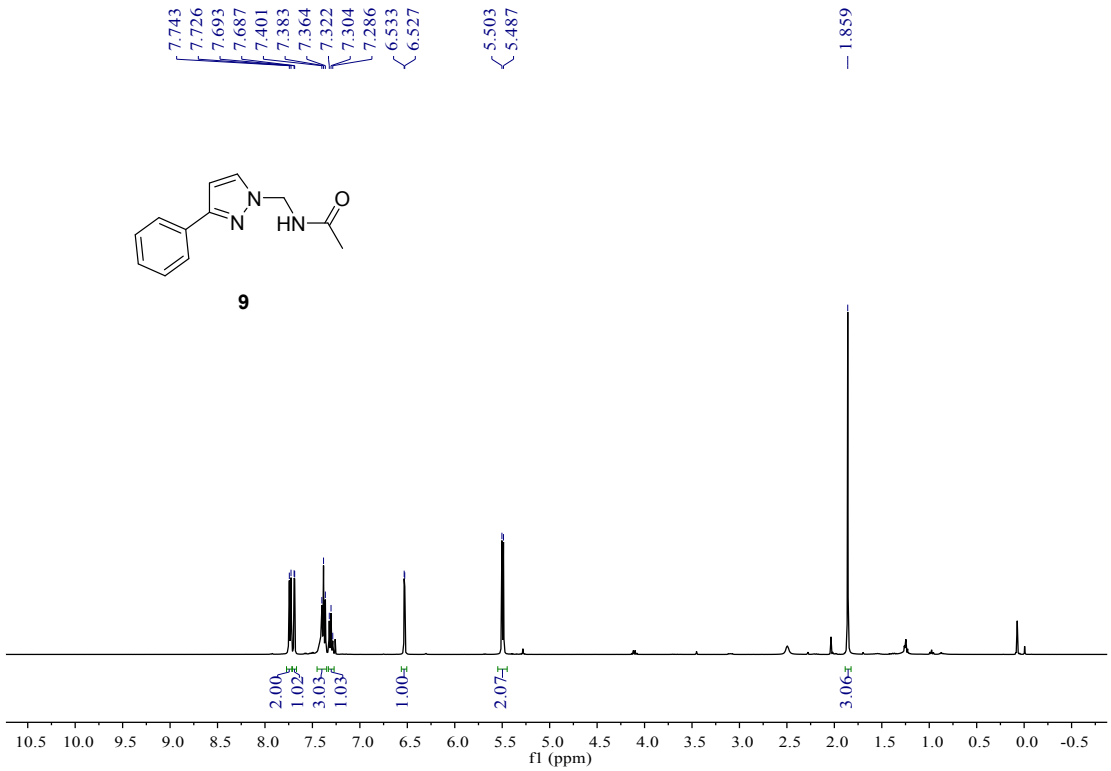
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 7



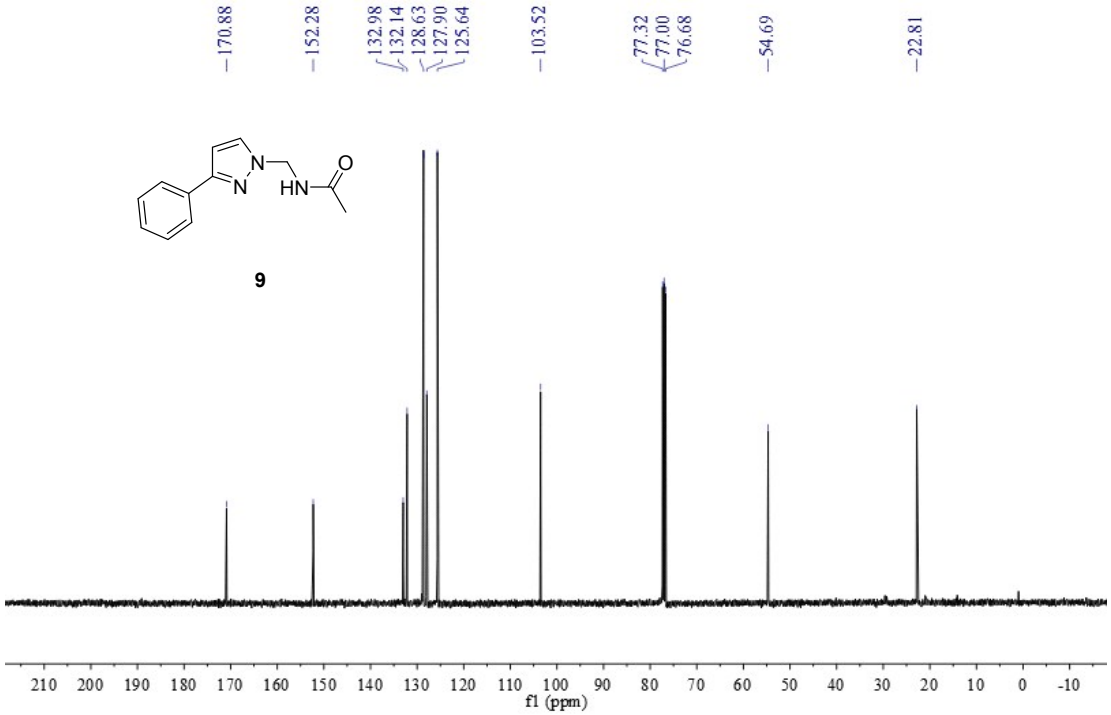
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8



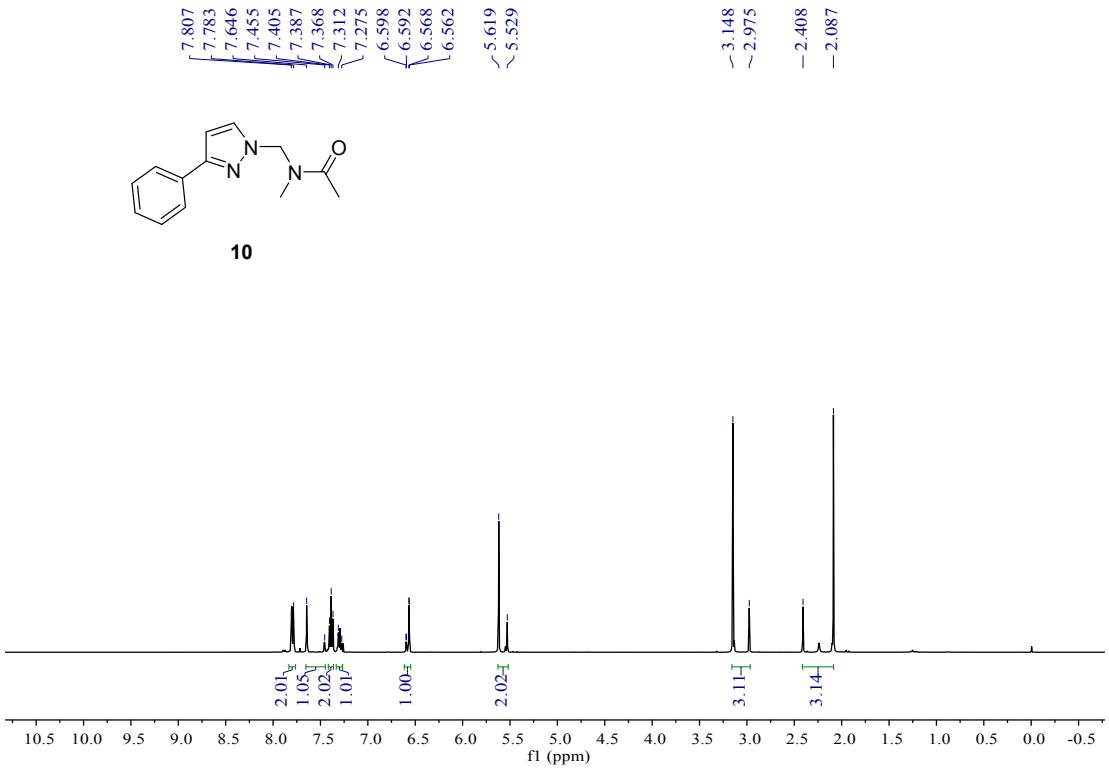
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 8



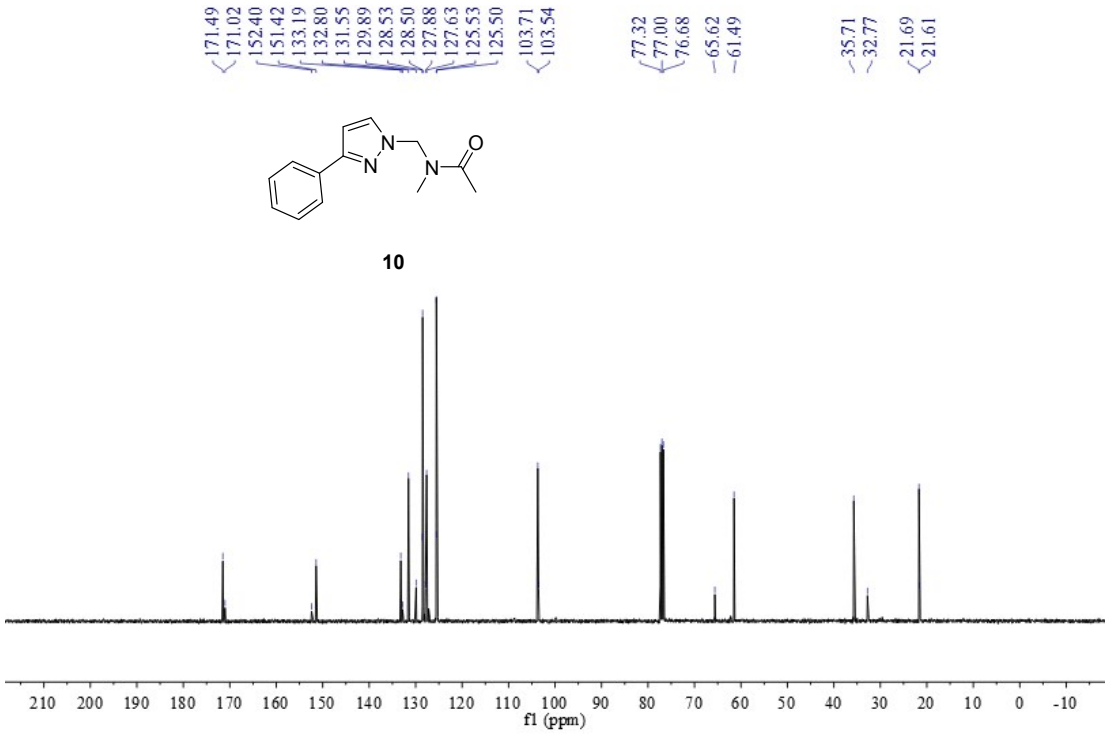
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 9



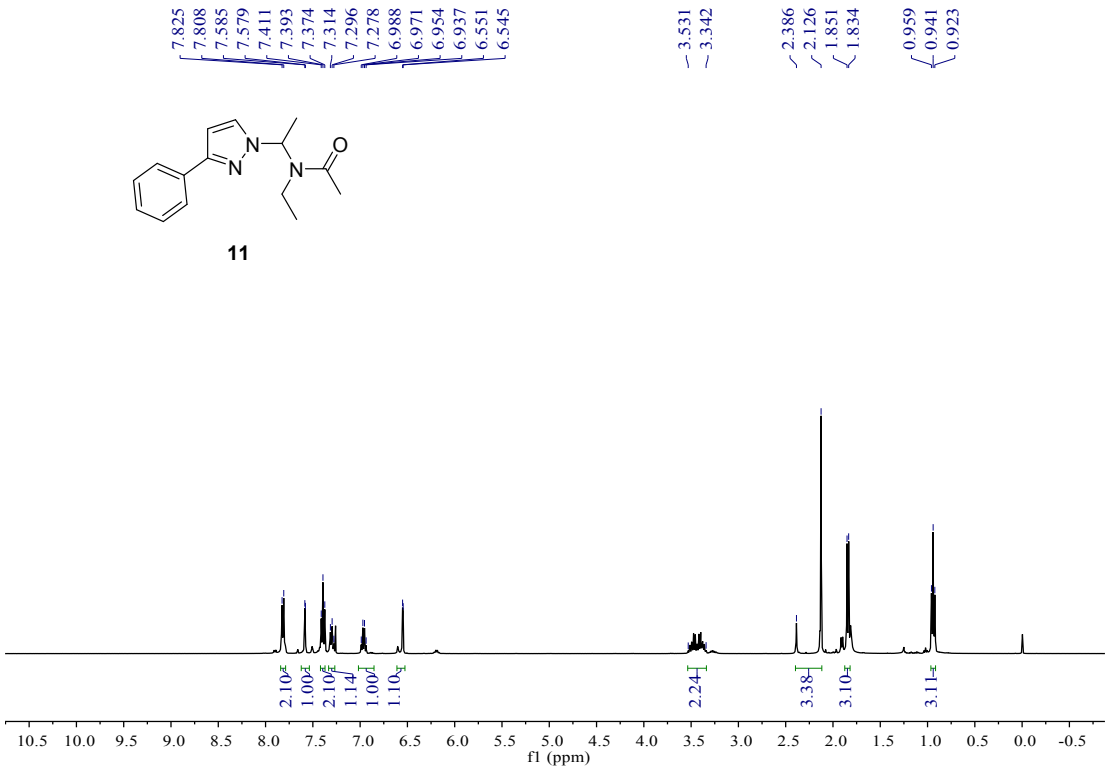
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 9



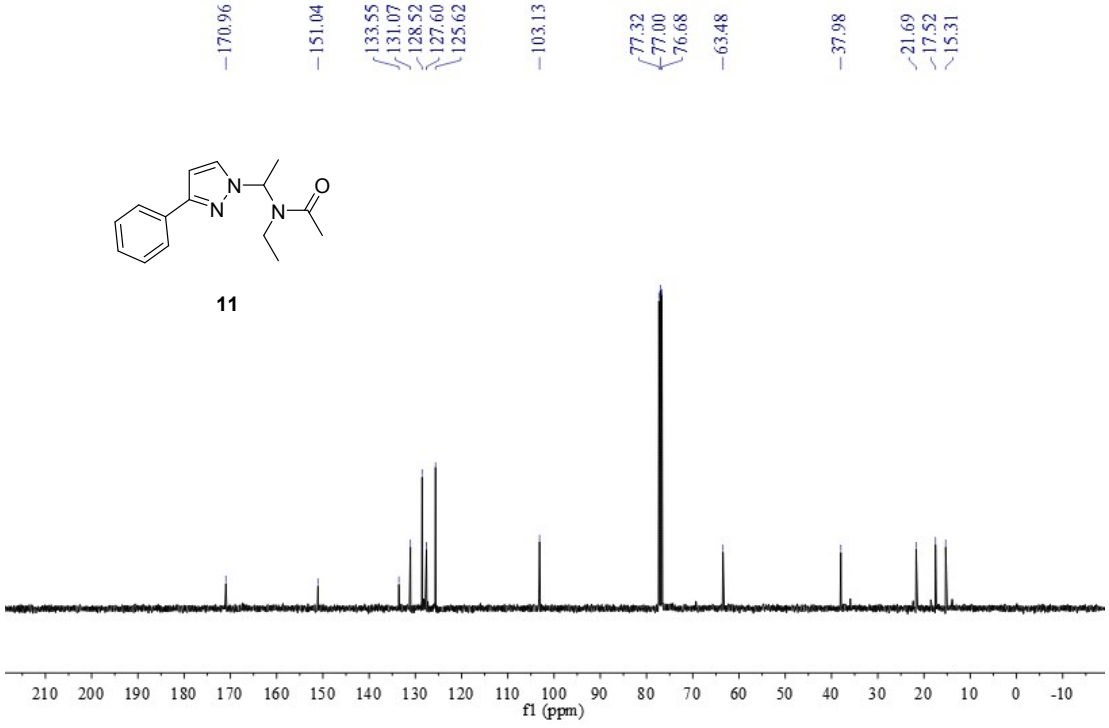
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 10



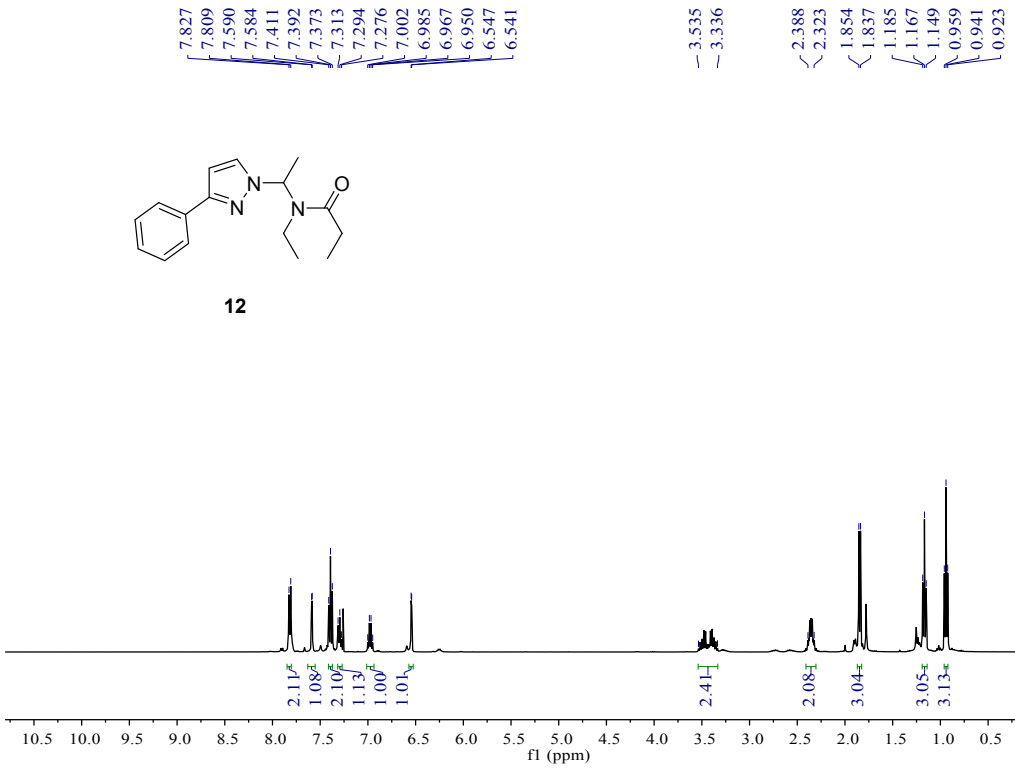
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 10



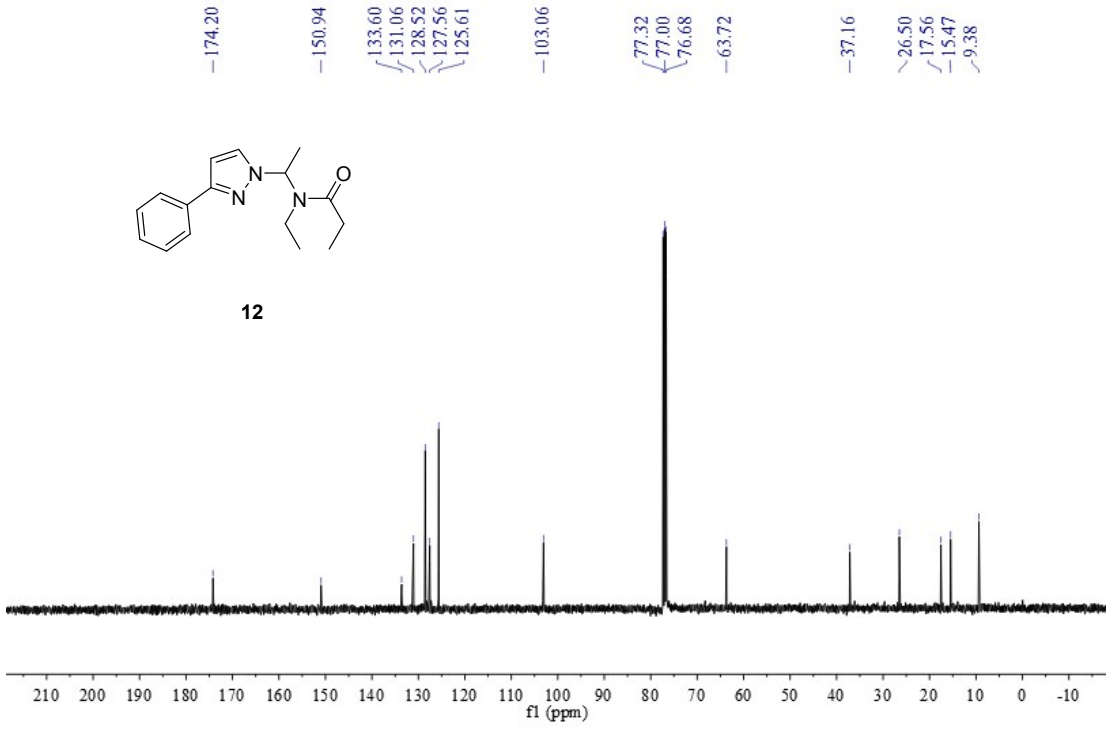
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 11



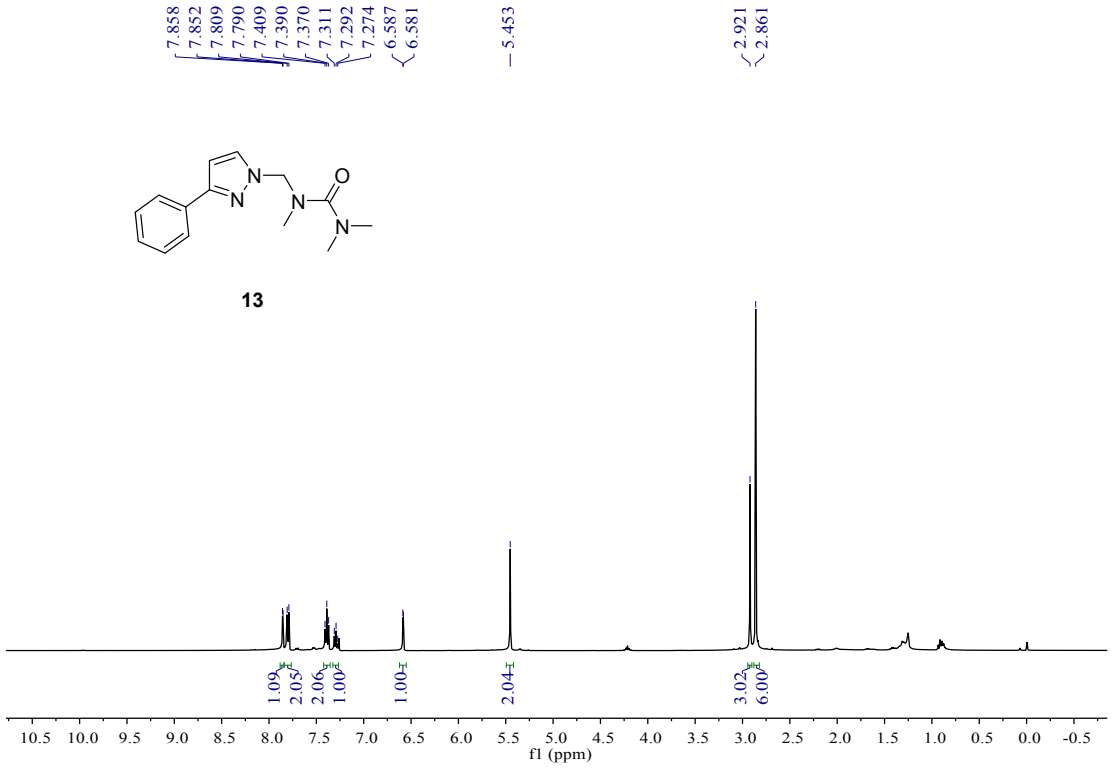
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 11



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

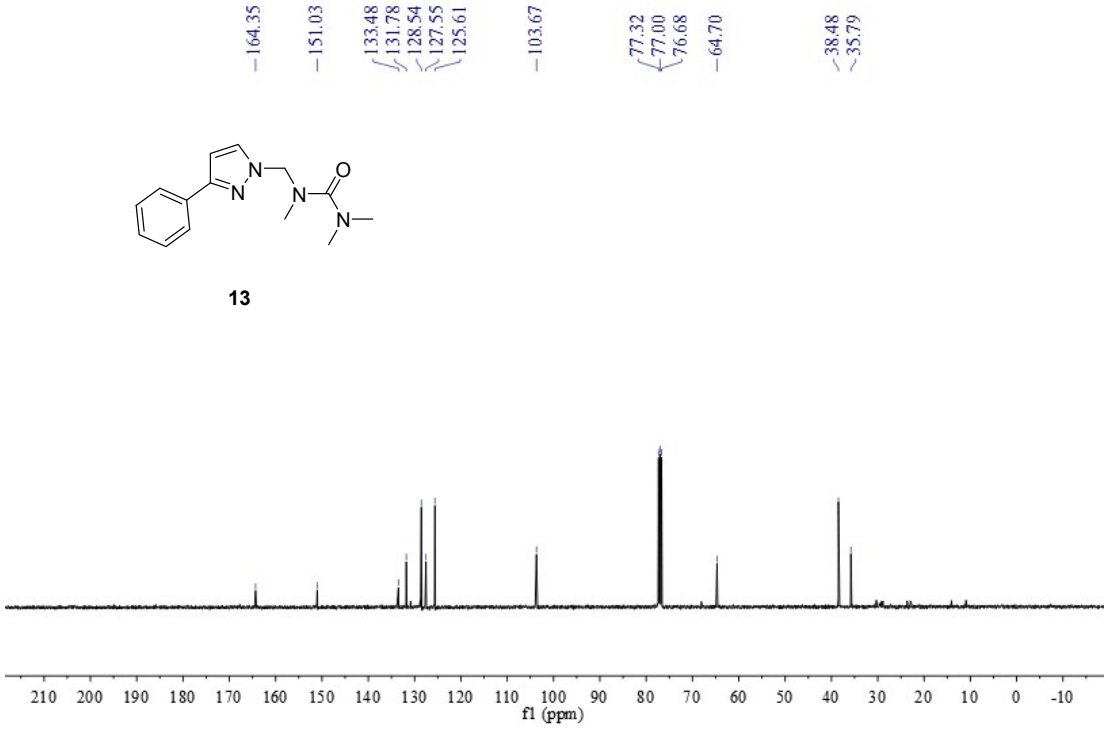


^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 12



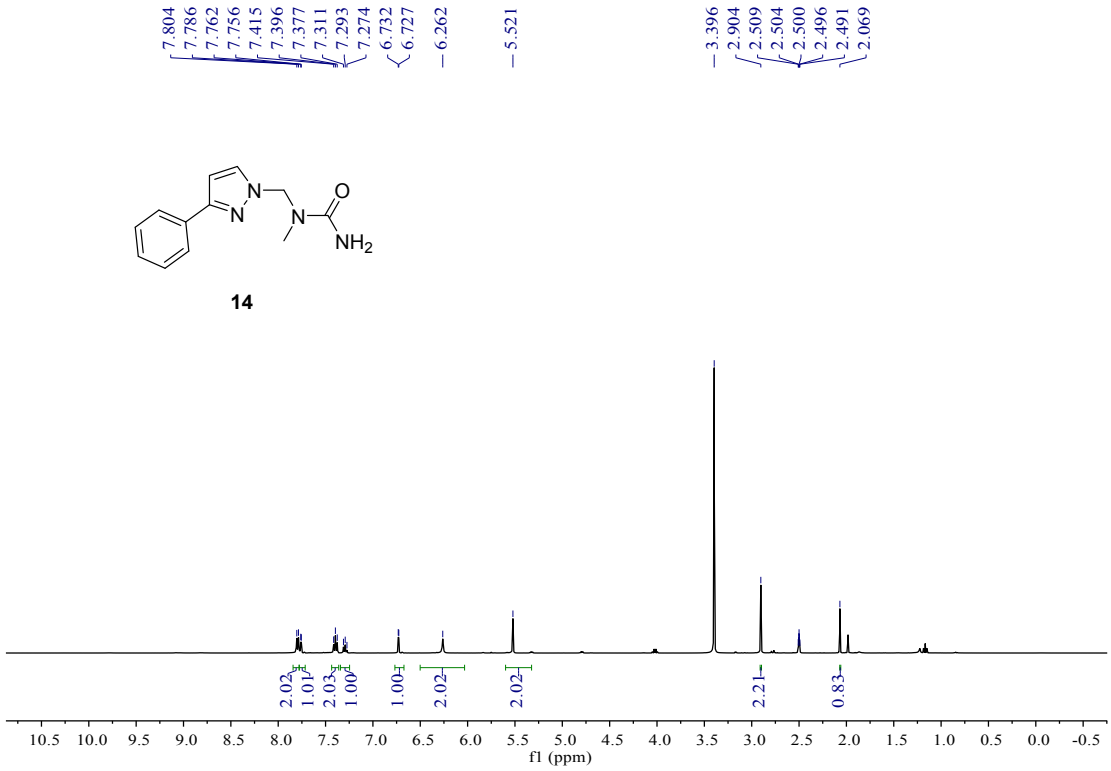
13

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

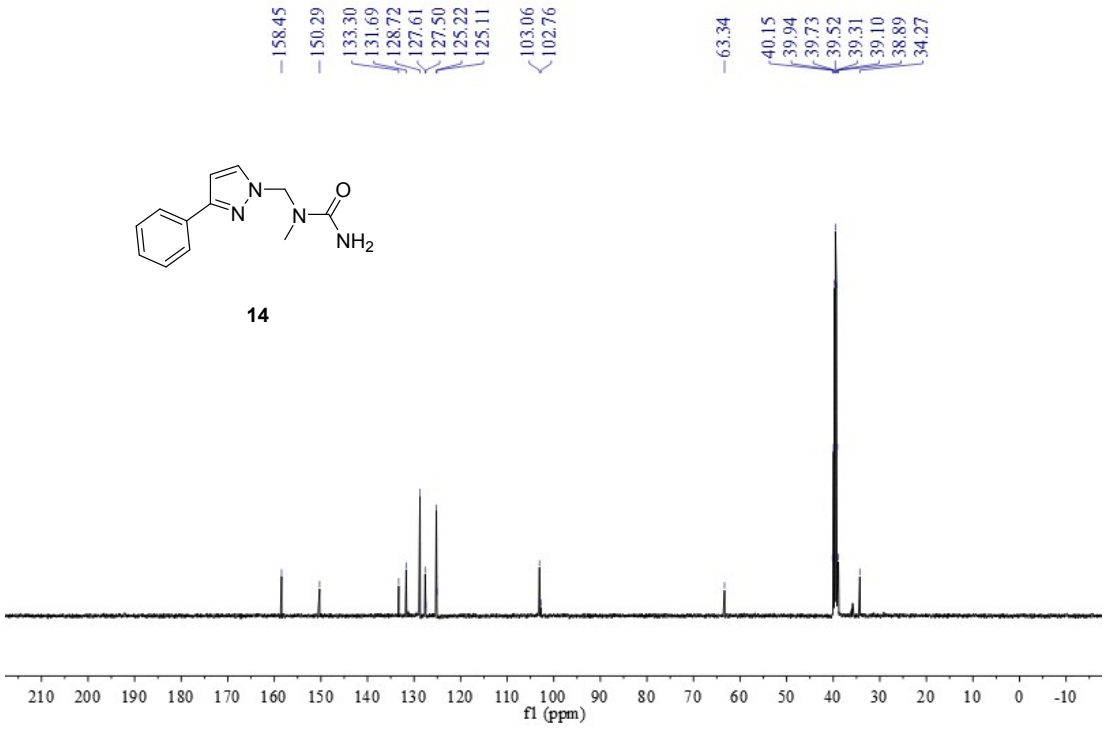


13

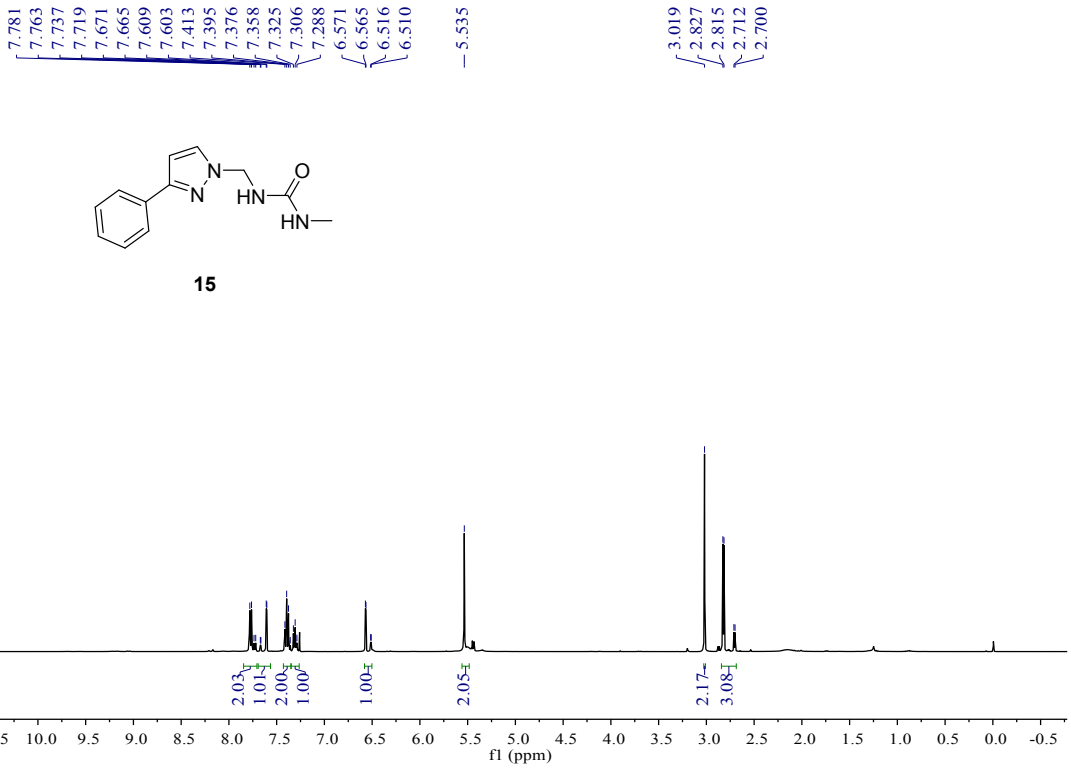
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 13



^{1}H NMR (400 MHz, DMSO-d$_6$) spectrum of 14

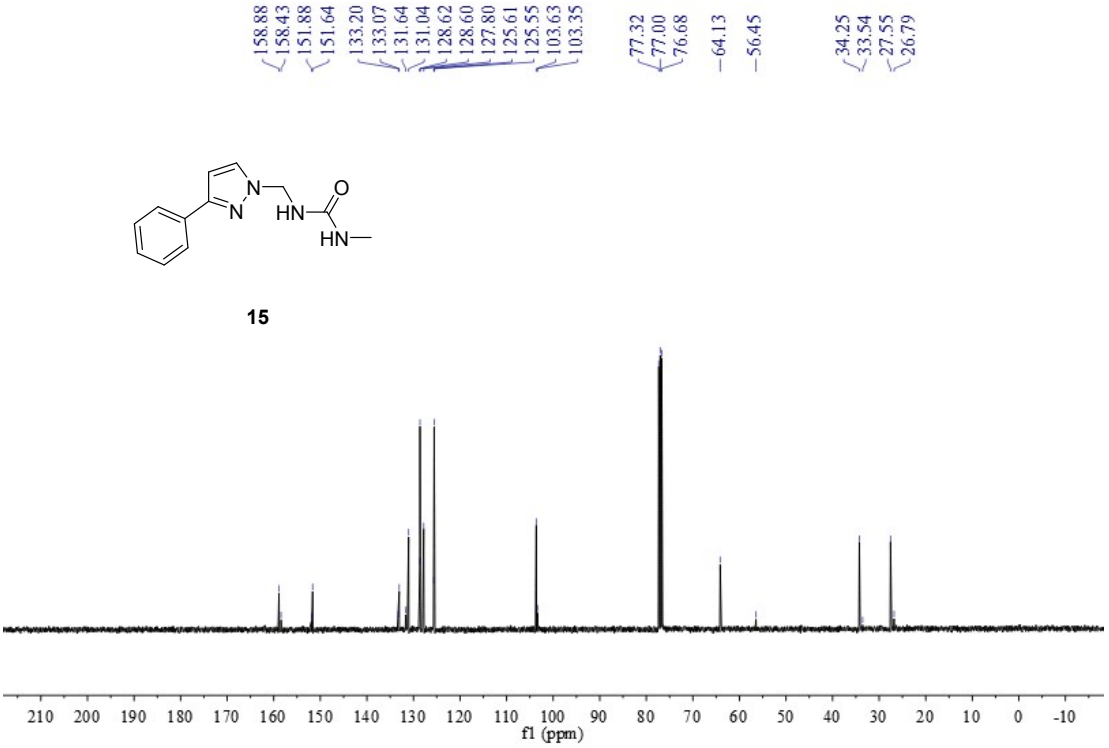


^{13}C NMR (101 MHz, DMSO-d$_6$) spectrum of 14



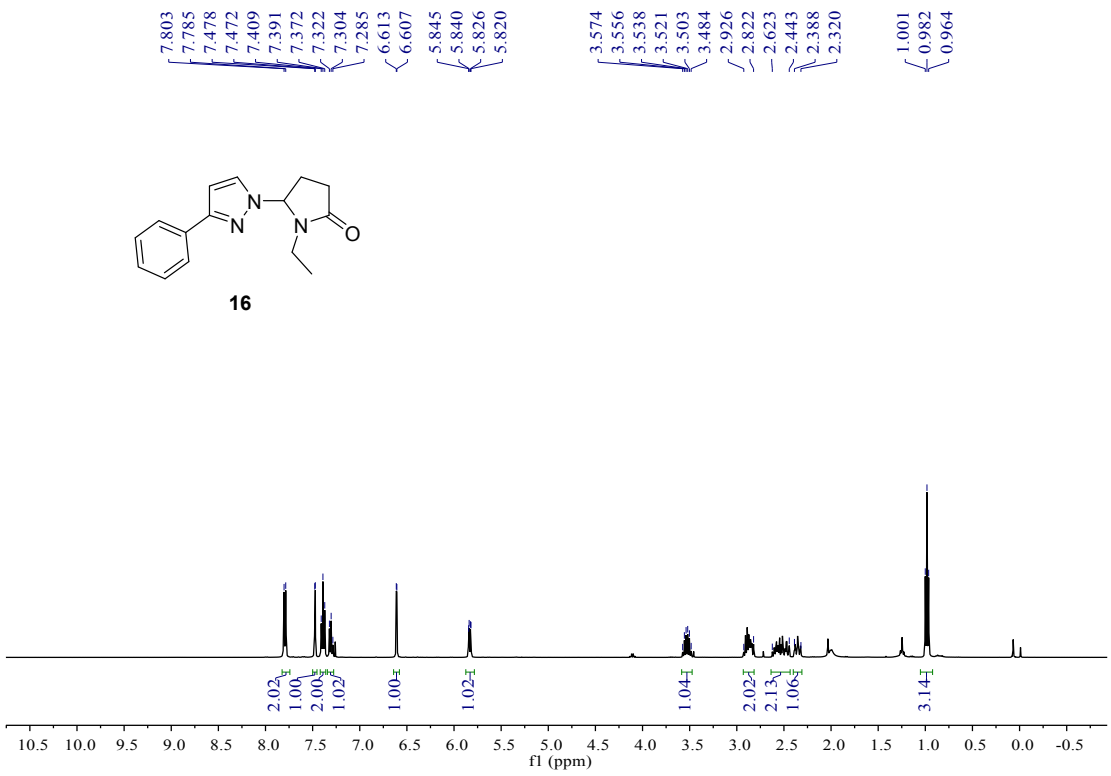
15

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

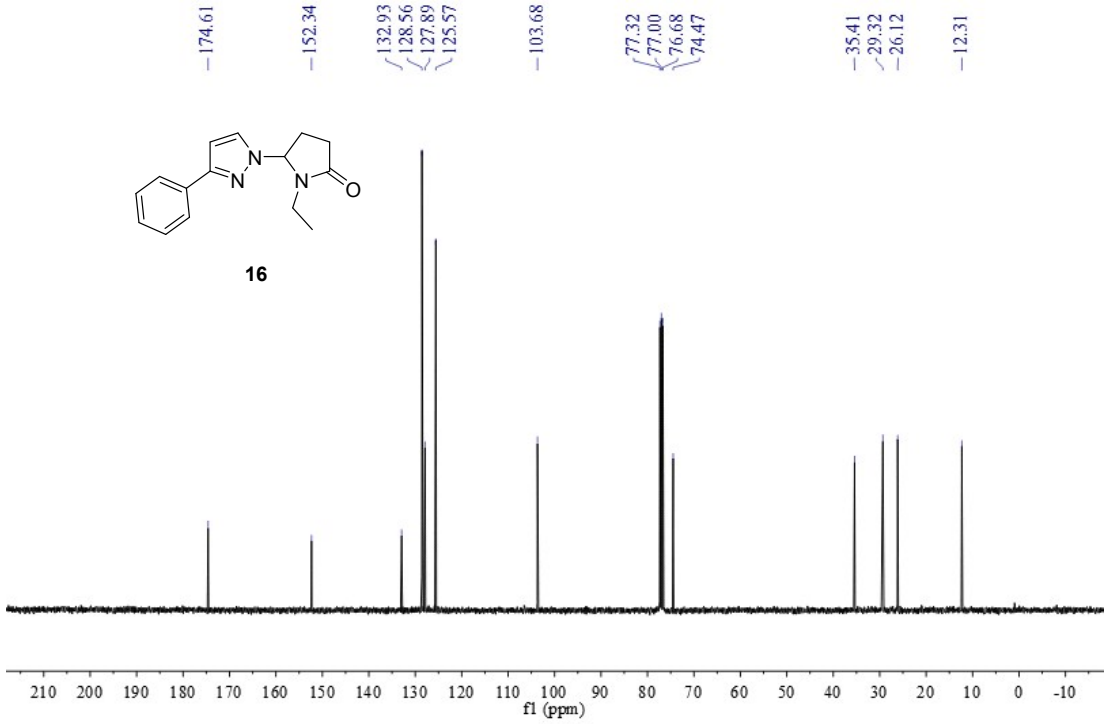


15

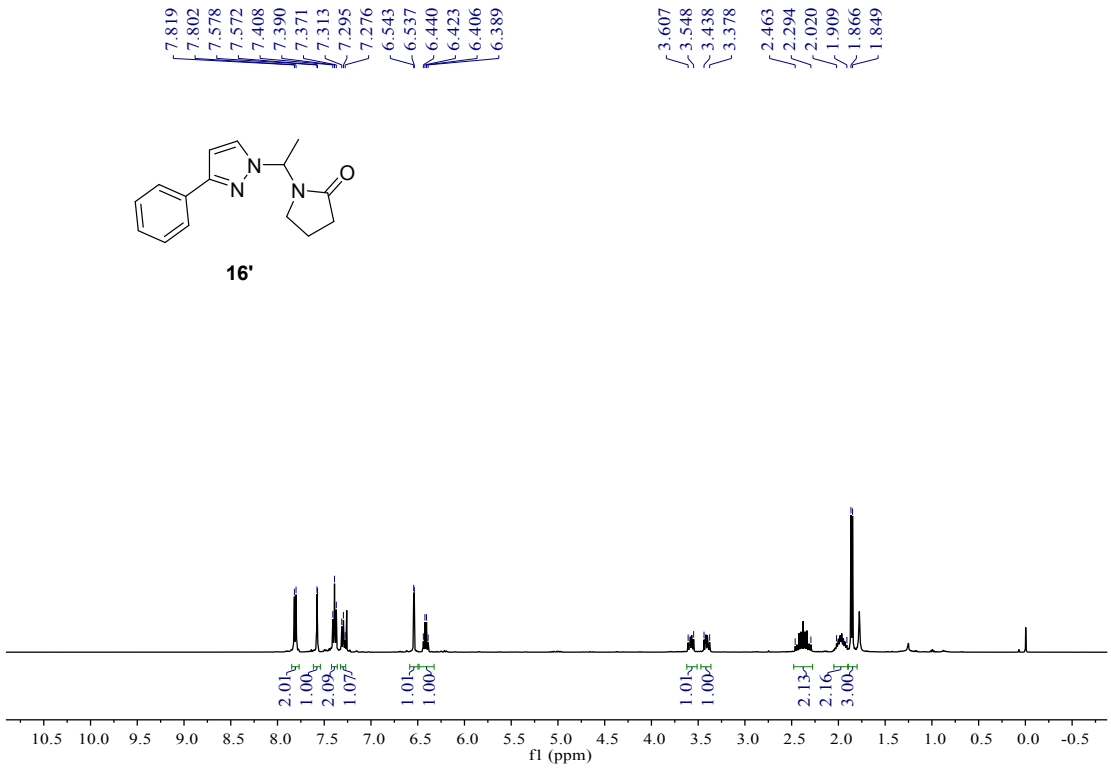
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 15



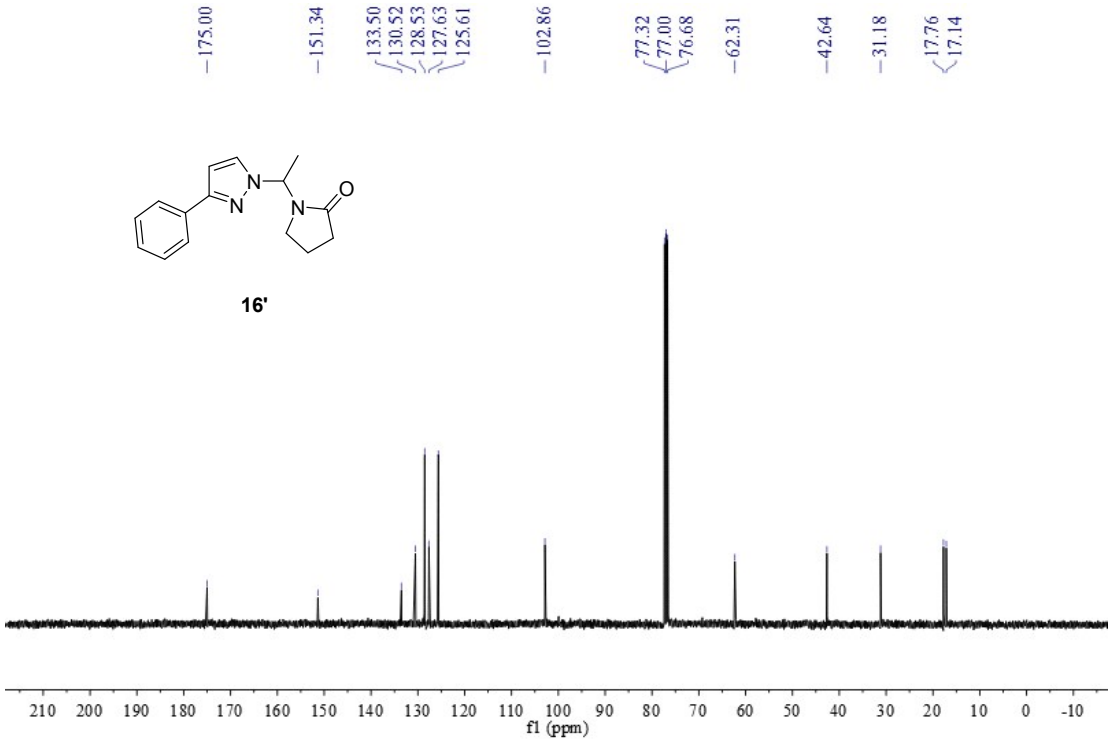
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 16



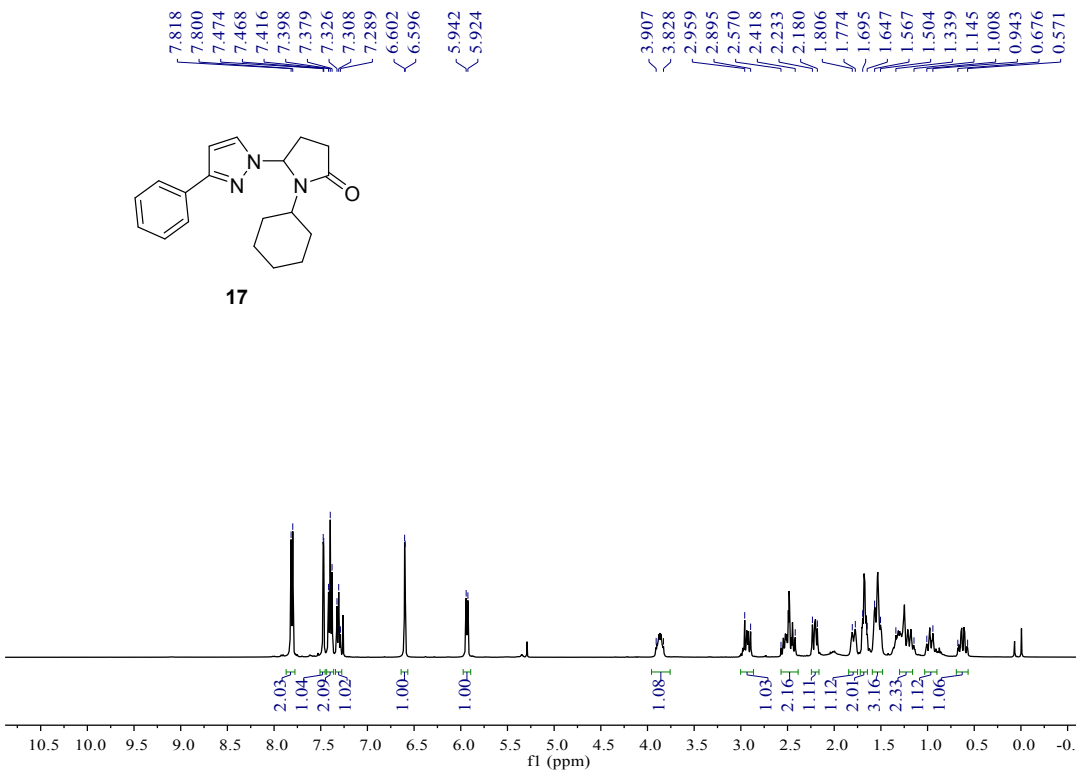
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 16



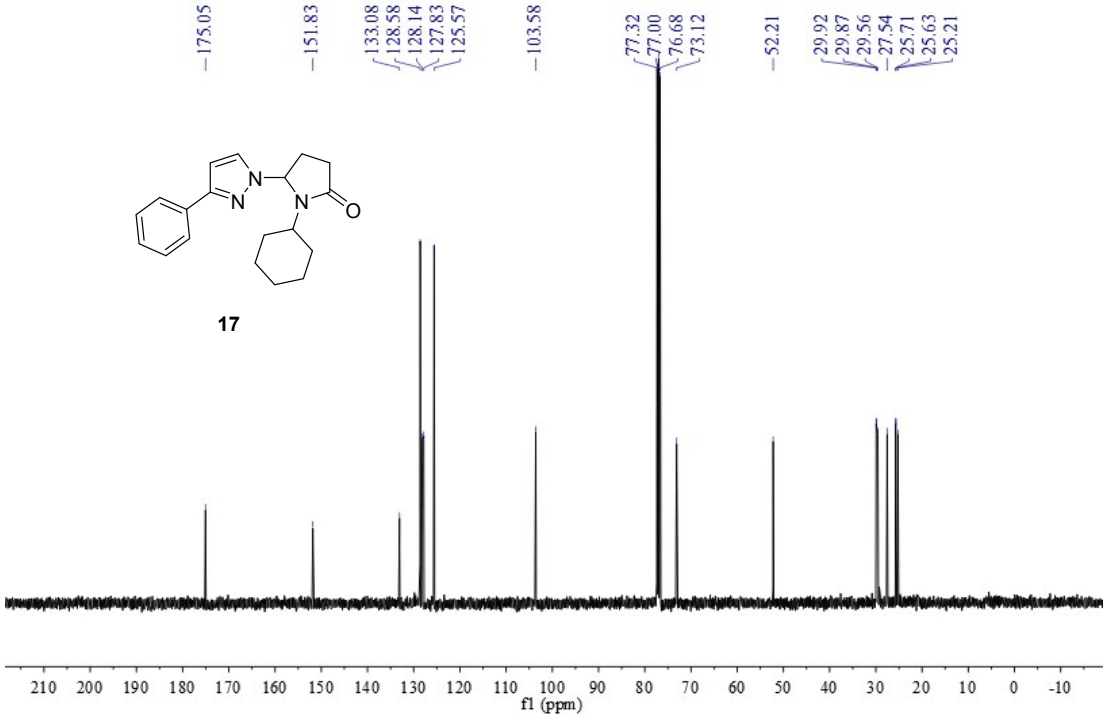
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 16'



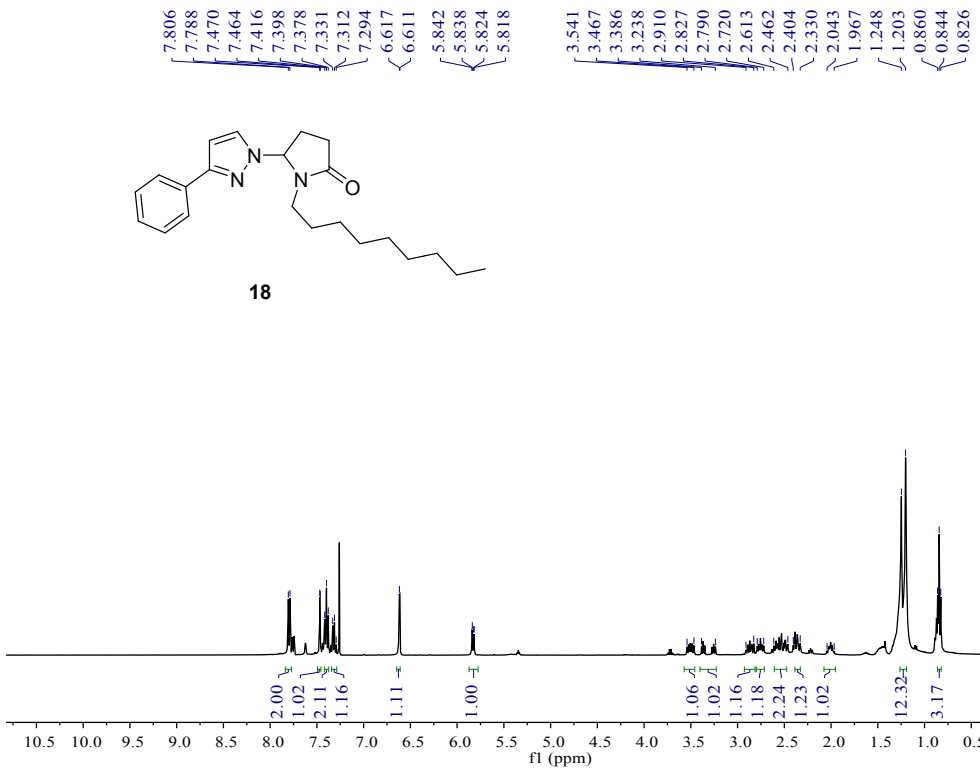
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 16'



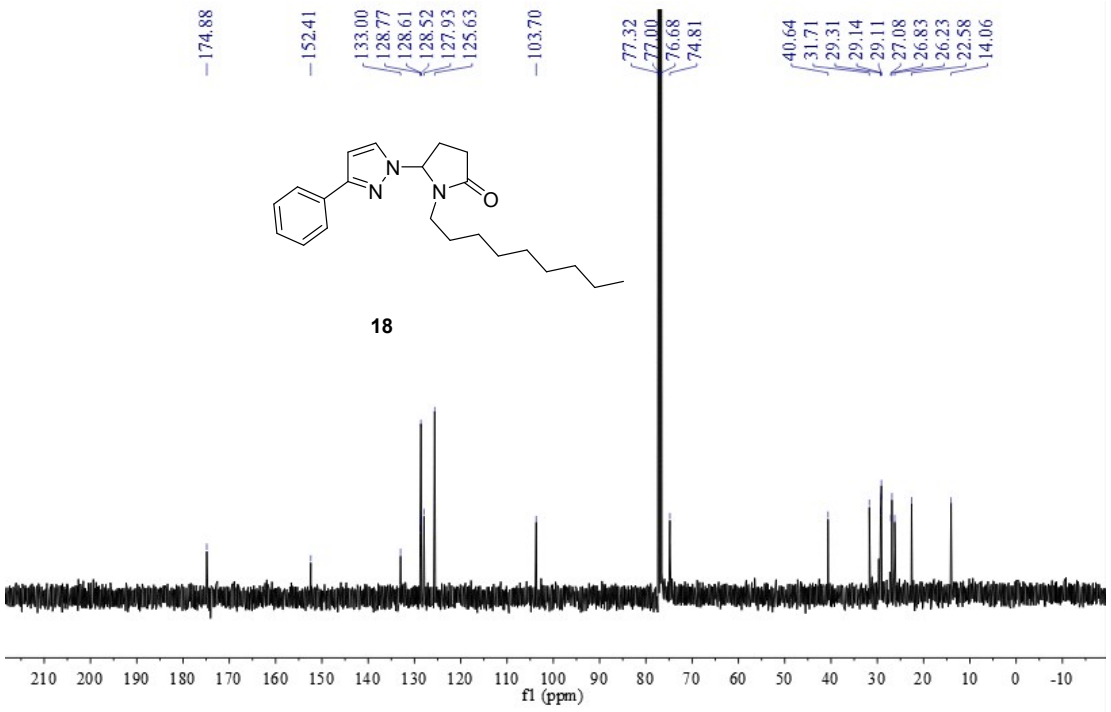
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 17



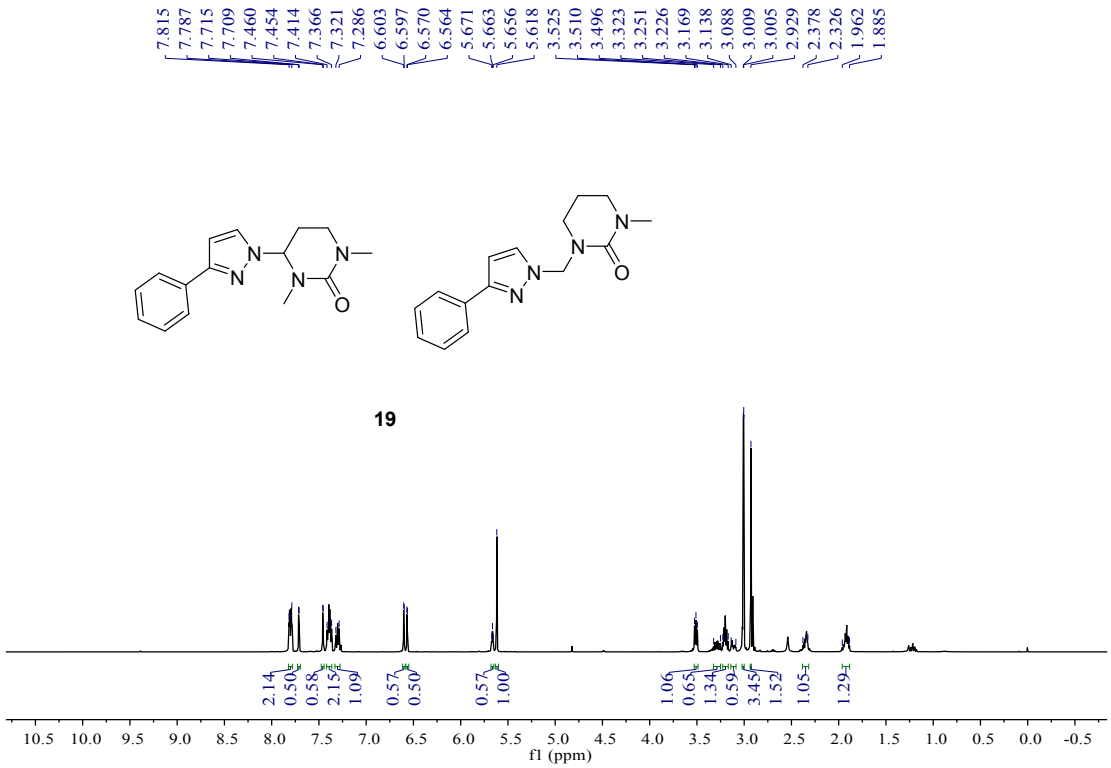
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 17



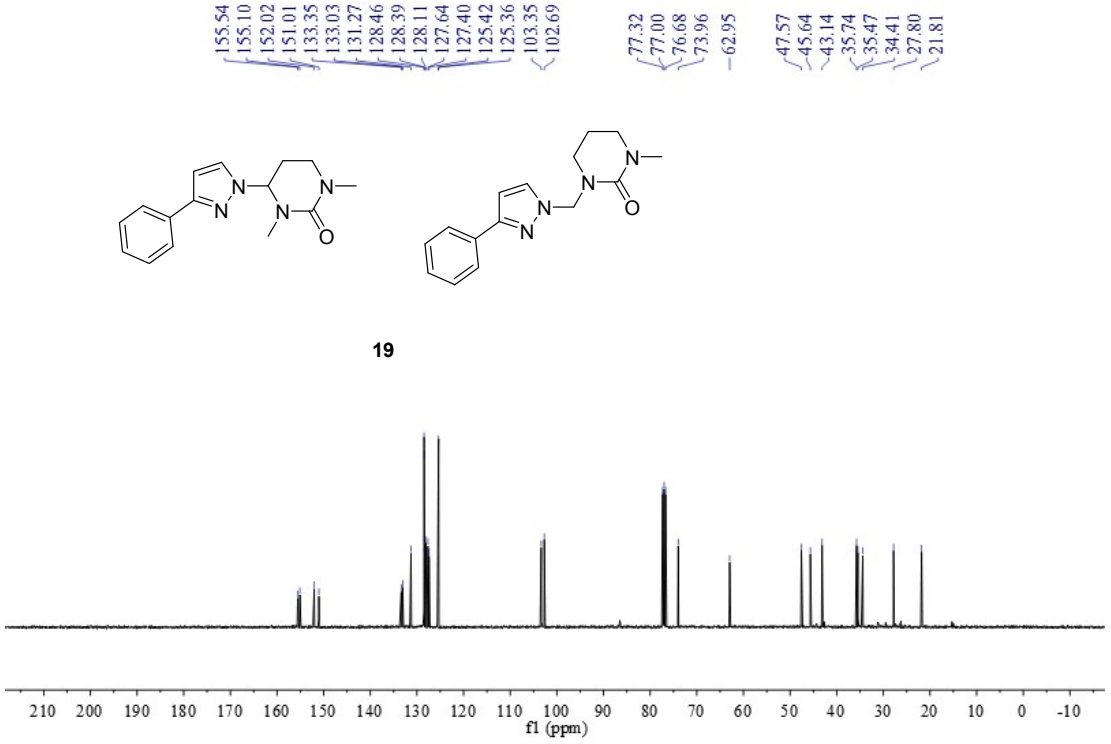
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 18



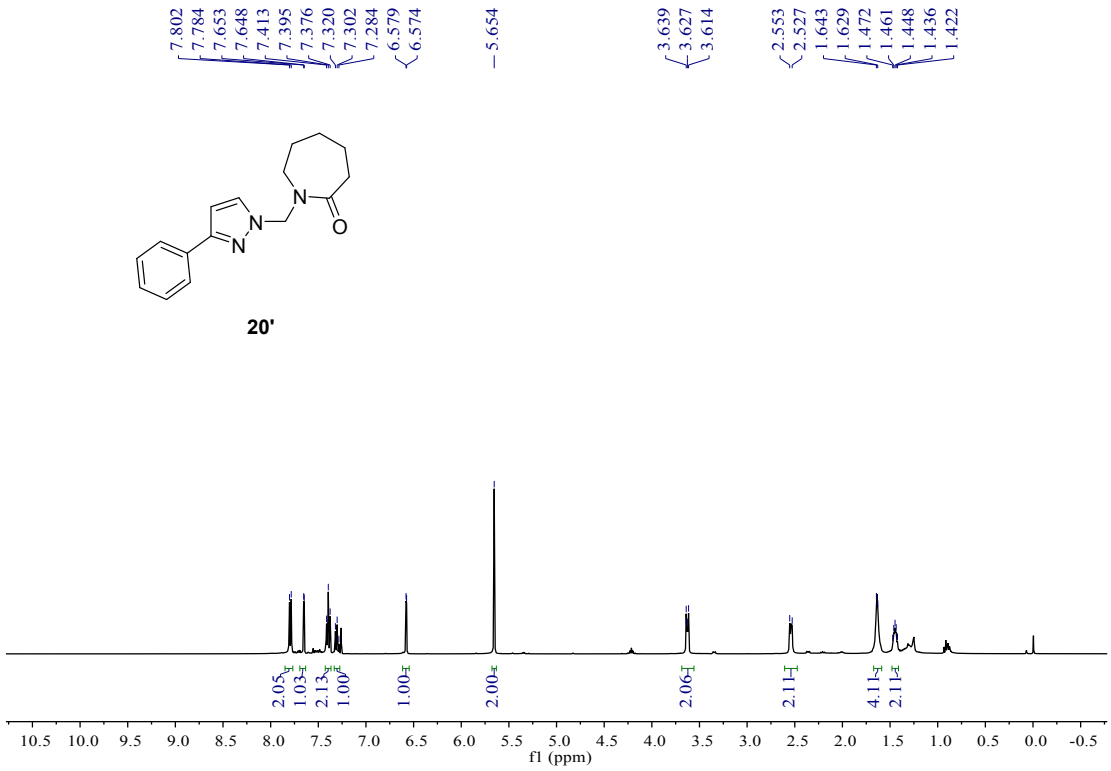
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 18



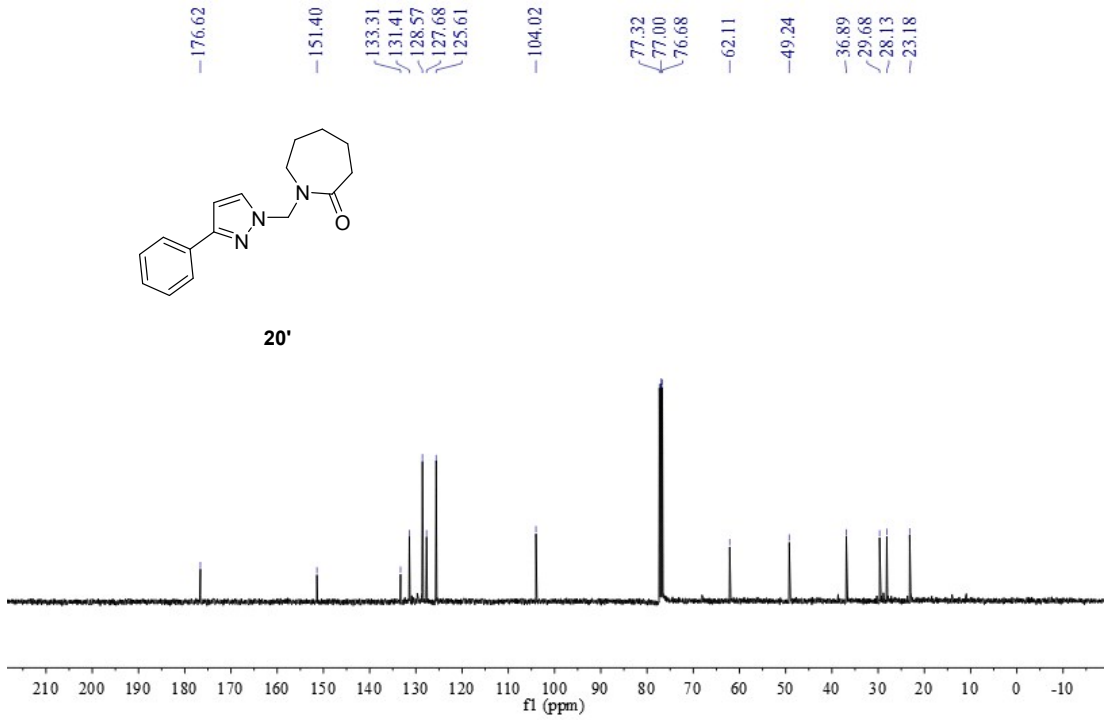
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 19



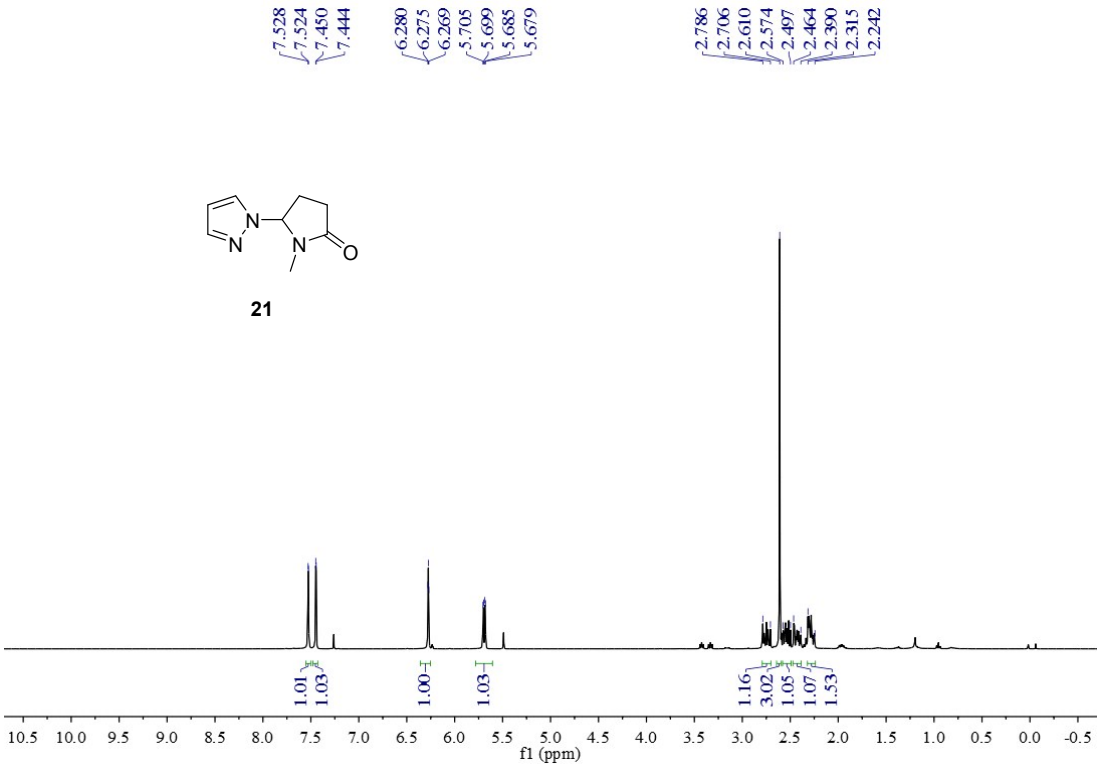
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 19



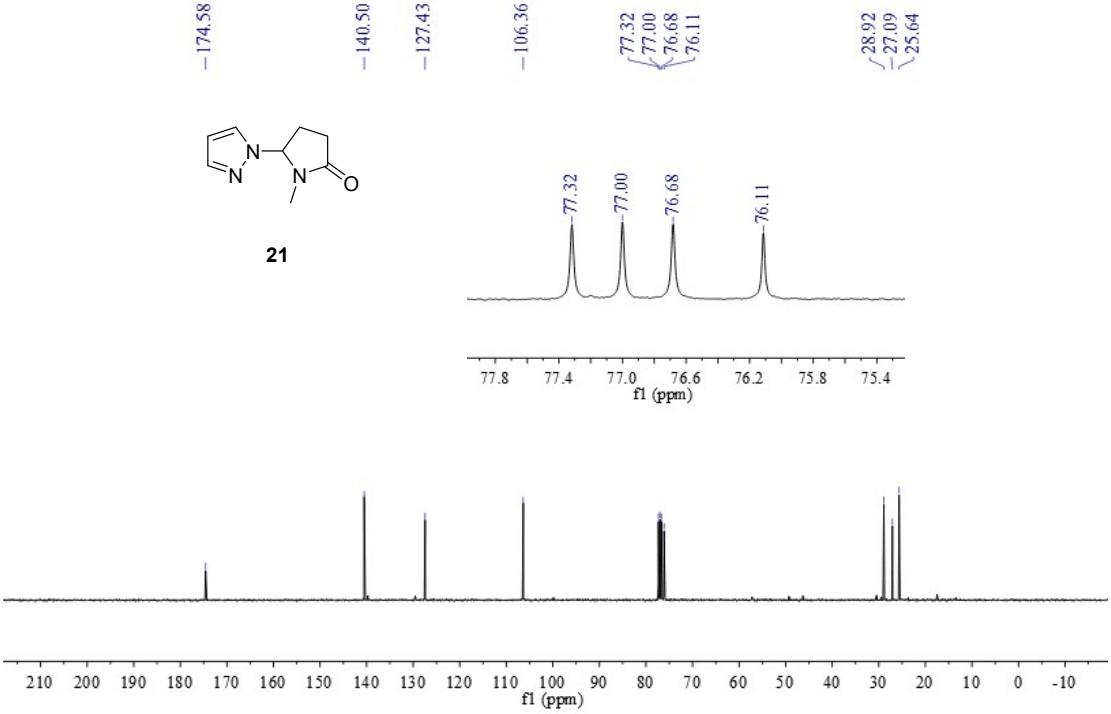
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 20'



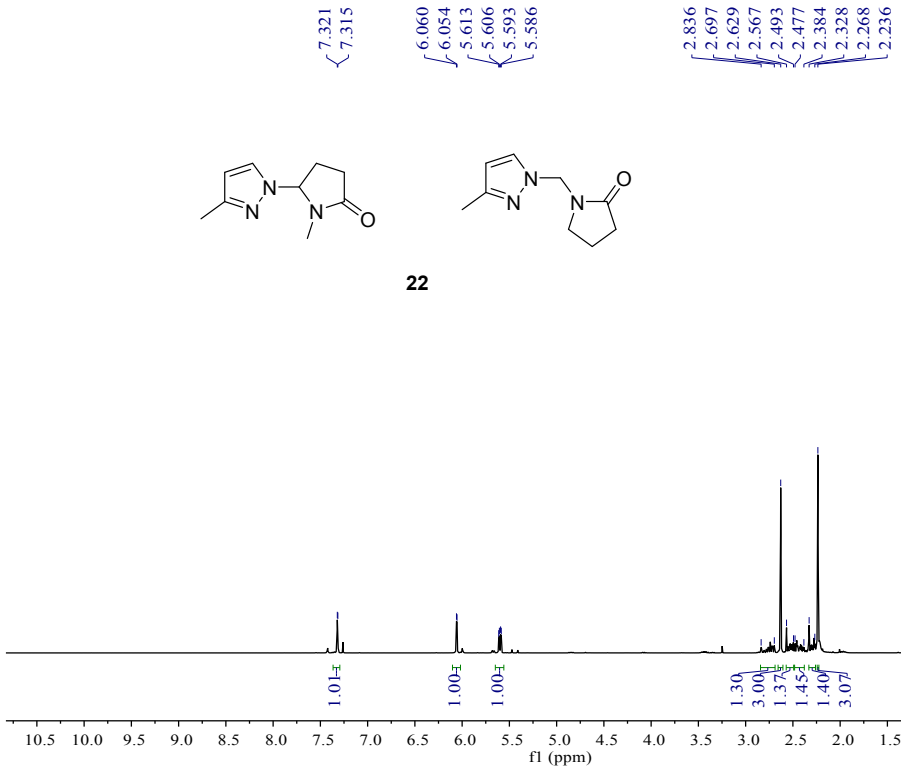
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 20'



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 21

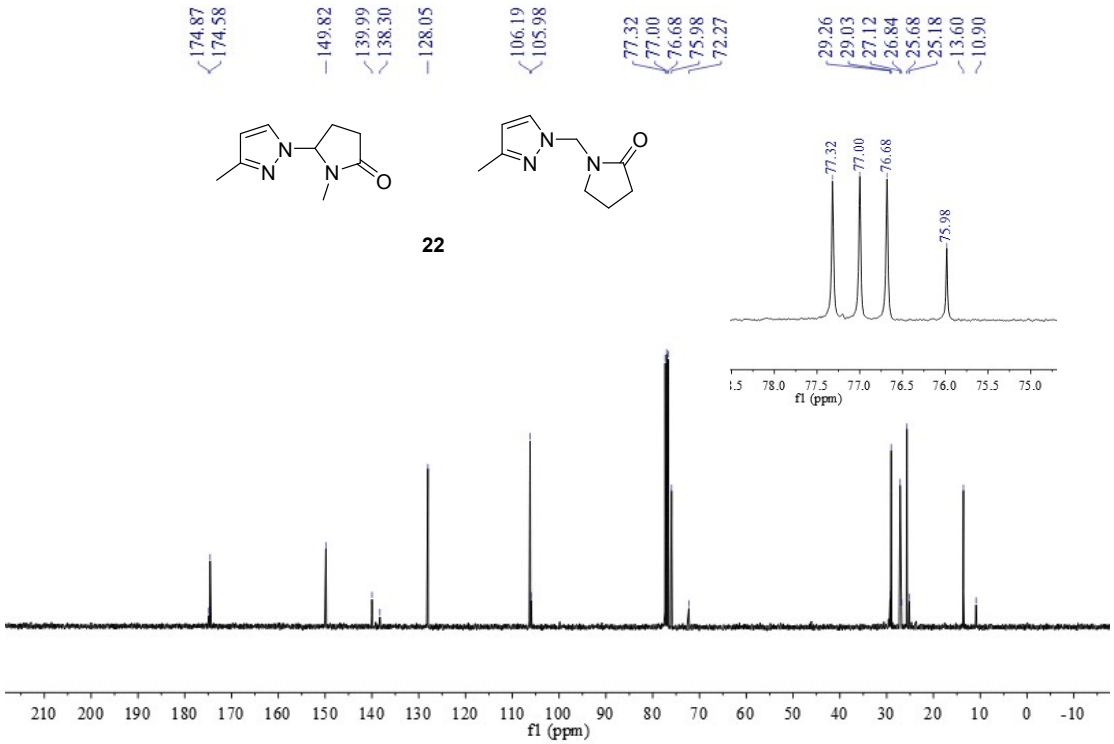


^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 21



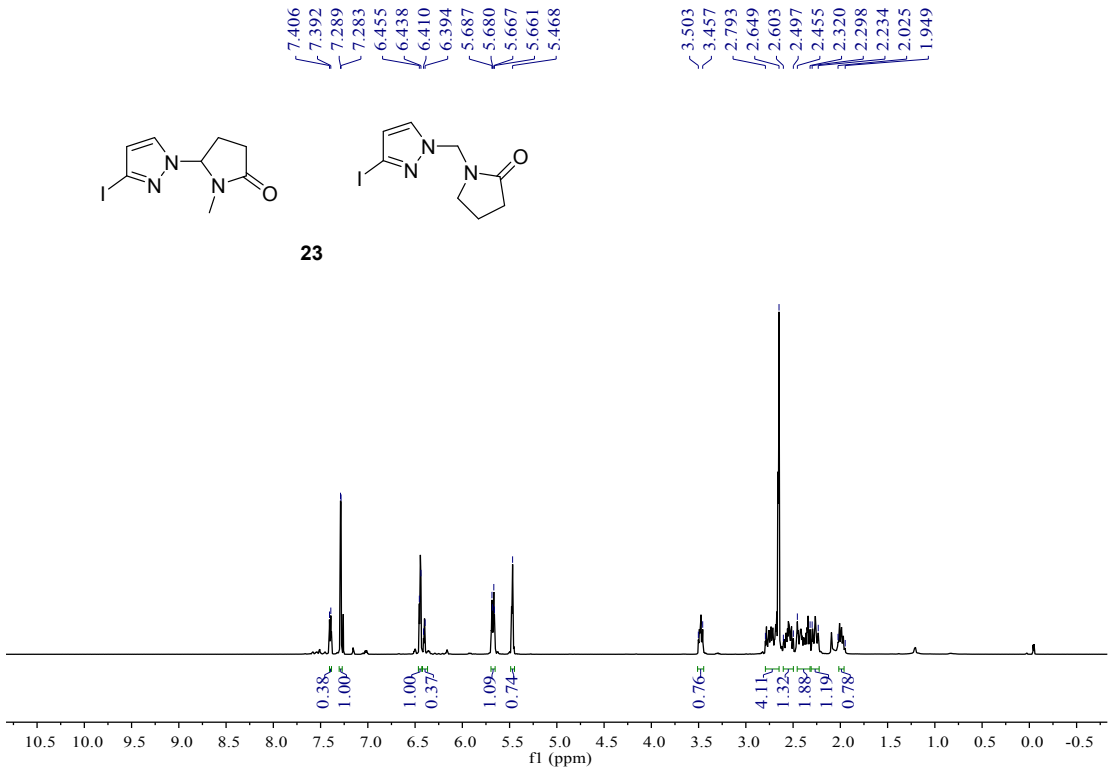
22

^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 22

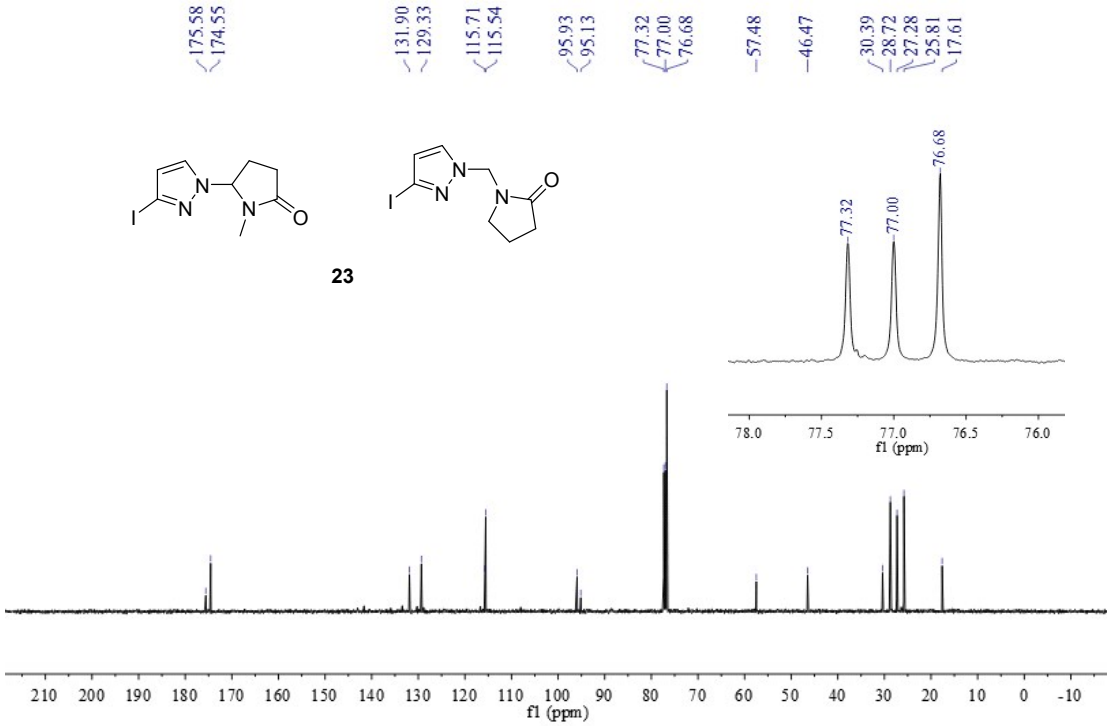


22

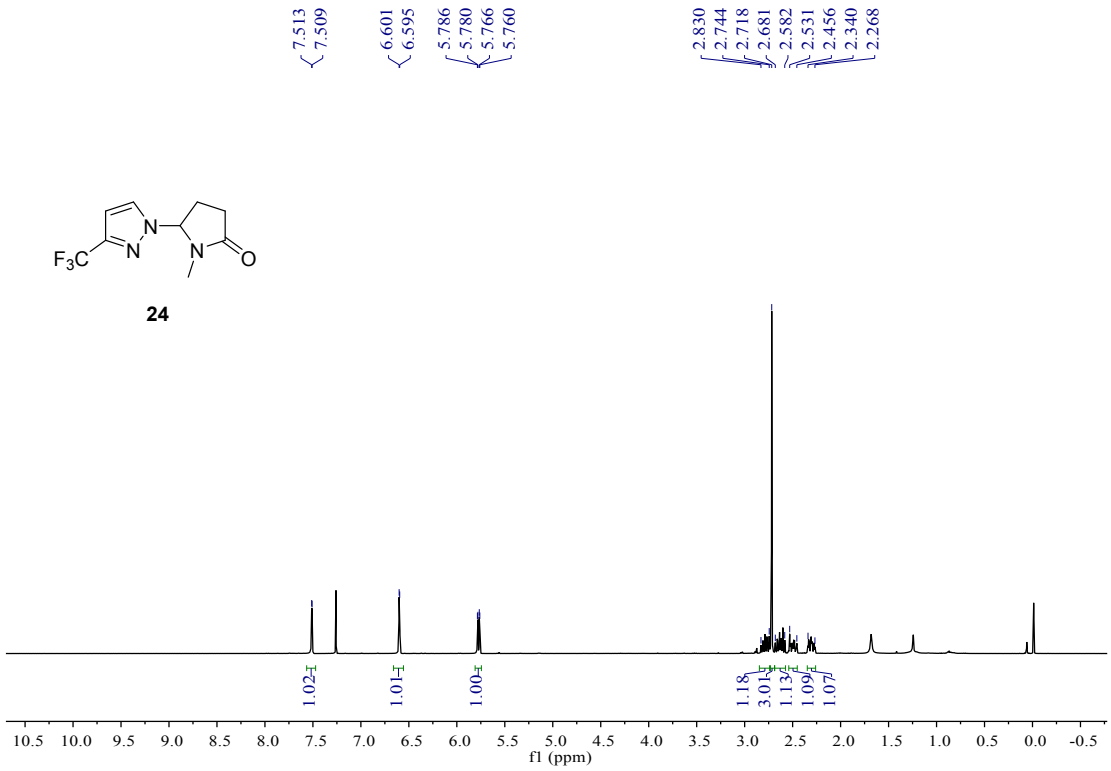
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 22



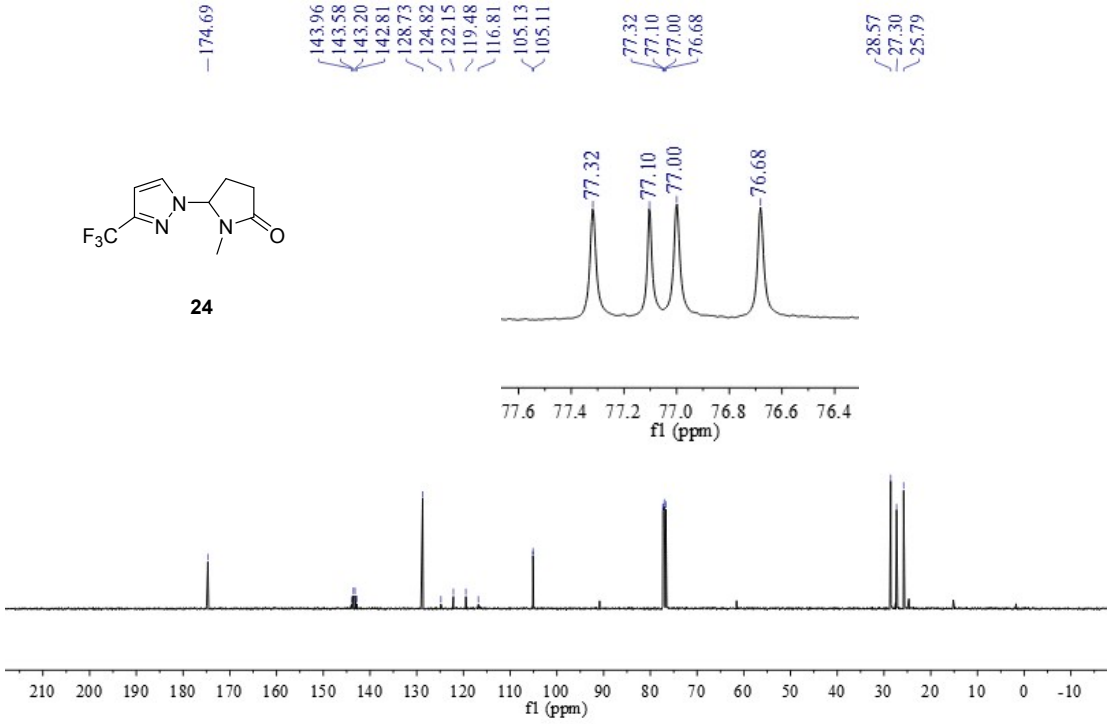
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 23



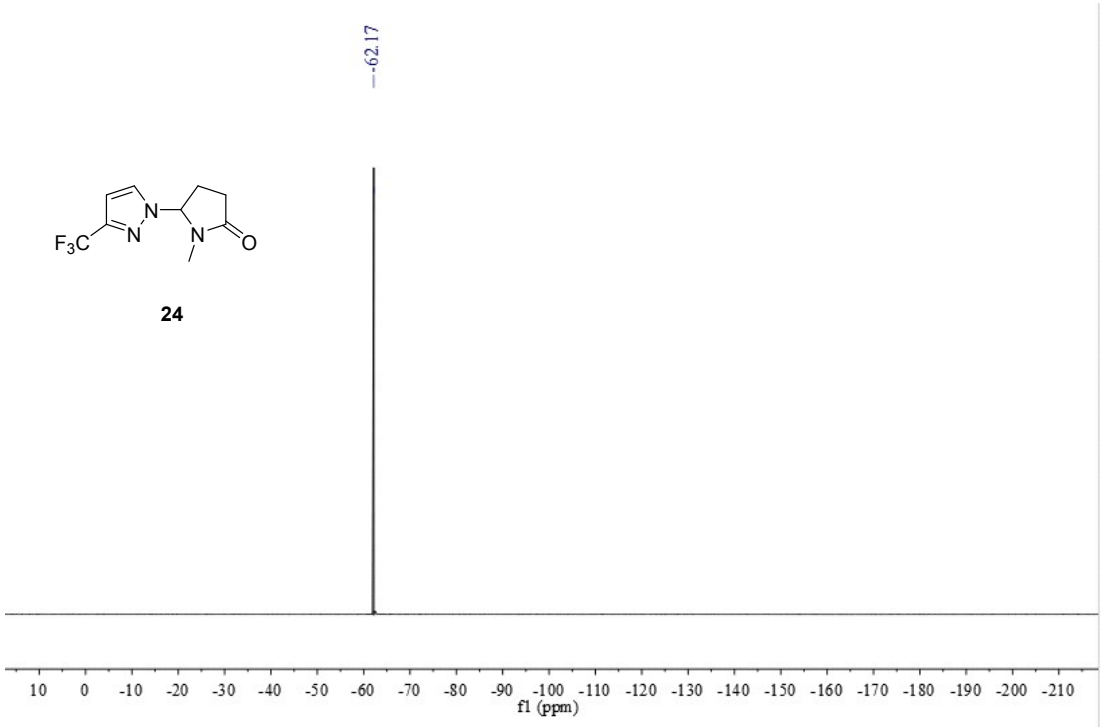
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 23



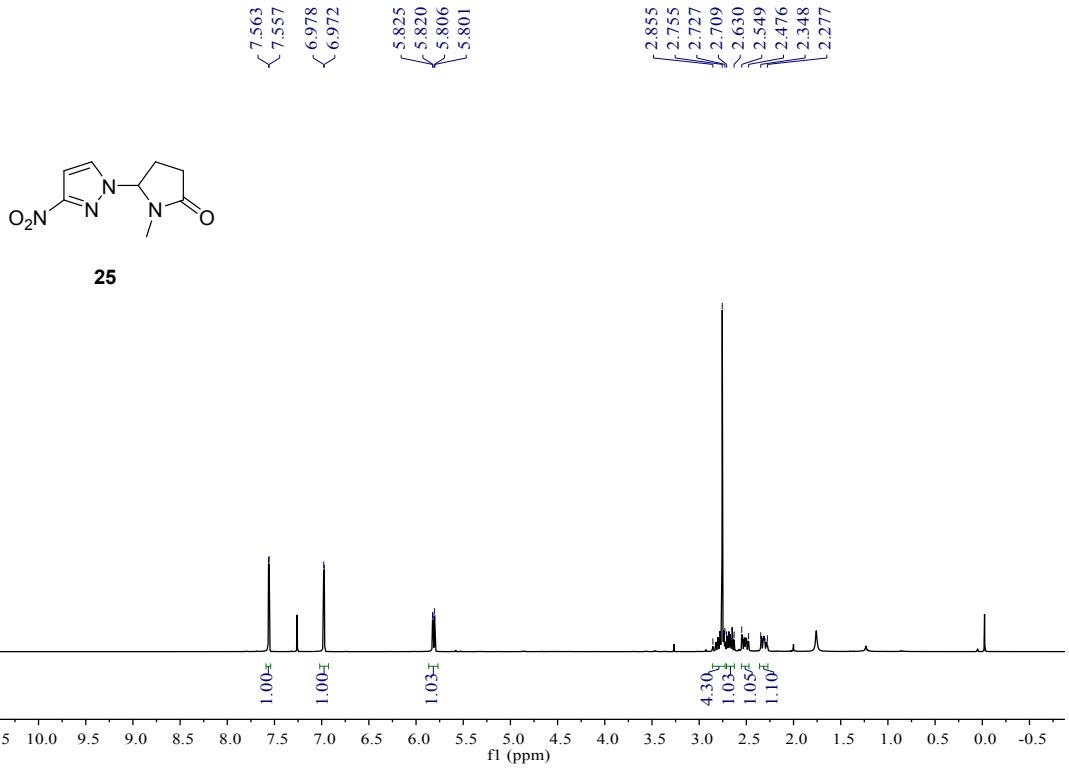
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 24



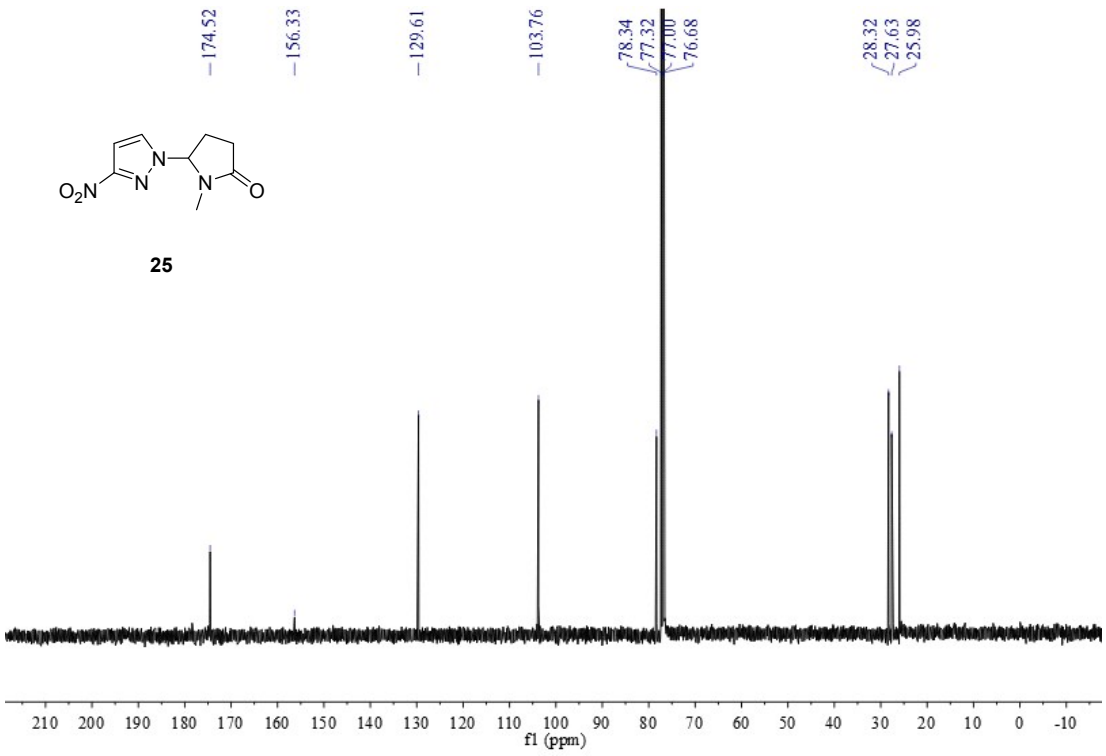
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 24



^{19}F NMR (373 MHz, $CDCl_3$) spectrum of 24

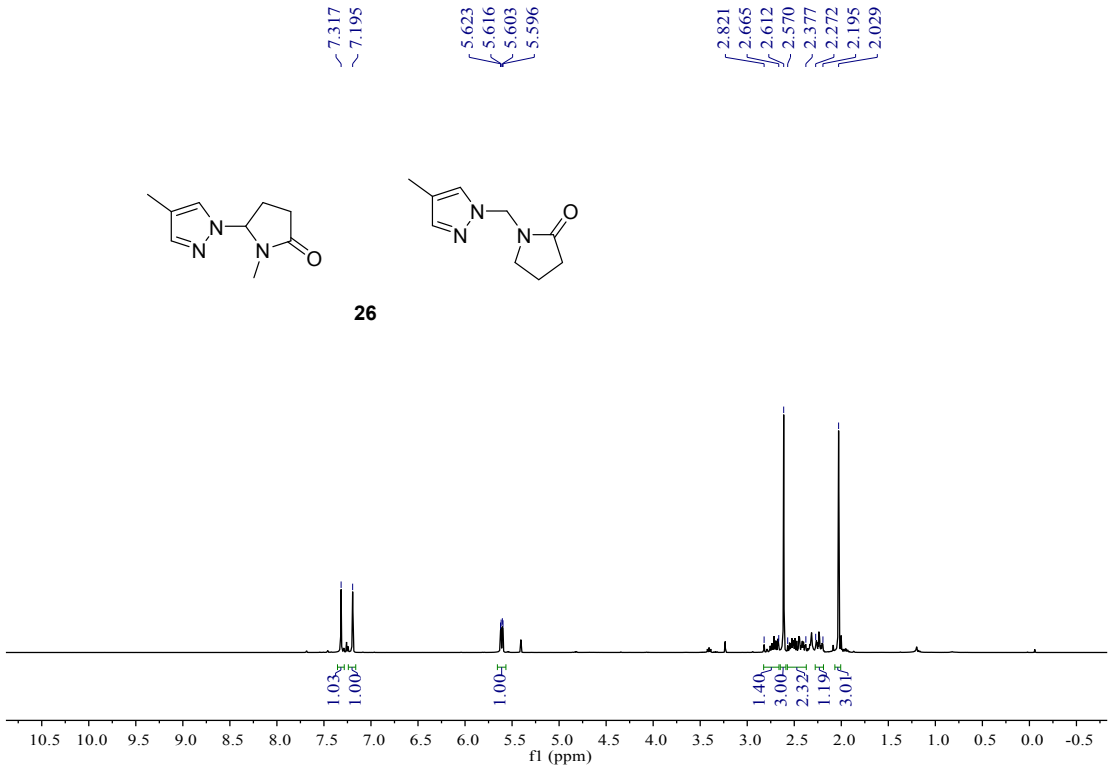


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 25



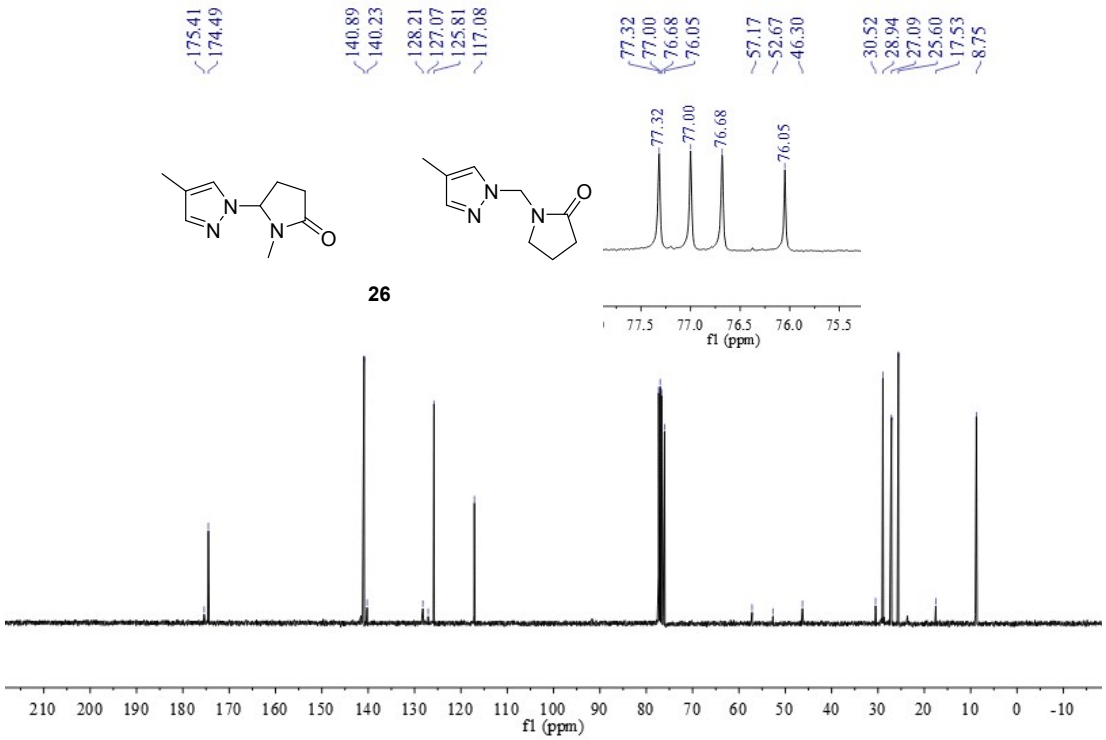
25

^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 25



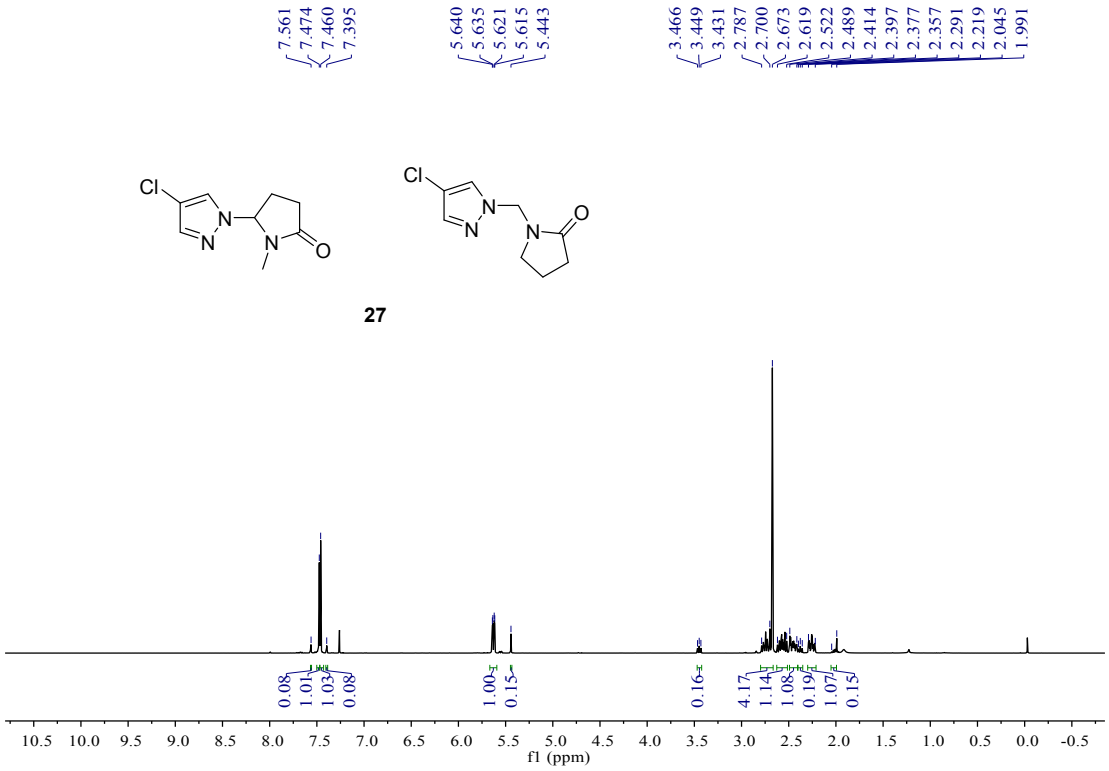
26

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



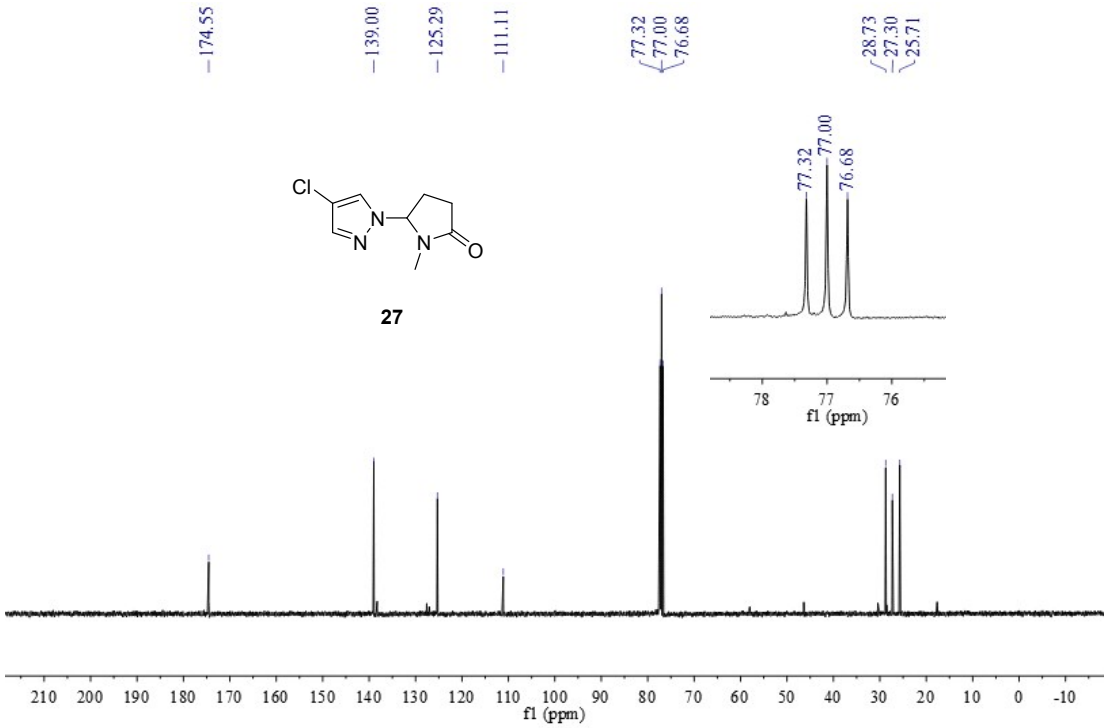
26

^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 26

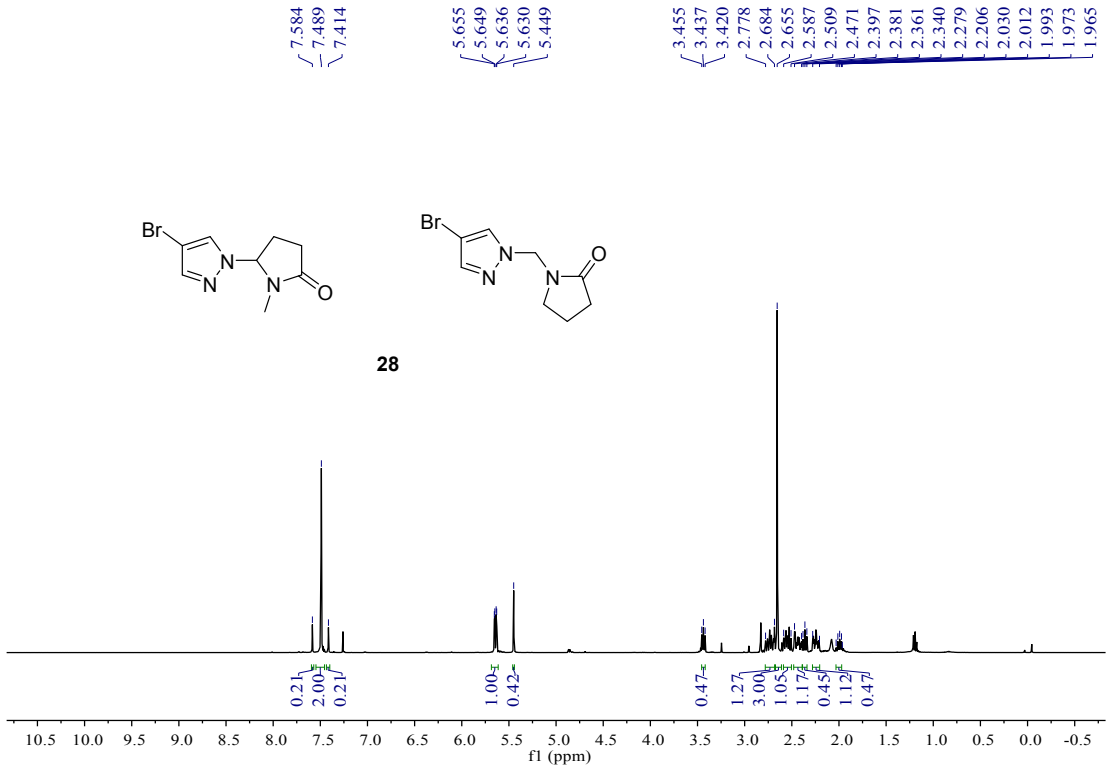


27

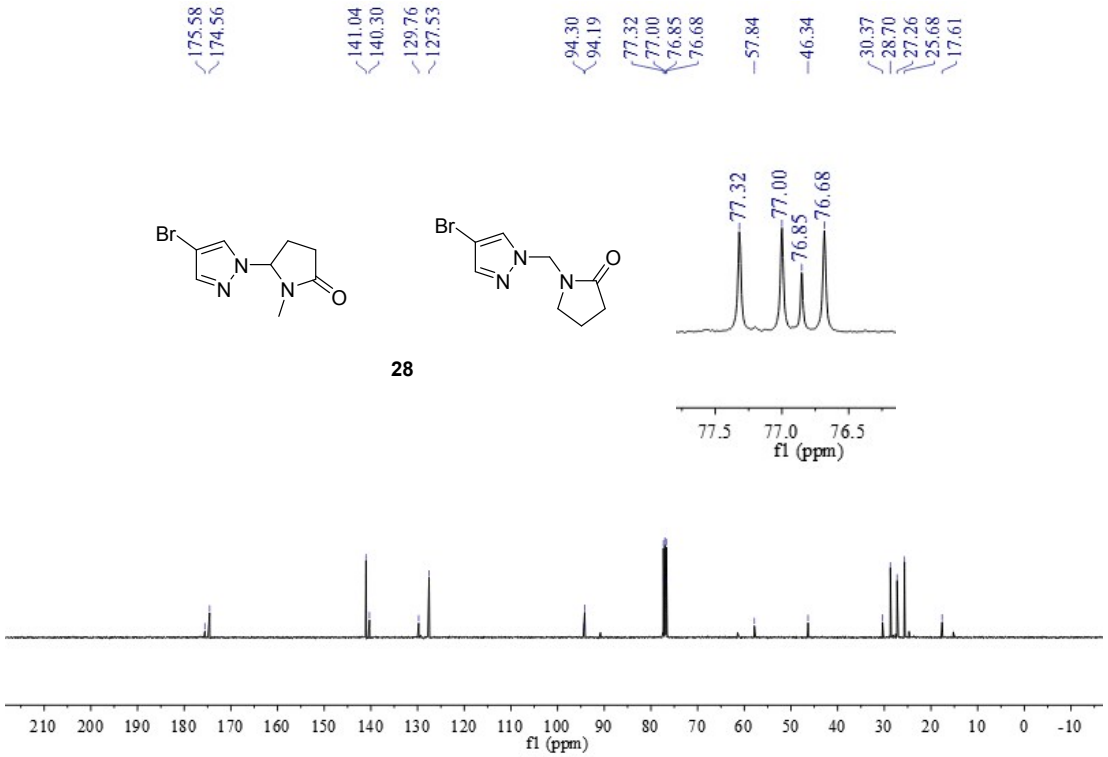
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 27



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

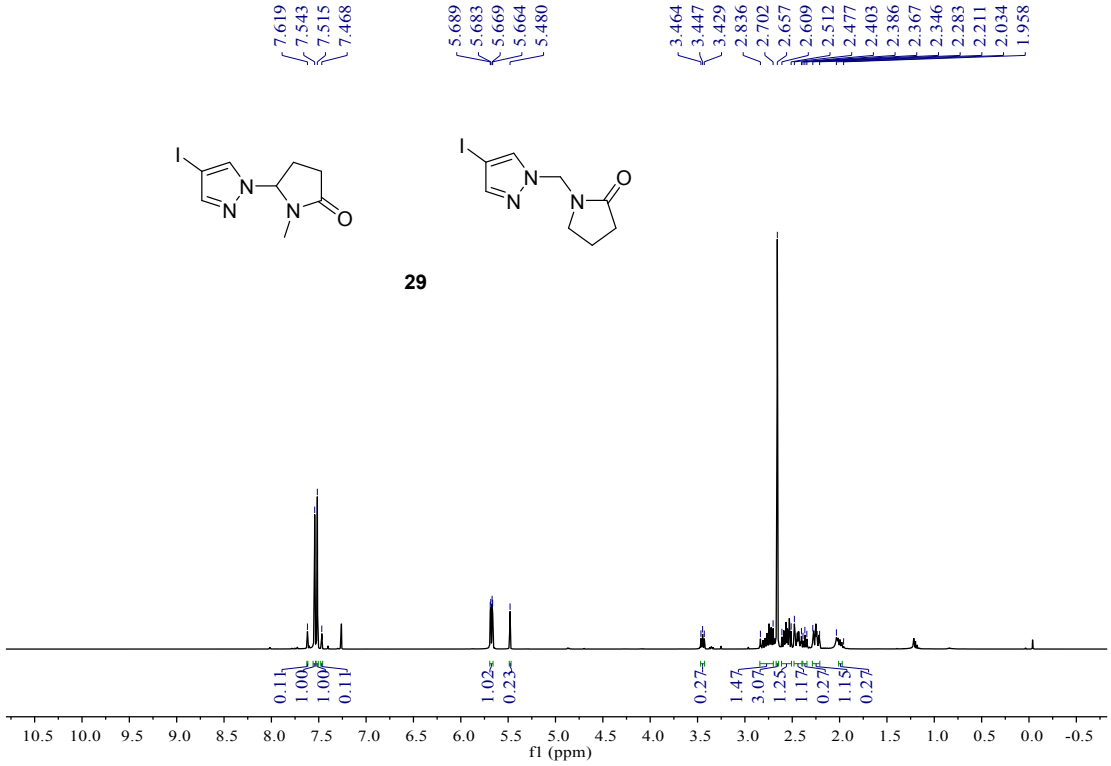


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 28



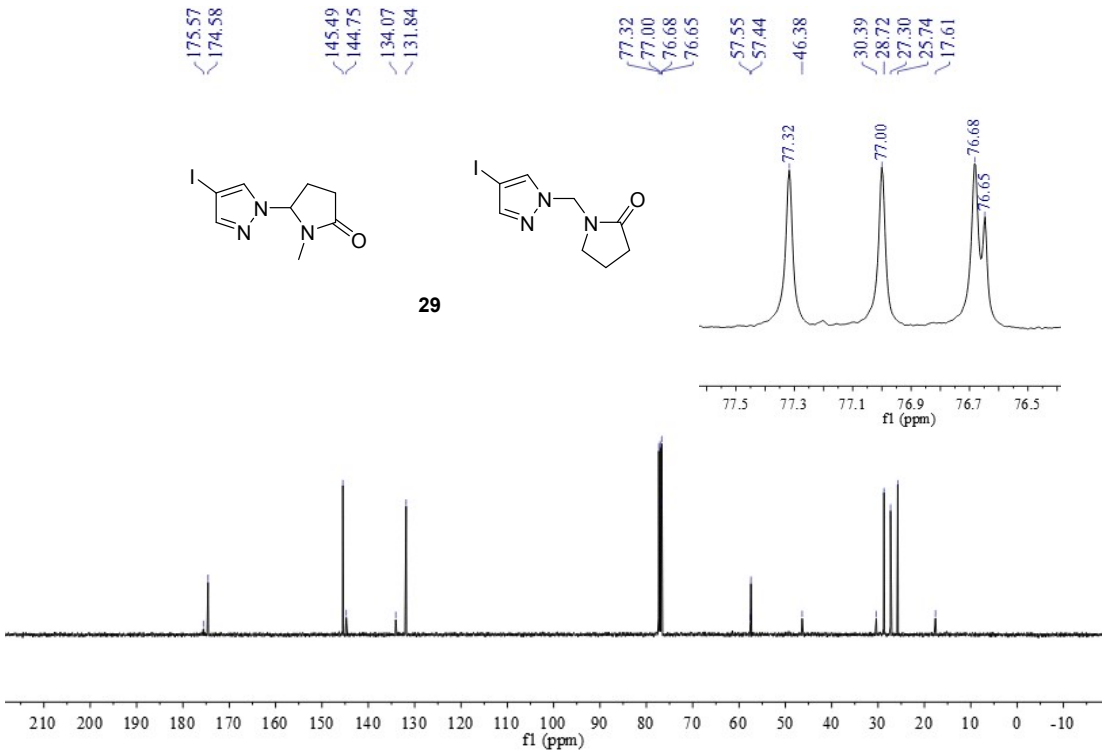
28

^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 28

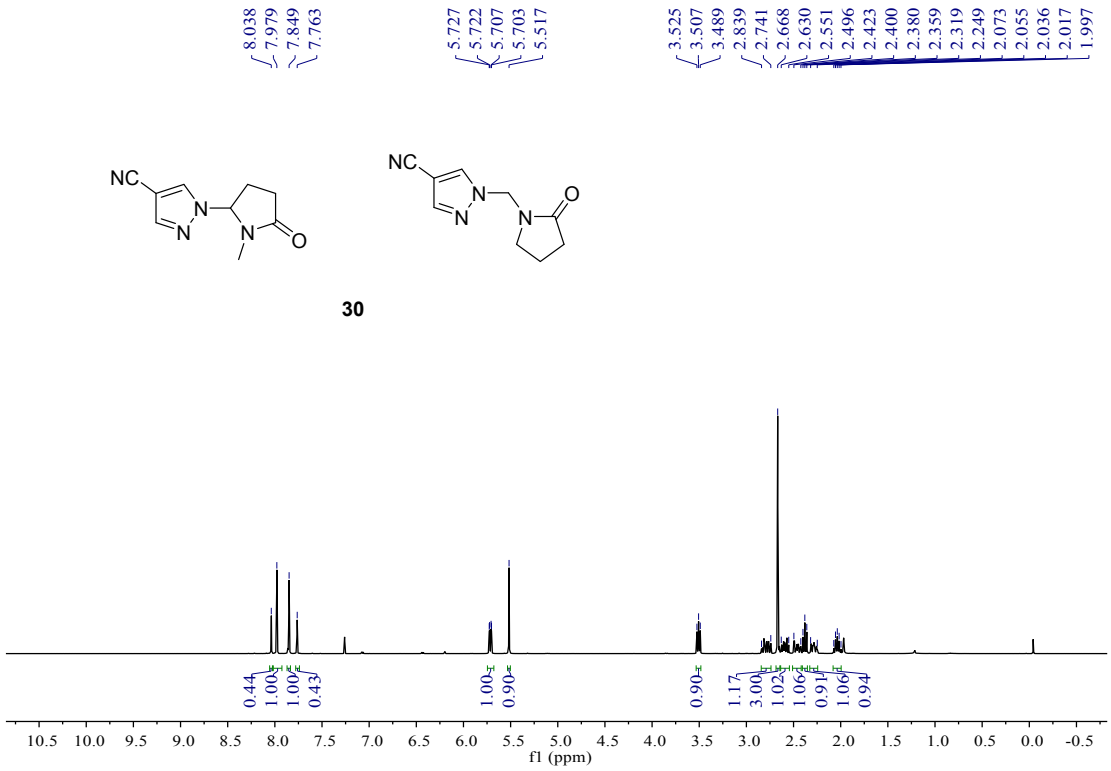


29

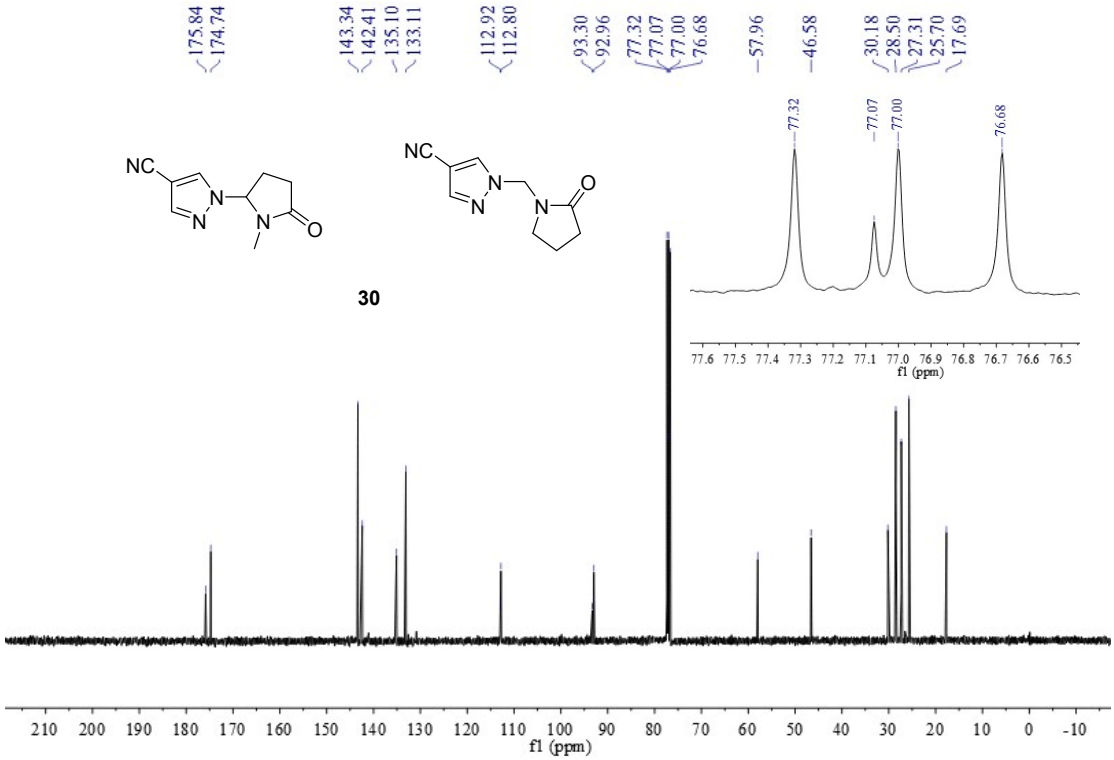
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 29



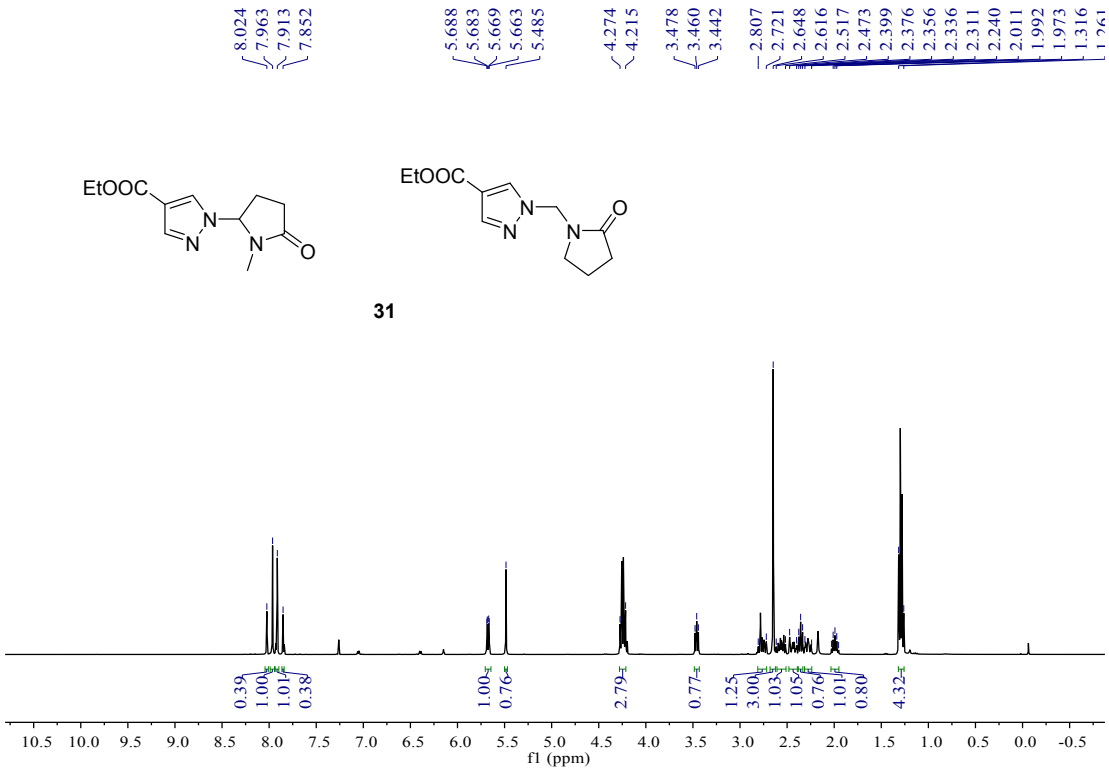
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 29



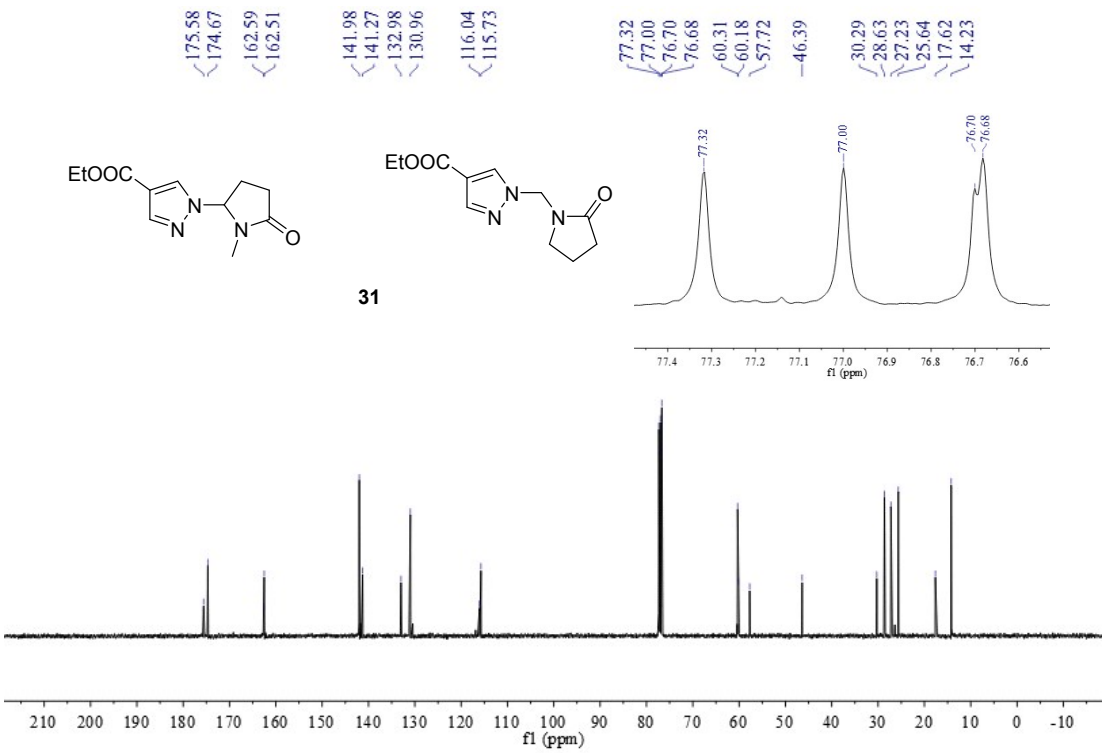
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 30



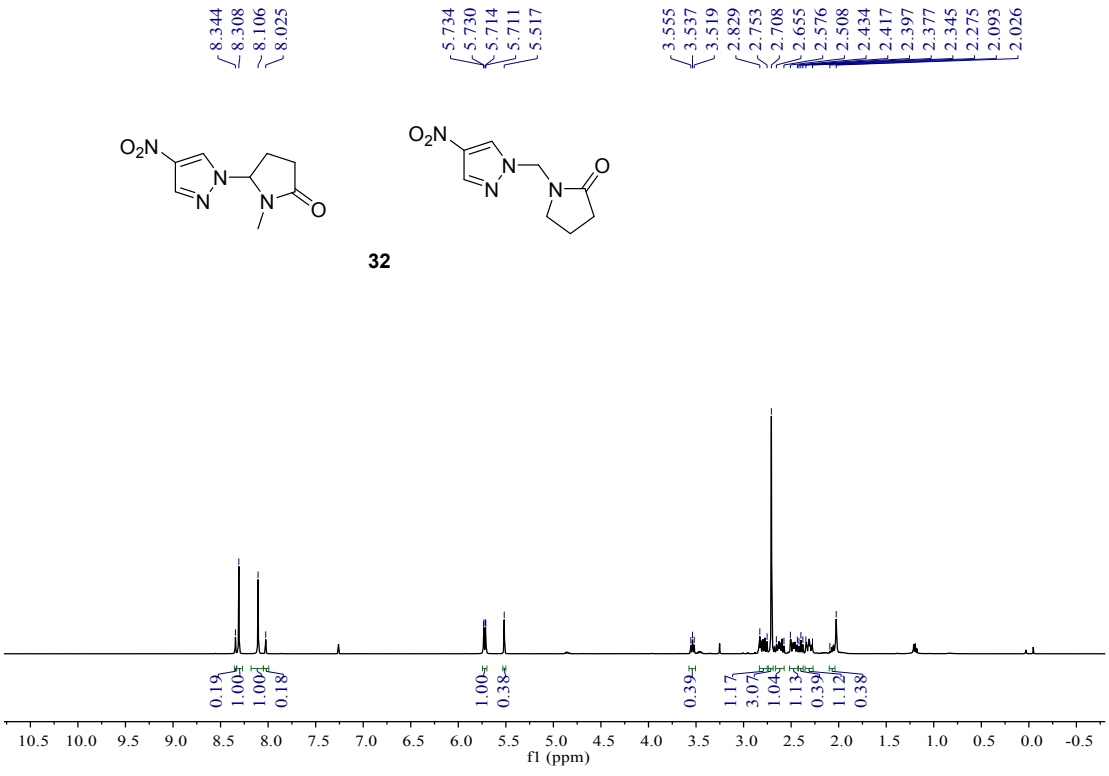
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 30



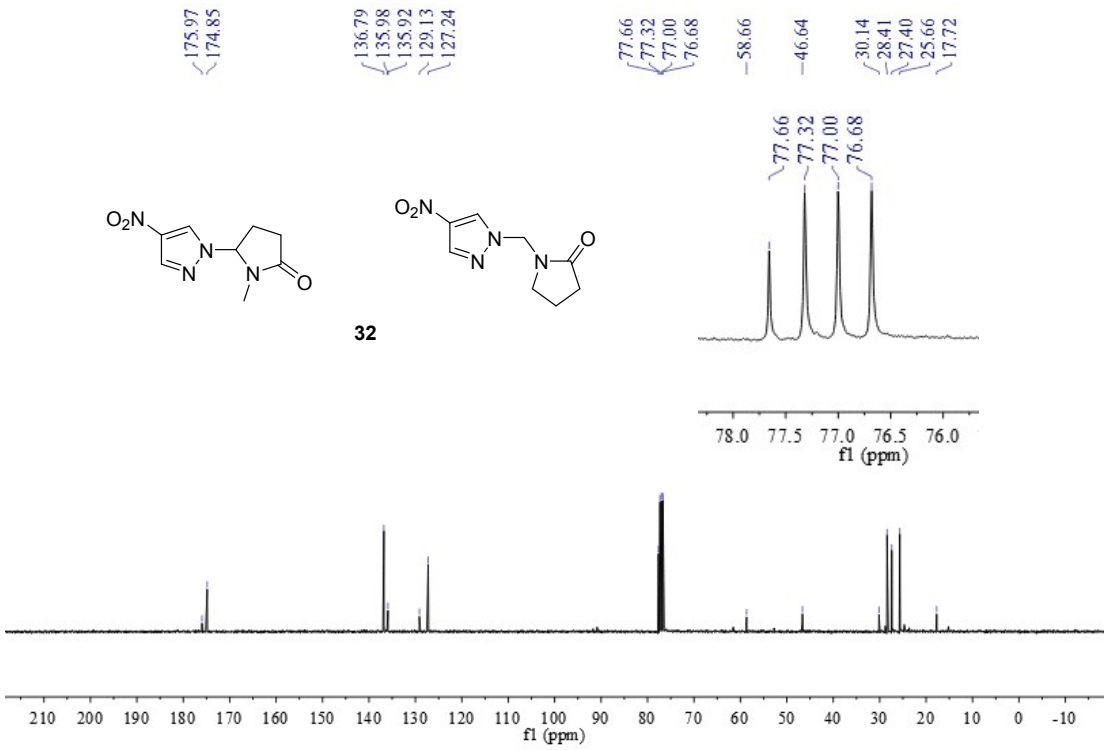
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 31



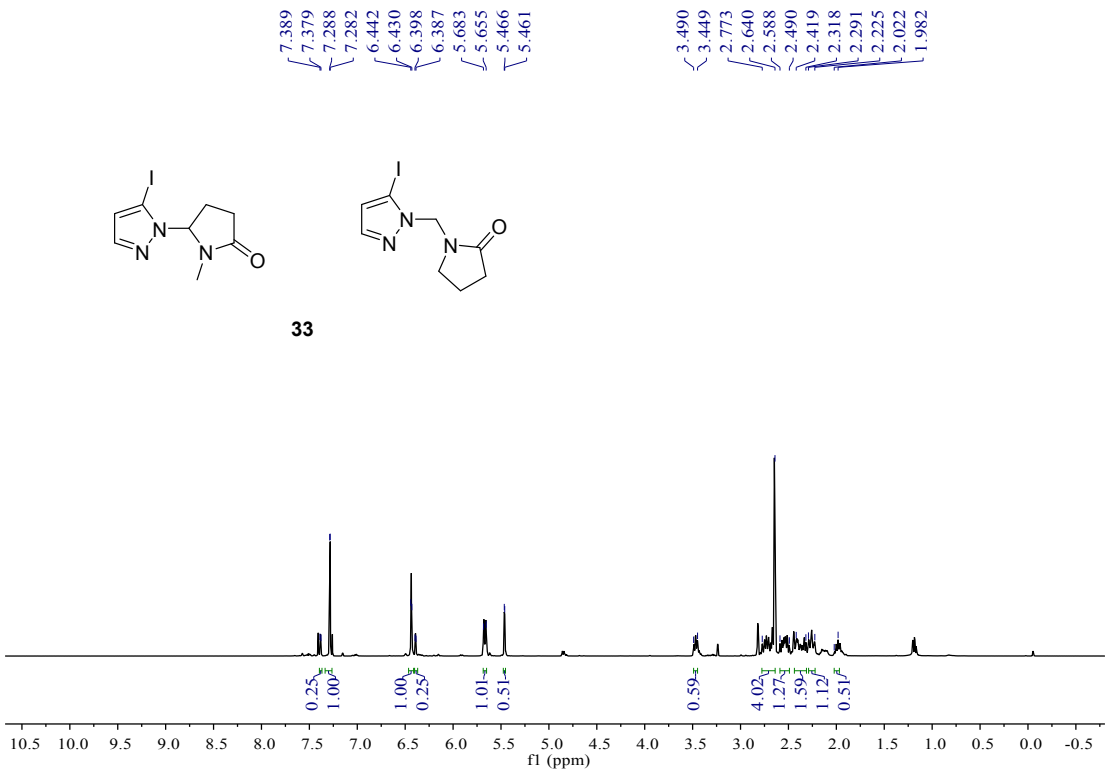
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 31



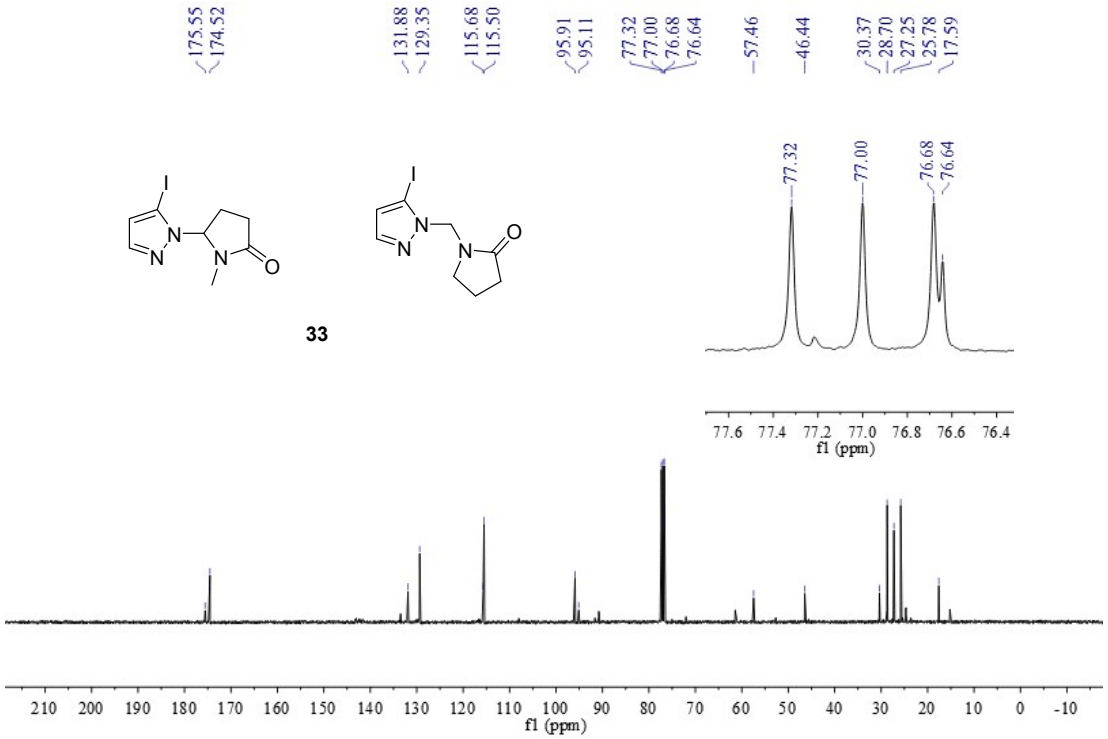
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 32



^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 32

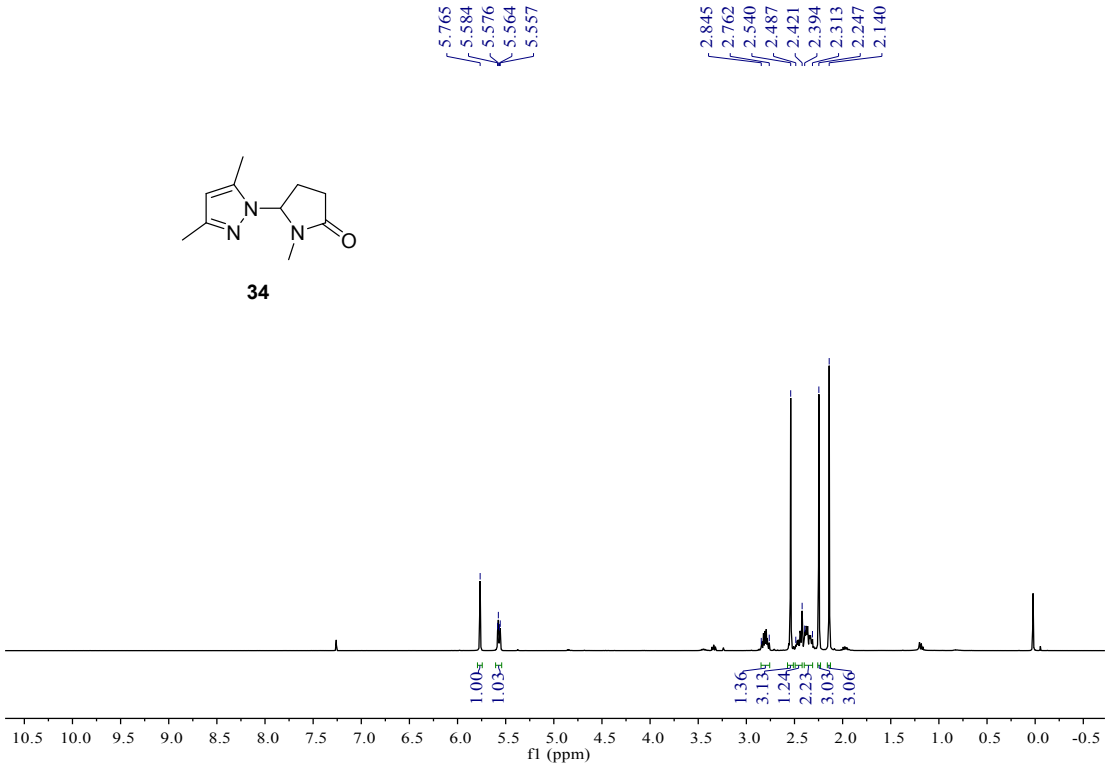


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 33



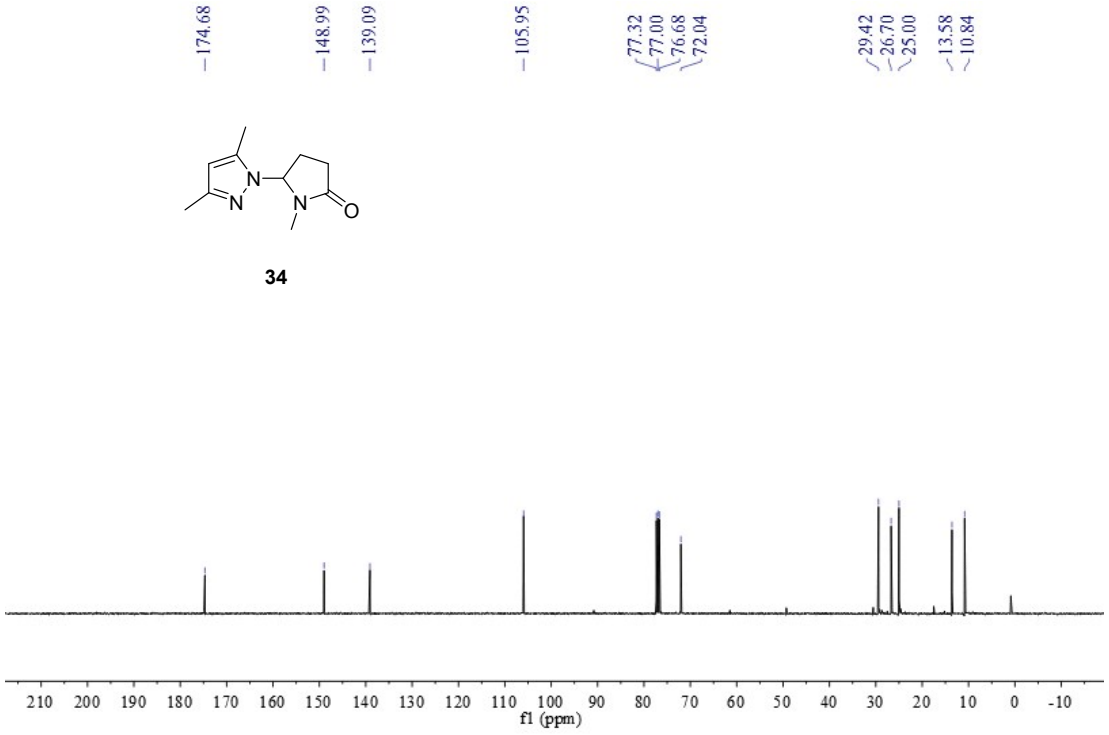
33

^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 33

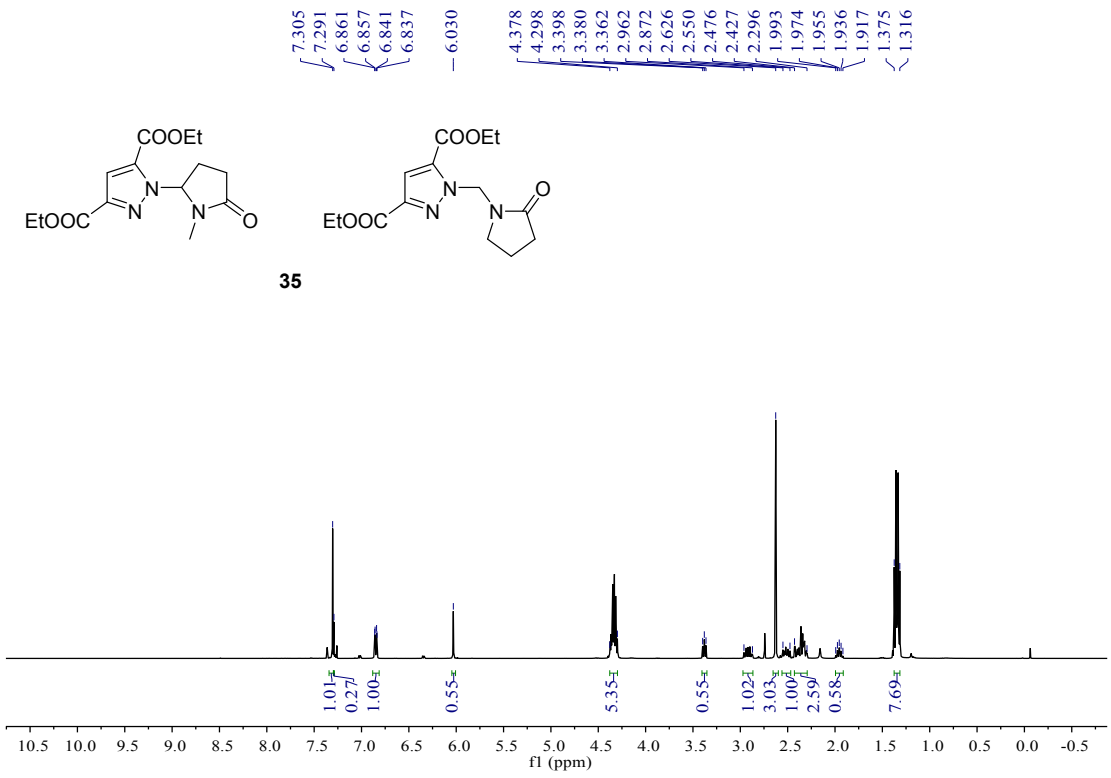


34

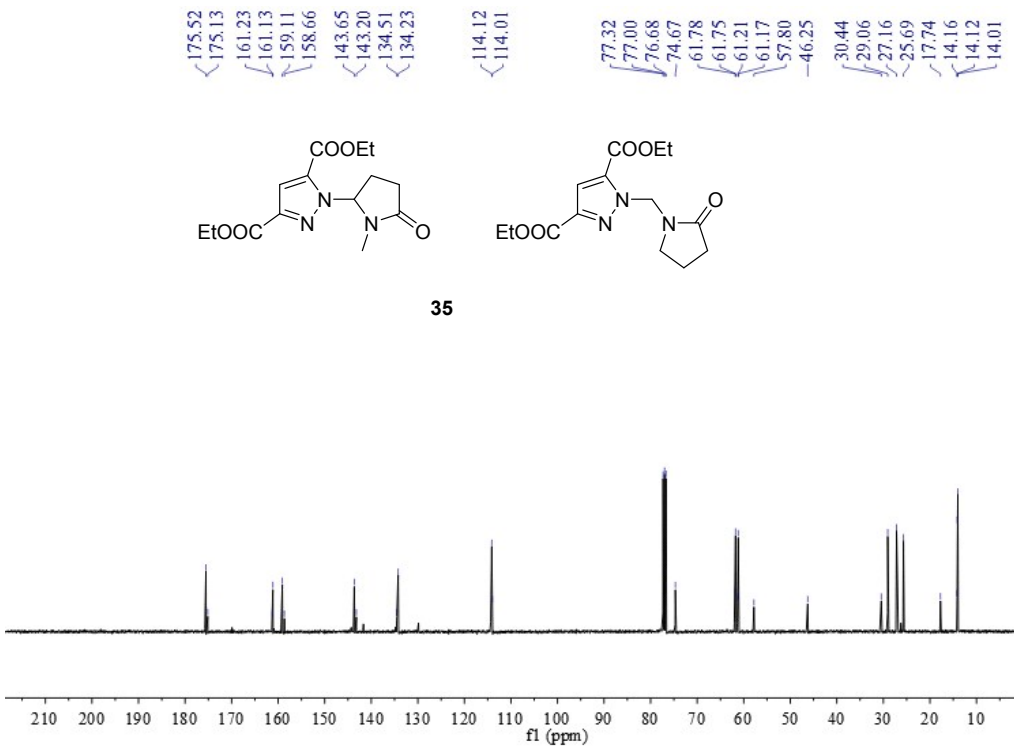
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 34



^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 34

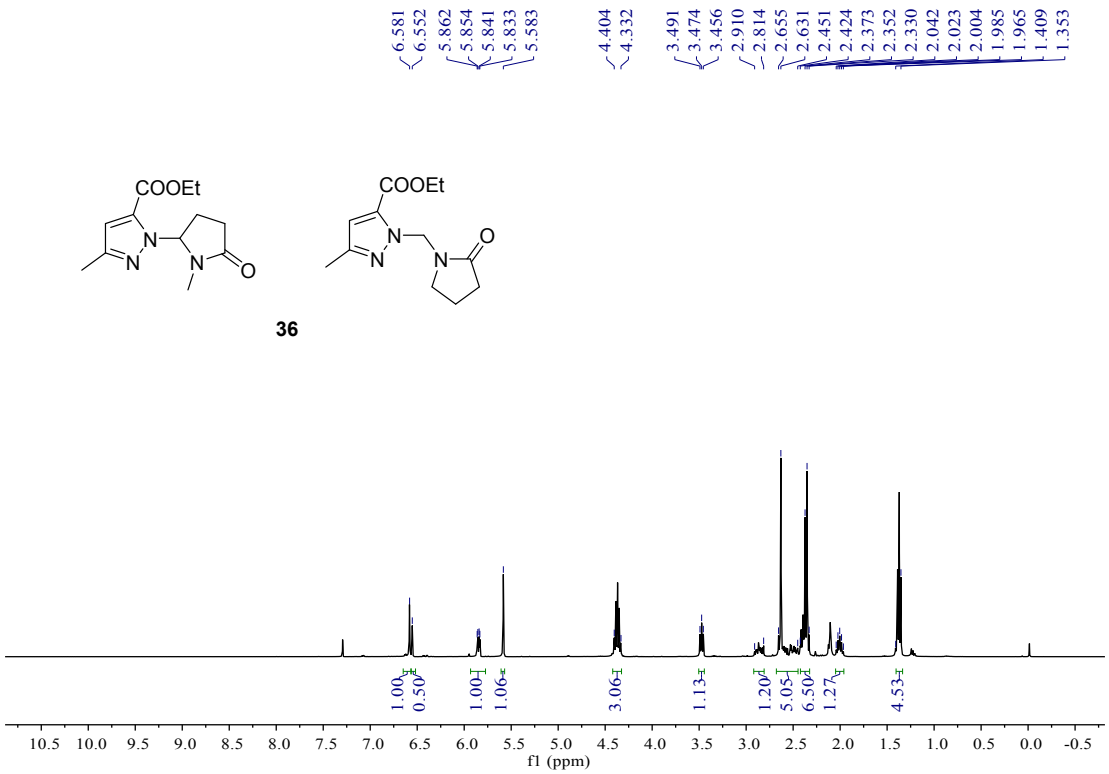


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 35



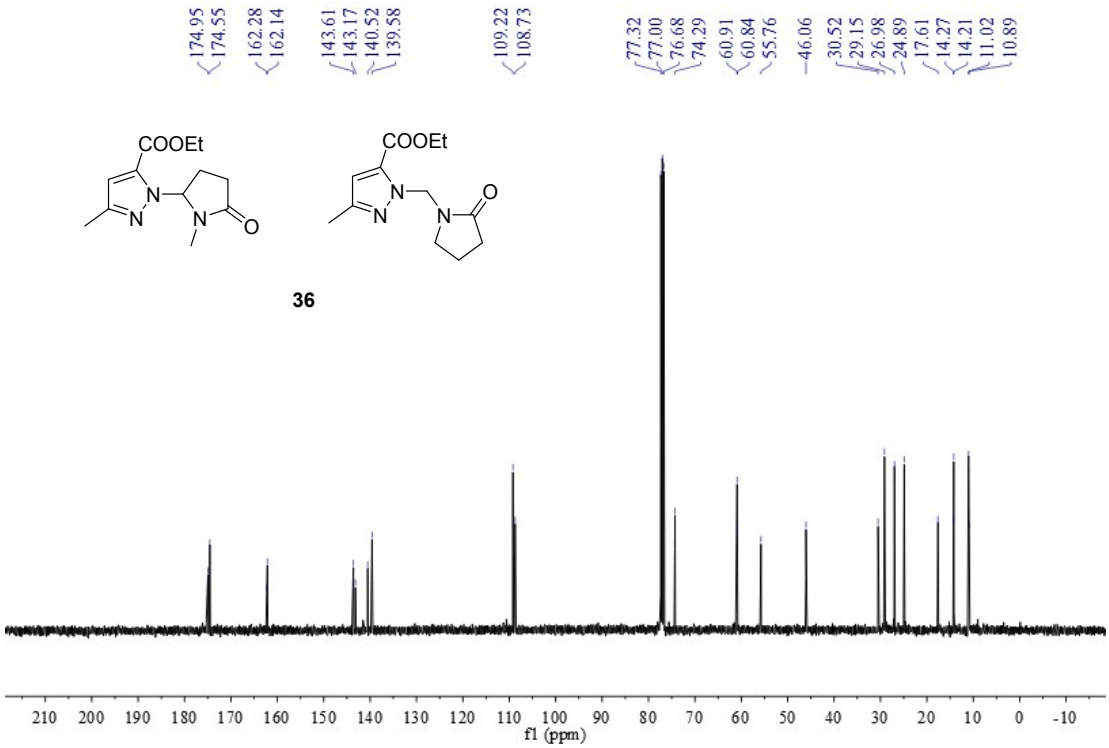
35

^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 35

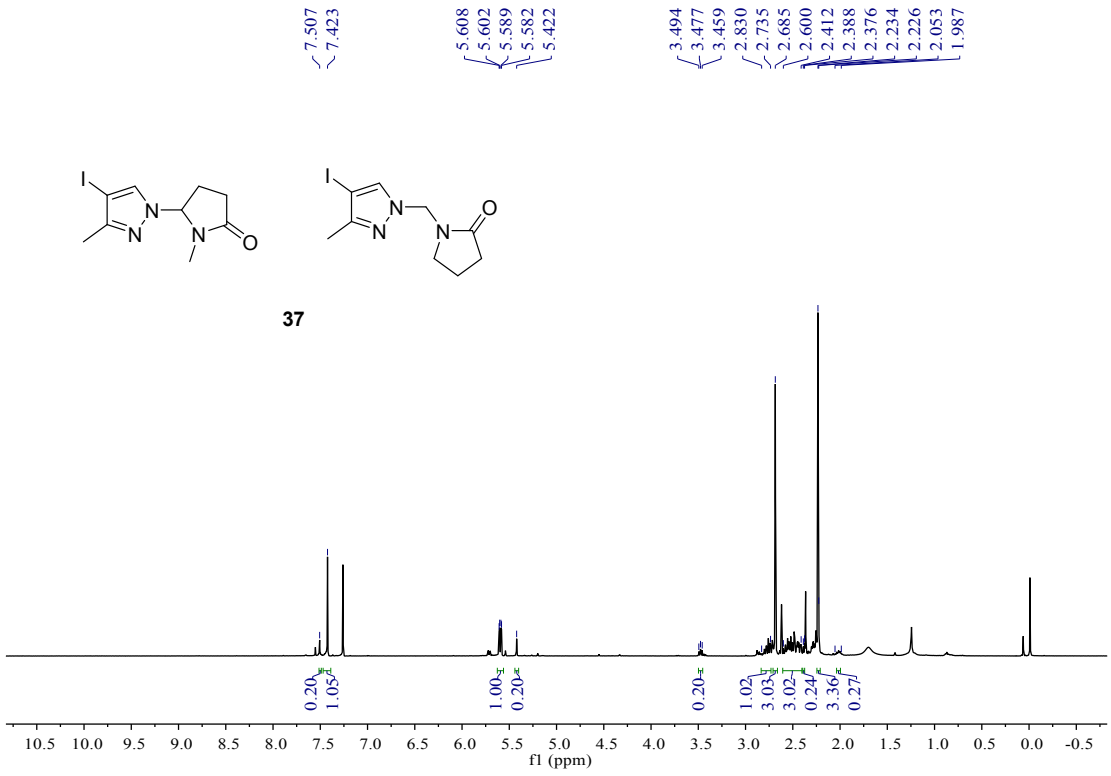


36

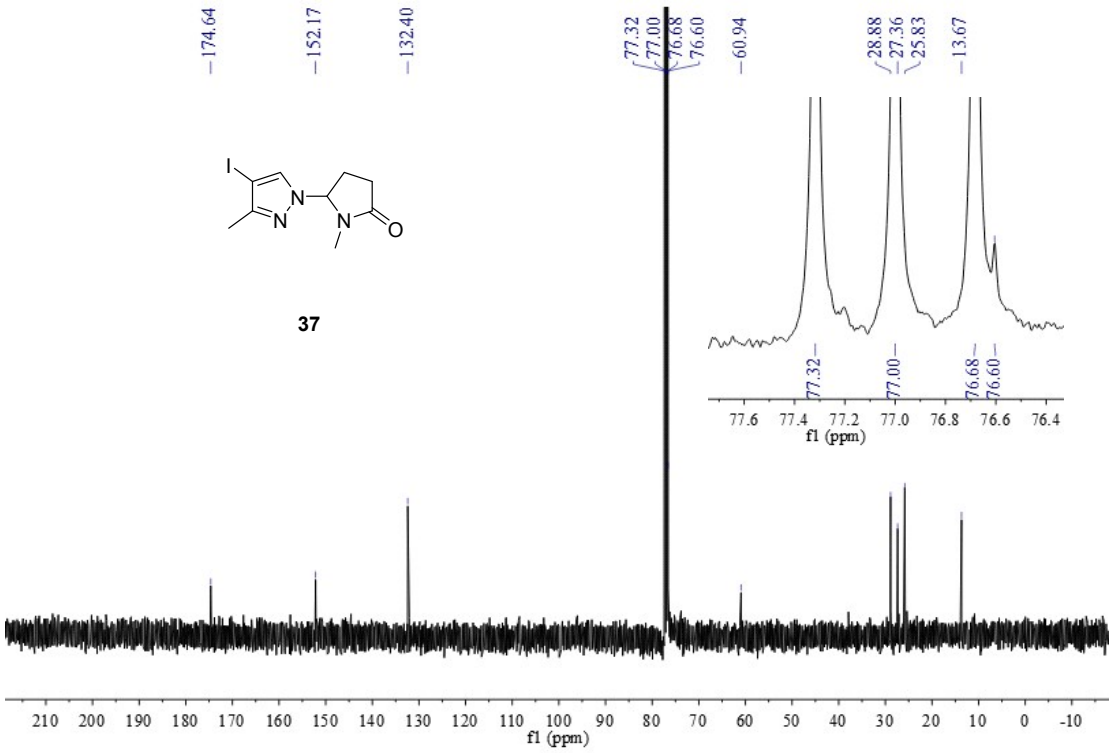
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 36



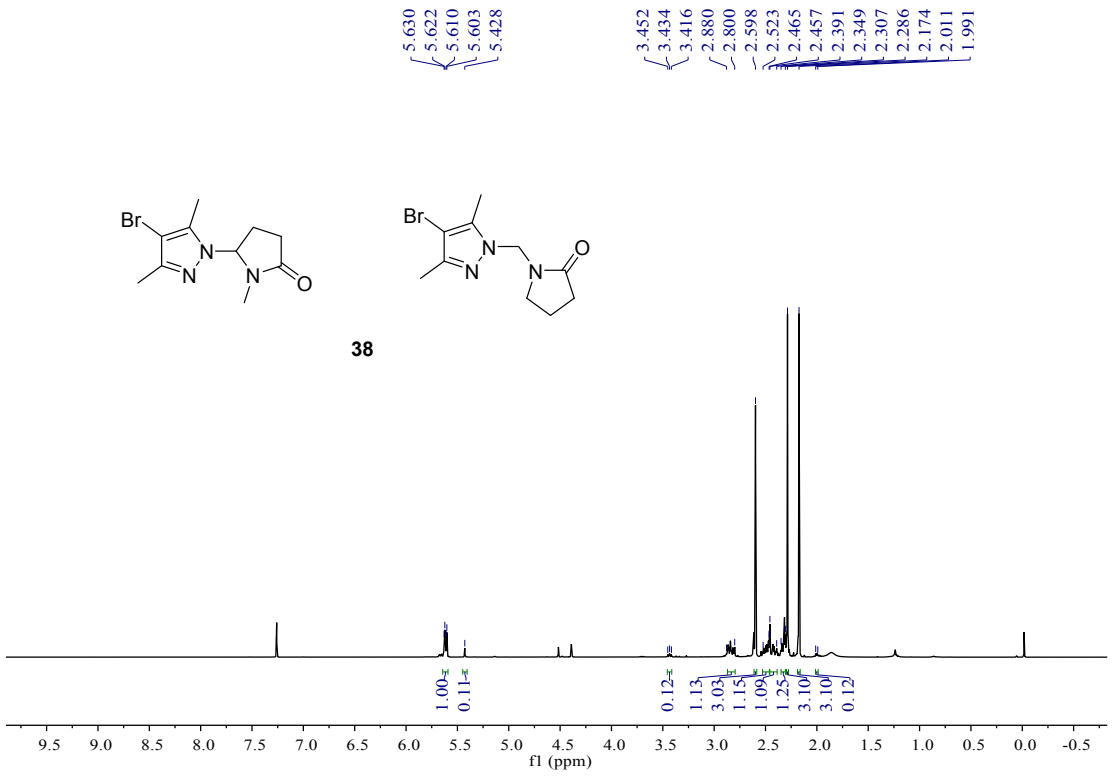
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 36



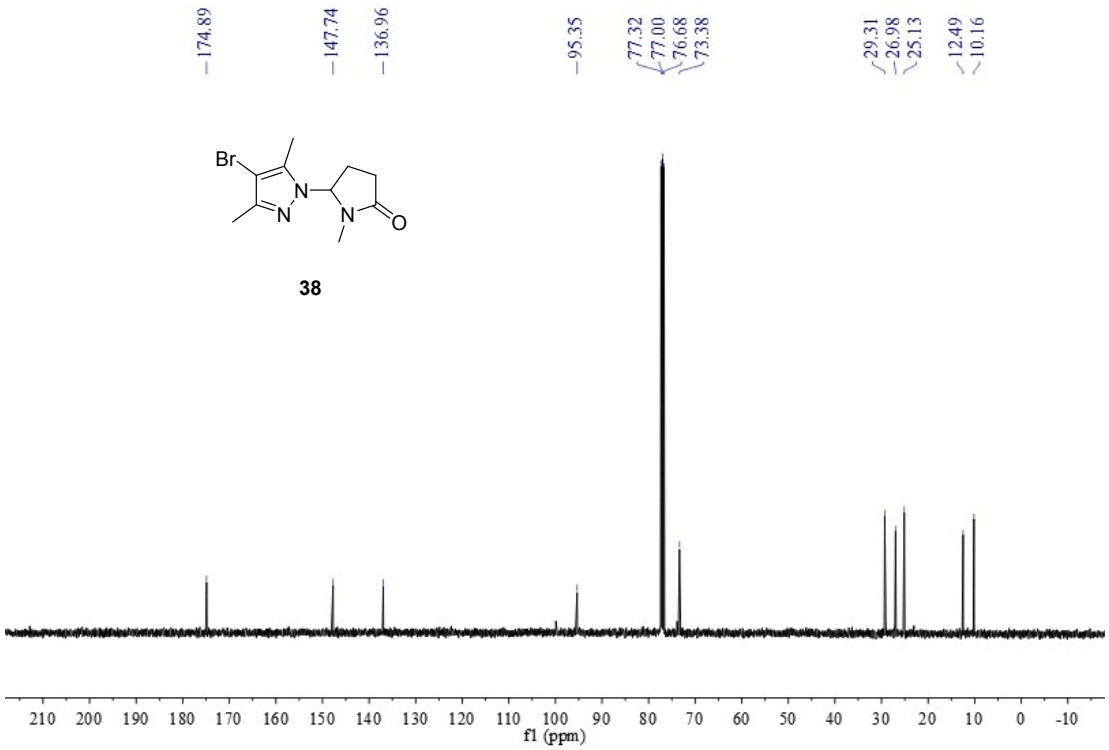
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 37



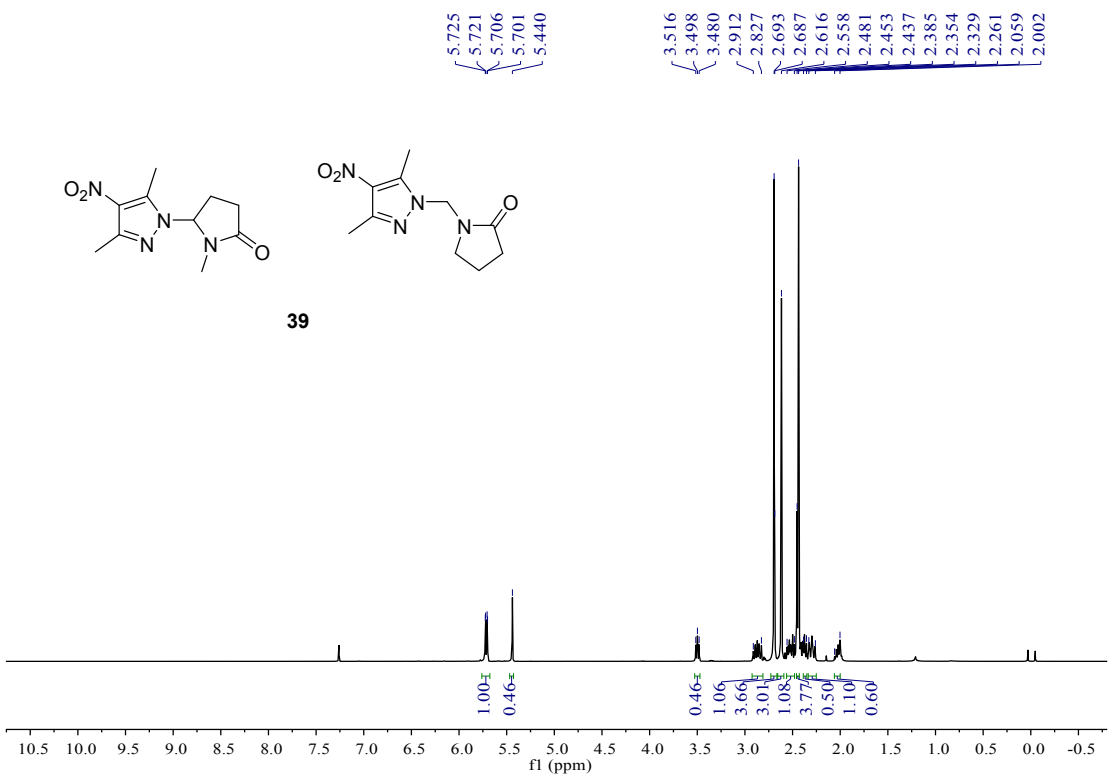
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 37



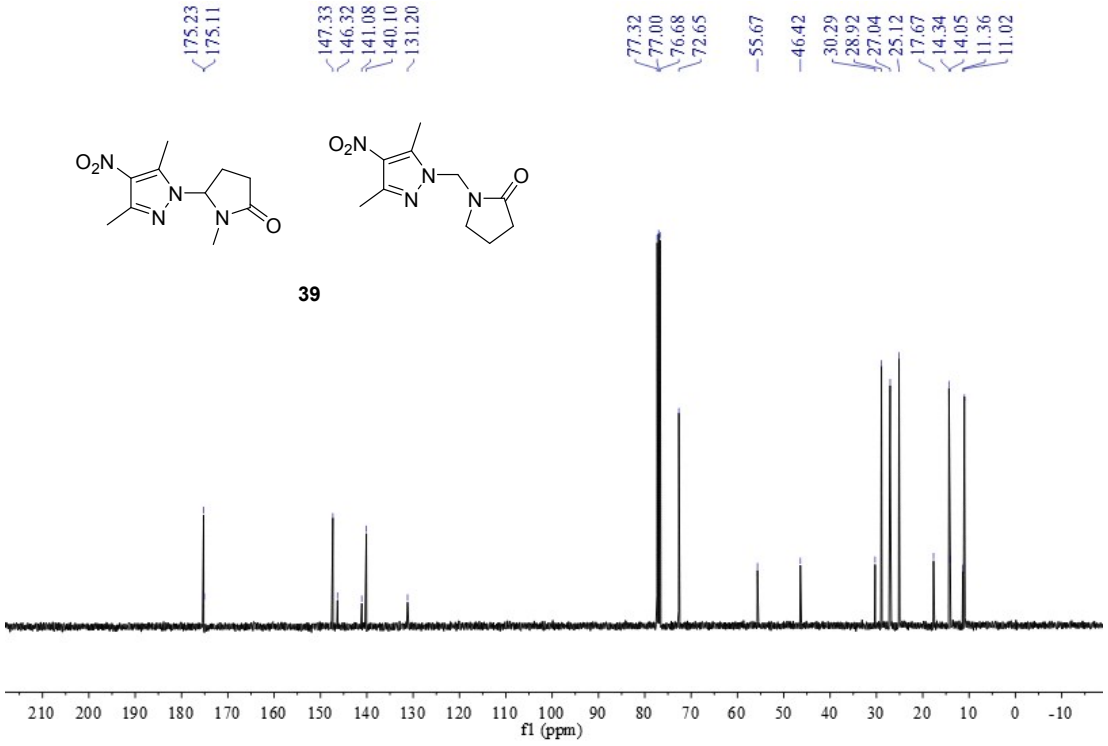
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 38



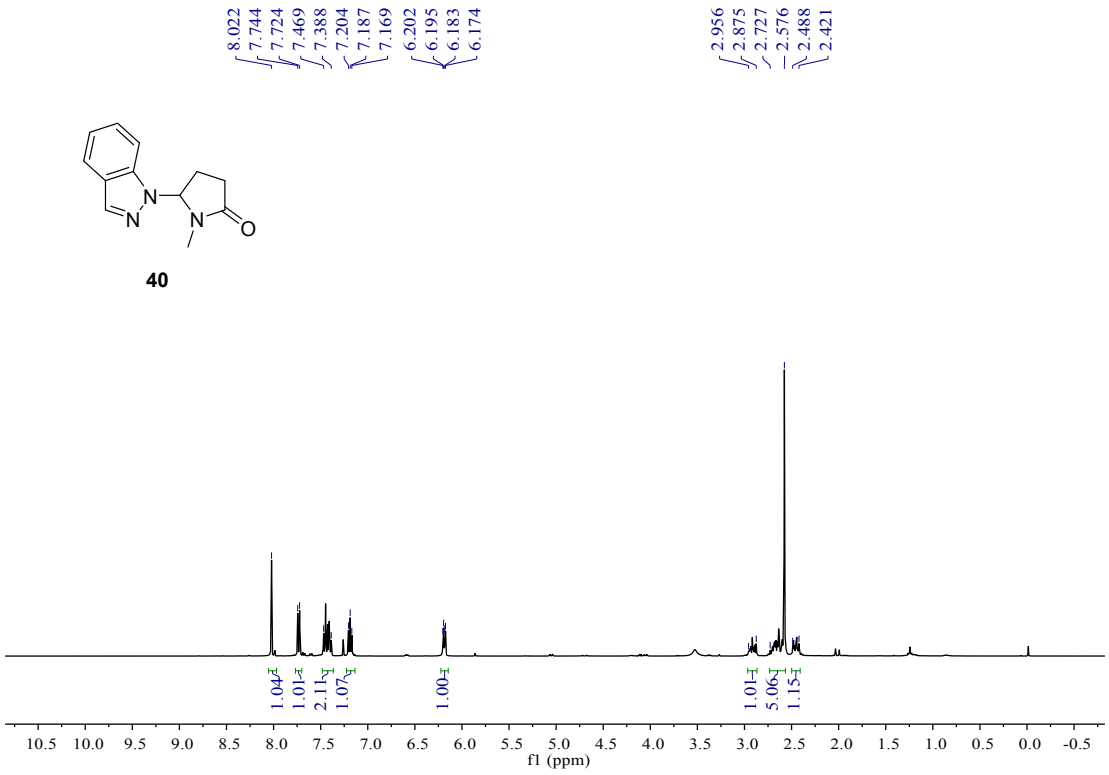
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 38



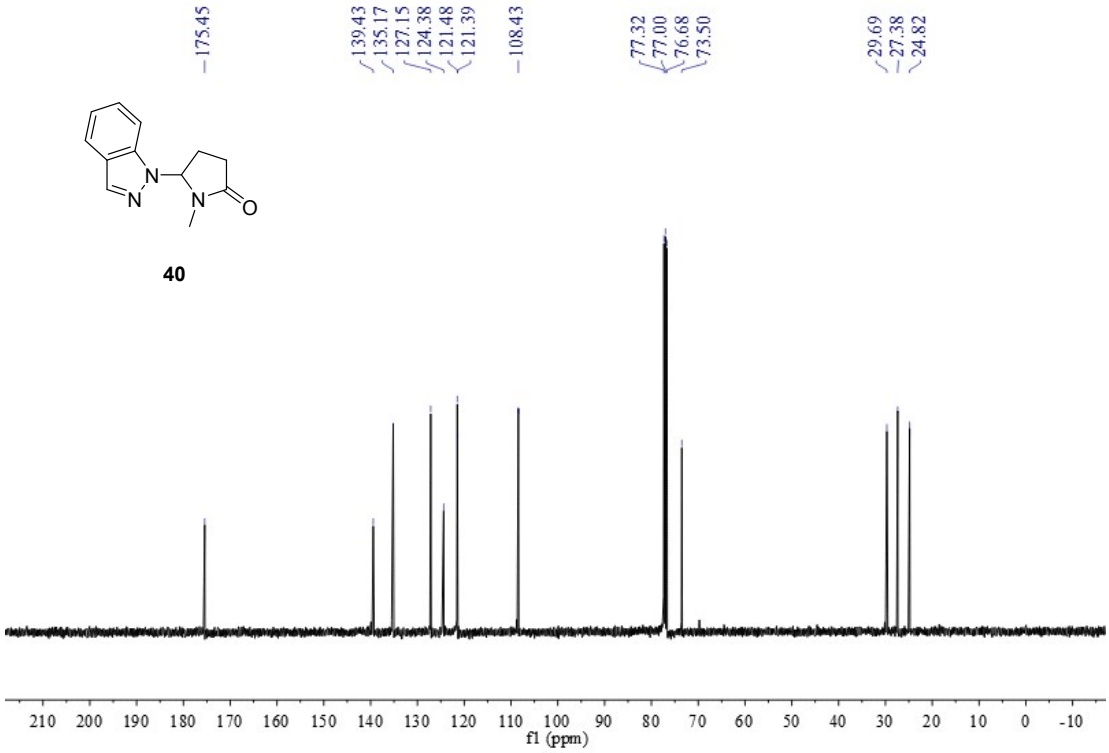
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 39



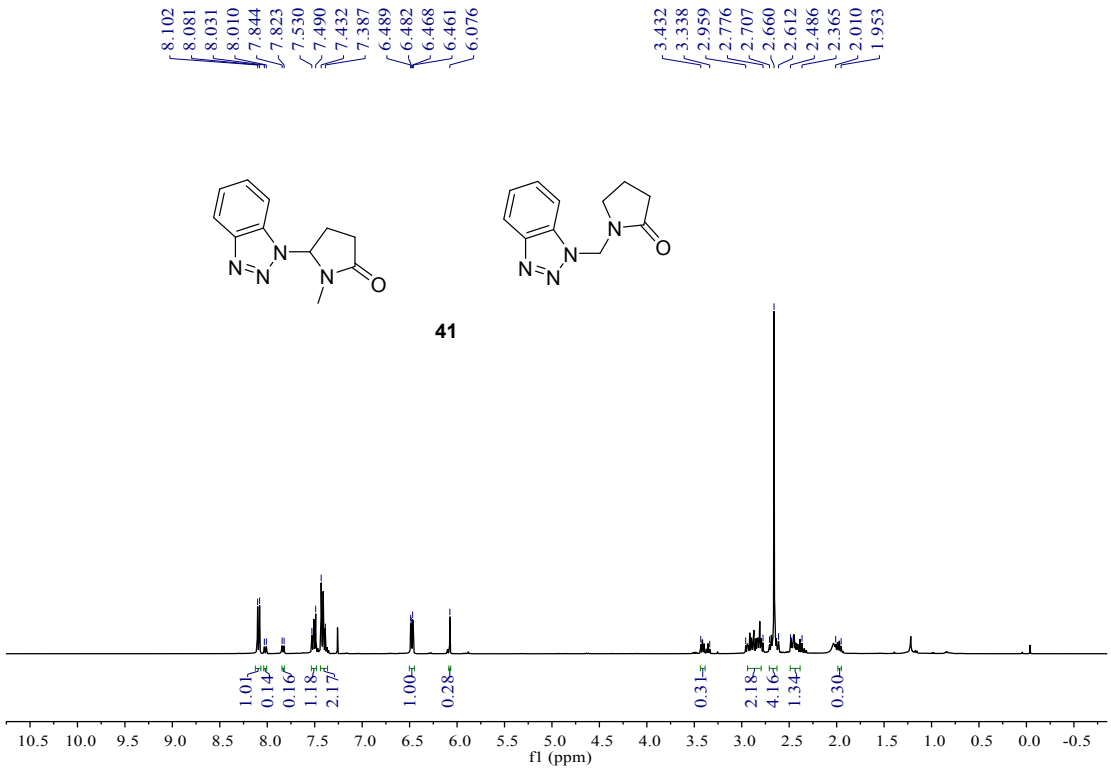
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 39



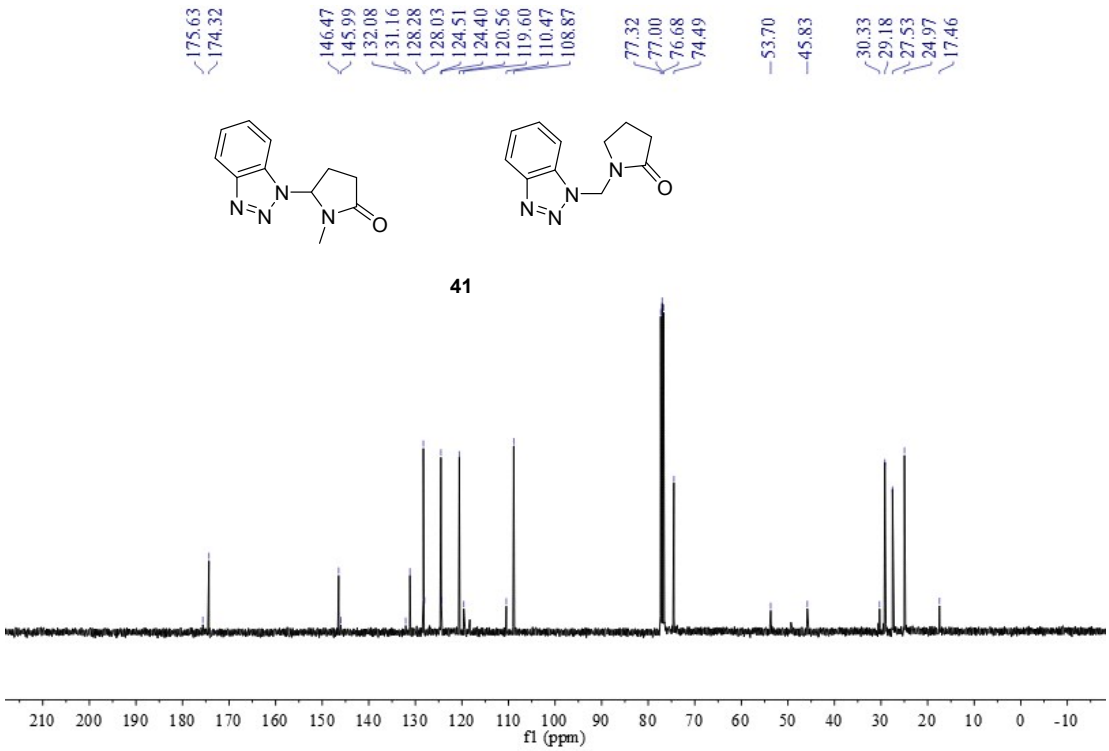
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 40



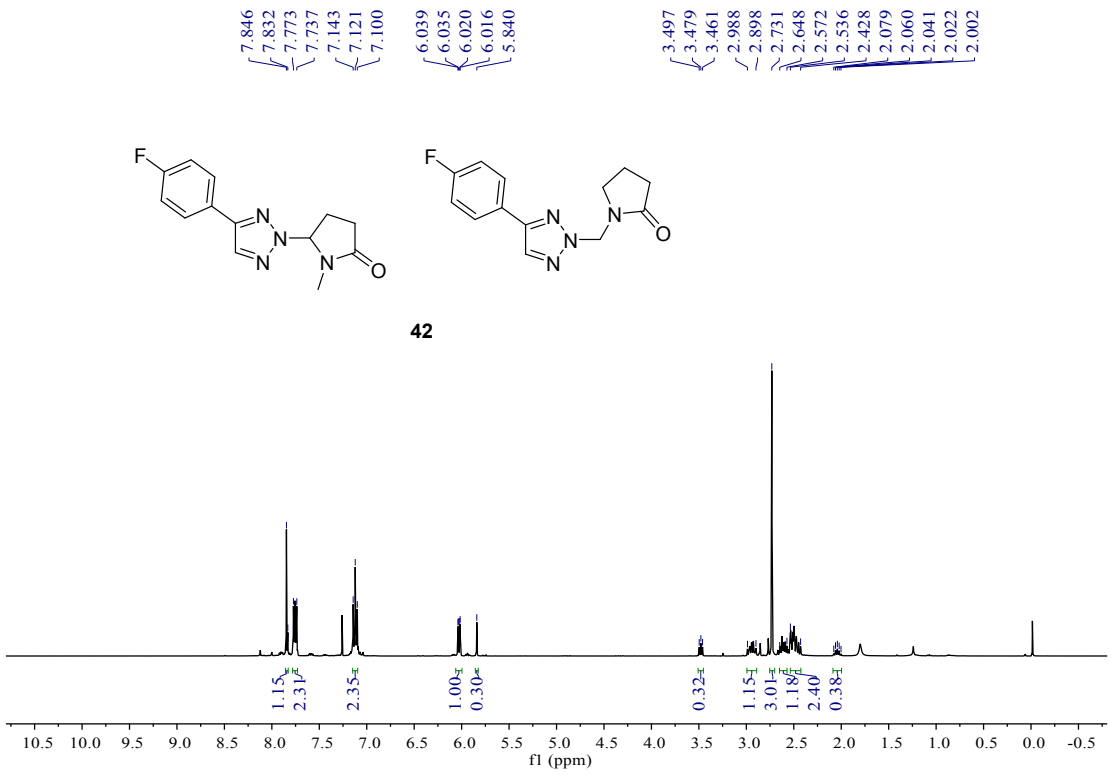
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 40



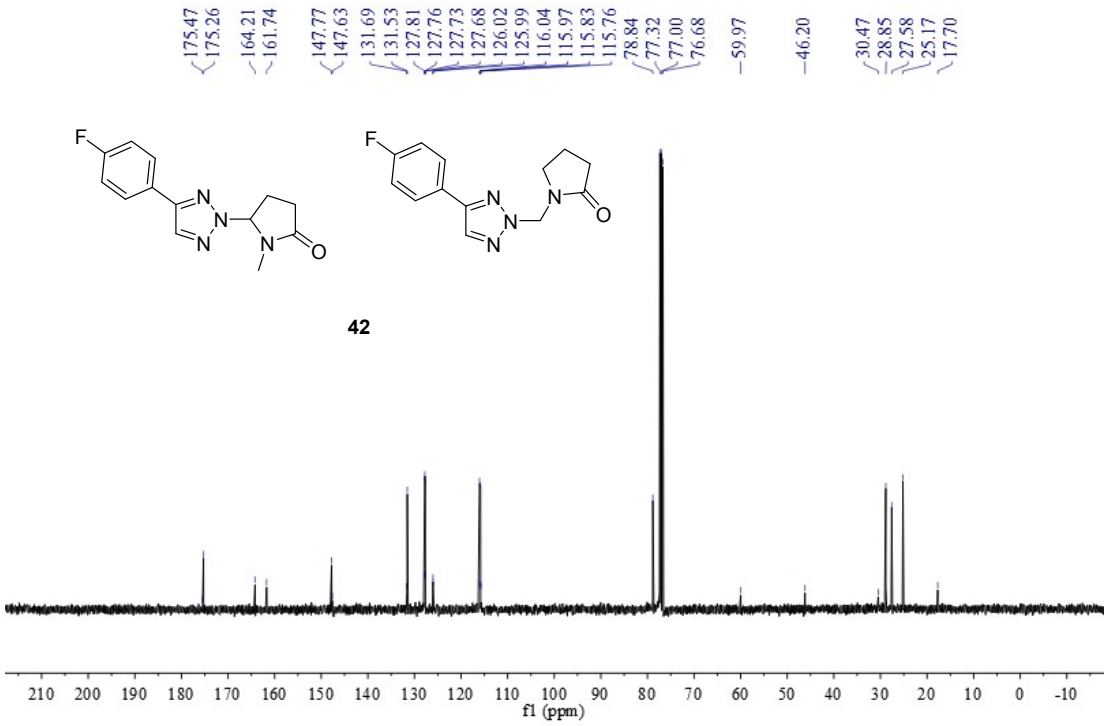
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 41



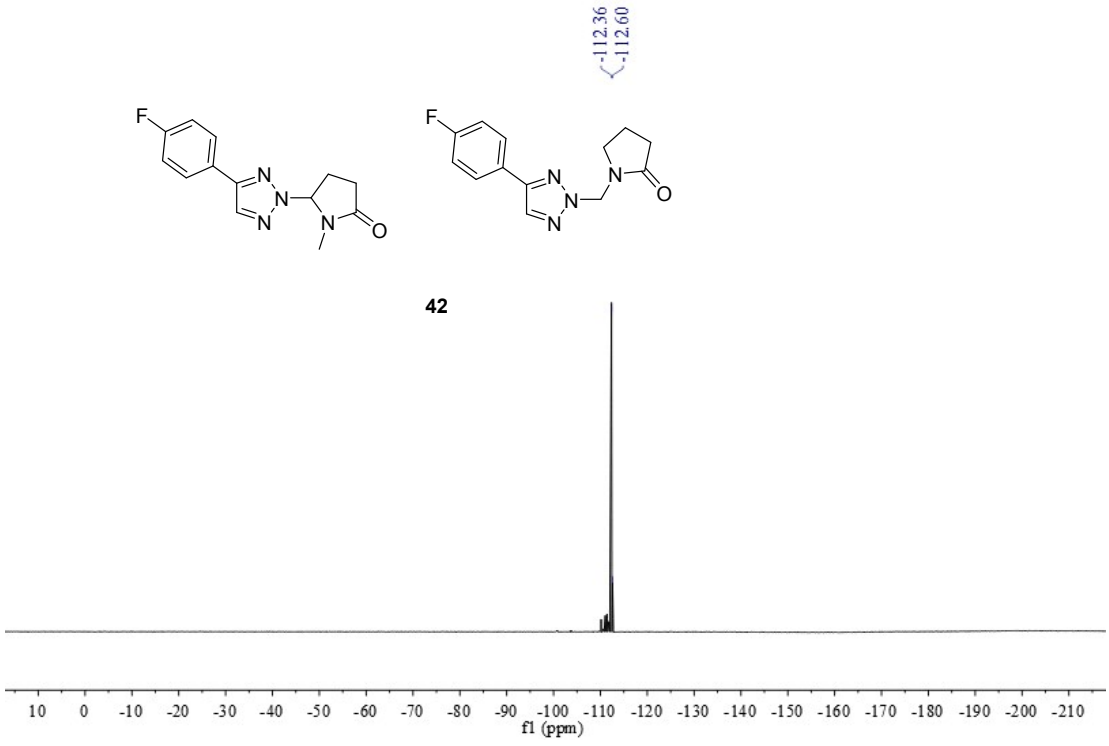
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 41



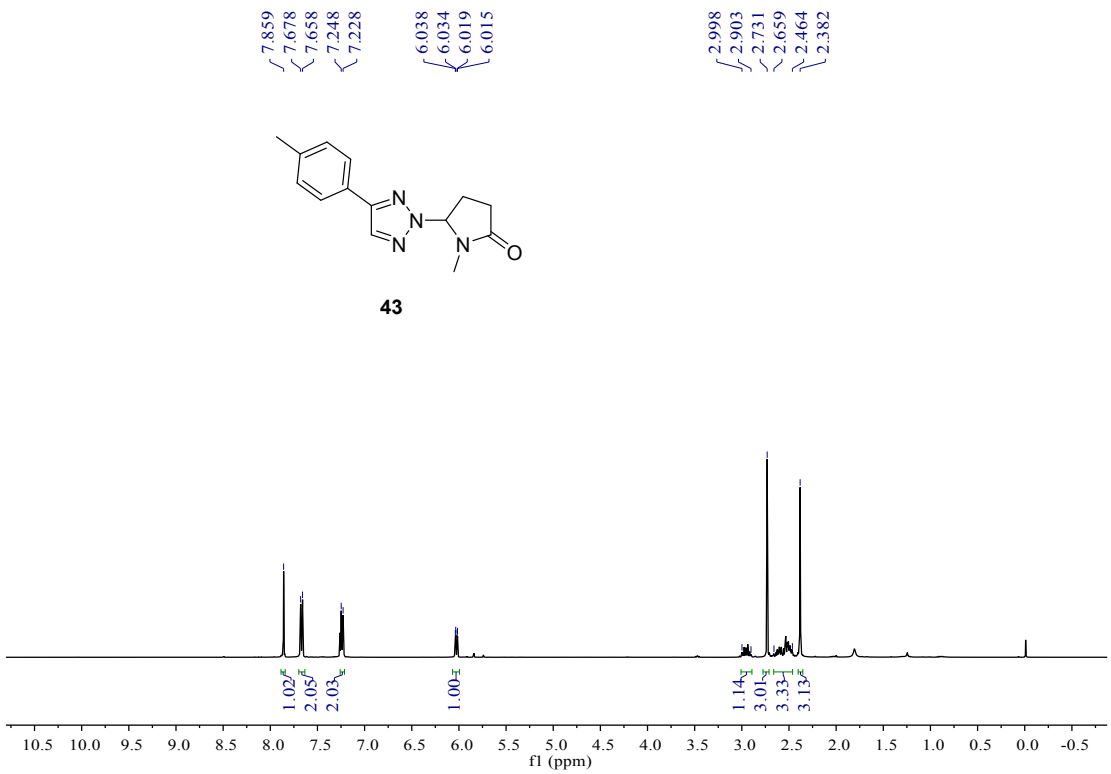
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 42



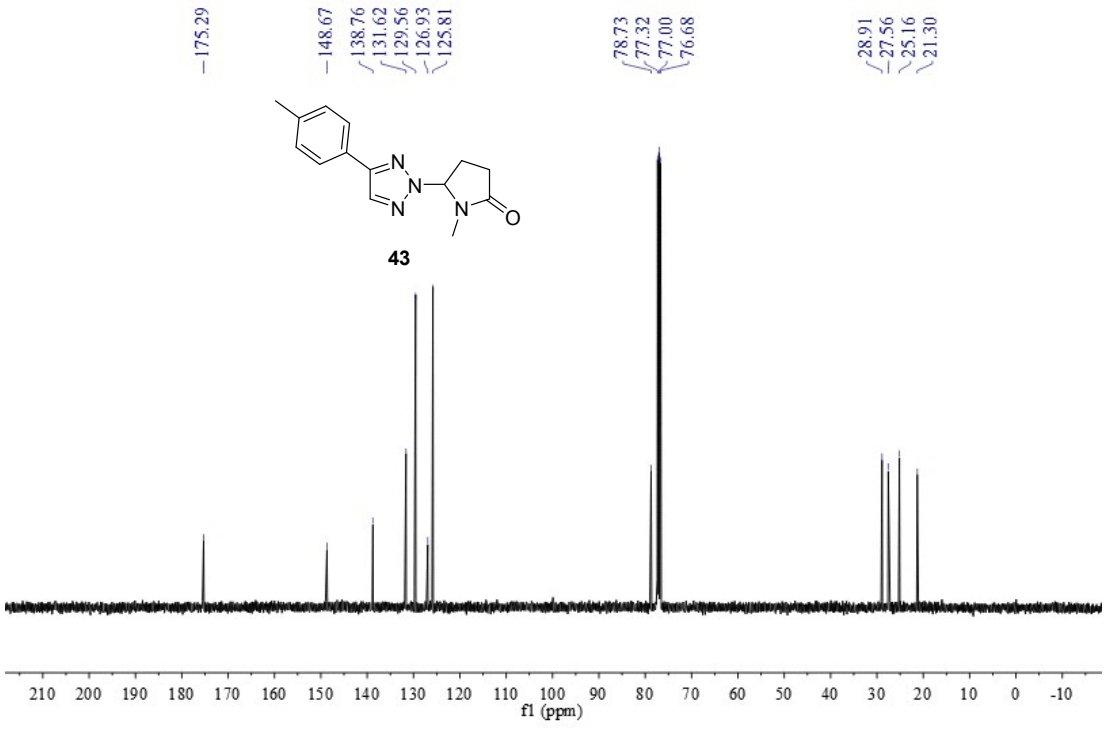
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 42



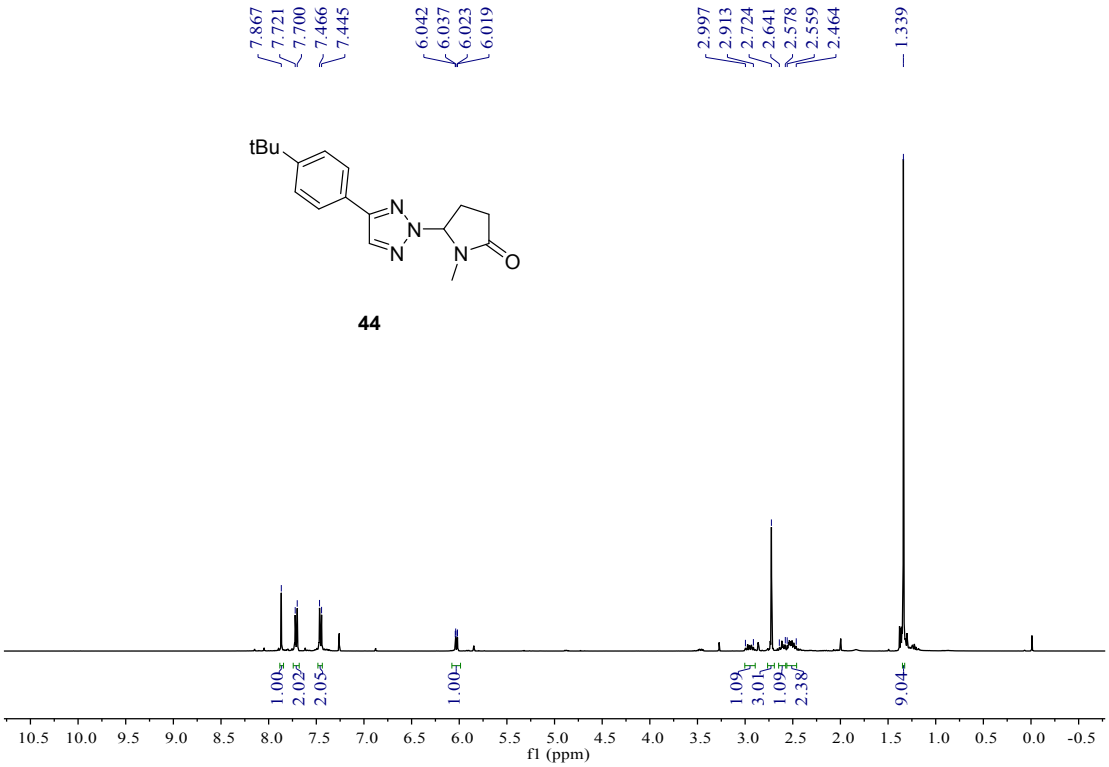
^{19}F NMR (373 MHz, $CDCl_3$) spectrum of 42



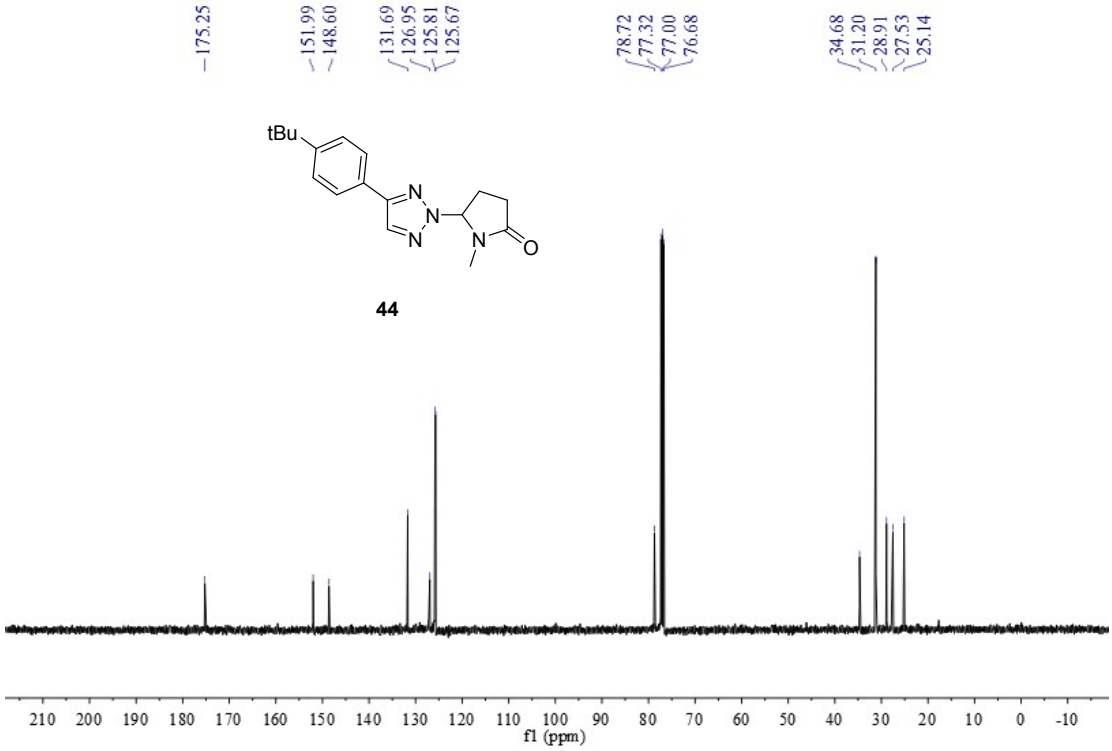
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 43



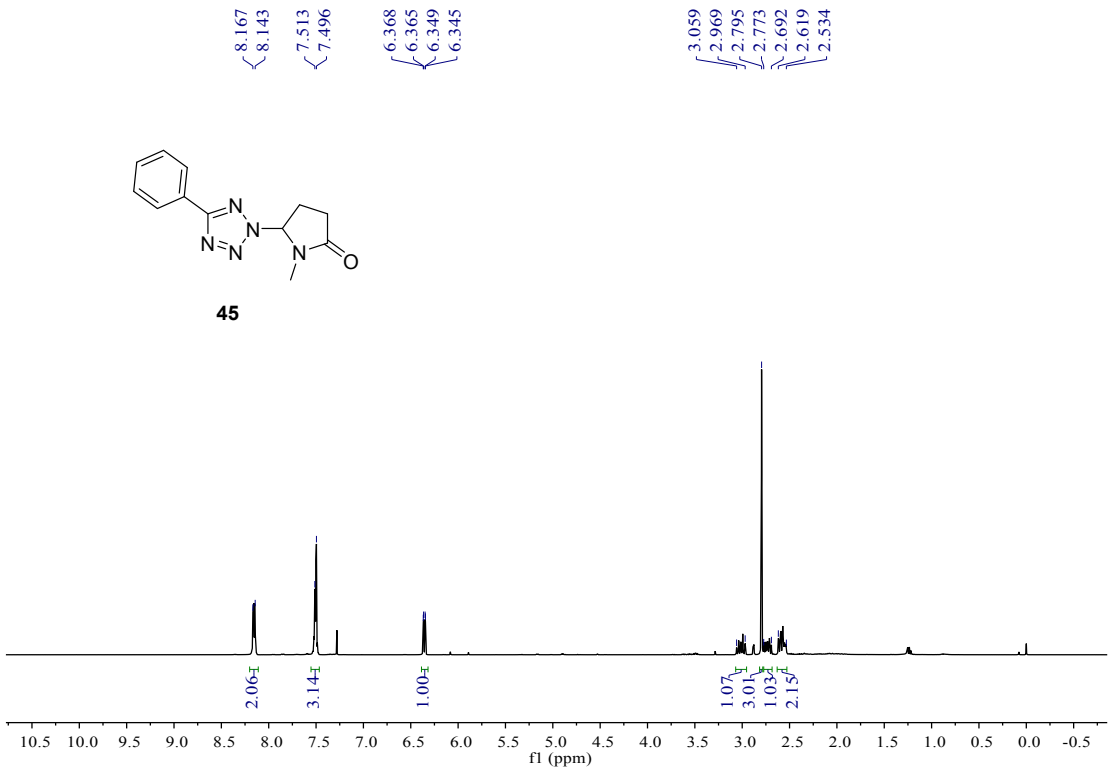
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 43



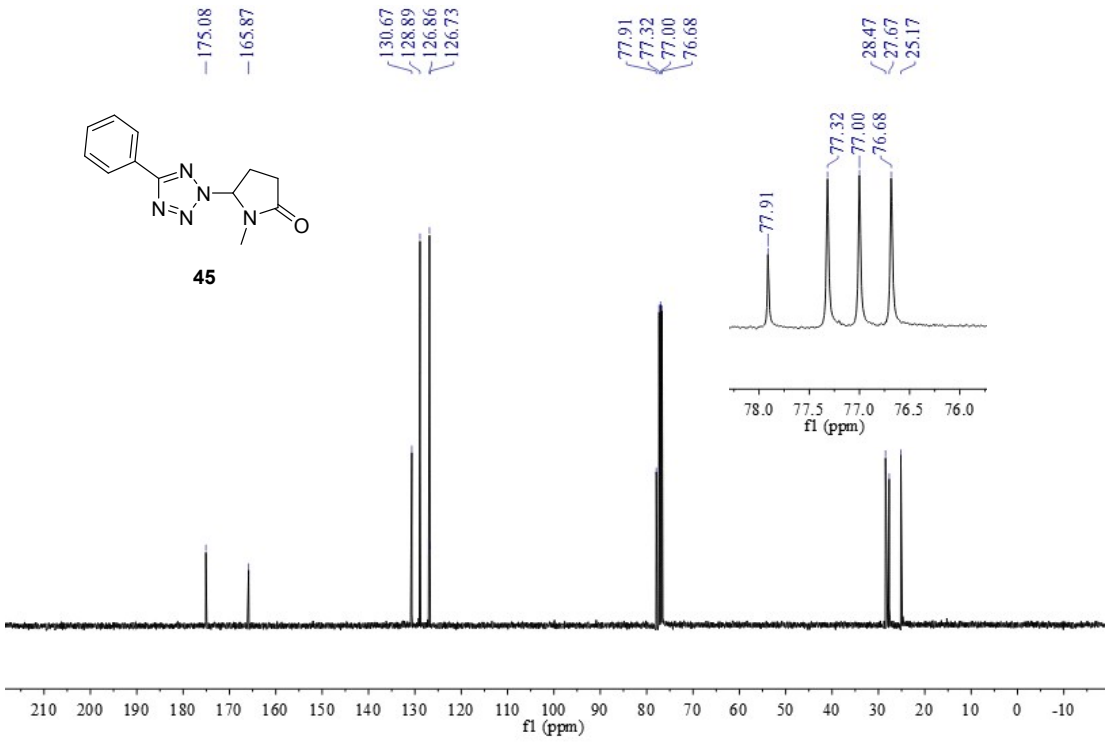
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 44



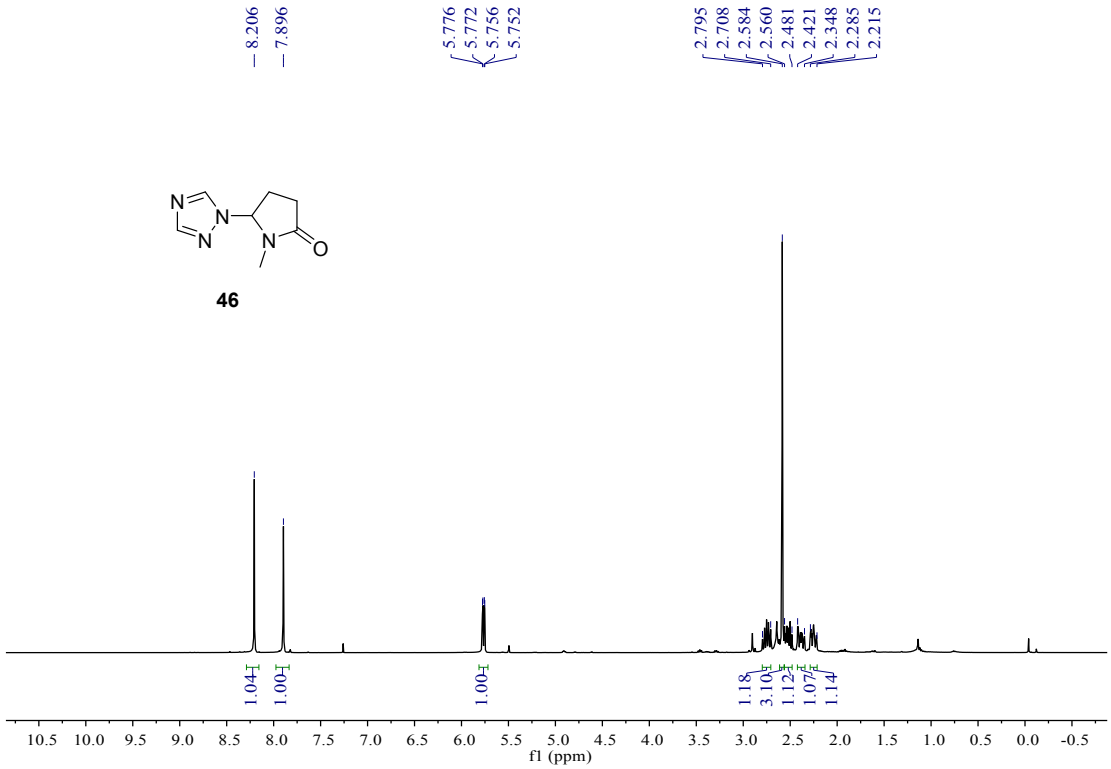
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 44



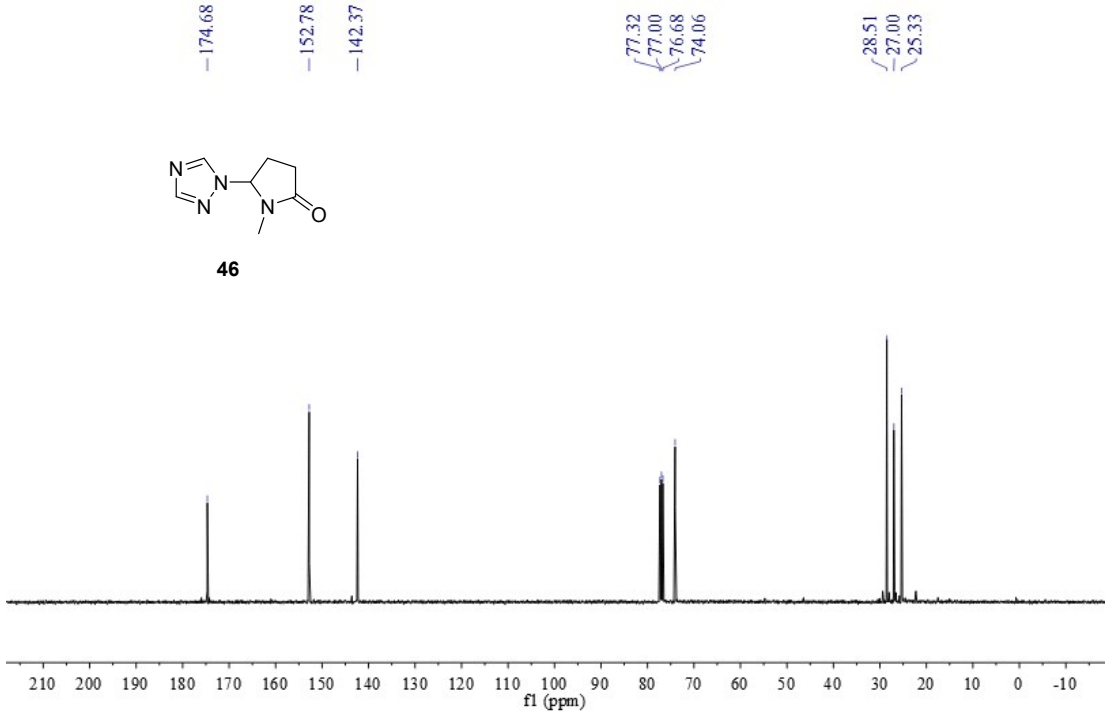
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 45



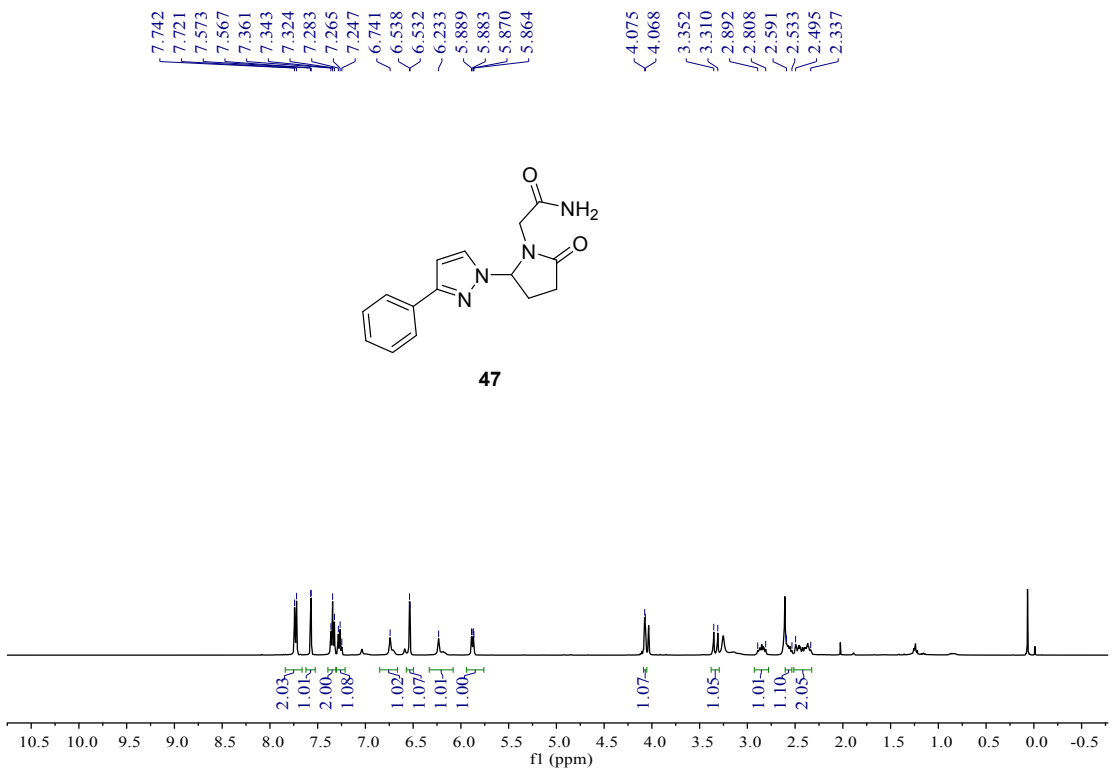
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 45



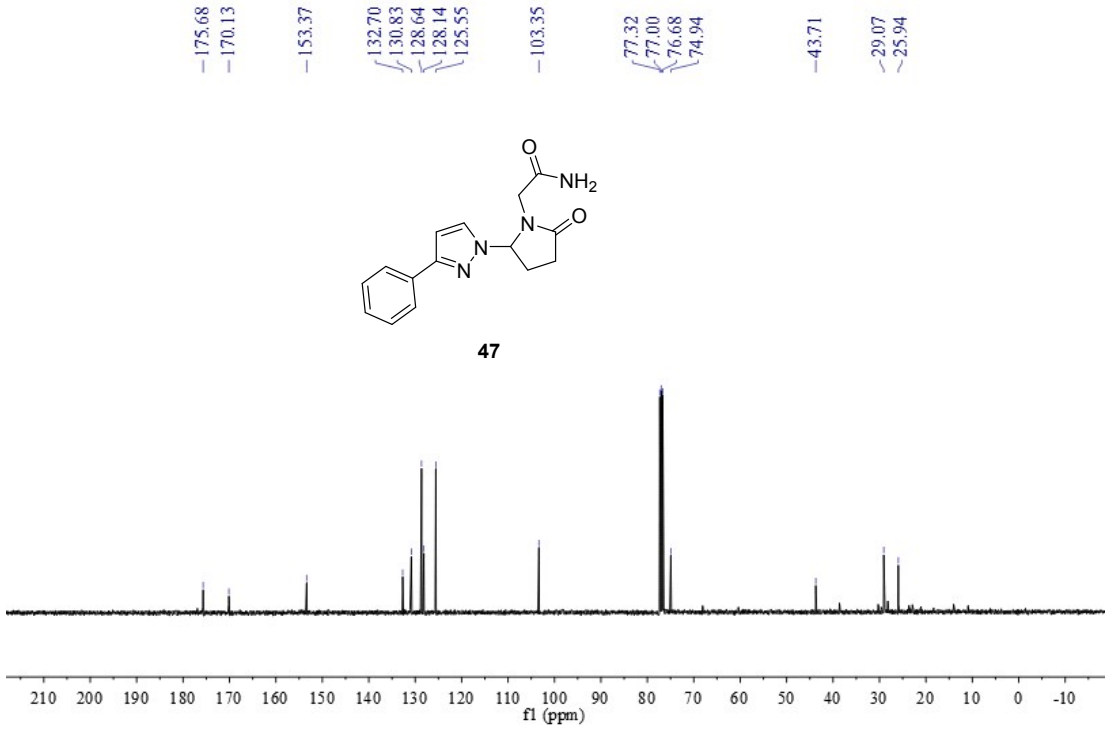
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 46



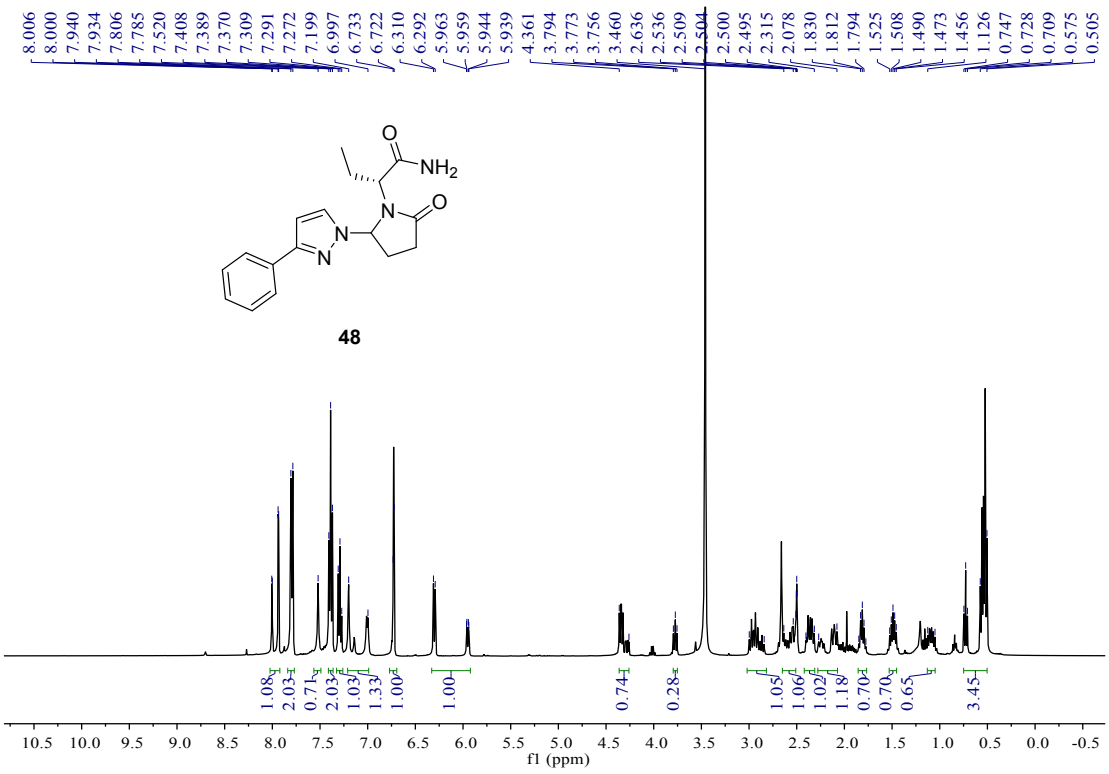
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 46



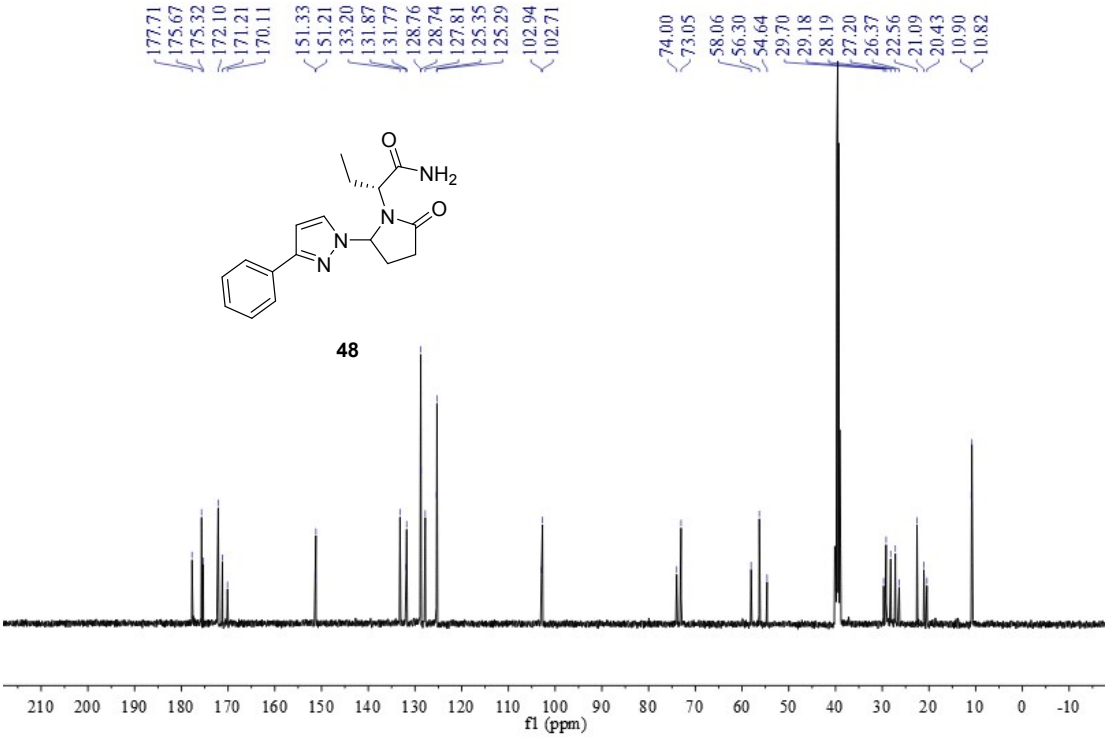
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 47



^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 47



^{1}H NMR (400 MHz, DMSO-d$_6$) spectrum of 48



^{13}C NMR (101 MHz, DMSO-d$_6$) spectrum of 48

6. References

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