Supporting Information

Visible-light-driven Anion Relay Chemistry (ARC): Construction of Fully Substituted Pyrazoles

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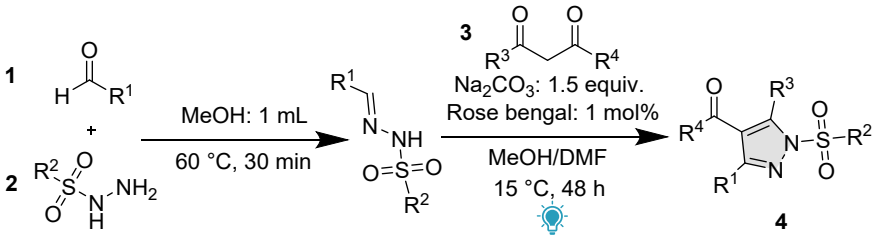
1. General information

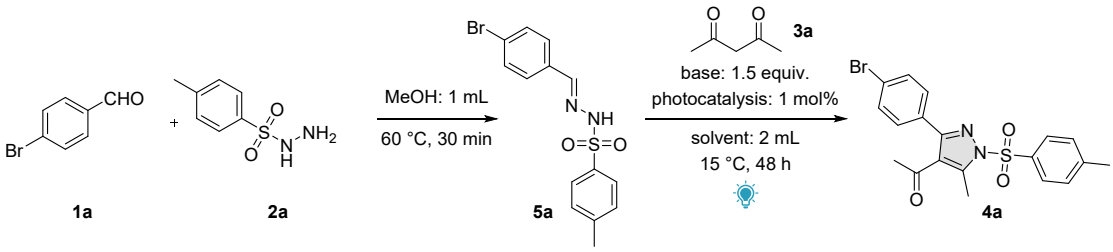
Column chromatography was generally performed on silica gel (300-400 mesh) and reactions were monitored by thin layer chromatography (TLC) using UV light to visualize the course of the reactions. The ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) and ^{19}F NMR (376 MHz) data were recorded with Chloroform-*d* or DMSO-d_6 as solvent at room temperature unless specified otherwise. The chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. ^{1}H NMR spectra was recorded with tetramethylsilane (δ= 0.00 ppm) or Chloroform-*d* (δ= 7.26 ppm) or DMSO-d_6 (δ = 2.50 ppm) as internal reference; ^{13}C NMR spectra was recorded with Chloroform-*d* (δ = 77.00 ppm) or DMSO (δ = 39.52 ppm) as internal reference. IR and HRMS were performed by the State-authorized Analytical Center in Soochow University.

2. General procedures



The first step is to add aldehyde **1** (0.2 mmol), sulfonydrazide **2** (0.4 mmol) and methanol (1 mL) to the reaction tube with magnetic stirring bar, stirring for 30 minutes at 60 ℃, then add 1,3-dicarbonyls **3** (0.5 mmol), sodium carbonate (0.3 mmol), Rose Bengal (1 mol%), *N, N*-dimethylformamide (1 mL), irradiation with 3W blue LED lamp for 48 hours. After confirming the finish of the reaction by TLC, the system was quenched with saturated sodium thiosulfate for three times, then extracted with ethyl acetate, merge the organic phase, dried with anhydrous sodium sulfate, then concentrated in vacuum and purified by column chromatography on silica gel to afford the desired products **4**.

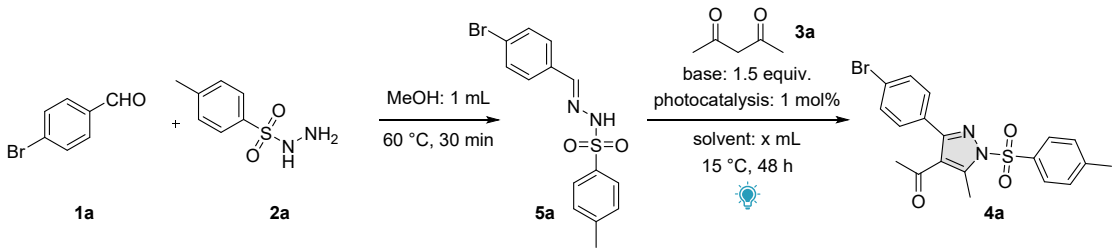
3. Optimization of the reaction conditions



Entry	Photocatalysis	Base	Solvents	Yield (%)
1	4CzIPN	Na_2CO_3	DMF	60
2	4CzIPN	Na_2CO_3	DMSO	54
3	4CzIPN	Na_2CO_3	MeOH	55
4	4CzIPN	Na_2CO_3	NMP	33
5	Rhodamine 6G	Na_2CO_3	DMF	65
6	$Ru(bpy)_3Cl_2·6H_2O$	Na_2CO_3	DMF	56
7	Rhodamine B	Na_2CO_3	DMF	7
8	Thioxanthone	Na_2CO_3	DMF	5
9	Rose Bengal	Na_2CO_3	DMF	57
10	Rose Bengal	Na_2CO_3	MeOH/DMSO	73
11	Rose Bengal	Na_2CO_3	DMSO/DMF	58
12	Rose Bengal	Na_2CO_3	NMP/DMF	45
13	Rose Bengal	Na_2CO_3	MeOH/DMF	82

Table S1. Optimization of the reaction conditions for the second step.

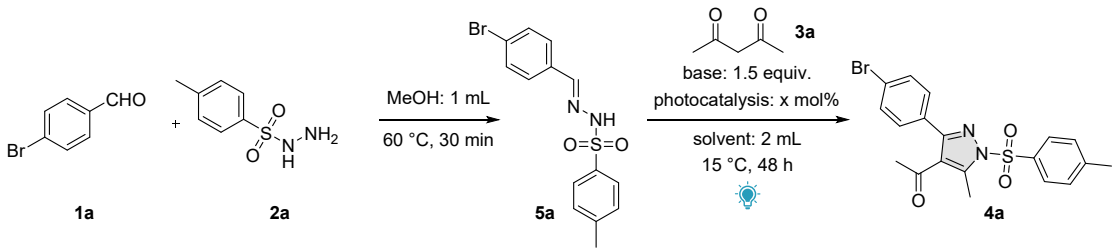
General reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), and MeOH (1 mL) were added at 60 °C for 30 minutes. **3a** (0.5 mmol), base (0.3 mmol), photocatalyst (1 mol%) were added, using 2 mL of the solvent and 3W blue LED at 15 °C for 48 h, yields of isolated product.



Entry	Photocatalysis	Base	Solvents (MeOH/DMF)	Yield (%)
1	Rose Bengal	Na_2CO_3	0.5 mL/0.5 mL	73
2	Rose Bengal	Na_2CO_3	0.5 mL/1.5 mL	68
3	Rose Bengal	Na_2CO_3	1.5 mL/0.5 mL	70
4	Rose Bengal	Na_2CO_3	1.0 mL/2.0 mL	75
5	Rose Bengal	Na_2CO_3	2.0 mL/1.0 mL	65

Table S2. Optimization of the reaction conditions for the second step.

General reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), and MeOH (1 mL) were added at 60 °C for 30 minutes. **3a** (0.5 mmol), base (0.3 mmol), photocatalyst (1 mol%) were added, using mixed solvent and 3W blue LED at 15 °C for 48 h, yields of isolated product.

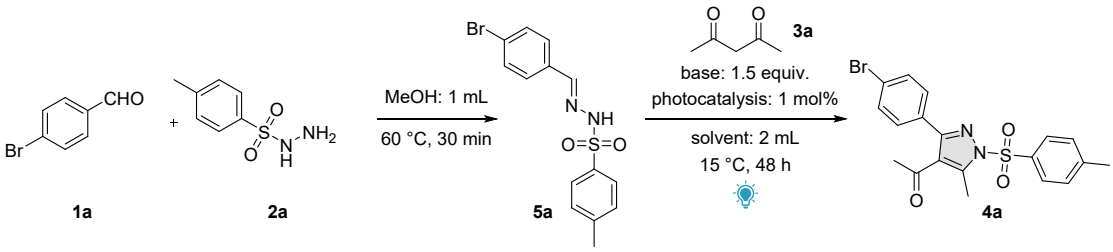


Entry	Photocatalysis (Rose Bengal)	Base	Solvents	Yield (%)
1	0.25 mol%	Na_2CO_3	MeOH/DMF	60
2	0.5 mol%	Na_2CO_3	MeOH/DMF	73
3	0.75 mol%	Na_2CO_3	MeOH/DMF	80
4	1 mol%	Na_2CO_3	MeOH/DMF	82

5	1.5 mol%	Na_2CO_3	MeOH/DMF	79
6	2 mol%	Na_2CO_3	MeOH/DMF	81
7	2.5 mol%	Na_2CO_3	MeOH/DMF	80

Table S3. Optimization of the reaction conditions for the second step.

General reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), and MeOH (1 mL) were added at 60 °C for 30 minutes. **3a** (0.5 mmol), base (0.3 mmol), photocatalyst (x mol%) were added, using using 2 mL of the solvent and 3W blue LED at 15 °C for 48 h, yields of isolated product.

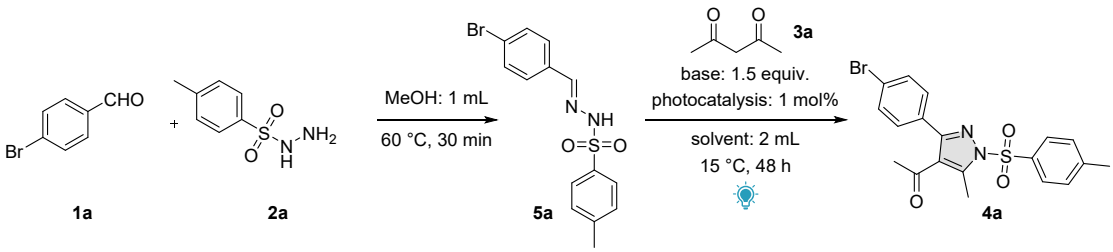


1a **2a** **5a** **4a**

Entry	Photocatalysis	Base	Solvents	Yield (%)
1	4CzIPN	Na_2CO_3	MeOH/DMF	78
2	Rhodamine 6G	Na_2CO_3	MeOH/DMF	67
3	$Ru(bpy)_3Cl_2·6H_2O$	Na_2CO_3	MeOH/DMF	69
4	Rhodamine B	Na_2CO_3	MeOH/DMF	17
5	Thioxanthone	Na_2CO_3	MeOH/DMF	5

Table S4. Optimization of the reaction conditions for the second step.

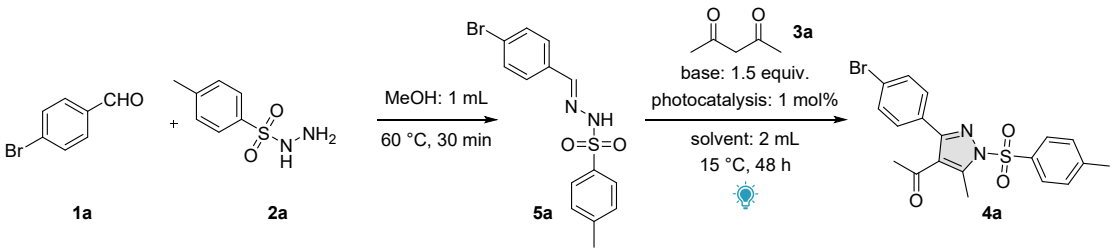
General reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), and MeOH (1 mL) were added at 60 °C for 30 minutes. **3a** (0.5 mmol), base (0.3 mmol), photocatalyst (1 mol%) were added, using using 2 mL of the solvent and 3W blue LED at 15 °C for 48 h, yields of isolated product.



Entry	Photocatalysis	Base	Solvents	Yield (%)
1	Rose Bengal	Li_2CO_3	MeOH/DMF	28
2	Rose Bengal	LiOH	MeOH/DMF	35
3	Rose Bengal	Cs_2CO_3	MeOH/DMF	73
4	Rose Bengal	$Mg(OH)_2$	MeOH/DMF	<5
5	Rose Bengal	NaOH	MeOH/DMF	46

Table S5. Optimization of the reaction conditions for the second step.

General reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), and MeOH (1 mL) were added at 60 °C for 30 minutes. **3a** (0.5 mmol), base (0.3 mmol), photocatalyst (1 mol%) were added, using 2 mL of the solvent and 3W blue LED at 15 °C for 48 h, yields of isolated product.

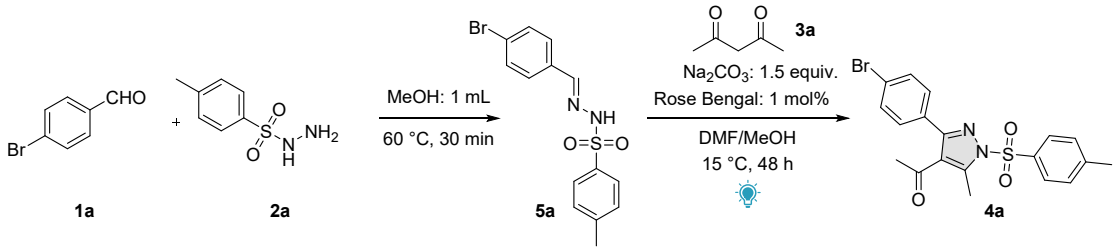


Entry	LED_S	Photocatalysis	Base	Solvents	Yield (%)
1	Blue LED: 24 W	Rose Bengal	Na_2CO_3	MeOH/DMF	81
2	Blue LED: 40 W	Rose Bengal	Na_2CO_3	MeOH/DMF	80
3	Blue LED: 60 W	Rose Bengal	Na_2CO_3	MeOH/DMF	80
4	Green LED: 3 W	Rose Bengal	Na_2CO_3	MeOH/DMF	76
5	Yellow LED: 3 W	Rose Bengal	Na_2CO_3	MeOH/DMF	60

Table S6. Optimization of the reaction conditions for the second step.

General reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), and MeOH (1 mL) were added at 60 °C for 30 minutes. **3a** (0.5 mmol), base (0.3 mmol), photocatalyst (1 mol%) were added, using using 2 mL of the solvent and blue LED at 15 °C for 48 h, yields of isolated product.

4. Control experiments



Entry	Controlled parameter	Yield (%)
1	Standard conditions	82
2	Without photocatalyst	0
3	Without light	0
4	Without base	0
5	Argon protects	0

Table S7. Optimization of the reaction conditions for the second step.

General reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), and MeOH (1 mL) were added at 60 °C for 30 minutes. **3a** (0.5 mmol), base (0.3 mmol), photocatalyst (1 mol%) were added, using 2 mL of the solvent and 3W blue LED at 15 °C for 48 h, yields of isolated product.

5. Mechanistic investigations

5.1 Ultraviolet visible absorption experiments

Ultraviolet-visible absorption experiments were performed using a UV-vis near-infrared spectrophotometer (UV3600). The samples were measured in 1.0 cm quartz cuvettes.

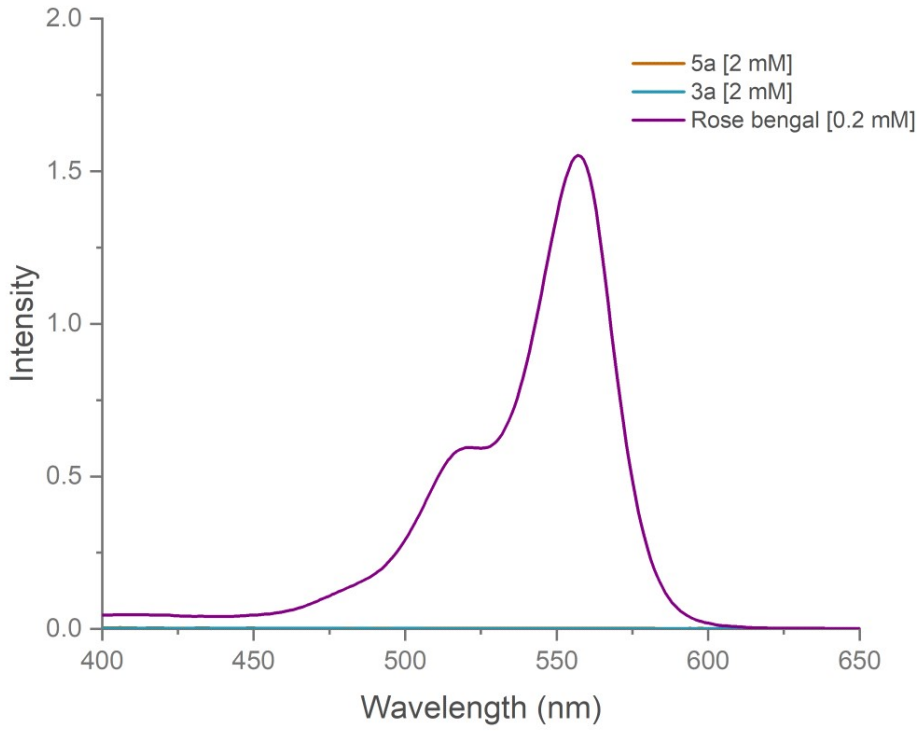


Figure S1: Ultraviolet-visible absorption experiments

The concentration of **3a** and **5a** were 2 $\times 10^{-3}$ M and the concentration of Rose Bengal was 2 $\times 10^{-4}$ M. The solvent was an equal volume of DMF and MeOH.

5.2 Stern Volmer quenching

Stern-Volmer luminescence quenching studies were performed using a FLS 980 spectrofluorometer using fluorescence quartz cuvettes. In each experiment, the following parameters were set: the excitation wavelength λ_{ex} = 521 nm, the luminescence was measured over a range of 541nm-751 nm (λ_{max} = 581 nm). The ratio of I_0/I was plotted as a function of the quencher concentration (I_0 = emission intensity of the photocatalyst (Rose Bengal) in isolation at the specified wavelength 521 nm; I = observed emission intensity of the photocatalyst (Rose Bengal) with added quencher.

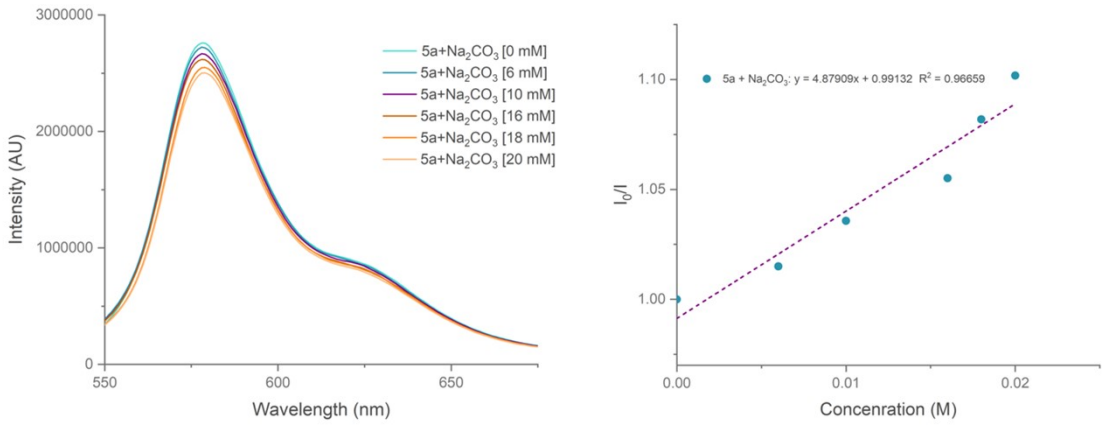


Figure S2: Stern-Volmer luminescence quenching studies

Using Rose Bengal as photocatalyst, **5a** and Na_2CO_3 as quencher can quench the fluorescence of the excited photocatalyst in an equal volume of DMF and MeOH.

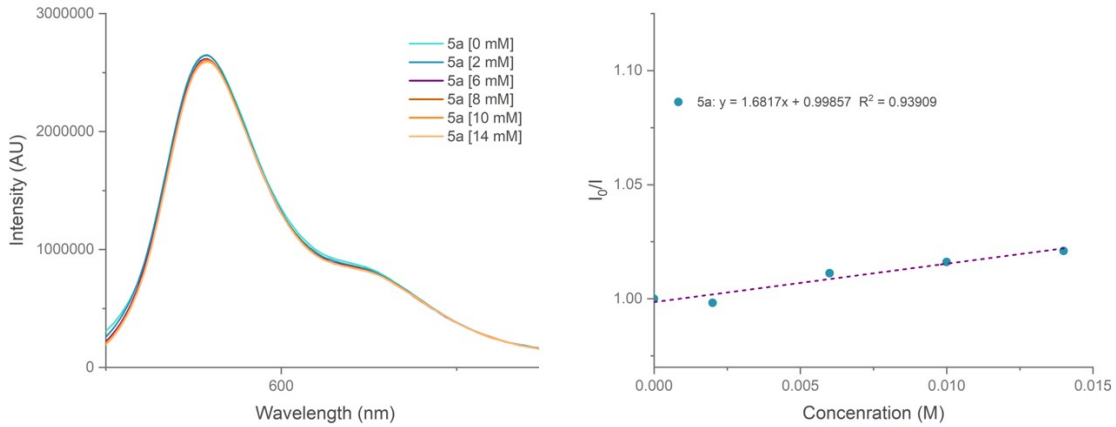


Figure S3: Stern-Volmer luminescence quenching studies

Using Rose Bengal as photocatalyst, **5a** as quencher can't quenches the fluorescence of the excited photocatalyst in an equal volume of DMF and MeOH.

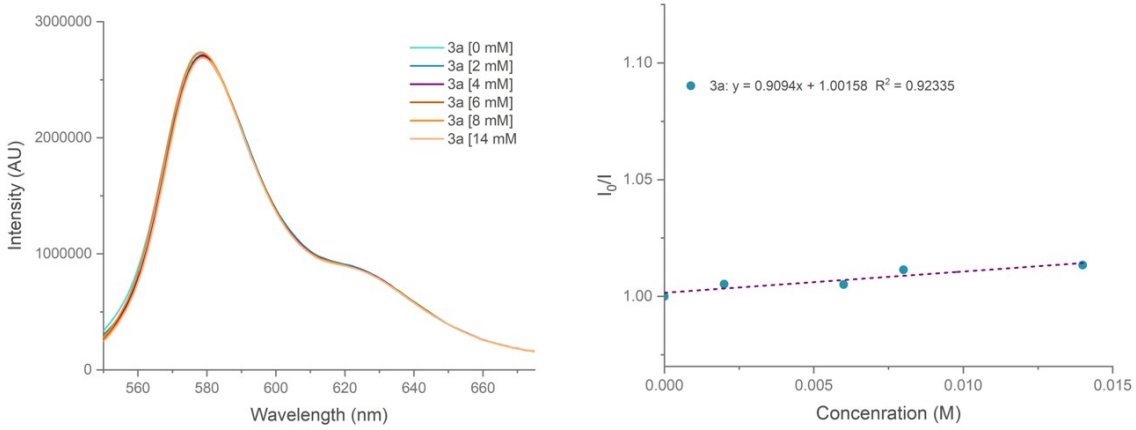


Figure S4: Stern-Volmer luminescence quenching studies

Using Rose Bengal as photocatalyst, **3a** as quencher can't quenches the fluorescence of the excited photocatalyst in an equal volume of DMF and MeOH.

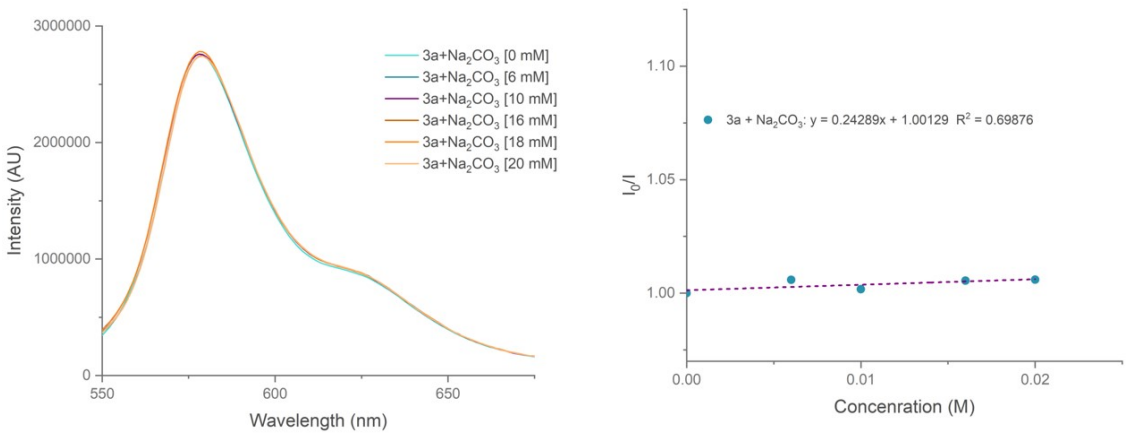


Figure S5: Stern-Volmer luminescence quenching studies

Using Rose Bengal as photocatalyst, **3a** and Na_2CO_3 as quencher can't quench the fluorescence of the excited photocatalyst in an equal volume of DMF and MeOH.

5.3 Radical quenching experiment

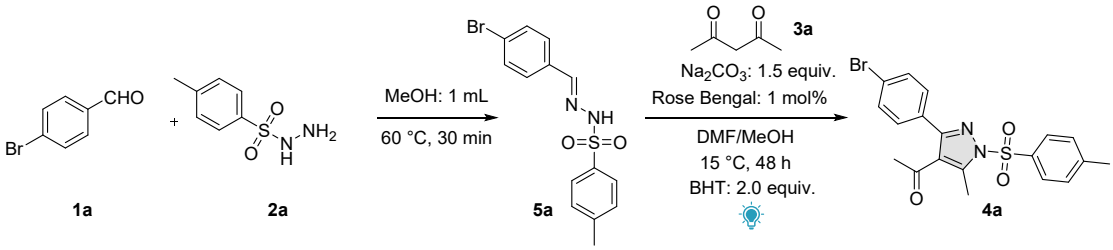


Figure S6: Radical quenching experiment with BHT

The first step was to add 4-dromobenzaldehyde **1a** (0.2 mmol), 4-methylbenzenesulfonhydrazide **2a** (0.4 mmol) and methanol (1 mL) to the reaction tube with magnetic stirring bar, stirring for 30 minutes at 60 ℃, then add acetylacetone **3a** (0.5 mmol), sodium carbonate (0.3 mmol), Rose Bengal (1 mol%), butylated hydroxytoluene (BHT) (0.4 mmol), *N, N*-dimethylformamide (1 mL), irradiation with 3W blue LED lamp for 48 hours. The desired products **4a** was afford in 73 % yield.

5.4 Triplet quenching experiment

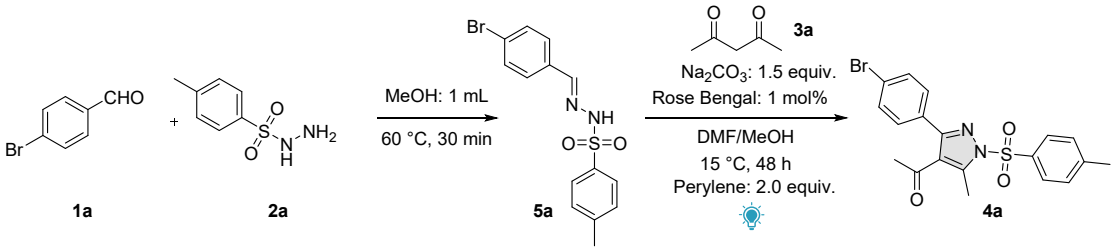


Figure S7: Triplet quenching experiment with perylene

The first step is to add 4-Bromobenzaldehyde **1a** (0.2 mmol), 4-Methylbenzenesulfonhydrazide **2a** (0.4 mmol) and methanol (1 mL) to the reaction tube with magnetic stirring bar, stirring for 30 minutes at 60 ℃, then add acetylacetone **3a** (0.5 mmol), sodium carbonate (0.3 mmol), Rose Bengal (1 mol%), perylene (0.4 mmol), *N, N*-dimethylformamide (1 mL), irradiation with 3W blue LED lamp for 48 hours. The desired products **4a** was afford in 29 % yield.

5.5 Replace the photocatalyst for the mechanism study

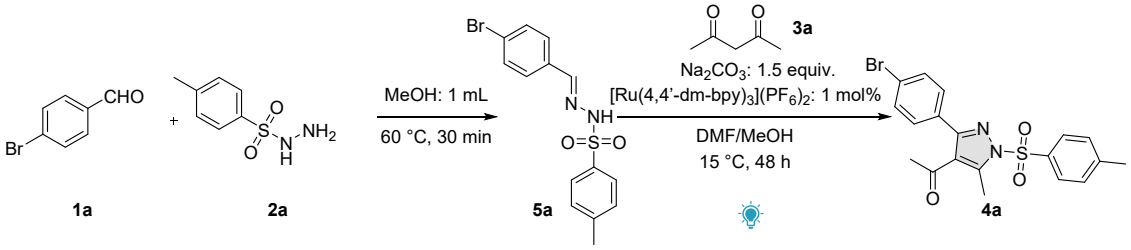


Figure S8: Replace the photocatalyst as $[Ru(4,4'\text{-dm-bpy})_3](PF_6)_2$ for the mechanism study

The first step is to add 4-Bromobenzaldehyde **1a** (0.2 mmol), 4-Methylbenzenesulfonhydrazide **2a** (0.4 mmol) and methanol (1 mL) to the reaction tube with magnetic stirring bar, stirring for 30 minutes at 60 ℃, then add acetylacetone **3a** (0.5 mmol), sodium carbonate (0.3 mmol), $[Ru(4,4'\text{-dm-bpy})_3](PF_6)_2$ (1 mol%), *N, N*-dimethylformamide (1 mL), irradiation with 3W blue LED lamp for 48 hours. The desired products **4a** was afford in 73 % yield.

5.6 Cyclic voltammetry (CV) measurements

Linear scan voltammetry measurements were performed on a photoelectrochemical analysis CHI760E electrical workstation (Shanghai Chenhua) using a three-electrode cell set-up: tetrabutylammonium hexafluorophosphate ([(n-Bu)$_4$N]PF$_6$) (0.1 M) was used as the supporting electrolyte, the working electrode is a glassy carbon, the counter electrode is a Pt wire and the reference electrode is Ag/AgCl.

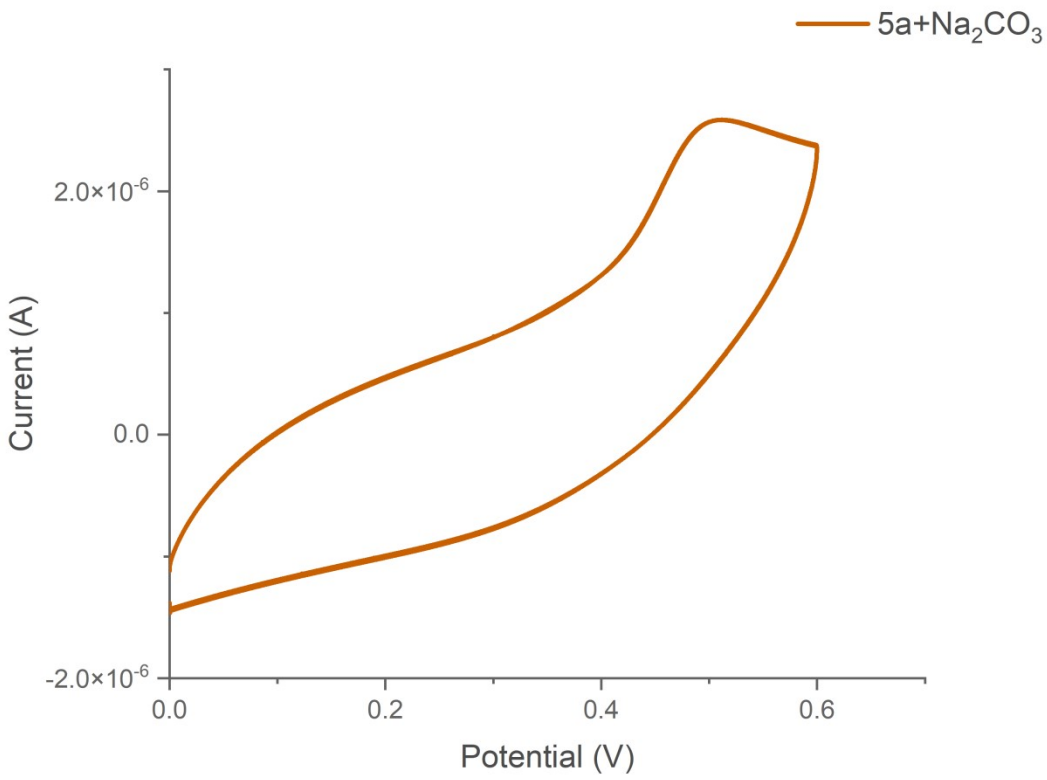


Figure S9: Cyclic voltammetry (CV) measurements

Cyclic voltammetry of [**5a** + Na_2CO_3] (0.1 mM)] in an equal volume of DMF and MeOH. The scan rate was 10 mV/s. It shows an oxidation at $E_{1/2}$ = 0.46 V vs SCE.

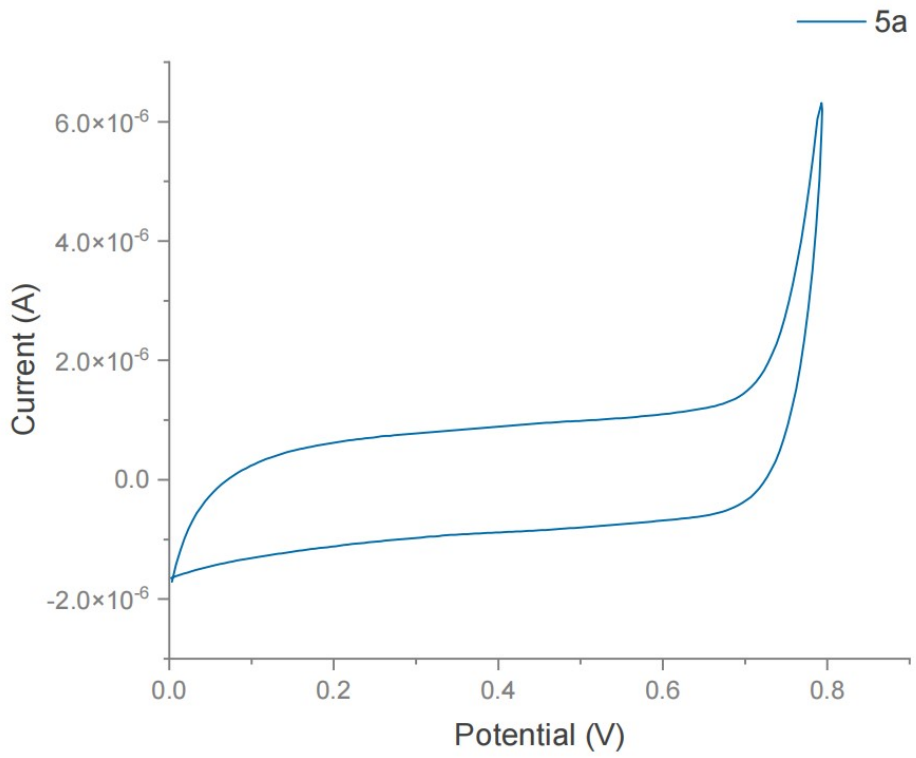


Figure S10: Cyclic voltammetry (CV) measurements

Cyclic voltammetry of **5a** (0.1 mM) in an equal volume of DMF and MeOH. The scan rate was 10 mV/s. It shows an oxidation at $E_{1/2}$ = 0.74 V vs SCE.

5.7 Singlet oxygen trapping experiment

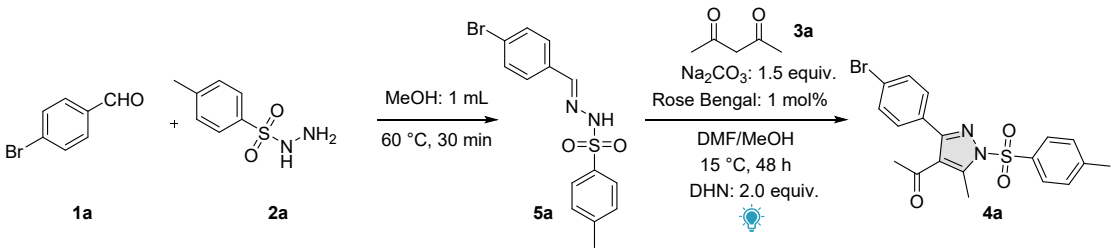


Figure S11: Singlet oxygen trapping with DHN

The first step is to add 4-Bromobenzaldehyde **1a** (0.2 mmol), 4-Methylbenzenesulfonhydrazide **2a** (0.4 mmol) and methanol (1 mL) to the reaction tube with magnetic stirring bar, stirring for 30 minutes at 60 ℃, then add acetylacetone **3a** (0.5 mmol), sodium carbonate (0.3 mmol), Rose Bengal (1 mol%), 1,5-Dihydroxy naphthalene (DHN) (0.4 mmol), *N, N*-dimethylformamide (1 mL), irradiation with 3W blue LED lamp for 48 hours. After confirming the finish of the reaction by TLC, the target point was found to be completely inhibited.

5.8 Replace the acetylacetone for the mechanism study

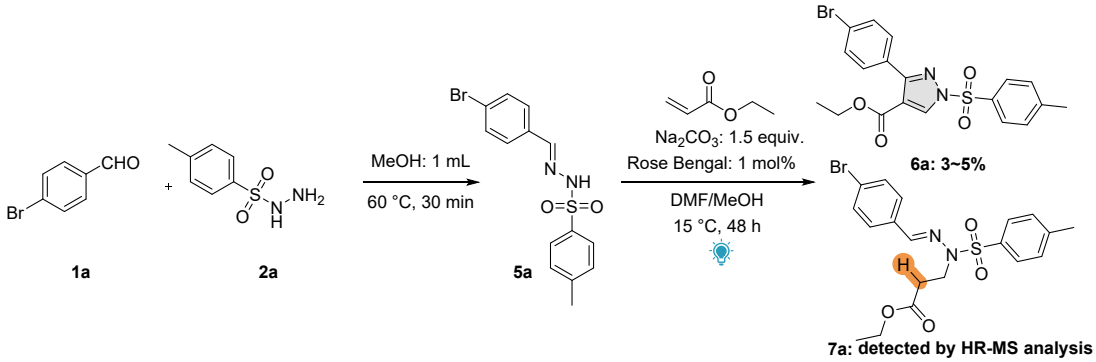


Figure S12: Replace the acetylacetone as ethyl acrylate for the mechanism study

The first step is to add 4-Bromobenzaldehyde **1a** (0.2 mmol), 4-Methylbenzenesulfonhydrazide **2a** (0.4 mmol) and methanol (1 mL) to the reaction tube with magnetic stirring bar, stirring for 30 minutes at 60 ℃, then add ethyl acrylate (0.5 mmol), sodium carbonate (0.3 mmol), Rose Bengal (1 mol%), *N, N*-dimethylformamide (1 mL), irradiation with 3W blue LED lamp for 48 hours.

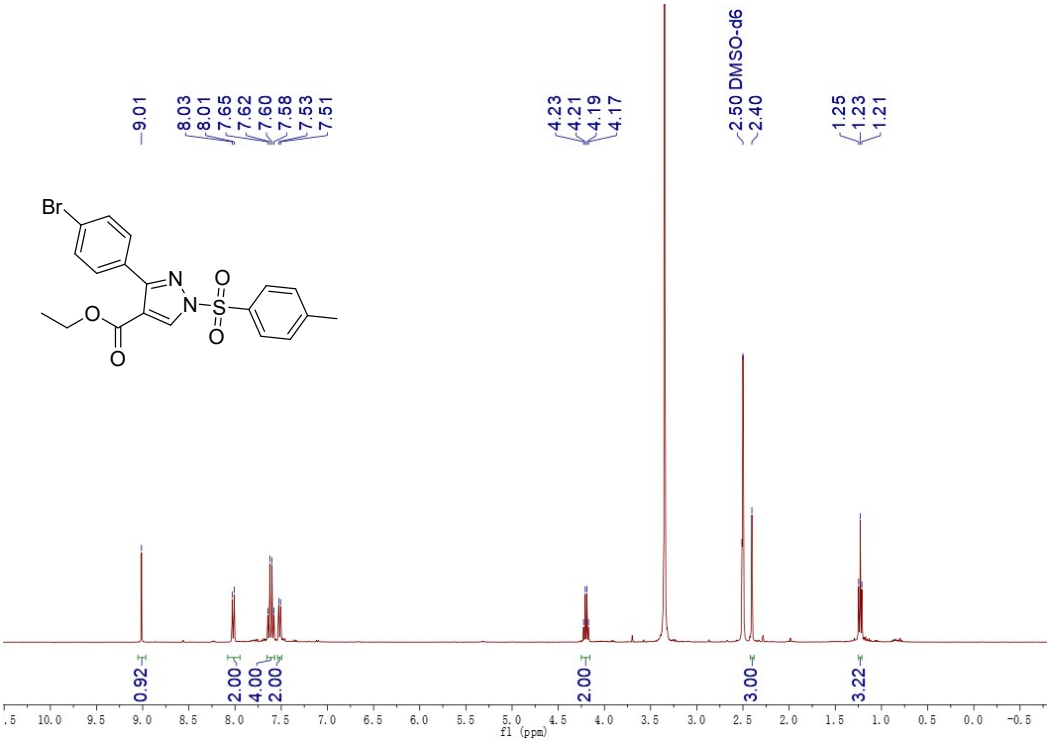
ethyl 3-(4-bromophenyl)-1-tosyl-1H-pyrazole-4-carboxylate (6a)

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.0 (s, 1H), 8.0 (d, J = 8.5 Hz, 2H), 7.6 (q, J = 8.7 Hz, 4H), 7.5 (d, J = 7.8 Hz, 2H), 4.2 (q, J = 7.1 Hz, 2H), 2.4 (s, 3H), 1.2 (t, J = 7.1 Hz, 3H).

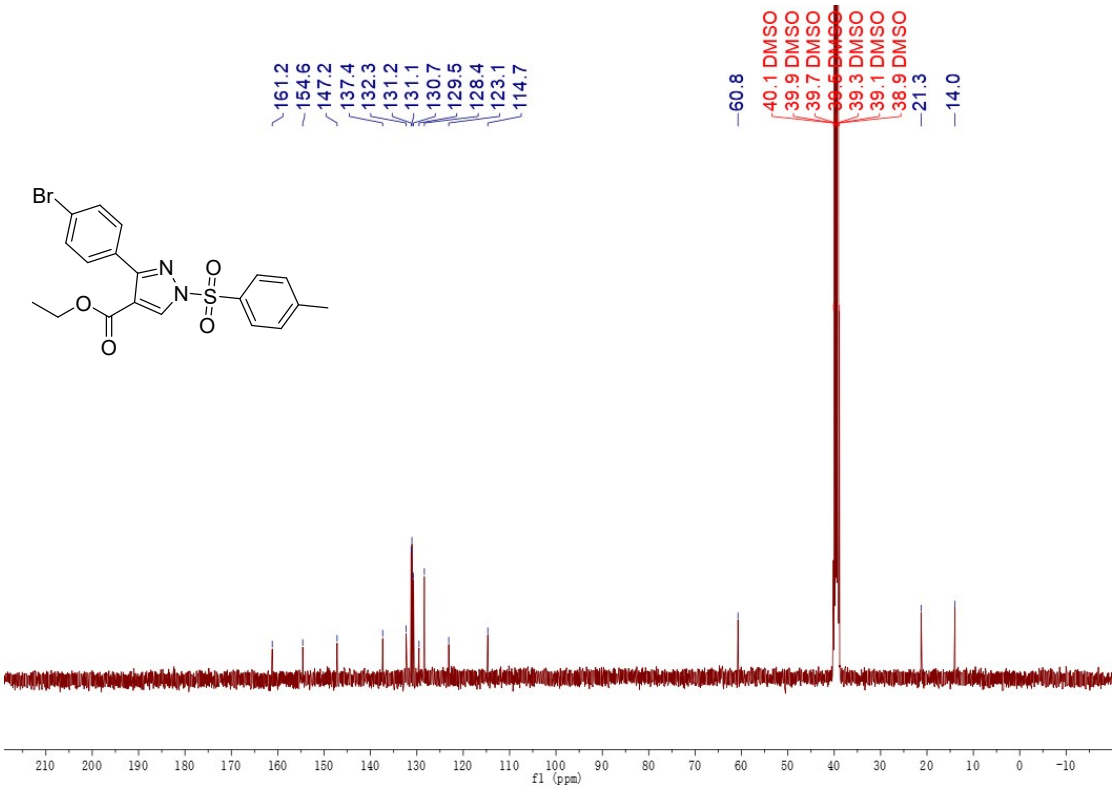
^{13}C NMR (100 MHz, DMSO-d_6) δ 161.2, 154.6, 147.2, 137.4, 132.3, 131.2, 131.1, 130.7, 129.5, 128.4, 123.1, 114.7, 60.8, 21.3, 14.0.

HRMS (ESI-TOF): Anal Calcd. For. $C_{19}H_{17}{}^{79}BrN_2O_4S$ $[M+H]^+$: 449.0166, Found: 449.0159. Anal Calcd. For. $C_{19}H_{17}{}^{81}BrN_2O_4S$ $[M+H]^+$: 451.0145, Found: 451.0117.

IR (neat, cm^{-1}): υ 2975, 1715, 1456, 1312, 1127, 1083, 1003, 835, 671, 667.



^{1}H NMR (400 MHz, DMSO-d_6)



^{13}C NMR (100 MHz, DMSO-d_6)

The detection of 7a in the reaction through HR-MS:

HRMS (ESI-TOF): Anal Calcd. For.$C_{19}H_{21}{}^{79}BrN_2O_4S[M+H]^+$: 453.0479, Found: 453.0482. Anal Calcd. For.$C_{19}H_{21}{}^{81}BrN_2O_4S[M+H]^+$: 455.0458, Found: 455.0426.

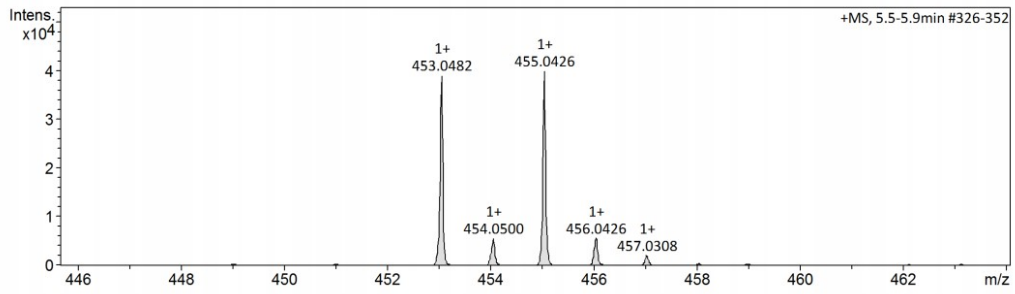


Figure S13: The detection of michael addition products in the reaction through HR-MS

6. X-ray data

Crystallography data for ***4b***

Empirical formula	$C_{21}H_{21}BrN_2O_3S$

Formula weight	461.36
Temperature/K	223
Crystal system	triclinic
Space group	P -1
a/Å	7.8985(5)
b/Å	8.7692(8)
c/Å	16.0272(7)
α/°	81.403(6)
β/°	81.187(5)
γ/°	73.244(7)
Volume/Å^3	1043.89(13)
Z	2
ρ_{calc}g/cm^3	1.468
μ/mm^{-1}	2.093
F(000)	472.0
Crystal size/mm^3	0.40 × 0.30 × 0.20
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.4140 to 29.1690
Index ranges	-11 ≤ h ≤ 11, -12≤ k ≤ 11, -19 ≤ l ≤ 22
Reflections collected	12614
Data/restraints/parameters	5519/0/256
Goodness-of-fit on F^2	1.019
Final R indexes (I>=2σ (I))	R_1 = 0.0523, wR_2 = 0.1134
Final R indexes (all data)	R_1 = 0.0936, wR_2 = 0.1394
Largest diff. peak/hole / e Å^{-3}	0.370/-0.614

7. DFT calculation

7.1 DFT computational details

All DFT calculations were performed with the Gaussian 16 software package.[1] All geometry optimizations of intermediates and transition states were achieved using M06-2X functional and def2-SVP basis set in the gas phase. Frequency calculations were also conducted at the same level of theory to obtain vibration frequencies to determine the identity of stationary points as an intermediate or transition state, and obtaining the zero-point energy (ZPE) and thermal corrections at 298 K. IRC (intrinsic reaction coordinates) analysis was also performed at the same level of theory as geometry optimization to verify the proposed process. The single-point

energies and solvent effects were computed at the same level of theory as geometry optimization with the def2-TZVP basis set. Since the optimal reaction condition is the use of a mixed solvent, two parameters under the mixed solvent are defined by volume ratio: dynamic dielectric constant (eps=35.6) and static dielectric constant (epsinf=1.9). Solvation energies were evaluated by a self-consistent reaction field (SCRF) using the SMD model. All structural figures were generated with CYL view.[2] The searching for minimal energy crossing points (MECPs) was conducted using a modified version of Harvey's code (sobMECP[3]) interfaced with Gaussian 16. The electron density distribution of the triplet structure obtained by Multiwfn software[4], as visualized by the VMD program[5].

7.2 DFT calculation for the intramolecular 1, 3-hydrogen migration of the Int3

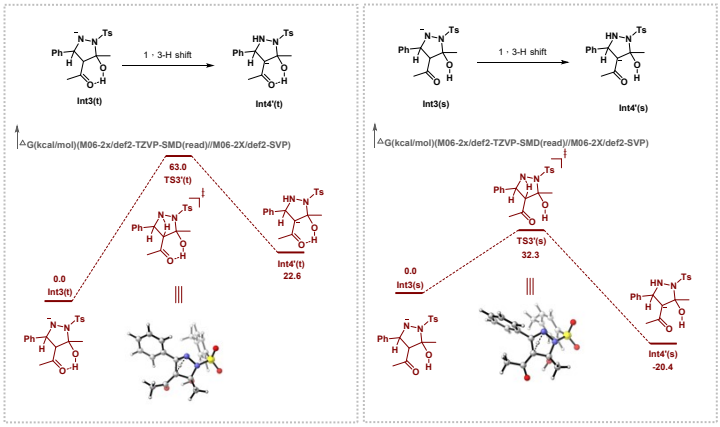


Figure S14: DFT calculations.

Calculated free Gibbs energies [SMD/M06-2x/def2-tzvp] are given in kcal/mol.

7.3 DFT calculation for the triplet excitation energies for the Int1'

1.Geometry optimizations of **Int1'** were achieved using def2-SVP basis set in the gas phase. Frequency calculations were also conducted at the same level of theory to obtain vibrational frequencies to determine the identity of stationary points as an intermediate, and obtaining the zero-point energy (ZPE) and thermal corrections at

298 K. The single-point energies and solvent effects were computed at the same level of theory as geometry optimization with the def2-TZVP basis set. Since the optimal reaction condition is the use of a mixed solvent, two parameters under the mixed solvent are defined by volume ratio: dynamic dielectric constant (eps=35.6) and static dielectric constant (epsinf=1.9). Solvation energies were evaluated by a self-consistent reaction field (SCRF) using the SMD model.

Entry	Functional	Triplet energy (kcal/mol)
1	B3LYP-D3	42.4
2	WB97XD	42.5
3	M06-2X	46.0

Table S8: DFT-computed triplet excitation energies for the **Int1'**

2. Geometry optimizations of **Int1'** were achieved using 6-311g(d,p) basis set in the gas phase. Frequency calculations were also conducted at the same level of theory to obtain vibrational frequencies to determine the identity of stationary points as an intermediate, and obtaining the zero-point energy (ZPE) and thermal corrections at 298 K. The single-point energies and solvent effects were computed at the same level of theory as geometry optimization with the 6-311+g** basis set. Since the optimal reaction condition is the use of a mixed solvent, two parameters under the mixed solvent are defined by volume ratio: dynamic dielectric constant (eps=35.6) and static dielectric constant (epsinf=1.9). Solvation energies were evaluated by a self-consistent reaction field (SCRF) using the SMD model.

Entry	Functional	Triplet energy (kcal/mol)
1	B3LYP-D3	40.9
2	WB97XD	42.5
3	M06-2X	46.1

Table S9: DFT-computed triplet excitation energies for the **Int1'**

7.4 Calculated Minimum Energy Crossing Points

Δ E is computed at the M06-2X/def2-SVP level.

Name	E / Hartree	Δ E/ kcal mol^{-1}
Int3(T)	-1543.67780007	/
MECP	-1543.67711716	0.42(8)

Table S10: Calculated Energies of MECPs.

7.5 The electron density distribution of the triplet structure

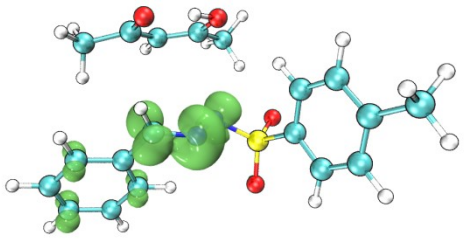


Figure S14: The electron density distribution of the **Int1(T)**. C (cyan); N (blue); O (red); S (yellow); H (white). The isovalue is 0.01 au. (green，positive)

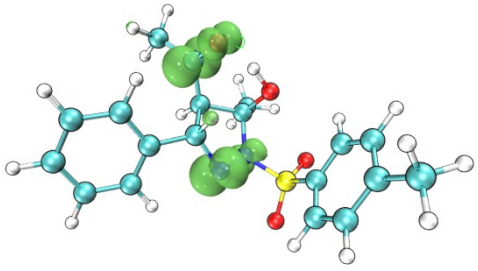


Figure S15: The electron density distribution of the **Int3(T)**. C (cyan); N (blue); O (red); S (yellow); H (white). The isovalue is 0.01 au. (green，positive)

7.6 DFT calculations for SET process

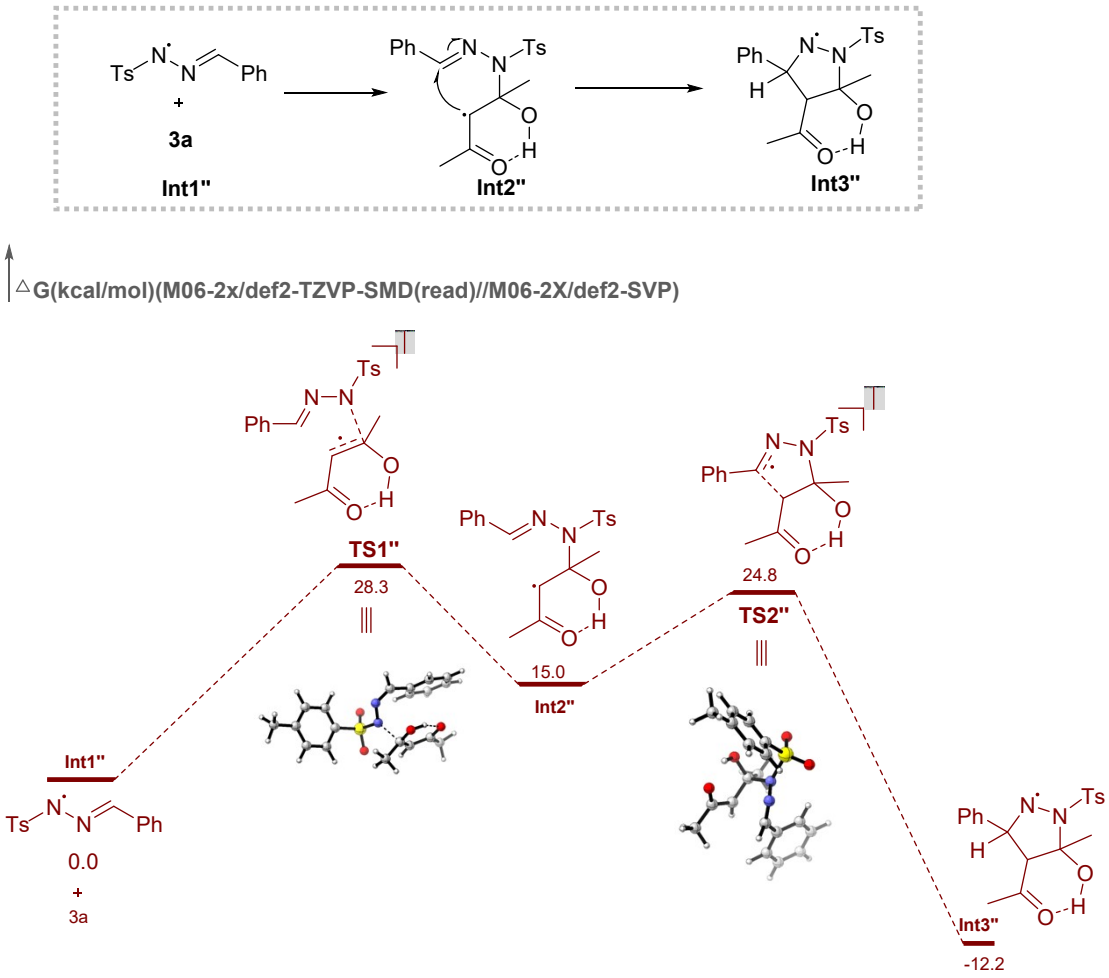


Figure S16: DFT calculations for SET process. The energy barrier increases to 28.3 kcal/mol for the formation of the Int2'', which is clearly unfavorable for this transformation.

7.7 Cartesian Coordinates for the Optimized Structures

Int1'(S)

C	-1.94976400	-1.06602900	-0.85802100
N	-0.84366100	-1.15760200	-0.19515900
N	0.08652800	-1.97294200	-0.66293500
C	-3.02184900	-0.18191500	-0.41689900
C	-2.91307800	0.59152200	0.75798300

C	-4.21129800	-0.07449700	-1.16040000
C	-3.94559700	1.42872700	1.15883800
H	-1.99319700	0.50371600	1.33753500
C	-5.24527700	0.76698100	-0.75475500
H	-4.31586300	-0.66658100	-2.07319700
C	-5.12272700	1.52714700	0.40782700
H	-3.83595100	2.01604900	2.07376600
H	-6.15693400	0.82919000	-1.35401000
H	-5.93161900	2.18671800	0.72766400
S	1.39521500	-1.97163000	0.31931700
O	1.07658400	-2.09169200	1.74451600
O	2.36513500	-2.89518600	-0.26757900
C	2.10773200	-0.32463900	0.14615200
C	3.08315500	-0.09522000	-0.81861900
C	1.64486000	0.71699900	0.94899100
C	3.59504700	1.19125500	-0.98457600
H	3.43184500	-0.93931900	-1.41610700
C	2.15891800	1.99805600	0.76914200
H	0.89569500	0.49522700	1.71028500
C	3.13715000	2.25558900	-0.20053900
H	4.36810300	1.37446800	-1.73579100
H	1.79819000	2.81849400	1.39561300
C	3.66399800	3.65390700	-0.40224400
H	4.59907800	3.64816600	-0.97919000
H	2.93698500	4.27387800	-0.95045800
H	3.85690800	4.15063100	0.55984900
H	-2.09812300	-1.66303800	-1.77114100

Thermal correction to Gibbs Free Energy= 0.199325

Esolv(RM062X) = -1199.52500492

Int1'(T)

C	1.78331500	-1.08203600	-0.94434700
N	0.68571500	-0.39524600	-0.54107900
N	0.36462300	0.79248900	-1.03850100
C	3.07527700	-0.81916900	-0.41171100
C	3.27577800	0.24049600	0.51919600
C	4.21137700	-1.58478800	-0.79008500
C	4.54024300	0.50732600	1.01958000
H	2.40740400	0.82892300	0.82417700
C	5.46939900	-1.30186300	-0.27993300
H	4.07955800	-2.40458800	-1.50160600
C	5.65259000	-0.25299900	0.63021300
H	4.66776100	1.32609300	1.73208100
H	6.32555600	-1.90564100	-0.59255500
H	6.64407300	-0.03278100	1.03001200
S	-0.68443000	1.56571200	-0.02899000
O	-0.16818700	1.66440400	1.34053500
O	-1.12030900	2.78361200	-0.70838600
C	-2.12814800	0.49937000	0.08593800
C	-3.24755900	0.78107000	-0.68779700
C	-2.09862200	-0.61821600	0.92141800
C	-4.35484000	-0.06601700	-0.62450300
H	-3.23206900	1.66920700	-1.32167700
C	-3.20627500	-1.45838100	0.96793600
H	-1.20450900	-0.80504500	1.51677100
C	-4.34861600	-1.19624700	0.19796300
H	-5.24165000	0.15501600	-1.22427900
H	-3.19016700	-2.33794900	1.61736000
C	-5.53521900	-2.12450700	0.25919800
H	-6.37844000	-1.73212800	-0.32533900

H	-5.28046600	-3.11833100	-0.14035400
H	-5.87540900	-2.26747900	1.29586900
H	1.65263900	-1.93575100	-1.62515100

Thermal correction to Gibbs Free Energy= 0.195024

Esolv(UM062X) = -1199.44739377

TS1(S)

C	-1.15292900	0.72407700	-0.65735100
N	-0.20523100	-0.02596400	-0.23885600
N	-0.25467500	-1.35394300	-0.46661500
C	-1.13837300	2.16701600	-0.37925500
C	-0.00451400	2.83163500	0.11385300
C	-2.31481200	2.89791900	-0.60157900
C	-0.05011000	4.19778600	0.37037200
H	0.90312100	2.24862100	0.28400000
C	-2.35655100	4.26641400	-0.33788600
H	-3.19670600	2.35912100	-0.96135300
C	-1.22466000	4.92274700	0.14539200
H	0.83860200	4.70763000	0.74921200
H	-3.28016000	4.82362000	-0.50832400
H	-1.25552000	5.99505400	0.34887900
S	0.98231100	-2.06964500	0.42243600
O	0.69226100	-2.10283400	1.85644700
O	1.35985700	-3.31550100	-0.23753900
C	2.35564000	-0.93899700	0.20333300
C	3.13698200	-1.05189100	-0.93882700
C	2.64210600	0.00312400	1.18681100
C	4.21814800	-0.18695600	-1.10690900
H	2.89064200	-1.81652100	-1.67701000
C	3.72480800	0.85725200	1.00663300

H	2.00503900	0.04914900	2.07104400
C	4.52329900	0.77940500	-0.14367100
H	4.83864900	-0.26526200	-2.00276300
H	3.95737900	1.60393100	1.77031700
C	5.67322800	1.73436900	-0.33622800
H	6.32435100	1.41361000	-1.16033600
H	5.30586300	2.74525800	-0.57174900
H	6.28326700	1.81133600	0.57544300
H	-2.01503700	0.35057000	-1.21422200
C	-2.63297900	-1.48509800	0.64990100
C	-1.54805700	-3.60165000	-0.21632700
H	-1.08459800	-3.76957300	0.76404600
H	-2.50027500	-4.14923100	-0.26244000
H	-0.87738600	-3.95755100	-1.00597700
C	-4.42751600	0.04318900	1.50439600
H	-5.50816300	-0.10891900	1.36434700
H	-4.12129300	-0.32939000	2.49046400
H	-4.24163100	1.12800700	1.45587400
C	-3.68052100	-0.62734400	0.36996400
C	-1.90211200	-2.14530600	-0.43342900
O	-4.06900700	-0.32852100	-0.81689800
O	-2.40013900	-1.93665400	-1.65985600
H	-3.15783500	-1.24154500	-1.53605800
H	-2.31618200	-1.68231700	1.67352500

Thermal correction to Gibbs Free Energy= 0.314614

Esolv(RM062X) = -1545.29636684

TS1(T)

C	1.69488200	0.26144700	-1.20345800
N	0.59313900	-0.38096500	-0.69734800

N	0.31268700	-0.34365800	0.58862600
C	2.99961100	-0.27466000	-1.05377600
C	3.22589200	-1.47992400	-0.32920600
C	4.13234100	0.39285500	-1.59548500
C	4.51270400	-1.96820700	-0.16184400
H	2.36384100	-2.01344800	0.07625400
C	5.41081700	-0.11003600	-1.41569400
H	3.97857200	1.32142700	-2.15120500
C	5.61909000	-1.29486600	-0.69663000
H	4.66116200	-2.89657200	0.39463600
H	6.26416900	0.42583800	-1.83846600
H	6.62778100	-1.68658000	-0.55590300
S	-0.81181800	-1.55766900	0.96715000
O	-0.35580000	-2.80874900	0.37511400
O	-1.07514400	-1.49772000	2.39569700
C	-2.29253600	-1.07710500	0.10113600
C	-3.20717900	-0.23771100	0.73275900
C	-2.49245100	-1.53204500	-1.19765700
C	-4.34844100	0.14685000	0.03695500
H	-2.99228700	0.10998800	1.74377900
C	-3.64075900	-1.13269700	-1.87876700
H	-1.74870500	-2.18911100	-1.64948800
C	-4.57881300	-0.28894300	-1.27481900
H	-5.07386800	0.80792800	0.51702900
H	-3.81090700	-1.48048500	-2.90040100
C	-5.80006700	0.17490700	-2.02576800
H	-6.69194000	0.16058700	-1.38311500
H	-5.66639200	1.20895300	-2.37982600
H	-5.99460600	-0.45737900	-2.90258800
H	1.53126100	1.13823300	-1.83637900

C	1.06859000	2.12548000	0.78593900
C	1.12376700	0.61469800	2.79917500
H	2.12927000	0.28466100	2.50379900
H	1.20930500	1.45038300	3.50911200
H	0.57982000	-0.21191100	3.26857300
C	1.05015600	4.06878100	-0.79943400
H	0.71706800	5.07914100	-0.51858300
H	2.14285400	3.99920900	-0.71295700
H	0.75675500	3.91553900	-1.84996800
C	0.32813500	3.04620500	0.05771400
C	0.37149000	1.11953500	1.58565900
O	-0.94352800	3.09440400	0.05001400
O	-0.92283900	1.39576000	1.83663800
H	-1.17655500	2.09958400	1.11977400
H	2.15682700	2.13214900	0.77209300

Thermal correction to Gibbs Free Energy= 0.310879

Esolv(UM062X) = -1545.22080584

Int2(S)

C	-0.90566700	1.12494000	-0.53655400
N	-0.26491400	0.03859200	-0.33044900
N	-0.81196500	-1.17758400	-0.48848600
C	-0.19891600	2.40381600	-0.34217800
C	1.18199500	2.47056400	-0.09623600
C	-0.93759900	3.59319900	-0.39805500
C	1.80199000	3.70107300	0.09070000
H	1.74792800	1.53695600	-0.05746700
C	-0.31232800	4.82525200	-0.20871800
H	-2.01337100	3.52695100	-0.58205200
C	1.05931200	4.88482800	0.03546800

H	2.87710000	3.74167600	0.28079300
H	-0.90045500	5.74434600	-0.25084400
H	1.55044700	5.84890300	0.18222200
S	0.16295400	-2.34520700	0.26701100
O	-0.17916300	-2.49837500	1.67837700
O	0.20596600	-3.53640600	-0.56965900
C	1.78141800	-1.58868200	0.18848900
C	2.49186900	-1.64210600	-1.00544200
C	2.31774800	-1.00612500	1.32938700
C	3.75679800	-1.06419500	-1.05977500
H	2.04261700	-2.12634900	-1.87370800
C	3.58818600	-0.43877500	1.26049000
H	1.72582700	-0.99503900	2.24535200
C	4.31901200	-0.44900000	0.06664000
H	4.32226200	-1.09013900	-1.99427100
H	4.01862400	0.02912100	2.14900200
C	5.66851400	0.21624400	-0.01675200
H	6.33060000	-0.30970300	-0.71843200
H	5.56724500	1.25380000	-0.37234200
H	6.15912500	0.24845600	0.96551000
H	-1.95301000	1.18684300	-0.84628700
C	-2.99562400	-0.70353500	0.66598200
C	-2.64639300	-2.87826700	-0.55038100
H	-2.32067200	-3.37415600	0.37423500
H	-3.73432900	-2.98435500	-0.64731000
H	-2.14987400	-3.34190700	-1.41172100
C	-4.43167300	1.02157200	1.76687400
H	-5.52058400	1.08130500	1.61539800
H	-4.21621000	0.45782200	2.68447200
H	-4.06760000	2.05509400	1.87946500

C	-3.79406000	0.40631900	0.53512300
C	-2.38667000	-1.37262500	-0.52859500
O	-4.04003000	1.00484000	-0.58127900
O	-2.79979800	-0.82645600	-1.71723300
H	-3.37788700	-0.01669200	-1.46237900
H	-2.80016500	-1.15248300	1.64027700

Thermal correction to Gibbs Free Energy= 0.317619

Esolv(RM062X) = -1545.30068586

Int2(T)

C	1.64827500	0.25961200	-1.17462300
N	0.55385700	-0.41579400	-0.67971700
N	0.27099300	-0.37791700	0.61028600
C	2.95521000	-0.28021900	-1.06347000
C	3.19680400	-1.49677000	-0.36390200
C	4.07667800	0.39807000	-1.61469600
C	4.48660800	-1.98822600	-0.23147800
H	2.34352700	-2.03780500	0.05019600
C	5.35843700	-0.10771600	-1.46970700
H	3.91166900	1.33684800	-2.14948900
C	5.58175200	-1.30541400	-0.77684700
H	4.64626100	-2.92614900	0.30560800
H	6.20300200	0.43643200	-1.89950200
H	6.59314100	-1.69901800	-0.66364600
S	-0.90743800	-1.56248800	0.96149900
O	-0.47361300	-2.80942800	0.35009600
O	-1.19199200	-1.52415800	2.38499900
C	-2.35159000	-1.01233700	0.07885300
C	-3.24484800	-0.14950800	0.70942400
C	-2.54816500	-1.44622200	-1.22739100

C	-4.36273900	0.28100800	0.00304700
H	-3.02950400	0.18090900	1.72597000
C	-3.67299300	-1.00027400	-1.91862400
H	-1.82009900	-2.12187200	-1.67726700
C	-4.58982900	-0.13207200	-1.31676800
H	-5.07150900	0.96138100	0.48093500
H	-3.84065100	-1.32993500	-2.94657000
C	-5.78425700	0.38183700	-2.07802100
H	-6.68486800	0.38931500	-1.44760400
H	-5.61093800	1.41522200	-2.41636800
H	-5.98739100	-0.23230000	-2.96566000
H	1.46425200	1.13137600	-1.80756600
C	1.19278400	1.96373200	0.84970600
C	1.09143300	0.43467600	2.82739900
H	2.08611800	0.04495800	2.56750000
H	1.20415400	1.28405600	3.51529500
H	0.49594300	-0.34895300	3.30732000
C	1.37622400	4.00823000	-0.58287600
H	1.08021400	5.01624200	-0.25537800
H	2.45624200	3.87077500	-0.43680300
H	1.14268900	3.94093500	-1.65763200
C	0.54572000	2.97558500	0.15824800
C	0.39761700	0.94744300	1.57453300
O	-0.71869500	3.09950800	0.07886100
O	-0.88682600	1.34040600	1.82694800
H	-1.06563600	2.07564200	1.13165000
H	2.27873400	1.92847200	0.91695500

Thermal correction to Gibbs Free Energy= 0.310101

Esolv(UM062X) = -1545.22187145

TS2(S)

C	-1.28023900	0.34611500	-0.23805000
N	-0.24950200	0.18319500	0.60155700
N	0.29154300	-1.03534100	0.14876900
C	-2.23997500	1.44346000	0.06501800
C	-2.28407500	2.02051800	1.34012100
C	-3.13402400	1.89170600	-0.91467700
C	-3.20013500	3.03106900	1.62362300
H	-1.57718800	1.64720700	2.08317700
C	-4.05727300	2.89668400	-0.62782400
H	-3.09903600	1.43107000	-1.90632700
C	-4.09214100	3.47179500	0.64299800
H	-3.22302800	3.47928300	2.61958400
H	-4.75147200	3.23460500	-1.40026700
H	-4.81261300	4.26065500	0.86920600
S	1.72354600	-1.37153100	0.91360500
O	1.68282300	-1.15578700	2.35644900
O	2.21900500	-2.65210600	0.41562700
C	2.76977400	-0.09038600	0.23672200
C	3.70744800	-0.43674300	-0.72624200
C	2.65831000	1.21865300	0.70597400
C	4.55164600	0.55084100	-1.23711300
H	3.76026600	-1.47442800	-1.05862700
C	3.50314000	2.19015900	0.18184500
H	1.89671700	1.44619200	1.45176300
C	4.45983800	1.87240700	-0.79398200
H	5.29389400	0.28875100	-1.99503600
H	3.42085500	3.22192900	0.53331500
C	5.35547000	2.94751300	-1.35449900
H	6.11117800	2.52493700	-2.03020900

H	4.77144500	3.68920100	-1.92073000
H	5.87772200	3.48772400	-0.55081400
H	-1.12406200	0.19759900	-1.33123400
C	-2.10051100	-1.34085600	-0.02380600
C	-0.76966700	-3.04489500	1.26802800
H	-0.80752900	-2.42781000	2.17649500
H	-1.62753900	-3.73116300	1.24193500
H	0.15830200	-3.63110000	1.26633600
C	-4.46360100	-1.26969900	-0.93313700
H	-4.90546500	-2.20209300	-0.54673100
H	-4.64986600	-0.47564300	-0.19582400
H	-4.94280000	-1.01940400	-1.88852400
C	-2.97491800	-1.47378600	-1.15841200
C	-0.80219000	-2.14410000	0.03706700
O	-2.54971800	-1.62729900	-2.31121800
O	-0.56268100	-2.91570800	-1.08118600
H	-0.99687100	-2.46768200	-1.83125500
H	-2.60063300	-1.24584000	0.94450500

Thermal correction to Gibbs Free Energy= 0.317443

Esolv(RM062X) = -1545.28039237

TS2(T)

C	-1.38377900	-0.59340500	0.30050500
N	-0.43140700	-0.60894400	-0.72933700
N	0.04154700	0.58200600	-1.09552100
C	-2.68140300	-1.13566800	0.07175100
C	-3.18041900	-1.36207100	-1.24067100
C	-3.56521100	-1.39020900	1.15599100
C	-4.47496500	-1.81527500	-1.44231800
H	-2.51346600	-1.18071800	-2.08589500

C	-4.85934500	-1.83763400	0.93697200
H	-3.20629400	-1.22448600	2.17502500
C	-5.33563700	-2.05846400	-0.36230200
H	-4.82717800	-1.98578300	-2.46310000
H	-5.51373500	-2.02204000	1.79303500
H	-6.35396100	-2.41288100	-0.52957400
S	1.55221000	0.38028800	-1.86472000
O	1.38032300	-0.59846600	-2.92119400
O	2.08929100	1.69408400	-2.17389900
C	2.57051100	-0.36183300	-0.60670400
C	3.28634900	0.46021200	0.26013000
C	2.61703100	-1.74816900	-0.51024400
C	4.07491200	-0.13433900	1.23950700
H	3.18770200	1.54185000	0.16582600
C	3.40867700	-2.32373700	0.48194400
H	2.03357600	-2.34839800	-1.20896600
C	4.14442800	-1.52849100	1.36674400
H	4.64240400	0.49550700	1.92868500
H	3.45360800	-3.41138800	0.57280900
C	4.97258900	-2.15044100	2.46118000
H	5.94251400	-1.64306600	2.56303100
H	4.45617500	-2.07033200	3.43036600
H	5.15711200	-3.21545900	2.26671000
H	-0.95979100	-0.67237700	1.31151900
C	-1.55361800	1.62325800	0.44686900
C	-0.44710800	3.00125200	-1.31474900
H	-1.23394200	2.74151800	-2.03705200
H	-0.74989200	3.90015500	-0.76036100
H	0.49226900	3.19551800	-1.84235300
C	-2.97130100	1.96916000	2.49986800

H	-3.05027800	2.96114400	2.97323000
H	-3.80499200	1.82490300	1.80047900
H	-3.04219700	1.22481200	3.30802600
C	-1.61709400	1.83843000	1.83315500
C	-0.26698900	1.87509500	-0.29695900
O	-0.59580900	1.85281100	2.58573300
O	0.79824500	2.14145700	0.53659100
H	0.45163900	2.00213300	1.48410100
H	-2.46977700	1.71824200	-0.13787600

Thermal correction to Gibbs Free Energy= 0.311961

Esolv(UM062X) = -1545.2175627

Int3(S)

C	-1.35558600	0.31098600	-0.27342600
N	-0.27965100	0.25622400	0.60897600
N	0.30286900	-0.97399400	0.16866000
C	-2.34608200	1.39790800	0.04528300
C	-2.36931100	1.97408300	1.32033400
C	-3.27615200	1.82696900	-0.90856100
C	-3.30856400	2.95602700	1.63256100
H	-1.62374500	1.61872400	2.03404200
C	-4.22245500	2.80304000	-0.59413300
H	-3.24667100	1.38559900	-1.90965600
C	-4.24132400	3.37154900	0.68000100
H	-3.31435600	3.40415000	2.62898300
H	-4.94322200	3.12643200	-1.34851800
H	-4.97748900	4.13928500	0.92797500
S	1.71367000	-1.29691100	0.96728700
O	1.65555300	-1.03176100	2.40083600
O	2.19942400	-2.60614100	0.53191700

C	2.78654600	-0.05959900	0.25253200
C	3.85164900	-0.48457600	-0.53049400
C	2.57810700	1.29475600	0.52365500
C	4.72695200	0.46396400	-1.06238900
H	3.97490700	-1.55293000	-0.71347500
C	3.45556000	2.22471000	-0.02362200
H	1.71073000	1.58051300	1.11860200
C	4.53996600	1.82680400	-0.81939300
H	5.56802800	0.13809900	-1.67946800
H	3.29777300	3.28921600	0.16915900
C	5.46883400	2.85897800	-1.40639600
H	6.32186300	2.38660200	-1.91216100
H	4.94398200	3.48693800	-2.14277700
H	5.86087000	3.52918800	-0.62685800
H	-1.10565100	0.35171100	-1.36824300
C	-2.02541100	-1.16835900	-0.12485000
C	-0.85739800	-2.87128600	1.35322500
H	-0.91006700	-2.18122400	2.20671500
H	-1.75166000	-3.51110200	1.32522100
H	0.03645100	-3.50216600	1.44613800
C	-4.37202000	-1.55603100	-1.07470800
H	-4.60960700	-2.38178800	-0.38654900
H	-4.71146700	-0.62310600	-0.59805200
H	-4.88534700	-1.70353800	-2.03266800
C	-2.87532600	-1.49564500	-1.29786400
C	-0.75735300	-2.05161000	0.07417100
O	-2.40686100	-1.61465600	-2.41778500
O	-0.49585000	-2.91961700	-0.97287400
H	-0.62666500	-2.42144800	-1.79333600
H	-2.61182000	-1.14278500	0.80256500

Thermal correction to Gibbs Free Energy= 0.317999

Esolv(RM062X) = -1545.28595404

Int3(T)

C	-1.35404300	-0.23742300	0.01365800
N	-0.36031500	-0.26406100	-1.04192500
N	0.20047300	0.95610500	-1.04032300
C	-2.55724900	-1.08394500	-0.25210900
C	-2.88112000	-1.54351700	-1.53179200
C	-3.42188700	-1.36581100	0.81643600
C	-4.05425400	-2.26841800	-1.74353700
H	-2.19412900	-1.32710800	-2.35166100
C	-4.59667800	-2.08277700	0.59978800
H	-3.14860500	-1.01296900	1.81476500
C	-4.91831900	-2.53655100	-0.68097000
H	-4.29612600	-2.62609500	-2.74687000
H	-5.26504300	-2.29303500	1.43759200
H	-5.83774300	-3.10125400	-0.84896100
S	1.79401700	0.95356800	-1.60131600
O	1.80214000	0.33641500	-2.91454900
O	2.31079800	2.29837700	-1.41690100
C	2.65332300	-0.14660400	-0.49467200
C	3.10188900	0.33379600	0.73437700
C	2.83967900	-1.46981000	-0.87658800
C	3.76580200	-0.54210900	1.58563900
H	2.88919900	1.36602000	1.01335100
C	3.50460800	-2.33265300	-0.00649700
H	2.46346700	-1.80045000	-1.84505200
C	3.97482100	-1.88244500	1.23078400
H	4.12022700	-0.18310400	2.55478900

H	3.65724500	-3.37585000	-0.29241000
C	4.66862300	-2.81863600	2.18605200
H	5.59652300	-2.37369300	2.57380300
H	4.02395100	-3.03810200	3.05097700
H	4.91866300	-3.77169500	1.70121000
H	-0.86283500	-0.58382700	0.94619100
C	-1.68585200	1.26245500	0.28859800
C	-0.32407200	3.32164700	-0.40710600
H	-0.79689400	3.40282100	-1.39626500
H	-0.92278700	3.87631200	0.33094500
H	0.68907400	3.73645800	-0.44653500
C	-3.59236900	1.93322000	1.97495200
H	-3.62451900	2.76109900	2.70829600
H	-4.12399700	2.25529300	1.06624700
H	-4.18477100	1.10989500	2.43122100
C	-2.17893700	1.53412200	1.67565000
C	-0.27573500	1.87928100	0.06515300
O	-1.38587900	1.14777500	2.64170700
O	0.50344400	1.73010300	1.18488200
H	-0.16461900	1.42929500	1.95774900
H	-2.37505100	1.62429200	-0.49059800

Thermal correction to Gibbs Free Energy= 0.315034

Esolv(UM062X) = -1545.24798104

Int3(S)-1

C	0.25785500	0.54117000	-0.04716100
N	0.17593200	-0.36007100	-1.14981100
N	-0.21730000	-1.57176500	-0.50468000
C	0.98072400	1.81867200	-0.38258700
C	2.19849300	1.78676600	-1.07789600

C	0.47464300	3.05536400	0.03127100
C	2.88903500	2.96909400	-1.33704600
H	2.60300600	0.82499900	-1.40155300
C	1.16577200	4.24055700	-0.23087300
H	-0.47751700	3.07603800	0.56839300
C	2.37856900	4.20062100	-0.91664000
H	3.84230100	2.92225400	-1.86799700
H	0.75374300	5.19694800	0.10193800
H	2.92679800	5.12400700	-1.12115200
S	-1.70521200	-2.12281100	-0.96891500
O	-1.70616400	-2.29040300	-2.41617100
O	-2.08787000	-3.26959300	-0.14251800
C	-2.81885900	-0.76565600	-0.64893600
C	-3.61349000	-0.76288000	0.49609300
C	-2.74195100	0.35104000	-1.48272000
C	-4.35198900	0.37320700	0.80645200
H	-3.60278200	-1.64847800	1.13316200
C	-3.45951300	1.49738600	-1.13140800
H	-2.09855000	0.30735100	-2.36019700
C	-4.26792900	1.52532300	0.00796800
H	-4.98537000	0.38453300	1.69838800
H	-3.38453400	2.39196600	-1.75577600
C	-5.02113400	2.77311800	0.39715600
H	-6.06860300	2.54702500	0.65066400
H	-4.56648500	3.24873300	1.28082300
H	-5.01662600	3.51074800	-0.41758700
H	-0.71819200	0.82061900	0.43937500
C	1.00418700	-0.33761200	1.02970600
C	0.85273200	-2.88196600	1.30090200
H	1.80035600	-2.92482200	0.74645800

H	1.07411400	-2.90327300	2.37944300
H	0.19753300	-3.72678000	1.04777500
C	2.57183400	0.81615500	2.63322200
H	3.30024900	0.03303400	2.36409300
H	2.76765100	1.65013300	1.93642600
H	2.66154800	1.16720600	3.66953900
C	1.17629600	0.32412200	2.35509500
C	0.12220400	-1.59334500	0.96466800
O	0.24869700	0.53130400	3.12791500
O	-1.02079900	-1.46494100	1.77774500
H	-0.90431400	-0.66209500	2.31502600
H	1.99761500	-0.58522000	0.63017100
C	4.41604400	-1.32954800	-0.56109900
O	3.84459000	-1.37689400	0.55670100
O	3.55481300	-1.23288000	-1.66850200
O	5.61124800	-1.35138800	-0.83924900
H	2.63378400	-1.23825300	-1.35770200

Thermal correction to Gibbs Free Energy= 0.339776

Esolv(RM062X) = -1809.88125971

TS3(S)

C	0.45969300	0.50183300	0.08335400
N	0.36894800	-0.38900000	-1.05911400
N	-0.13807500	-1.57998100	-0.44836000
C	1.17236800	1.78740000	-0.25352000
C	2.33413300	1.80943400	-1.03895200
C	0.66354600	3.00919200	0.20588900
C	2.97919300	3.01468500	-1.31259000
H	2.71316400	0.87252600	-1.44461600
C	1.30894900	4.21651400	-0.06450200

H	-0.26154100	3.00012500	0.78955600
C	2.47925700	4.22301000	-0.82216700
H	3.88704600	3.00545100	-1.92023800
H	0.89262000	5.15423300	0.31339200
H	2.99305500	5.16341600	-1.03832900
S	-1.62560700	-2.02008300	-0.99889100
O	-1.57878000	-2.12226300	-2.45092900
O	-2.11516500	-3.17110000	-0.24110100
C	-2.68333400	-0.61608300	-0.66559100
C	-3.51309900	-0.61469600	0.45230800
C	-2.55720400	0.51110700	-1.47755700
C	-4.23987900	0.53279400	0.75457100
H	-3.53870700	-1.50907800	1.07623300
C	-3.26911900	1.66306700	-1.14032700
H	-1.87713900	0.46761400	-2.32787300
C	-4.11607100	1.69022700	-0.02753000
H	-4.89997800	0.54426000	1.62693900
H	-3.15902800	2.56298100	-1.75173500
C	-4.85356600	2.95050100	0.35215400
H	-5.85656300	2.72545200	0.74510300
H	-4.31081500	3.50408800	1.13547300
H	-4.96421000	3.62314500	-0.51037600
H	-0.55147700	0.79782500	0.46156400
C	1.06899100	-0.42777700	1.17156000
C	0.87404000	-2.98391600	1.30919400
H	1.77777500	-3.07408200	0.69234600
H	1.15681900	-3.00341900	2.37244000
H	0.17458000	-3.80283200	1.08845300
C	2.13693900	1.24292500	2.74618500
H	2.93689800	1.29870500	1.99483600

H	1.51048100	2.14189600	2.63667900
H	2.55063200	1.21770000	3.76358100
C	1.29428200	-0.00679100	2.53591400
C	0.18283500	-1.66300800	1.00407600
O	0.90936900	-0.63139400	3.53584600
O	-1.00009600	-1.54390300	1.78337500
H	-0.64829800	-1.32063600	2.66302900
H	2.29305400	-0.70694500	0.68126800
C	3.69985700	-1.38183700	-0.95395000
O	3.46397800	-0.93980900	0.24853100
O	2.69480100	-1.31604200	-1.83724400
O	4.78435600	-1.82484900	-1.30992800
H	1.77665700	-0.91483100	-1.49268300

Thermal correction to Gibbs Free Energy= 0.337022

Esolv(RM062X) = -1809.86435791

Int4(S)

C	0.41881000	0.62039500	-0.04883500
N	0.37303600	-0.35104300	-1.16310900
N	-0.16898400	-1.51609600	-0.57483400
C	1.26082400	1.82995000	-0.38243400
C	2.56873600	1.70813800	-0.87010100
C	0.73222500	3.11149000	-0.18955500
C	3.32476200	2.85007600	-1.13426000
H	2.97899000	0.70901100	-1.05745400
C	1.49198400	4.25310200	-0.44531500
H	-0.29235100	3.20596900	0.18081700
C	2.79766900	4.12477700	-0.91759600
H	4.34310600	2.73441100	-1.51157400
H	1.06248700	5.24383500	-0.27522700

H	3.40084100	5.01383100	-1.11923100
S	-1.63872500	-1.94536400	-1.17501400
O	-1.58275300	-1.88161800	-2.62794300
O	-2.06954500	-3.17579000	-0.53227500
C	-2.77306200	-0.64095100	-0.69500000
C	-3.46347900	-0.72877100	0.51205700
C	-2.89157600	0.47586600	-1.51668600
C	-4.28820800	0.32567000	0.89151400
H	-3.30555800	-1.60917800	1.13544900
C	-3.71460100	1.52816700	-1.11537500
H	-2.32352400	0.50314600	-2.44752400
C	-4.41966000	1.46870100	0.09081700
H	-4.83225900	0.27116700	1.83850700
H	-3.80559700	2.41523100	-1.74780500
C	-5.27769700	2.62241600	0.54597400
H	-6.23016600	2.27000800	0.96920700
H	-4.76674400	3.20489100	1.32896000
H	-5.50134700	3.30554900	-0.28540100
H	-0.62042800	0.99764700	0.06266300
C	0.77283000	-0.23413400	1.15433600
C	1.16157200	-2.77121900	1.06607000
H	1.98322600	-2.67949300	0.34387300
H	1.55131800	-2.72864800	2.09338700
H	0.61687800	-3.71443400	0.90532600
C	1.26596900	1.54997900	2.88371700
H	1.88530100	2.05094500	2.12901400
H	0.36961000	2.16685200	3.07290100
H	1.82004700	1.47631600	3.83076500
C	0.84919000	0.13669300	2.48988200
C	0.18643100	-1.61649300	0.88274400

O	0.55639600	-0.65027400	3.44815200
O	-0.96667000	-1.82830200	1.66657700
H	-0.63175400	-1.50966900	2.54751400
H	3.06326200	-0.73285600	0.82099200
C	4.19313100	-1.40480000	-0.58852400
O	3.99790600	-0.98822400	0.72570700
O	3.18285200	-1.29488200	-1.33854200
O	5.32027900	-1.81055100	-0.85721800
H	1.34308000	-0.61590800	-1.40556900

Thermal correction to Gibbs Free Energy= 0.342478

Esolv(RM062X) = -1809.90475883

Int4(S)-1

C	-1.70299000	-0.19660600	-0.50206800
N	-2.28084800	1.13399700	-0.14711400
N	-1.56322600	1.70708700	0.91137100
C	-2.81658800	-1.22931200	-0.59416600
C	-3.89771200	-0.98583300	-1.45362700
C	-2.79755900	-2.41715600	0.14030900
C	-4.94161300	-1.90138700	-1.56458900
H	-3.91178800	-0.06353200	-2.04066500
C	-3.84009500	-3.33826500	0.02616700
H	-1.95127200	-2.60673800	0.80370100
C	-4.91531700	-3.08363200	-0.82310100
H	-5.77688600	-1.69507600	-2.23667600
H	-3.80960200	-4.26227600	0.60662000
H	-5.72956600	-3.80521800	-0.91098100
S	-0.63764900	3.04461600	0.40729900
O	-1.47644200	3.76980800	-0.53192000
O	-0.13131600	3.70433800	1.59308700

C	0.72211500	2.35457100	-0.51141700
C	1.93066500	2.09676700	0.13133800
C	0.50932800	1.98456800	-1.83655900
C	2.93008900	1.42452900	-0.56335500
H	2.04863900	2.40147000	1.17140200
C	1.51764000	1.30039700	-2.51298400
H	-0.44767600	2.21913700	-2.30626700
C	2.73350000	1.00127500	-1.88603100
H	3.87283500	1.18484200	-0.06682500
H	1.35706900	0.98344200	-3.54632100
C	3.81814900	0.23497900	-2.59463200
H	4.67621000	0.88857200	-2.81637300
H	4.17904600	-0.58062100	-1.95056300
H	3.45665900	-0.18474400	-3.54321500
H	-1.25289600	-0.12315400	-1.50851300
C	-0.63335800	-0.40485900	0.53157100
C	-1.90948000	0.07225300	2.68469000
H	-2.86255000	-0.20192100	2.20806700
H	-1.49205700	-0.81633200	3.17916300
H	-2.08101800	0.86225300	3.42885500
C	0.79366600	-1.98175400	-0.80189800
H	-0.03787500	-2.00019200	-1.51776300
H	1.70482400	-1.62760900	-1.30984300
H	0.99252800	-3.01115800	-0.46437300
C	0.51918700	-1.10573300	0.39741900
C	-0.89065000	0.57757500	1.66272700
O	1.48197900	-1.06216000	1.30422800
O	0.25491100	0.99706400	2.30584100
C	3.96822800	-2.69405500	0.63867000
O	2.96716000	-3.17854800	1.37388400

O	4.92222000	-3.34606500	0.32046000
O	3.81901500	-1.41243000	0.27893500
H	2.94099400	-1.06773700	0.63275600
H	0.92801600	0.29685100	2.10959700
H	2.27674100	-2.46340500	1.50571300
H	-3.25292300	1.04570500	0.13902100

Thermal correction to Gibbs Free Energy= 0.3603

Esolv(RM062X) = -1810.38945895

TS4(S)

C	1.52581100	-0.06033700	-0.23971100
N	1.09048000	-1.42168100	-0.62959900
N	0.33407300	-1.93154600	0.45510100
C	2.92045100	0.17849600	-0.77915500
C	3.11076500	0.93051800	-1.94068400
C	4.03574500	-0.38343400	-0.14731000
C	4.39042300	1.12235800	-2.46270100
H	2.24018500	1.37355100	-2.42969600
C	5.31465100	-0.19745600	-0.66756100
H	3.88021300	-0.94487200	0.77750800
C	5.49561300	0.55743400	-1.82809600
H	4.52454200	1.71763500	-3.36786200
H	6.17723600	-0.63504000	-0.16110700
H	6.49797400	0.70964400	-2.23280700
S	-1.11943700	-2.65905200	-0.05730800
O	-0.70699300	-3.59960400	-1.08190300
O	-1.79810100	-3.12081600	1.13994100
C	-2.04711500	-1.36563200	-0.83163500
C	-3.13347200	-0.80288100	-0.16441500
C	-1.62356400	-0.88804700	-2.07085600

C	-3.77222600	0.29064600	-0.73272400
H	-3.42008700	-1.19655000	0.81005000
C	-2.27085700	0.21715700	-2.61373000
H	-0.78180000	-1.36537600	-2.57153300
C	-3.33176900	0.83691900	-1.94554000
H	-4.59712300	0.77095500	-0.20255700
H	-1.92854000	0.62614600	-3.56688100
C	-3.93414300	2.11328200	-2.45572900
H	-5.02717300	2.11780700	-2.33542600
H	-3.51486400	2.92932200	-1.84379300
H	-3.69160600	2.28223900	-3.51386700
H	0.83460100	0.67044400	-0.69882200
C	1.35600800	-0.05757500	1.27101600
C	0.39363100	-1.79530300	2.93667800
H	1.25182700	-2.48078700	2.98897000
H	0.48074900	-1.04844300	3.73384200
H	-0.53451400	-2.37080600	3.02442300
C	2.01956600	2.35722300	1.43500700
H	3.03378700	2.13938700	1.07289400
H	1.41107200	2.68204000	0.57368600
H	2.03933800	3.15939100	2.18264600
C	1.34222900	1.14017000	2.03097900
C	0.45401900	-1.10437300	1.60268900
O	0.69210500	1.28009900	3.09093200
O	-1.21705700	-0.25582600	1.78930500
C	-1.66906900	2.68942300	0.68965300
O	-1.40340000	3.04411700	1.98365000
O	-2.44741800	3.38332500	0.06425600
O	-1.05434000	1.63815600	0.27057400
H	-1.16071800	0.58231400	1.06976400

H	-0.97157900	0.20569600	2.61111000
H	-0.69342100	2.48914000	2.35113200
H	1.91046400	-2.02354500	-0.70435600

Thermal correction to Gibbs Free Energy= 0.357246

Esolv(RM062X) = -1810.35096825

Int5(S)

C	-0.94923300	0.69092800	-0.38463700
N	-0.25657200	1.75697400	-1.13738500
N	0.63820200	2.38304200	-0.23640500
C	-2.36845400	0.50326100	-0.86209300
C	-2.81816700	-0.78360400	-1.17870100
C	-3.25114800	1.58444500	-0.95706100
C	-4.13874400	-0.97284700	-1.58796500
H	-2.13784700	-1.63733600	-1.06337100
C	-4.56786600	1.39199900	-1.37196300
H	-2.91455600	2.58735800	-0.67687300
C	-5.01420900	0.10864700	-1.68897900
H	-4.48467800	-1.98060900	-1.82486000
H	-5.24868800	2.24291000	-1.43928500
H	-6.04611000	-0.04752400	-2.00989400
S	2.25615400	2.13240400	-0.76830700
O	2.34560000	2.76188600	-2.07004800
O	3.10968900	2.56446100	0.32588800
C	2.35141500	0.38032500	-0.95615800
C	2.57655800	-0.40125200	0.17380300
C	2.07392100	-0.18889200	-2.19911100
C	2.52360000	-1.78616600	0.04920100
H	2.75867900	0.04881600	1.15005200
C	2.02804500	-1.57392100	-2.29937800

H	1.88554700	0.46120600	-3.05364200
C	2.24476500	-2.39480800	-1.18052100
H	2.66736000	-2.40043300	0.93804500
H	1.80384700	-2.03710600	-3.26273600
C	2.12724100	-3.88858800	-1.29226700
H	2.72919100	-4.39135300	-0.52440800
H	1.07324800	-4.16739200	-1.12601400
H	2.44205100	-4.23628500	-2.28681400
H	-0.42629000	-0.26763800	-0.51758500
C	-0.73428600	1.11755700	1.06844900
C	0.97627600	2.62002500	2.26279700
H	1.53836000	3.50841600	1.96030300
H	0.24577800	2.84536700	3.04929700
H	1.67229300	1.87900000	2.68358200
C	-2.79143600	0.03478100	2.18550900
H	-3.48025200	0.70806100	1.65554600
H	-2.70277100	-0.89456900	1.60677800
H	-3.15669900	-0.17563200	3.19745600
C	-1.41451000	0.63641000	2.29742200
C	0.27696600	2.01303000	1.09323300
O	-0.88397500	0.76770200	3.38815000
O	1.33862600	-1.06833000	2.82518200
C	-0.40348500	-2.88617700	0.69592300
O	0.48506400	-3.64682300	1.43304800
O	-0.85449000	-3.39823400	-0.32466600
O	-0.62865800	-1.73321700	1.16007900
H	0.64083000	-1.17344300	2.12741400
H	0.85947100	-0.56055900	3.49276700
H	0.76525700	-3.09094300	2.17764300
H	-0.91223300	2.47063500	-1.45006100

Thermal correction to Gibbs Free Energy= 0.358974

Esolv(RM062X) = -1810.39643258

Int5(S)-1

C	0.96546200	0.08461800	-0.21438000
N	0.32914100	-0.66716600	-1.31741700
N	-0.42082000	-1.72459600	-0.75341700
C	2.41233000	0.38429300	-0.54529600
C	2.82621400	1.68917600	-0.81674900
C	3.34903800	-0.65457100	-0.59993500
C	4.15941400	1.95857800	-1.12718300
H	2.09562700	2.50060900	-0.77991600
C	4.68000200	-0.38851800	-0.91194900
H	3.03170800	-1.67727800	-0.37792400
C	5.08813000	0.92061000	-1.17392600
H	4.47290900	2.98270900	-1.33471400
H	5.40386100	-1.20406300	-0.94531300
H	6.13138300	1.13015500	-1.41430300
S	-2.09817800	-1.49032300	-1.10978900
O	-2.20678100	-1.50486000	-2.54863300
O	-2.82053000	-2.42409100	-0.26902100
C	-2.36713600	0.16200700	-0.52449000
C	-2.62545600	0.36277500	0.82986500
C	-2.20840600	1.22904100	-1.40678100
C	-2.71454600	1.66774800	1.30809200
H	-2.75953500	-0.49485000	1.49143900
C	-2.30653500	2.52457600	-0.91061100
H	-2.00248400	1.02598300	-2.45813300
C	-2.55578200	2.76286000	0.44914300
H	-2.91486200	1.83992400	2.36744400

H	-2.18585600	3.37142700	-1.58947400
C	-2.68834000	4.16980500	0.96717700
H	-2.42066700	4.23129300	2.03002300
H	-2.05039000	4.86391000	0.40427400
H	-3.72757700	4.51869100	0.86507600
H	0.43815800	1.04577200	-0.06062200
C	0.74933200	-0.83430700	0.97832000
C	-0.57338700	-2.99610000	1.42706000
H	-0.97035000	-3.77754400	0.77269300
H	0.23345500	-3.36974600	2.06719400
H	-1.38167200	-2.66417500	2.09500200
C	2.05947800	0.64358100	2.59715500
H	3.05636900	0.55786500	2.13822000
H	1.56833200	1.51525900	2.13940100
H	2.16510100	0.78593100	3.67833900
C	1.27092300	-0.62318500	2.34680900
C	-0.06686800	-1.85101000	0.61634700
O	1.06157300	-1.41929000	3.23761400
H	1.03176800	-1.08030800	-1.92794500

Thermal correction to Gibbs Free Energy= 0.305846

Esolv(RM062X) = -1469.35570836

Int6(S)

C	-1.51606900	0.20799900	-1.12909300
N	-0.06284500	-0.05154900	-1.01711300
N	0.13970700	-1.37791300	-0.55654100
C	-1.95838700	1.42185200	-0.33057400
C	-2.50920700	2.53069300	-0.97463600
C	-1.81849400	1.43595300	1.06147600
C	-2.93282200	3.64016100	-0.24214700

H	-2.61659600	2.52421300	-2.06288500
C	-2.23701200	2.54533100	1.79316600
H	-1.36900400	0.57807700	1.56737000
C	-2.79893600	3.64724400	1.14476400
H	-3.36721100	4.49914800	-0.75597000
H	-2.12601900	2.54885700	2.87864100
H	-3.13057900	4.51178400	1.72194000
S	1.16631400	-1.38675700	0.85540500
O	0.49142600	-0.69450900	1.94182400
O	1.60105000	-2.76100100	1.01521700
C	2.52259600	-0.40213400	0.29568400
C	3.58878200	-1.04006000	-0.32980900
C	2.51177000	0.97378000	0.52029000
C	4.67096300	-0.27034000	-0.75090300
H	3.56583900	-2.12184600	-0.46857200
C	3.60204600	1.72172100	0.09374700
H	1.65447900	1.43286200	1.01429300
C	4.69397600	1.11378800	-0.54491100
H	5.51693400	-0.75462900	-1.24225800
H	3.61049500	2.80119900	0.25812400
C	5.87611400	1.94060500	-0.97336000
H	5.55199800	2.87103700	-1.45949300
H	6.48516000	2.22066700	-0.10041000
H	6.51974600	1.38898500	-1.67009000
H	-1.76023500	0.40190700	-2.18863400
C	-2.11784500	-1.11158800	-0.67598100
C	-1.19575200	-3.34173500	0.24089400
H	-0.98278000	-3.30223900	1.32044400
H	-2.19808400	-3.74935900	0.09114000
H	-0.42339600	-3.97372300	-0.21384700

C	-4.51390400	-0.30672900	-1.07313700
H	-4.17996200	0.18419300	-1.99867800
H	-5.51418800	-0.73334900	-1.20565500
H	-4.54367200	0.46751500	-0.29139300
C	-3.57128100	-1.41364200	-0.65251900
C	-1.12792200	-1.96621800	-0.32846100
O	-4.00444300	-2.49198500	-0.30815300
H	0.39206700	0.01892200	-1.92303500

Thermal correction to Gibbs Free Energy= 0.306522

Esolv(RM062X) = -1469.34828527

Int6(S)-1

C	1.42613000	0.28065400	0.77441200
N	-0.02242600	-0.00960500	0.70035900
N	-0.20865000	-1.24345600	0.02508500
C	1.79122700	1.63431400	0.19026500
C	2.38880100	2.61223100	0.98713100
C	1.52066700	1.91288200	-1.15376700
C	2.72721600	3.85505900	0.45022000
H	2.59682500	2.39762600	2.03902500
C	1.85379700	3.15536000	-1.68841500
H	1.03370000	1.15677000	-1.77433700
C	2.46031800	4.12714400	-0.88990800
H	3.19745100	4.61098100	1.08098800
H	1.64030600	3.36599000	-2.73746100
H	2.72351800	5.09752700	-1.31368800
S	-1.35140000	-1.06723100	-1.28331000
O	-0.81275900	-0.13151100	-2.25574800
O	-1.70716800	-2.41695100	-1.67382600
C	-2.70865100	-0.31519600	-0.44121300

C	-3.66971100	-1.14033600	0.13469300
C	-2.80187400	1.07492600	-0.39588200
C	-4.75083500	-0.54910100	0.78365400
H	-3.56791800	-2.22396100	0.06111300
C	-3.88974600	1.64302800	0.25563100
H	-2.02454500	1.68334000	-0.85979800
C	-4.87689000	0.84356000	0.85178000
H	-5.51465700	-1.18087200	1.24083000
H	-3.97848000	2.73015600	0.30507200
C	-6.06230100	1.47943300	1.52612500
H	-5.76070400	2.36022500	2.10901200
H	-6.79459500	1.81552600	0.77613600
H	-6.56832700	0.77322300	2.19642800
H	1.73389700	0.29131700	1.84046500
C	2.03645800	-0.90868500	0.07203100
C	1.14007200	-2.98855300	-1.16134200
H	0.88776000	-2.78020400	-2.21281300
H	2.16400300	-3.36967100	-1.12081900
H	0.40920400	-3.71699000	-0.79120700
C	4.38242900	-0.35930600	0.88422300
H	4.02368100	-0.41776500	1.92416700
H	5.40760500	-0.73883200	0.81649400
H	4.35418600	0.69741900	0.58001500
C	3.49483800	-1.18302500	-0.01879800
C	1.04869200	-1.73061200	-0.37281900
O	3.94581400	-2.03793100	-0.74733500
O	2.01542800	-2.32028500	2.21730400
O	1.88739800	-1.49879300	3.07662300
H	-0.41652100	-0.12356700	1.63095400

Thermal correction to Gibbs Free Energy= 0.306081

Esolv(RM062X) = -1619.62381256

TS5(S)

C	1.47191300	0.16720000	0.61272800
N	0.07219600	0.02667400	0.42549200
N	-0.23630000	-1.32486700	0.30954800
C	2.07662800	1.35697900	-0.10020100
C	2.57094900	2.45452900	0.60304700
C	2.12770500	1.33841400	-1.49830100
C	3.14555600	3.52234800	-0.08761100
H	2.49660100	2.46948400	1.69275500
C	2.70159800	2.40539400	-2.18452800
H	1.70998000	0.48336600	-2.03653700
C	3.21670500	3.49553800	-1.47917700
H	3.53602500	4.37846700	0.46434700
H	2.74651600	2.38856300	-3.27449800
H	3.66891400	4.32919800	-2.01854000
S	-1.39483000	-1.58616000	-0.98579600
O	-0.77560000	-1.15602400	-2.22393100
O	-1.86483100	-2.94290500	-0.80898600
C	-2.64959200	-0.44243800	-0.51440000
C	-3.58339700	-0.83629300	0.44234700
C	-2.68390900	0.81456900	-1.11196800
C	-4.57142800	0.06848400	0.81311000
H	-3.53295600	-1.83710100	0.87353300
C	-3.68409600	1.70178800	-0.72768700
H	-1.93553000	1.07865800	-1.86014700
C	-4.63423200	1.34641000	0.23899100
H	-5.31369300	-0.22225700	1.55887200
H	-3.72952200	2.69093000	-1.18688100

C	-5.69027200	2.32491100	0.67502400
H	-5.87003400	3.08773800	-0.09305800
H	-6.63833700	1.81546500	0.89235600
H	-5.37349000	2.84188100	1.59391500
H	1.60281700	0.41148600	1.77839500
C	2.01202800	-1.20505900	0.38043600
C	0.92759500	-3.51574900	-0.05552100
H	0.69025100	-3.69145900	-1.11610200
H	1.91099200	-3.94089700	0.15957700
H	0.13710200	-3.99252400	0.53586600
C	4.43119700	-0.52300600	0.85545900
H	4.08050200	0.03994000	1.73305200
H	5.39548400	-0.99834500	1.06540700
H	4.54677200	0.19917700	0.03299600
C	3.44341100	-1.59591100	0.45811100
C	0.95778500	-2.05097300	0.21187000
O	3.80838200	-2.72491600	0.21623700
O	-0.29627400	0.64928800	2.77340000
O	0.91530200	0.86033000	2.97177000
H	-0.47507800	0.48515800	1.21384400

Thermal correction to Gibbs Free Energy= 0.302984

Esolv(RM062X) = -1619.61272925

4e with hydrogen peroxide

C	1.56333500	-0.21325000	-0.34004100
N	0.36448400	-0.23401000	-0.88439100
N	-0.17277500	-1.41503700	-0.52848100
C	2.39636400	1.00877100	-0.46657500
C	2.50840700	1.88152600	0.62194000
C	3.04439500	1.30654500	-1.66856900
C	3.28769900	3.03105200	0.51065600

H	1.96516500	1.65570100	1.54234900
C	3.82467700	2.45718600	-1.77409500
H	2.93648400	0.62864500	-2.51724300
C	3.95091900	3.31654600	-0.68334100
H	3.37105300	3.71220600	1.35870400
H	4.33378900	2.68405900	-2.71190300
H	4.56198300	4.21666900	-0.76634900
S	-1.77535500	-1.73138900	-1.10906600
O	-1.72648000	-1.62497200	-2.54444800
O	-2.18358500	-2.94110800	-0.43098300
C	-2.64179000	-0.34570300	-0.44859600
C	-3.08816000	-0.40232500	0.86993300
C	-2.84740900	0.77090300	-1.25417200
C	-3.71671100	0.71866300	1.40329400
H	-2.94863900	-1.31377900	1.45470600
C	-3.48691100	1.87550800	-0.70300300
H	-2.49733900	0.76176200	-2.28721200
C	-3.90663600	1.87559400	0.63285300
H	-4.07851000	0.69625900	2.43365600
H	-3.64946400	2.76376400	-1.31610200
C	-4.51600700	3.10784200	1.23921100
H	-5.10632400	3.66665900	0.50144200
H	-5.15963500	2.86176600	2.09342700
H	-3.71523700	3.77256800	1.59893000
H	-1.21250600	0.69530800	2.11571600
C	1.81634100	-1.42272900	0.38216300
C	0.32059600	-3.54447600	0.74630800
H	0.01004800	-4.19874500	-0.07742900
H	1.19796200	-3.94781500	1.25661400
H	-0.52288300	-3.49871700	1.44806300

C	4.30333200	-1.03186400	0.92208400
H	4.20059200	-0.06739400	1.43961000
H	5.14010400	-1.59251200	1.35302600
H	4.48954500	-0.80557100	-0.13669200
C	3.04734900	-1.85406300	1.09872400
C	0.65414900	-2.17967700	0.24310100
O	3.05417100	-2.84642400	1.79316400
O	-0.66688500	1.87816400	0.78308800
O	-0.33835000	0.91240900	1.76137300
H	-0.44706800	1.39388000	-0.03695800

Thermal correction to Gibbs Free Energy= 0.30994

Esolv(RM062X) = -1619.7497503

TS3'(S)

C	0.95884400	-0.16235300	-0.18197100
N	0.36439200	-0.66741900	-1.45105700
N	-0.65363400	-1.53500400	-0.94418400
C	2.16148900	0.69109300	-0.45893500
C	3.05023800	0.37821100	-1.49708400
C	2.42008200	1.82494200	0.31812500
C	4.18257700	1.15827900	-1.72093600
H	2.82844900	-0.48128000	-2.13104800
C	3.55482000	2.60642600	0.09846600
H	1.71490100	2.09044900	1.11010000
C	4.44581600	2.27150300	-0.91967200
H	4.86593600	0.89920700	-2.53265200
H	3.74072100	3.48334800	0.72237700
H	5.33520100	2.87979800	-1.09636100
S	-2.20646700	-1.04477500	-1.18427000
O	-2.38578300	-0.77739900	-2.60094900

O	-3.08780400	-1.99406800	-0.51407600
C	-2.34451500	0.53917000	-0.37069400
C	-2.87975100	0.61724700	0.91147300
C	-1.80156000	1.65670700	-1.00193700
C	-2.87918600	1.84498000	1.56730100
H	-3.25451800	-0.29512400	1.37680700
C	-1.79279500	2.87382100	-0.32251500
H	-1.37057000	1.54190800	-1.99700700
C	-2.33272000	2.98600400	0.96391800
H	-3.29601800	1.92042900	2.57503200
H	-1.35092100	3.75327800	-0.79746600
C	-2.35018300	4.31267500	1.67996900
H	-1.56075100	4.97775100	1.30377700
H	-3.31437100	4.82607900	1.53558200
H	-2.20566100	4.18311700	2.76189600
H	0.24568700	0.40453900	0.44662800
C	1.21207500	-1.58028100	0.36753800
C	-0.33183400	-3.67291600	0.23813200
H	0.24504800	-4.04450800	-0.61944500
H	0.04141600	-4.13902800	1.15870800
H	-1.39496200	-3.90817500	0.09165000
C	3.33771700	-1.19892400	1.75288000
H	3.14986100	-0.18078900	2.12714800
H	3.91540200	-1.75478700	2.50211800
H	3.90256300	-1.09340400	0.81752100
C	2.01317400	-1.91593600	1.54065700
C	-0.20433000	-2.15903300	0.33088600
O	1.66649600	-2.76155000	2.36383100
O	-0.97581100	-1.68114600	1.42305600
H	-0.49168300	-1.99619900	2.20013500

H	1.32590200	-1.64963400	-0.98899000

Thermal correction to Gibbs Free Energy= 0.315587

Esolv(RM062X) = -1545.23211702

TS3'(T)

C	0.95953000	-0.04575600	-0.25612400
N	0.38841000	-0.66613200	-1.48105600
N	-0.54477800	-1.59017400	-0.92483000
C	2.06275400	0.92818000	-0.50471400
C	2.34337300	1.44830700	-1.76952700
C	2.84568200	1.31508100	0.59372900
C	3.39321300	2.35462300	-1.93749700
H	1.73039300	1.13223100	-2.61506300
C	3.89083700	2.21839000	0.42076700
H	2.62408400	0.87315600	1.57057000
C	4.16763700	2.74154900	-0.84544500
H	3.60674400	2.75921400	-2.92929300
H	4.50004800	2.51254700	1.27802000
H	4.98976400	3.44788700	-0.97895300
S	-2.14692200	-1.25908200	-1.12433500
O	-2.38150400	-1.00064800	-2.53385600
O	-2.86503600	-2.31300900	-0.42757400
C	-2.45012000	0.28143100	-0.27654800
C	-2.76691700	0.26911200	1.08040000
C	-2.29128700	1.47316800	-0.97706100
C	-2.92646300	1.48396300	1.73839500
H	-2.84615400	-0.68798000	1.59619200
C	-2.44741900	2.68028600	-0.29804100
H	-2.04636400	1.43644400	-2.03943700
C	-2.76214900	2.70239400	1.06466700

H	-3.17153100	1.49041200	2.80319200
H	-2.31906900	3.62267800	-0.83534500
C	-2.89113800	4.00629400	1.80862400
H	-3.73547100	3.98135300	2.51211000
H	-1.98075000	4.20952400	2.39365800
H	-3.03949200	4.84733800	1.11810000
H	0.18007400	0.39058300	0.38881800
C	1.42217800	-1.44163600	0.19202300
C	0.07993200	-3.65569300	0.27265200
H	0.56404100	-4.00374400	-0.65040200
H	0.64207700	-4.02300700	1.14248000
H	-0.95540200	-4.02019500	0.31138000
C	3.87562700	-1.85648600	1.08582900
H	4.28650400	-2.63763100	1.75200100
H	4.11301000	-2.12679300	0.04552000
H	4.43514700	-0.92578400	1.32509300
C	2.39680100	-1.72076500	1.27434300
C	0.05698000	-2.14134100	0.33137300
O	1.86944000	-1.43080500	2.43615900
O	-0.56255400	-1.69961600	1.50058600
H	0.22946500	-1.52121700	2.10145700
H	1.40115600	-1.51155800	-1.24911800

Thermal correction to Gibbs Free Energy= 0.31099

Esolv(UM062X) = -1545.14357229

Int4'(S)

C	1.22561200	0.18468100	-0.37820100
N	0.95699800	-1.20449600	-0.87671800
N	0.11768200	-1.88543400	0.01828500
C	2.72675200	0.44577200	-0.43963900

C	3.44944600	0.86620500	0.67914600
C	3.40822500	0.27267300	-1.65321300
C	4.82291200	1.09885000	0.59160500
H	2.90271400	1.00194300	1.61529400
C	4.78012900	0.49938400	-1.74234300
H	2.84525600	-0.04531900	-2.53521400
C	5.49373900	0.91475200	-0.61668300
H	5.37366200	1.42629900	1.47602200
H	5.29542200	0.35597800	-2.69454600
H	6.56825500	1.09673500	-0.68342900
S	-1.42018900	-2.13021900	-0.63588000
O	-1.21649600	-2.54144900	-2.01763600
O	-2.16967000	-2.98506600	0.26337400
C	-2.18585500	-0.51812000	-0.68682900
C	-2.94162000	-0.07512500	0.39424600
C	-1.94468100	0.29711300	-1.79058000
C	-3.44020400	1.22336200	0.37584200
H	-3.09155900	-0.74283700	1.24236400
C	-2.45376400	1.59334900	-1.79218700
H	-1.35623000	-0.09747800	-2.62034800
C	-3.19793300	2.07503600	-0.70797900
H	-4.00173700	1.59258700	1.23642800
H	-2.26579800	2.24798500	-2.64698400
C	-3.69177400	3.49836000	-0.68274600
H	-3.72322200	3.93026600	-1.69253600
H	-4.69762700	3.56445200	-0.24438400
H	-3.02527200	4.12614800	-0.06957200
H	0.75895700	0.89912200	-1.08350200
C	0.54573200	0.22823700	0.95435200
C	1.42998500	-1.90499900	2.06347900

H	2.33375400	-1.89118700	1.43445400
H	1.64571200	-1.37952500	3.00462300
H	1.14422100	-2.94485400	2.27851600
C	0.04542800	2.69108900	0.98491300
H	-0.93739500	3.06579000	0.65845200
H	0.38390100	3.34091100	1.80650600
H	0.76283000	2.76229700	0.15576000
C	-0.13448600	1.28244200	1.52610700
C	0.25517000	-1.19740100	1.38210200
O	-0.94475900	1.16240400	2.51003100
O	-0.87358800	-1.30760400	2.15315900
H	-1.05924300	-0.34339300	2.45672400
H	1.82287900	-1.73315000	-0.95130400

Thermal correction to Gibbs Free Energy= 0.321711

Esolv(RM062X) = -1545.32223232

Int4'(T)

C	1.15127500	-0.02541000	-0.28463400
N	0.36789200	-0.40076400	-1.46344900
N	-0.43107000	-1.48927400	-1.02252400
C	2.36608400	0.80274400	-0.55381300
C	2.79398200	1.15449600	-1.83584600
C	3.11392500	1.22728300	0.55877500
C	3.96676100	1.89256900	-2.01407300
H	2.19893300	0.87020200	-2.70590800
C	4.28451300	1.95826200	0.37548300
H	2.74519300	0.97839800	1.55796200
C	4.72013600	2.28814900	-0.91044800
H	4.28792800	2.16249900	-3.02230700
H	4.86135500	2.27878600	1.24558000

H	5.63869300	2.86187300	-1.04947300
S	-2.05356800	-1.21552300	-1.28042600
O	-2.21228500	-0.90622800	-2.69283800
O	-2.77002800	-2.33338800	-0.68927200
C	-2.46592200	0.27556700	-0.39327300
C	-2.96459100	0.18946800	0.90472400
C	-2.25316100	1.50363900	-1.01179100
C	-3.25443400	1.36485600	1.58823800
H	-3.08508100	-0.79475200	1.35688100
C	-2.53774300	2.67156400	-0.30535000
H	-1.86744100	1.52422300	-2.03104500
C	-3.03784500	2.61860100	0.99939000
H	-3.64367800	1.31242600	2.60783100
H	-2.36710100	3.64242400	-0.77630800
C	-3.31009800	3.88019700	1.77697300
H	-4.24849100	3.80323600	2.34458300
H	-2.50238200	4.06984300	2.50090700
H	-3.37670400	4.75270200	1.11312600
H	0.48048900	0.54815800	0.38818100
C	1.40113500	-1.35353400	0.43942300
C	0.10243300	-3.56476200	0.21372600
H	0.68875000	-3.89140500	-0.65672700
H	0.57253600	-3.93669700	1.13514300
H	-0.92420600	-3.94712600	0.13632400
C	3.41003300	-1.82319100	2.06477900
H	3.45494300	-2.53070700	2.91513500
H	3.85891000	-2.31016000	1.18509600
H	4.06657600	-0.97165500	2.34907900
C	2.00081400	-1.39837900	1.78230000
C	0.05175200	-2.05005000	0.29104900

O	1.27562700	-0.79529900	2.68925600
O	-0.75151700	-1.64027100	1.35605200
H	-0.11179400	-1.22309600	2.03590300
H	1.00324900	-0.79146400	-2.16071100

Thermal correction to Gibbs Free Energy= 0.316825

Esolv(UM062X) = -1545.21384216

Int1''

C	0.65148300	-1.48848400	-1.35744600
N	-0.37602900	-0.75160000	-1.18903800
N	-0.64151900	0.17195800	-0.34063500
C	1.85296800	-1.55730400	-0.51385600
C	1.97255200	-0.91081100	0.72561600
C	2.91898000	-2.33820000	-0.98660300
C	3.14366300	-1.04615700	1.46542900
H	1.16172300	-0.30115300	1.12359800
C	4.08885400	-2.46316600	-0.24773700
H	2.82654400	-2.84164900	-1.95120400
C	4.20156600	-1.81729200	0.98324900
H	3.22605500	-0.54116800	2.42913100
H	4.91397500	-3.06393400	-0.63166700
H	5.11564800	-1.91825100	1.57109800
S	-1.57087200	-0.37040500	1.00555200
O	-1.32731200	-1.78669900	1.21743900
O	-1.27561800	0.61568100	2.03045500
C	-3.23437800	-0.15031300	0.45024000
C	-3.85199700	1.08512500	0.62905400
C	-3.88150400	-1.21235000	-0.17715500
C	-5.15093000	1.25407100	0.16062400
H	-3.31680700	1.88861500	1.13677500

C	-5.17966300	-1.02136600	-0.63915900
H	-3.36849300	-2.16883400	-0.28649200
C	-5.83156200	0.20860100	-0.47770000
H	-5.64961800	2.21622800	0.29348000
H	-5.70089700	-1.84375900	-1.13323300
C	-7.24815400	0.39210800	-0.95141800
H	-7.44955800	1.43980100	-1.20996400
H	-7.45802900	-0.23134600	-1.83037800
H	-7.95743700	0.10182800	-0.16090300
H	0.62565000	-2.13524300	-2.24048600
C	3.27374300	2.21089800	0.15951400
C	0.87986600	3.02009300	0.10107900
H	1.21854100	3.79081200	0.80230400
H	0.34064600	3.47711000	-0.73941900
H	0.17814600	2.34049300	0.60955800
C	5.64220300	1.31026400	0.30362500
H	6.25885500	0.52447000	-0.14692100
H	6.14130200	2.28421700	0.18835200
H	5.51802900	1.12671500	1.38039500
C	4.29850700	1.34906200	-0.37972400
C	2.02810000	2.22294200	-0.42125600
O	4.10184100	0.64964400	-1.38320200
O	1.76246600	1.48794700	-1.47590600
H	2.62233100	0.99544300	-1.68926800
H	3.47337200	2.82467400	1.03558200

Thermal correction to Gibbs Free Energy= 0.311284

Esolv(UM062X) = -1545.1431999

TS1''

C	0.80597800	-1.82778800	-0.94865300

N	-0.21707200	-1.09279900	-0.74331200
N	-0.17629900	0.14401300	-0.24306500
C	2.18522100	-1.64855800	-0.44398600
C	2.38578500	-1.30036300	0.89987600
C	3.28117800	-1.97210300	-1.25017700
C	3.67806400	-1.26741500	1.41683600
H	1.52327900	-1.08217100	1.53442300
C	4.57294300	-1.91430600	-0.73236900
H	3.11863400	-2.26394000	-2.29011500
C	4.77163500	-1.56523000	0.60170800
H	3.83198700	-1.01524900	2.46750100
H	5.42568900	-2.15032100	-1.37007800
H	5.78245400	-1.53295500	1.01159600
S	-1.11136900	0.35657100	1.13913900
O	-0.74475400	-0.65611000	2.11661000
O	-1.02457300	1.77088600	1.46942200
C	-2.75804800	0.00547900	0.58242400
C	-3.57914200	1.05748100	0.18992900
C	-3.19477800	-1.31820600	0.54483600
C	-4.86571000	0.77068200	-0.26144200
H	-3.21560100	2.08364700	0.25723400
C	-4.47988800	-1.58307300	0.08784700
H	-2.53099100	-2.11571700	0.87978900
C	-5.33146200	-0.54712400	-0.32377900
H	-5.52329200	1.58732300	-0.56537100
H	-4.83634600	-2.61483200	0.05352100
C	-6.71832600	-0.86084300	-0.81731100
H	-7.27684200	0.05388200	-1.05201600
H	-6.67681200	-1.47955400	-1.72582200
H	-7.28360700	-1.42538700	-0.06182000

H	0.59250200	-2.75704100	-1.49156500
C	1.61625200	1.89442700	0.00880900
C	-0.35132000	2.38592500	-1.54587500
H	0.05644700	3.23804700	-2.11044800
H	-1.01215900	1.80623600	-2.20245600
H	-0.89683200	2.75420400	-0.67100900
C	3.84279600	2.10187700	1.18607300
H	4.85343200	1.68429100	1.11575300
H	3.89970300	3.20080300	1.17744300
H	3.36984100	1.79930800	2.13058400
C	3.02603700	1.62725200	0.01085200
C	0.80888400	1.53009500	-1.12785000
O	3.58352300	1.05888100	-0.94339100
O	1.39226600	0.89598600	-2.12349100
H	2.36068200	0.75884700	-1.85226000
H	1.14502400	2.44054000	0.82385100

Thermal correction to Gibbs Free Energy= 0.31435

Esolv(UM062X) = -1545.10109285

Int2''

C	0.94241200	-2.07105700	-0.61990800
N	-0.13837600	-1.40878200	-0.49032000
N	0.02850700	-0.10387200	0.00640600
C	2.31517000	-1.69300300	-0.20584300
C	2.55231600	-1.15120000	1.06713400
C	3.39074200	-1.94353900	-1.06308700
C	3.85461400	-0.84953800	1.45735900
H	1.71051900	-0.98719100	1.74233900
C	4.68851600	-1.61348500	-0.67716100
H	3.20530700	-2.37997100	-2.04713000

C	4.92137000	-1.06547600	0.58255500
H	4.03845000	-0.44595200	2.45474600
H	5.51980500	-1.78659500	-1.36157100
H	5.93823700	-0.81423400	0.88836800
S	-1.06504300	0.20946900	1.23437300
O	-0.84521200	-0.83775700	2.21355800
O	-0.89094200	1.61359100	1.58449400
C	-2.70598200	-0.00104100	0.58796000
C	-3.50914500	1.11933400	0.39621000
C	-3.17696300	-1.28795500	0.31923100
C	-4.79852000	0.94844600	-0.10306700
H	-3.12698800	2.10769300	0.65461100
C	-4.46321500	-1.43567400	-0.18573800
H	-2.53648000	-2.14878000	0.50638800
C	-5.29012900	-0.32496800	-0.40865000
H	-5.43788400	1.82108700	-0.25003900
H	-4.84109100	-2.43671800	-0.40459900
C	-6.67536800	-0.51176100	-0.96685500
H	-7.25105100	0.42169900	-0.93101700
H	-6.62867300	-0.84250300	-2.01534400
H	-7.22540400	-1.27981600	-0.40506100
H	0.81415000	-3.06122000	-1.07660400
C	1.45352200	1.82001100	-0.18304800
C	-0.68370700	1.78405100	-1.51975700
H	-0.29888400	2.49086100	-2.26715700
H	-1.38427500	1.09490000	-2.01226900
H	-1.19409900	2.33520400	-0.72248500
C	3.71149400	2.64887300	0.58721300
H	4.77151900	2.55073800	0.32853800
H	3.41244800	3.70651200	0.54769000

H	3.54188500	2.29359200	1.61386600
C	2.88801500	1.83572200	-0.38112000
C	0.49558200	0.97643700	-0.98903200
O	3.42709100	1.21590500	-1.30014000
O	1.08868800	0.34234900	-2.05311200
H	2.06299600	0.43012400	-1.96834700
H	1.01791700	2.38988000	0.63772500

Thermal correction to Gibbs Free Energy= 0.317107

Esolv(UM062X) = -1545.12508728

Ts2''

C	1.63210900	0.62193900	-1.29320500
N	0.49309800	-0.00009200	-1.13563700
N	0.38422800	-0.60488700	0.06258600
C	2.97606000	0.14285600	-0.85517300
C	3.20742800	-1.22377900	-0.64326500
C	4.05350200	1.03471900	-0.80005400
C	4.49103200	-1.67504500	-0.34698100
H	2.37545700	-1.92647000	-0.71288100
C	5.33425000	0.58078800	-0.49423500
H	3.88469500	2.09699900	-0.99525300
C	5.55511100	-0.77636900	-0.26095500
H	4.66049500	-2.74064300	-0.18648300
H	6.16329500	1.28805000	-0.44400600
H	6.55735200	-1.13502100	-0.02286400
S	-0.80998800	-1.83577700	0.07860000
O	-0.52963600	-2.61129200	-1.11127400
O	-0.75351000	-2.42199700	1.40089500
C	-2.35421100	-1.00343100	-0.14815000
C	-3.16148500	-0.75604700	0.96047300

C	-2.72628200	-0.61593900	-1.43307400
C	-4.36594500	-0.08919500	0.76855600
H	-2.82825800	-1.07804100	1.94774300
C	-3.93299600	0.05771400	-1.59970300
H	-2.07596700	-0.84610400	-2.27714600
C	-4.76442600	0.33358100	-0.50776300
H	-5.01375300	0.10755300	1.62529900
H	-4.23908700	0.37117900	-2.59963700
C	-6.05161700	1.09123900	-0.69206700
H	-6.82556200	0.73543300	0.00108000
H	-5.89580500	2.16291400	-0.49356900
H	-6.42959900	0.99338900	-1.71793200
H	1.64140800	1.33048600	-2.13117000
C	1.19917800	1.57553500	0.80629000
C	1.51842200	-0.44158600	2.28605200
H	1.61982700	0.18272500	3.18345700
H	1.05956600	-1.39843600	2.56113200
H	2.50626500	-0.61494000	1.84084400
C	0.99532700	3.98050400	0.02594900
H	0.25786700	4.64671300	-0.43459200
H	1.38392000	4.44445000	0.94478600
H	1.84549600	3.83099500	-0.65492100
C	0.33451000	2.66385600	0.36325200
C	0.60242800	0.26761800	1.30290600
O	-0.87619100	2.51630200	0.24594000
O	-0.61468900	0.47071900	1.92925600
H	-1.11997700	1.10651300	1.38549700
H	2.22872100	1.80594200	1.08272500

Thermal correction to Gibbs Free Energy= 0.317587

Esolv(UM062X) = -1545.11001032

Int3''

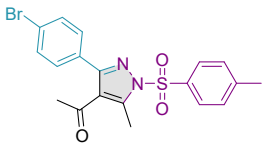
C	1.64294200	0.82639800	-0.76505800
N	0.64449600	-0.19023700	-1.02978400
N	0.28563500	-0.63185000	0.17299600
C	3.04918800	0.23720700	-0.70394200
C	3.26629400	-1.13440900	-0.85824200
C	4.14243800	1.08565900	-0.50016900
C	4.56258500	-1.64716500	-0.78929900
H	2.41566900	-1.79707400	-1.02597600
C	5.43528500	0.57263400	-0.43541100
H	3.98210500	2.16228400	-0.39109000
C	5.64759000	-0.79939400	-0.57698200
H	4.72175200	-2.72029000	-0.90476500
H	6.27970800	1.24478700	-0.27545800
H	6.65893800	-1.20487400	-0.52412100
S	-0.86494300	-1.89320600	0.21219900
O	-0.54281900	-2.75154700	-0.90388500
O	-0.87153200	-2.37182800	1.57803400
C	-2.38183000	-1.04984100	-0.12764200
C	-3.23206800	-0.72928700	0.92667100
C	-2.66640400	-0.69070700	-1.44424600
C	-4.39770900	-0.02113100	0.64684800
H	-2.96547300	-1.02859600	1.94127500
C	-3.83346900	0.02077800	-1.69828200
H	-1.97700400	-0.96984900	-2.24234500
C	-4.71097200	0.36801000	-0.66152600
H	-5.08037600	0.23303000	1.46009500
H	-4.07340800	0.31109900	-2.72320900

C	-5.95372100	1.16531100	-0.95284800
H	-6.69008200	1.06813500	-0.14486900
H	-5.70773700	2.23326500	-1.05713100
H	-6.42171200	0.84127400	-1.89224000
H	1.61392100	1.55521100	-1.59118400
C	1.20162200	1.47112400	0.58526200
C	1.47470600	-0.37480900	2.34030700
H	1.64621200	0.31845200	3.17466200
H	0.99255500	-1.28464000	2.71814400
H	2.43183600	-0.63003200	1.86713100
C	0.86937900	3.95690600	0.03040400
H	0.13920600	4.63702200	-0.42117000
H	1.18298100	4.34973500	1.00988100
H	1.76989600	3.88671700	-0.59654300
C	0.24721500	2.59962300	0.23622300
C	0.54006600	0.28232100	1.34119800
O	-0.93906200	2.41215900	0.08553000
O	-0.63093300	0.59149400	2.00518000
H	-1.19749100	1.09970600	1.40002600
H	2.06261700	1.86296700	1.14276300

Thermal correction to Gibbs Free Energy= 0.320949

Esolv(UM062X) = -1545.17231943

8. Characterization data of products



1-(3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4a)

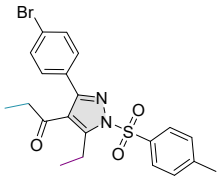
petroleum ether/ ethyl acetate = 8:1, white solid, 82% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 (d, J = 8.1 Hz, 2H), 7.66 (d, J = 8.5 Hz, 2H), 7.50 (d, J = 8.1 Hz, 2H), 7.40 (d, J = 8.4 Hz, 2H), 2.73 (s, 3H), 2.40 (s, 3H), 2.13 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 195.0, 152.7, 146.7, 146.1, 133.4, 131.5, 130.9, 130.7, 130.6, 127.9, 122.9, 122.2, 31.1, 21.2, 12.0.

HRMS (ESI-TOF): Anal Calcd. For. $C_{19}H_{17}{}^{79}BrN_2O_3S[M+H]^+$: 433.0217, Found:433.0219 .Anal Calcd. For. $C_{19}H_{17}{}^{81}BrN_2O_3S[M+H]^+$: 435.0196, Found:435.0218 .

IR (neat, cm^{-1}): υ 2361, 2341, 1674, 1529, 1412, 1312, 1190, 1179, 1111, 1081, 1014, 840, 829, 817, 705, 688, 673, 656, 611.



1-(3-(4-bromophenyl)-5-ethyl-1-tosyl-1*H*-pyrazol-4-yl)propan-1-one (4b)

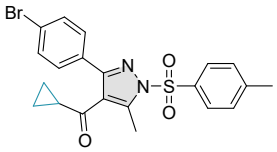
petroleum ether/ ethyl acetate = 10:1, white solid, 76% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 (d, J = 8.5 Hz, 2H), 7.67 (d, J = 8.5 Hz, 2H), 7.51 (d, J = 8.2 Hz, 2H), 7.38 (d, J = 8.5 Hz, 2H), 3.10 (q, J = 7.3 Hz, 2H), 2.44 – 2.36 (m, 5H), 1.24 (t, J = 7.3 Hz, 3H), 0.88 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 198.6, 152.3, 151.1, 146.7, 133.5, 131.7, 130.7, 130.6, 128.0, 123.0, 121.5, 36.1, 21.2, 18.8, 14.7, 8.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{21}H_{21}{}^{79}BrN_2O_3S[M+H]^+$: 461.0530, Found: 461.0538. Anal Calcd. For.$C_{21}H_{21}{}^{81}BrN_2O_3S[M+H]^+$: 463.0509, Found: 463.0541.

IR (neat, cm^{-1}): υ 2978, 1673, 1380, 1195, 1178, 1095, 1071, 838, 811, 675.



(3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)(cyclopropyl)methanone (4c)

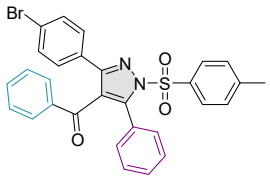
petroleum ether/ ethyl acetate = 10:1, white solid, 50% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, J = 8.3 Hz, 2H), 7.54 (d, J = 8.5 Hz, 2H), 7.45 (d, J = 8.5 Hz, 2H), 7.35 (d, J = 8.1 Hz, 2H), 2.72 (s, 3H), 2.43 (s, 3H), 1.79 – 1.70 (m, 1H), 1.21 – 1.14 (m, 2H), 0.84 – 0.76 (m, 2H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 198.8, 152.9, 146.2, 145.7, 134.4, 131.5, 130.6, 130.6, 130.1, 128.2, 123.7, 122.8, 22.8, 21.7, 13.5, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{21}H_{19}{}^{79}BrN_2O_3S[M+H]^+$: 459.0373, Found: 459.0368. Anal Calcd. For.$C_{21}H_{19}{}^{81}BrN_2O_3S[M+H]^+$: 461.0353, Found: 461.0318.

IR (neat, cm^{-1}): υ 2922, 1667, 1389, 1373, 1192, 1177, 1101, 1084, 1069, 1009, 961, 837, 811, 702, 681, 665.



(3-(4-bromophenyl)-5-phenyl-1-tosyl-1*H*-pyrazol-4-yl)(phenyl)methanone (4d)

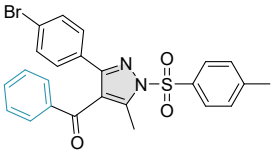
petroleum ether/ ethyl acetate = 8:1, white solid, 71% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 (d, *J* = 8.4 Hz, 2H), 7.61 – 7.54 (m, 2H), 7.46 (d, *J* = 8.6 Hz, 2H), 7.38 (d, *J* = 8.6 Hz, 2H), 7.38 – 7.34 (m, 1H), 7.33 – 7.26 (m, 4H), 7.25 – 7.17 (m, 5H), 2.39 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 191.6, 152.3, 147.5, 146.1, 136.6, 134.1, 133.6, 131.6, 130.5, 129.8, 129.8, 129.6, 129.6, 129.5, 128.3, 128.2, 127.6, 127.2, 123.6, 122.6, 21.7.

HRMS (ESI-TOF): Anal Calcd. For.$C_{29}H_{21}{}^{79}BrN_2O_3S[M+H]^+$: 557.0530, Found: 557.0522. Anal Calcd. For.$C_{29}H_{21}{}^{81}BrN_2O_3S[M+H]^+$: 559.0509, Found: 559.0533.

IR (neat, cm^{-1}): υ 1661, 1423, 1390, 1192, 1173, 1132, 1010, 914, 828, 699, 677, 664.



(3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)(phenyl)methanone (4e)

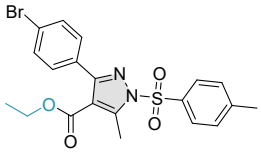
petroleum ether/ ethyl acetate = 8:1, white solid, 71% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 8.4 Hz, 2H), 7.72 – 7.64 (m, 2H), 7.52 – 7.46 (m, 1H), 7.39 – 7.24 (m, 8H), 2.56 (s, 3H), 2.44 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 191.7, 152.6, 146.2, 145.4, 134.3, 133.7, 131.3, 130.1, 129.8, 129.8, 129.6, 128.6, 128.2, 123.2, 120.8, 21.7, 12.3.

HRMS (ESI-TOF): Anal Calcd. For.$C_{24}H_{19}{}^{79}BrN_2O_3S[M+H]^+$: 495.0373, Found: 495.0373. Anal Calcd. For.$C_{24}H_{19}{}^{81}BrN_2O_3S[M+H]^+$: 497.0353, Found: 497.0415.

IR (neat, cm^{-1}): υ 2919, 1651, 1375, 1190, 1176, 1083, 1010, 914, 833, 744, 673, 603.



ethyl 3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4f)

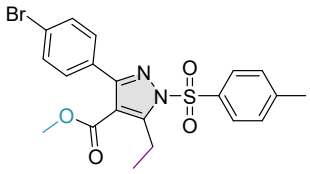
petroleum ether/ ethyl acetate = 8:1, white solid, 55% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 (d, *J* = 8.4 Hz, 2H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.50 (d, *J* = 8.2 Hz, 2H), 7.44 (d, *J* = 8.5 Hz, 2H), 4.13 (q, *J* = 7.1 Hz, 2H), 2.80 (s, 3H), 2.39 (s, 3H), 1.09 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 162.1, 153.3, 148.3, 146.8, 133.3, 131.0, 130.9, 130.6, 130.4, 128.0, 122.7, 113.1, 60.6, 21.2, 13.7, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{20}H_{19}{}^{79}BrN_2O_4S[M+H]^+$: 463.0322, Found: 463.0321. Anal Calcd. For.$C_{20}H_{19}{}^{81}BrN_2O_4S[M+H]^+$: 465.0302, Found: 465.0295.

IR (neat, cm^{-1}): υ 2977, 1705, 1492, 1448, 1300, 1158, 1120, 1097, 1070, 1009, 820, 785, 680.



methyl 3-(4-bromophenyl)-5-ethyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4g)

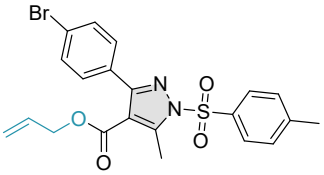
petroleum ether/ ethyl acetate = 10:1, white solid, 45% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 (d, J = 8.3 Hz, 2H), 7.61 (d, J = 8.5 Hz, 2H), 7.50 (d, J = 8.2 Hz, 2H), 7.45 (d, J = 8.5 Hz, 2H), 3.67 (s, 3H), 3.25 (q, J = 7.3 Hz, 2H), 2.40 (s, 3H), 1.25 (t, J = 7.4 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 153.9, 153.2, 146.8, 133.4, 131.0, 130.9, 130.6, 130.3, 128.0, 122.7, 112.2, 51.7, 21.2, 19.0, 14.4.

HRMS (ESI-TOF): Anal Calcd. For.$C_{20}H_{19}{}^{79}BrN_2O_4S[M+H]^+$: 463.0322, Found: 463.0319. Anal Calcd. For.$C_{20}H_{19}{}^{81}BrN_2O_4S[M+H]^+$: 465.0302, Found: 465.0301.

IR (neat, cm^{-1}): υ 2955, 1717, 1548, 1389, 1293, 1190, 1123, 1071, 1017, 1002, 837, 811, 703, 675.



allyl 3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4h)

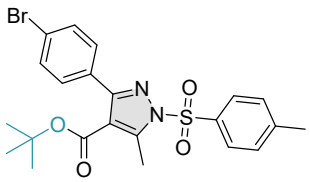
petroleum ether/ ethyl acetate = 10:1, white solid, 41% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 (d, J = 8.3 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 8.1 Hz, 2H), 7.44 (d, J = 8.5 Hz, 2H), 5.89 – 5.76 (m, 1H), 5.18 – 5.04 (m, 2H), 4.67 – 4.60 (m, 2H), 2.81 (s, 3H), 2.39 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 161.8, 153.4, 148.5, 146.8, 133.3, 131.9, 131.0, 131.0, 130.6, 130.4, 128.0, 122.7, 118.3, 112.8, 65.1, 21.2, 12.1.

HRMS (ESI-TOF): Anal Calcd. For.$C_{21}H_{19}{}^{79}BrN_2O_4S[M+H]^+$: 475.0322, Found: 475.0324. Anal Calcd. For.$C_{21}H_{19}{}^{81}BrN_2O_4S[M+H]^+$: 477.0302, Found: 477.0289.

IR (neat, cm^{-1}): υ 2921, 1709, 1552, 1393, 1315, 1174, 1134, 1013, 922, 832, 703, 687, 668.



tert-butyl 3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4i)

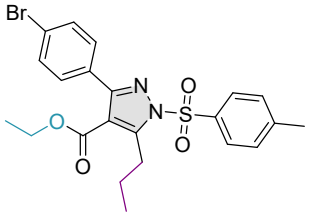
petroleum ether/ ethyl acetate = 10:1, white solid, 51% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.0 Hz, 2H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.40 – 7.32 (m, 4H), 2.83 (s, 3H), 2.44 (s, 3H), 1.37 (s, 9H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 162.2, 154.1, 147.9, 146.2, 134.4, 131.1, 130.9, 130.9, 130.1, 128.2, 123.1, 114.8, 82.0, 28.0, 21.7, 12.2.

HRMS (ESI-TOF): Anal Calcd. For.$C_{22}H_{23}{}^{79}BrN_2O_4S[M+H]^+$: 491.0635, Found: 491.0625. Anal Calcd. For.$C_{22}H_{23}{}^{81}BrN_2O_4S[M+H]^+$: 493.0615, Found: 493.0602.

IR (neat, cm^{-1}): υ 2976, 1709, 1386, 1313, 1184, 1133, 1084, 1013, 842, 818, 704, 688, 669.



ethyl 3-(4-bromophenyl)-5-propyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4j)

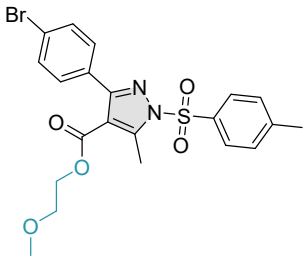
petroleum ether/ ethyl acetate = 10:1, white solid, 66% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 4.20 (q, *J* = 7.1 Hz, 2H), 3.38 – 3.15 (m, 2H), 2.43 (s, 3H), 1.85 – 1.68 (m, 2H), 1.19 (t, *J* = 7.1 Hz, 3H), 1.06 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 162.9, 154.1, 153.1, 146.2, 134.5, 130.9, 130.9, 130.8, 130.0, 128.3, 123.3, 112.8, 60.7, 27.8, 23.8, 21.7, 14.1, 13.9.

HRMS (ESI-TOF): Anal Calcd. For.$C_{22}H_{23}{}^{79}BrN_2O_4S[M+H]^+$: 491.0635, Found: 491.0628. Anal Calcd. For.$C_{22}H_{23}{}^{81}BrN_2O_4S[M+H]^+$: 493.0615, Found: 493.0609.

IR (neat, cm^{-1}): υ 2970, 2934, 2875, 1071, 1429, 1378, 1302, 1193, 1138, 1108, 1074, 1022, 816, 671.



2-methoxyethyl 3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4k)

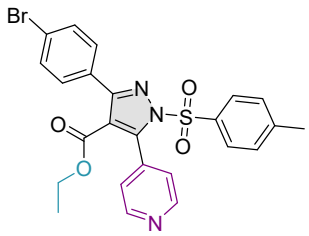
petroleum ether/ ethyl acetate = 10:1, white solid, 67% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.6 Hz, 2H), 7.42 (d, *J* = 8.6 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 4.31 – 4.25 (m, 2H), 3.50 – 3.45 (m, 2H), 3.27 (s, 3H), 2.86 (s, 3H), 2.43 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 162.9, 154.1, 148.7, 146.3, 134.2, 131.0, 130.9, 130.7, 130.1, 128.2, 123.3, 113.1, 69.9, 63.6, 58.8, 21.7, 12.3.

HRMS (ESI-TOF): Anal Calcd. For.$C_{21}H_{21}{}^{79}BrN_2O_5S[M+H]^+$: 493.0428, Found: 493.0419. Anal Calcd. For.$C_{21}H_{21}{}^{81}BrN_2O_5S[M+H]^+$: 495.0407, Found: 495.0440.

IR (neat, cm^{-1}): υ 2920, 2878, 1713, 1394, 1314, 1176, 1145, 1123, 1011, 831, 686, 668.



ethyl 3-(4-bromophenyl)-5-(pyridin-4-yl)-1-tosyl-1*H*-pyrazole-4-carboxylate (4l)

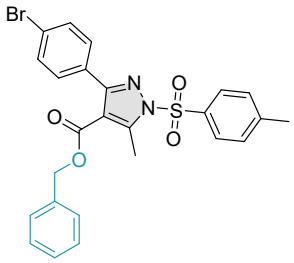
petroleum ether/ ethyl acetate = 3:1, white solid, 58% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.75 (d, *J* = 4.9 Hz, 2H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.60 – 7.51 (m, 4H), 7.35 – 7.30 (m, 2H), 7.28 – 7.25 (m, 2H), 3.97 (q, *J* = 7.1 Hz, 2H), 2.45 (s, 3H), 0.87 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 161.8, 153.8, 149.2, 146.7, 146.2, 137.1, 133.8, 131.2, 130.8, 130.1, 129.6, 128.5, 124.6, 123.9, 115.4, 61.0, 21.8, 13.3.

HRMS (ESI-TOF): Anal Calcd. For. $C_{24}H_{20}{}^{79}BrN_3O_4S[M+H]^+$: 526.0431, Found: 526.0433. Anal Calcd. For.$C_{24}H_{20}{}^{81}BrN_3O_4S[M+H]^+$: 528.0411, Found: 528.0406.

IR (neat, cm^{-1}): υ 2984, 1718, 1430, 1391, 1318, 1192, 1171, 1118, 1005, 843, 814, 702, 685, 667.



benzyl 3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4m)

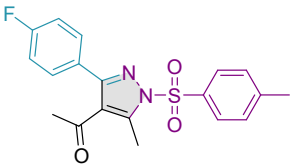
petroleum ether/ ethyl acetate = 10:1, white solid, 40% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.41 – 7.23 (m, 9H), 7.17 – 7.09 (m, 2H), 5.15 (s, 2H), 2.86 (s, 3H), 2.43 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 162.7, 154.2, 148.7, 146.3, 134.9, 134.2, 130.9, 130.7, 130.1, 128.5, 128.4, 128.4, 128.2, 123.2, 113.1, 66.5, 21.7, 12.4.

HRMS (ESI-TOF): Anal Calcd. For.$C_{25}H_{21}{}^{79}BrN_2O_4S[M+H]^+$: 525.0479, Found: 525.0480. Anal Calcd. For.$C_{25}H_{21}{}^{81}BrN_2O_4S[M+H]^+$: 527.0458, Found: 527.0449.

IR (neat, cm^{-1}): υ 1705, 1547, 1394, 1313, 1192, 1175, 1132, 1013, 831, 732, 704, 686, 668.



1-(3-(4-fluorophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4n)

petroleum ether/ ethyl acetate = 8:1, white solid, 70% yield.

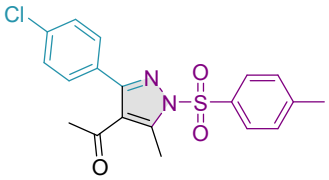
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.45 – 7.39 (m, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.13 – 7.07 (m, 2H), 2.75 (s, 3H), 2.43 (s, 3H), 2.06 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9, 163.4 (d, *J* = 249.6 Hz), 153.3, 146.2, 134.3, 130.9 (d, *J* = 8.4 Hz), 130.1, 128.1, 128.0, 128.0, 122.6, 115.6 (d, *J* = 21.8 Hz), 31.1, 21.7, 12.0.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -111.5.

HRMS (ESI-TOF): Anal Calcd. For.$C_{19}H_{17}FN_2O_3S[M+H]^+$: 373.1017, Found: 373.1008.

IR (neat, cm^{-1}): υ 1672, 1520, 1395, 1227, 1191, 1163, 1112, 843, 816, 739, 673, 661, 617.



1-(3-(4-chlorophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4o)

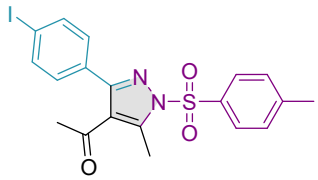
petroleum ether/ ethyl acetate = 8:1, white solid, 62% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 (d, J = 8.0 Hz, 2H), 7.54 – 7.45 (m, 6H), 2.74 (s, 3H), 2.37 (s, 3H), 2.12 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 194.9, 152.7, 146.7, 146.1, 134.3, 133.4, 130.6, 130.6, 130.3, 128.6, 127.9, 122.2, 31.1, 21.2, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{19}H_{17}ClN_2O_3S[M+H]^+$: 389.0722, Found: 389.0724.

IR (neat, cm^{-1}): υ 2926, 1660, 1417, 1090, 1015, 839, 830, 703, 667, 657, 611.



1-(3-(4-iodophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4p)

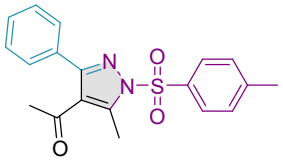
petroleum ether/ ethyl acetate = 10:1, white solid, 60% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 (d, J = 8.4 Hz, 2H), 7.82 (d, J = 8.3 Hz, 2H), 7.49 (d, J = 8.1 Hz, 2H), 7.24 (d, J = 8.4 Hz, 2H), 2.72 (s, 3H), 2.39 (s, 3H), 2.13 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 195.0, 152.9, 146.7, 146.1, 137.3, 133.4, 130.9, 130.8, 130.6, 127.9, 122.2, 96.3, 31.1, 21.2, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{19}H_{17}IN_2O_3S[M+H]^+$: 481.0078, Found: 481.0072.

IR (neat, cm^{-1}): υ 1672, 1411, 1393, 1312, 1190, 1179, 1110, 1007, 827, 680, 671, 653, 611.



1-(5-methyl-3-phenyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4q)

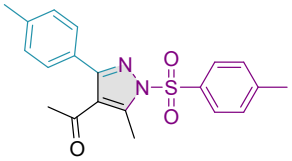
petroleum ether/ ethyl acetate = 8:1, white solid, 82% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, J = 8.2 Hz, 2H), 7.45 – 7.38 (m, 5H), 7.34 (d, J = 8.0 Hz, 2H), 2.75 (s, 3H), 2.41 (s, 3H), 2.04 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.3, 154.3, 146.2, 146.1, 134.3, 131.9, 130.1, 129.3, 129.0, 128.4, 128.1, 122.7, 31.2, 21.7, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{19}H_{18}N_2O_3S[M+H]^+$: 355.1111, Found: 355.1106.

IR (neat, cm^{-1}): υ 1671, 1393, 1308, 1188, 1178, 1112, 772, 705, 672, 648, 611.



1-(5-methyl-3-(p-tolyl)-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4r)

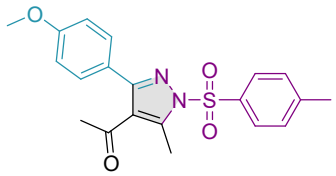
petroleum ether/ ethyl acetate = 8:1, white solid, 65% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 3.5 Hz, 2H), 7.32 (d, *J* = 3.2 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 2.74 (s, 3H), 2.42 (s, 3H), 2.38 (s, 3H), 2.06 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.5, 154.4, 146.1, 146.0, 139.3, 134.4, 130.0, 129.1, 128.9, 128.8, 128.1, 122.7, 31.1, 21.6, 21.3, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{20}H_{20}N_2O_3S[M+H]^+$: 369.1268, Found: 369.1261.

IR (neat, cm^{-1}): υ 2920, 1666, 1518, 1396, 1365, 1190, 1110, 1020, 960, 824, 817, 736, 671, 661, 619.



1-(3-(4-methoxyphenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4s)

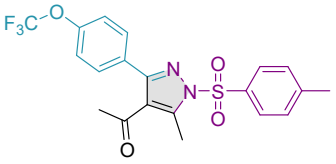
petroleum ether/ ethyl acetate = 3:1, white solid, 60% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 8.7 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 6.94 (d, *J* = 8.7 Hz, 2H), 3.84 (s, 3H), 2.73 (s, 3H), 2.43 (s, 3H), 2.07 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.7, 160.5, 154.2, 146.1, 146.1, 134.5, 130.3, 130.1, 128.2, 124.2, 122.7, 113.9, 55.3, 31.2, 21.7, 12.1.

HRMS (ESI-TOF): Anal Calcd. For.$C_{20}H_{20}N_2O_4S[M+H]^+$:385.1217, Found: 385.1214.

IR (neat, cm^{-1}): υ 2361, 2342, 1665, 1517, 1395, 1250, 1190, 1178, 1108, 1030, 957, 836, 816, 730, 671, 659, 619.



1-(5-methyl-1-tosyl-3-(4-(trifluoromethoxy)phenyl)-1*H*-pyrazol-4-yl)ethan-1-one (4t)

petroleum ether/ ethyl acetate = 8:1, white solid, 65% yield.

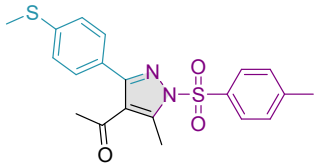
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, *J* = 8.0 Hz, 2H), 7.50 (d, *J* = 8.2 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 7.8 Hz, 2H), 2.77 (s, 3H), 2.44 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.8, 152.9, 150.0 (q, *J* = 1.9 Hz), 146.4, 146.3, 134.2, 130.6, 130.6, 130.2, 128.2, 122.6, 120.8, 120.3 (q, *J* = 259.2 Hz), 31.3, 21.7, 12.1.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.8.

HRMS (ESI-TOF): Anal Calcd. For.$C_{20}H_{17}F_3N_2O_4S[M+H]^+$: 439.0934, Found: 439.0931.

IR (neat, cm^{-1}): υ 2361, 2341, 1677, 1517, 1262, 1219, 1157, 1111, 1020, 858, 815, 671, 612.



1-(5-methyl-3-(4-(methylthio)phenyl)-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4u)

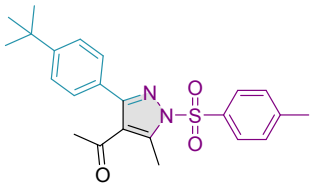
petroleum ether/ ethyl acetate = 8:1, white solid, 56% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 (d, J = 8.3 Hz, 2H), 7.49 (d, J = 8.1 Hz, 2H), 7.38 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 8.4 Hz, 2H), 2.71 (s, 3H), 2.50 (s, 3H), 2.39 (s, 3H), 2.12 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 195.3, 153.3, 146.6, 145.9, 140.2, 133.5, 130.6, 129.2, 127.9, 127.6, 125.4, 122.2, 31.1, 21.2, 14.3, 11.9.

HRMS (ESI-TOF): Anal Calcd. For.$C_{20}H_{20}N_2O_3S_2$[M+H]$^+$: 401.0989, Found: 401.0987.

IR (neat, cm^{-1}): υ 2361, 1668, 1391, 1367, 1311, 1190, 1109, 1017, 967, 819, 702, 668, 655, 612.



1-(3-(4-(tert-butyl)phenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4v)

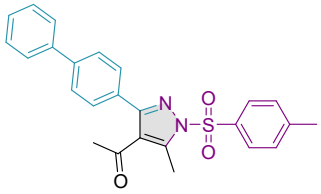
petroleum ether/ ethyl acetate = 8:1, white solid, 60% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, J = 8.2 Hz, 2H), 7.42 (d, J = 8.2 Hz, 2H), 7.37 (d, J = 8.3 Hz, 2H), 7.33 (d, J = 8.1 Hz, 2H), 2.75 (s, 3H), 2.42 (s, 3H), 2.08 (s, 3H), 1.32 (s, 9H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.7, 154.4, 152.5, 146.1, 146.0, 134.4, 130.0, 128.9, 128.6, 128.2, 125.4, 122.7, 34.7, 31.3, 31.2, 21.7, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{23}H_{26}N_2O_3S$[M+H]$^+$: 411.1737, Found: 411.1735.

IR (neat, cm^{-1}): υ 2360, 2342, 1681, 1384, 1192, 1115, 969, 846, 706, 665, 622.



1-(3-([1,1'-biphenyl]-4-yl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4w)

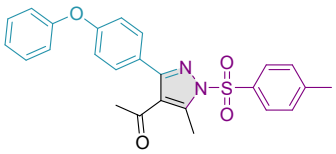
petroleum ether/ ethyl acetate = 8:1, white solid, 72% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.98 (d, J = 8.4 Hz, 2H), 7.75 (d, J = 8.4 Hz, 2H), 7.72-7.70 (m, 2H), 7.57 – 7.44 (m, 6H), 7.42 – 7.35 (m, 1H), 2.74 (s, 3H), 2.39 (s, 3H), 2.16 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 195.4, 153.5, 146.7, 146.0, 141.1, 139.3, 133.5, 130.6, 130.5, 129.4, 129.1, 128.0, 127.9, 126.8, 126.8, 122.4, 31.2, 21.2, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{25}H_{22}N_2O_3S$[M+H]$^+$: 431.1424, Found: 431.1428.

IR (neat, cm^{-1}): υ 2361, 2342, 1672, 1393, 1189, 1179, 1111, 969, 774, 743, 700, 671, 657, 614.



1-(5-methyl-3-(4-phenoxyphenyl)-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4x）

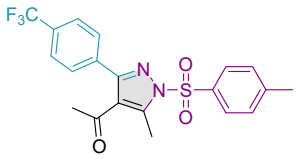
petroleum ether/ ethyl acetate = 8:1, white solid, 63% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, J = 8.1 Hz, 2H), 7.40 (d, J = 8.6 Hz, 2H), 7.37 – 7.33 (m, 4H), 7.15 (t, J = 7.4 Hz, 1H), 7.06 – 7.00 (m, 4H) 2.75 (s, 3H), 2.44 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.3, 158.6, 156.3, 153.8, 146.2, 146.2, 134.4, 130.5, 130.1, 129.9, 128.2, 126.5, 123.9, 122.7, 119.4, 118.3, 31.2, 21.7, 12.1.

HRMS (ESI-TOF): Anal Calcd. For.$C_{25}H_{22}N_2O_4S$[M+H]$^+$: 447.1374, Found: 447.1372.

IR (neat, cm^{-1}): υ 1666, 1515, 1489, 1409, 1396, 1360, 1312, 1235, 1191, 1171, 1113, 841, 765, 674, 614.



1-(5-methyl-1-tosyl-3-(4-(trifluoromethyl)phenyl)-1*H*-pyrazol-4-yl)ethan-1-one (4y)

petroleum ether/ ethyl acetate = 8:1, white solid, 50% yield.

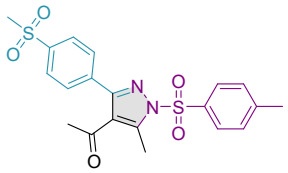
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.97 (d, J = 7.9 Hz, 2H), 7.81 (d, J = 8.0 Hz, 2H), 7.69 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 8.1 Hz, 2H), 2.76 (s, 3H), 2.40 (s, 3H), 2.16 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 194.8, 152.5, 146.8, 146.2, 135.6, 133.4, 130.6, 129.7, 129.4, 128.0, 125.3 (q, J = 4.7 Hz), 122.7, 122.3, 31.1, 21.2, 12.0.

^{19}F NMR (376 MHz, DMSO-d_6) δ -61.3.

HRMS (ESI-TOF): Anal Calcd. For. $C_{20}H_{17}F_3N_2O_3S[M+H]^+$: 423.0985, Found: 423.0980.

IR (neat, cm^{-1}): υ 2923, 2852, 1675, 1397, 1325, 1191, 1168, 1110, 1068, 1019, 850, 814, 670, 657.



1-(5-methyl-3-(4-(methylsulfonyl)phenyl)-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4z)

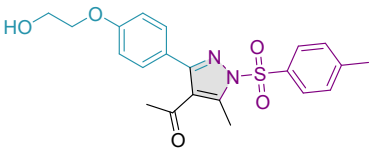
petroleum ether/ ethyl acetate = 1:1, white solid, 55% yield.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.98 (d, J = 8.3 Hz, 2H), 7.92 (d, J = 8.3 Hz, 2H), 7.66 (d, J = 8.3 Hz, 2H), 7.36 (d, J = 8.1 Hz, 2H), 3.07 (s, 3H), 2.76 (s, 3H), 2.43 (s, 3H), 2.12 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-d) δ 195.3, 152.2, 146.6, 146.4, 141.1, 137.4, 134.0, 130.2, 130.0, 128.2, 127.5, 122.6, 44.4, 31.4, 21.7, 12.2.

HRMS (ESI-TOF): Anal Calcd. For.$C_{20}H_{20}N_2O_5S_2[M+H]^+$: 433.0887, Found: 433.0887.

IR (neat, cm^{-1}): υ 2360, 1674, 1537, 1391, 1311, 1191, 1148, 1111, 1019, 961, 846, 785, 760, 670, 658.



1-(3-(4-(2-hydroxyethoxy)phenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4aa)

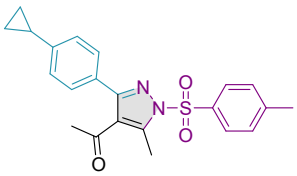
petroleum ether/ ethyl acetate = 1:1, white solid, 42% yield.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.92 (d, J = 8.4 Hz, 2H), 7.38 (d, J = 8.7 Hz, 2H), 7.34 (d, J = 8.2 Hz, 2H), 6.96 (d, J = 8.7 Hz, 2H), 4.14 – 4.10 (m, 2H), 4.01 – 3.95 (m, 3H), 2.74 (s, 3H), 2.43 (s, 3H), 2.07 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-d) δ 196.7, 159.6, 154.0, 146.1, 146.1, 134.5, 130.4, 130.1, 128.2, 124.7, 122.7, 114.5, 69.2, 61.4, 31.2, 21.7, 12.1.

HRMS (ESI-TOF): Anal Calcd. For.$C_{21}H_{22}N_2O_5S[M+H]^+$: 415.1323, Found: 415.1319.

IR (neat, cm^{-1}): υ 3435, 2920, 2360, 1656, 1520, 1406, 1390, 1310, 1251, 1186, 1115, 1077, 811, 744, 674, 637.



1-(3-(4-cyclopropylphenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ab)

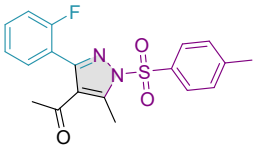
petroleum ether/ ethyl acetate = 8:1, white solid, 55% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 8.2 Hz, 2H), 7.31 (d, J = 8.2 Hz, 2H), 7.16 (d, J = 8.3 Hz, 2H), 2.71 (s, 3H), 2.40 (s, 3H), 2.09 (s, 3H), 2.02 – 1.91 (m, 1H), 1.03 – 0.96 (m, 2H), 0.74 – 0.68 (m, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 195.5, 153.8, 146.6, 145.8, 145.5, 133.6, 130.6, 128.6, 128.3, 127.9, 125.4, 122.2, 31.1, 21.2, 15.0, 11.9, 9.9.

HRMS (ESI-TOF): Anal Calcd. For.$C_{22}H_{22}N_2O_3S[M+H]^+$: 395.1424, Found: 395.1425.

IR (neat, cm^{-1}): υ 2922, 2852, 1666, 1518, 1410, 1366, 1310, 1190, 1173, 1110, 1016, 969, 815, 716, 618, 657, 622.



1-(3-(2-fluorophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ac)

petroleum ether/ ethyl acetate = 8:1, white solid, 52% yield.

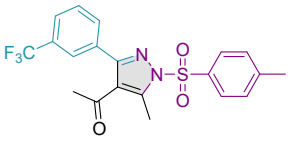
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, J = 8.4 Hz, 2H), 7.51 (td, J = 7.4, 1.8 Hz, 1H), 7.48 – 7.38 (m, 1H), 7.35 (d, J = 8.1 Hz, 2H), 7.24 (td, J = 7.5, 1.1 Hz, 1H), 7.14 – 7.08 (m, 1H), 2.79 (s, 3H), 2.44 (s, 3H), 2.07 (d, J = 1.2 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.1, 160.0 (d, J = 248.5 Hz), 148.9, 146.4, 146.3, 134.3, 131.5 (d, J = 8.2 Hz), 131.2 (d, J = 2.8 Hz), 130.2, 128.2, 124.5 (d, J = 3.6 Hz), 123.1, 120.4 (d, J = 14.7 Hz), 115.7 (d, J = 21.2 Hz), 29.9 (d, J = 2.0 Hz), 21.7, 12.1.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -114.1.

HRMS (ESI-TOF): Anal Calcd. For. $C_{19}H_{17}FN_2O_3S[M+H]^+$: 373.1017, Found: 373.1019.

IR (neat, cm^{-1}): υ 2360, 1666, 1536, 1395, 1369, 1318, 1189, 1179, 1116, 1106, 972, 816, 759, 750, 672, 648, 615.



1-(5-methyl-1-tosyl-3-(3-(trifluoromethyl)phenyl)-1*H*-pyrazol-4-yl)ethan-1-one (4ad)

petroleum ether/ ethyl acetate = 8:1, white solid, 50% yield.

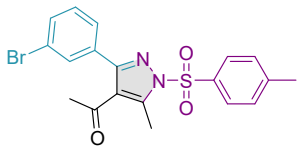
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, J = 8.0 Hz, 2H), 7.76 – 7.67 (m, 2H), 7.66 – 7.62 (m, 1H), 7.58 – 7.52 (m, 1H), 7.37 (d, J = 8.1 Hz, 2H), 2.77 (s, 3H), 2.44 (s, 3H), 2.07 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.5, 152.8, 146.6, 146.5, 134.1, 132.8, 132.4, 131.2, 130.8, 130.2, 129.0, 128.2, 126.0 (q, J = 3.9 Hz), 122.6, 122.4, 31.2, 21.7, 12.2.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.7.

HRMS (ESI-TOF): Anal Calcd. For.$C_{20}H_{17}F_3N_2O_3S[M+H]^+$: 423.0985, Found: 423.0983.

IR (neat, cm^{-1}): υ 2364, 1673, 1531, 1414, 1333, 1305, 1272, 1191, 1162, 1113, 1074, 981, 822, 808, 746, 706, 673, 658, 640.



1-(3-(3-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ae)

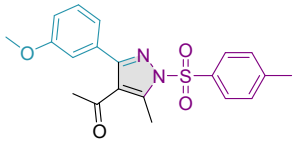
petroleum ether/ ethyl acetate = 10:1, white solid, 65% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.5 Hz, 2H), 7.63 (t, *J* = 1.8 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.39 – 7.32 (m, 3H), 7.28 (t, *J* = 7.8 Hz, 1H), 2.75 (s, 3H), 2.44 (s, 3H), 2.08 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.7, 152.7, 146.4, 146.3, 134.2, 133.9, 132.3, 131.8, 130.2, 129.9, 128.2, 127.7, 122.6, 122.5, 31.3, 21.7, 12.1.

HRMS (ESI-TOF): Anal Calcd. For. $C_{19}H_{17}{}^{79}BrN_2O_3S[M+H]^+$: 433.0217, Found: 433.0221. Anal Calcd. For. $C_{19}H_{17}{}^{81}BrN_2O_3S[M+H]^+$: 435.0196, Found: 435.0194.

IR (neat, cm^{-1}): υ 1668, 1534, 1394, 1367, 1310, 1190, 1178, 1113, 801, 704, 689, 670, 650, 620.



1-(3-(3-methoxyphenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4af)

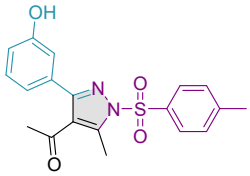
petroleum ether/ ethyl acetate = 10:1, white solid, 71% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.41 – 7.34 (m, 1H), 7.07 – 7.03 (m, 1H), 7.00 – 6.95 (m, 2H), 3.77 (s, 3H), 2.71 (s, 3H), 2.40 (s, 3H), 2.08 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 195.2, 159.1, 153.7, 146.7, 145.9, 133.5, 132.8, 130.6, 129.8, 127.9, 122.3, 121.1, 115.0, 114.2, 55.2, 31.0, 21.2, 11.9.

HRMS (ESI-TOF): Anal Calcd. For.$C_{20}H_{20}N_2O_4S[M+H]^+$: 385.1217, Found: 385.1208.

IR (neat, cm^{-1}): υ 2923, 2852, 1675, 1591, 1536, 1409, 1311, 1244, 1188, 1179, 1112, 985, 862, 797, 705, 670, 655, 634.



1-(3-(3-hydroxyphenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ag)

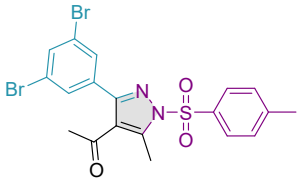
petroleum ether/ ethyl acetate = 3:1, white solid, 76% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.27 – 7.22 (m, 1H), 6.94 – 6.91 (m, 2H), 6.90 – 6.86 (m, 1H), 5.88 (s, 1H), 2.75 (s, 3H), 2.43 (s, 3H), 2.08 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.8, 156.0, 154.2, 146.4, 146.3, 134.3, 133.0, 130.2, 129.8, 128.2, 122.7, 121.3, 116.7, 115.9, 31.2, 21.7, 12.1.

HRMS (ESI-TOF): Anal Calcd. For. $C_{19}H_{18}N_2O_4S[M+H]^+$: 371.1061, Found: 371.1059.

IR (neat, cm^{-1}): υ 3280, 2360, 1657, 1536, 1380, 1318, 1190, 1181, 1114, 993, 866, 804, 711, 672, 656.



1-(3-(3,5-dibromophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ah)

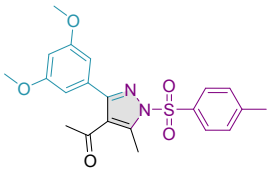
petroleum ether/ ethyl acetate = 10:1, white solid, 50% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.97 (d, J = 8.4 Hz, 2H), 7.95 (d, J = 1.4 Hz, 1H), 7.68 (d, J = 1.8 Hz, 2H), 7.51 (d, J = 8.1 Hz, 2H), 2.76 (s, 3H), 2.40 (s, 3H), 2.20 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 194.2, 151.1, 146.8, 146.2, 135.5, 134.1, 133.3, 130.7, 130.6, 128.0, 122.3, 122.2, 31.2, 21.2, 12.2.

HRMS (ESI-TOF): Anal Calcd. For. $C_{19}H_{16}{}^{79}Br_2N_2O_3S[M+H]^+$: 510.9322, Found:510.9293. Anal Calcd. For. $C_{19}H_{16}{}^{79}Br^{81}BrN_2O_3S[M+H]^+$: 512.9301, Found: 512.9309. $C_{19}H_{16}{}^{81}Br_2N_2O_3S[M+H]^+$: 514.9281, Found:514.9303.

IR (neat, cm^{-1}): υ 1674, 1546, 1529, 1395, 1310, 1192, 1179, 1114, 983, 857, 813, 725, 684, 670, 653, 624.



1-(3-(3,5-dimethoxyphenyl)-5-methyl-1-tosyl-1H-pyrazol-4-yl)ethan-1-one (4ai)

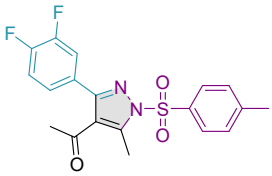
petroleum ether/ ethyl acetate = 3:1, white solid, 71% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 (d, J = 8.5 Hz, 2H), 7.50 (d, J = 8.2 Hz, 2H), 6.61 (t, J = 2.3 Hz, 1H), 6.54 (d, J = 2.3 Hz, 2H), 3.76 (s, 6H), 2.71 (s, 3H), 2.40 (s, 3H), 2.09 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 195.2, 160.4, 153.7, 146.7, 145.8, 133.5, 133.5, 130.6, 127.9, 122.2, 106.9, 101.1, 55.4, 30.9, 21.2, 11.8.

HRMS (ESI-TOF): Anal Calcd. For.$C_{21}H_{22}N_2O_5S[M+H]^+$: 415.1323, Found: 415.1323.

IR (neat, cm^{-1}): υ 2921, 2850, 1673, 1601, 1319, 1192, 1181, 1156, 1114, 1024, 995, 840, 814, 717, 697, 670, 656.



1-(3-(3,4-difluorophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4aj)

petroleum ether/ ethyl acetate = 8:1, white solid, 58% yield.

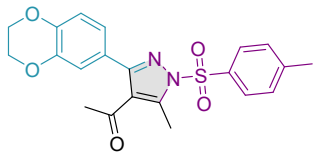
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, J = 8.5 Hz, 2H), 7.36 (d, J = 8.2 Hz, 2H), 7.34 – 7.27 (m, 1H), 7.24 – 7.13 (m, 2H), 2.75 (s, 3H), 2.44 (s, 3H), 2.11 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.5, 152.1, 151.8 (dd, J = 93.7, 11.8 Hz), 149.3 (dd, J = 93.4, 11.9 Hz), 146.4, 146.3, 134.1, 130.2, 128.9, 128.2, 125.5 (q, J = 5.0, 4.3 Hz), 122.5, 118.2 (d, J = 18.3 Hz), 117.4 (d, J = 17.4 Hz), 31.2, 21.7, 12.1.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -136.1 (d, J = 21.3 Hz), -136.7 (d, J = 21.2 Hz).

HRMS (ESI-TOF): Anal Calcd. For.$C_{19}H_{16}F_2N_2O_3S[M+H]^+$: 391.0923, Found: 391.0920.

IR (neat, cm^{-1}): υ 1669, 1517, 1399, 1314, 1268, 1190, 1180, 1107, 989, 889, 825, 813, 777, 671, 655.



1-(3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ak)

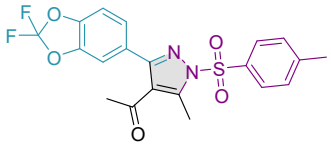
petroleum ether/ ethyl acetate = 3:1, white solid, 55% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.94 (d, J = 8.1 Hz, 2H), 7.50 (d, J = 8.1 Hz, 2H), 6.96 – 6.89 (m, 2H), 6.89 – 6.83 (m, 1H), 4.27 (s, 4H), 2.68 (s, 3H), 2.40 (s, 3H), 2.12 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 195.5, 153.3, 146.6, 145.7, 144.5, 143.2, 133.6, 130.6, 127.9, 124.3, 122.2, 121.9, 117.3, 117.2, 64.2, 64.1, 31.1, 21.2, 11.9.

HRMS (ESI-TOF): Anal Calcd. For.$C_{21}H_{20}N_2O_5S[M+H]^+$: 413.1166, Found: 413.1160.

IR (neat, cm^{-1}): υ 2360, 2342, 1664, 1517, 1283, 1189, 1109, 1067, 893, 864, 863, 826, 741, 671, 657.



1-(3-(2,2-difluorobenzo[d][1,3]dioxol-5-yl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4al)

petroleum ether/ ethyl acetate = 8:1, white solid, 62% yield.

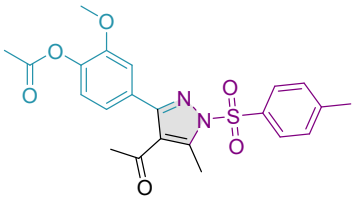
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, J = 8.3 Hz, 2H), 7.36 (d, J = 8.1 Hz, 2H), 7.22 (d, J = 1.6 Hz, 1H), 7.17 – 7.08 (m, 2H), 2.76 (s, 3H), 2.44 (s, 3H), 2.12 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.8, 152.7, 146.4, 146.3, 144.5, 143.8, 134.2, 131.6, 130.2, 128.3, 128.0, 124.9, 122.5, 110.3, 109.4, 31.3, 21.7, 12.1.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -49.8.

HRMS (ESI-TOF): Anal Calcd. For.$C_{20}H_{16}F_2N_2O_5S[M+H]^+$: 435.0821, Found: 435.0823.

IR (neat, cm^{-1}): υ 2361, 2342, 1674, 1463, 1237, 1192, 1149, 1108, 1031, 914, 816, 702, 676, 655, 640.



4-(4-acetyl-5-methyl-1-tosyl-1*H*-pyrazol-3-yl)-2-methoxyphenyl acetate (4am)

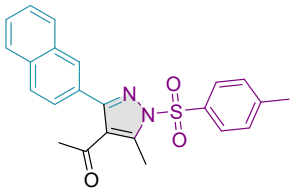
petroleum ether/ ethyl acetate = 3:1, white solid, 51% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, J = 8.1 Hz, 2H), 7.34 (d, J = 8.2 Hz, 2H), 7.12 – 7.03 (m, 2H), 7.00 – 6.93 (m, 1H), 3.84 (s, 3H), 2.73 (s, 3H), 2.42 (s, 3H), 2.31 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.3, 168.5, 153.4, 151.0, 146.2, 146.0, 140.6, 134.1, 130.5, 130.0, 128.1, 122.8, 122.6, 121.4, 112.9, 55.9, 31.2, 21.6, 20.5, 11.9.

HRMS (ESI-TOF): Anal Calcd. For.$C_{22}H_{22}N_2O_6S[M+H]^+$: 443.1272, Found: 443.1276.

IR (neat, cm^{-1}): υ 2360, 2342, 1764, 1664, 1397, 1367, 1316, 1217, 1190, 1176, 1111, 988, 869, 821, 670, 658.



1-(5-methyl-3-(naphthalen-2-yl)-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4an)

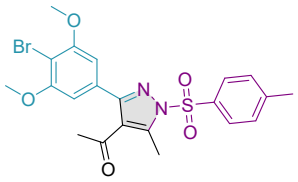
petroleum ether/ ethyl acetate = 8:1, white solid, 66% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.06 – 7.95 (m, 6H), 7.62 – 7.55 (m, 3H), 7.51 (d, J = 7.9 Hz, 2H), 2.76 (s, 3H), 2.40 (s, 3H), 2.11 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 195.3, 153.8, 146.7, 146.1, 133.6, 133.0, 132.5, 130.6, 128.9, 128.3, 128.2, 128.1, 127.9, 127.7, 127.1, 126.8, 126.2, 122.5, 31.1, 21.2, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{23}H_{20}N_2O_3S[M+H]^+$: 405.1268, Found: 405.1265.

IR (neat, cm^{-1}): υ 2360, 1669, 1528, 1408, 1364, 1307, 1190, 1177, 1108, 985, 860, 827, 747, 681, 669, 659, 625.



1-(3-(4-bromo-3,5-dimethoxyphenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ao)

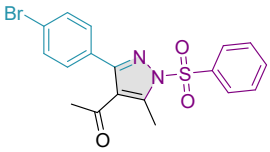
petroleum ether/ ethyl acetate = 3:1, white solid, 73% yield.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.91 (d, J = 8.4 Hz, 2H), 7.34 (d, J = 8.1 Hz, 2H), 6.62 (s, 2H), 3.87 (s, 6H), 2.73 (s, 3H), 2.41 (s, 3H), 2.09 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-d) δ 196.2, 157.0, 153.5, 146.3, 146.1, 134.2, 132.2, 130.1, 128.2, 122.6, 105.4, 102.3, 56.5, 31.2, 21.7, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{21}H_{21}{}^{79}BrN_2O_5S[M+H]^+$: 493.0428, Found: 493.0423. Anal Calcd. For.$C_{21}H_{21}{}^{81}BrN_2O_5S[M+H]^+$: 495.0407, Found: 495.0425.

IR (neat, cm^{-1}): υ 2361, 2342, 1670, 1579, 1404, 1390, 1241, 1189, 1179, 1118, 1001, 846, 719, 679, 660, 630.



1-(3-(4-bromophenyl)-5-methyl-1-(phenylsulfonyl)-1*H*-pyrazol-4-yl)ethan-1-one (4ap)

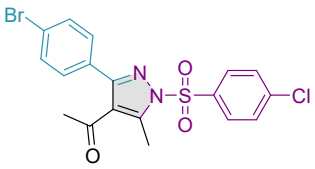
petroleum ether/ ethyl acetate = 8:1, white solid, 68% yield.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.05 (d, J = 7.5 Hz, 2H), 7.71 – 7.66 (m, 1H), 7.59 – 7.54 (m, 4H), 7.32 (d, J = 8.4 Hz, 2H), 2.76 (s, 3H), 2.09 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-d) δ 196.0, 153.3, 146.5, 137.3, 134.9, 131.8, 130.8, 130.5, 129.5, 128.2, 123.9, 122.7, 31.3, 12.1.

HRMS (ESI-TOF): Anal Calcd. For.$C_{18}H_{15}{}^{79}BrN_2O_3S[M+H]^+$: 419.0060, Found: 419.0065. Anal Calcd. For.$C_{18}H_{15}{}^{81}BrN_2O_3S[M+H]^+$: 421.0040, Found: 421.0047.

IR (neat, cm^{-1}): υ 2361, 1674, 1416, 1394, 1313, 1189, 1168, 1108, 1013, 967, 838, 755, 727, 683, 653, 619.



1-(3-(4-bromophenyl)-1-((4-chlorophenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4aq)

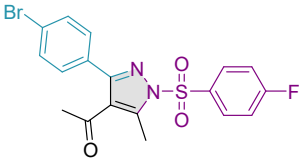
petroleum ether/ ethyl acetate = 10:1, white solid, 66% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 8.3 Hz, 2H), 7.58 – 7.52 (m, 4H), 7.32 (d, *J* = 8.0 Hz, 2H), 2.76 (s, 3H), 2.09 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9, 153.6, 146.6, 141.9, 135.6, 131.8, 130.6, 130.5, 129.9, 129.7, 124.0, 122.8, 31.3, 12.1.

HRMS (ESI-TOF): Anal Calcd. For.$C_{18}H_{14}{}^{79}BrClN_2O_3S[M+H]^+$: 452.9670, Found: 452.9663. Anal Calcd. For.$C_{18}H_{14}{}^{81}BrClN_2O_3S[M+H]^+$: 454.9650, Found: 454.9653.

IR (neat, cm^{-1}): υ 1673, 1532, 1394, 1311, 1188, 1164, 1113, 1010, 833, 768, 755, 702, 657, 630, 620, 608.



1-(3-(4-bromophenyl)-1-((4-fluorophenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4ar)

petroleum ether/ ethyl acetate = 10:1, white solid, 57% yield.

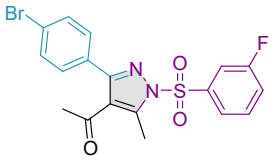
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 (dd, *J* = 8.7, 4.9 Hz, 2H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 7.6 Hz, 2H), 2.80 (s, 3H), 2.13 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9, 166.4 (d, *J* = 259.4 Hz), 153.5, 146.5, 133.2 (d, *J* = 3.0 Hz), 131.8, 131.3 (d, *J* = 10.0 Hz), 130.7, 130.5, 124.0, 122.7, 117.0 (d, *J* = 23.0 Hz), 31.3, 12.1.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -100.4.

HRMS (ESI-TOF): Anal Calcd. For.$C_{18}H_{14}{}^{79}BrFN_2O_3S[M+H]^+$: 436.9966, Found: 436.9958. Anal Calcd. For.$C_{18}H_{14}{}^{81}BrFN_2O_3S[M+H]^+$: 438.9949, Found: 438.9939.

IR (neat, cm^{-1}): υ 2358, 1674, 1394, 1313, 1188, 1155, 1112, 1081, 1011, 836, 828, 708, 690, 674, 654, 612.



1-(3-(4-bromophenyl)-1-((3-fluorophenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4as)

petroleum ether/ ethyl acetate = 8:1, white solid, 50% yield.

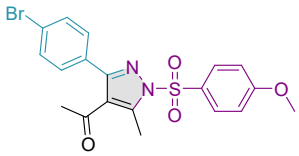
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.81 (m, 1H), 7.78 – 7.71 (m, 1H), 7.62 – 7.52 (m, 3H), 7.43 – 7.34 (m, 1H), 7.32 (d, *J* = 8.4 Hz, 2H), 2.76 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9, 162.3 (d, *J* = 253.4 Hz), 153.6, 146.7, 139.0 (d, *J* = 7.2 Hz), 131.8, 131.4 (d, *J* = 7.8 Hz), 130.5, 130.5, 124.0 (d, *J* = 1.8 Hz), 124.0, 122.9, 122.3 (d, *J* = 21.2 Hz), 115.6 (d, *J* = 25.1 Hz), 31.3, 12.1.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -107.8.

HRMS (ESI-TOF): Anal Calcd. For.$C_{18}H_{14}{}^{79}BrFN_2O_3S[M+H]^+$: 439.9966, Found: 436.9968. Anal Calcd. For.$C_{18}H_{14}{}^{81}BrFN_2O_3S[M+H]^+$: 438.9945, Found: 438.9952.

IR (neat, cm^{-1}): υ 2361, 1674, 1428, 1396, 1313, 1228, 1182, 1109, 1072, 1011, 968, 838, 699, 672, 653, 618, 607.



1-(3-(4-bromophenyl)-1-((4-methoxyphenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4at)

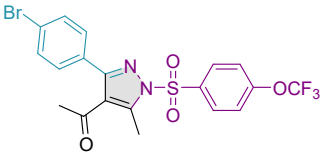
petroleum ether/ ethyl acetate = 5:1, white solid, 65% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 9.0 Hz, 2H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 6.99 (d, *J* = 9.0 Hz, 2H), 3.86 (s, 3H), 2.75 (s, 3H), 2.08 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9, 164.7, 153.0, 146.1, 131.7, 130.9, 130.6, 130.6, 128.4, 123.7, 122.4, 114.7, 55.8, 31.3, 12.1.

HRMS (ESI-TOF): Anal Calcd. For.$C_{19}H_{17}{}^{79}BrN_2O_4S[M+H]^+$: 449.0166, Found: 449.0162. Anal Calcd. For.$C_{19}H_{17}{}^{81}BrN_2O_4S[M+H]^+$: 451.0145, Found: 451.0139.

IR (neat, cm^{-1}): υ 2361, 1667, 1594, 1391, 1370, 1314, 1267, 1192, 1161, 1112, 1083, 1010, 840, 833, 806, 689, 677, 656.



1-(3-(4-bromophenyl)-5-methyl-1-((4-(trifluoromethoxy)phenyl)sulfonyl)-1H-pyrazol-4-yl)ethan-1-one (4au)

petroleum ether/ ethyl acetate = 10:1, white solid, 40% yield.

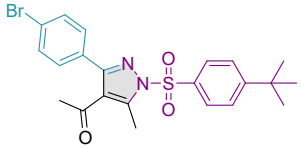
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.11 (d, *J* = 8.8 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.6 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 2.76 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9, 153.7, 146.5, 142.0, 135.1, 134.4, 131.9, 130.7, 130.5, 127.3, 124.1, 123.0, 121.0, 31.4, 12.2.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.6.

HRMS (ESI-TOF): Anal Calcd. For.$C_{19}H_{14}{}^{79}BrF_3N_2O_4S[M+H]^+$: 502.9883, Found: 502.9886. Anal Calcd. For.$C_{19}H_{14}{}^{81}BrF_3N_2O_4S[M+H]^+$: 504.9863, Found: 504.9866.

IR (neat, cm^{-1}): υ 3435, 2920, 2360, 1656, 1520, 1406, 1310, 1251, 1186, 1115, 1077, 970, 811, 744, 674, 637.



1-(3-(4-bromophenyl)-1-((4-(tert-butyl)phenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4av)

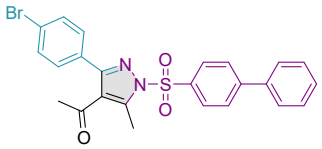
petroleum ether/ ethyl acetate = 10:1, white solid, 58% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 8.7 Hz, 2H), 7.59– 7.53 (m, 4H), 7.34 (d, *J* = 8.5 Hz, 2H), 2.75 (s, 3H), 2.09 (s, 3H), 1.33 (s, 9H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.1, 159.1, 153.1, 146.3, 134.2, 131.7, 130.9, 130.6, 128.1, 126.6, 123.8, 122.6, 35.4, 31.3, 30.9, 12.1.

HRMS (ESI-TOF): Anal Calcd. For. $C_{22}H_{23}{}^{79}BrN_2O_3S[M+H]^+$: 475.0686, Found: 475.0680. Anal Calcd. For.$C_{22}H_{23}{}^{81}BrN_2O_3S[M+H]^+$: 477.0666, Found: 477.0668.

IR (neat, cm^{-1}): υ 2956, 2362, 1681, 1374, 1184, 1115, 1103, 833, 658, 627, 610.



1-(1-([1,1'-biphenyl]-4-ylsulfonyl)-3-(4-bromophenyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4aw)

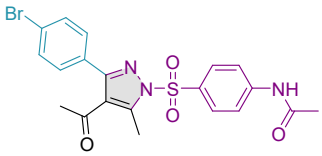
petroleum ether/ ethyl acetate = 8:1, white solid, 56% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.10 (d, *J* = 8.5 Hz, 2H), 7.76 (d, *J* = 8.6 Hz, 2H), 7.60 – 7.53 (m, 4H), 7.51 – 7.40 (m, 3H), 7.34 (d, *J* = 8.4 Hz, 2H), 2.80 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9, 153.3, 147.8, 146.4, 138.5, 135.5, 131.7, 130.8, 130.5, 129.1, 129.0, 128.7, 128.0, 127.3, 123.8, 122.6, 31.3, 12.1.

HRMS (ESI-TOF): Anal Calcd. For.$C_{24}H_{19}{}^{79}BrN_2O_3S[M+H]^+$: 495.0373, Found: 495.0370. Anal Calcd. For.$C_{24}H_{19}{}^{81}BrN_2O_3S[M+H]^+$: 497.0353, Found: 497.0350.

IR (neat, cm^{-1}): υ 2361, 1668, 1391, 1367, 1311, 1190, 1179, 1109, 1017, 967, 819, 702, 668, 655, 612.



N-(4-((4-acetyl-3-(4-bromophenyl)-5-methyl-1*H*-pyrazol-1-yl)sulfonyl)phenyl)acetamide (4ax)

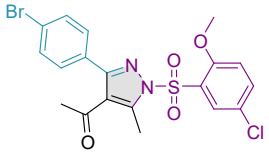
petroleum ether/ ethyl acetate = 1:1, white solid, 60% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 (s, 1H), 7.92 (d, *J* = 8.5 Hz, 2H), 7.71 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.3 Hz, 2H), 2.75 (s, 3H), 2.17 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.0, 169.1, 153.3, 146.4, 144.2, 131.8, 130.9, 130.6, 130.4, 129.6, 123.9, 122.6, 119.4, 31.3, 24.6, 12.1.

HRMS (ESI-TOF): Anal Calcd. For. $C_{20}H_{18}{}^{79}BrN_3O_4S[M+H]^+$: 476.0275, Found: 476.0272. Anal Calcd. For.$C_{20}H_{18}{}^{81}BrN_3O_4S[M+H]^+$: 478.0254, Found: 478.0247.

IR (neat, cm^{-1}): υ 2362, 1705, 1658, 1528, 1406, 1369, 1316, 1192, 1173, 1108, 1010, 836, 822, 652, 634, 627, 620, 606.



1-(3-(4-bromophenyl)-1-((5-chloro-2-methoxyphenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4ay)

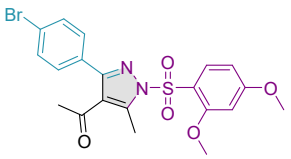
petroleum ether/ ethyl acetate = 3:1, colorless oil, 58% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.10 (d, *J* = 2.6 Hz, 1H), 7.55 (d, *J* = 2.7 Hz, 1H), 7.52 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 6.91 (d, *J* = 8.9 Hz, 1H), 3.81 (s, 3H), 2.82 (s, 3H), 2.12 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.0, 155.9, 153.2, 148.6, 136.5, 131.7, 131.0, 130.7, 130.5, 126.3, 126.0, 123.8, 121.8, 113.9, 56.6, 31.4, 12.2.

HRMS (ESI-TOF): Anal Calcd. For.$C_{19}H_{16}{}^{79}BrClN_2O_4S[M+H]^+$: 482.9776, Found: 482.9776. Anal Calcd. For.$C_{19}H_{16}{}^{81}BrClN_2O_4S[M+H]^+$: 484.9755, Found: 484.9773.

IR (neat, cm^{-1}): υ 2923, 2361, 2341, 1673, 1478, 1274, 1187, 1111, 1010, 961, 829, 814, 725, 654, 645, 615.



1-(3-(4-bromophenyl)-1-((2,4-dimethoxyphenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4az)

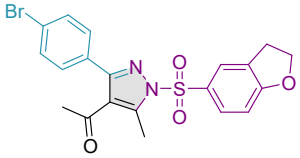
petroleum ether/ ethyl acetate = 3:1, white solid, 64% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 (d, *J* = 9.0 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 6.58 (dd, *J* = 9.0, 2.3 Hz, 1H), 6.42 (d, *J* = 2.3 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 2.81 (s, 3H), 2.11 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9, 166.6, 159.1, 152.4, 147.8, 133.4, 131.5, 131.1, 130.5, 123.4, 121.4, 116.9, 105.1, 99.2, 56.1, 55.8, 31.3, 12.1.

HRMS (ESI-TOF): Anal Calcd. For.$C_{20}H_{19}{}^{79}BrN_2O_5S[M+H]^+$: 479.0271, Found: 479.0271. Anal Calcd. For.$C_{20}H_{19}{}^{81}BrN_2O_5S[M+H]^+$: 481.0251, Found: 481.0233.

IR (neat, cm^{-1}): υ 2360, 1671, 1413, 1364, 1299, 1186, 1168, 1104, 1075, 1012, 842, 678, 655, 608.



1-(3-(4-bromophenyl)-1-((2,3-dihydrobenzofuran-5-yl)sulfonyl)-5-methyl-1H-pyrazol-4-yl)ethan-1-one (4ba)

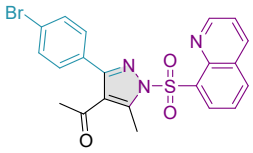
petroleum ether/ ethyl acetate = 10:1, white solid, 71% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 – 7.80 (m, 2H), 7.55 (d, *J* = 8.5 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 1H), 4.69 (t, *J* = 8.9 Hz, 2H), 3.26 (t, *J* = 8.8 Hz, 2H), 2.75 (s, 3H), 2.08 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.0, 165.8, 152.8, 146.0, 131.7, 131.0, 130.6, 130.5, 129.1, 128.2, 125.6, 123.7, 122.4, 110.0, 72.7, 31.3, 28.8, 12.1.

HRMS (ESI-TOF): Anal Calcd. For. $C_{20}H_{17}{}^{79}BrN_2O_4S[M+H]^+$: 461.0166, Found: 461.0164. Anal Calcd. For.$C_{20}H_{17}{}^{81}BrN_2O_4S[M+H]^+$: 463.0145, Found: 463.0146.

IR (neat, cm^{-1}): υ 2955, 2895, 1666, 1393, 1366, 1243, 1187, 1159, 1107, 1060, 1010, 893, 828, 702, 656, 614, 605.



1-(3-(4-bromophenyl)-5-methyl-1-(quinolin-8-ylsulfonyl)-1*H*-pyrazol-4-yl)ethan-1-one (4bb)

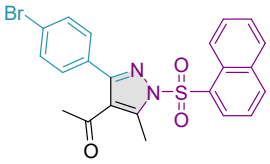
petroleum ether/ ethyl acetate = 3:1, white solid, 51% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.93 (d, *J* = 3.3 Hz, 1H), 8.71 (d, *J* = 7.4 Hz, 1H), 8.22 (d, *J* = 8.3 Hz, 1H), 8.14 (d, *J* = 8.2 Hz, 1H), 7.70 (t, *J* = 7.9 Hz, 1H), 7.51 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 3.14 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.1, 153.1, 151.5, 150.0, 143.6, 136.5, 135.7, 134.2, 133.6, 131.5, 131.0, 130.5, 128.7, 125.5, 123.6, 122.5, 121.5, 31.4, 12.9.

HRMS (ESI-TOF): Anal Calcd. For.$C_{21}H_{16}{}^{79}BrN_3O_3S[M+H]^+$: 470.0169, Found: 470.0163. Anal Calcd. For.$C_{21}H_{16}{}^{81}BrN_3O_3S[M+H]^+$: 472.0149, Found: 472.0130.

IR (neat, cm^{-1}): υ 1674, 1384, 1371, 1309, 1183, 1113, 1091, 1008, 831, 792, 690, 676, 658, 631.



1-(3-(4-bromophenyl)-5-methyl-1-(naphthalen-1-ylsulfonyl)-1*H*-pyrazol-4-yl)ethan-1-one (4bc)

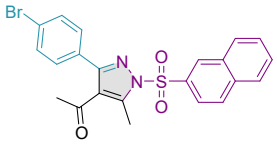
petroleum ether/ ethyl acetate = 8:1, white solid, 64% yield.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.77 – 8.70 (m, 1H), 8.61 – 8.54 (m, 1H), 8.47 (d, *J* = 8.2 Hz, 1H), 8.17 (d, *J* = 8.2 Hz, 1H), 7.87 – 7.78 (m, 2H), 7.75 – 7.70 (m, 1H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 2.66 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 194.7, 151.9, 145.6, 137.4, 133.8, 131.7, 131.5, 131.3, 130.8, 130.7, 129.5, 129.3, 127.7, 127.3, 124.9, 123.5, 122.9, 122.4, 31.0, 12.1.

HRMS (ESI-TOF): Anal Calcd. For.$C_{22}H_{17}{}^{79}BrN_2O_3S[M+H]^+$: 469.0217, Found: 469.0214. Anal Calcd. For.$C_{22}H_{17}{}^{81}BrN_2O_3S[M+H]^+$: 471.0196, Found: 471.0213.

IR (neat, cm^{-1}): υ 2921, 2851, 1670, 1632, 1419, 1372, 1310, 1182, 1106, 1010, 968, 838, 806, 766, 689, 645, 628, 617.



1-(3-(4-bromophenyl)-5-methyl-1-(naphthalen-2-ylsulfonyl)-1*H*-pyrazol-4-yl)ethan-1-one (4bd)

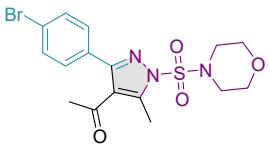
petroleum ether/ ethyl acetate = 8:1, white solid, 50% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.66 (s, 1H), 8.03 – 7.87 (m, 4H), 7.72 – 7.62 (m, 2H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 2.81 (s, 3H), 2.07 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9, 153.3, 146.5, 135.6, 134.0, 131.8, 131.7, 130.8, 130.5, 130.3, 130.1, 130.0, 129.6, 128.1, 128.0, 123.8, 122.7, 122.3, 31.3, 12.2.

HRMS (ESI-TOF): Anal Calcd. For.$C_{22}H_{17}{}^{79}BrN_2O_3S[M+H]^+$:469.0217, Found: 469.0214. Anal Calcd. For.$C_{22}H_{17}{}^{81}BrN_2O_3S[M+H]^+$: 471.0196, Found: 471.0195.

IR (neat, cm^{-1}): υ 2360, 1666, 1536, 1395, 1369, 1318, 1189, 1179, 1116, 1106, 972, 759, 750, 672, 648, 615.



1-(3-(4-bromophenyl)-5-methyl-1-(morpholinosulfonyl)-1*H*-pyrazol-4-yl)ethan-1-one (4be)

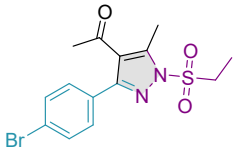
petroleum ether/ ethyl acetate = 8:1, white solid, 47% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 (d, *J* = 8.5 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 3.81 – 3.74 (m, 4H), 3.56 – 3.49 (m, 4H), 2.71 (s, 3H), 2.14 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.7, 152.0, 146.3, 131.8, 131.1, 130.5, 123.8, 121.5, 66.0, 47.5, 31.2, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{16}H_{18}{}^{79}BrN_3O_4S[M+H]^+$: 428.0275, Found: 428.0271. Anal Calcd. For.$C_{16}H_{18}{}^{81}BrN_3O_4S[M+H]^+$: 430.0254, Found: 430.0245.

IR (neat, cm^{-1}): υ 2361, 1671, 1533, 1393, 1372, 1308, 1188, 1178, 1166, 1112, 772, 705, 672, 648, 611.



1-(3-(4-bromophenyl)-1-(ethylsulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4bf)

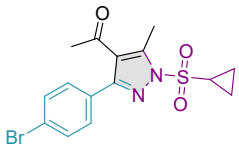
petroleum ether/ ethyl acetate = 10:1, white solid, 69% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 3.60 (q, *J* = 7.4 Hz, 2H), 2.74 (s, 3H), 2.13 (s, 3H), 1.35 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.8, 153.3, 147.5, 131.8, 130.7, 130.5, 124.0, 122.2, 49.3, 31.3, 11.9, 7.6.

HRMS (ESI-TOF): Anal Calcd. For. $C_{14}H_{15}{}^{79}BrN_2O_3S[M+H]^+$: 371.0060, Found: 371.0058. Anal Calcd. For.$C_{14}H_{15}{}^{81}BrN_2O_3S[M+H]^+$: 373.0040, Found: 373.0034.

IR (neat, cm^{-1}): υ 2988, 2939, 1679, 1445, 1246, 1149, 1071, 1035, 1012, 830, 741, 624.



1-(3-(4-bromophenyl)-1-(cyclopropylsulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4bg)

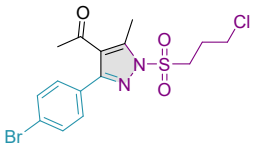
petroleum ether/ ethyl acetate = 8:1, white solid, 73% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 8.1 Hz, 2H), 3.03 – 2.90 (m, 1H), 2.73 (s, 3H), 2.14 (s, 3H), 1.55 – 1.48 (m, 2H), 1.27 – 1.18 (m, 2H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.0, 153.0, 146.5, 131.8, 130.9, 130.5, 123.9, 122.3, 32.0, 31.3, 12.0, 7.1.

HRMS (ESI-TOF): Anal Calcd. For.$C_{15}H_{15}{}^{79}BrN_2O_3S[M+H]^+$: 383.0060, Found: 383.0056. Anal Calcd. For.$C_{15}H_{15}{}^{81}BrN_2O_3S[M+H]^+$: 385.0040, Found: 385.0033.

IR (neat, cm^{-1}): υ 2360, 2341, 1686, 1426, 1382, 1308, 1178, 1114, 1069, 1008, 880, 836, 716, 652, 616.



1-(3-(4-bromophenyl)-1-((2-chloroethyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4bh)

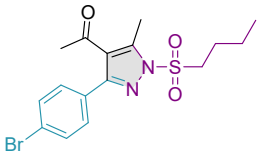
petroleum ether/ ethyl acetate = 10:1, white solid, 52% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 8.5 Hz, 2H), 3.80 – 3.74 (m, 2H), 3.65 (t, *J* = 6.1 Hz, 2H), 2.76 (s, 3H), 2.35 – 2.23 (m, 2H), 2.15 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.8, 153.5, 147.3, 131.9, 130.5, 124.1, 122.5, 52.0, 41.9, 31.4, 26.0, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{15}H_{16}{}^{79}BrClN_2O_3S[M+H]^+$: 418.9827, Found: 418.9821. Anal Calcd. For.$C_{15}H_{16}{}^{81}BrClN_2O_3S[M+H]^+$: 420.9806, Found: 420.9797.

IR (neat, cm^{-1}): υ 1665, 1367, 1313, 1161, 1111, 1038, 1010, 967, 832, 659, 616.



1-(3-(4-bromophenyl)-1-(butylsulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4bi)

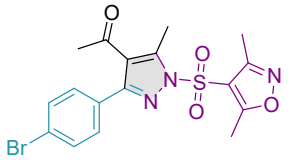
petroleum ether/ ethyl acetate = 10:1, white solid, 52% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 2H), 3.58 – 3.51 (m, 2H), 2.74 (s, 3H), 2.14 (s, 3H), 1.80 – 1.70 (m, 2H), 1.44 (h, *J* = 7.4 Hz, 2H), 0.92 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9, 153.3, 147.3, 131.8, 130.7, 130.5, 124.0, 122.2, 54.3, 31.3, 24.6, 21.1, 13.3, 12.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{16}H_{19}{}^{79}BrN_2O_3S[M+H]^+$: 399.0373, Found: 399.0370. Anal Calcd. For.$C_{16}H_{19}{}^{81}BrN_2O_3S[M+H]^+$: 401.0353, Found: 401.0345.

IR (neat, cm^{-1}): υ 2961, 2934, 1681, 1444, 1149, 1070, 1034, 1012, 830, 736.



1-(3-(4-bromophenyl)-1-((3,5-dimethylisoxazol-4-yl)sulfonyl)-5-methyl-1H-pyrazol-4-yl)ethan-1-one (4bj)

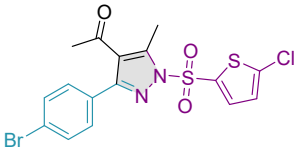
petroleum ether/ ethyl acetate = 10:1, white solid, 63% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 2.77 (s, 3H), 2.76 (s, 3H), 2.46 (s, 3H), 2.12 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.7, 176.6, 158.0, 153.2, 146.3, 131.9, 130.5, 130.3, 124.1, 122.5, 114.4, 31.3, 13.2, 12.0, 11.0.

HRMS (ESI-TOF): Anal Calcd. For.$C_{17}H_{16}{}^{79}BrN_3O_4S[M+Na]$+: 459.9938, Found: 559.9947. Anal Calcd. For.$C_{17}H_{16}{}^{81}BrN_3O_4S[M+Na]$+: 461.9917, Found: 461.9999.

IR (neat, cm^{-1}): υ 2361, 1672, 1587, 1536, 1398, 1395, 1309, 1271, 1202, 1133, 1106, 1010, 968, 847, 824, 689, 677, 662, 639, 612.



1-(3-(4-bromophenyl)-1-((5-chlorothiophen-2-yl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4bk)

petroleum ether/ ethyl acetate = 10:1, white solid, 50% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 4.2 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.5 Hz, 2H), 6.99 (d, *J* = 4.2 Hz, 1H), 2.76 (s, 3H), 2.12 (s, 3H).

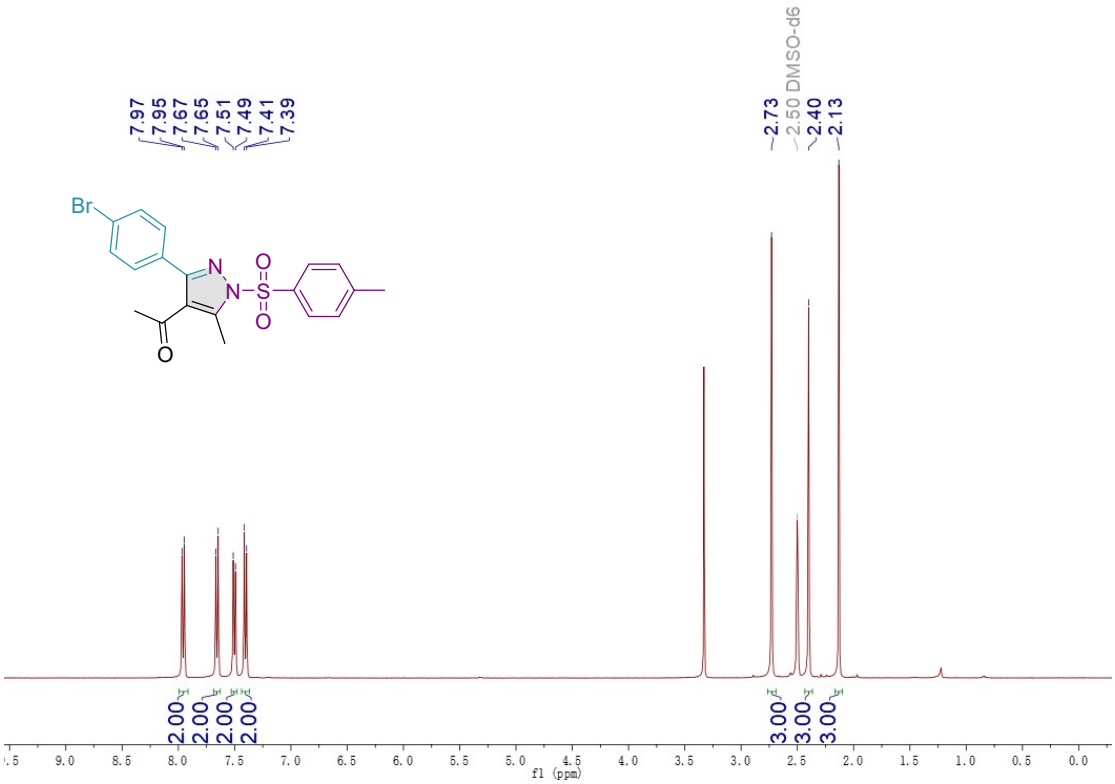
^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.8, 153.7, 146.5, 142.0, 135.1, 134.4, 131.9, 130.5, 130.5, 127.3, 124.1, 122.9, 31.3, 12.2.

HRMS (ESI-TOF): Anal Calcd. For.$C_{16}H_{12}{}^{79}BrClN_2O_3S_2[M+H]^+$: 458.9234, Found: 458.9226. Anal Calcd. For.$C_{20}H_{19}{}^{81}BrN_2O_3S_2[M+H]^+$: 460.9214, Found: 460.9201.

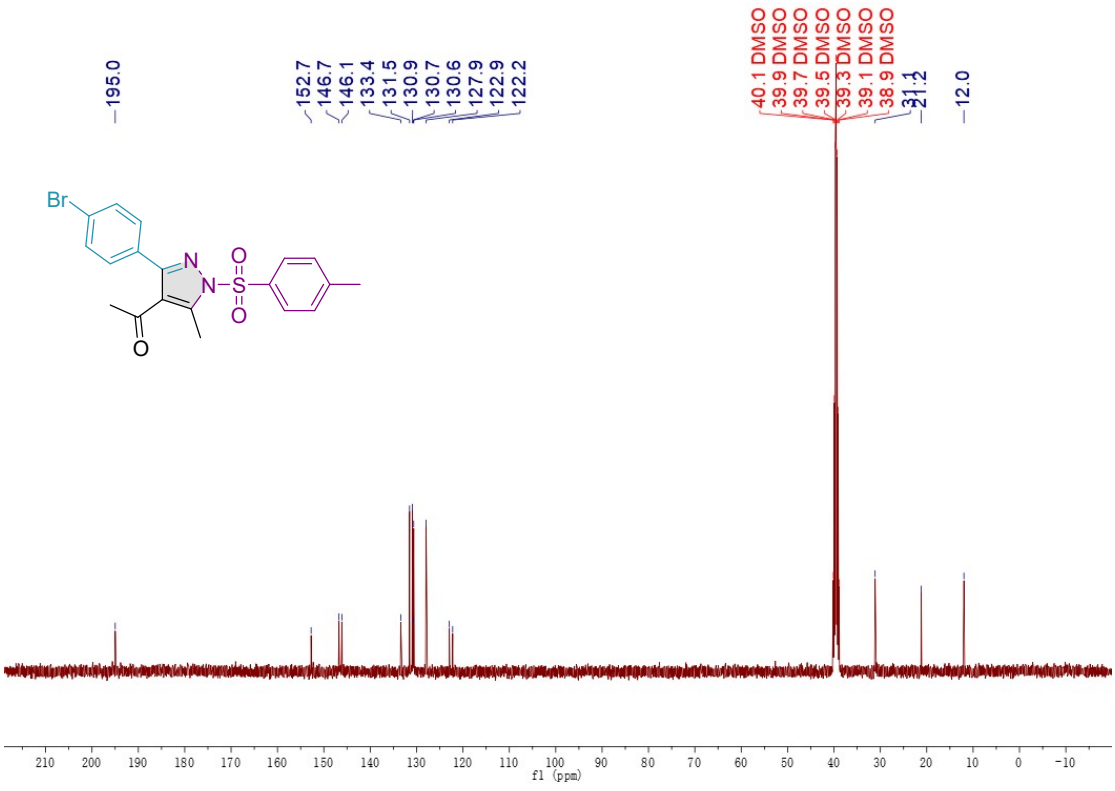
IR (neat, cm^{-1}): υ 2361, 2341, 1676, 1525, 1500, 1397, 1310, 1182, 1113, 1014, 1002, 967, 826, 683, 656, 630, 621, 609.

Spectra

1-(3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4a)

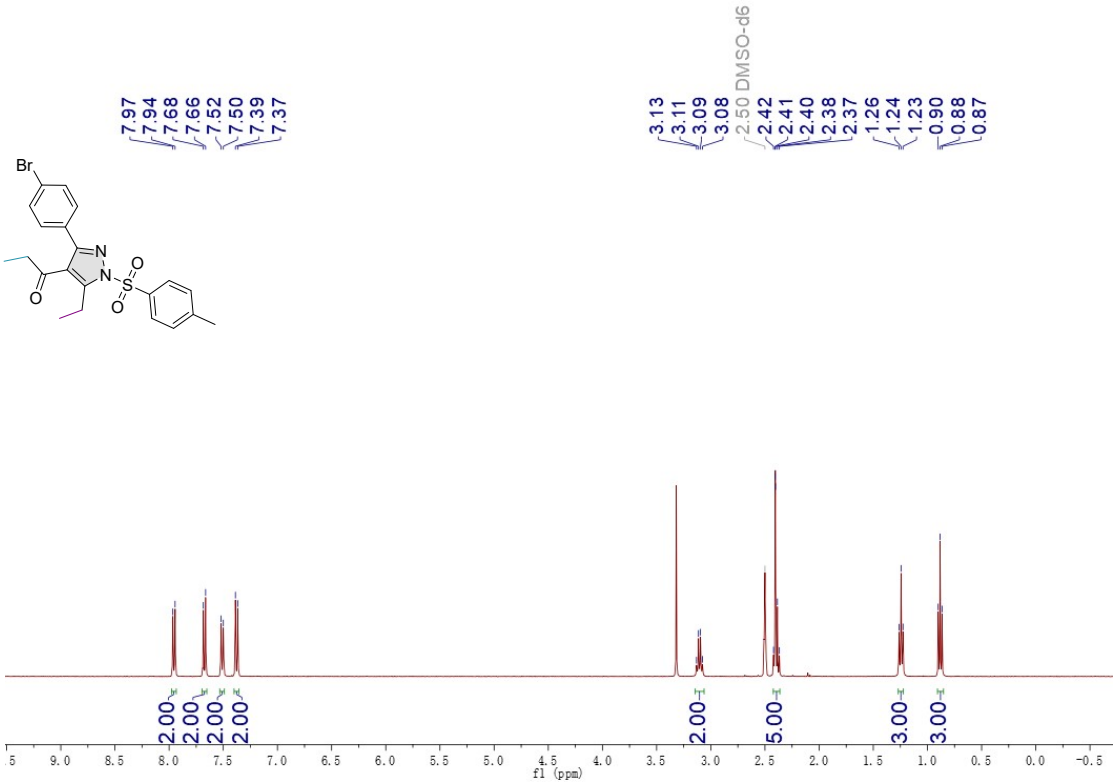


^{1}H NMR (400 MHz, DMSO-d_6)

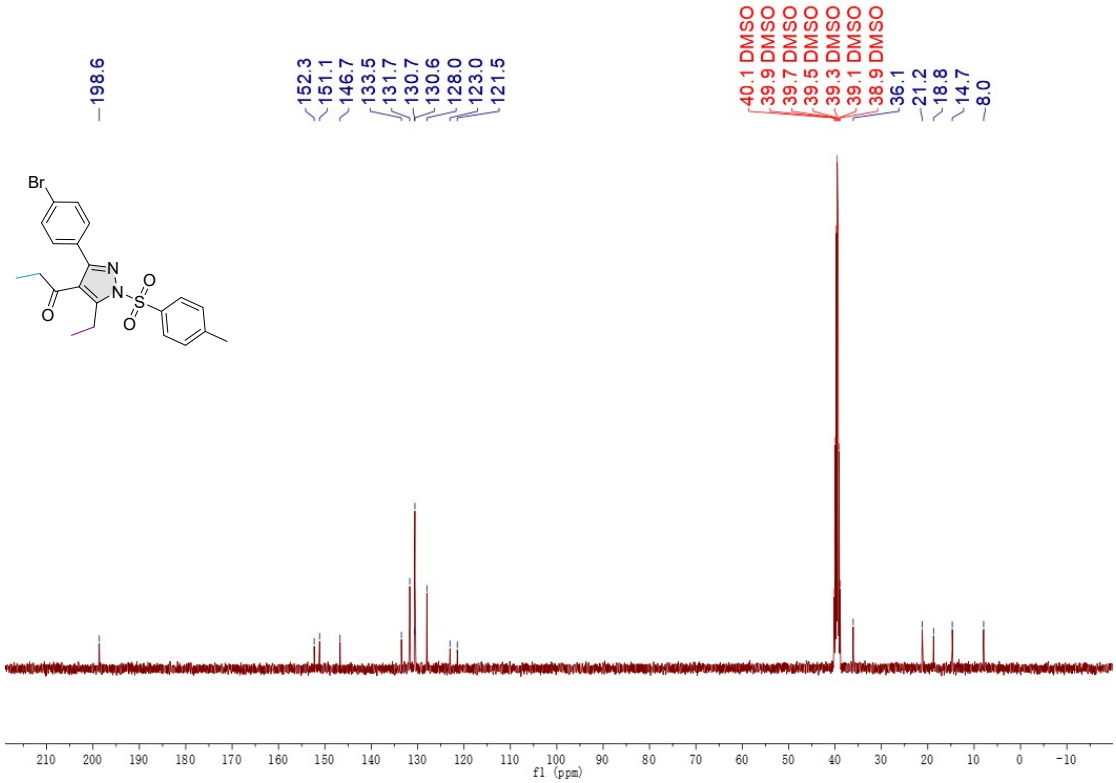


^{13}C NMR (100 MHz, DMSO-d_6)

1-(3-(4-bromophenyl)-5-ethyl-1-tosyl-1*H*-pyrazol-4-yl)propan-1-one (4b)

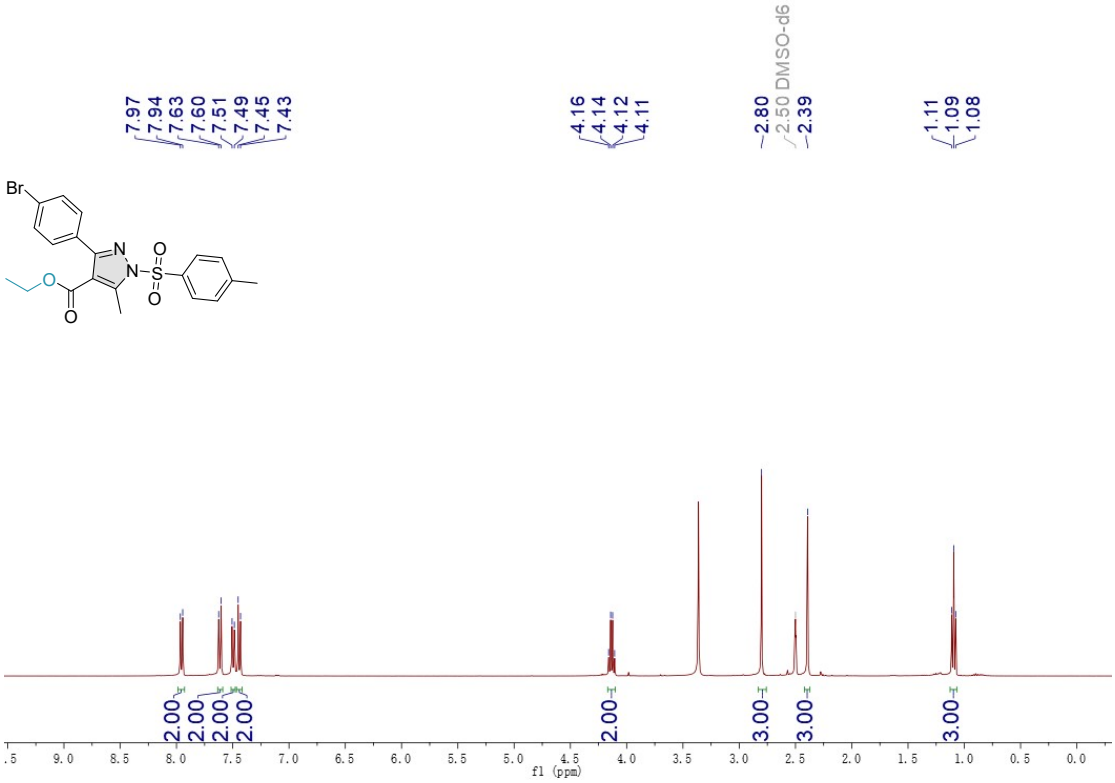


^{1}H NMR (400 MHz, DMSO-d_6)

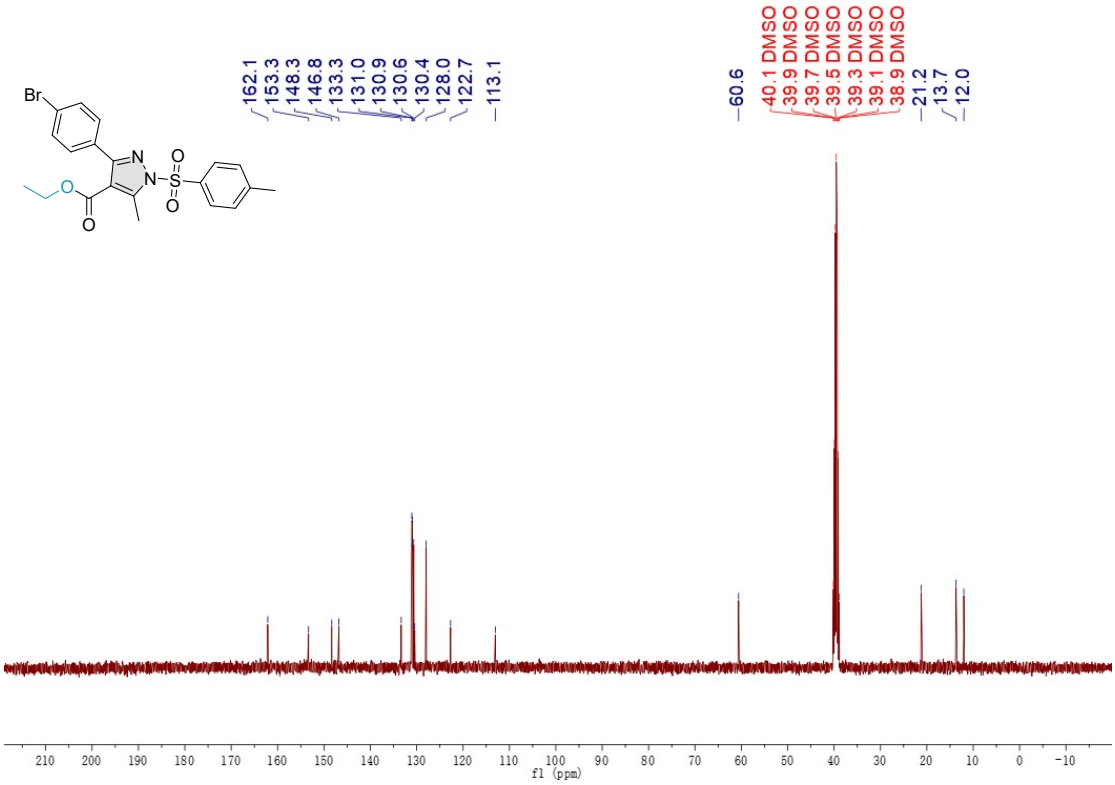


^{13}C NMR (100 MHz, DMSO-d_6)

ethyl 3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4c)

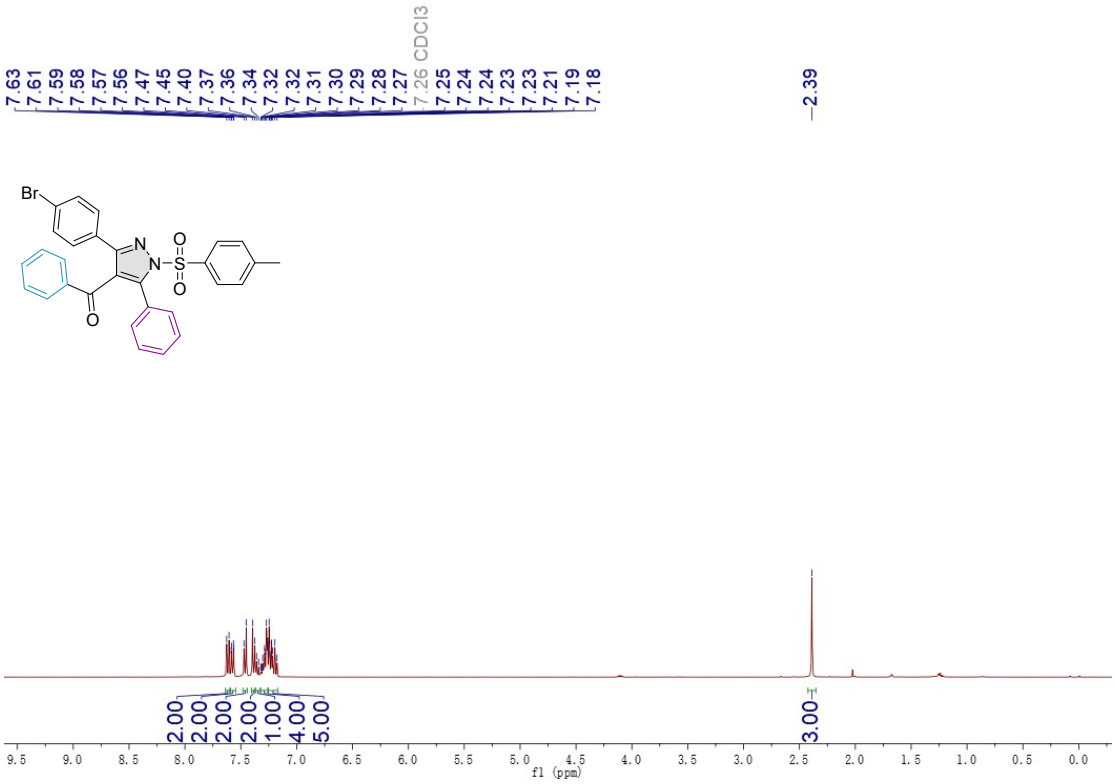


^{1}H NMR (400 MHz, DMSO-d_6)

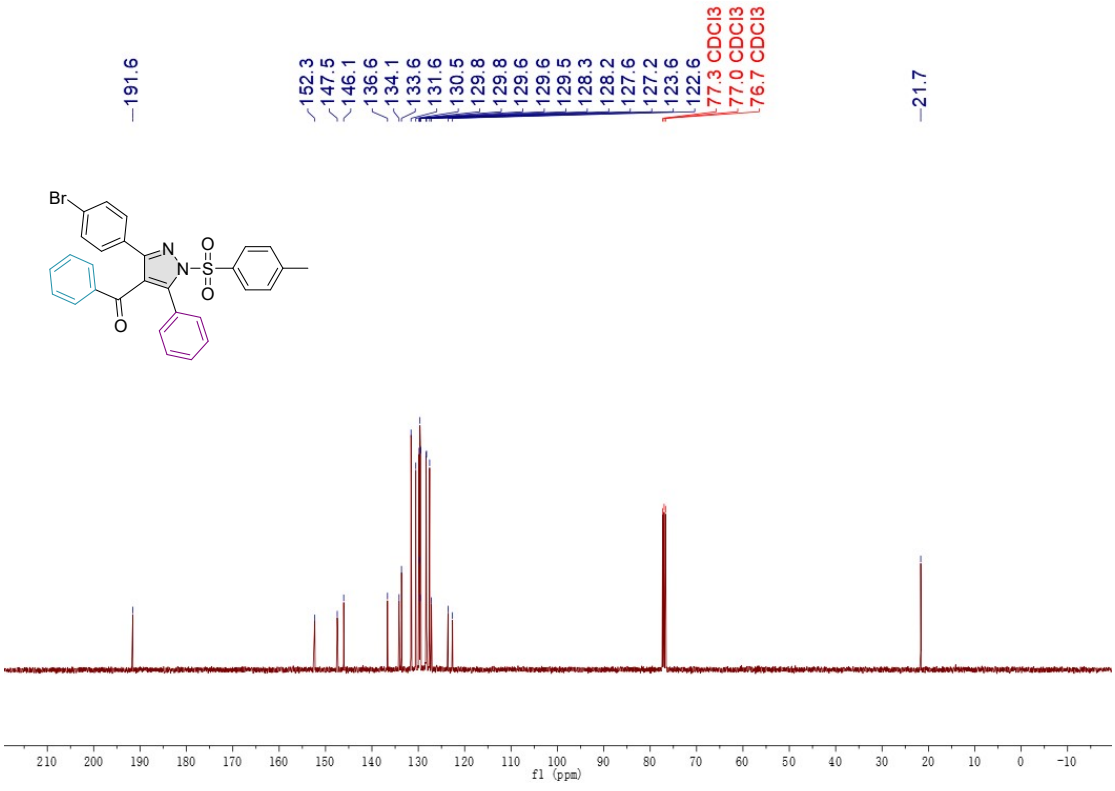


^{13}C NMR (100 MHz, DMSO-d_6)

(3-(4-bromophenyl)-5-phenyl-1-tosyl-1*H*-pyrazol-4-yl)(phenyl)methanone (4d)

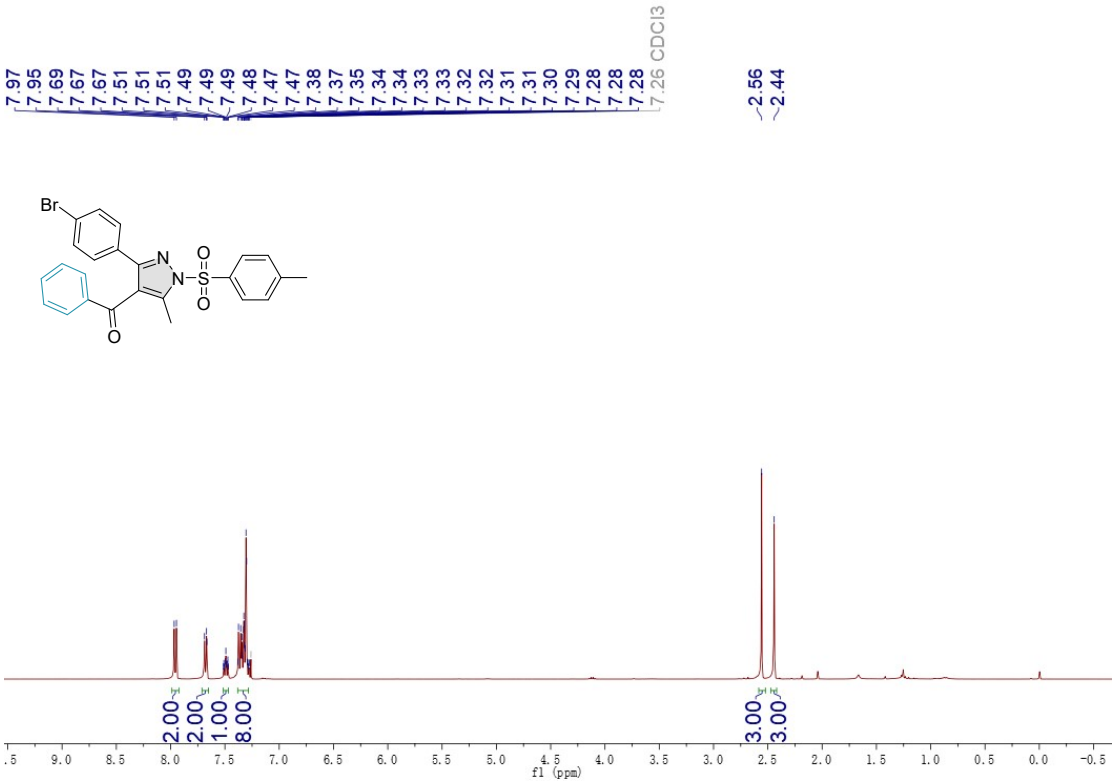


^{1}H NMR (400 MHz, $CDCl_3$)

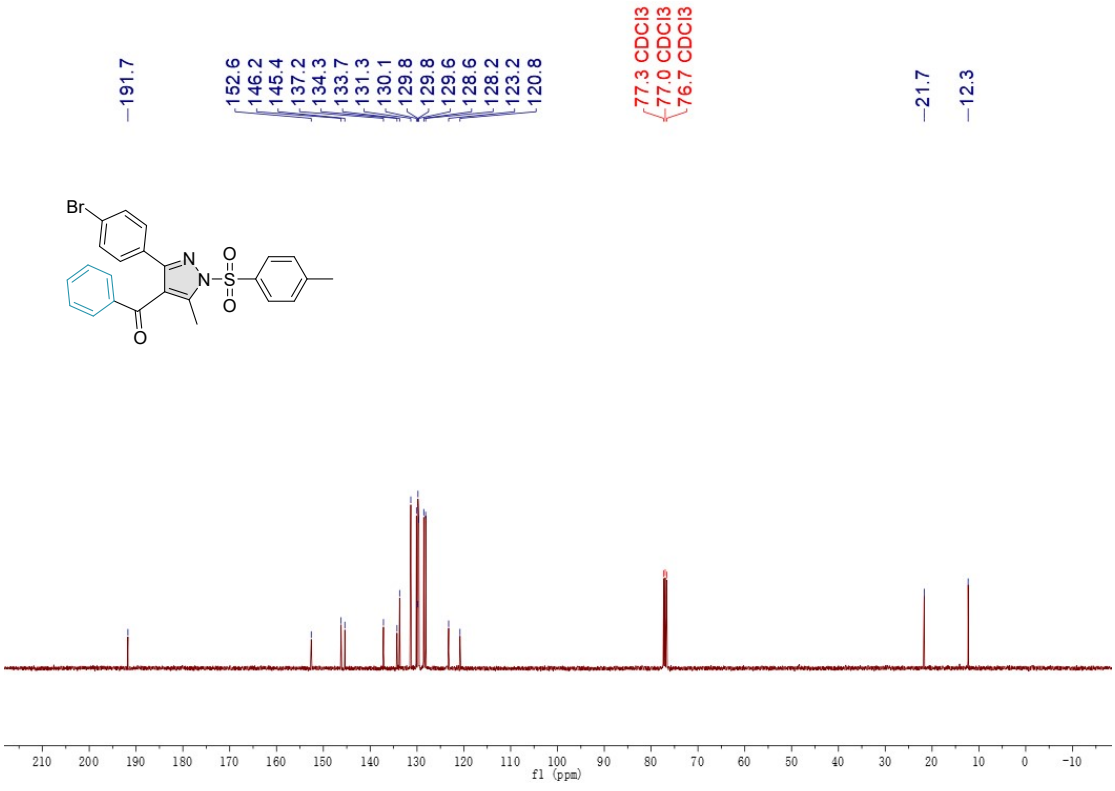


^{13}C NMR (100 MHz, $CDCl_3$)

(3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)(phenyl)methanone (4e)

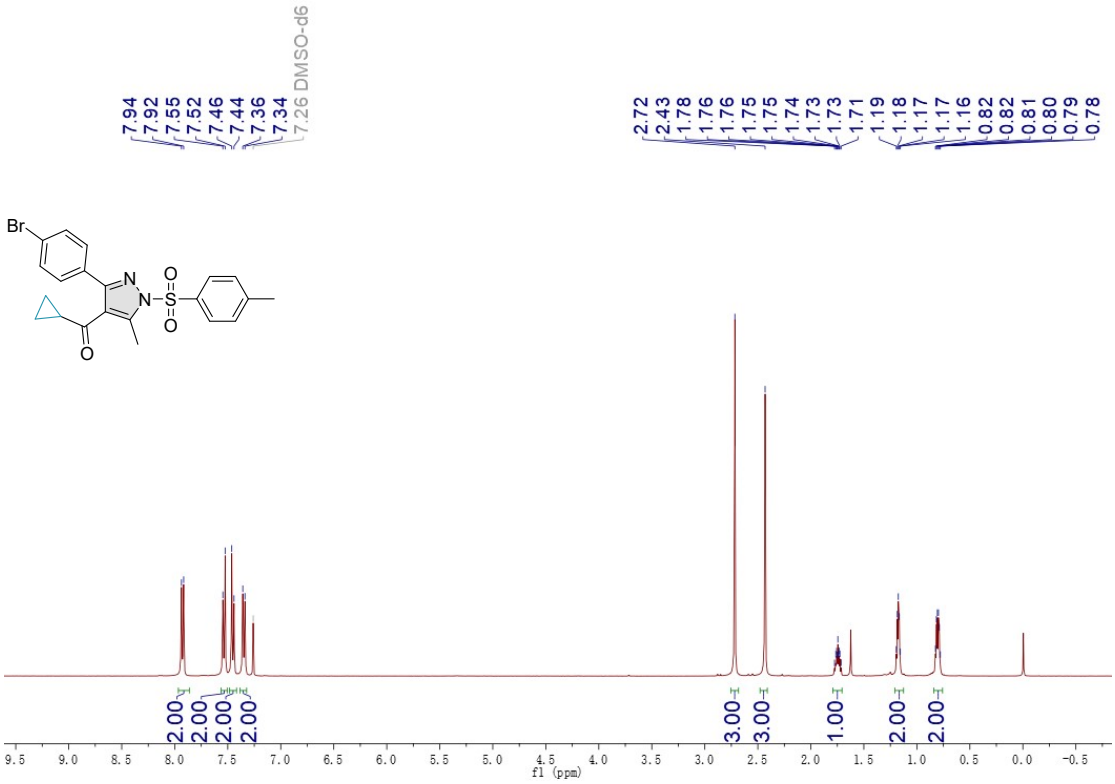


^{1}H NMR (400 MHz, $CDCl_3$)

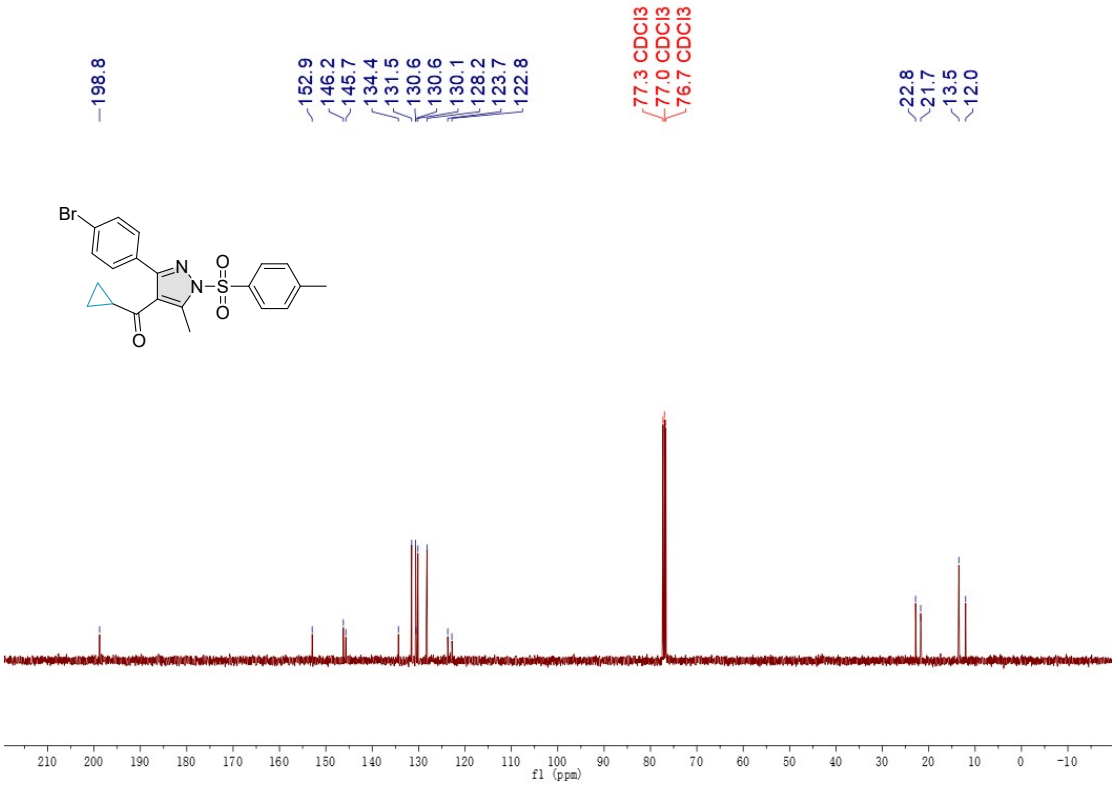


^{13}C NMR (100 MHz, $CDCl_3$)

(3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)(cyclopropyl)methanone (4f)

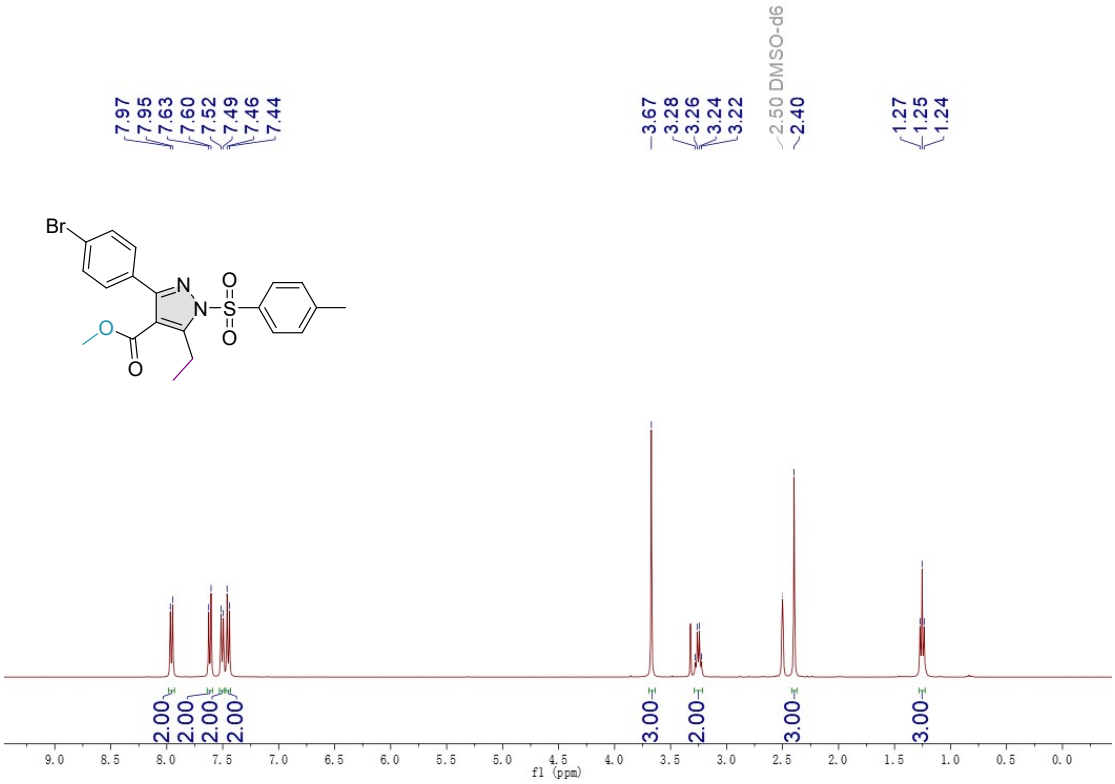


^{1}H NMR (400 MHz, DMSO-d_6)

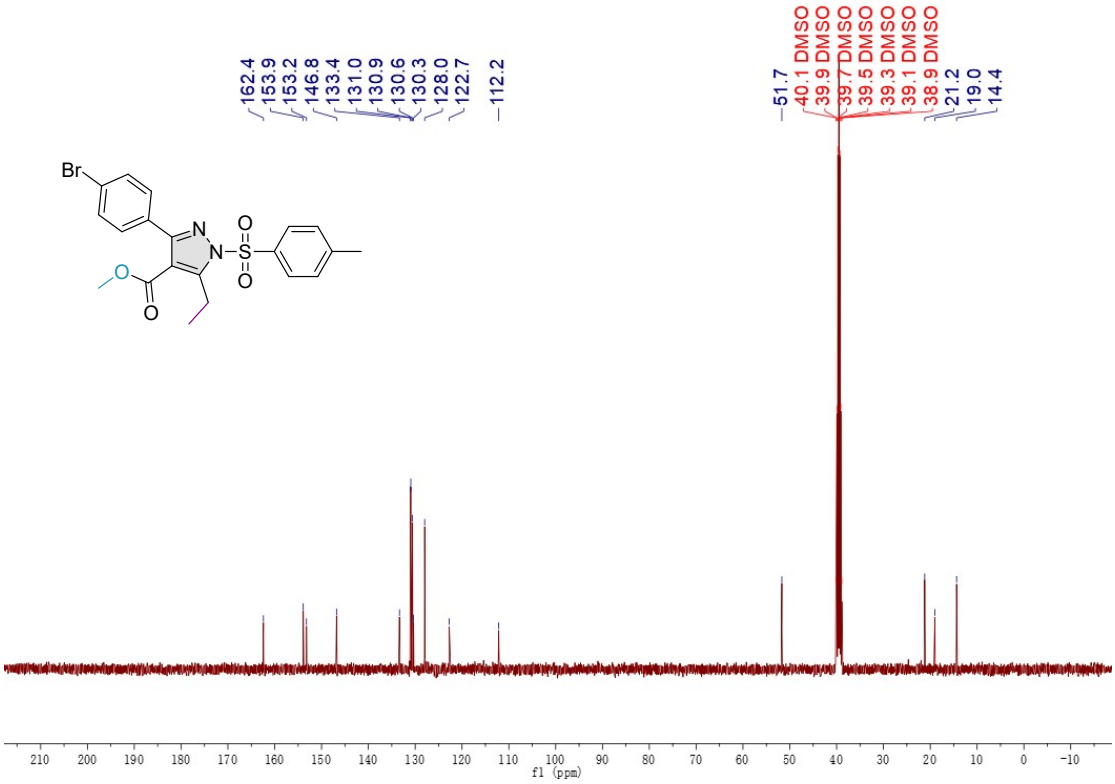


^{13}C NMR (100 MHz, DMSO-d_6)

methyl 3-(4-bromophenyl)-5-ethyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4g)

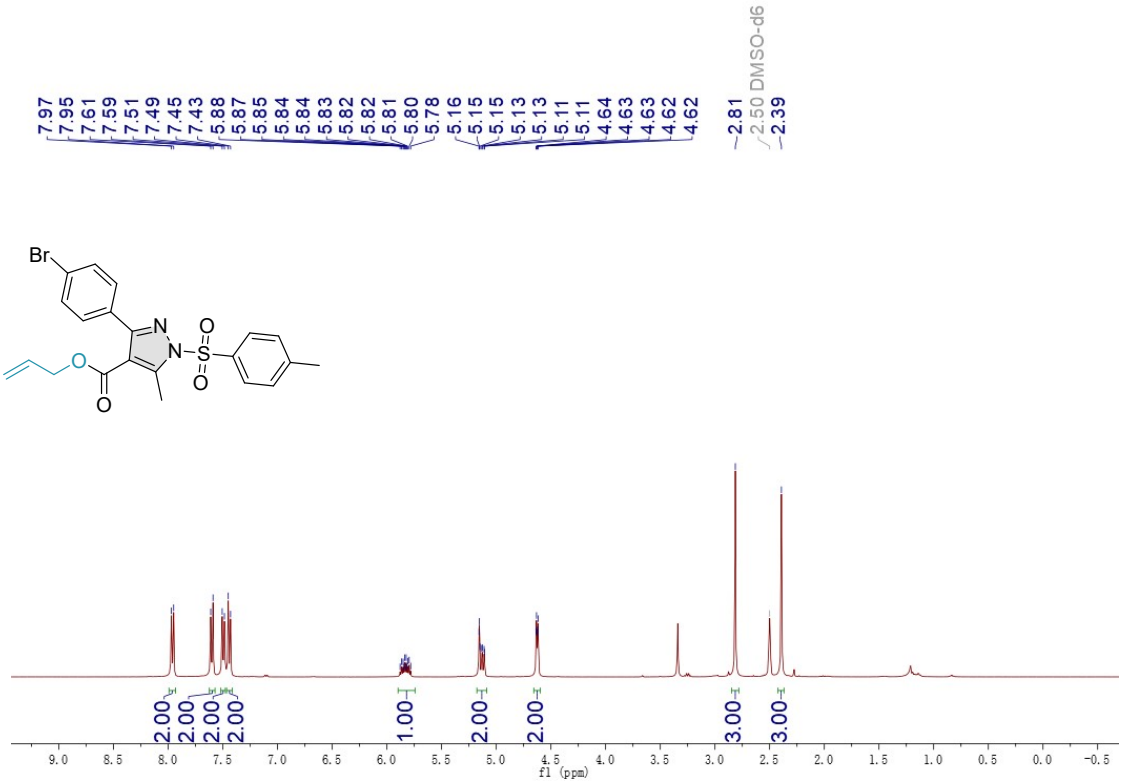


^{1}H NMR (400 MHz, DMSO-*d*$_6$)

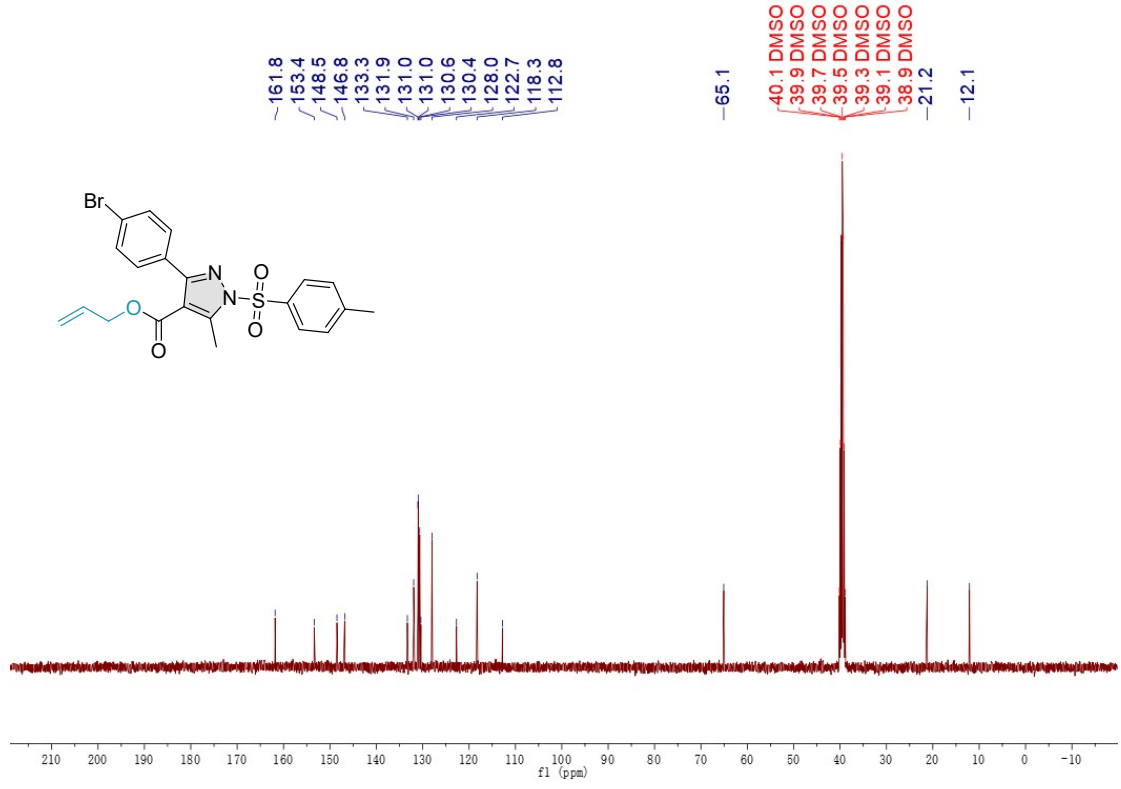


^{13}C NMR (100 MHz, DMSO-*d*$_6$)

allyl 3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4h)

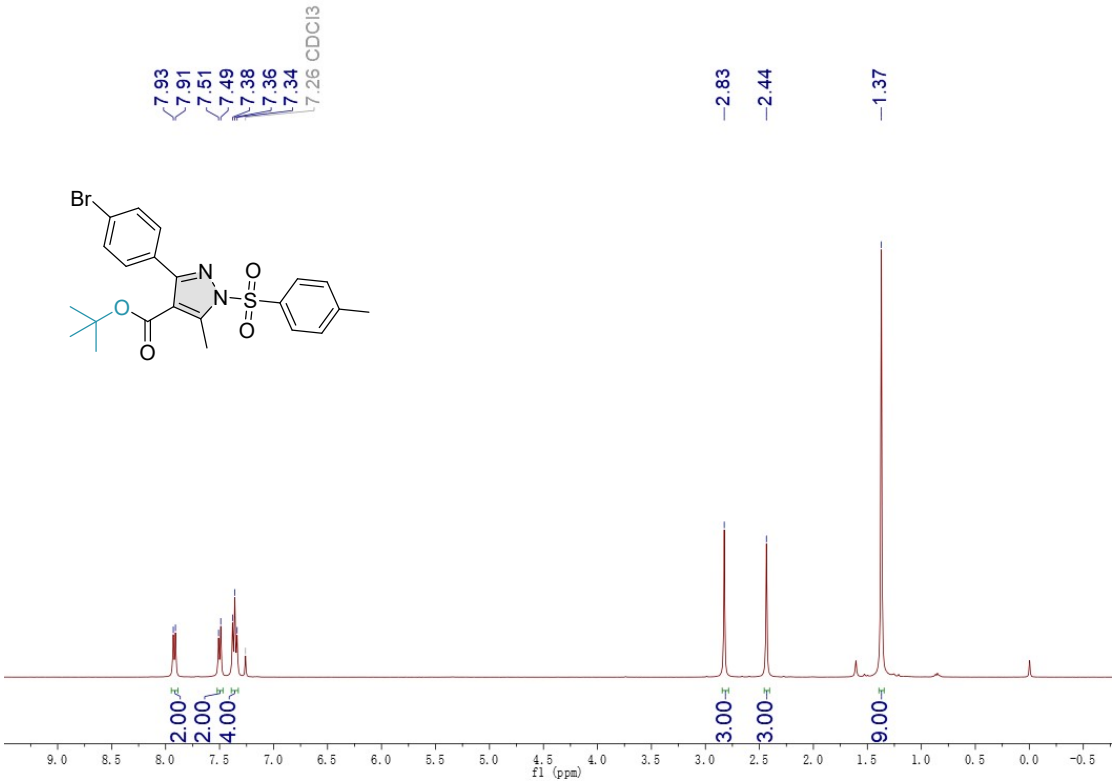


^{1}H NMR (400 MHz, DMSO-d_6)

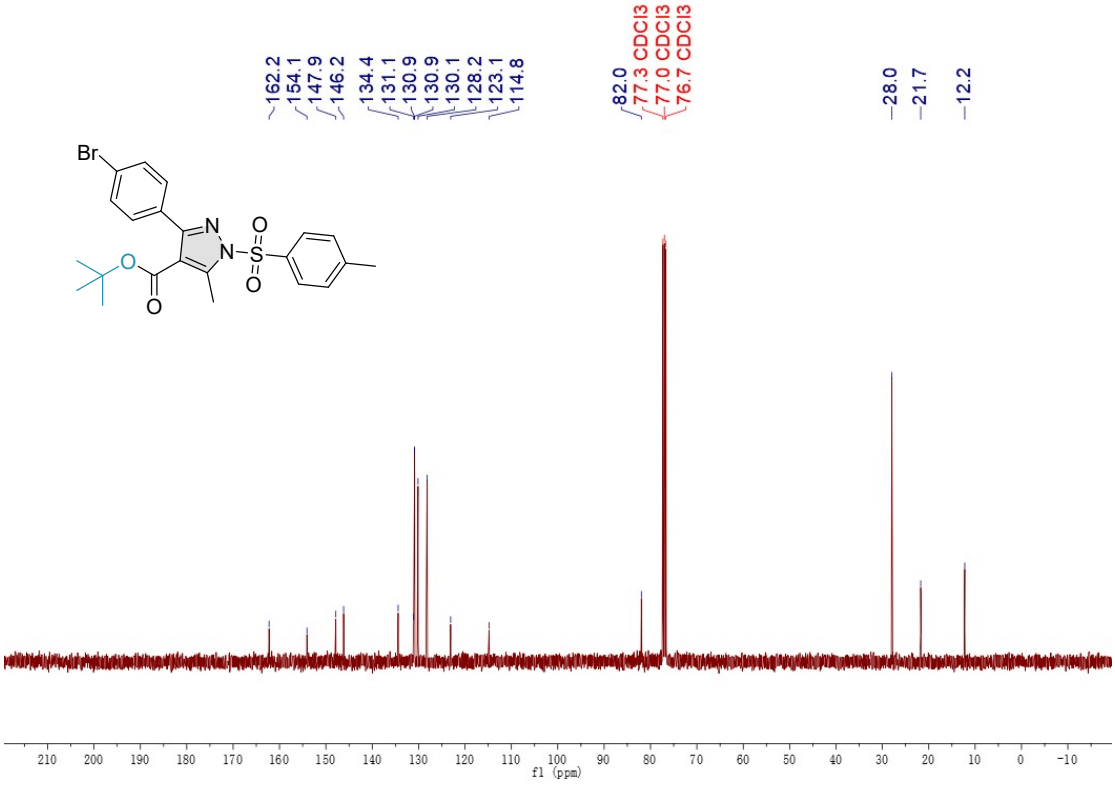


^{13}C NMR (100 MHz, DMSO-d_6)

tert-butyl 3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4i)

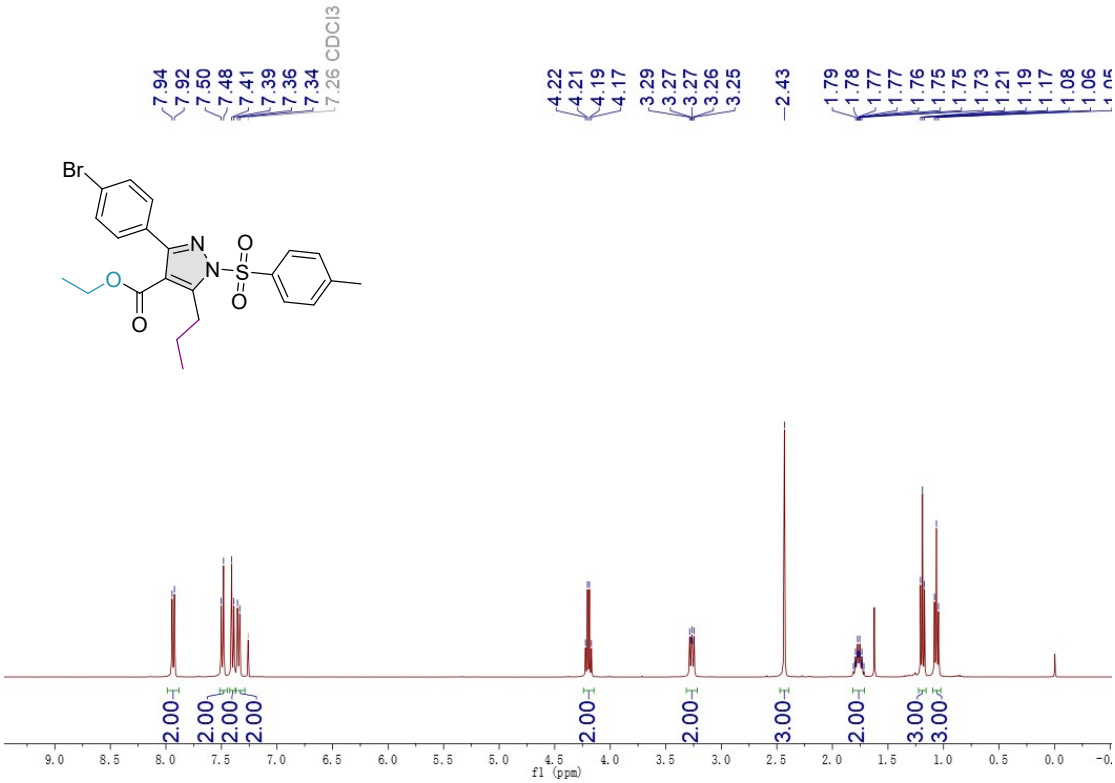


^{1}H NMR (400 MHz, $CDCl_3$)

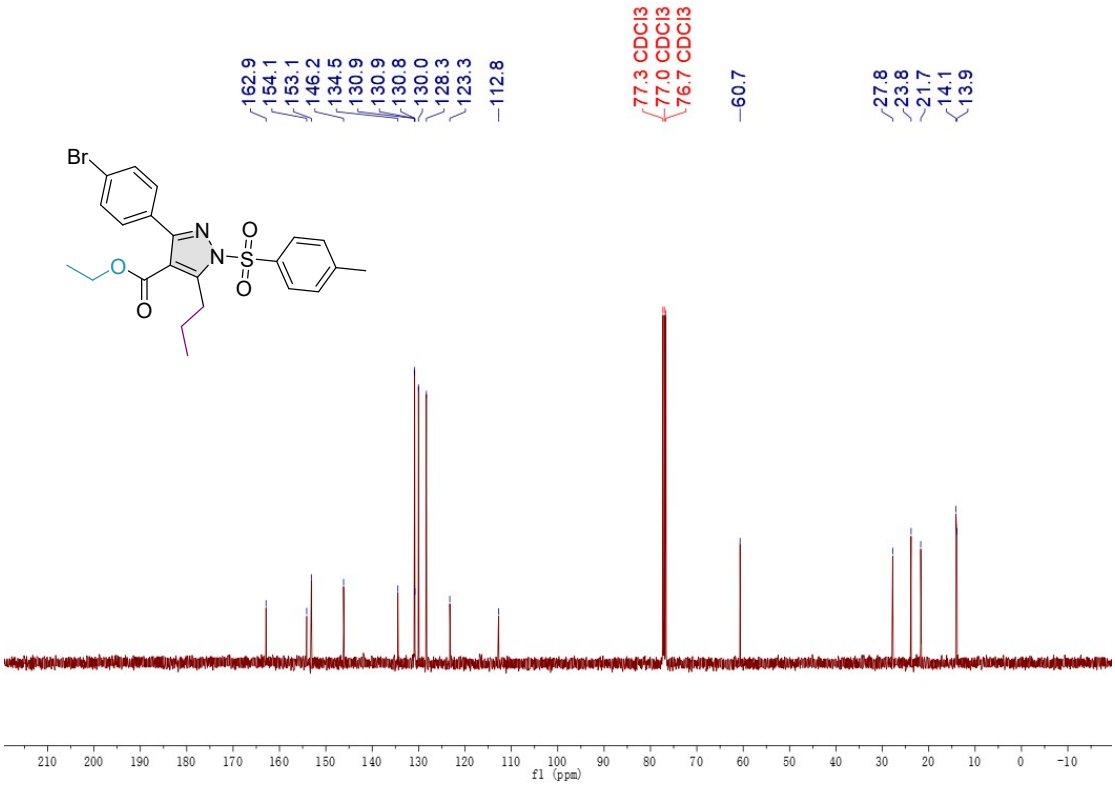


^{13}C NMR (100 MHz, $CDCl_3$)

ethyl 3-(4-bromophenyl)-5-propyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4j)

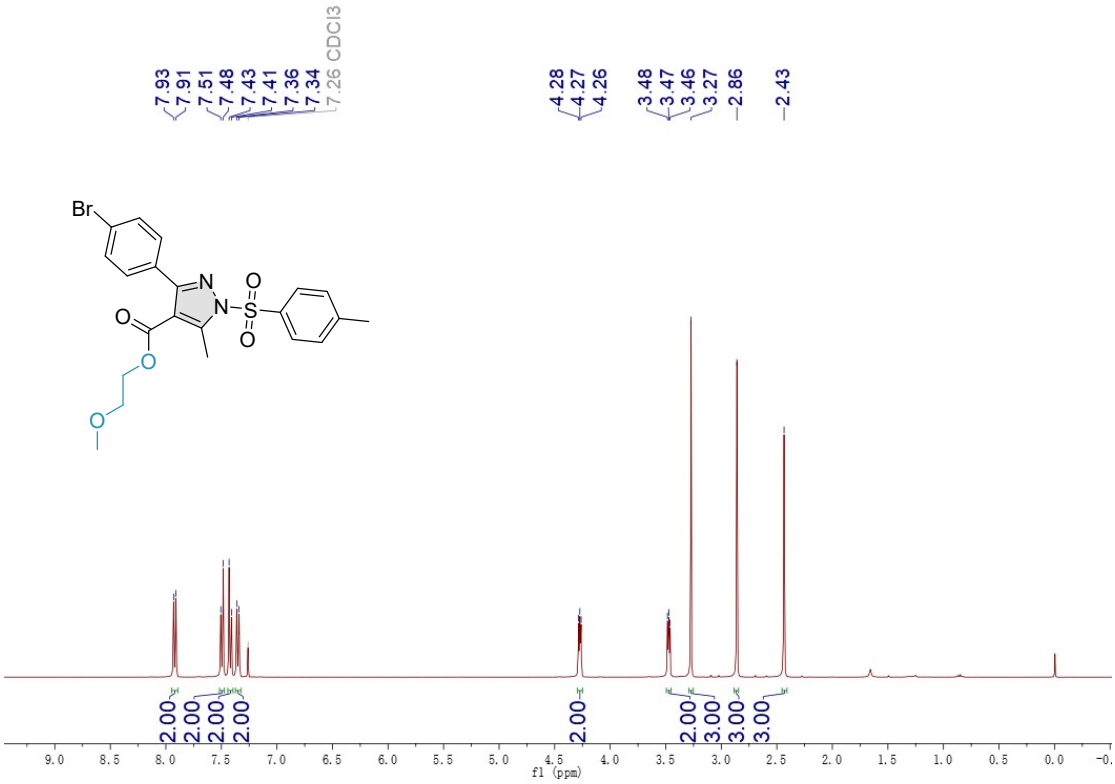


^{1}H NMR (400 MHz, $CDCl_3$)

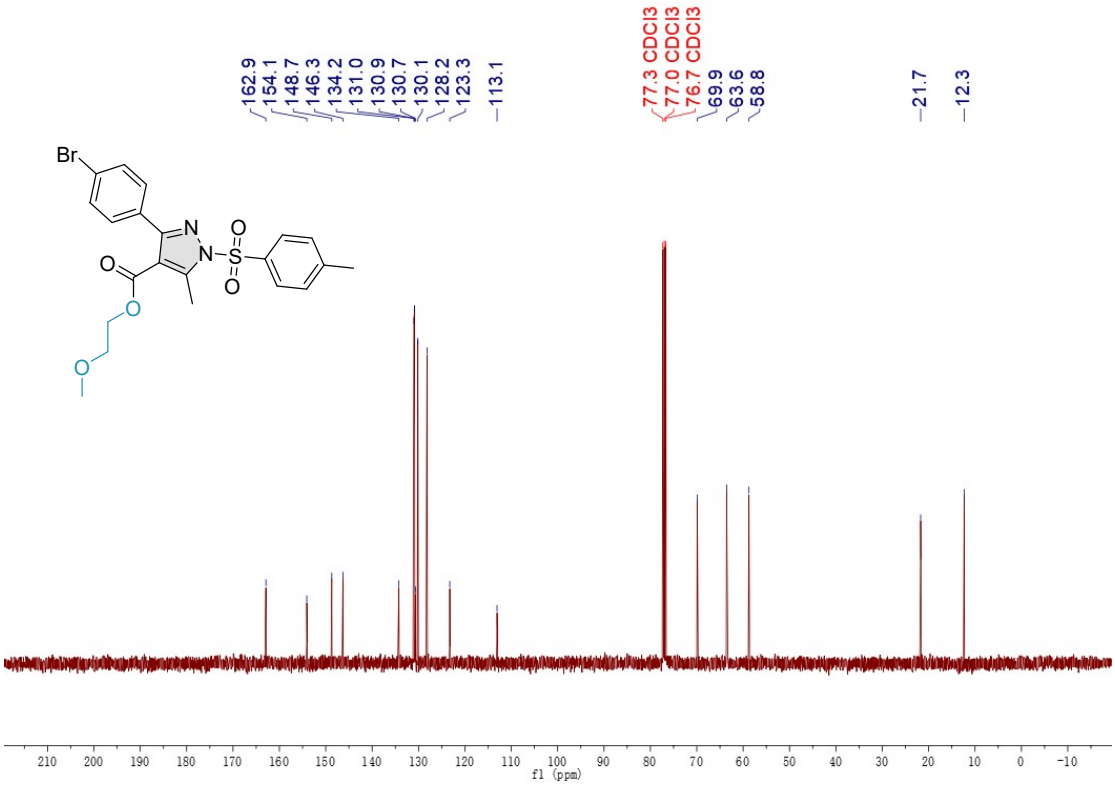


^{13}C NMR (100 MHz, $CDCl_3$)

2-methoxyethyl 3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4k)

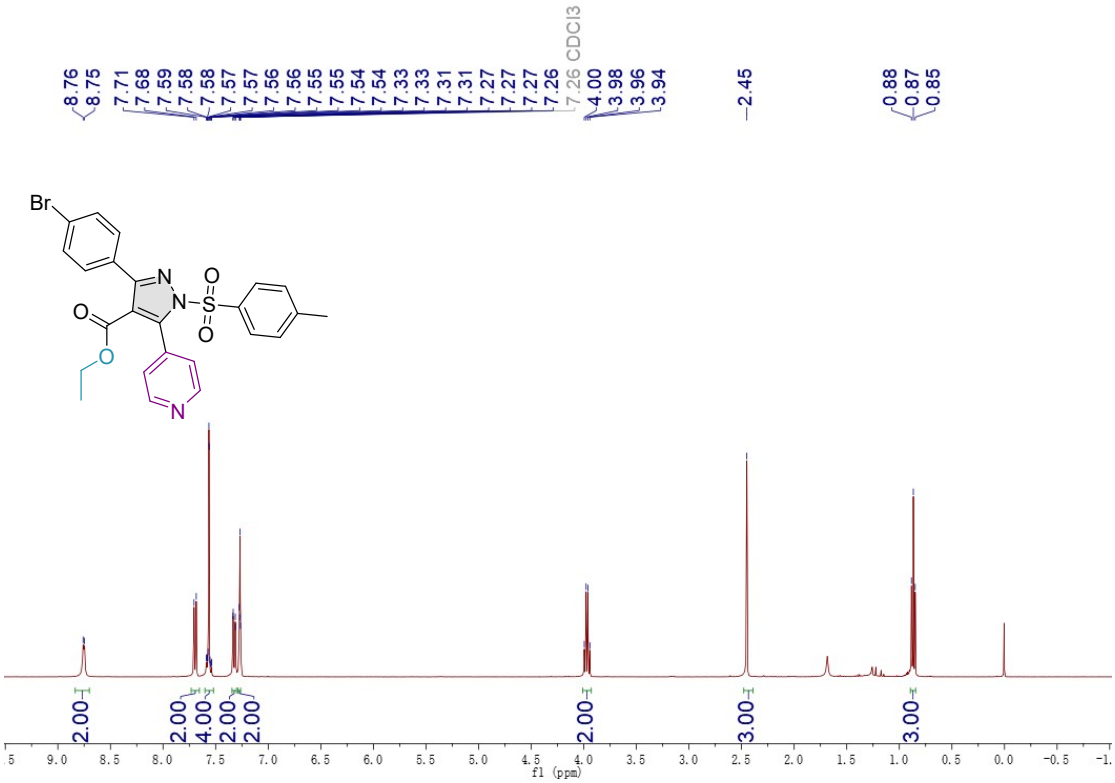


^{1}H NMR (400 MHz, $CDCl_3$)

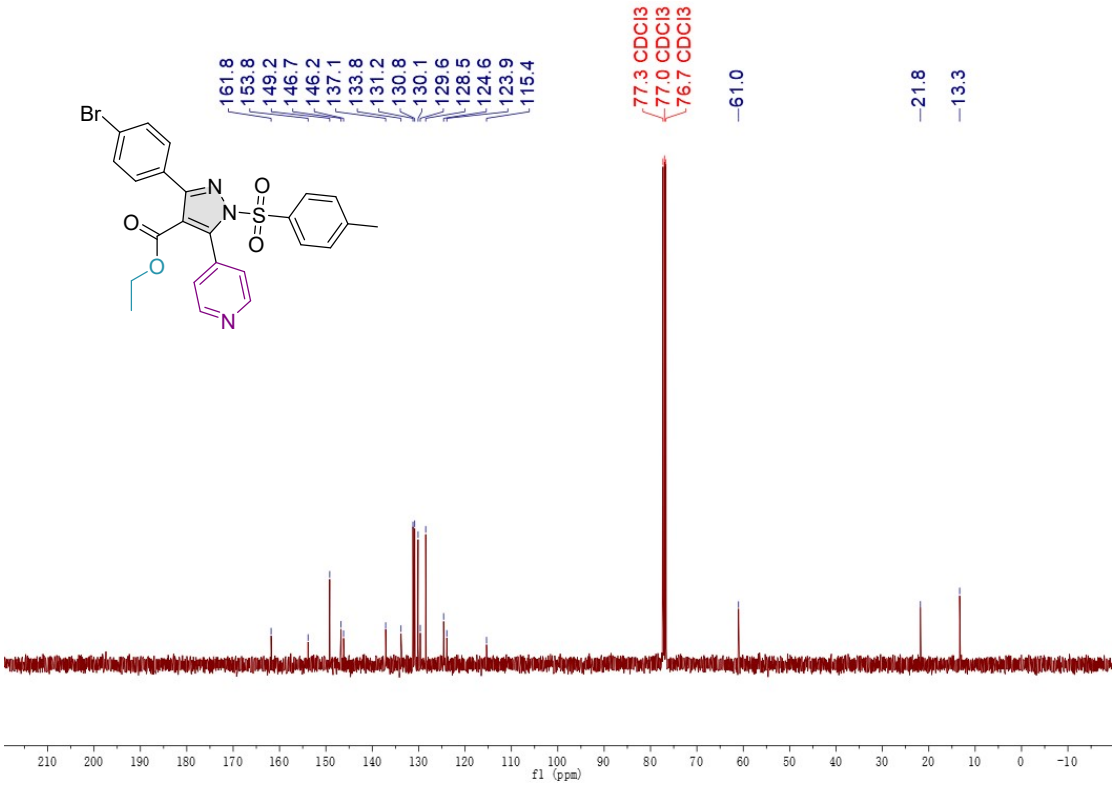


^{13}C NMR (100 MHz, $CDCl_3$)

ethyl 3-(4-bromophenyl)-5-(pyridin-4-yl)-1-tosyl-1*H*-pyrazole-4-carboxylate (4l)

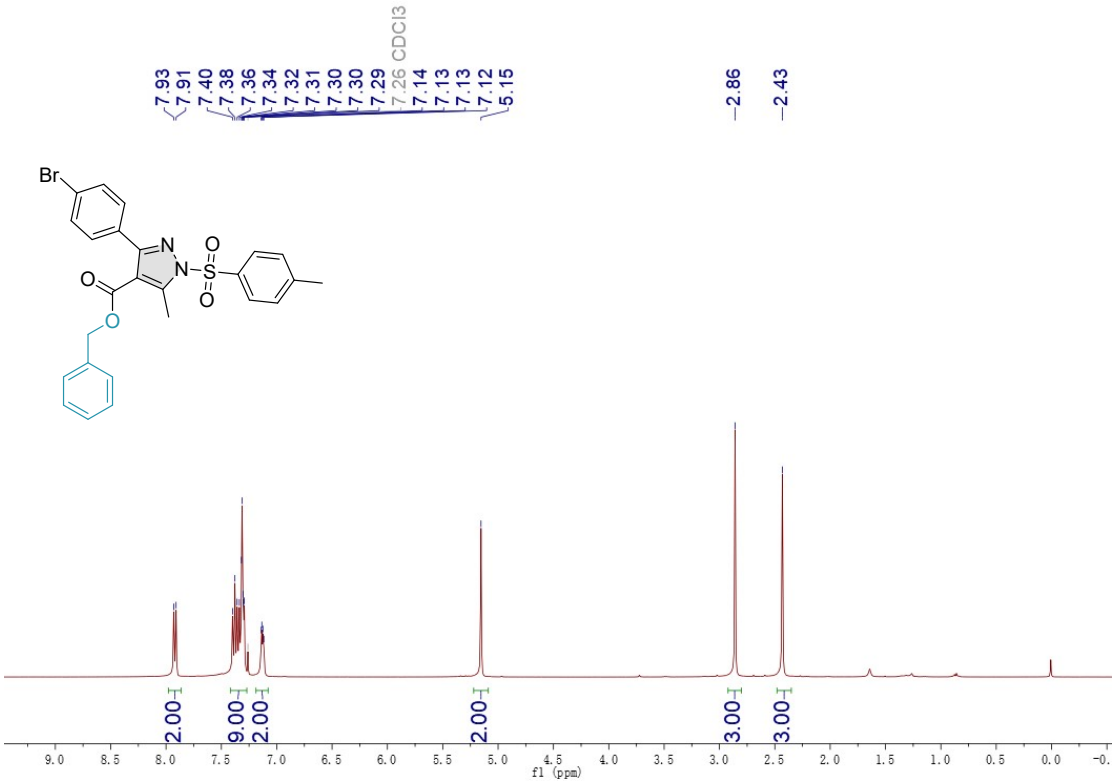


^{1}H NMR (400 MHz, $CDCl_3$)

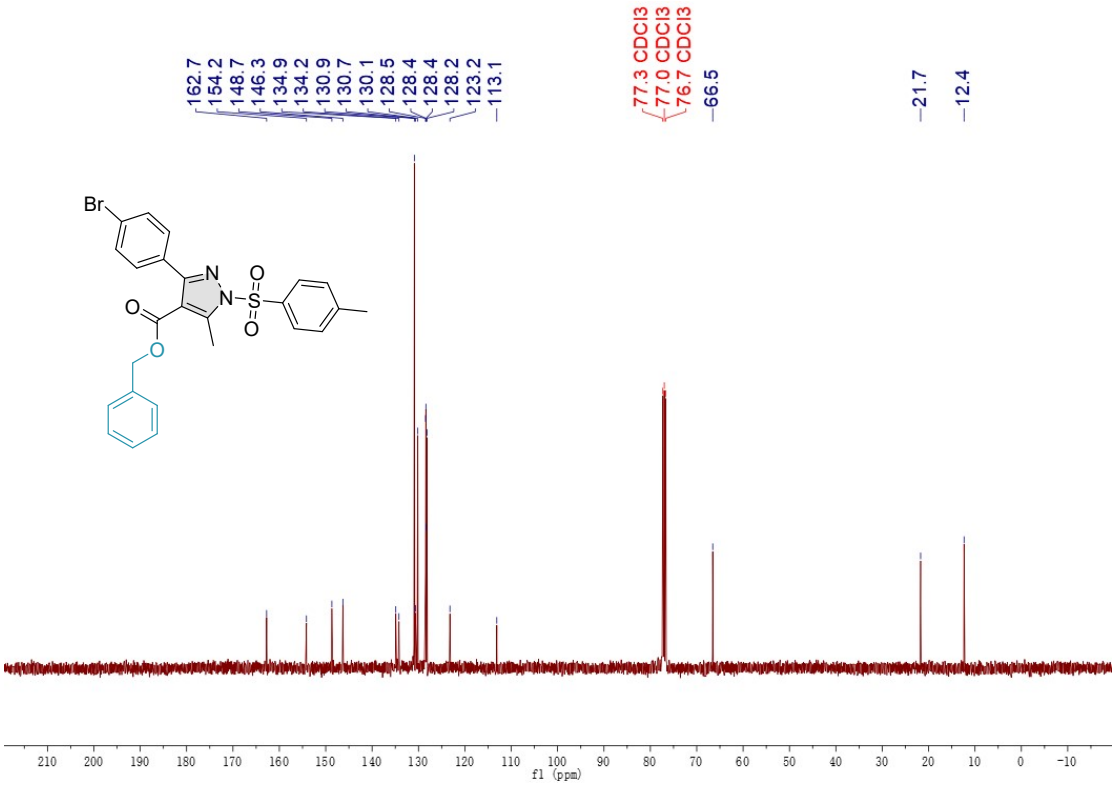


^{13}C NMR (100 MHz, $CDCl_3$)

benzyl 3-(4-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazole-4-carboxylate (4m)

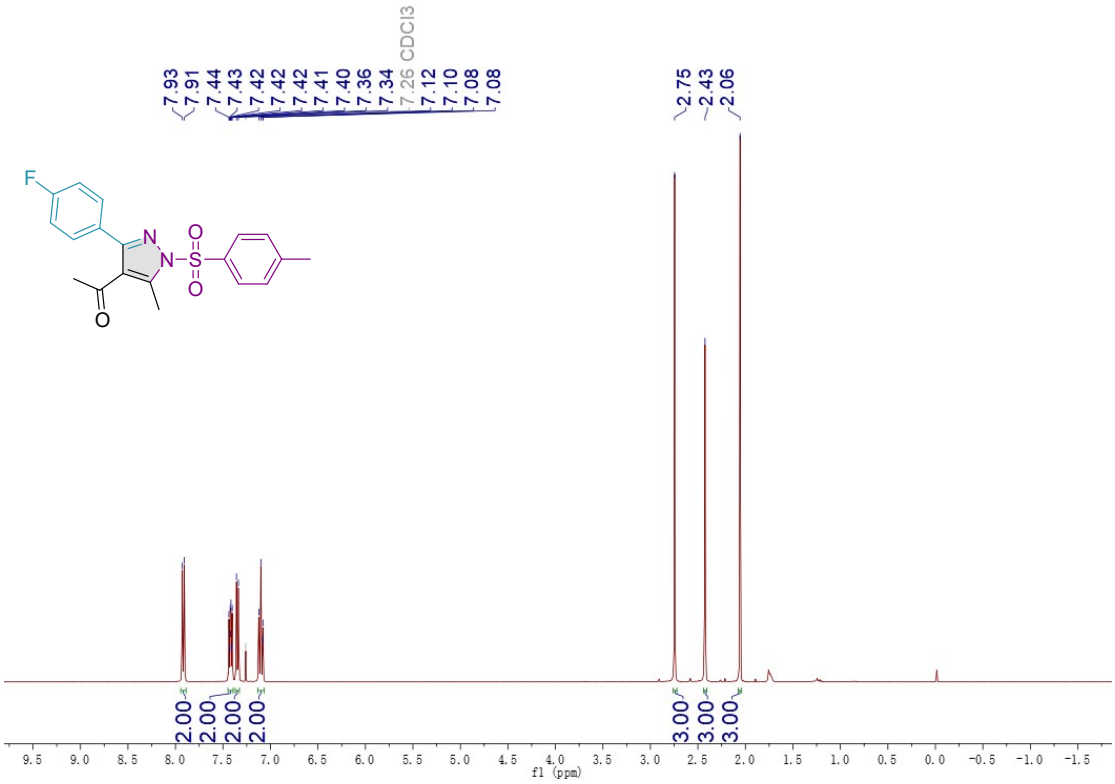


^{1}H NMR (400 MHz, $CDCl_3$)

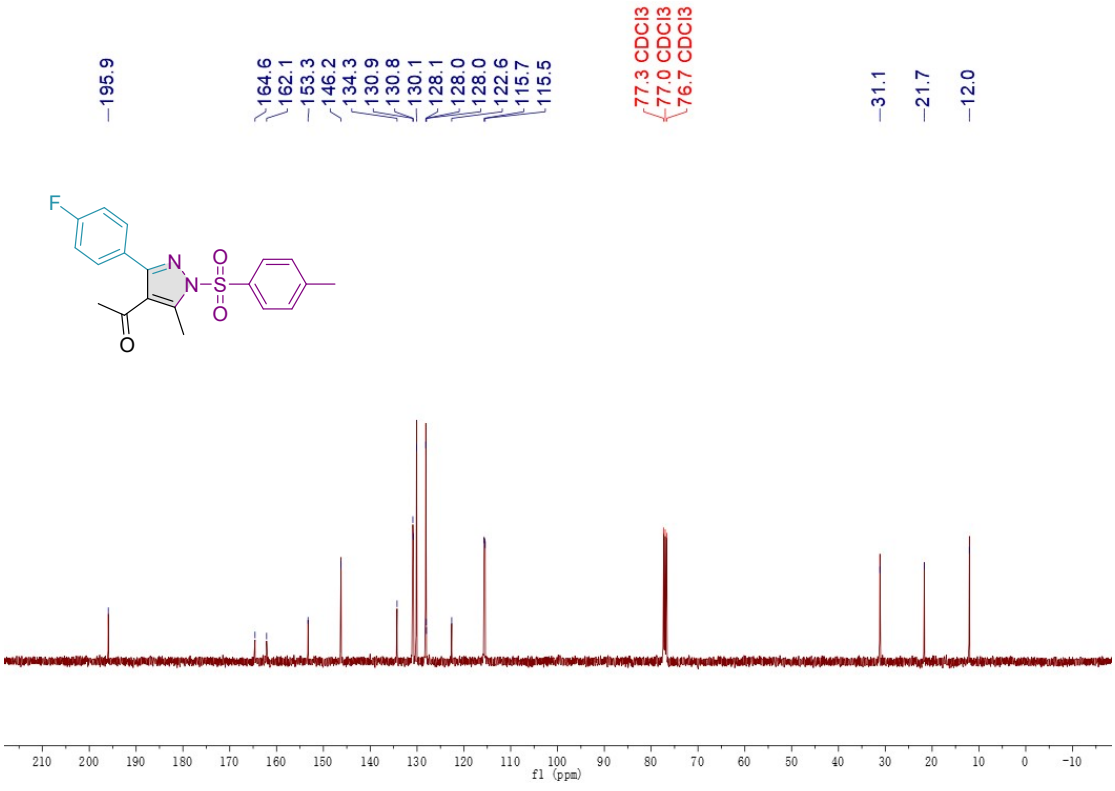


^{13}C NMR (100 MHz, $CDCl_3$)

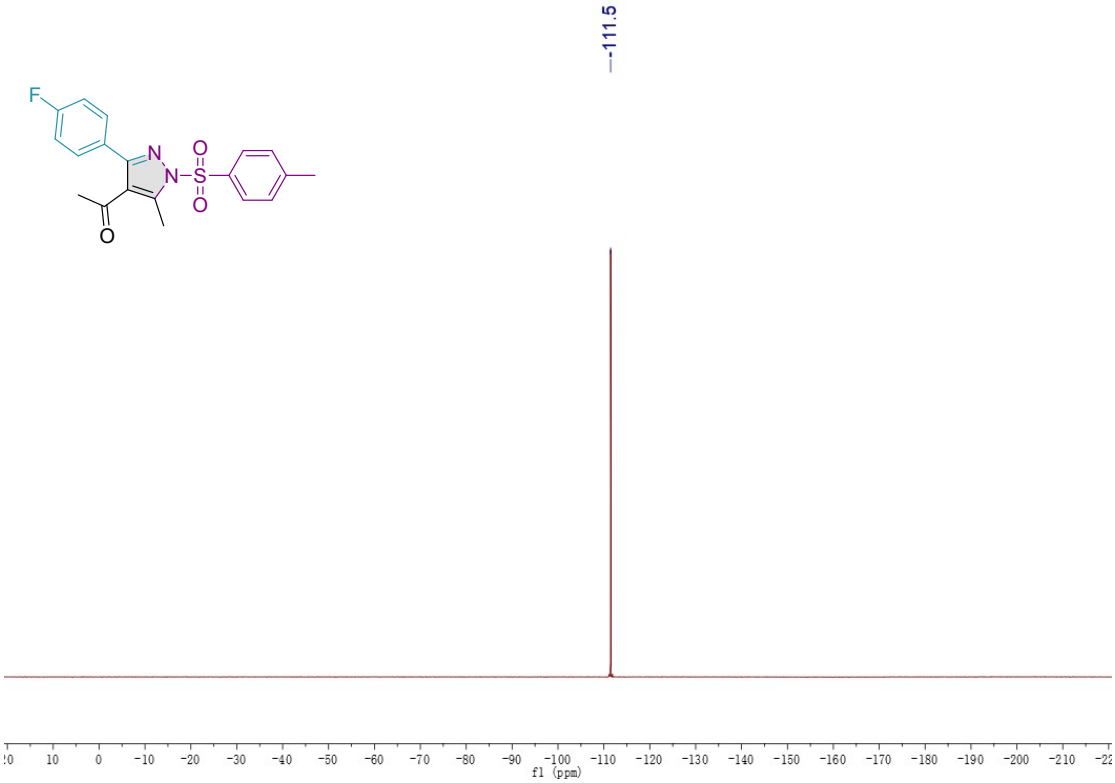
1-(3-(4-fluorophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4n)



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

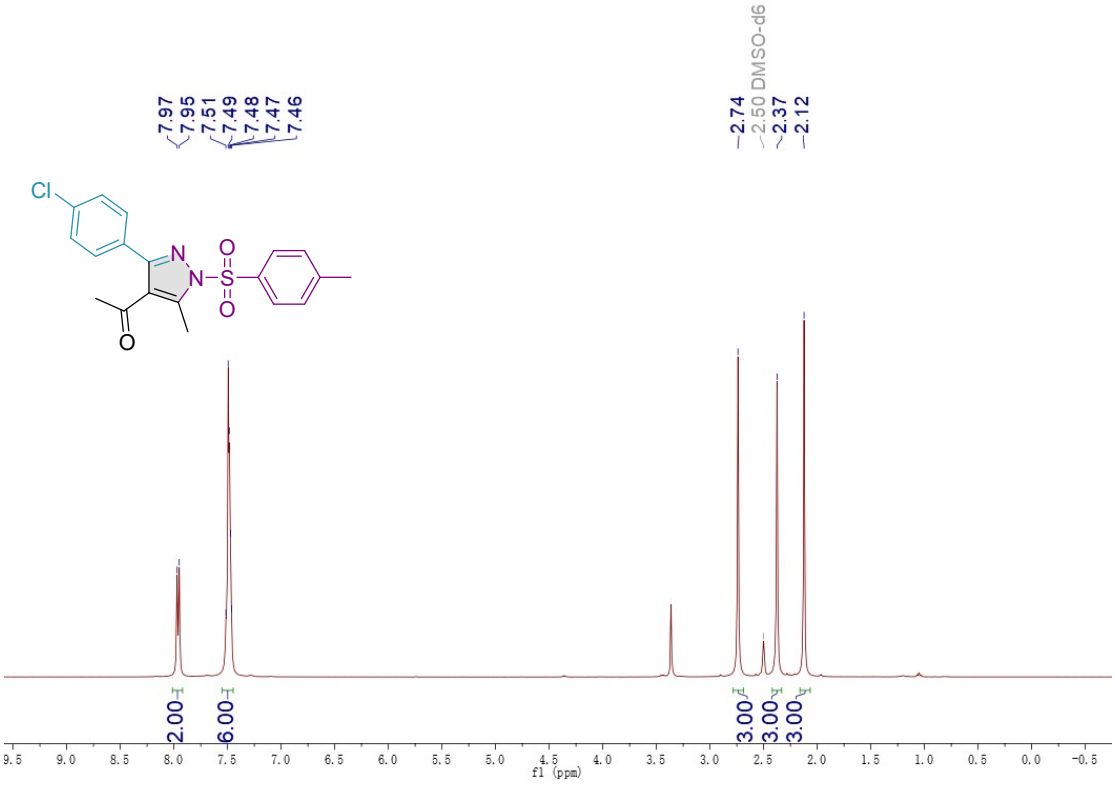


^{13}C NMR (100 MHz, $CDCl_3$)

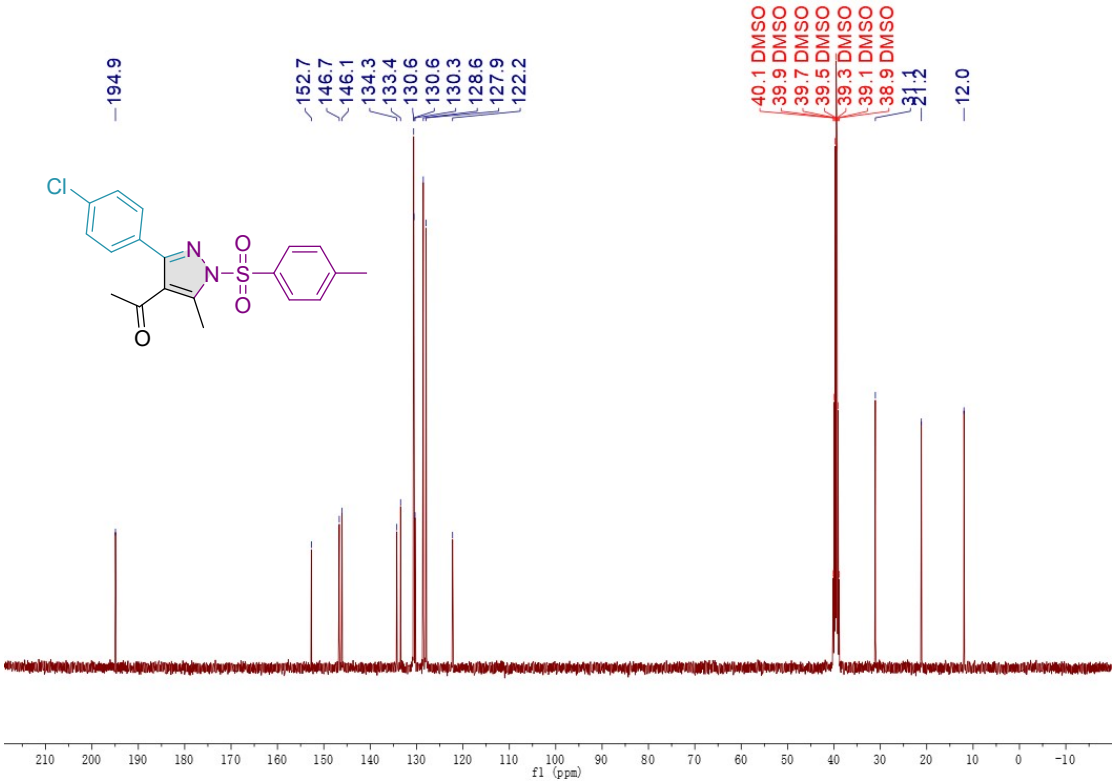


^{19}F NMR (376 MHz, $CDCl_3$)

1-(3-(4-chlorophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4o)

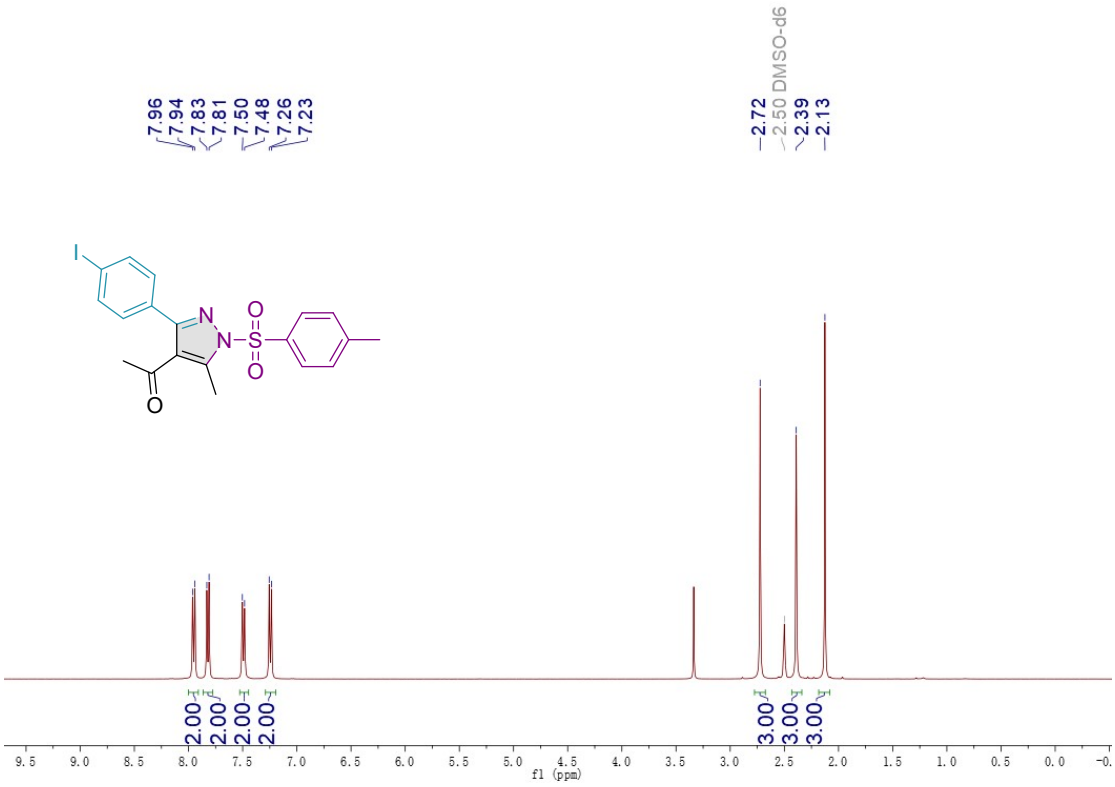


^{1}H NMR (400 MHz, DMSO-d_6)

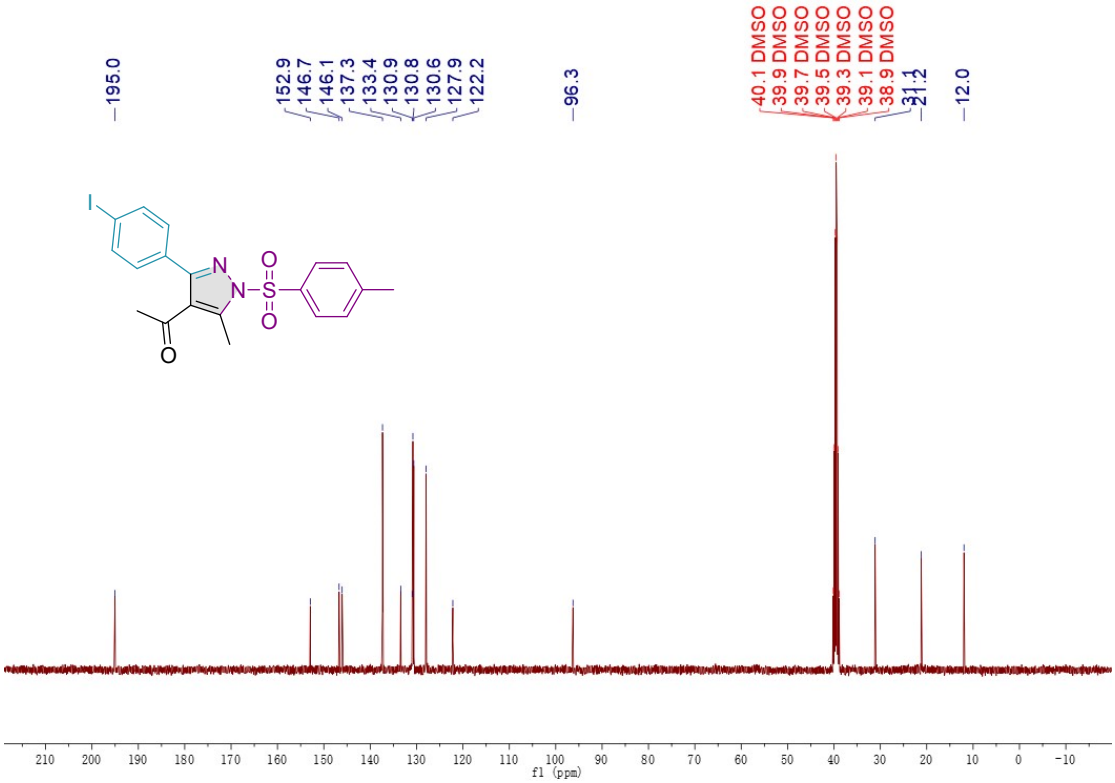


^{13}C NMR (100 MHz, DMSO-d_6)

1-(3-(4-iodophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4p)

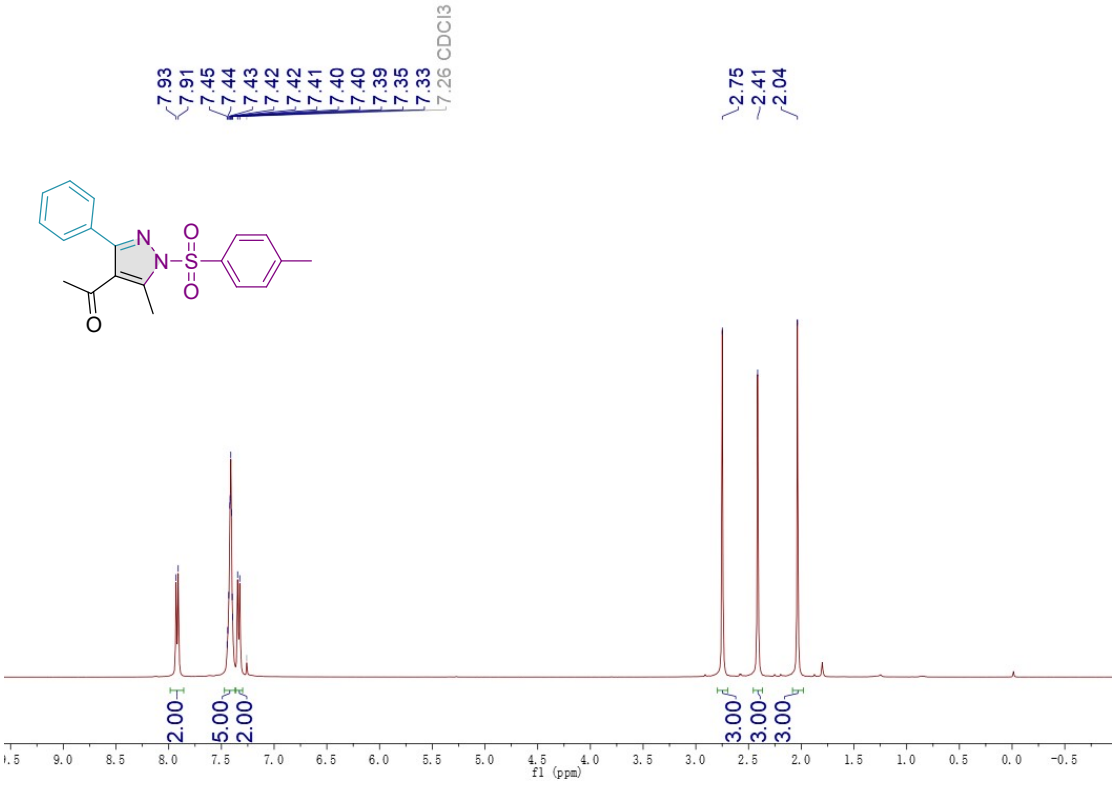


^{1}H NMR (400 MHz, DMSO-d_6)

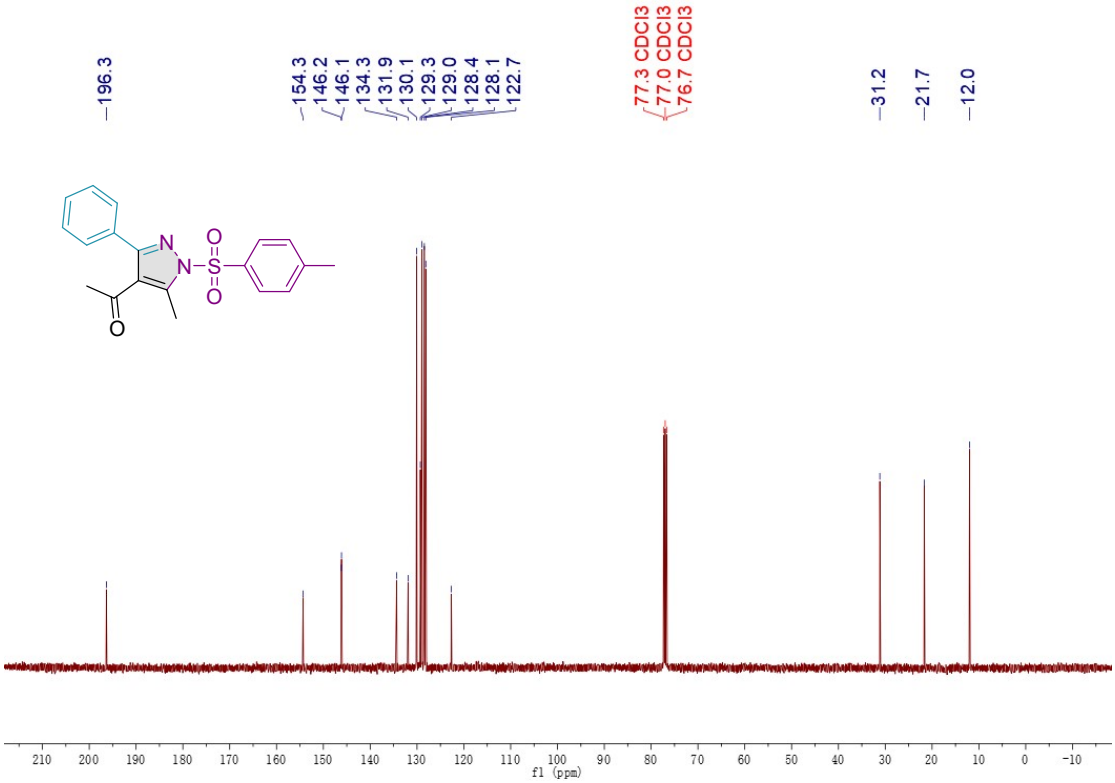


^{13}C NMR (100 MHz, DMSO-d_6)

1-(5-methyl-3-phenyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4q)

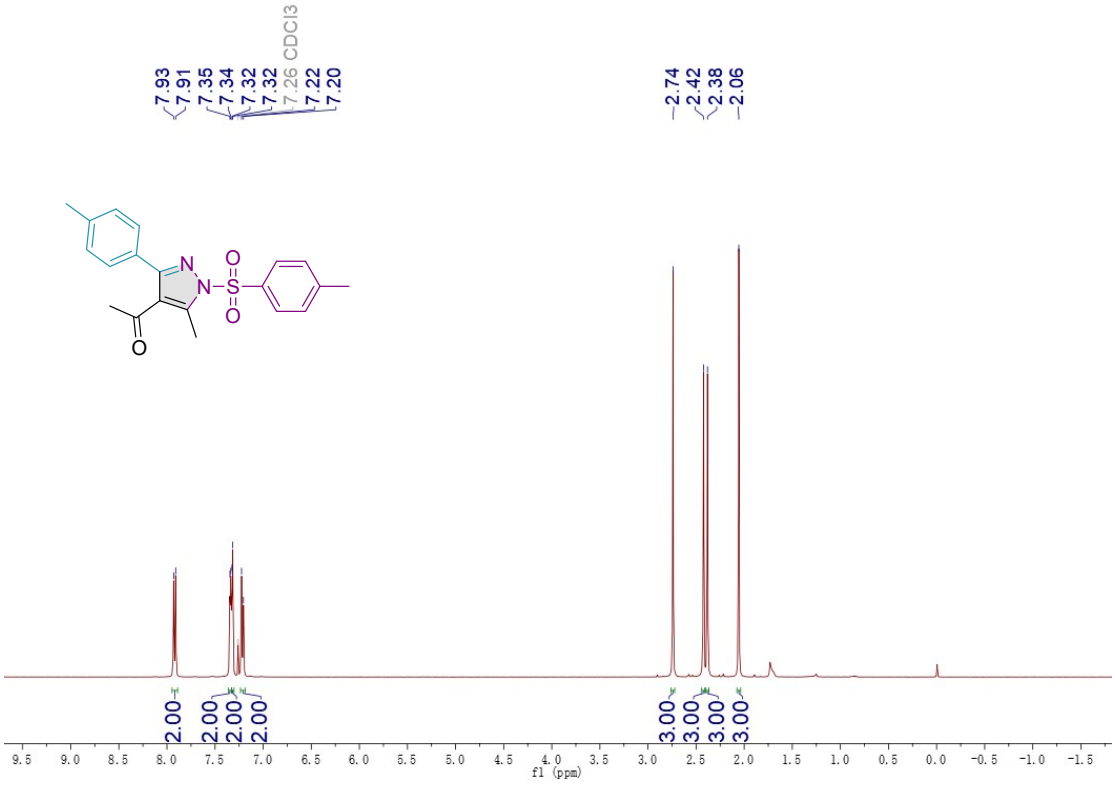


^{1}H NMR (400 MHz, $CDCl_3$)

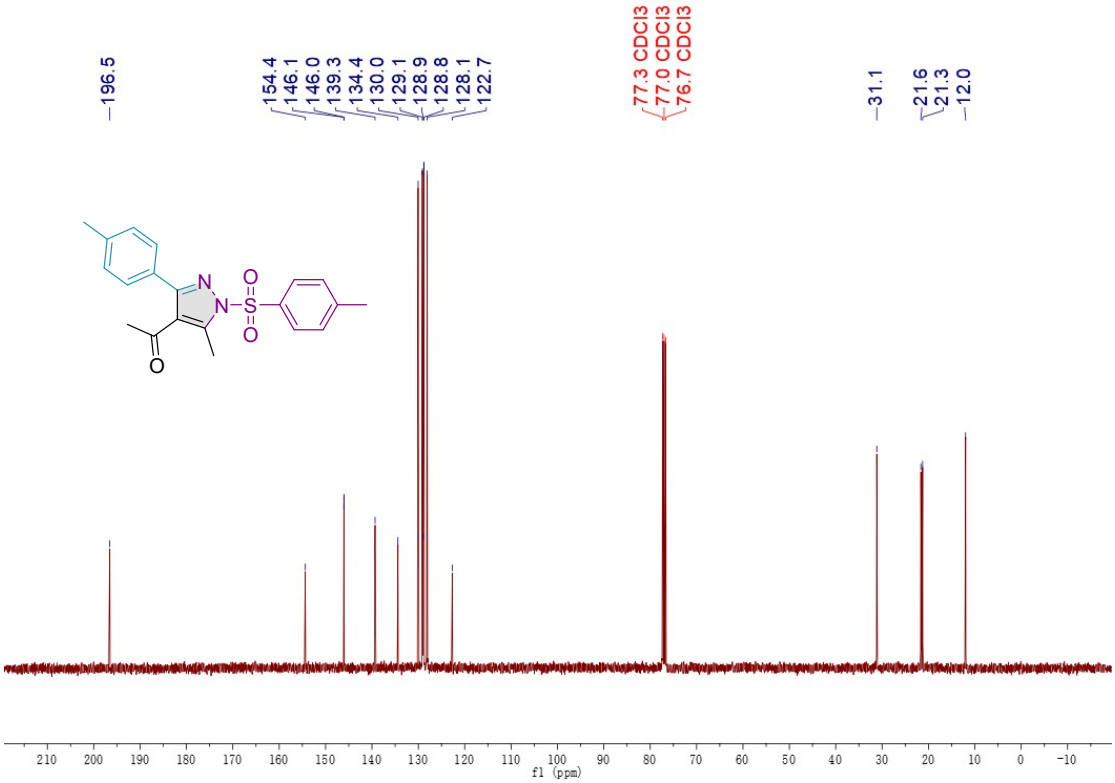


^{13}C NMR (100 MHz, $CDCl_3$)

1-(5-methyl-3-(p-tolyl)-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4r)

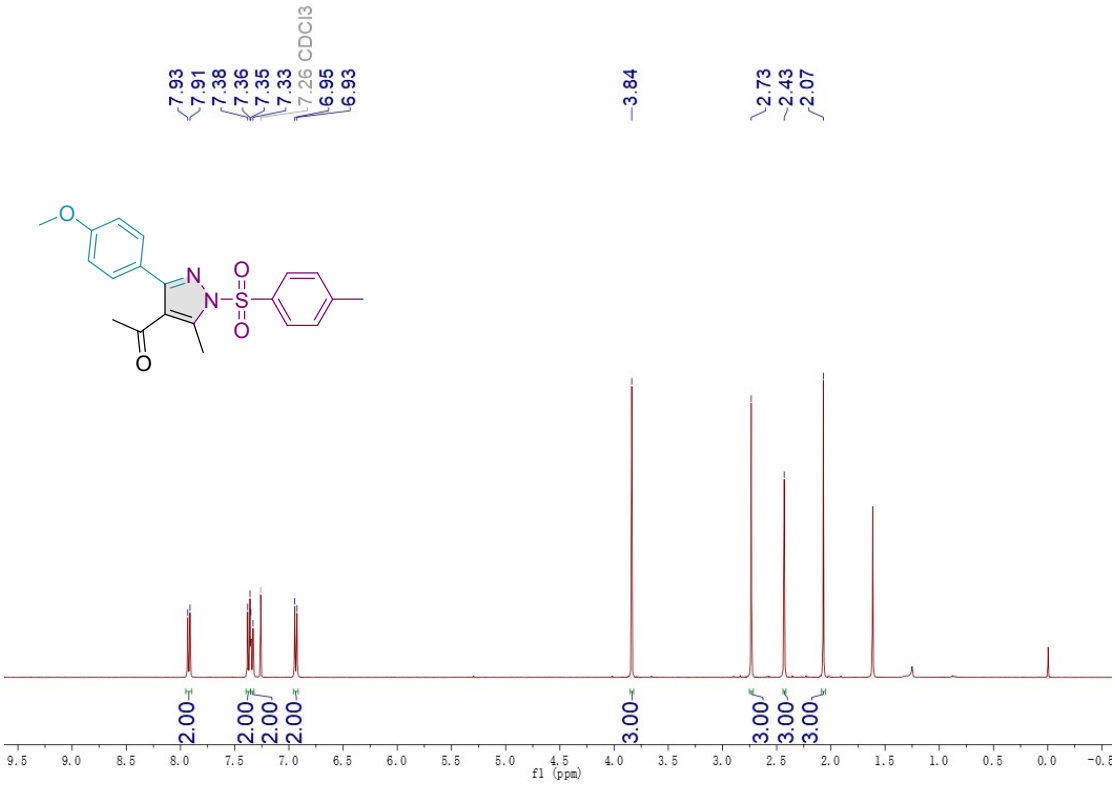


^{1}H NMR (400 MHz, $CDCl_3$)

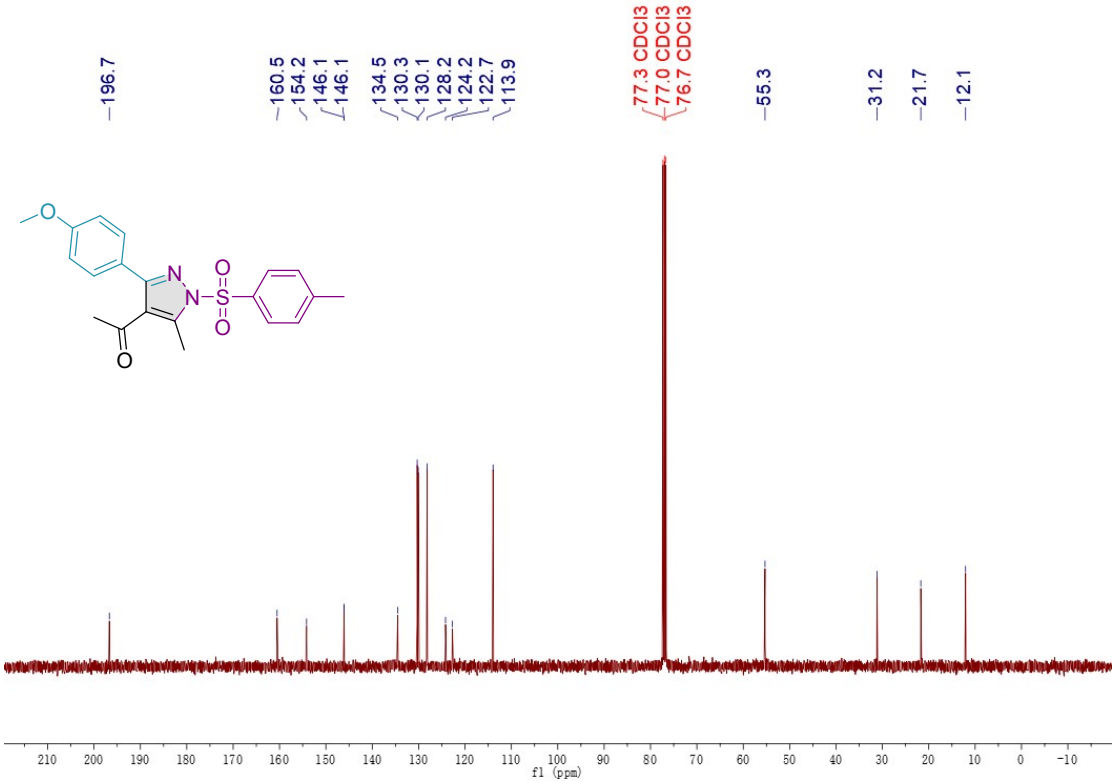


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-methoxyphenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4s)

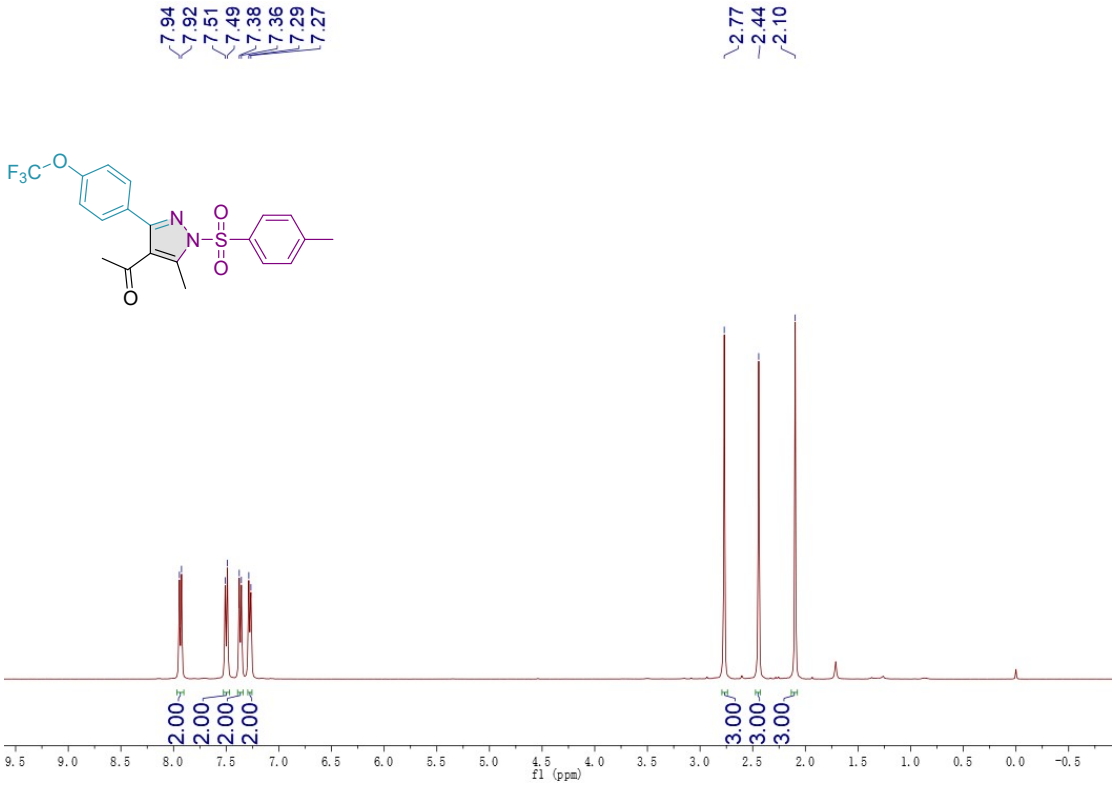


^{1}H NMR (400 MHz, $CDCl_3$)

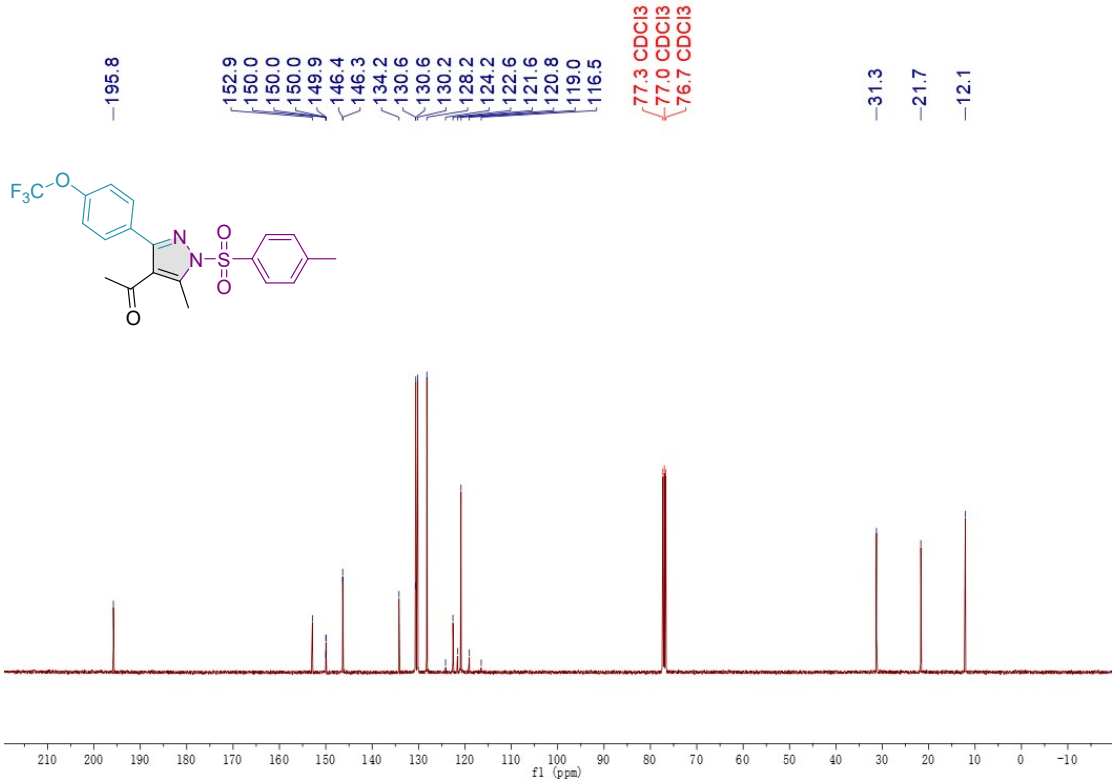


^{13}C NMR (100 MHz, $CDCl_3$)

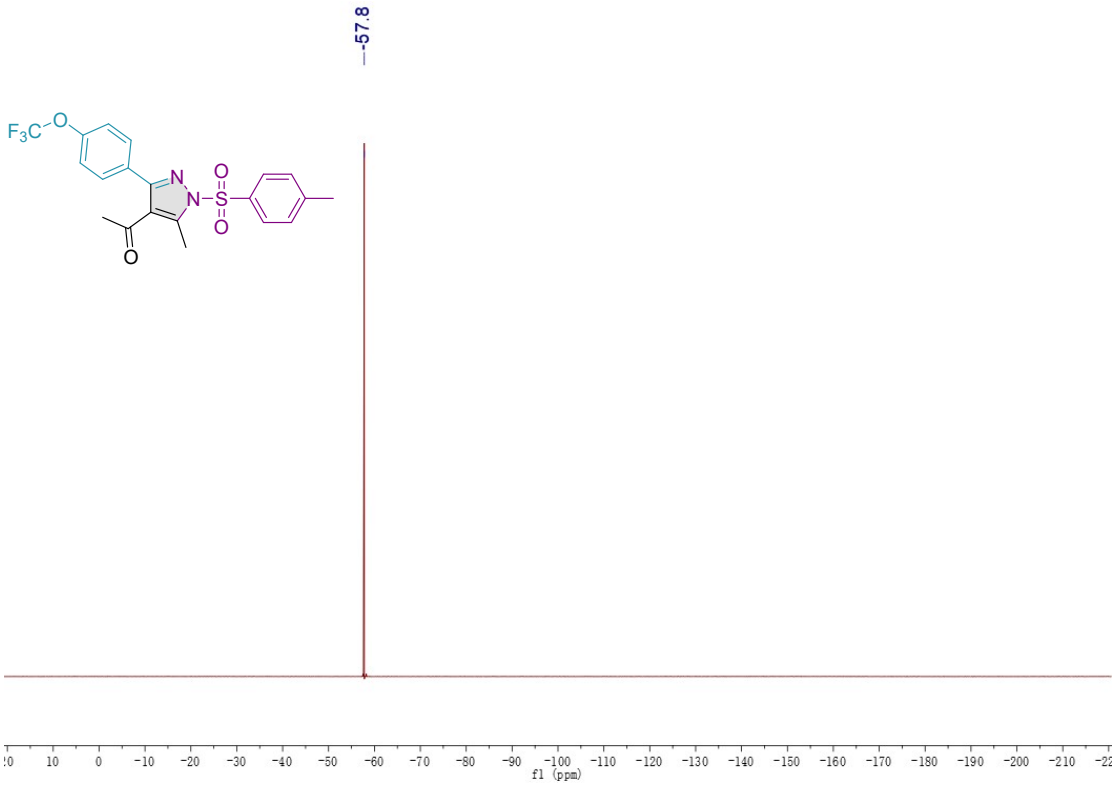
1-(5-methyl-1-tosyl-3-(4-(trifluoromethoxy)phenyl)-1*H*-pyrazol-4-yl)ethan-1-one (4t)



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

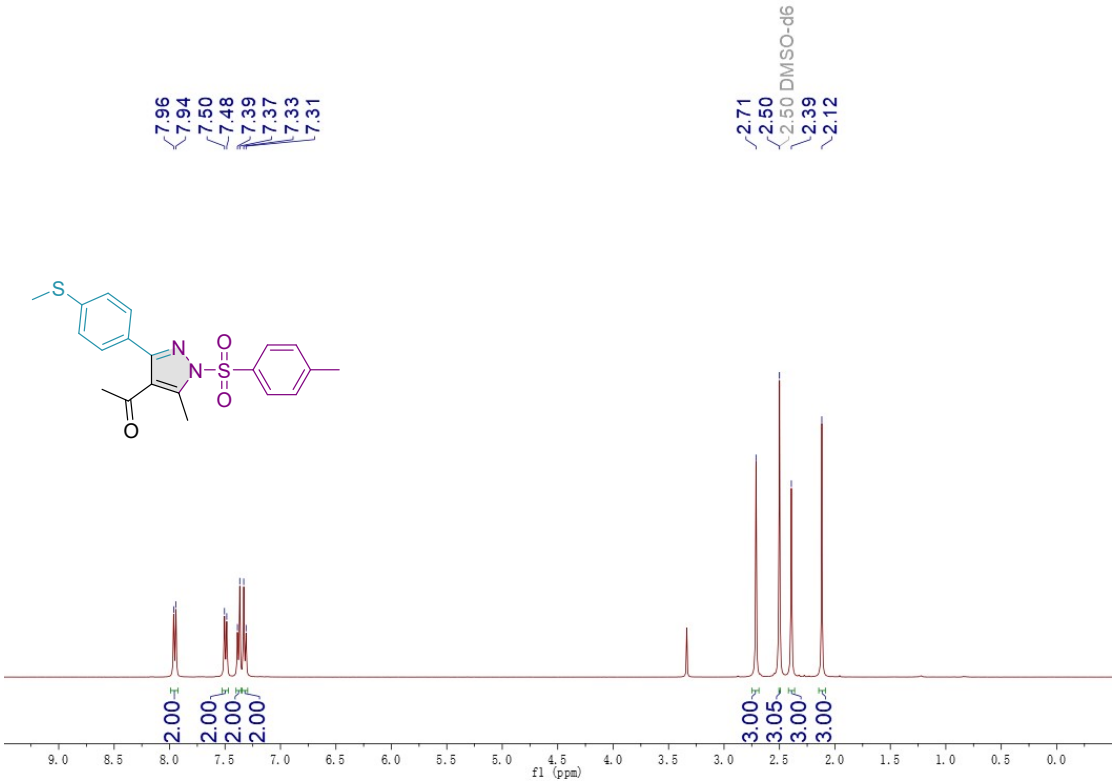


^{13}C NMR (100 MHz, $CDCl_3$)

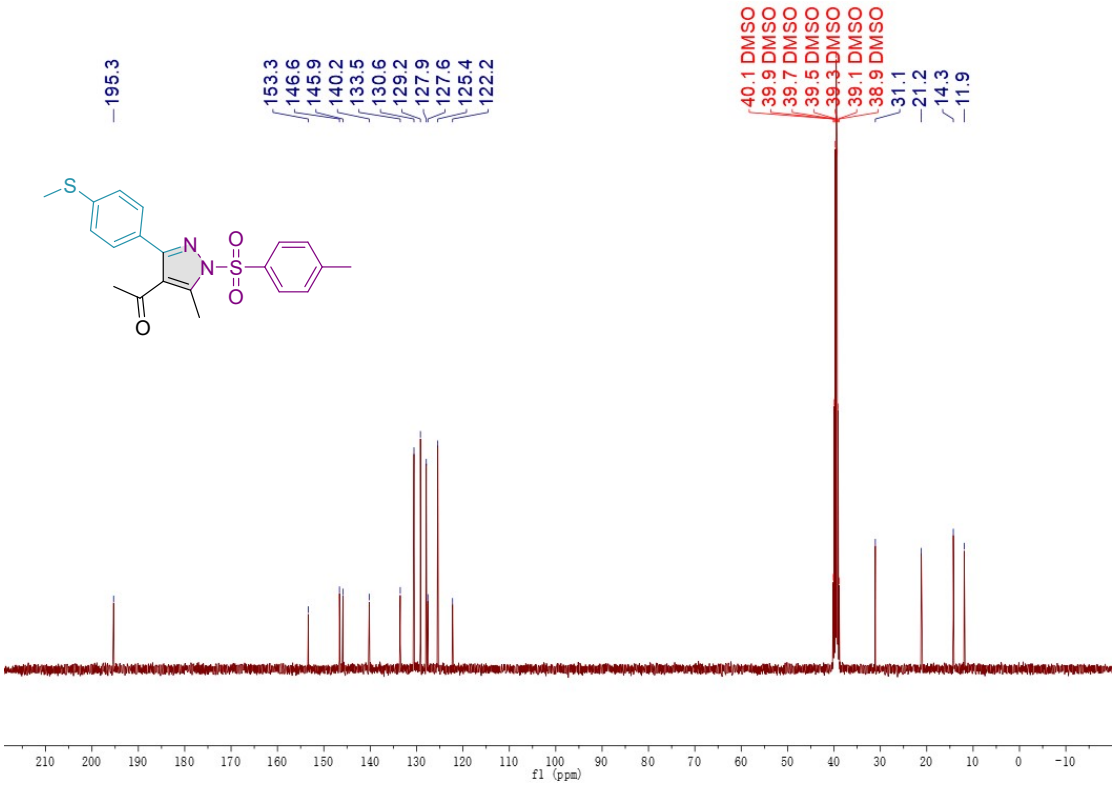


^{19}F NMR (376 MHz, $CDCl_3$)

1-(5-methyl-3-(4-(methylthio)phenyl)-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4u)

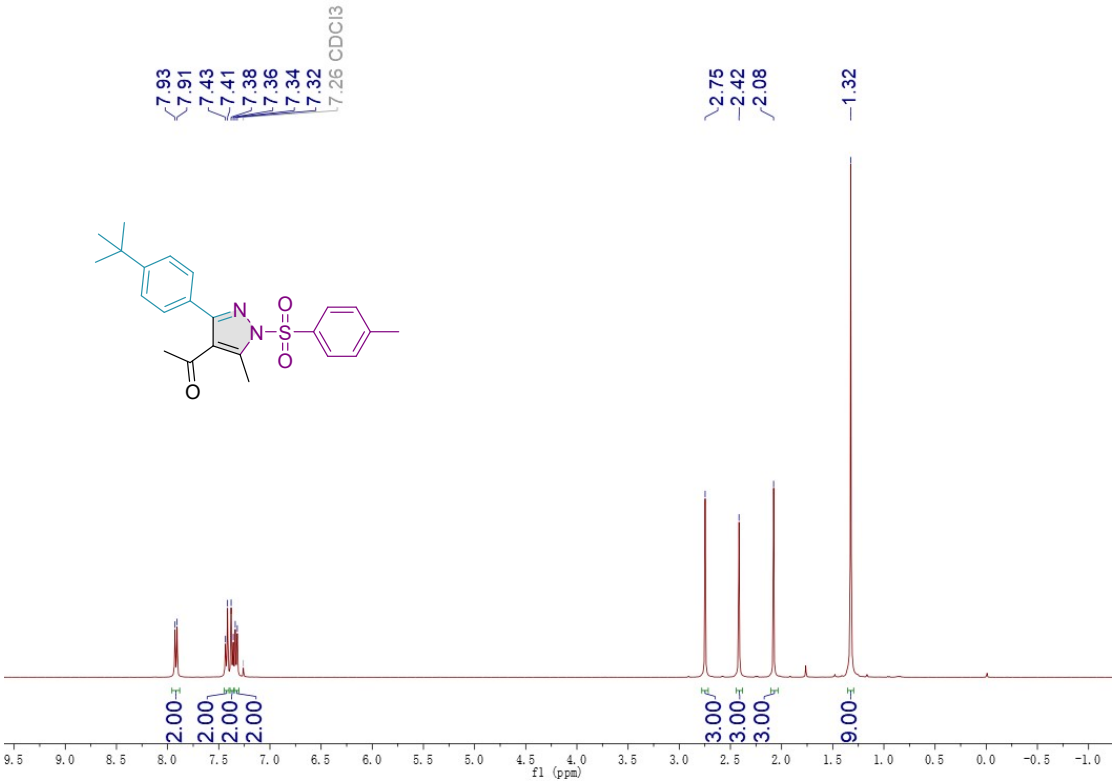


^{1}H NMR (400 MHz, DMSO-d_6)

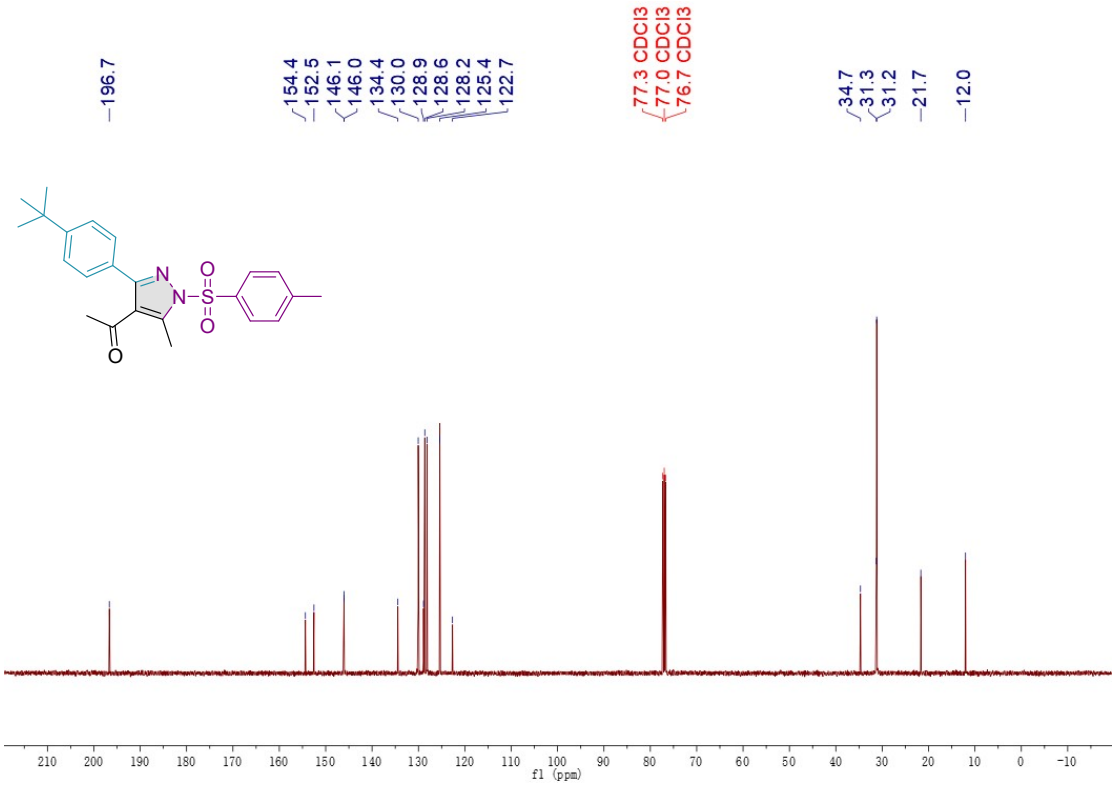


^{13}C NMR (100 MHz, DMSO-d_6)

1-(3-(4-(tert-butyl)phenyl-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4v)

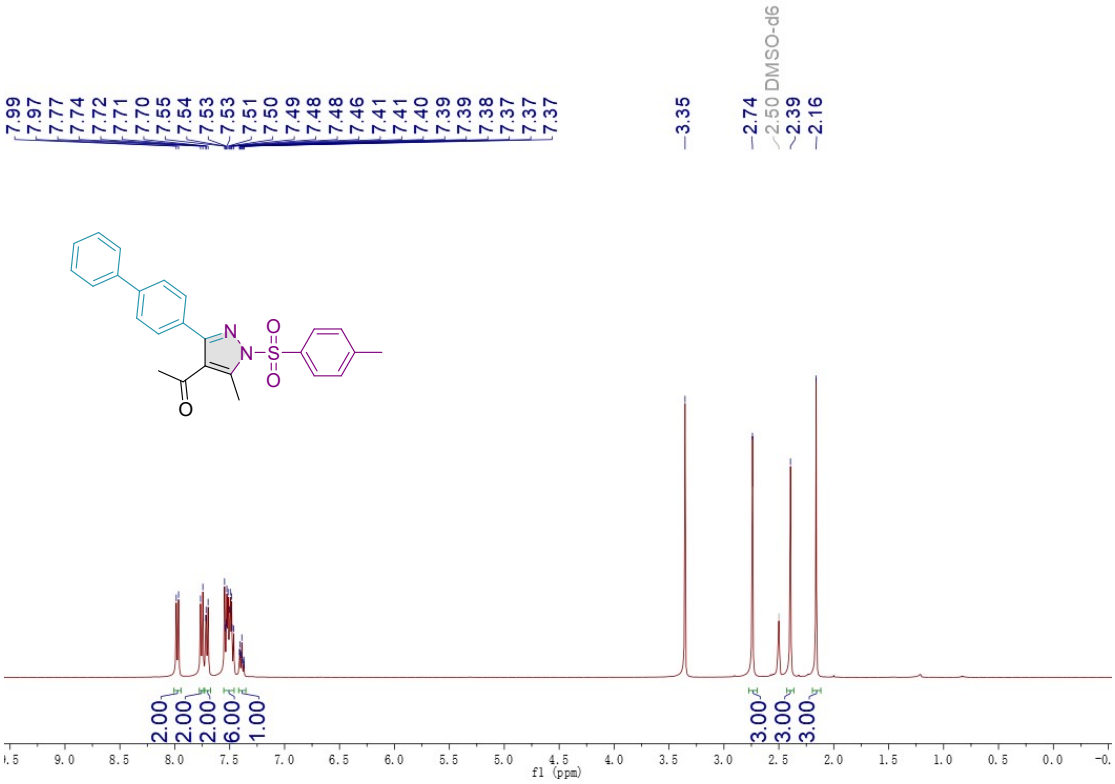


^{1}H NMR (400 MHz, $CDCl_3$)

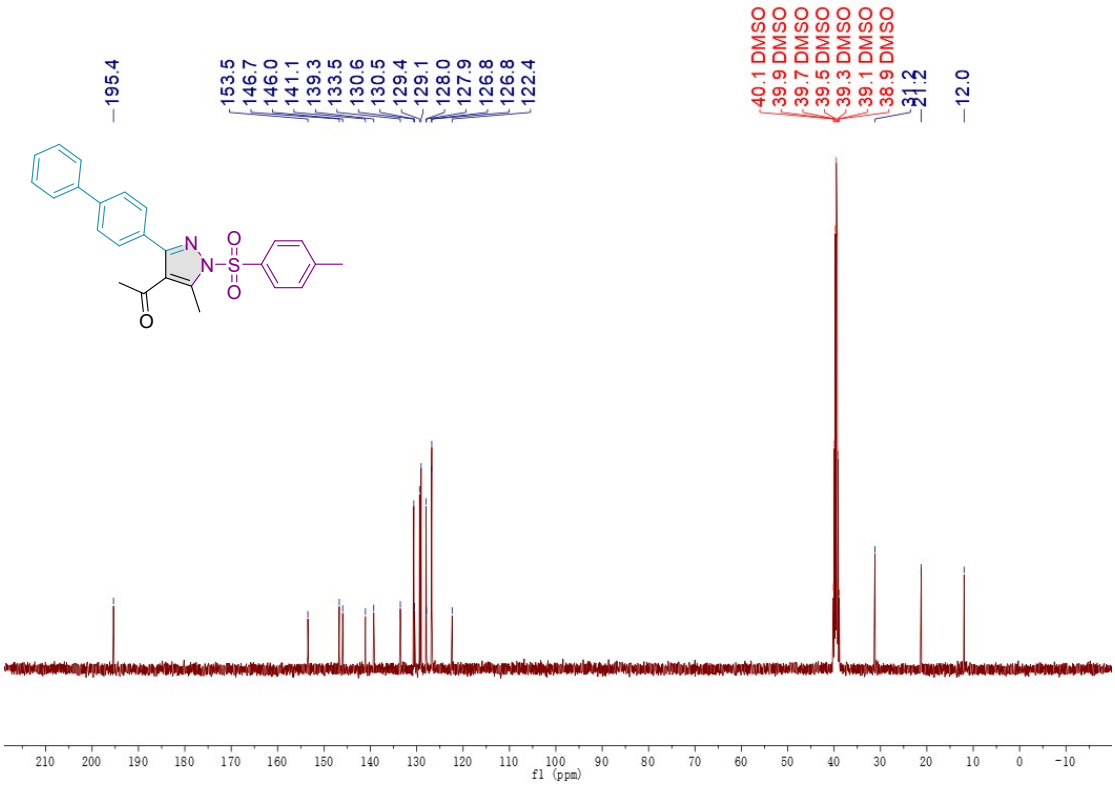


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-([1,1'-biphenyl]-4-yl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4w)

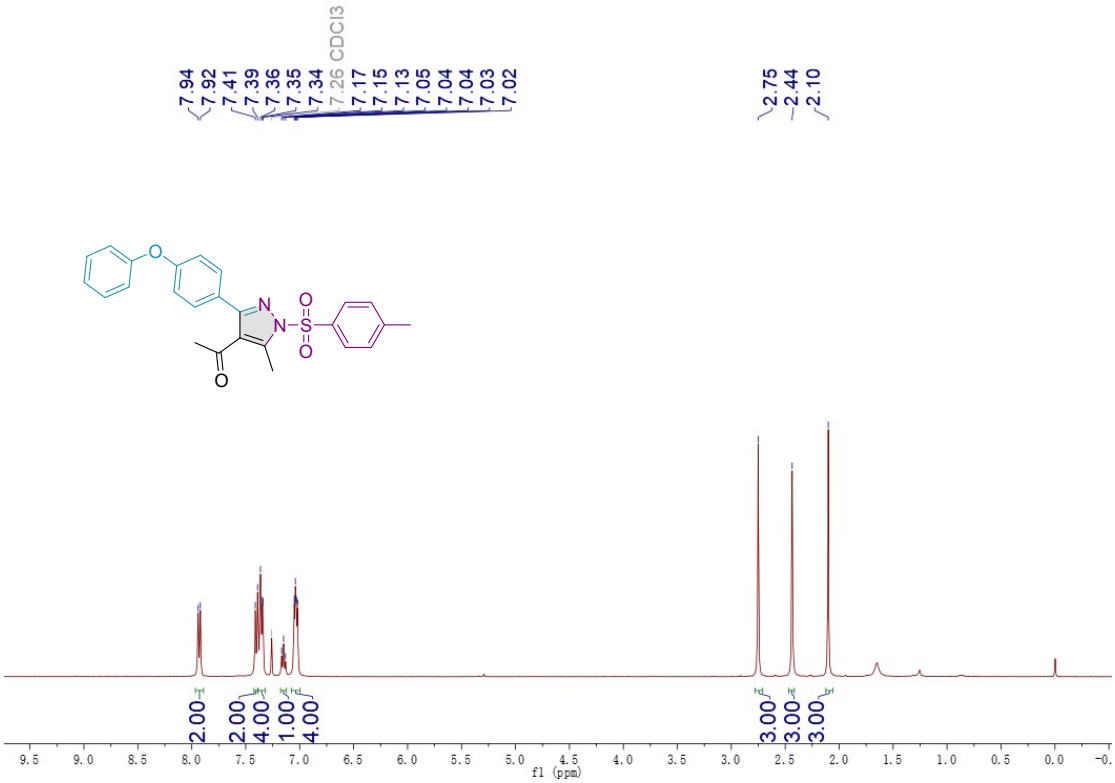


^{1}H NMR (400 MHz, DMSO-d_6)

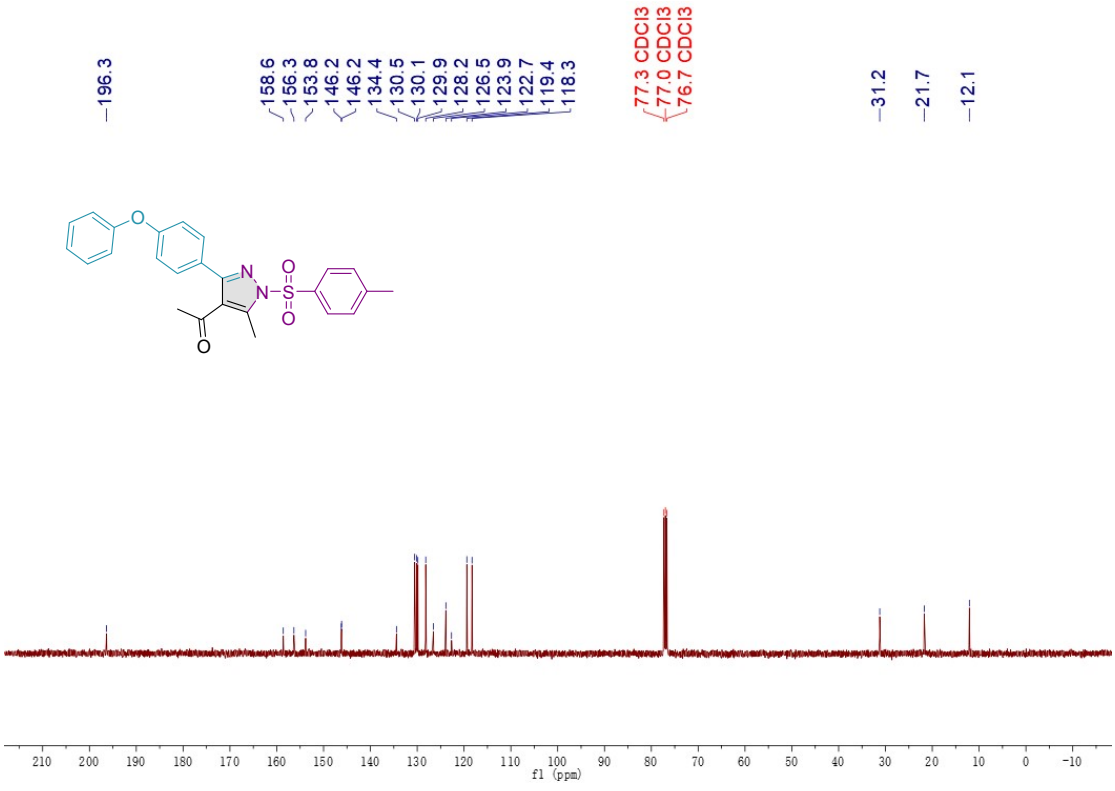


^{13}C NMR (100 MHz, DMSO-d_6)

1-(5-methyl-3-(4-phenoxyphenyl)-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4x）

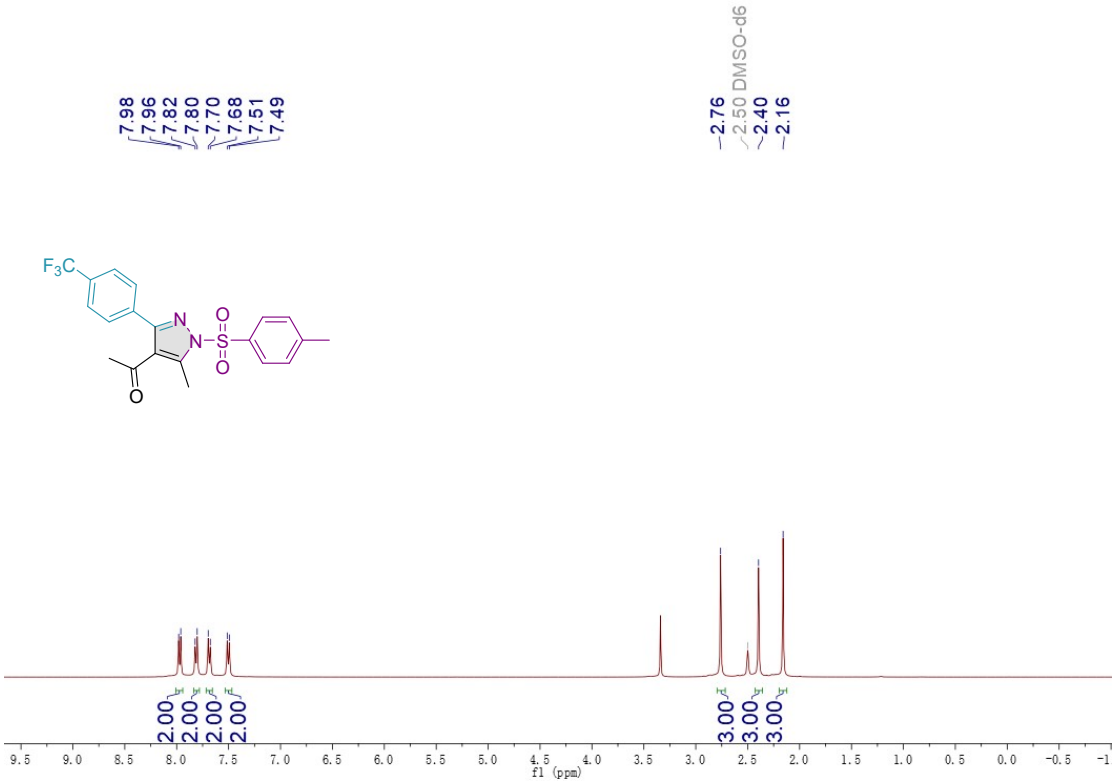


^{1}H NMR (400 MHz, $CDCl_3$)

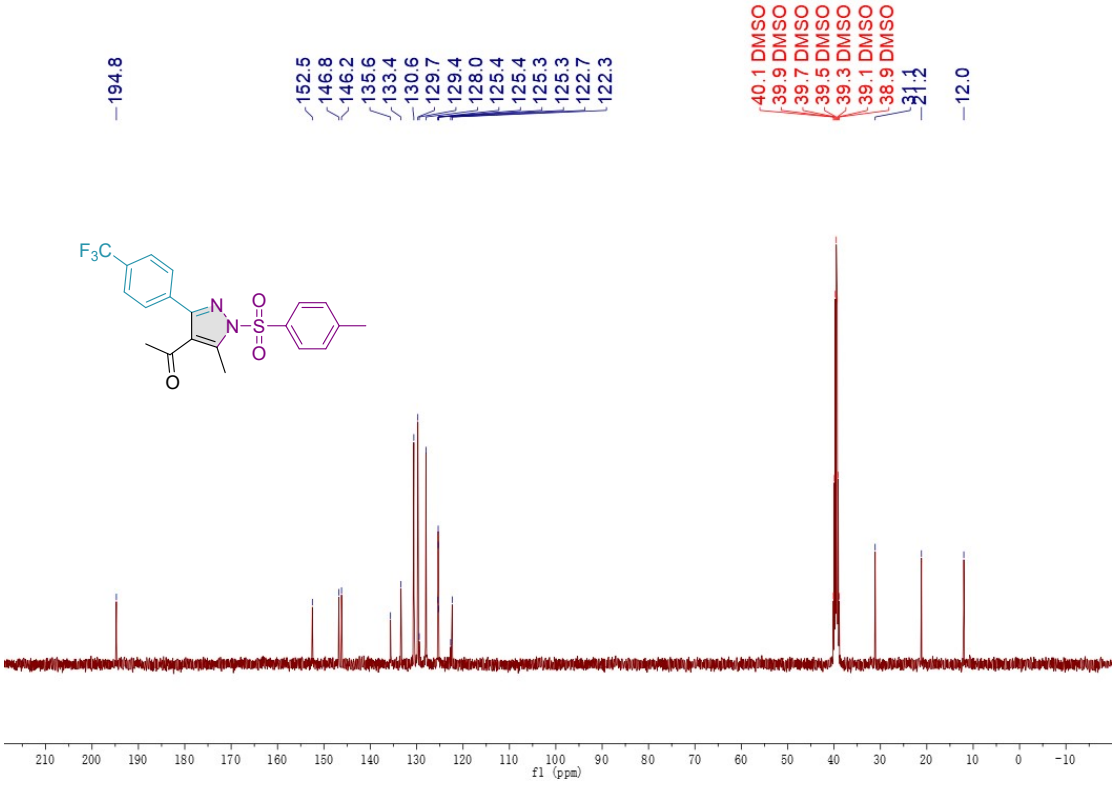


^{13}C NMR (100 MHz, $CDCl_3$)

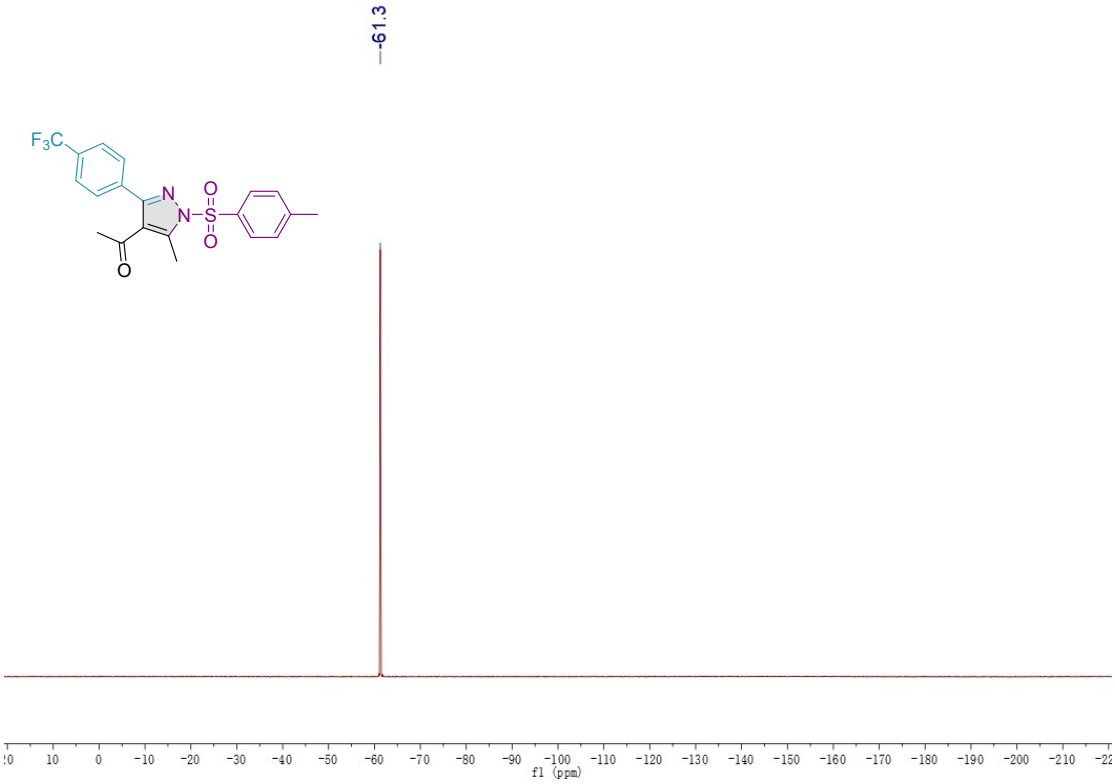
1-(5-methyl-1-tosyl-3-(4-(trifluoromethyl)phenyl)-1*H*-pyrazol-4-yl)ethan-1-one (4y)



^{1}H NMR (400 MHz, DMSO-d_6)

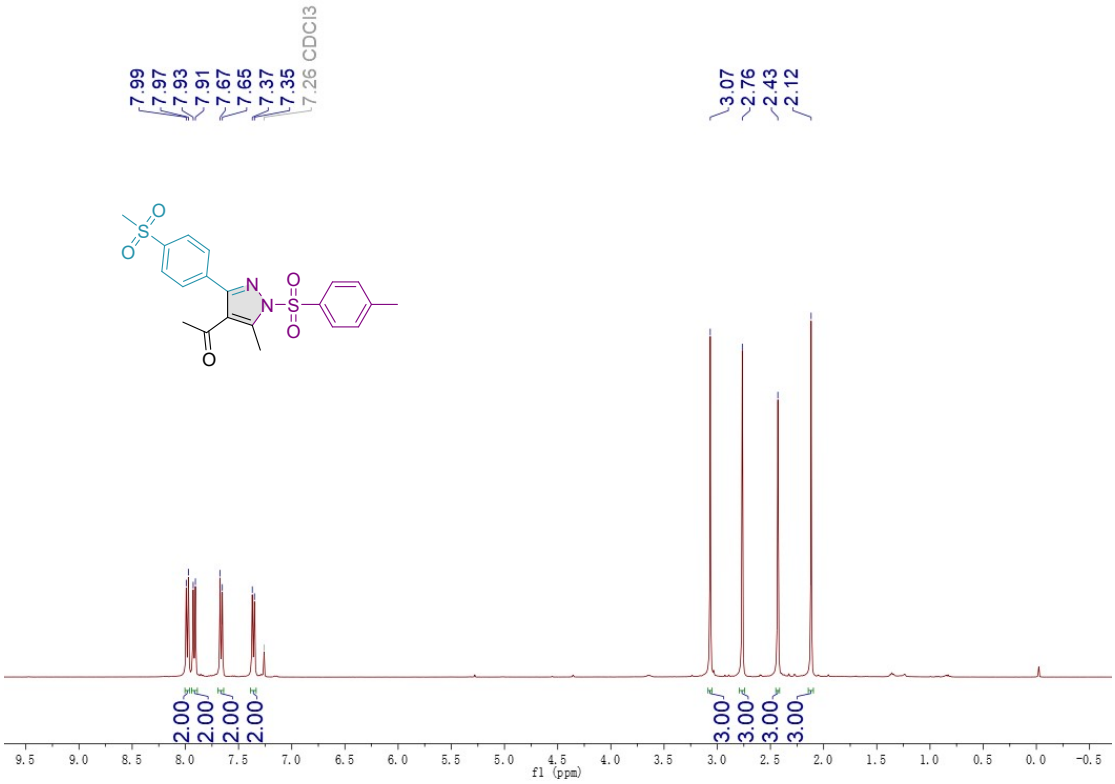


^{13}C NMR (100 MHz, DMSO-d_6)

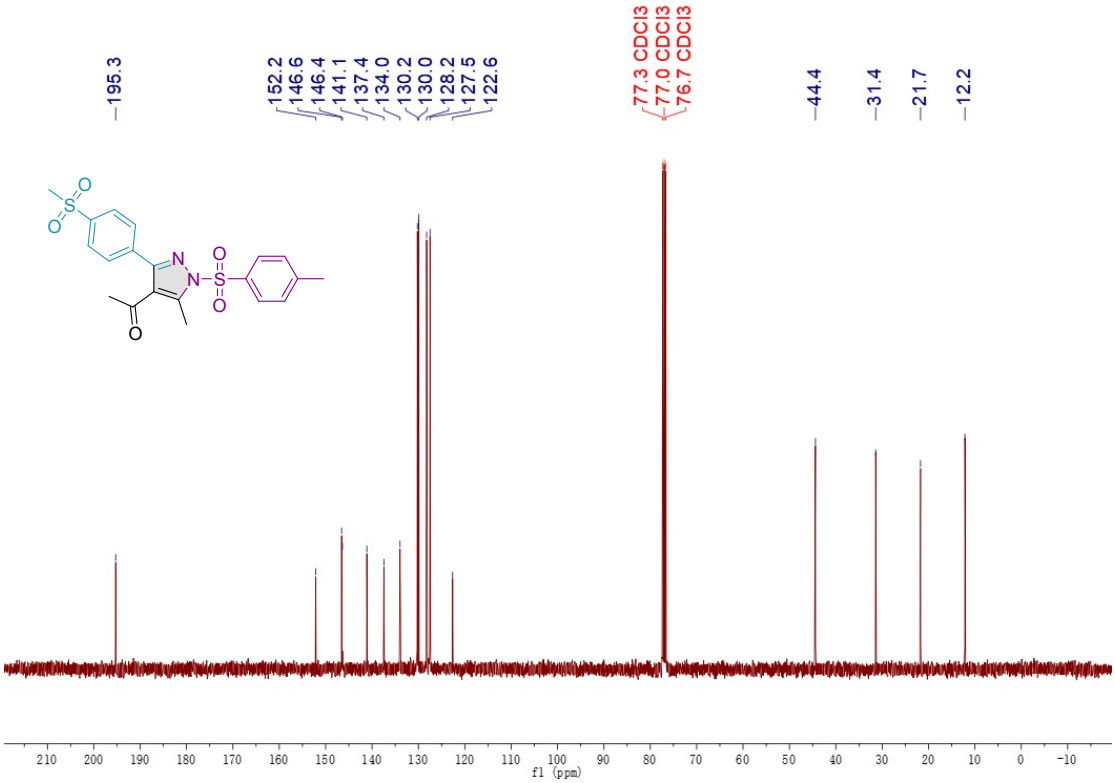


^{19}F NMR (376 MHz, DMSO-d_6)

1-(5-methyl-3-(4-(methylsulfonyl)phenyl)-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4z)

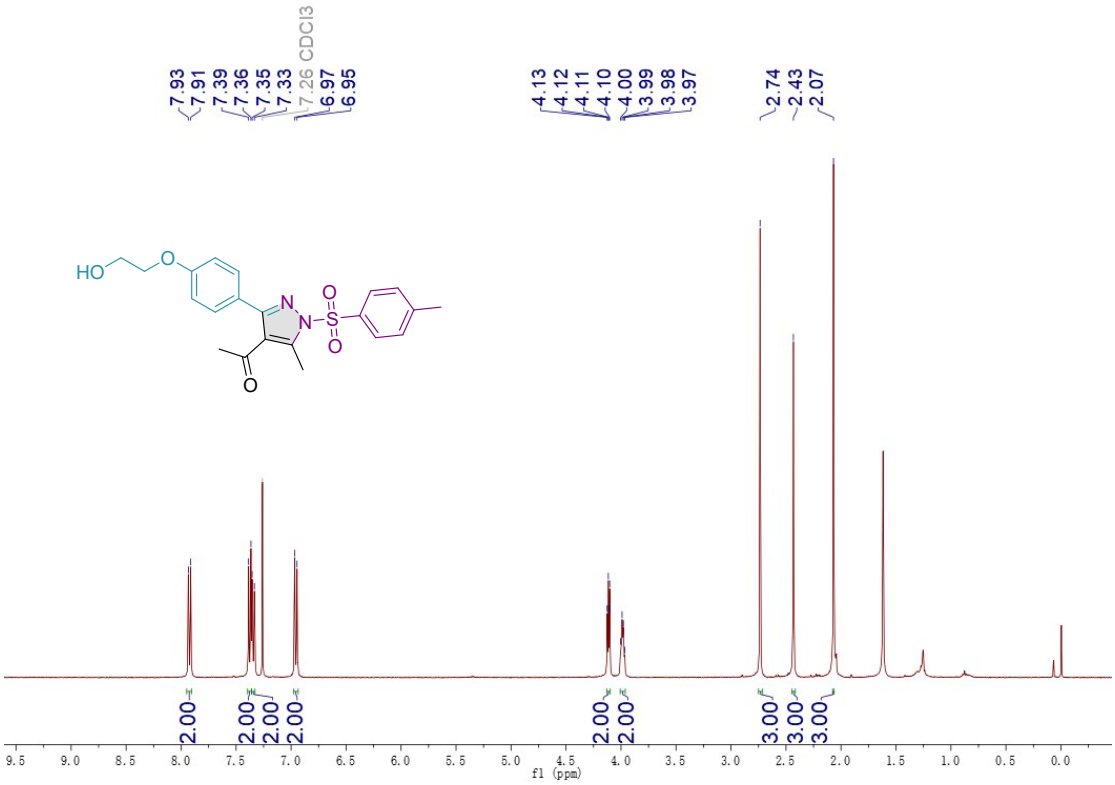


^{1}H NMR (400 MHz, $CDCl_3$)

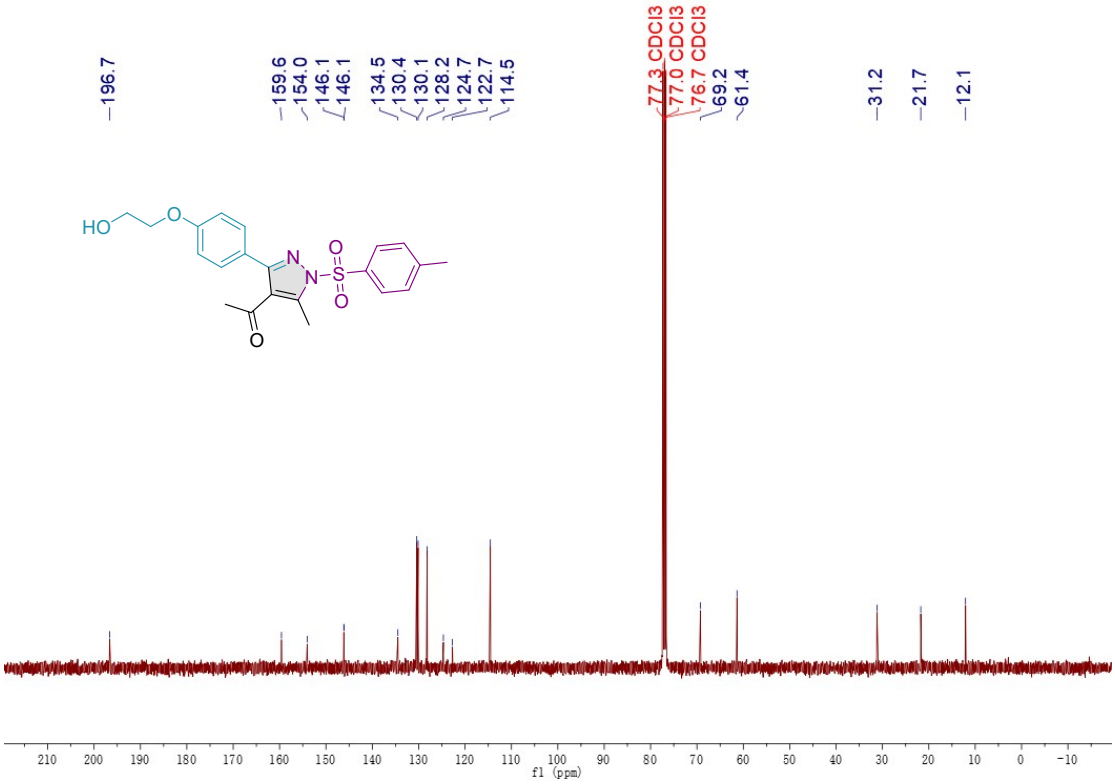


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-(2-hydroxyethoxy)phenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4aa)

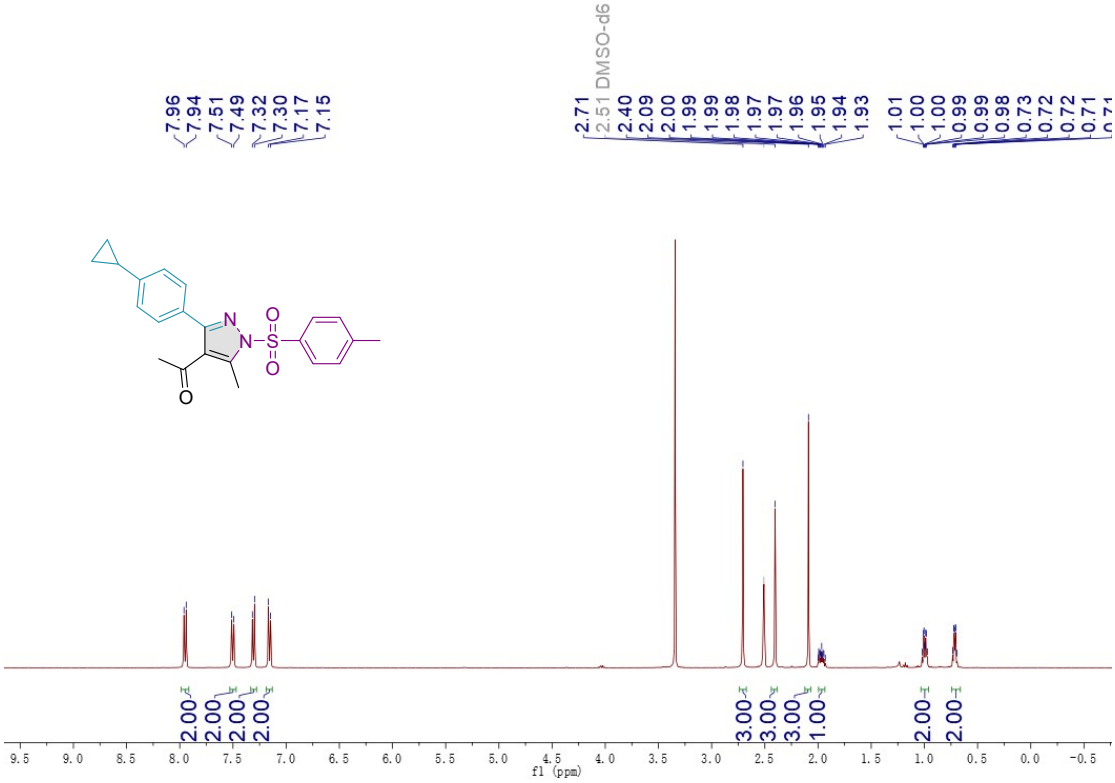


^{1}H NMR (400 MHz, $CDCl_3$)

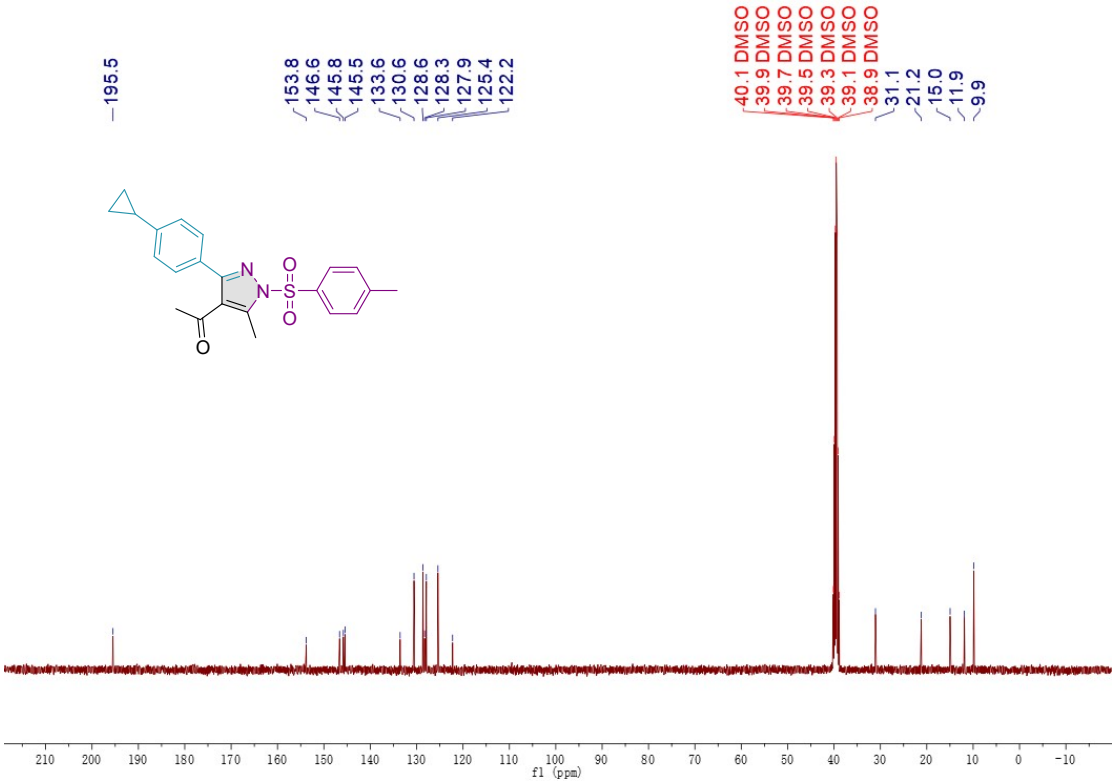


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-cyclopropylphenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ab)

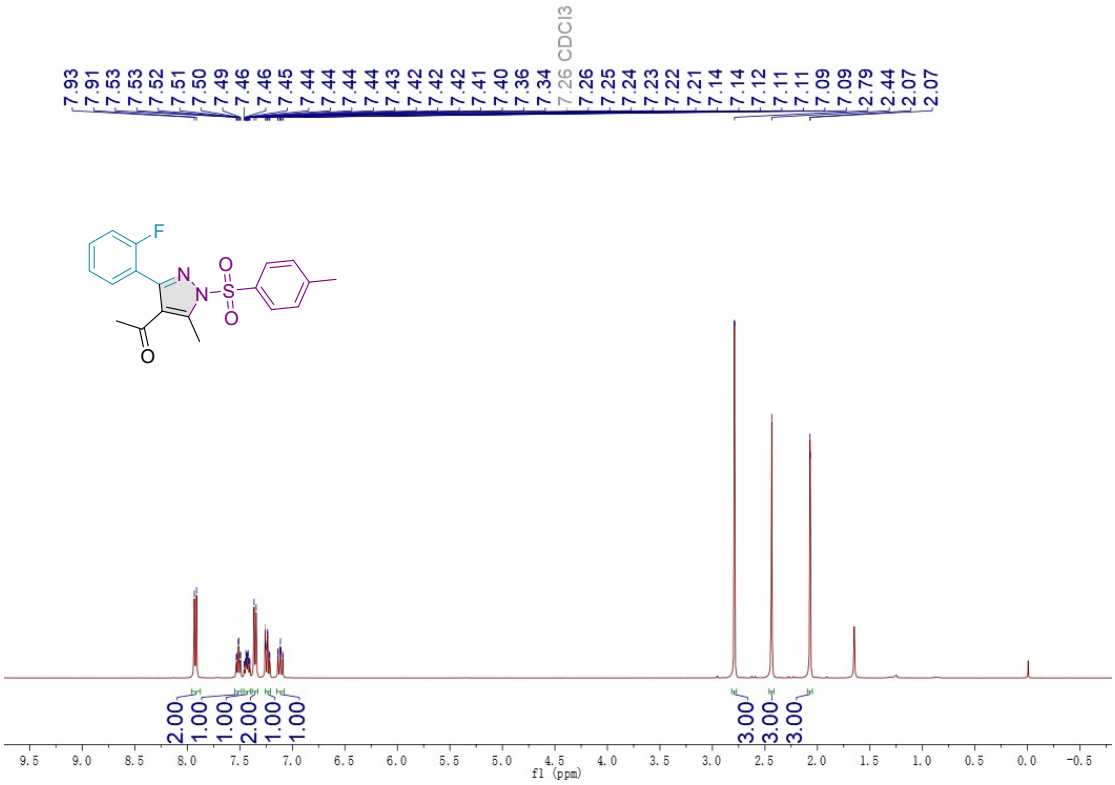


^{1}H NMR (400 MHz, DMSO-d_6)

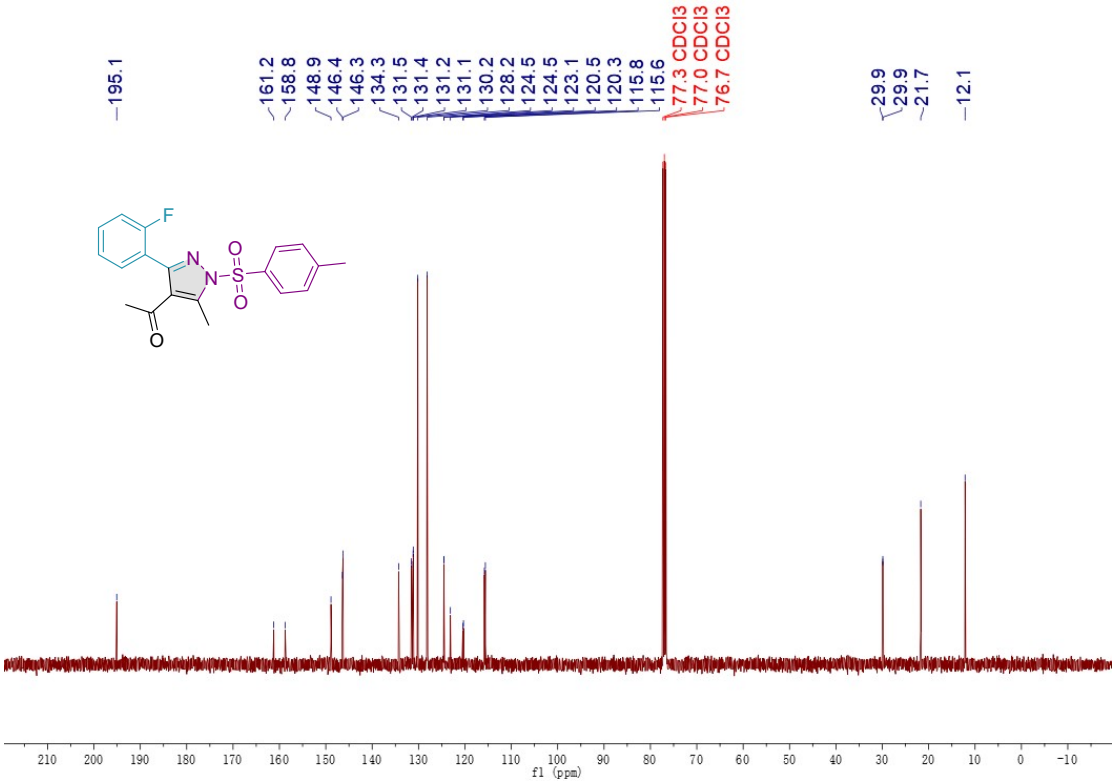


^{13}C NMR (100 MHz, DMSO-d_6)

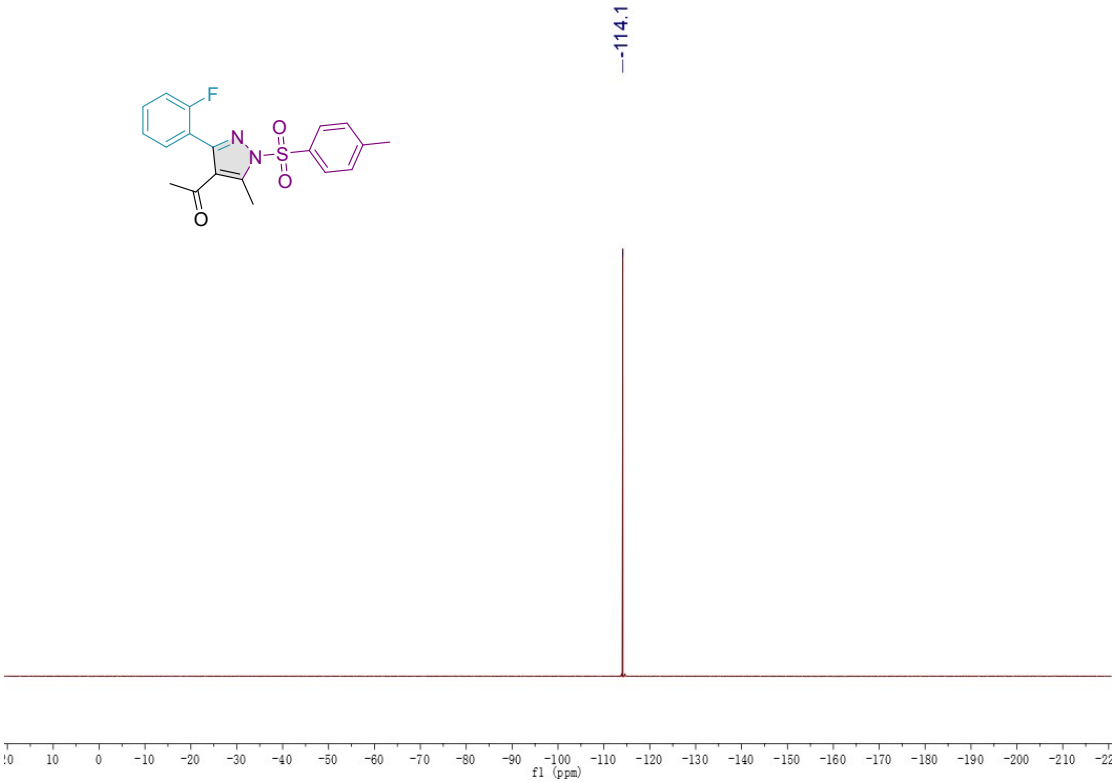
1-(3-(2-fluorophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ac)



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

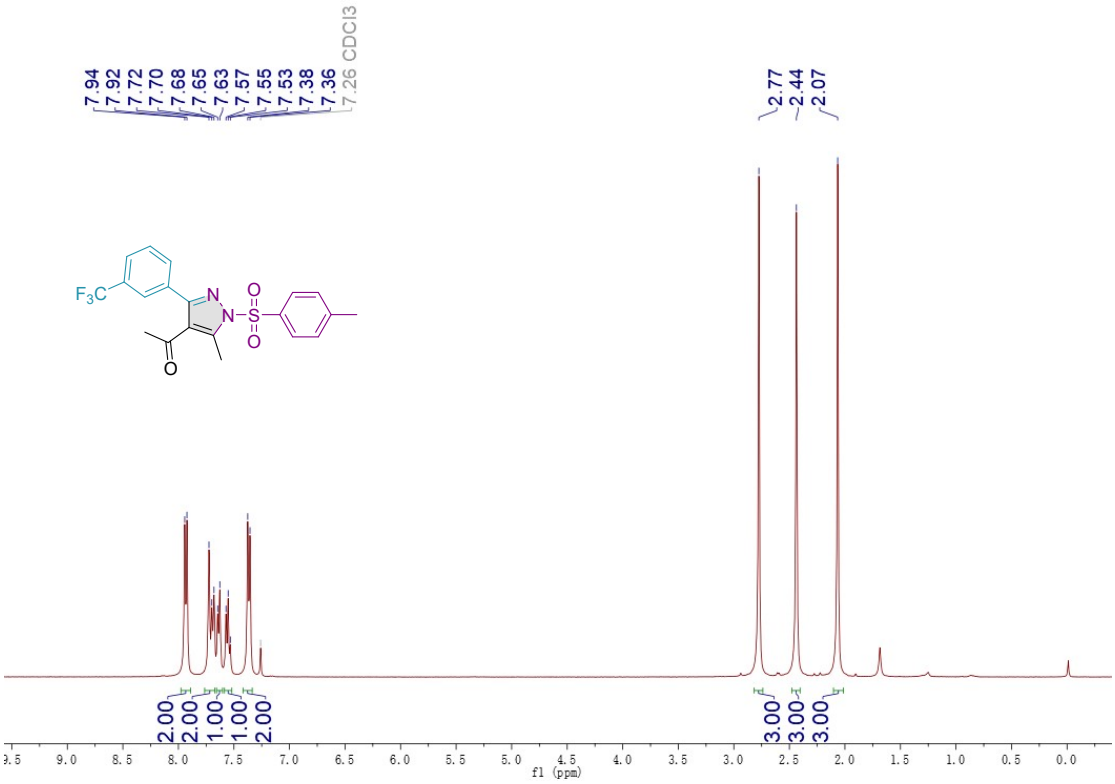


^{13}C NMR (100 MHz, $CDCl_3$)

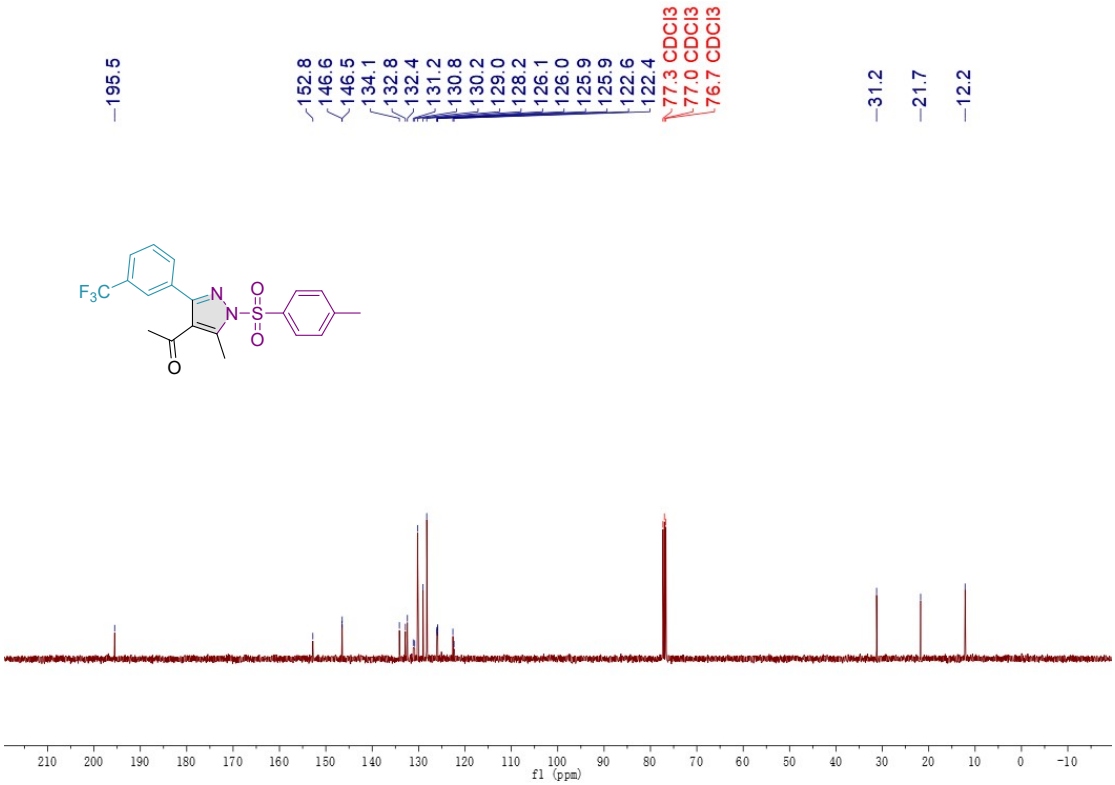


^{19}F NMR (376 MHz, $CDCl_3$)

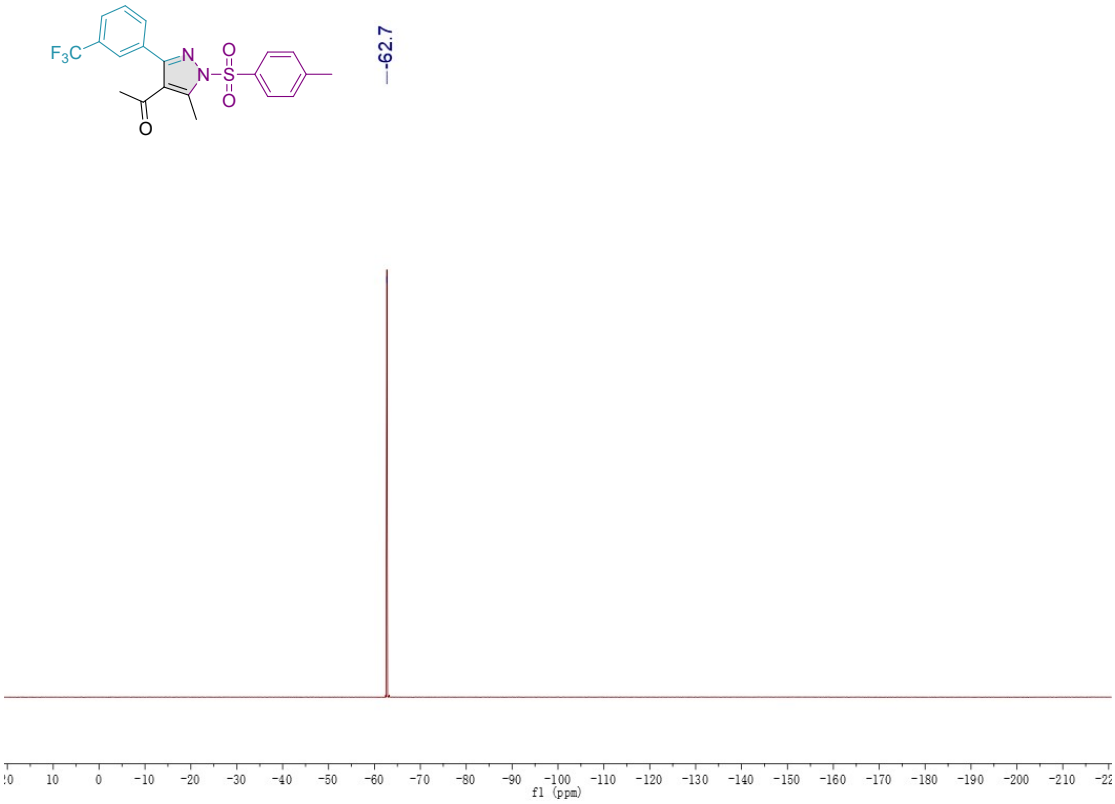
1-(5-methyl-1-tosyl-3-(3-(trifluoromethyl)phenyl)-1*H*-pyrazol-4-yl)ethan-1-one (4ad)



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

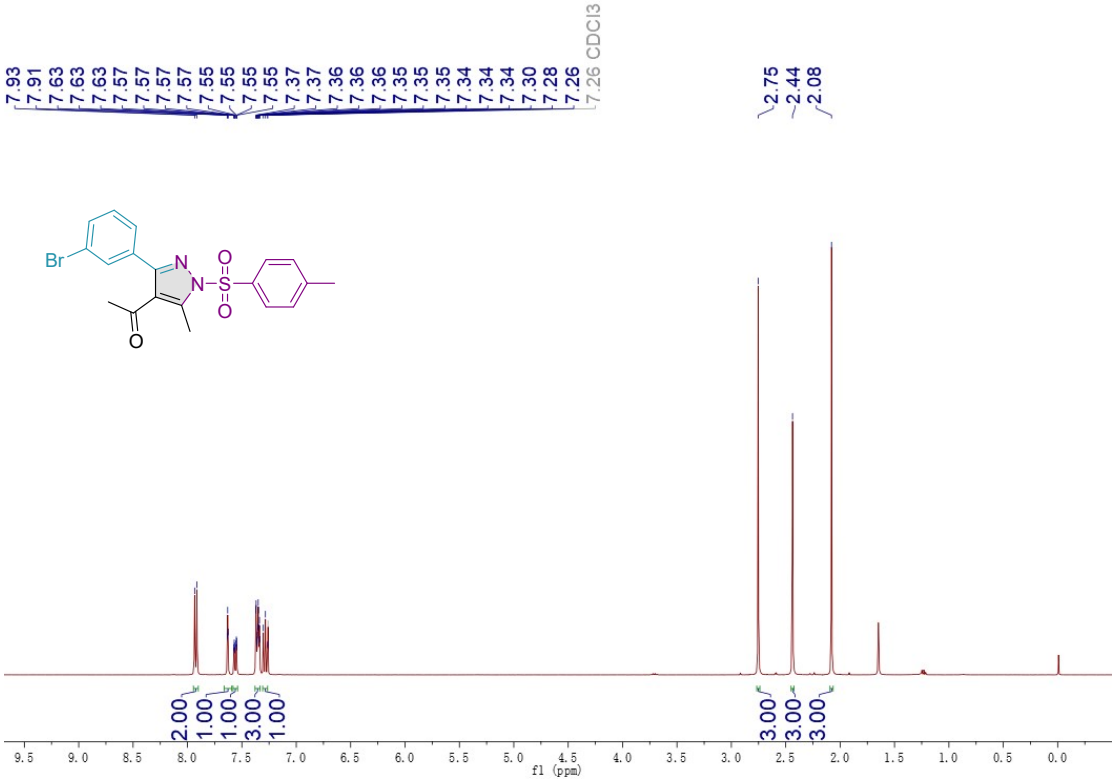


^{13}C NMR (100 MHz, $CDCl_3$)

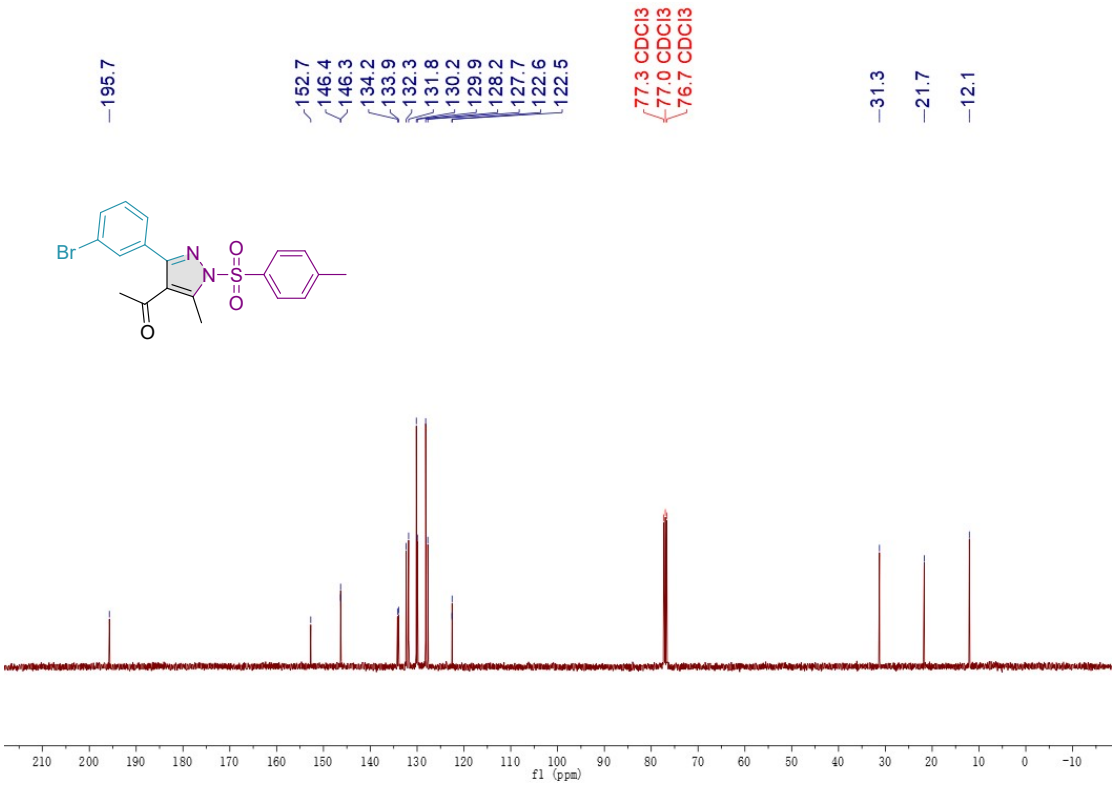


^{19}F NMR (376 MHz, $CDCl_3$)

1-(3-(3-bromophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ae)

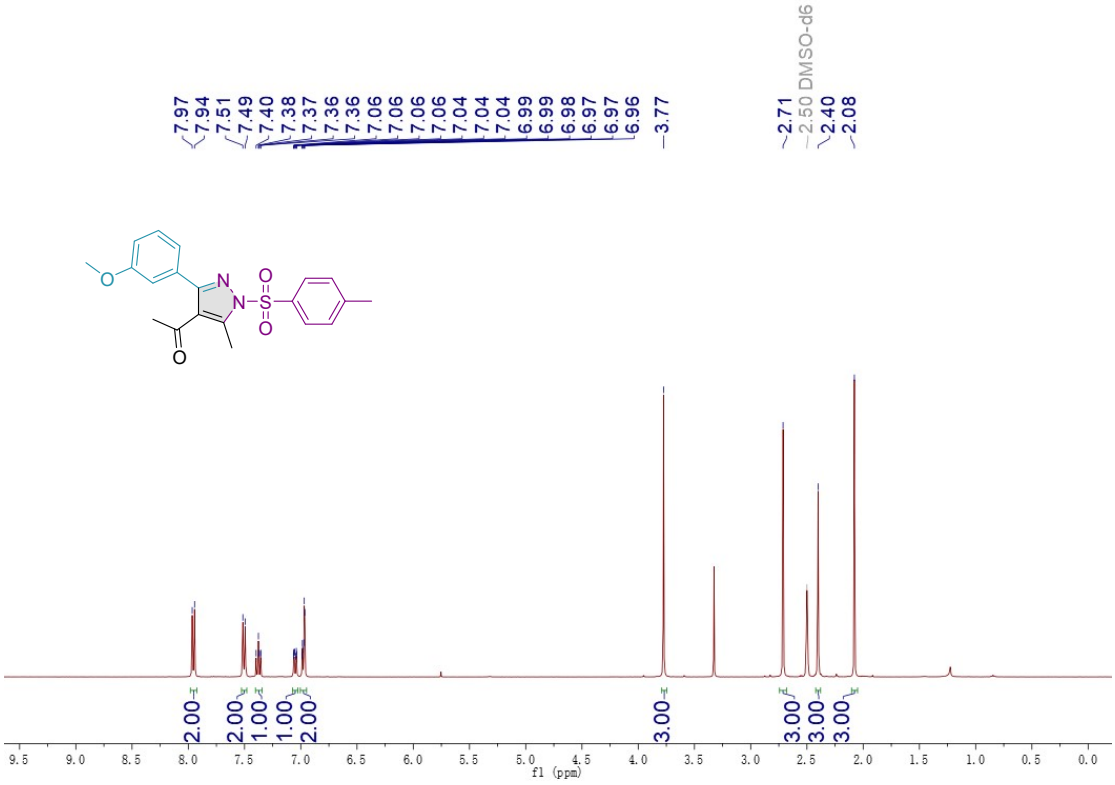


^{1}H NMR (400 MHz, $CDCl_3$)

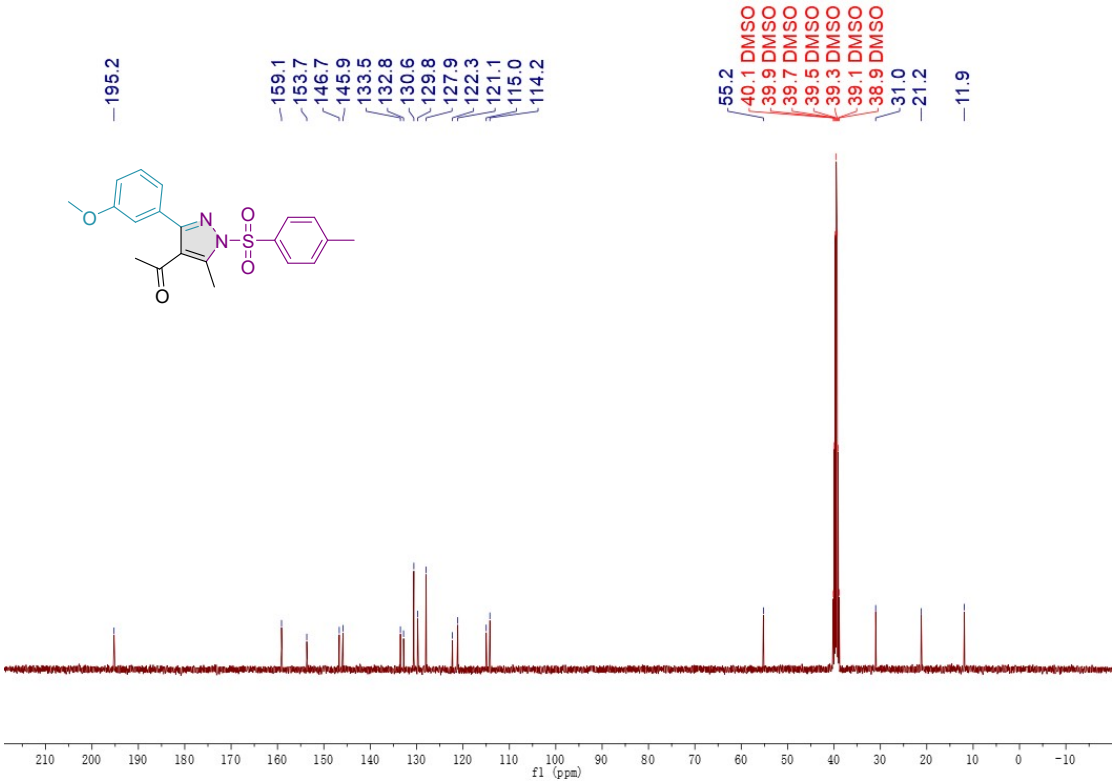


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(3-methoxyphenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4af)

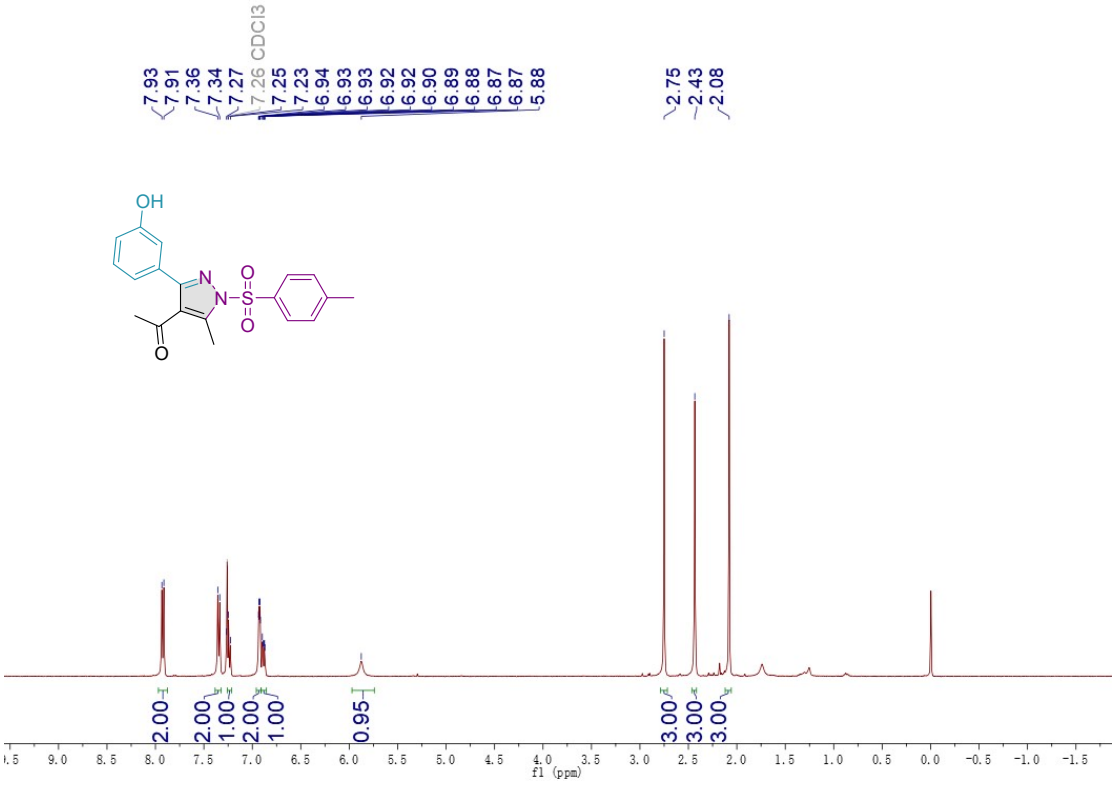


^{1}H NMR (400 MHz, DMSO-d_6)

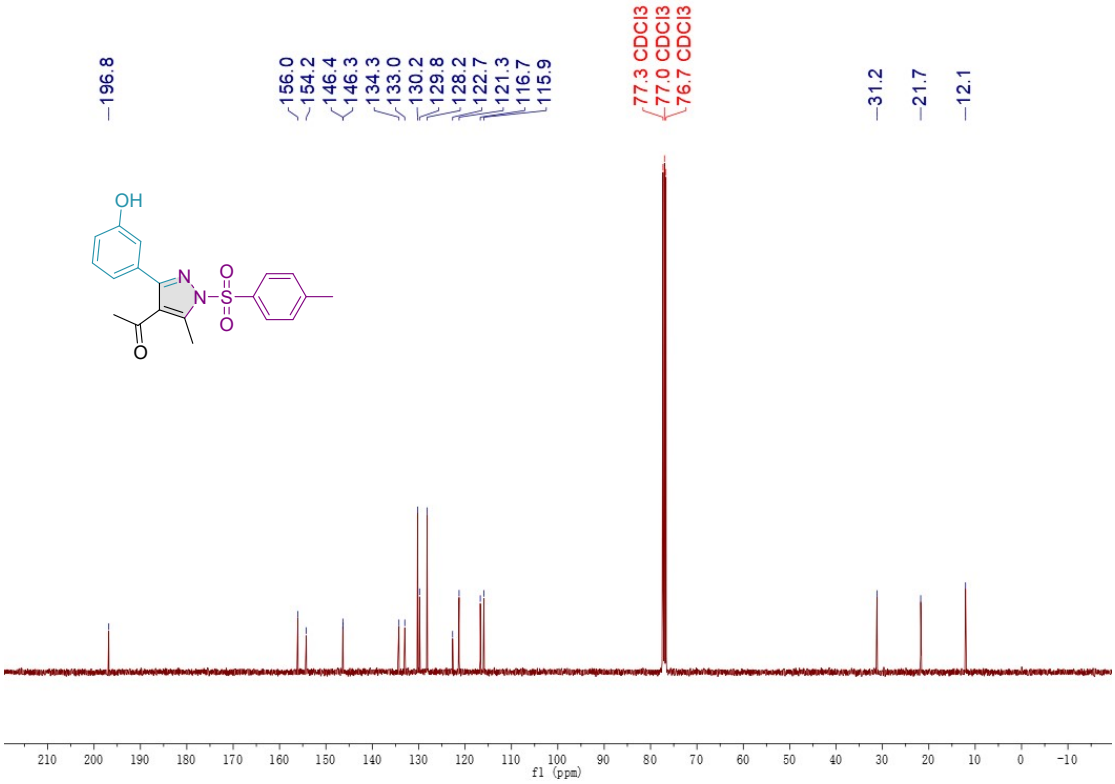


^{13}C NMR (100 MHz, DMSO-d_6)

1-(3-(3-hydroxyphenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ag)

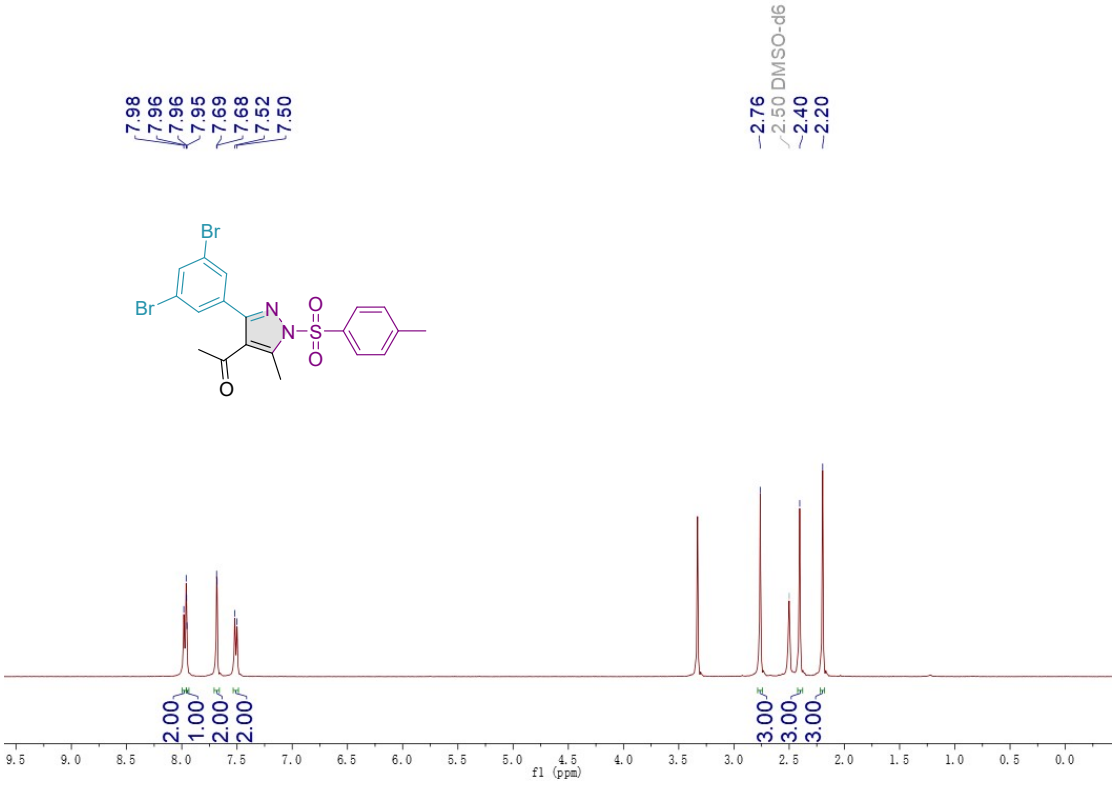


^{1}H NMR (400 MHz, $CDCl_3$)

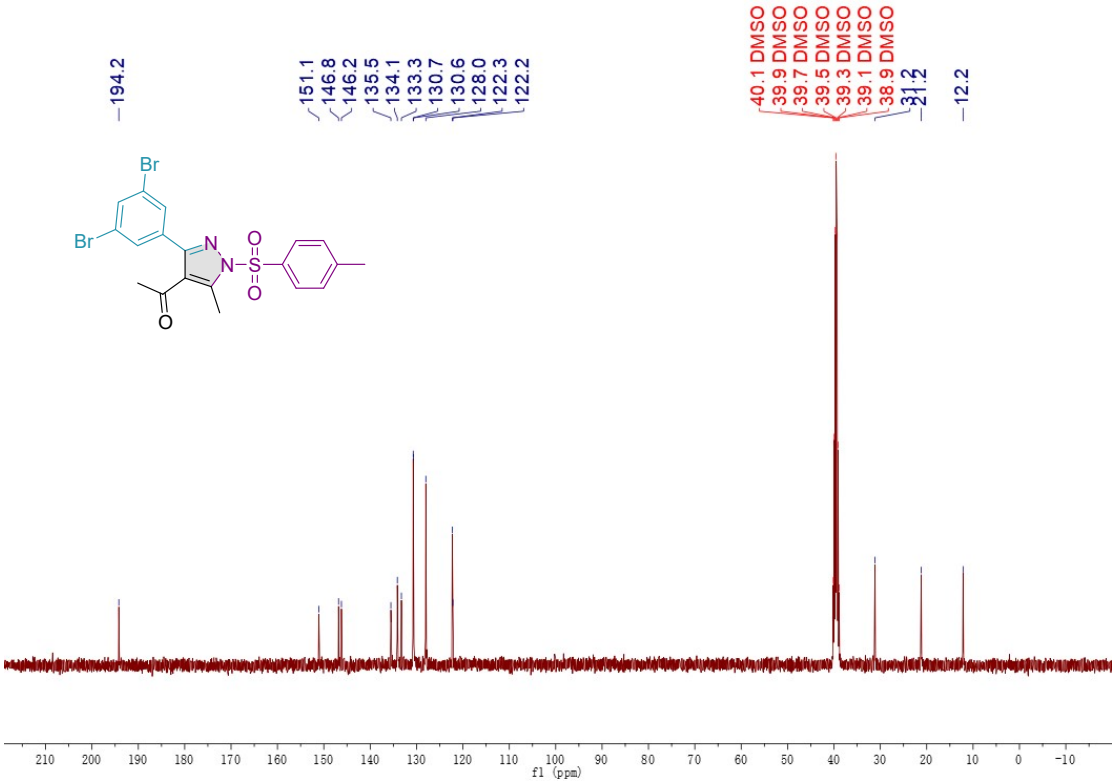


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(3,5-dibromophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ah)

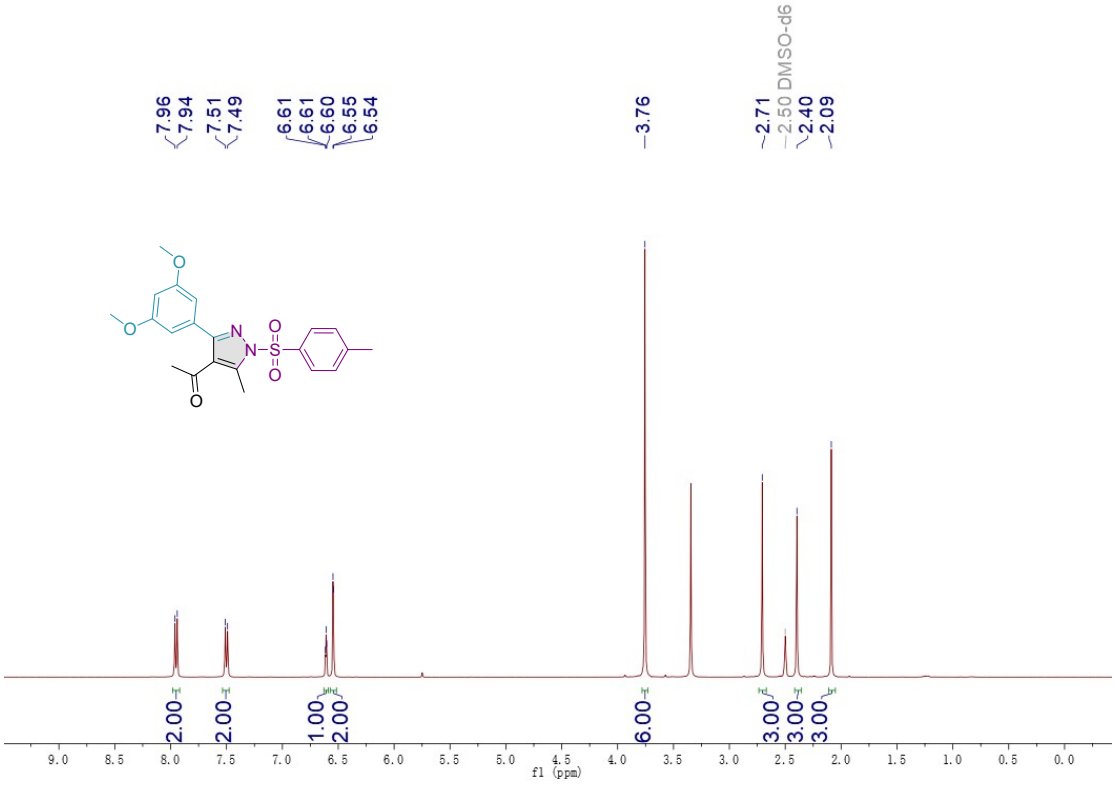


^{1}H NMR (400 MHz, DMSO-d_6)

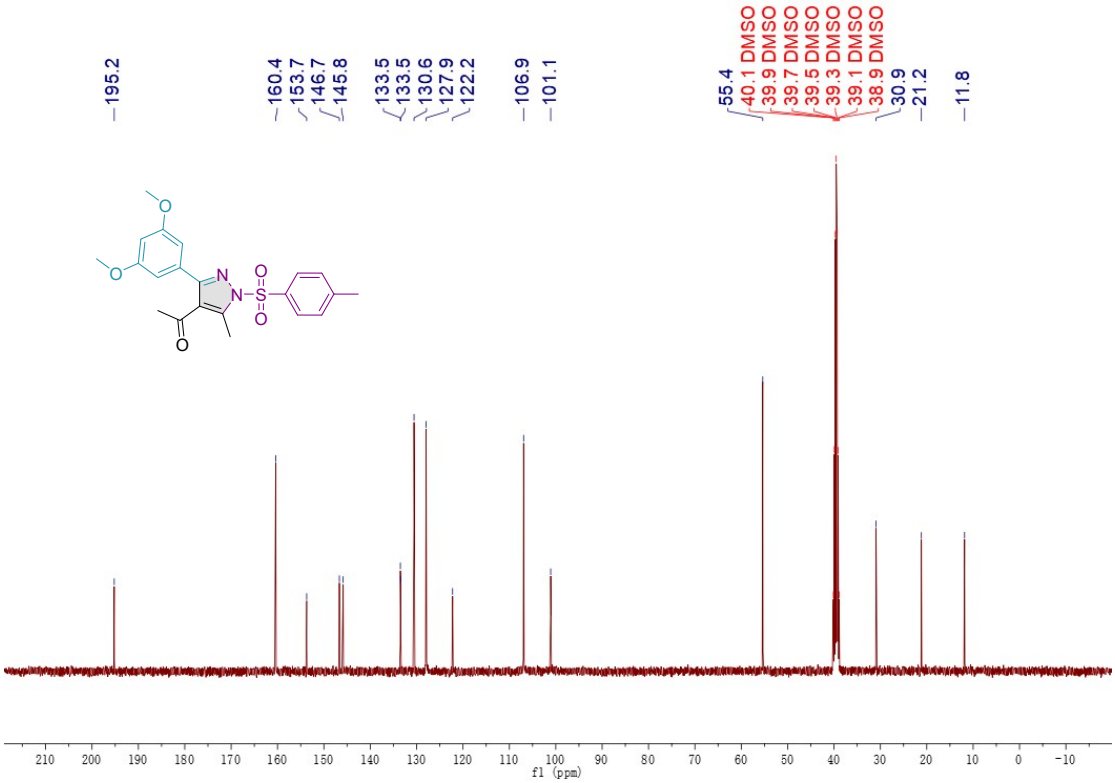


^{13}C NMR (100 MHz, DMSO-d_6)

1-(3-(3,5-dimethoxyphenyl)-5-methyl-1-tosyl-1H-pyrazol-4-yl)ethan-1-one (4ai)

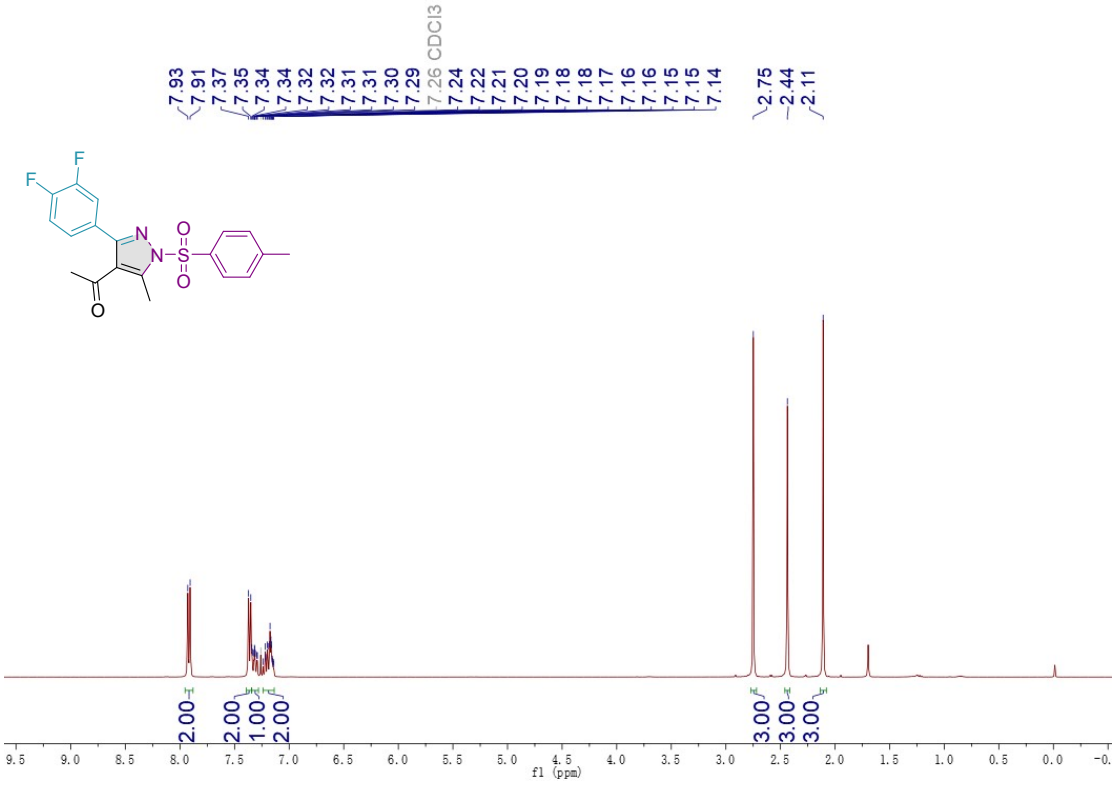


^{1}H NMR (400 MHz, DMSO-d_6)

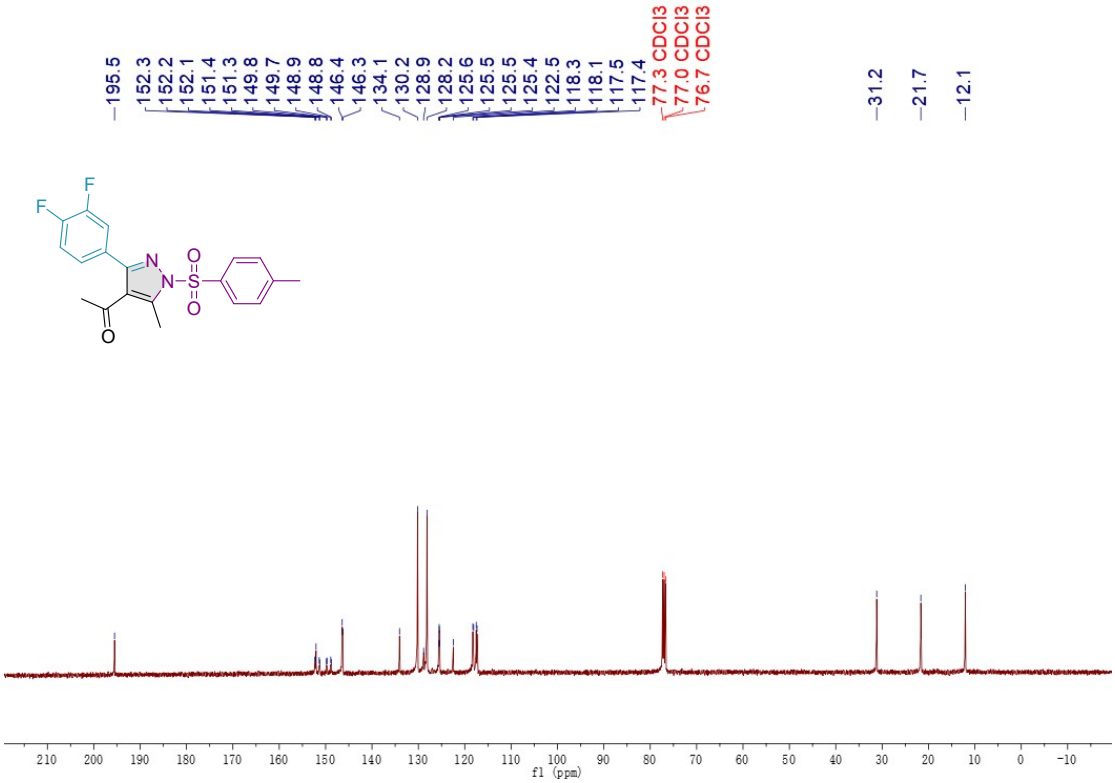


^{13}C NMR (100 MHz, DMSO-d_6)

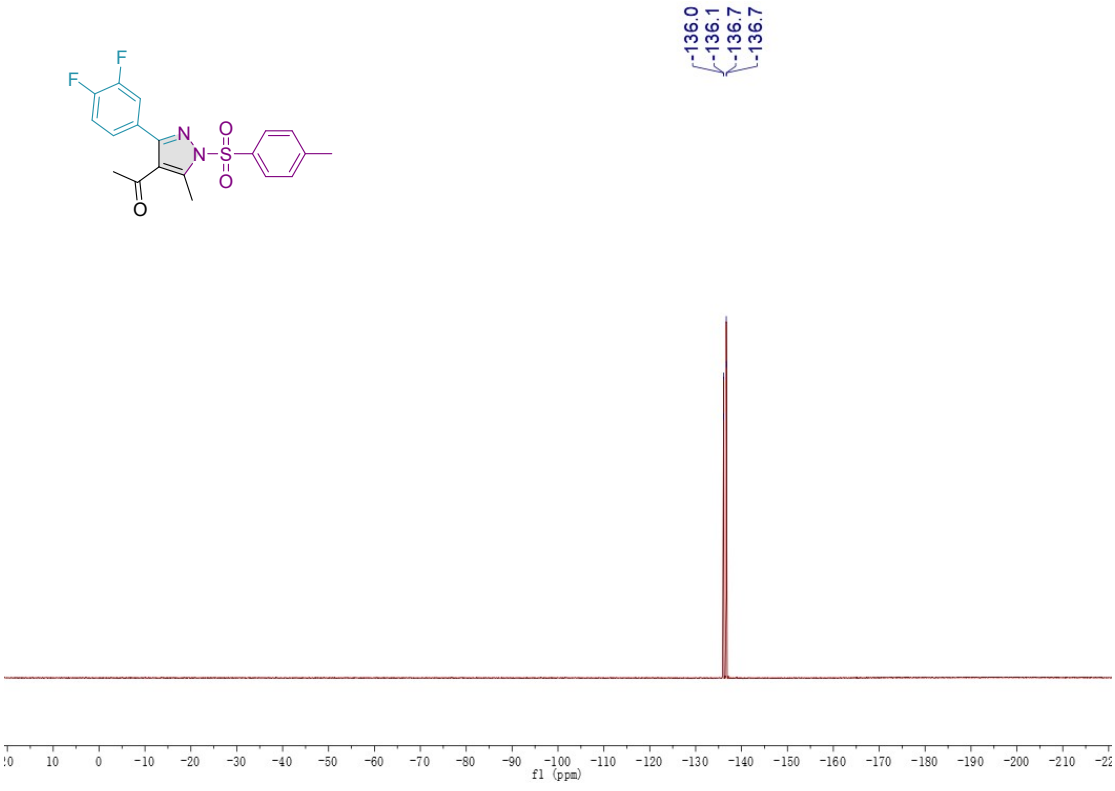
1-(3-(3,4-difluorophenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4aj)



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

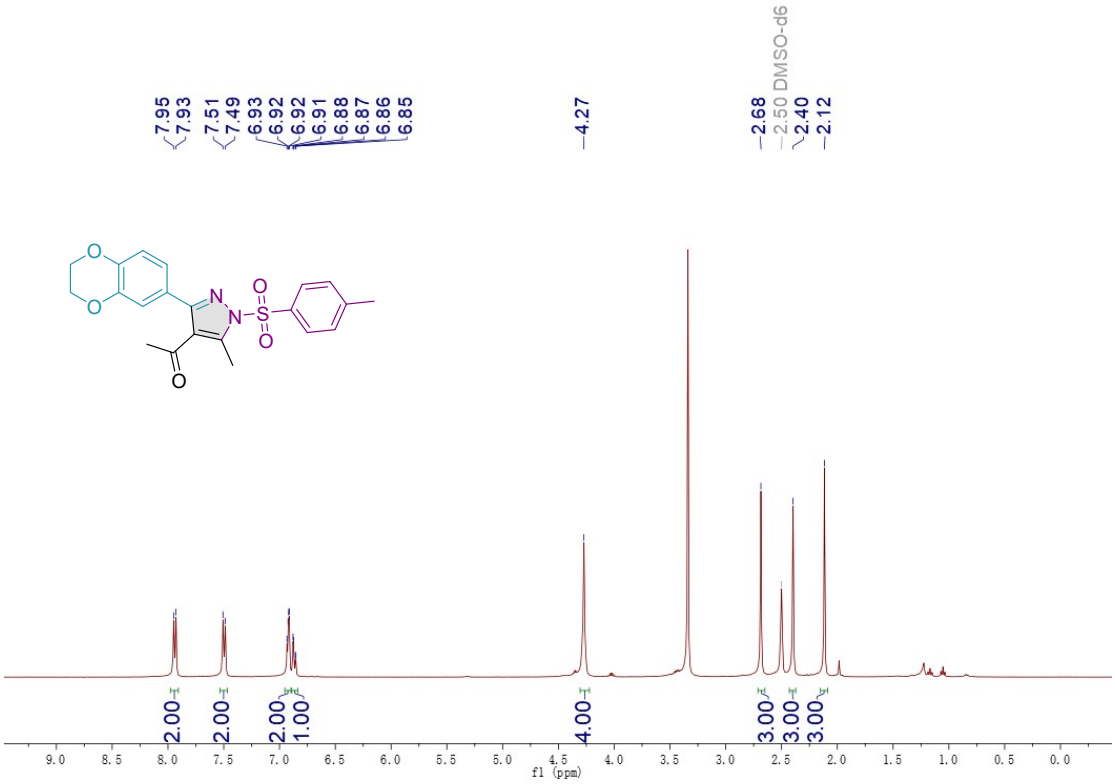


^{13}C NMR (100 MHz, $CDCl_3$)

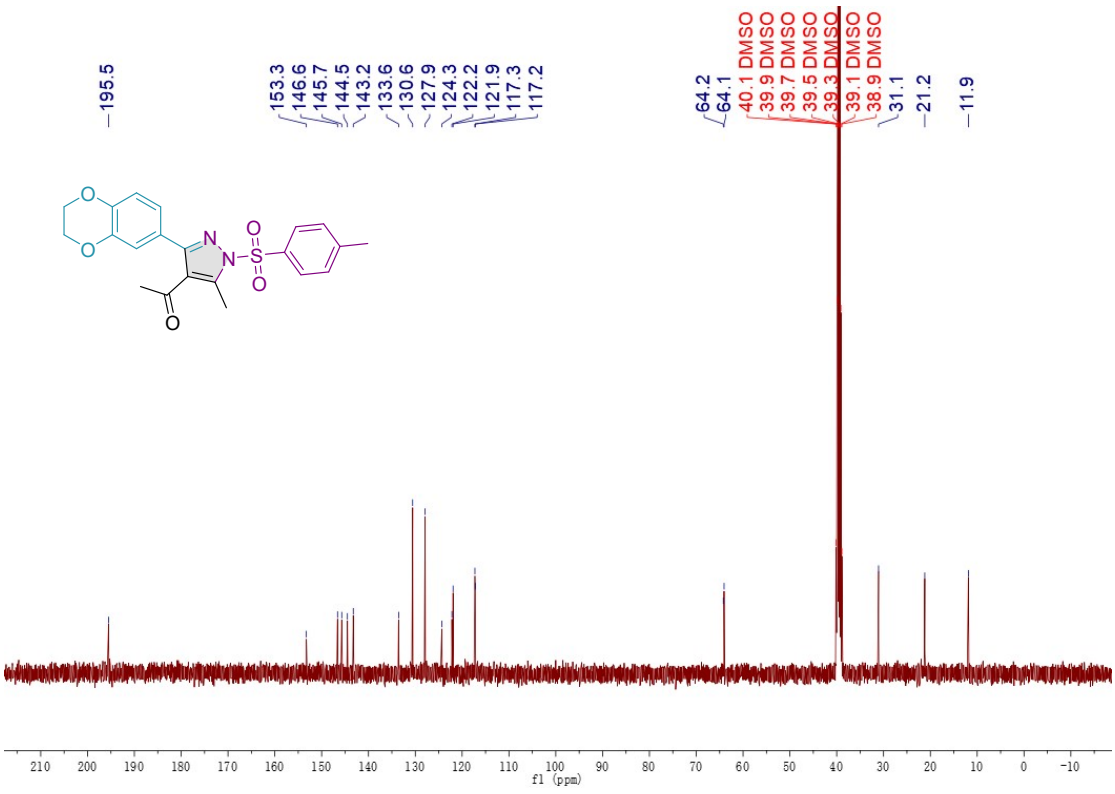


^{19}F NMR (376 MHz, $CDCl_3$)

1-(3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ak)

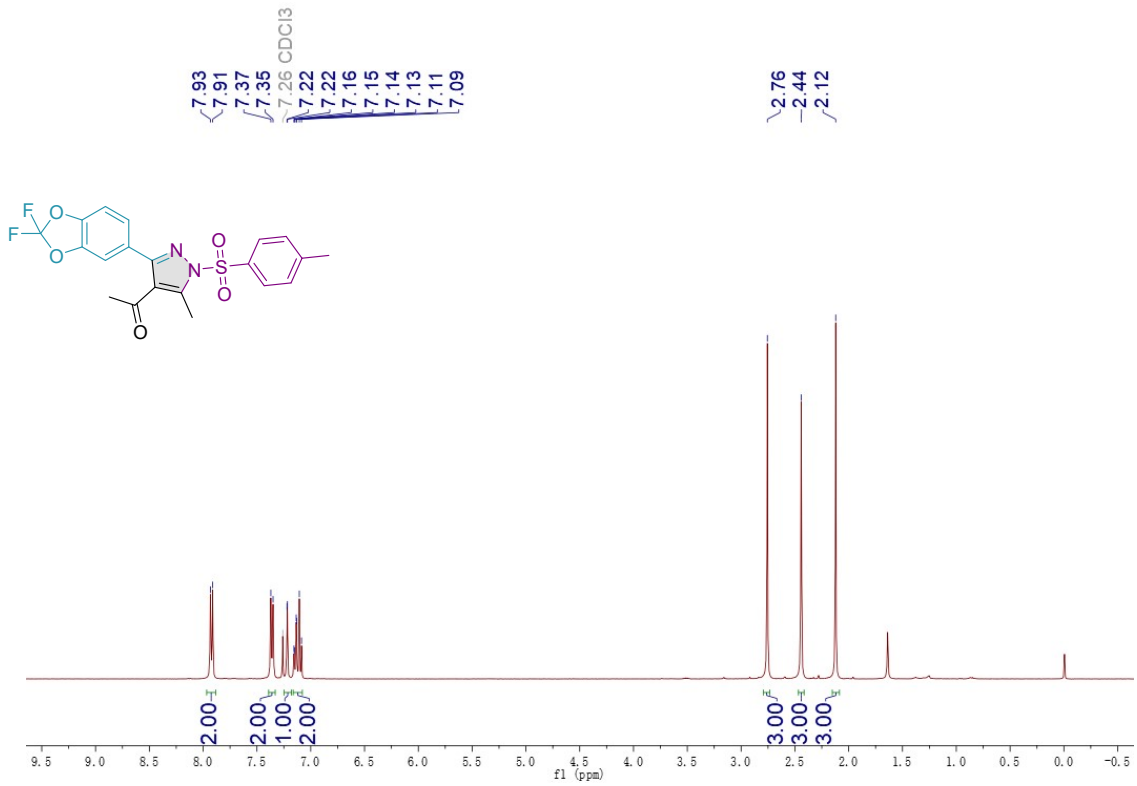


^{1}H NMR (400 MHz, DMSO-d_6)

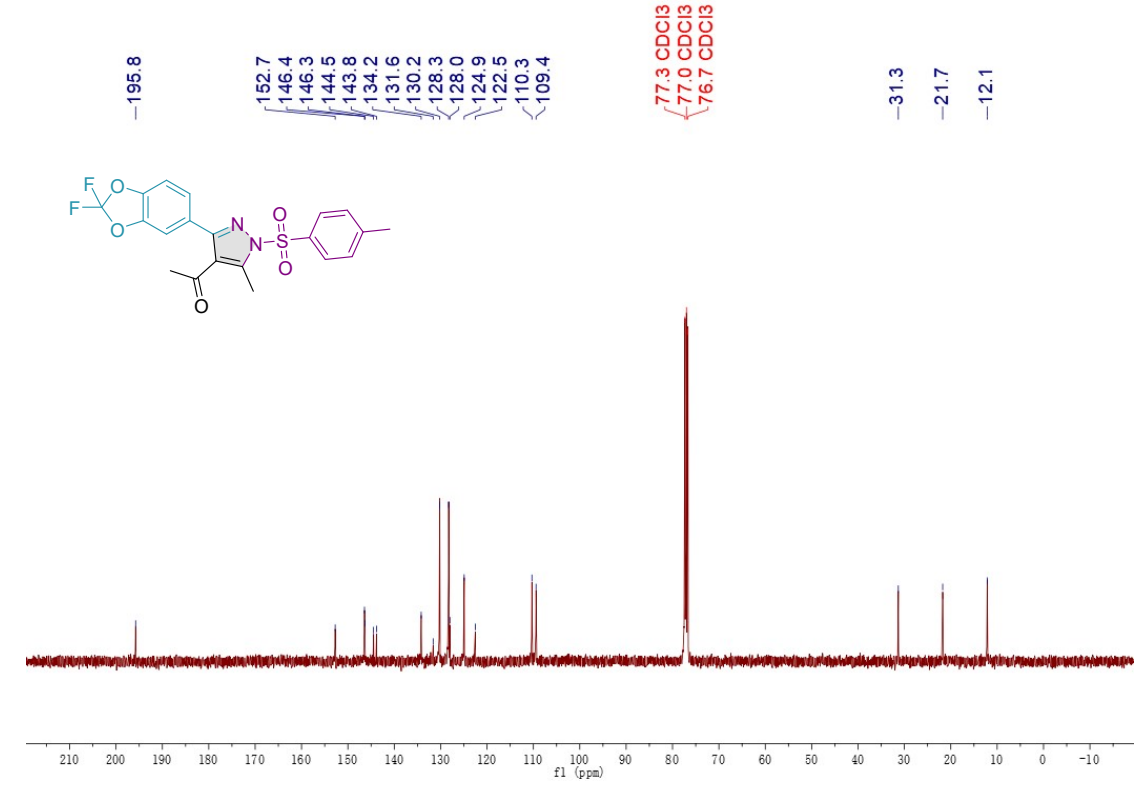


^{13}C NMR (100 MHz, DMSO-d_6)

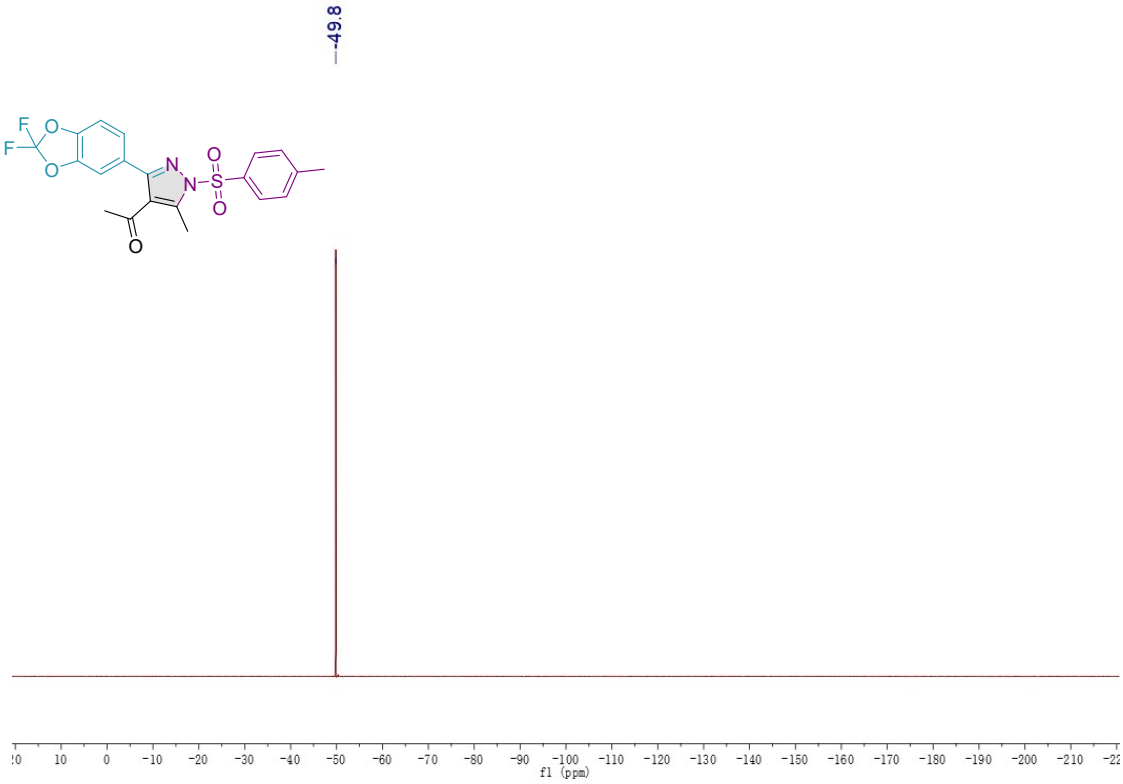
1-(3-(2,2-difluorobenzo[d][1,3]dioxol-5-yl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4al)



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

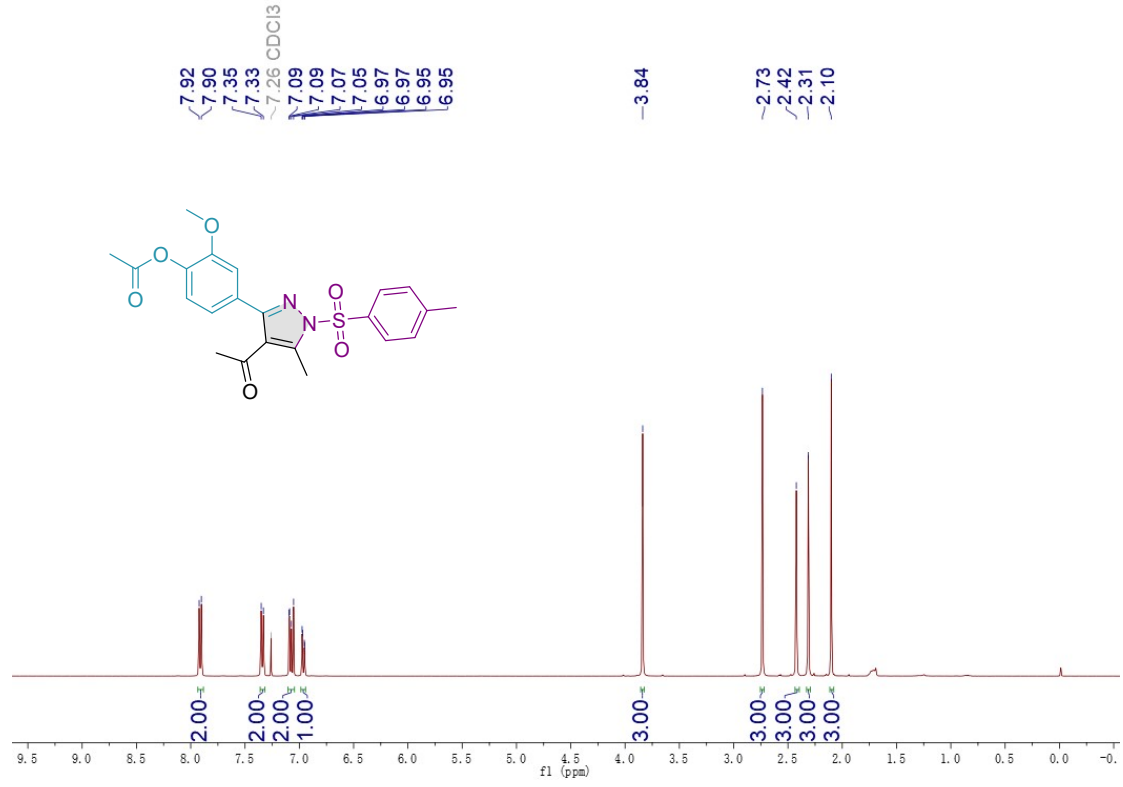


^{13}C NMR (100 MHz, $CDCl_3$)

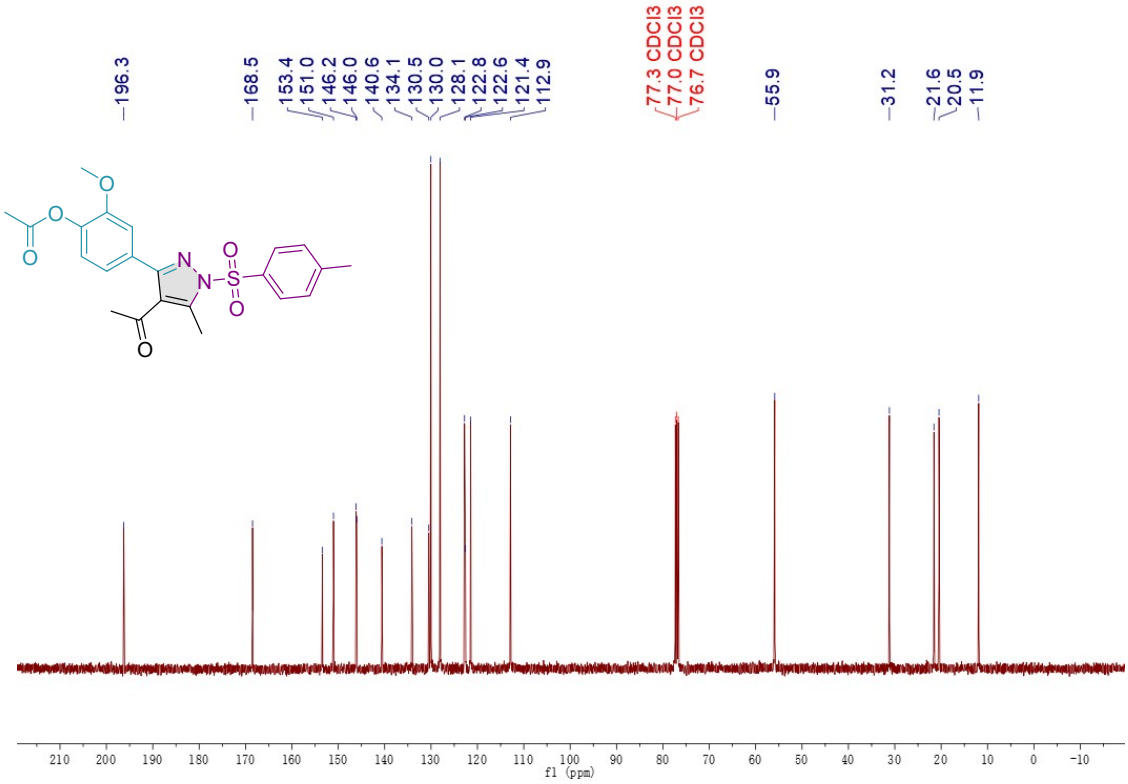


^{19}F NMR (376 MHz, $CDCl_3$)

4-(4-acetyl-5-methyl-1-tosyl-1*H*-pyrazol-3-yl)-2-methoxyphenyl acetate (4am)

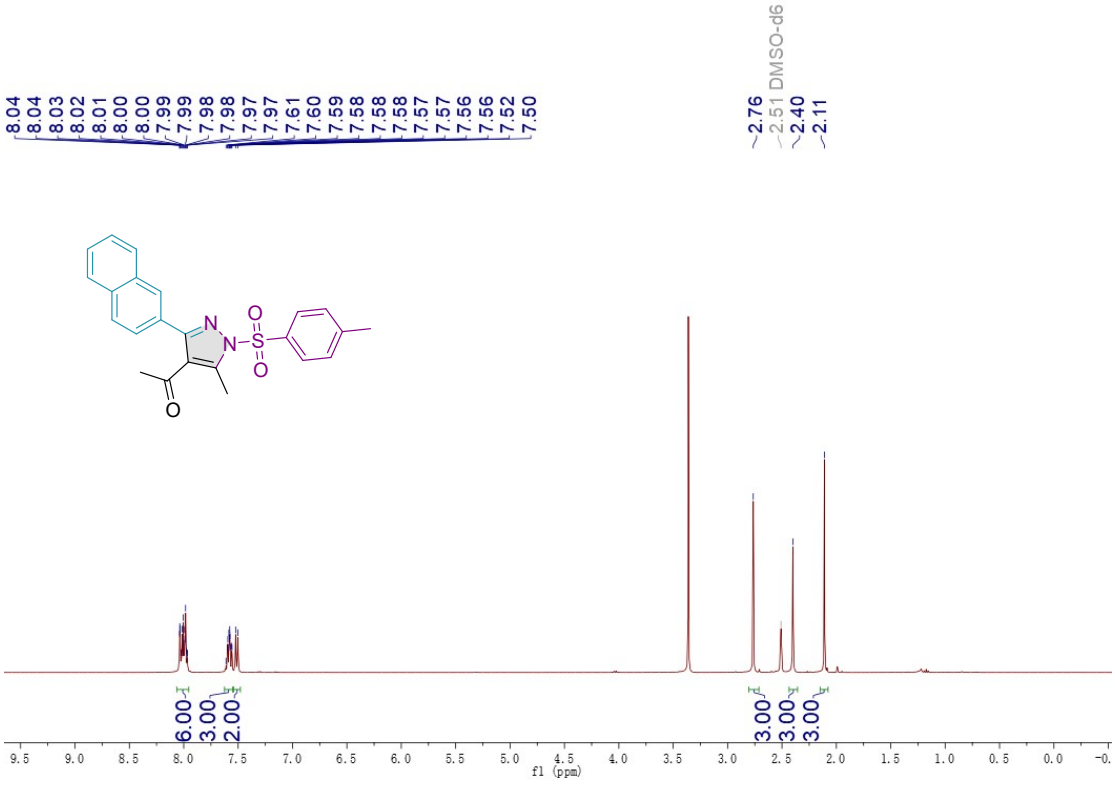


^{1}H NMR (400 MHz, $CDCl_3$)

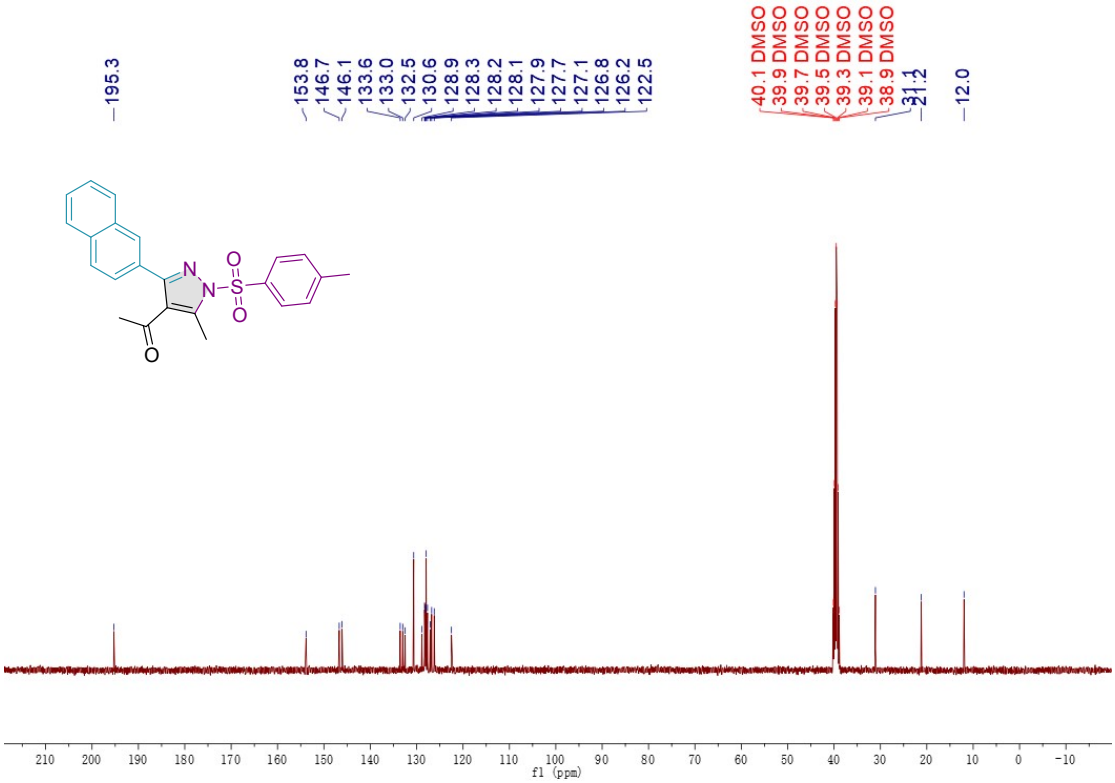


^{13}C NMR (100 MHz, $CDCl_3$)

1-(5-methyl-3-(naphthalen-2-yl)-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4an)

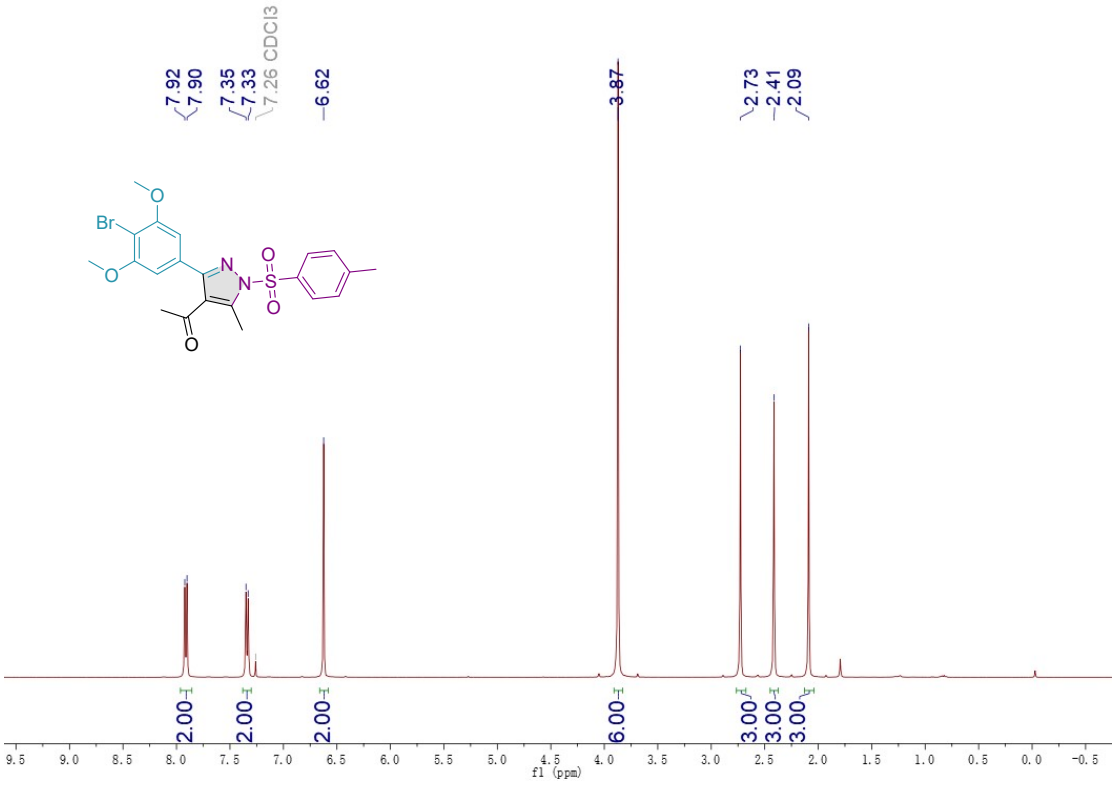


^{1}H NMR (400 MHz, DMSO-d_6)

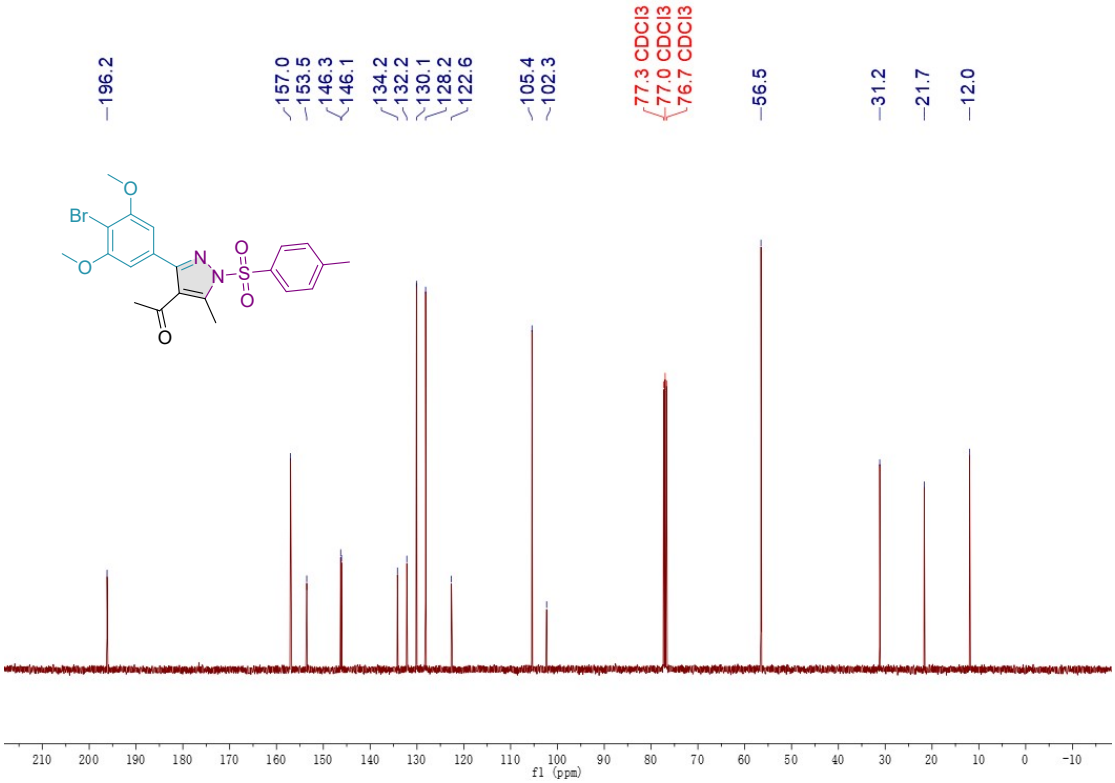


^{13}C NMR (100 MHz, DMSO-d_6)

1-(3-(4-bromo-3,5-dimethoxyphenyl)-5-methyl-1-tosyl-1*H*-pyrazol-4-yl)ethan-1-one (4ao)

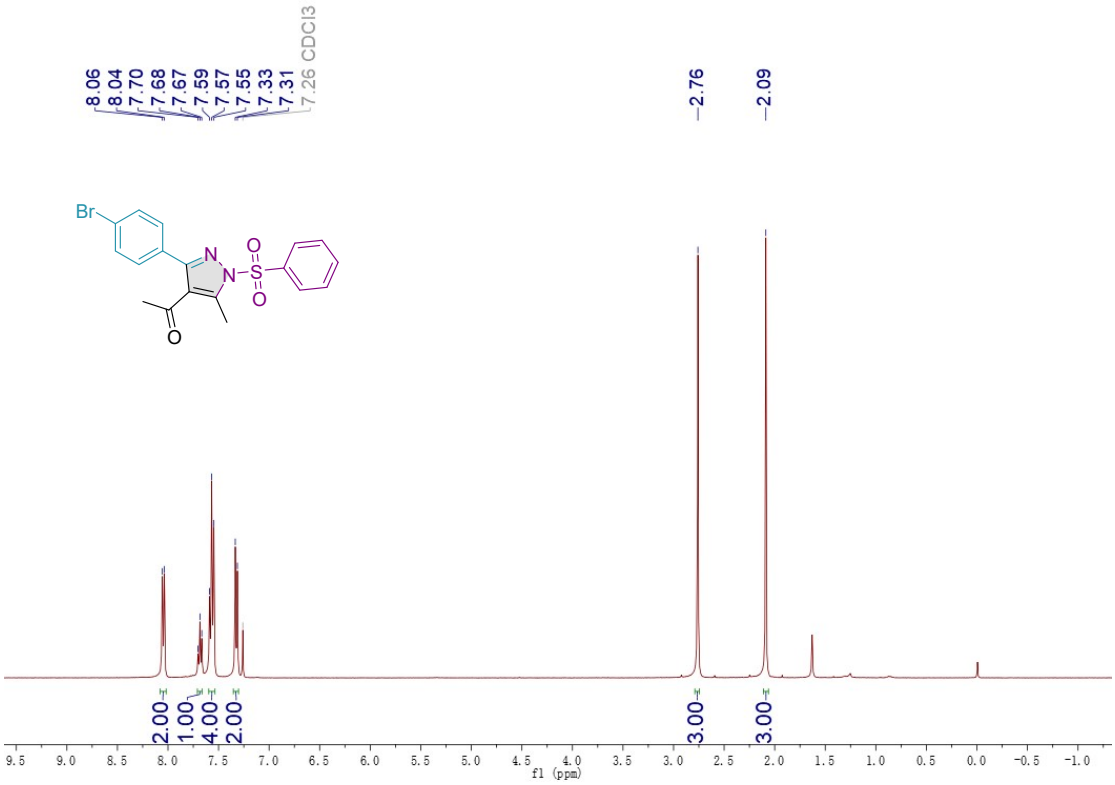


^{1}H NMR (400 MHz, $CDCl_3$)

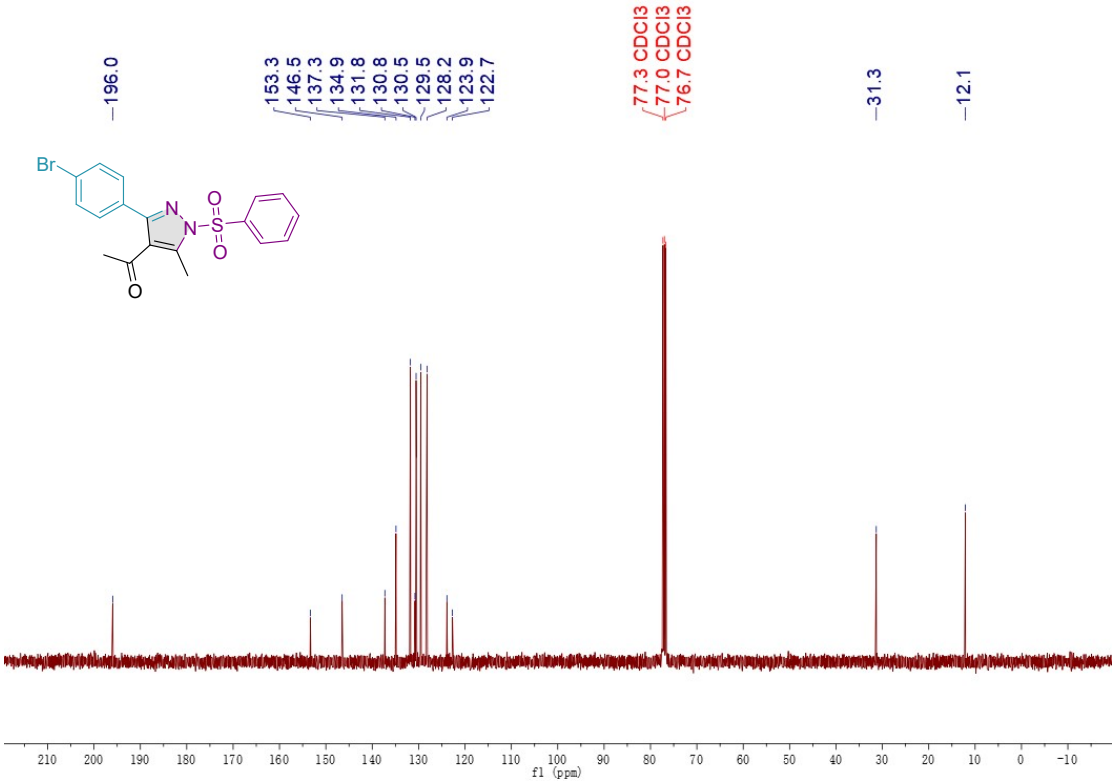


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-5-methyl-1-(phenylsulfonyl)-1*H*-pyrazol-4-yl)ethan-1-one (4ap)

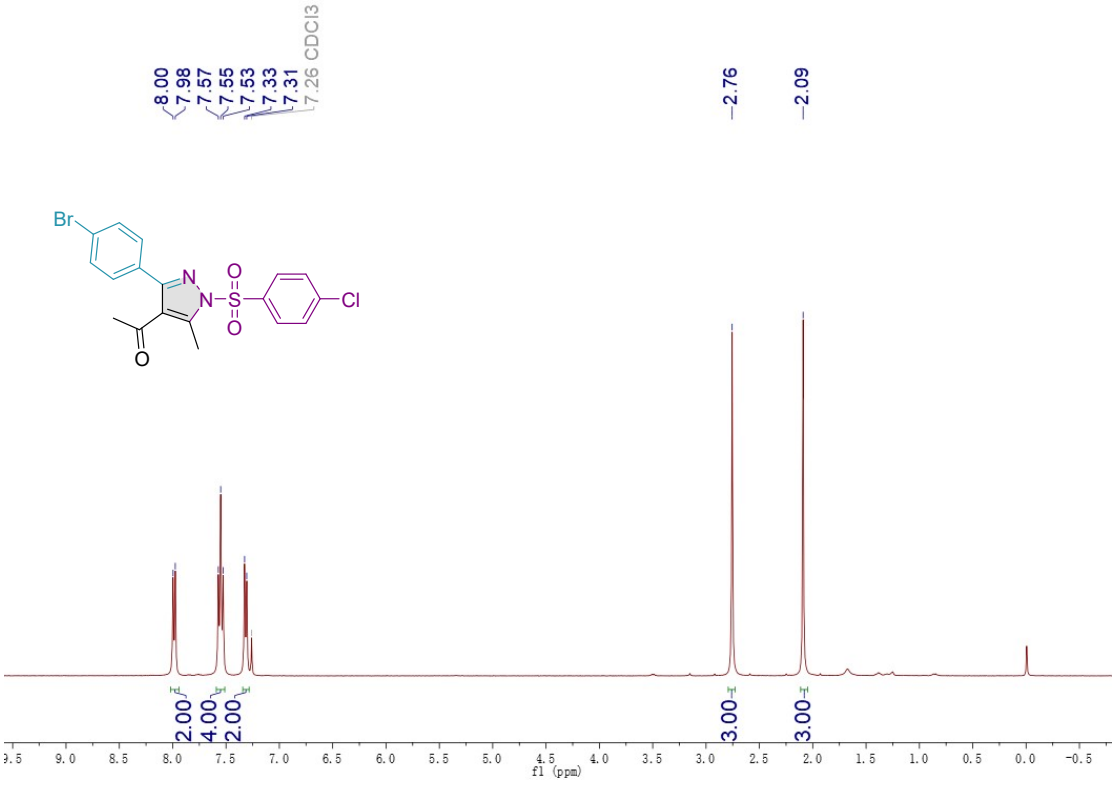


^{1}H NMR (400 MHz, $CDCl_3$)

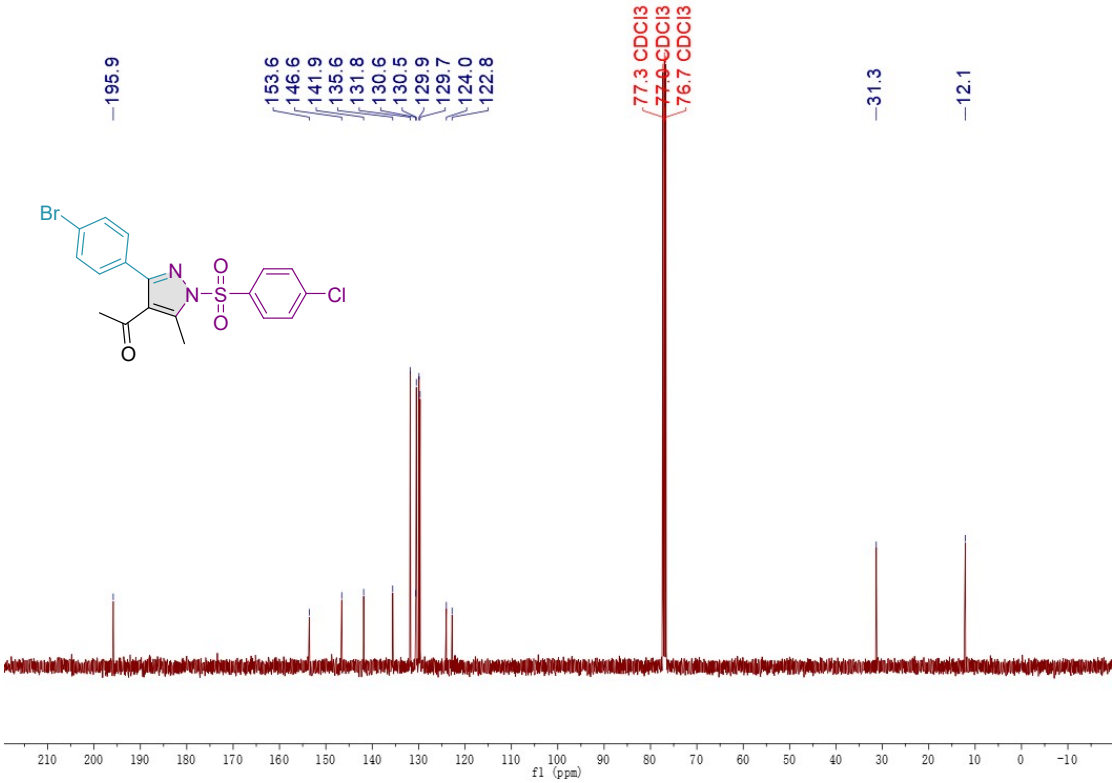


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-((4-chlorophenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4aq)

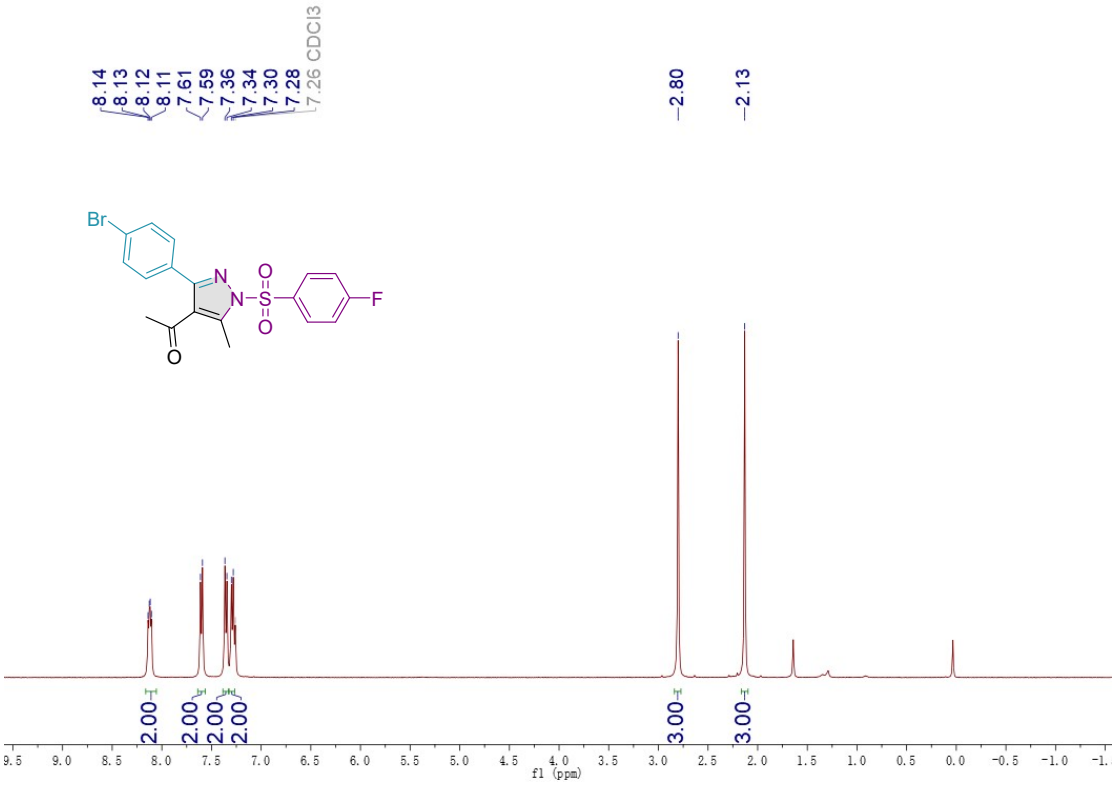


^{1}H NMR (400 MHz, $CDCl_3$)

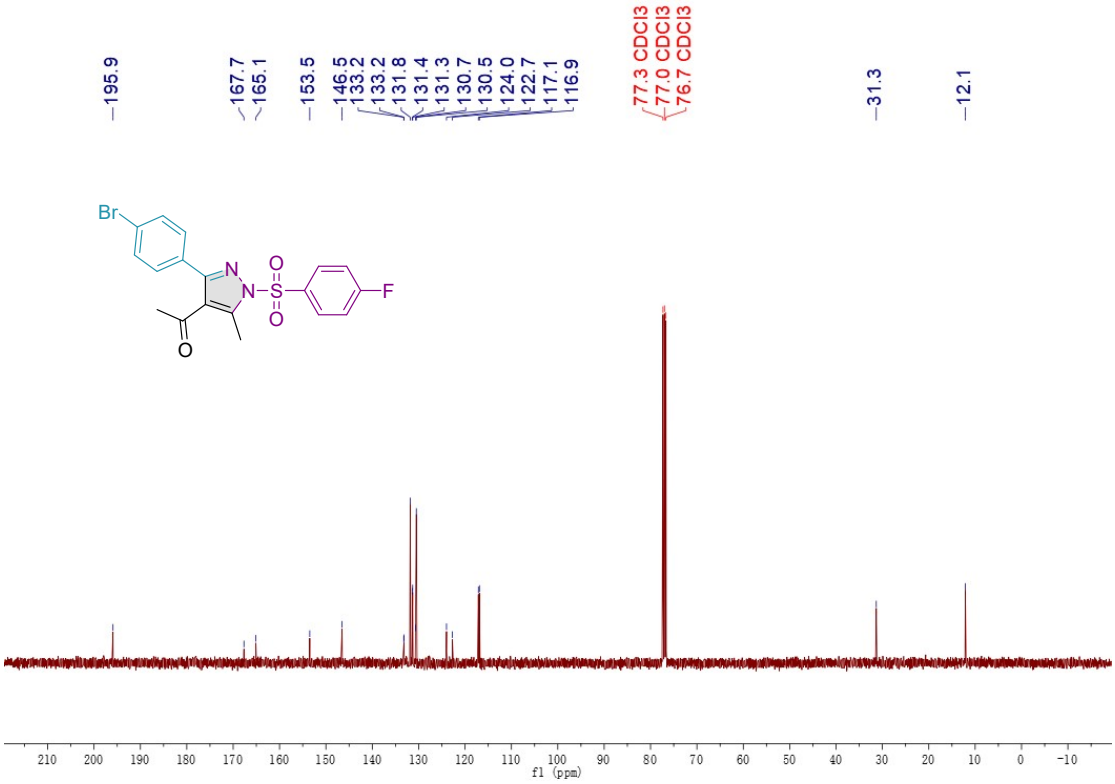


^{13}C NMR (100 MHz, $CDCl_3$)

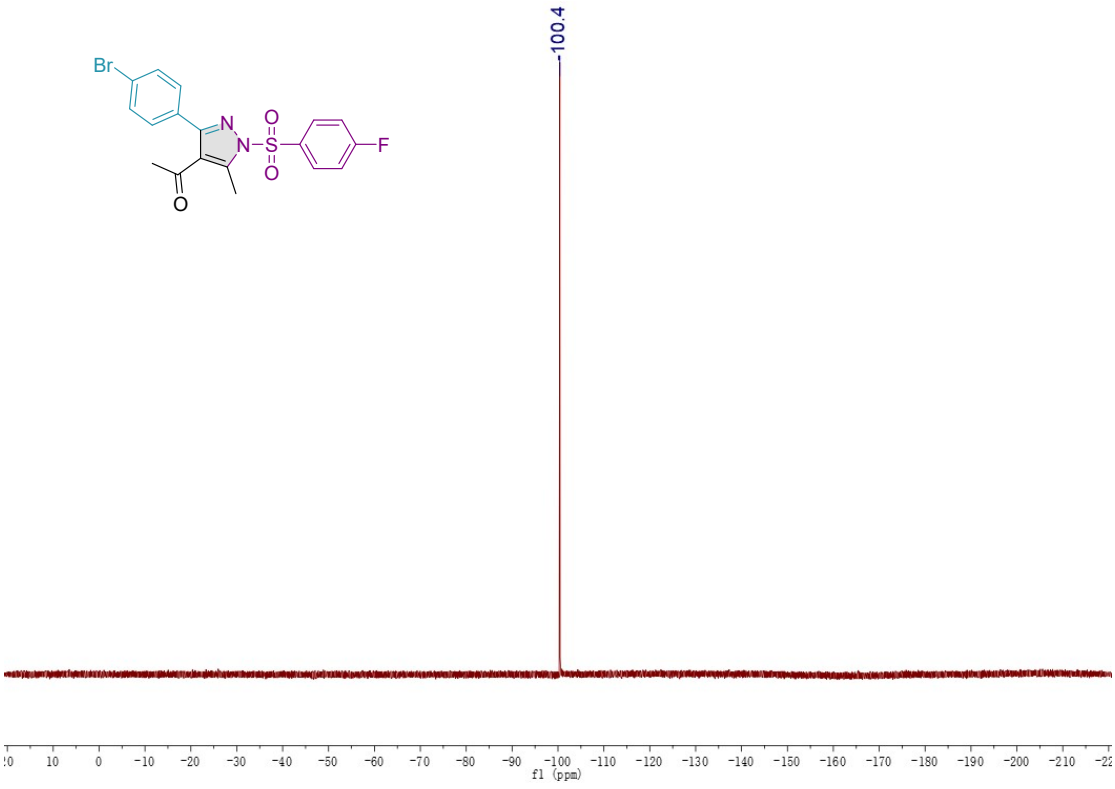
1-(3-(4-bromophenyl)-1-((4-fluorophenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4ar)



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

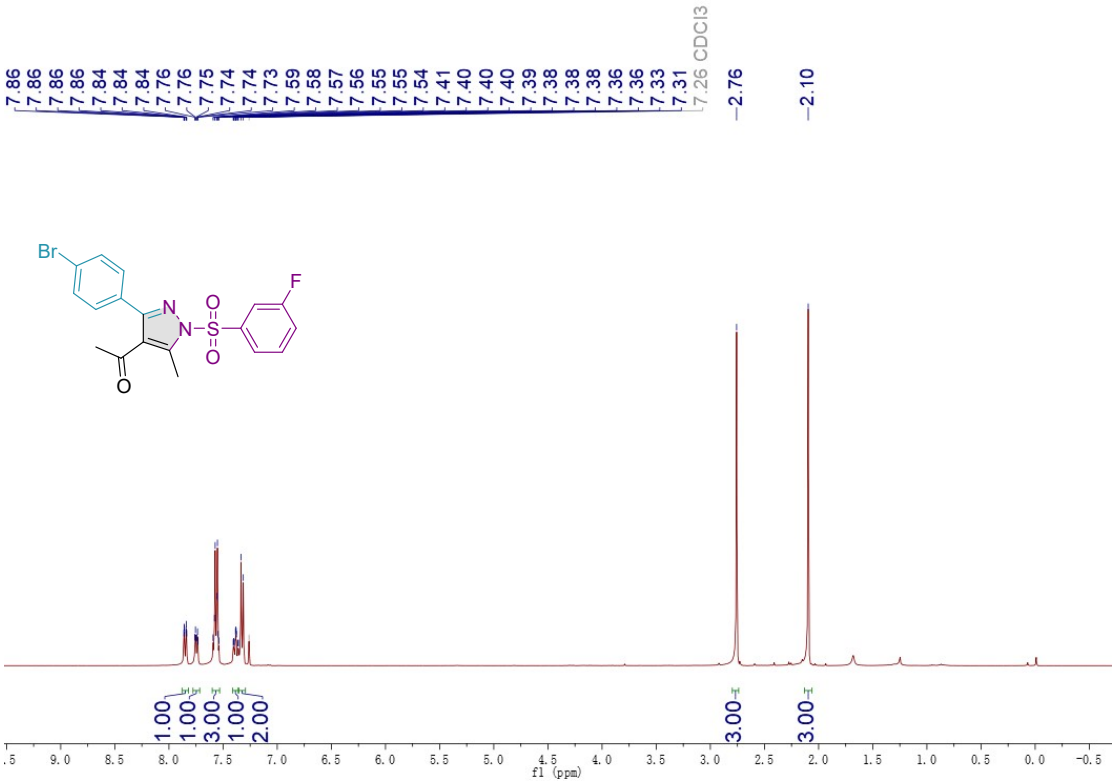


^{13}C NMR (100 MHz, $CDCl_3$)

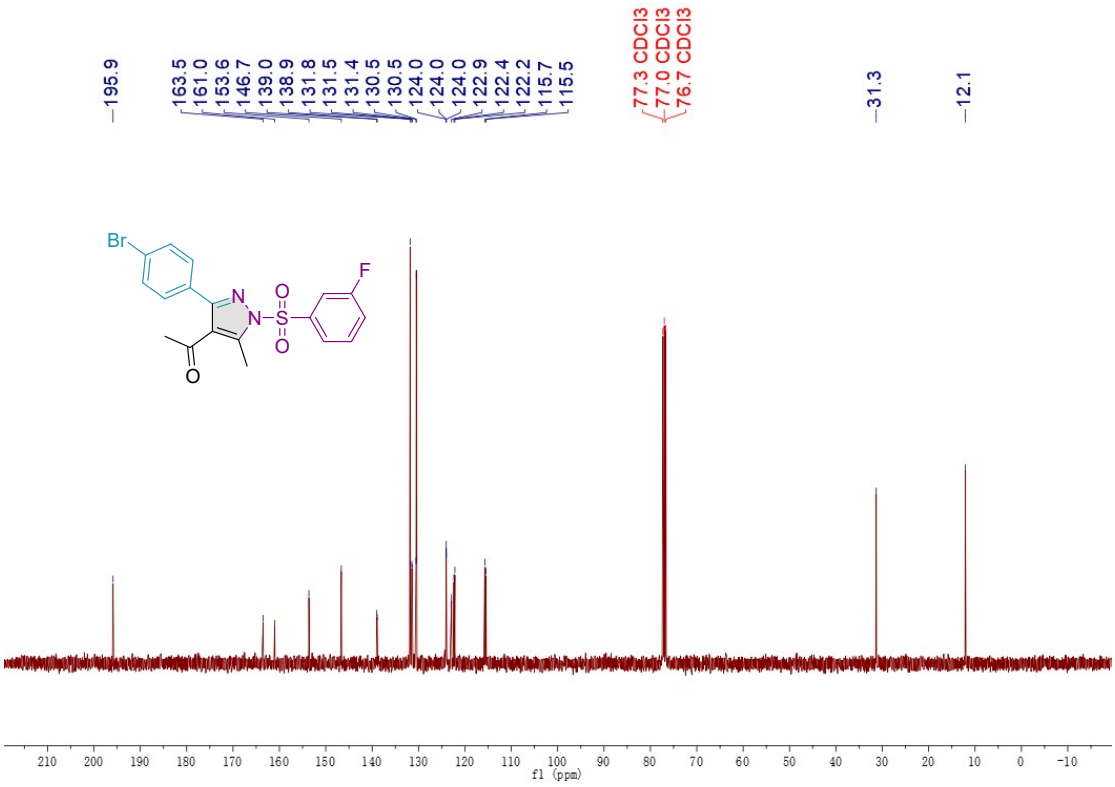


^{19}F NMR (376 MHz, $CDCl_3$)

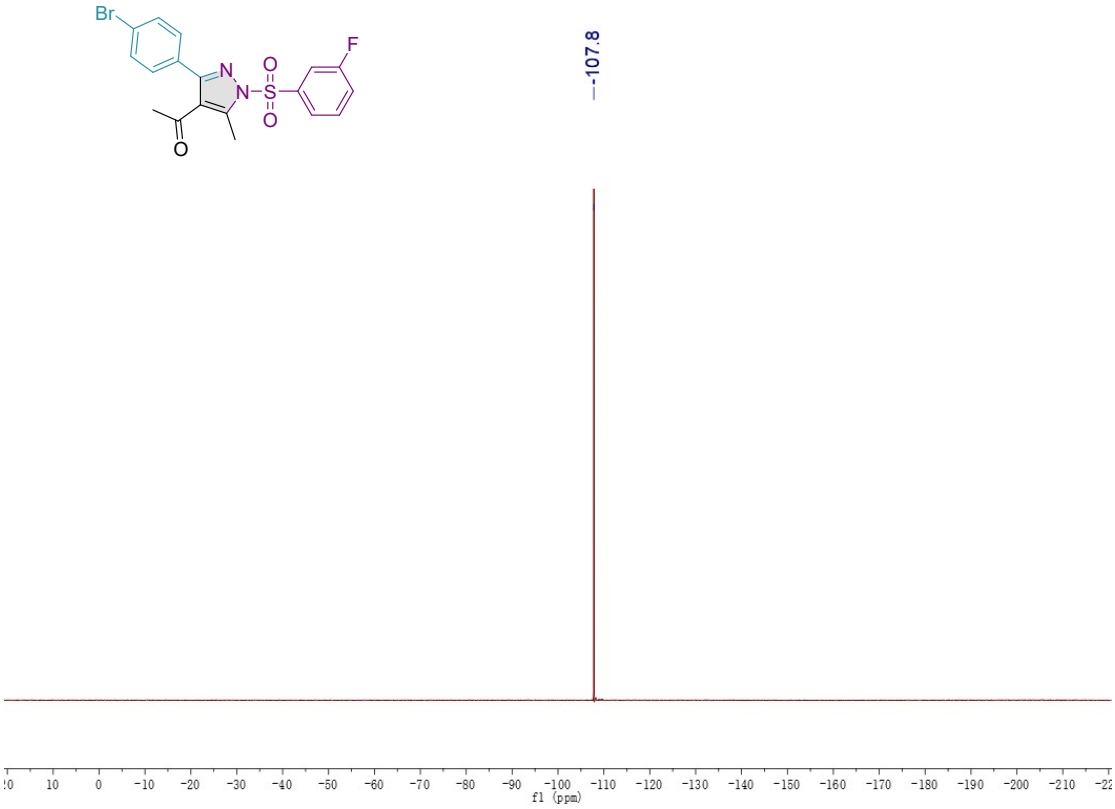
1-(3-(4-bromophenyl)-1-((3-fluorophenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4as)



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

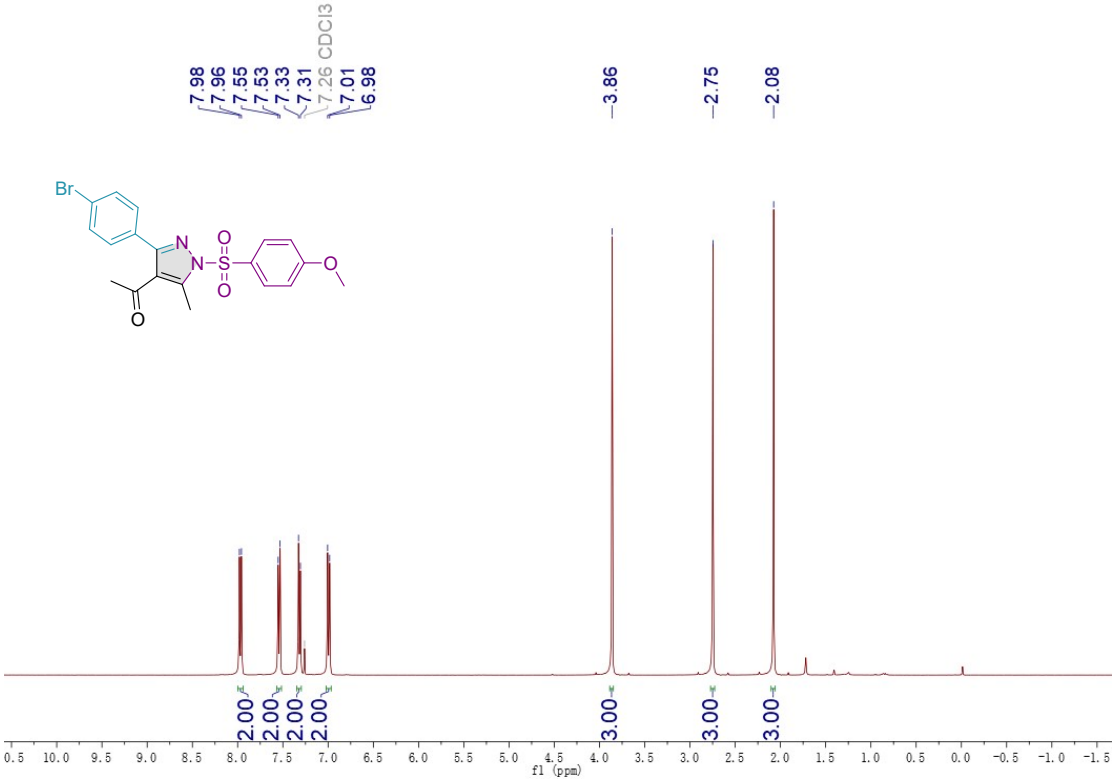


^{13}C NMR (100 MHz, $CDCl_3$)

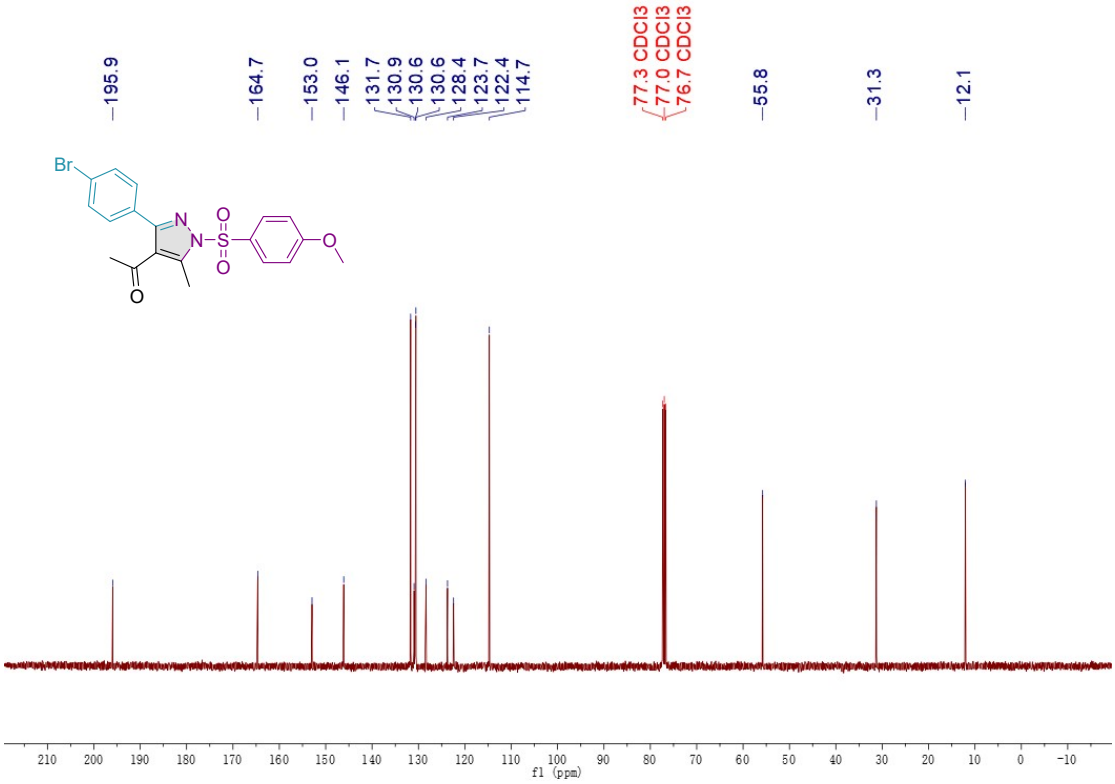


^{19}F NMR (376 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-((4-methoxyphenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4at)

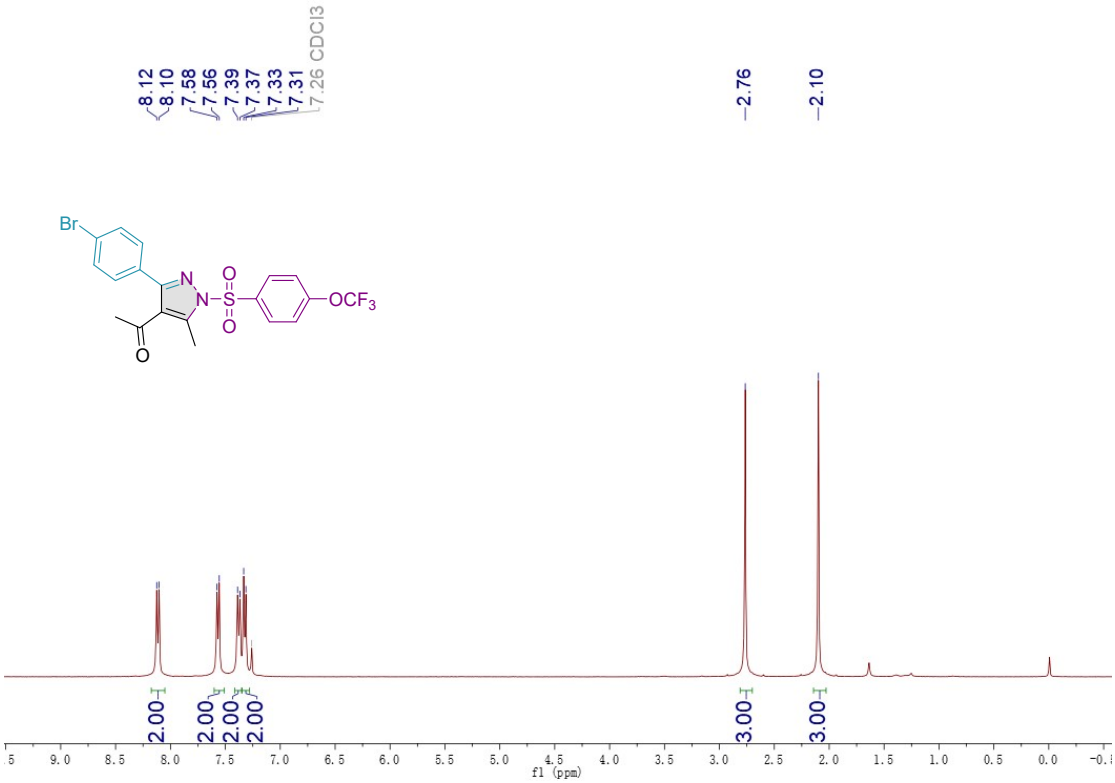


^{1}H NMR (400 MHz, $CDCl_3$)

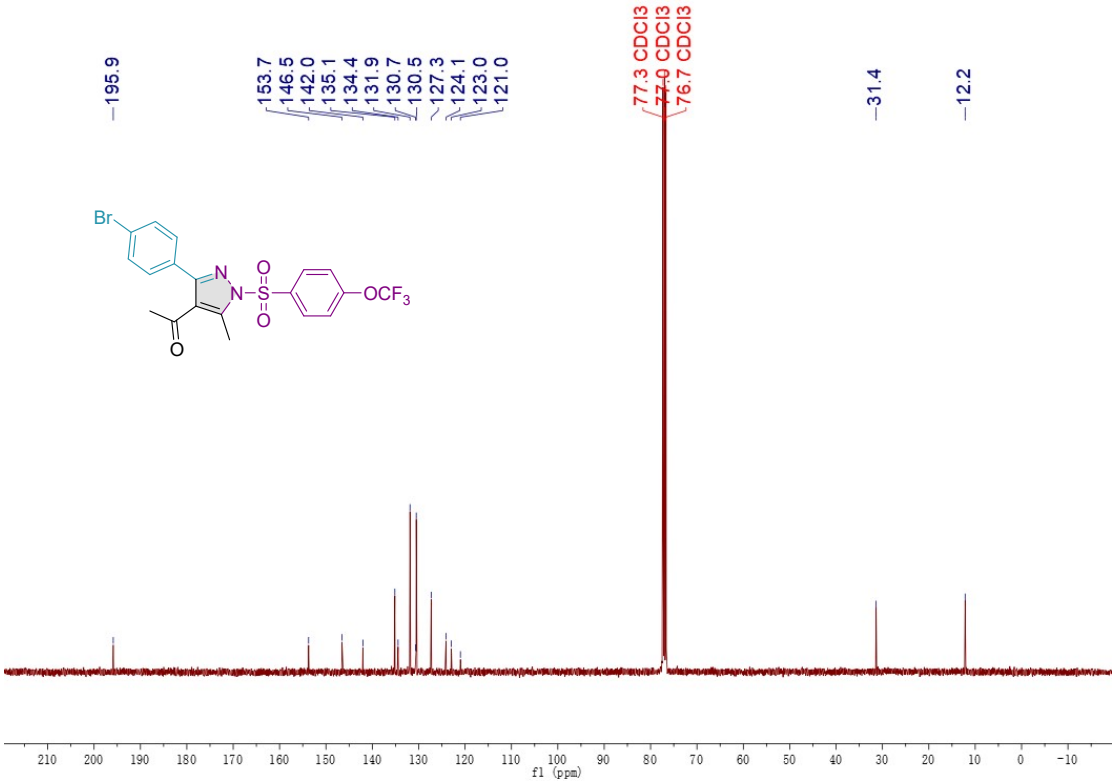


^{13}C NMR (100 MHz, $CDCl_3$)

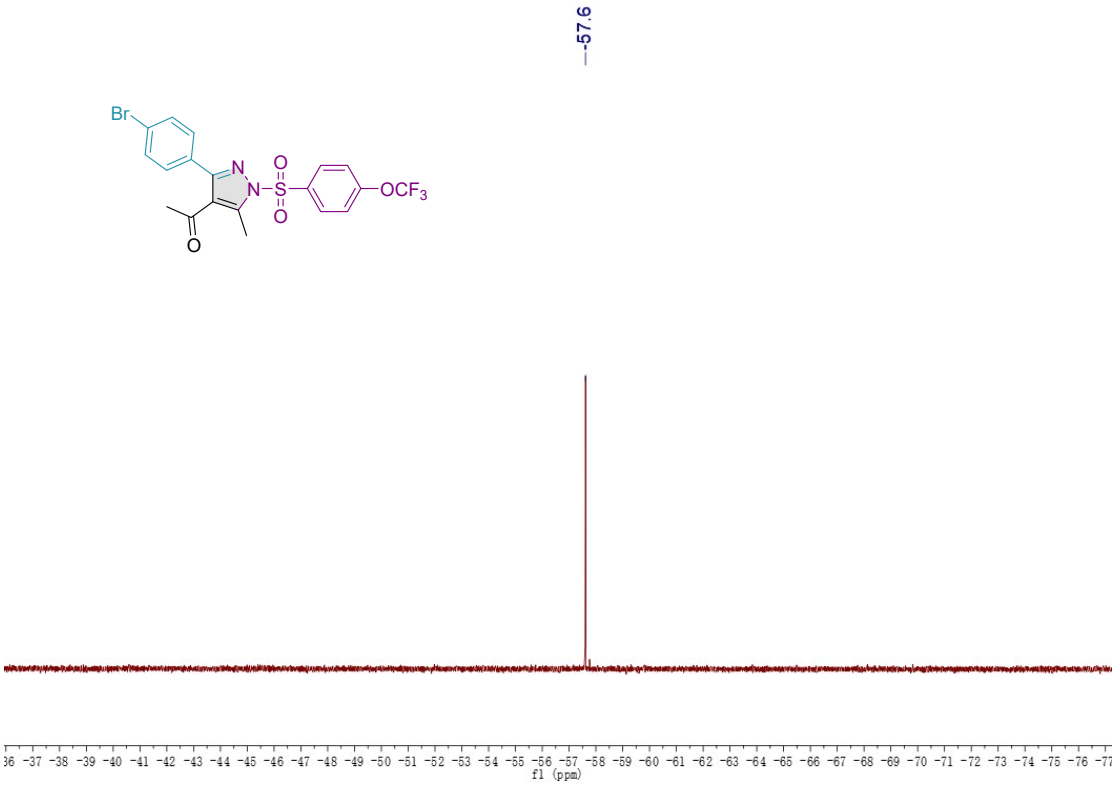
1-(3-(4-bromophenyl)-5-methyl-1-((4-(trifluoromethoxy)phenyl)sulfonyl)-1H-pyrazol-4-yl)ethan-1-one (4au)



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

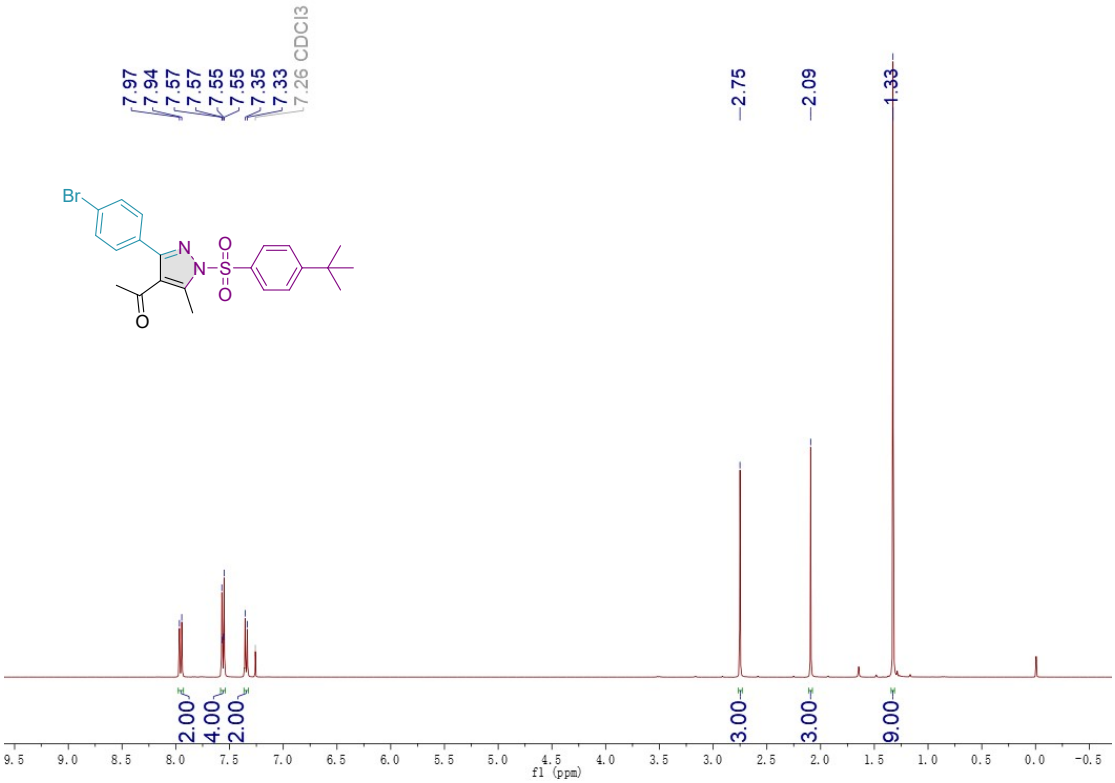


^{13}C NMR (100 MHz, $CDCl_3$)

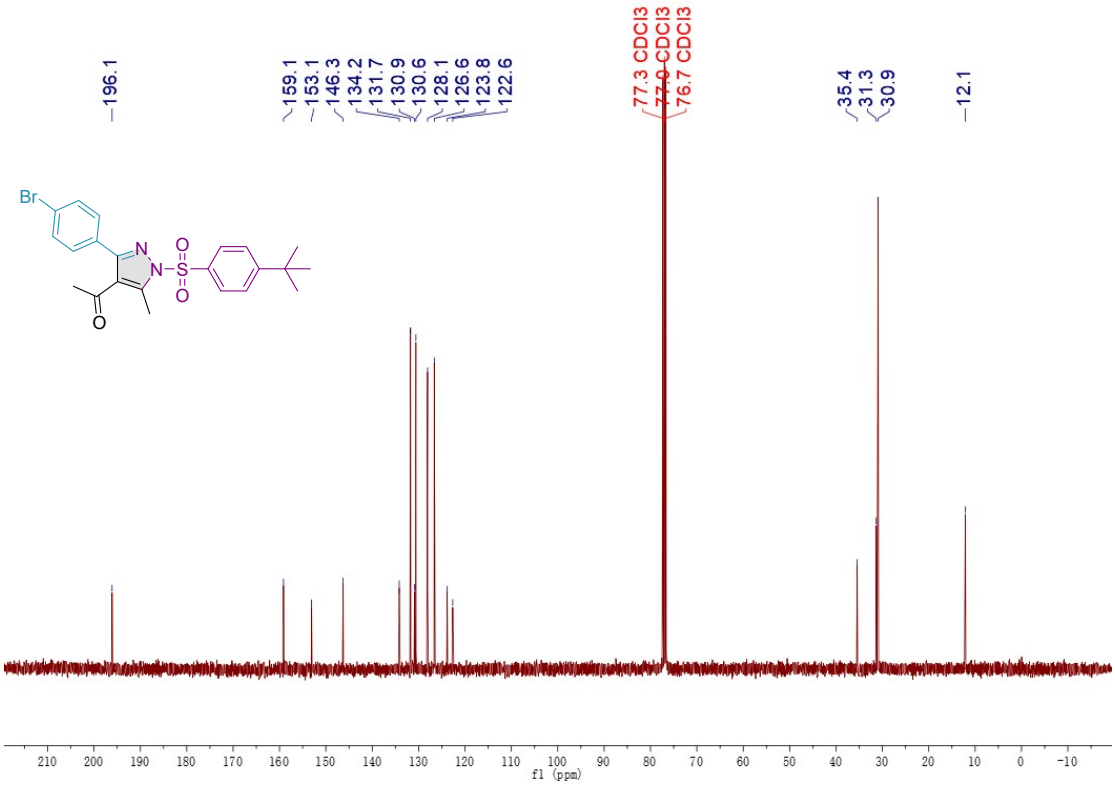


^{19}F NMR (376 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-((4-(tert-butyl)phenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4av)

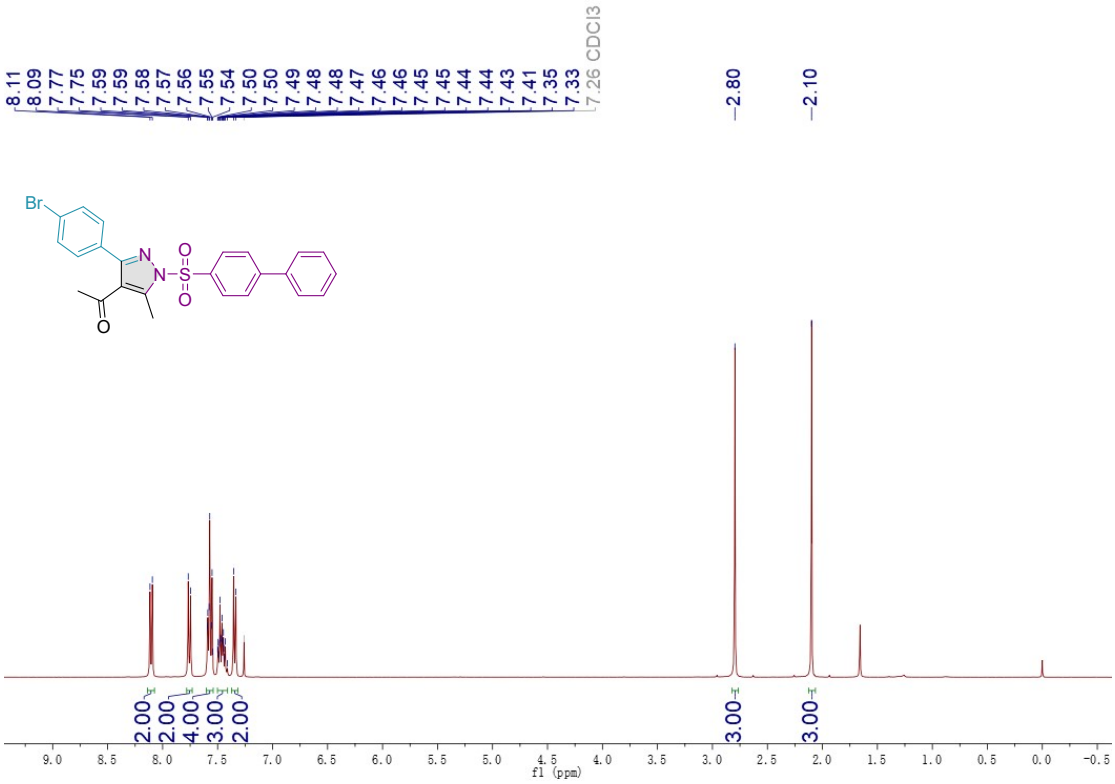


^{1}H NMR (400 MHz, $CDCl_3$)

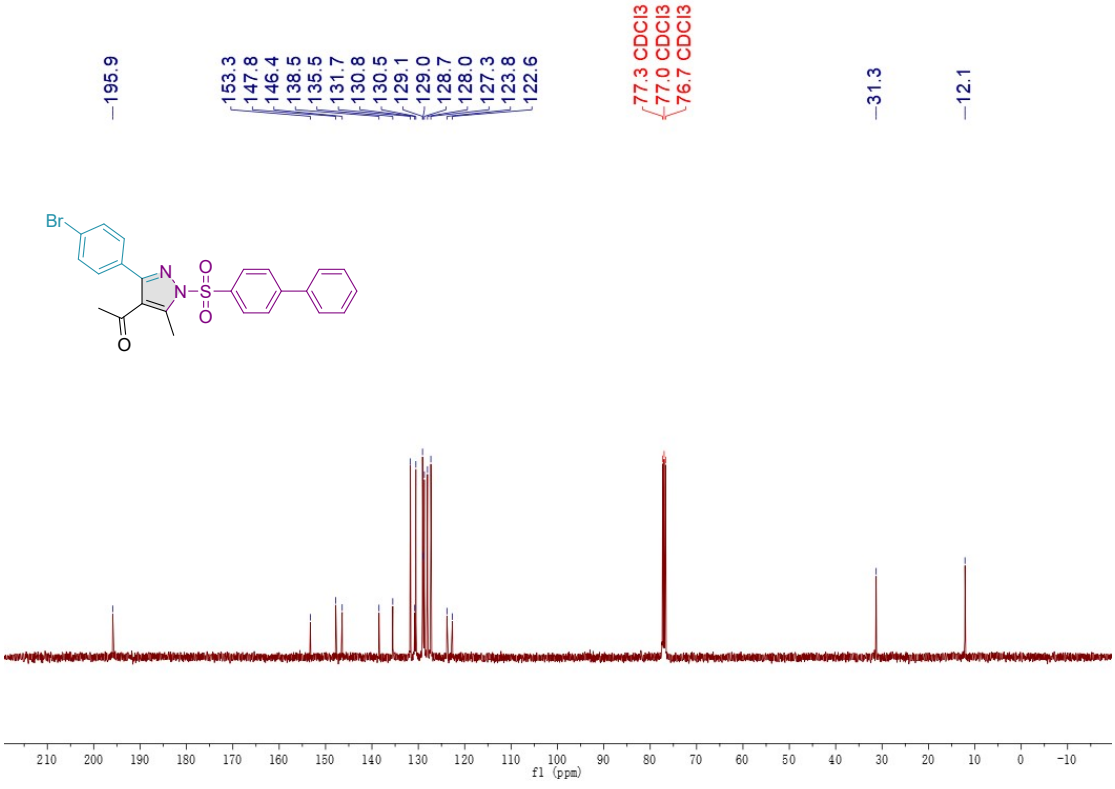


^{13}C NMR (100 MHz, $CDCl_3$)

1-(1-([1,1'-biphenyl]-4-ylsulfonyl)-3-(4-bromophenyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4aw)

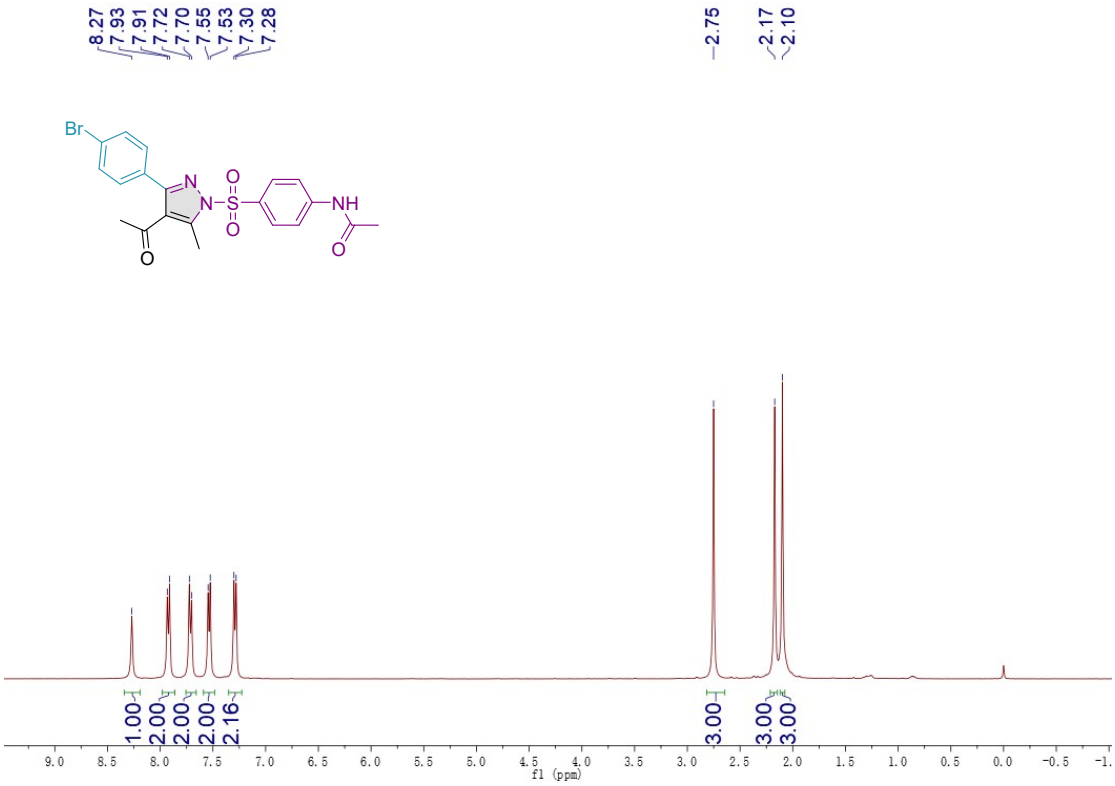


^{1}H NMR (400 MHz, $CDCl_3$)

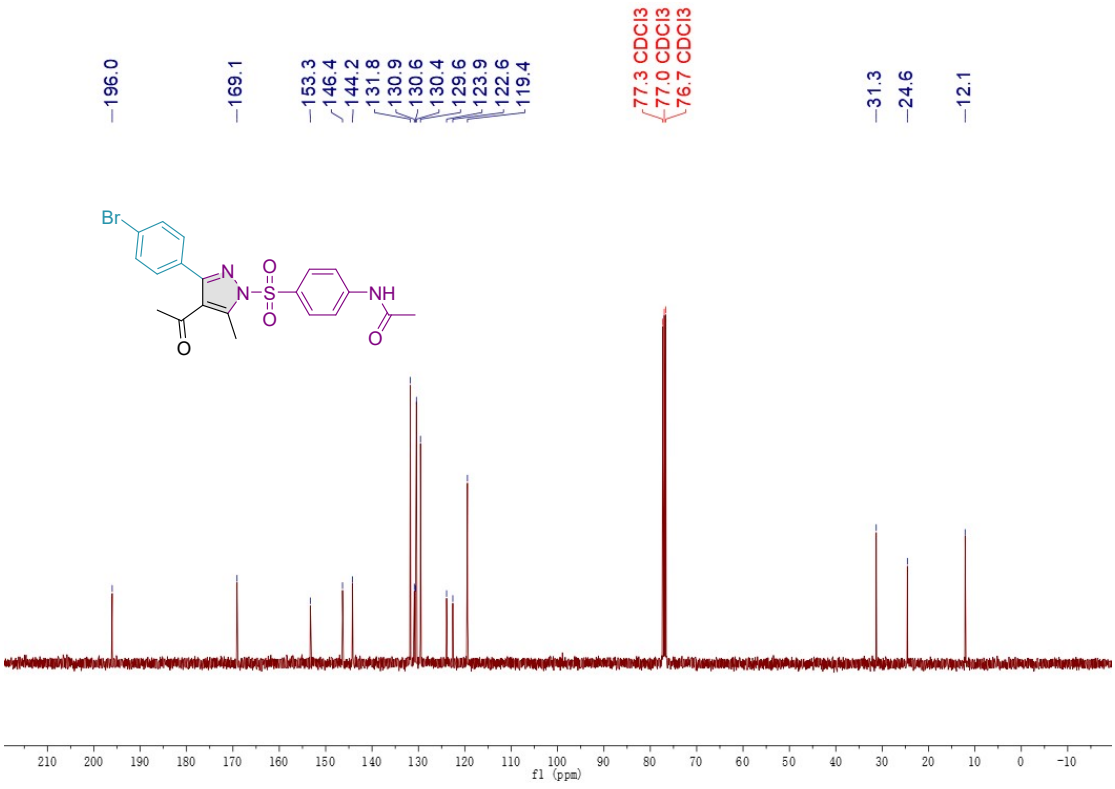


^{13}C NMR (100 MHz, $CDCl_3$)

N-(4-((4-acetyl-3-(4-bromophenyl)-5-methyl-1*H*-pyrazol-1-yl)sulfonyl)phenyl)acetamide (4ax)

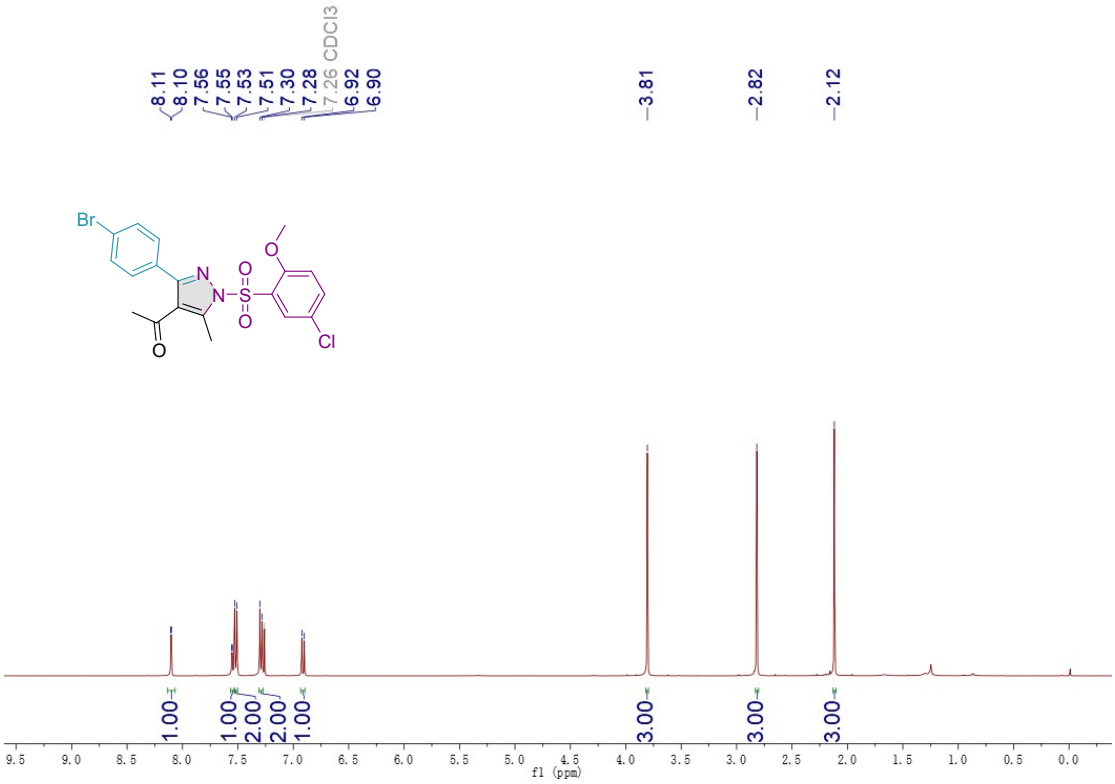


^{1}H NMR (400 MHz, $CDCl_3$)

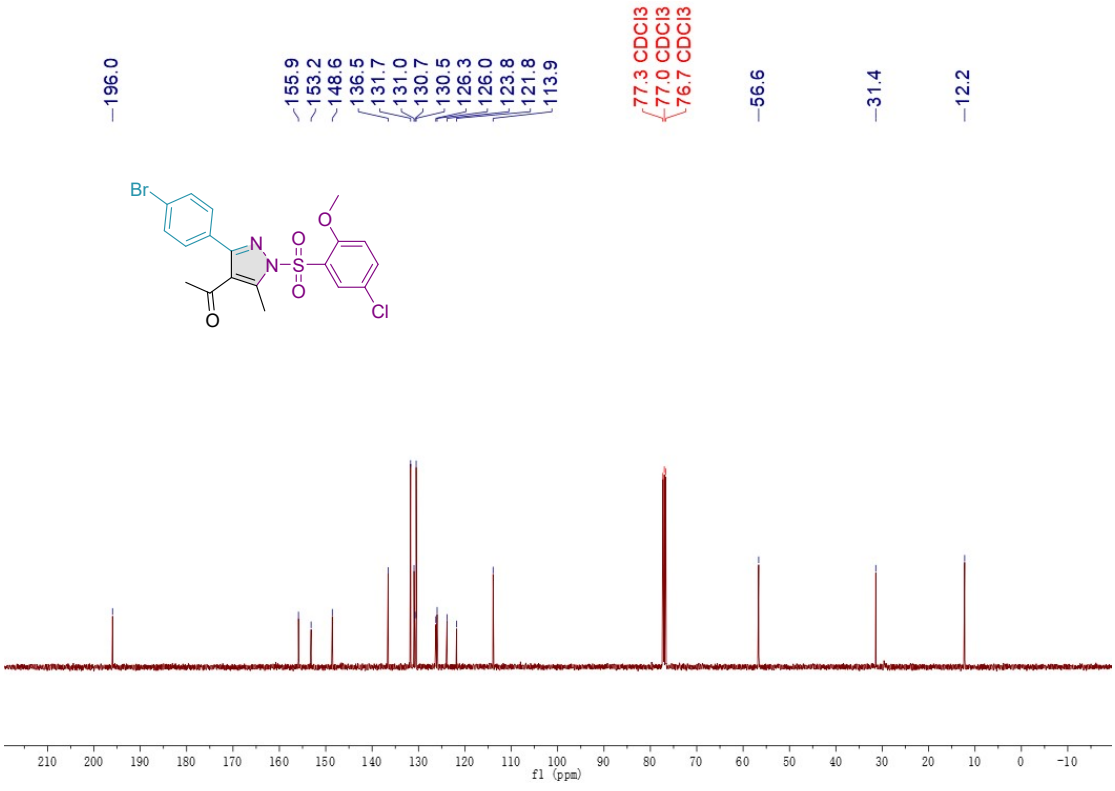


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-((5-chloro-2-methoxyphenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4ay)

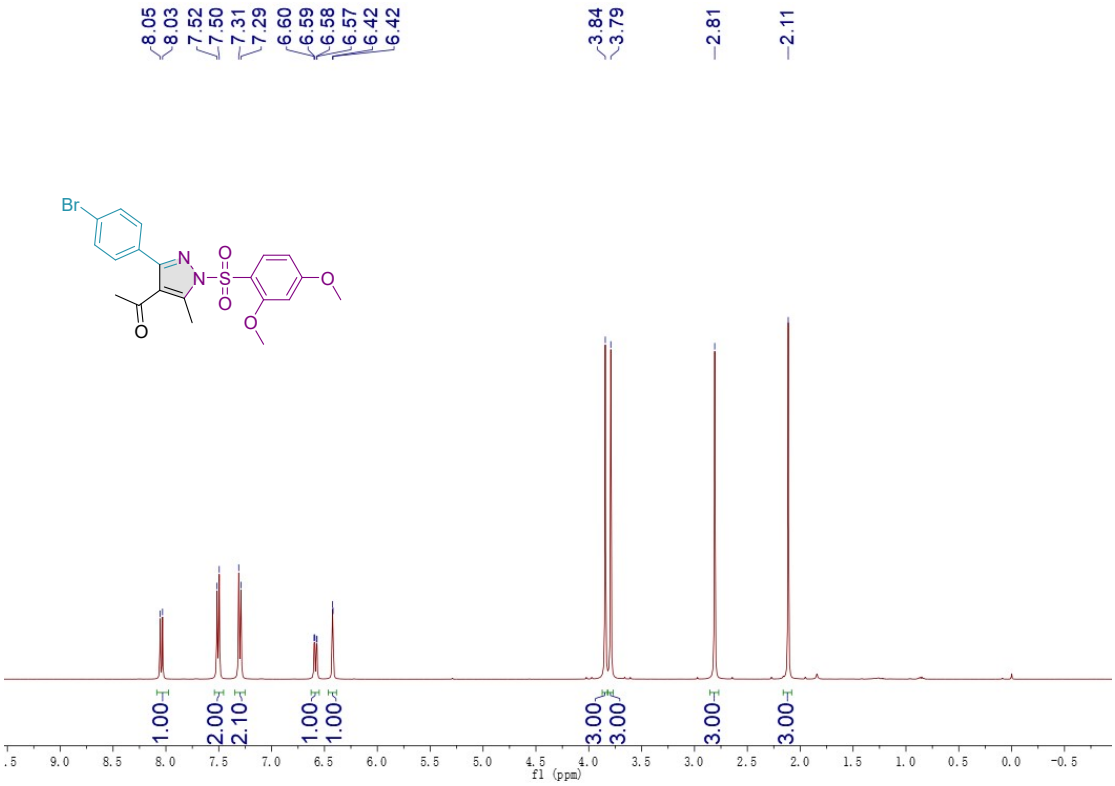


^{1}H NMR (400 MHz, $CDCl_3$)

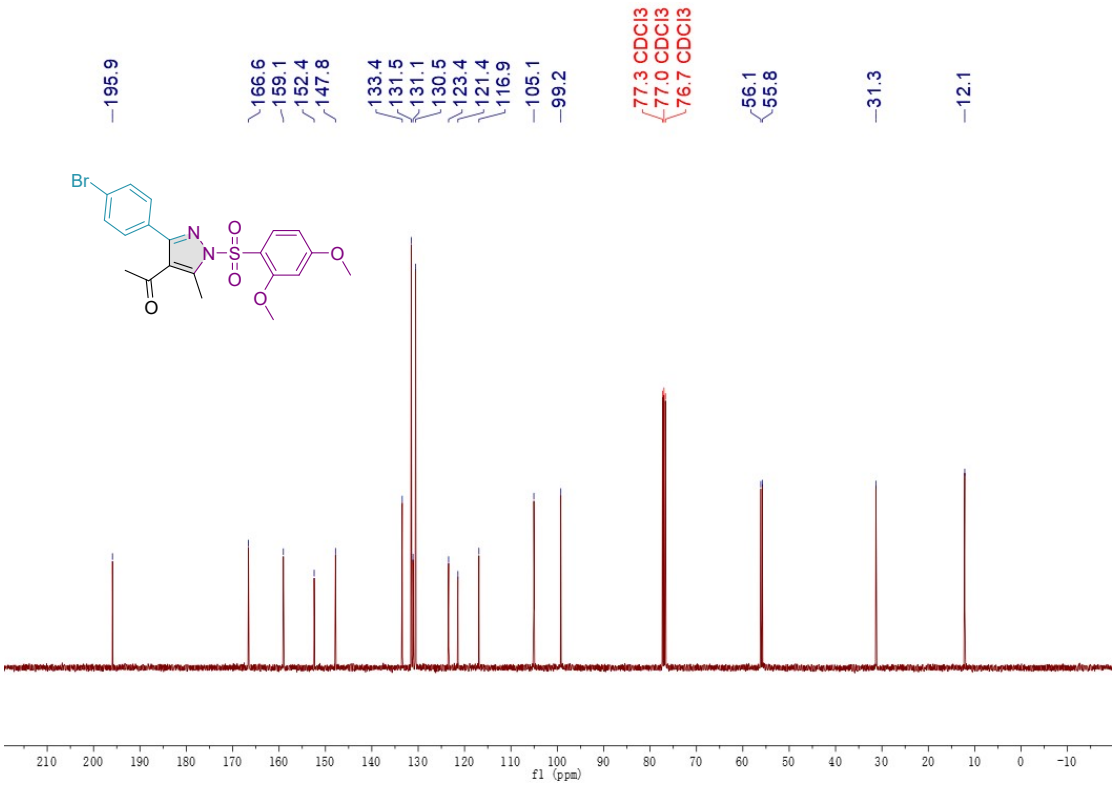


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-((2,4-dimethoxyphenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4az)

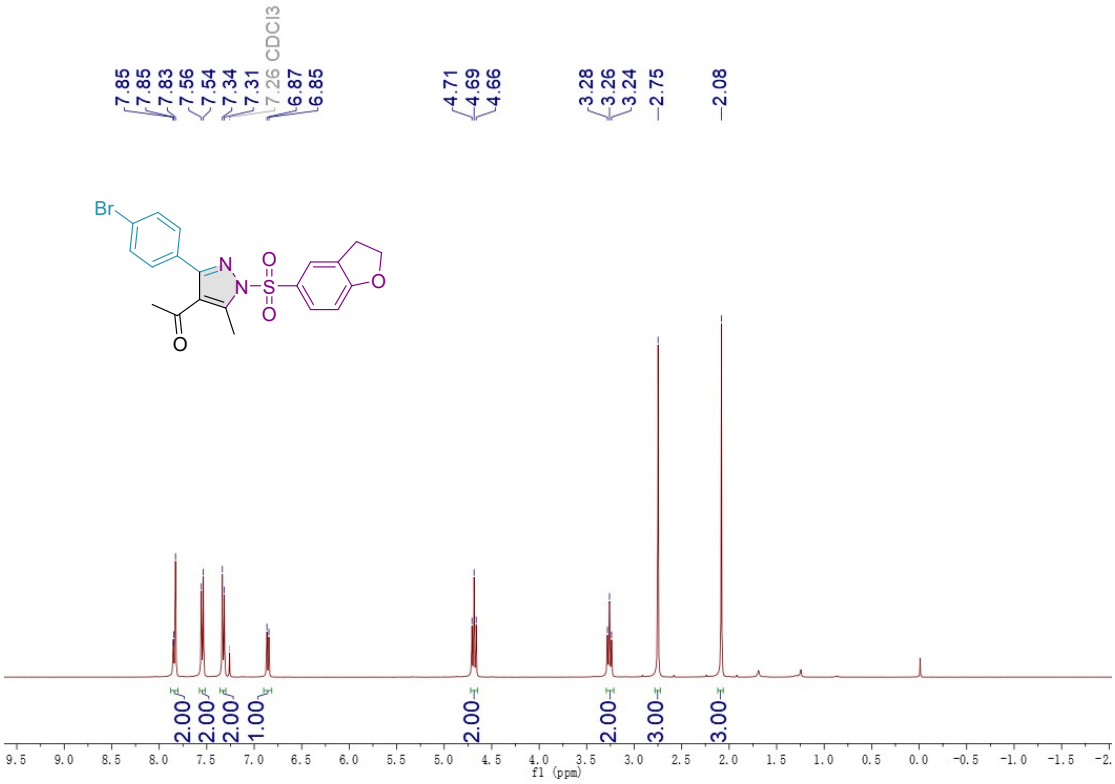


^{1}H NMR (400 MHz, $CDCl_3$)

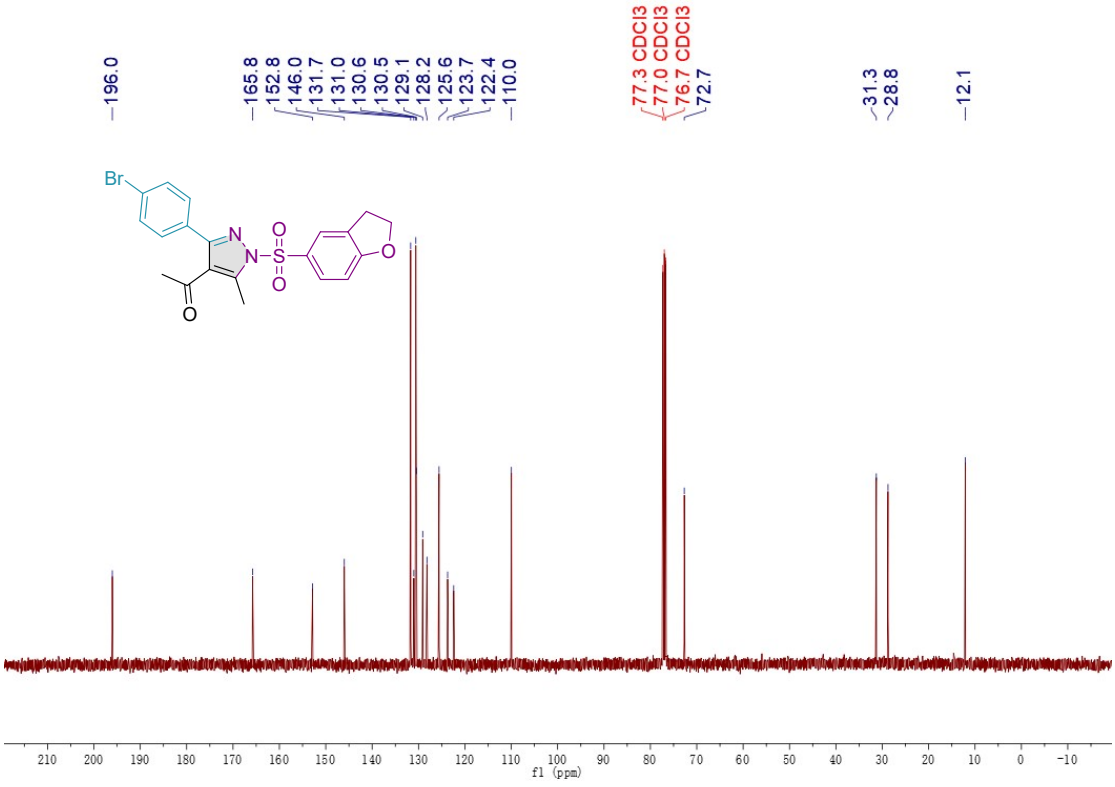


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-((4-chlorophenyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4ba)

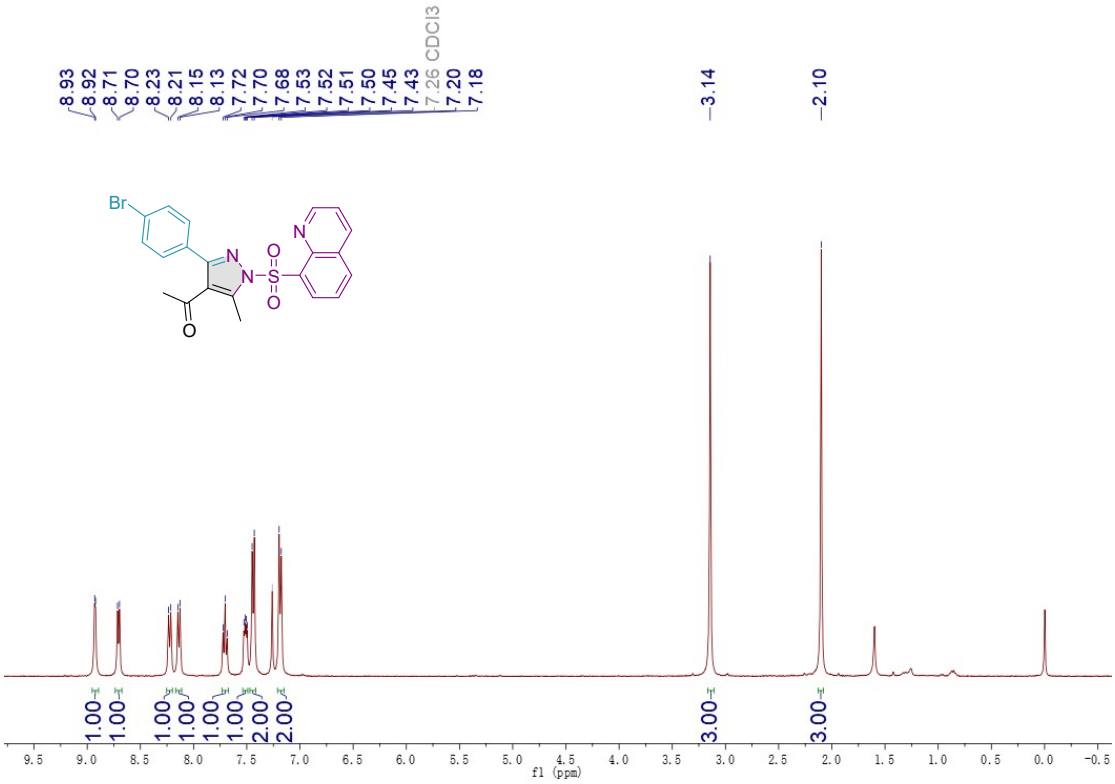


^{1}H NMR (400 MHz, $CDCl_3$)

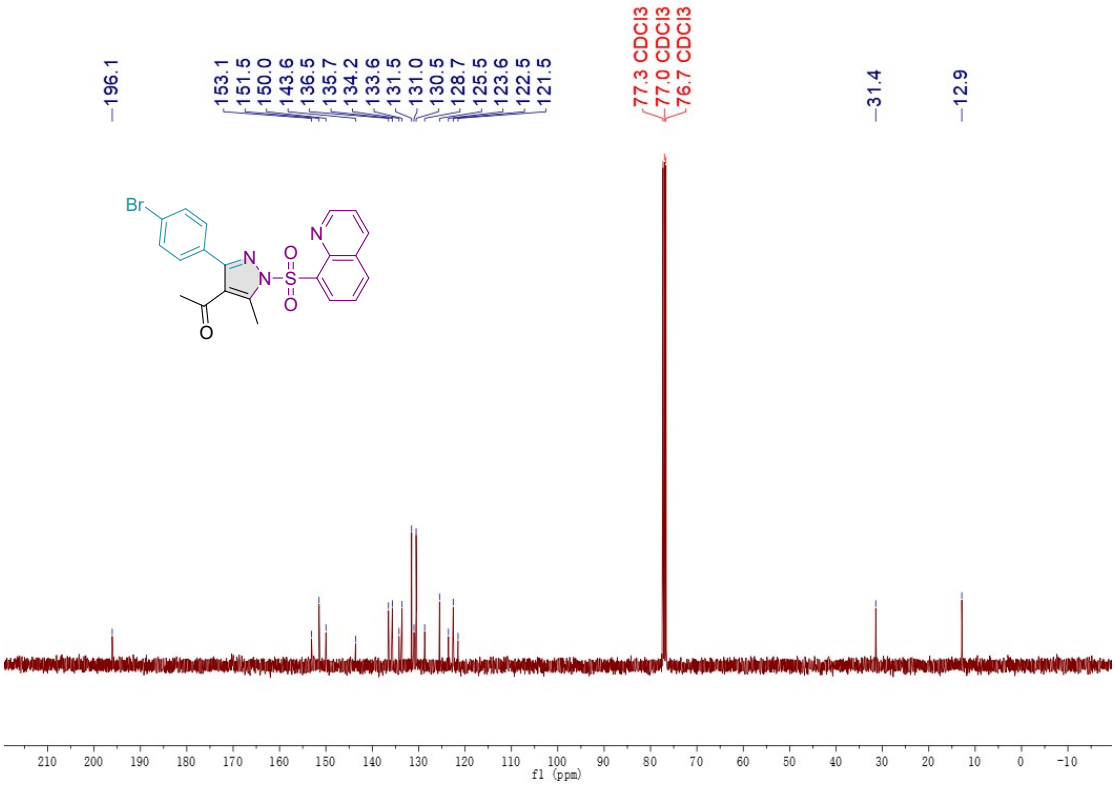


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-5-methyl-1-(quinolin-8-ylsulfonyl)-1*H*-pyrazol-4-yl)ethan-1-one (4bb)

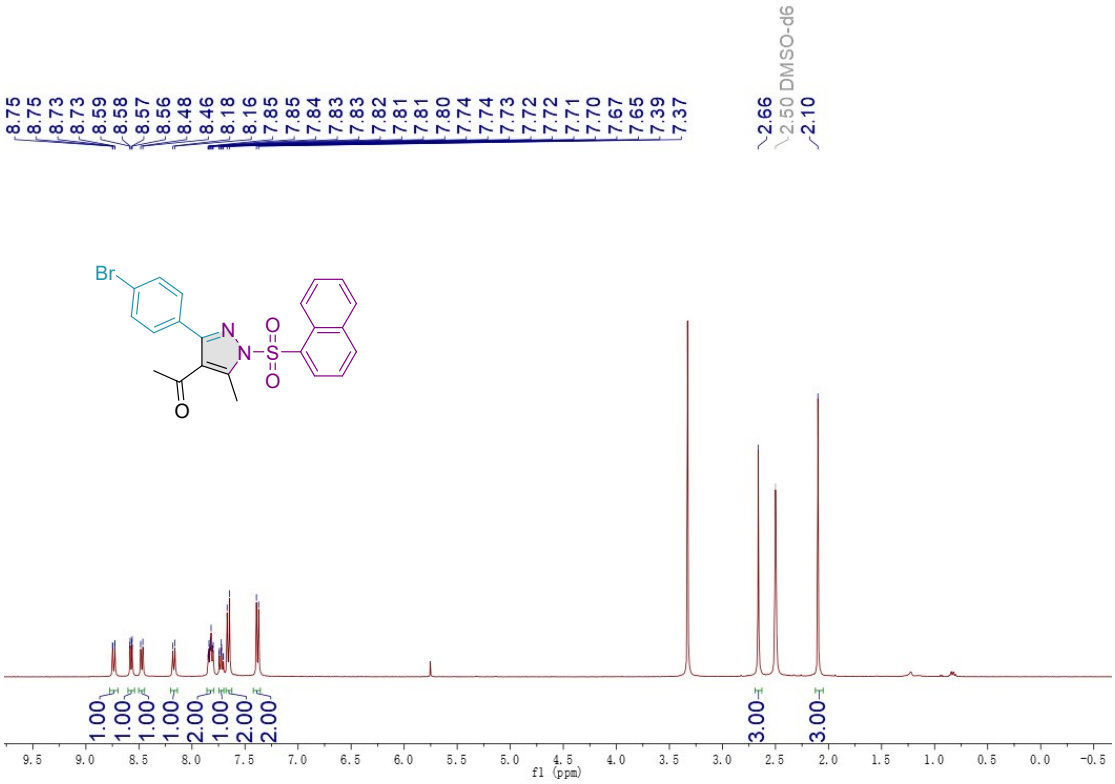


^{1}H NMR (400 MHz, $CDCl_3$)

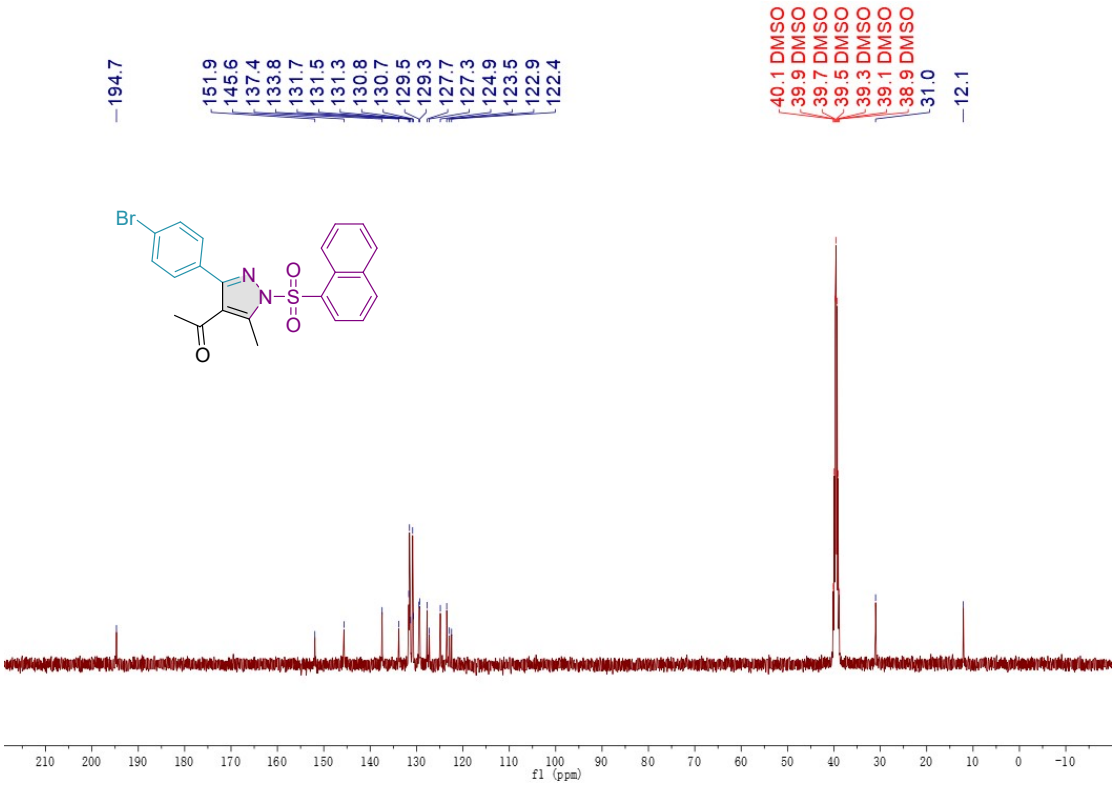


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-5-methyl-1-(naphthalen-1-ylsulfonyl)-1*H*-pyrazol-4-yl)ethan-1-one (4bc)

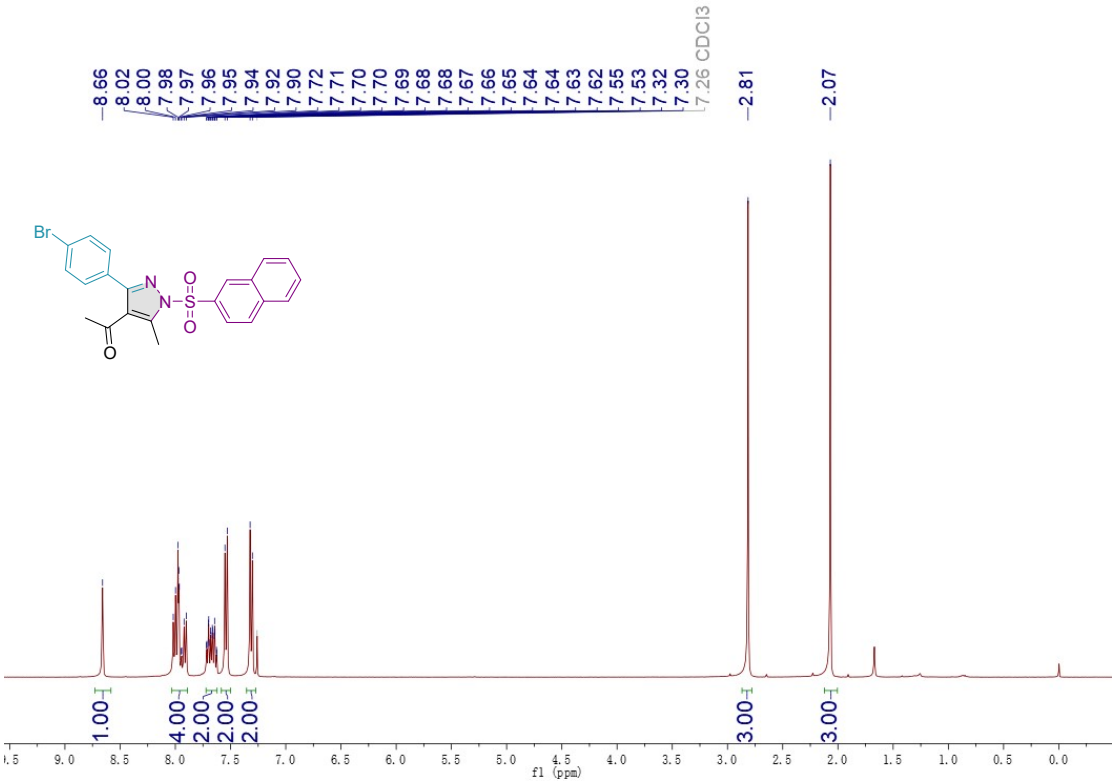


^{1}H NMR (400 MHz, DMSO-d_6)

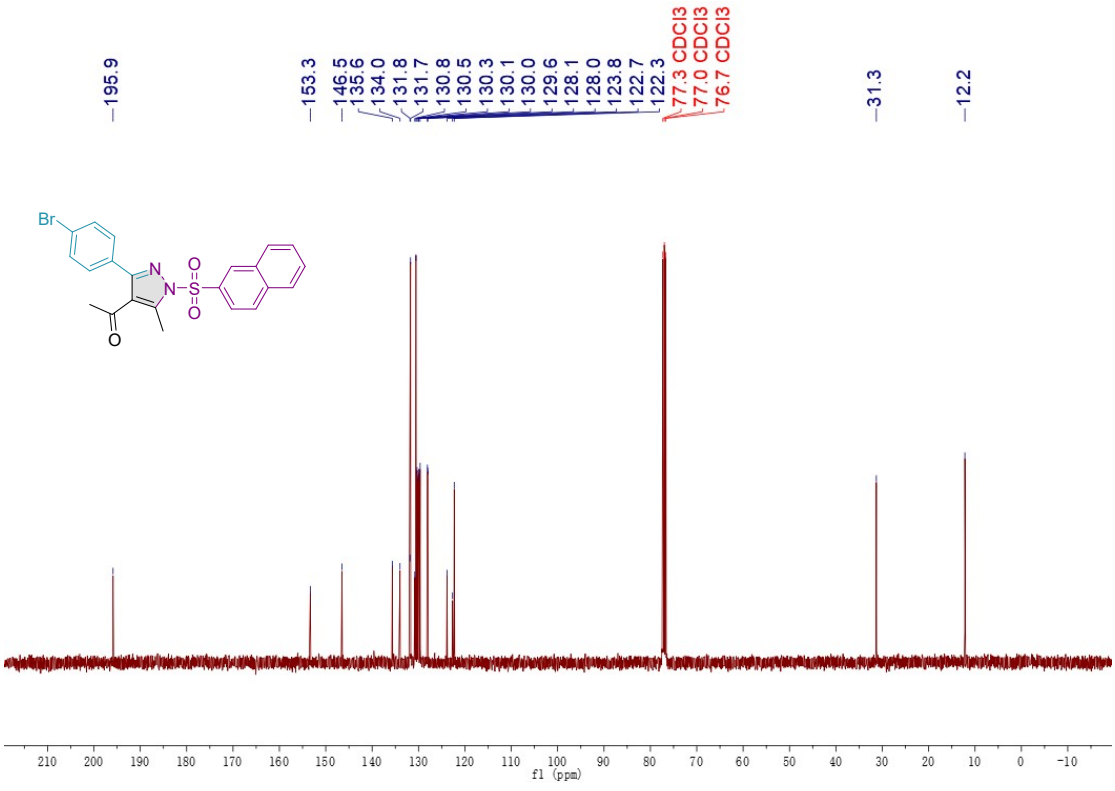


^{13}C NMR (100 MHz, DMSO-d_6)

1-(3-(4-bromophenyl)-5-methyl-1-(naphthalen-2-ylsulfonyl)-1*H*-pyrazol-4-yl)ethan-1-one (4bd)

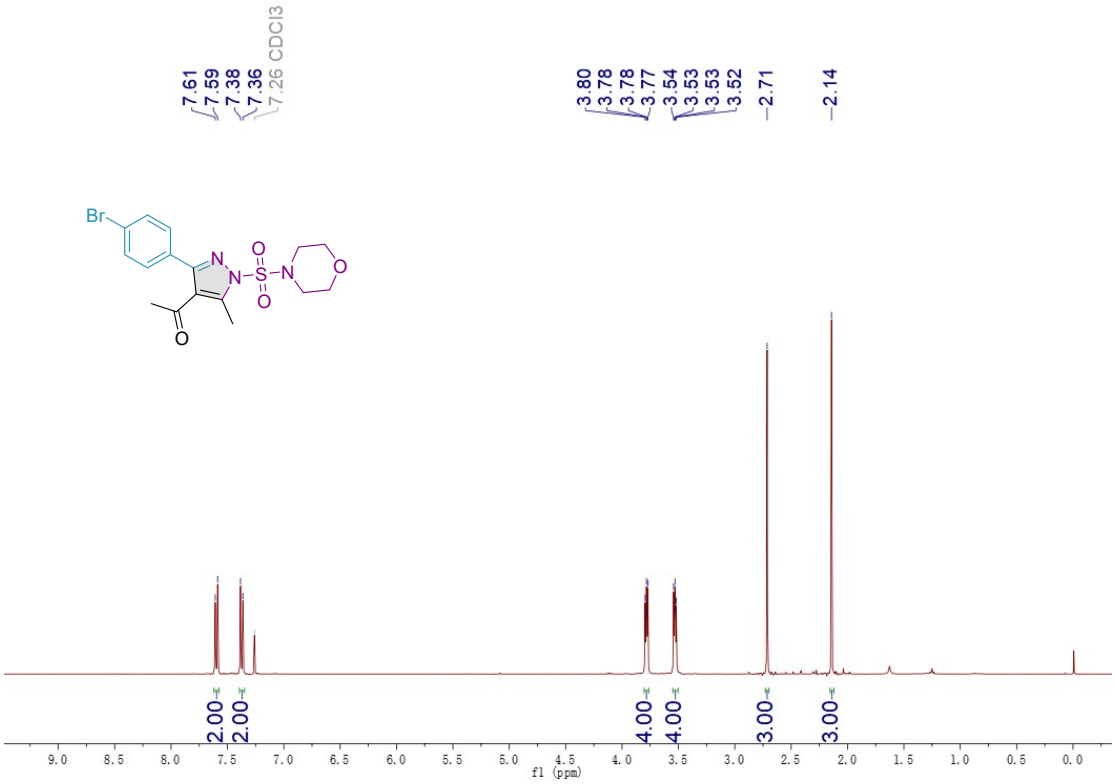


^{1}H NMR (400 MHz, $CDCl_3$)

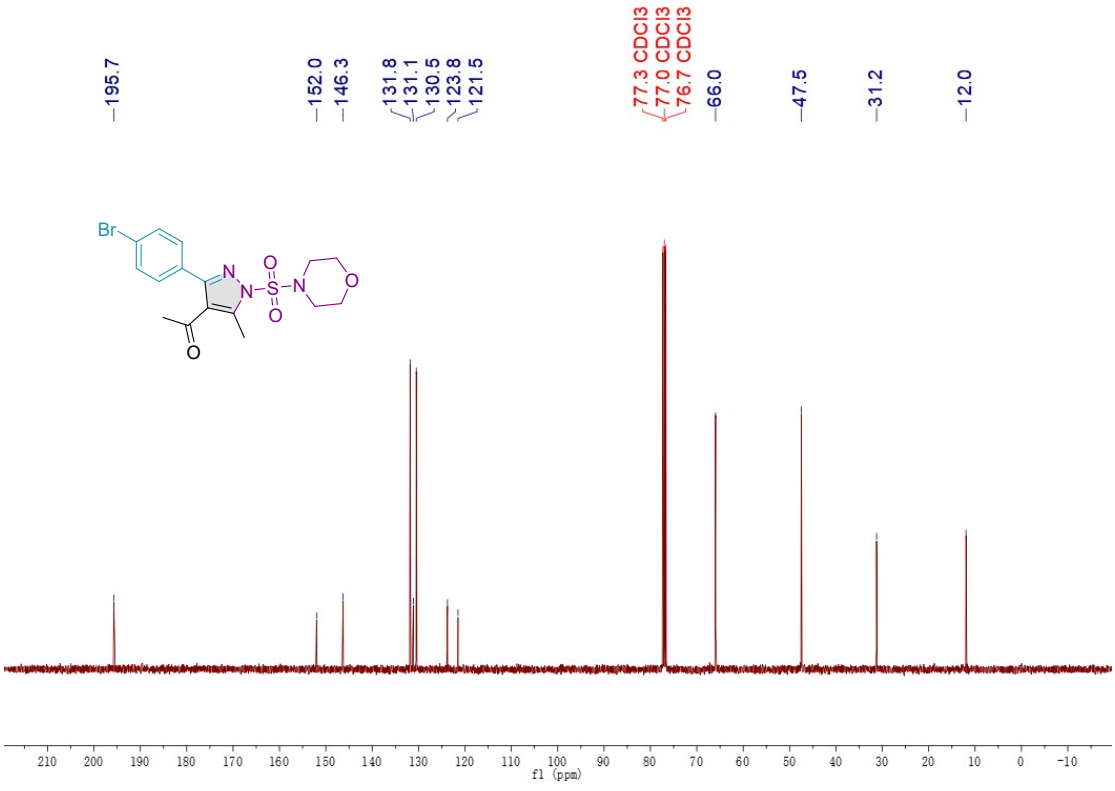


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-5-methyl-1-(morpholinosulfonyl)-1*H*-pyrazol-4-yl)ethan-1-one (4be)

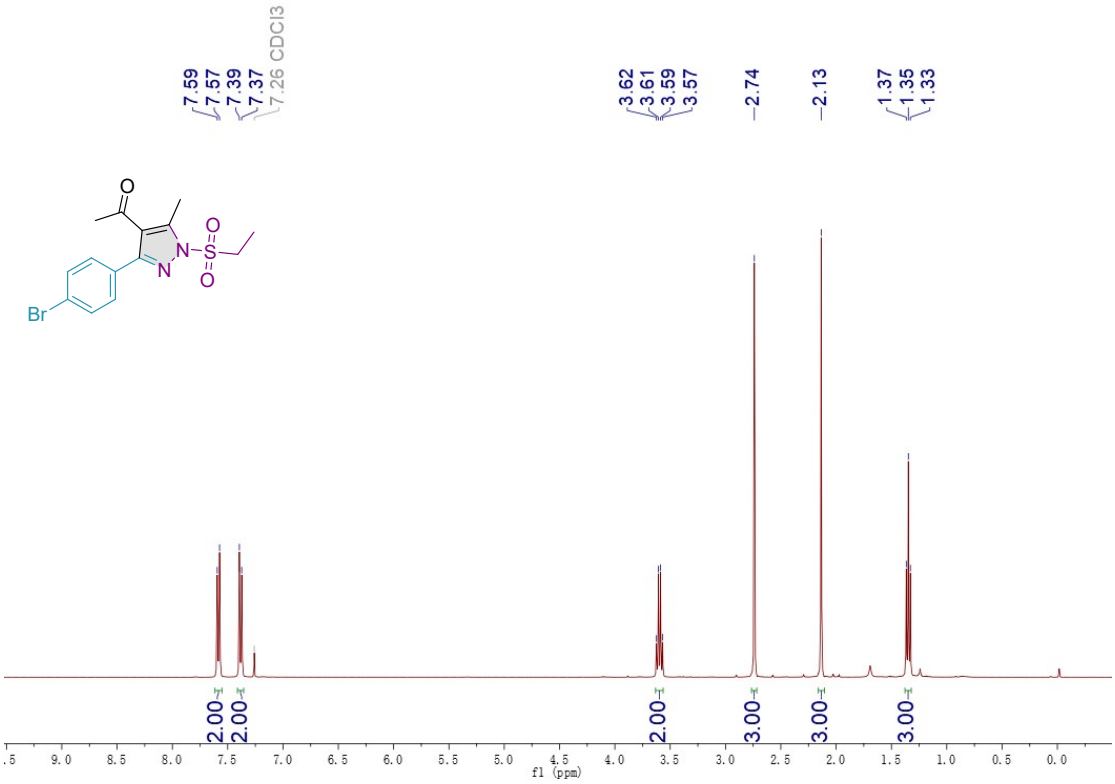


^{1}H NMR (400 MHz, $CDCl_3$)

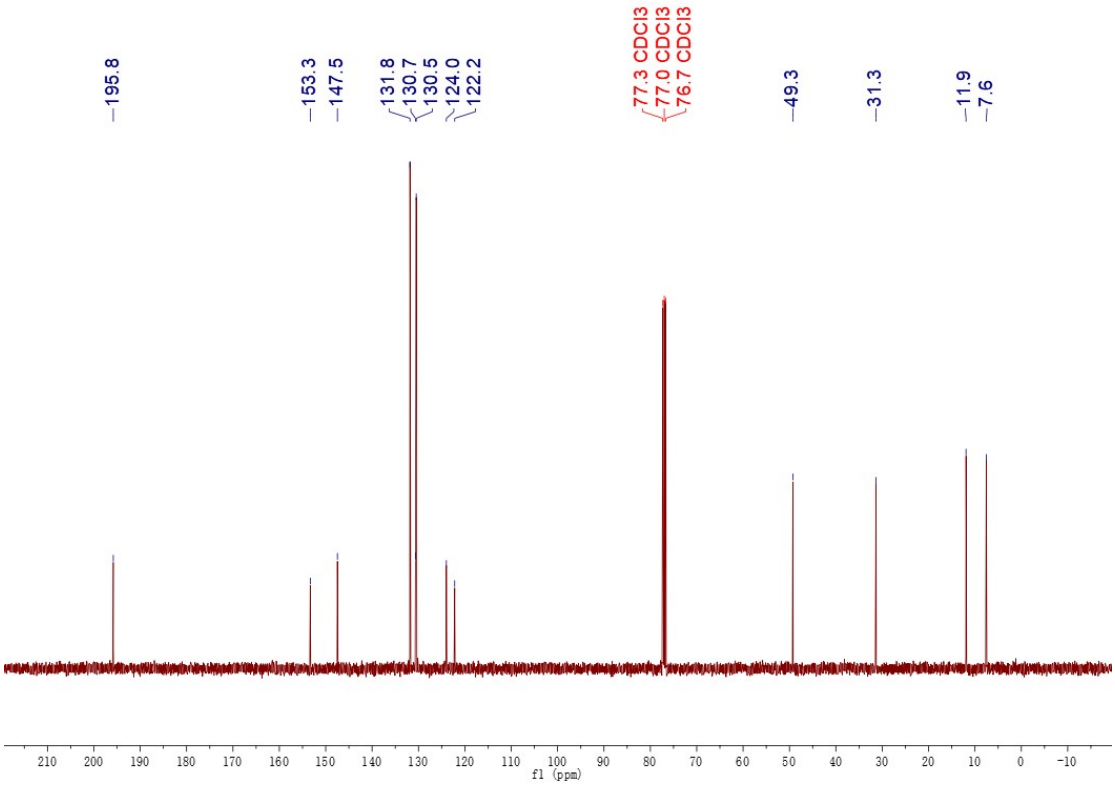


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-(ethylsulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4bf)

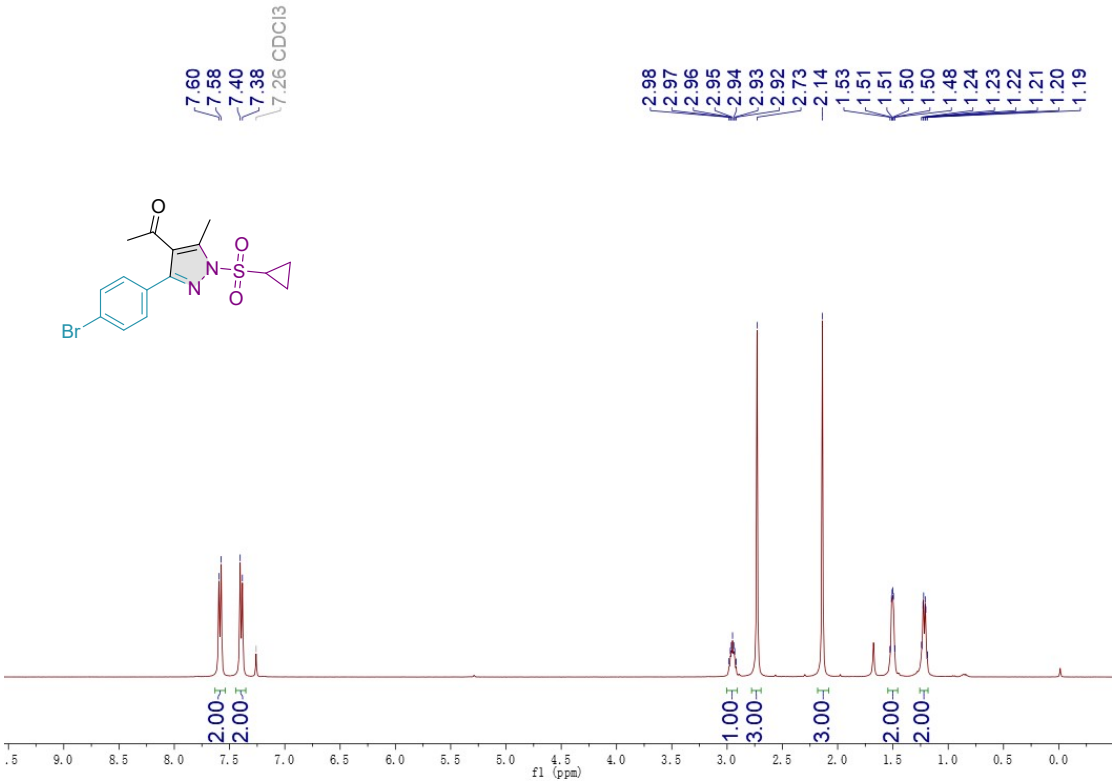


^{1}H NMR (400 MHz, $CDCl_3$)

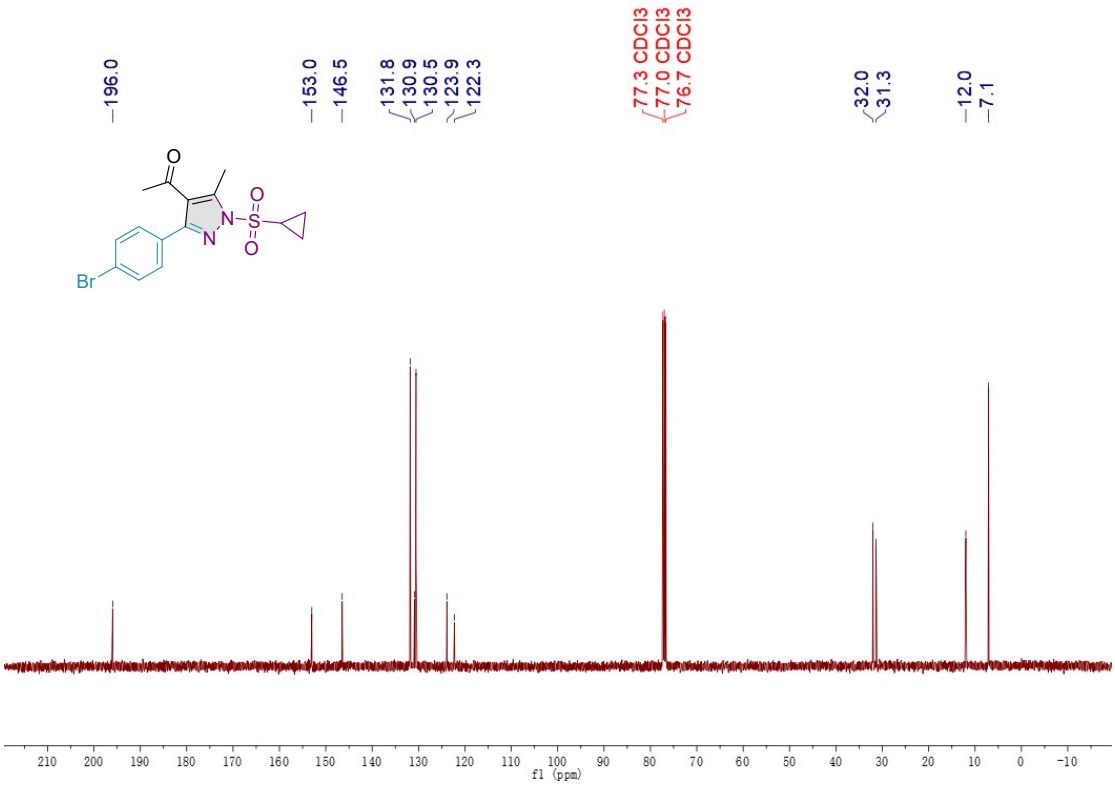


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-(cyclopropylsulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4bg)

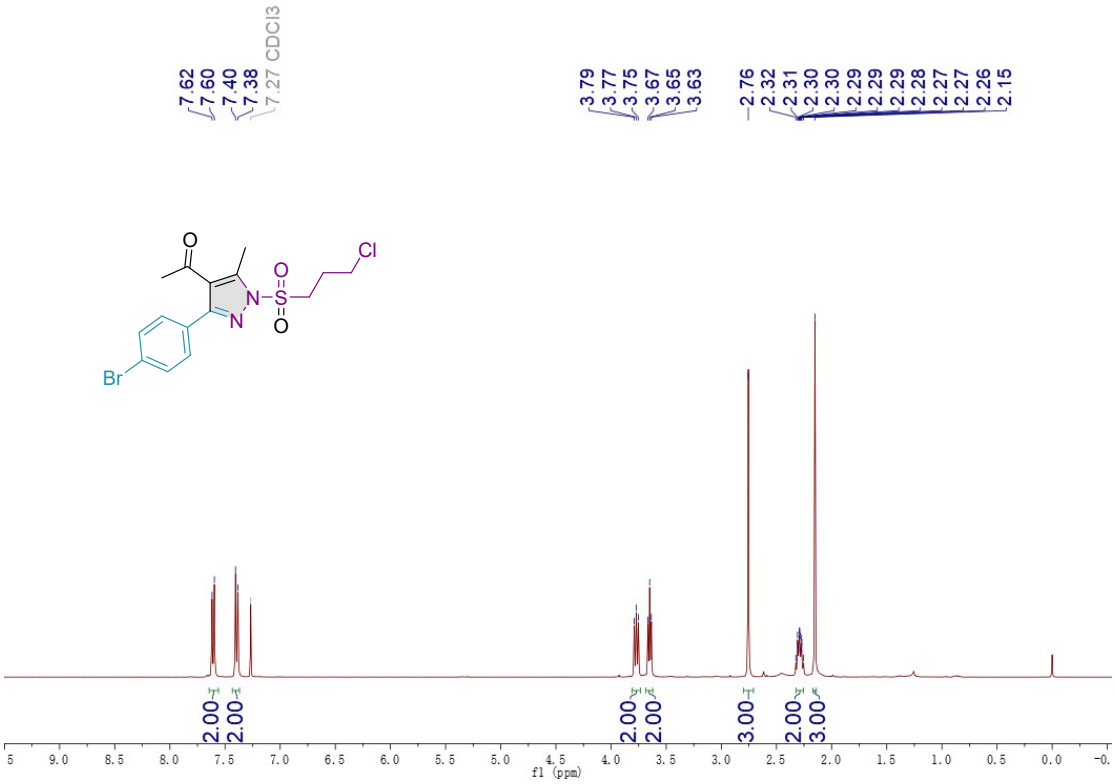


^{1}H NMR (400 MHz, $CDCl_3$)

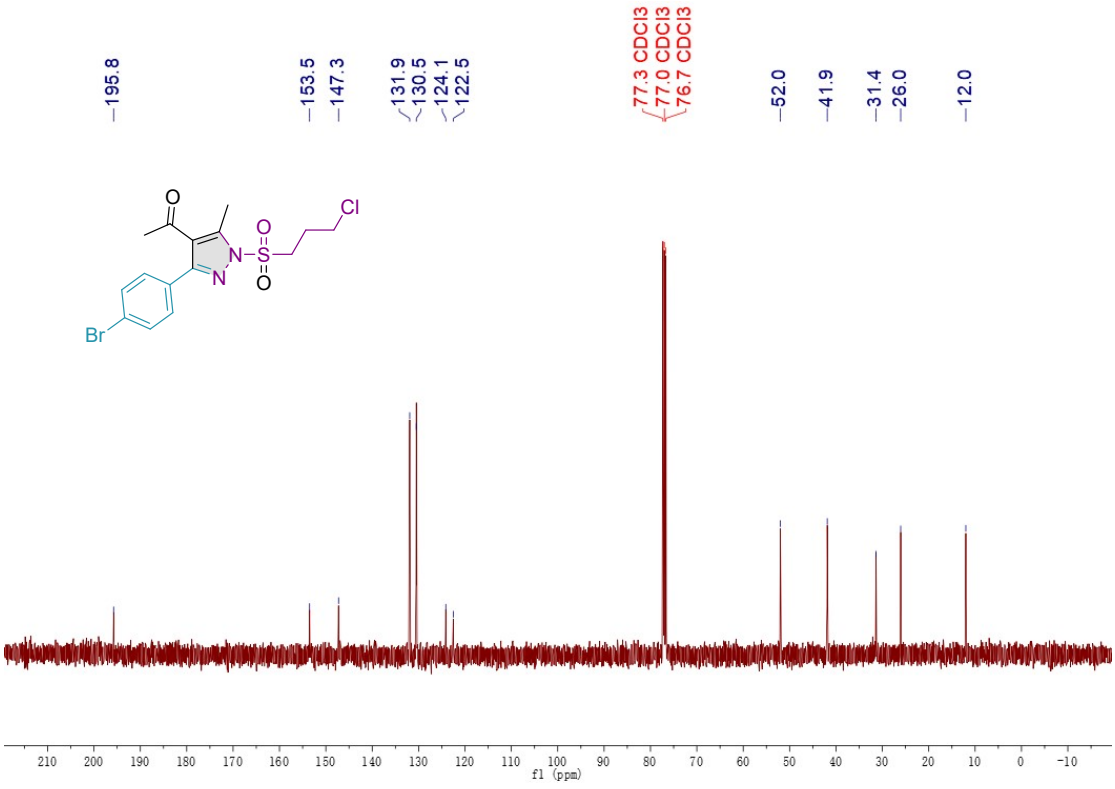


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-((2-chloroethyl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4bh)

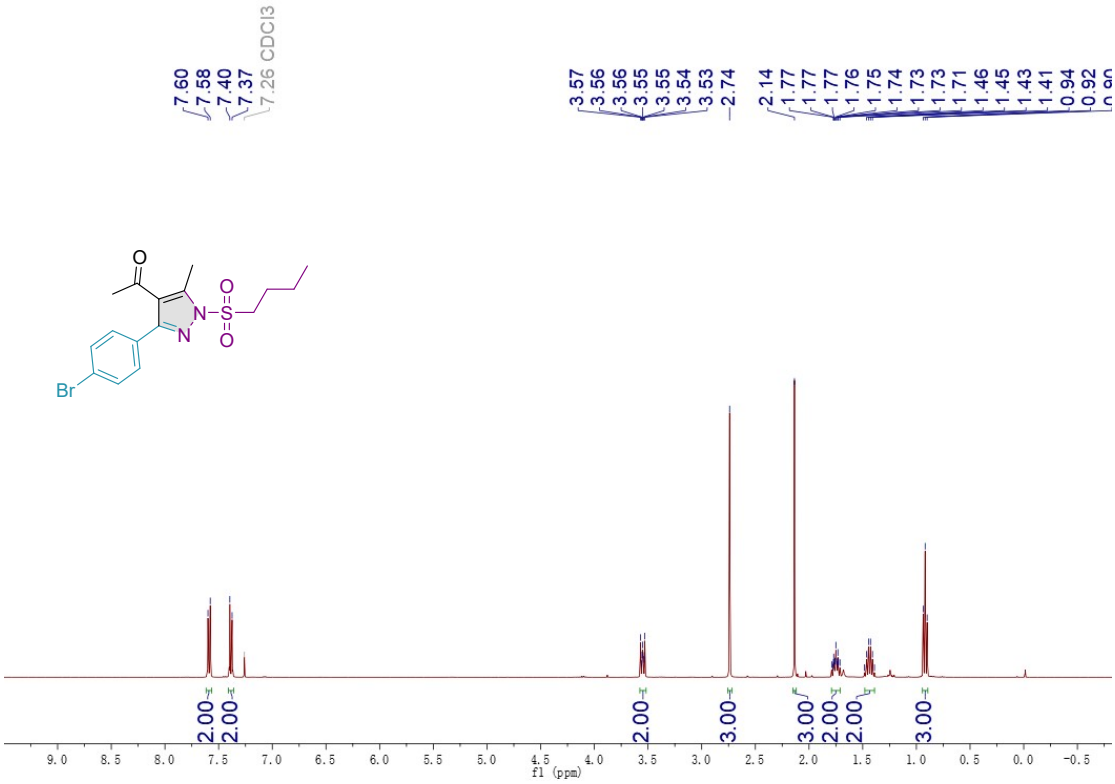


^{1}H NMR (400 MHz, $CDCl_3$)

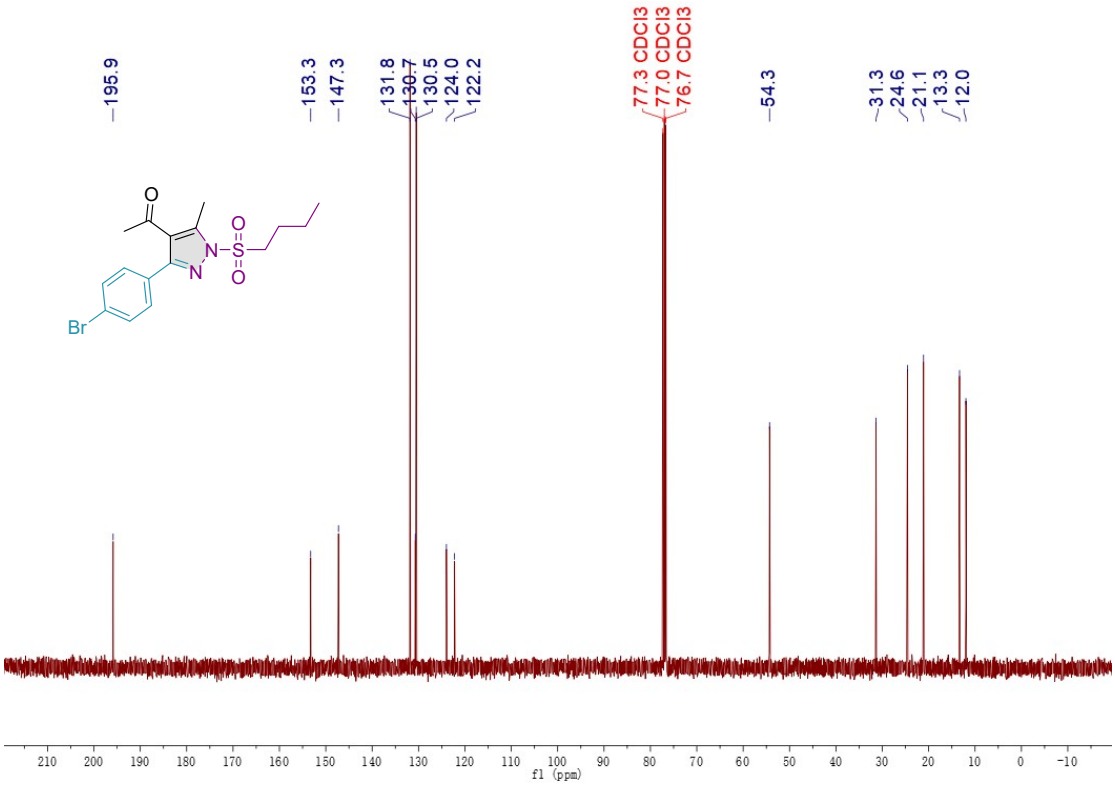


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-(butylsulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4bi)

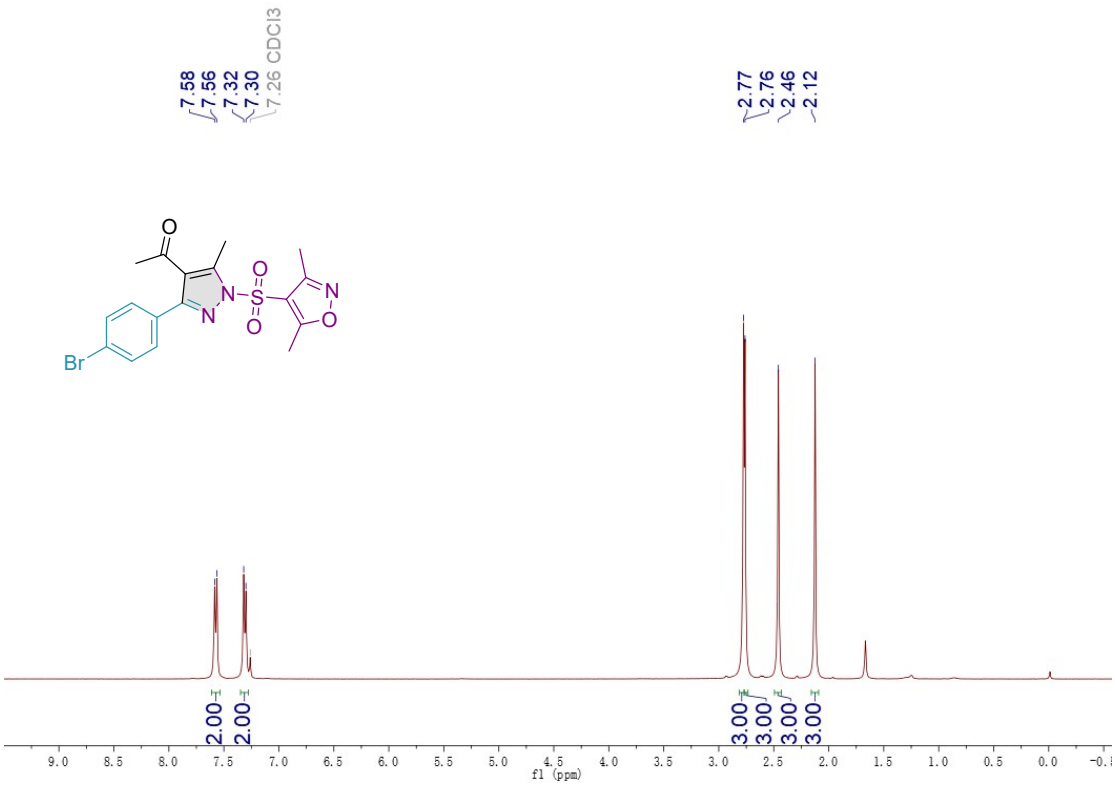


^{1}H NMR (400 MHz, $CDCl_3$)

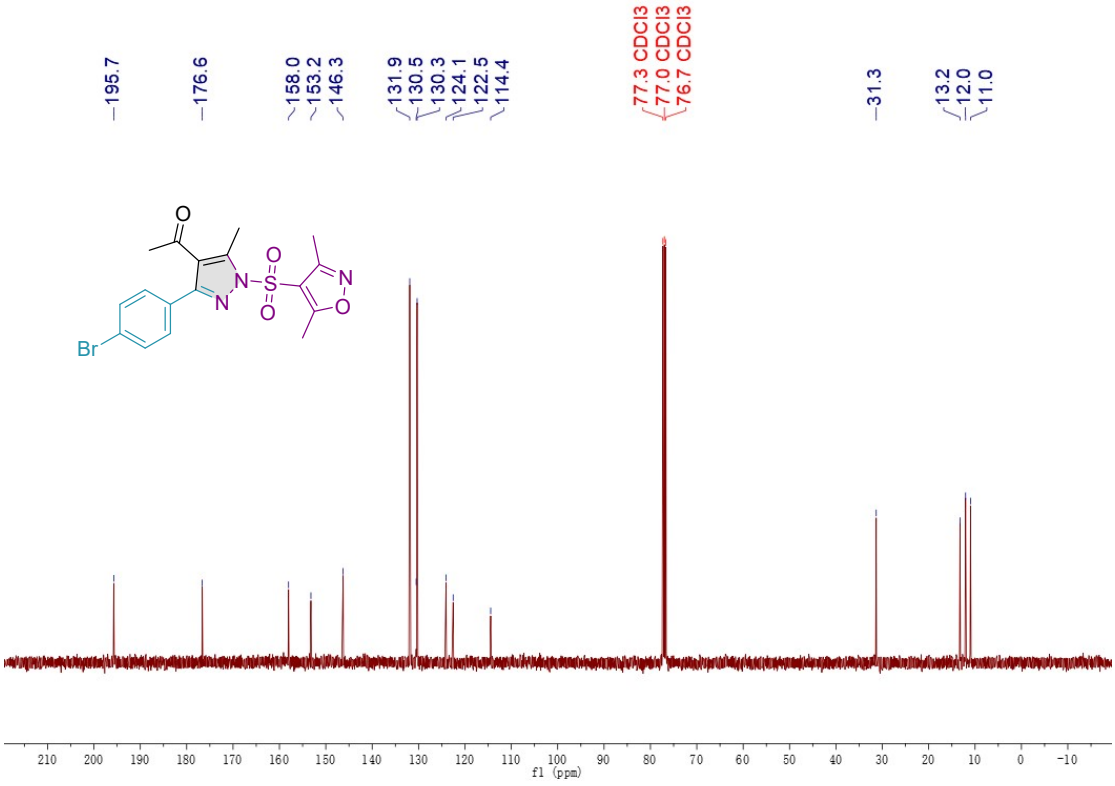


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-((3,5-dimethylisoxazol-4-yl)sulfonyl)-5-methyl-1H-pyrazol-4-yl)ethan-1-one(4bj)

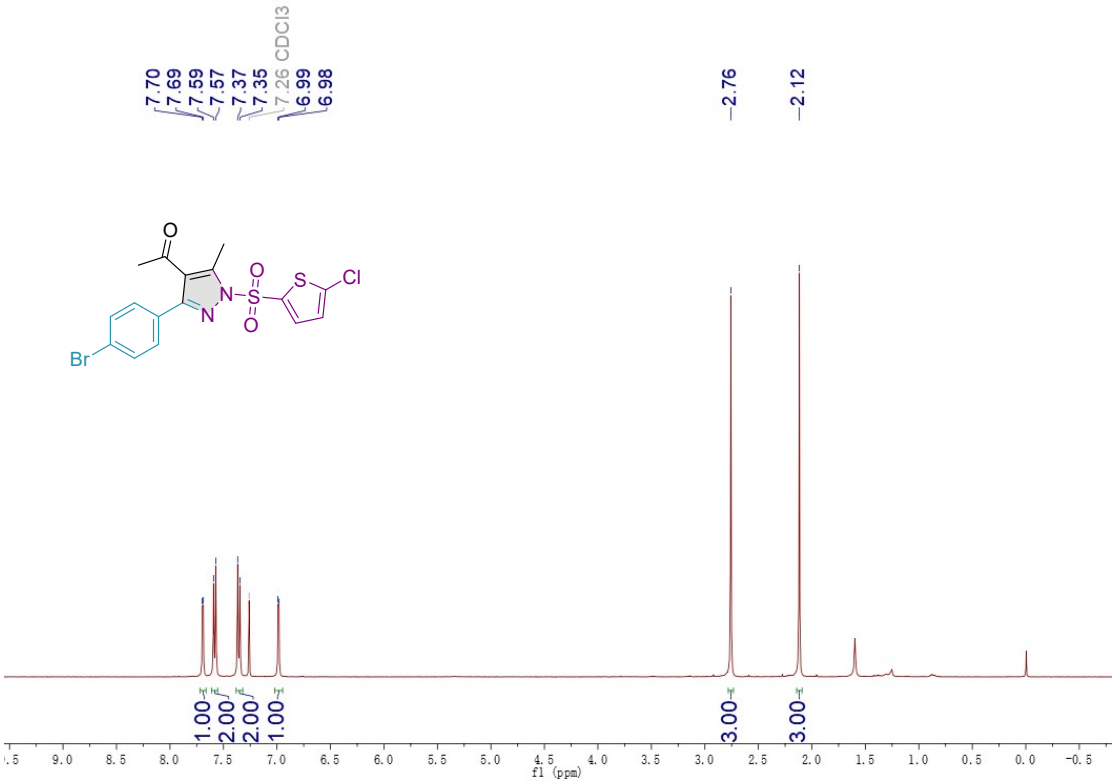


^{1}H NMR (400 MHz, $CDCl_3$)

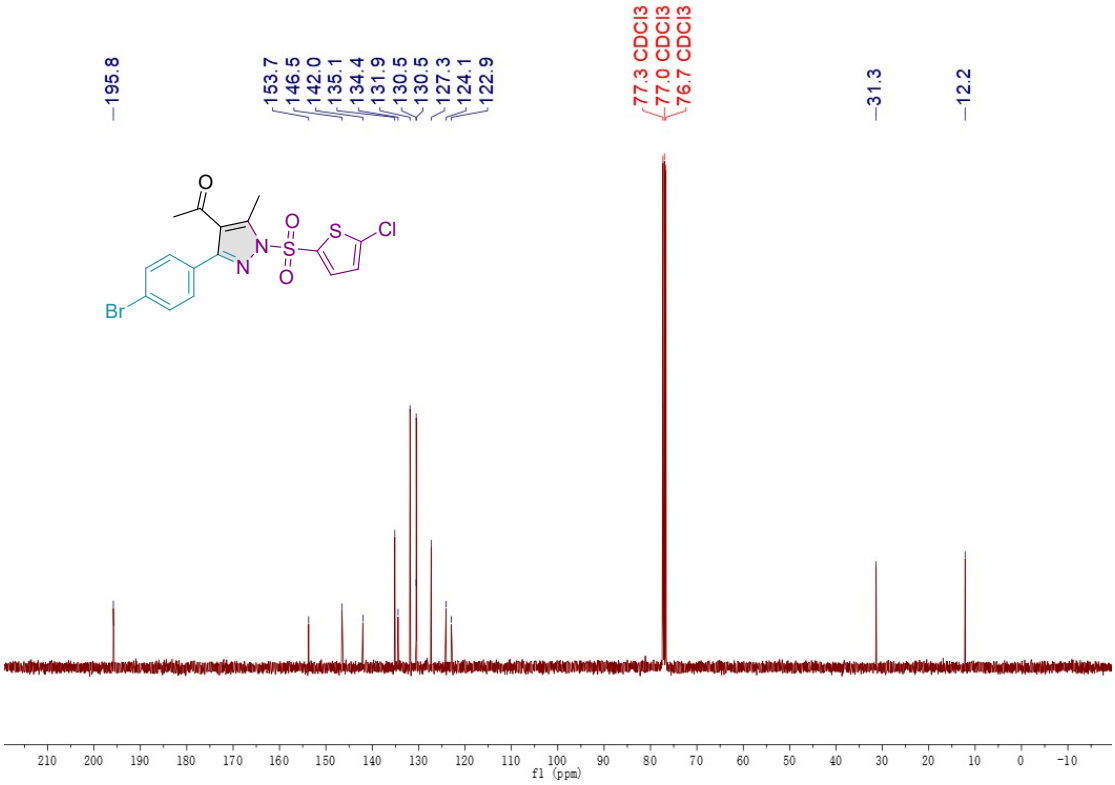


^{13}C NMR (100 MHz, $CDCl_3$)

1-(3-(4-bromophenyl)-1-((5-chlorothiophen-2-yl)sulfonyl)-5-methyl-1*H*-pyrazol-4-yl)ethan-1-one (4bk)



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



^{13}C NMR (100 MHz, $CDCl_3$)

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