Direct oxidation of *N*-ynylsulfonamides into *N*-sulfonyloxoacetamides with DMSO as a nucleophilic oxidant

Jun Dong,[a,b] Duo Fu,[a] Dongning Sheng,[a] Jiayi Wang,[a] and Jiaxi Xu[a]*

[a]State Key Laboratory of Chemical Resource Engineering, Department of Organic Chemistry, College of Chemistry, Beijing University of Chemical Technology, Beijing 100029, People's Republic of China E-mail: jxxu@mail.buct.edu.cn

[b]School of Chemistry and Environmental Engineering, Yancheng Teachers University, Yancheng 224007, People's Republic of China

Electronic Supporting Information

Contents

Details of calculation

All of the DFT calculations were performed with the Gaussian 09 program package.[1] The geometry optimization of all the minima and transition states involved were performed at the B3LYP levels of theory[2] with the 6-31+G(d,p) basis set for all atoms. The solution condition is given by IEFPCM model.[3-5] The vibrational frequencies were computed at the same level of theory to check whether every optimized geometrical structure is an energy minimum or a transition state and to get the correction of Gibbs free energy. IRC calculations[6-7] were used to confirm that the transition states found from the optimization calculations connect the related reactants and products. The high accurate zero-point energy is given under the level M06-2X/def2-TZVPP.[8] Solvent effects were computed by the uESE software[9-12] at the B3LYP/def2-TZVP level using the optimized structures. CM5 charges is given by Multiwfn program.[13-15]

References

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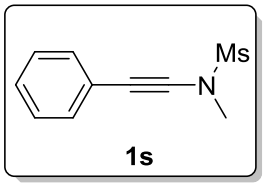
Coordinates of All Stationary Points



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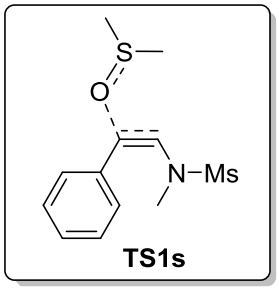

TS1s

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13	6	0	-0.550448	-0.031978	0.073864
14	7	0	-1.239994	-1.185621	-0.241011
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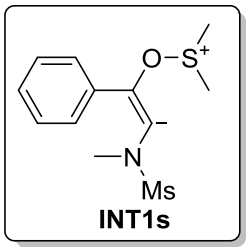

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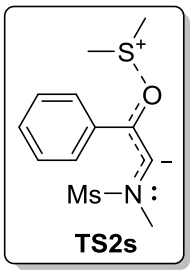

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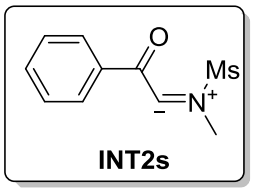

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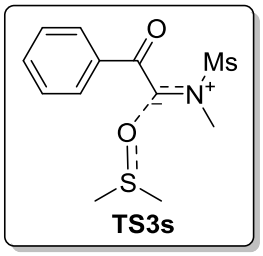

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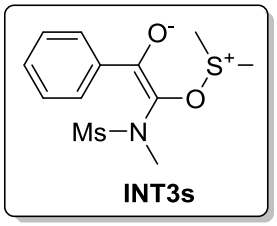

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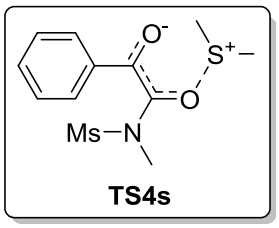
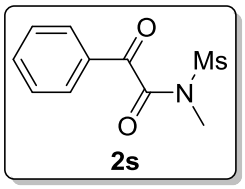
29	6	0	-3.998357	-0.948553	-0.664523
30	1	0	-3.909700	-0.008031	-1.208310
31	1	0	-4.629570	-1.639796	-1.228196
32	1	0	-4.393738	-0.791419	0.340460
33	6	0	-2.720258	-3.180552	0.363300
34	1	0	-3.310436	-3.825149	-0.292478
35	1	0	-1.759608	-3.632735	0.600519
36	1	0	-3.282941	-2.914272	1.259163



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.328189	-1.532395	0.487240
2	6	0	2.955033	-1.752718	0.613975
3	6	0	2.029156	-0.923673	-0.043167
4	6	0	2.512177	0.115504	-0.852641
5	6	0	3.888060	0.328741	-0.990609
6	6	0	4.800477	-0.488892	-0.317511

7	1	0	5.028820	-2.175260	1.012963
8	1	0	2.591590	-2.570786	1.229198
9	1	0	1.813203	0.746456	-1.390183
10	1	0	4.245107	1.133026	-1.628020
11	1	0	5.868287	-0.319036	-0.422012
12	6	0	0.565398	-1.250218	0.092216
13	6	0	-0.351820	-0.319314	0.575525
14	7	0	-0.123858	1.025766	0.873640
15	16	0	-0.463433	2.246825	-0.276302
16	8	0	0.538431	3.324069	-0.122707
17	8	0	-0.582941	1.573551	-1.583845
18	6	0	-0.138631	1.468516	2.284623
19	1	0	0.553652	0.833166	2.840017
20	1	0	0.212455	2.500343	2.352618
21	1	0	-1.136331	1.390729	2.731271
22	6	0	-2.061770	2.969456	0.151417
23	1	0	-1.984935	3.435196	1.133964
24	1	0	-2.275055	3.721948	-0.609909
25	1	0	-2.819250	2.187279	0.148188
26	8	0	0.181659	-2.431416	-0.219844
27	16	0	-2.470789	-1.509860	-0.600631
28	8	0	-1.664410	-0.787077	0.767573
29	6	0	-4.083686	-0.707980	-0.409535
30	1	0	-4.009141	0.291326	-0.837834
31	1	0	-4.818075	-1.293204	-0.968300
32	1	0	-4.345541	-0.666606	0.649405
33	6	0	-2.820027	-3.129718	0.114127
34	1	0	-3.459059	-3.671258	-0.587094
35	1	0	-1.850741	-3.614058	0.221525
36	1	0	-3.317677	-2.997932	1.076260



Standard orientation:

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1	6	0	-3.390299	-1.785257	0.231928
2	6	0	-2.191602	-1.103128	0.023786
3	6	0	-2.196283	0.294776	-0.133719
4	6	0	-3.413592	1.000216	-0.080073
5	6	0	-4.607045	0.314275	0.122936
6	6	0	-4.596254	-1.078776	0.279459
7	1	0	-3.384071	-2.863527	0.353913
8	1	0	-1.260621	-1.659054	-0.018442
9	1	0	-3.405299	2.078390	-0.199260
10	1	0	-5.545493	0.858322	0.160705
11	1	0	-5.528787	-1.611696	0.438849
12	6	0	-0.942681	1.050566	-0.324649
13	6	0	0.365923	0.264136	-0.556729
14	7	0	1.316806	0.313501	0.430523
15	16	0	2.872832	-0.445296	0.140805
16	8	0	3.671105	-0.117682	1.329484
17	8	0	2.647880	-1.853531	-0.199916
18	6	0	1.116191	1.041308	1.703215
19	1	0	0.082095	0.914046	2.024210
20	1	0	1.765281	0.608088	2.460440
21	1	0	1.344107	2.102366	1.583832
22	8	0	0.518052	-0.283226	-1.645584
23	8	0	-0.873283	2.271816	-0.409496
24	6	0	3.530850	0.435318	-1.277555
25	1	0	4.508412	-0.009683	-1.473713
26	1	0	2.853204	0.286177	-2.116666
27	1	0	3.626926	1.487177	-1.007898

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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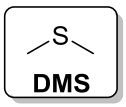
2	6	0	0.264667	-0.781162	1.375441
3	6	0	0.264667	-0.781162	-1.375441
4	1	0	0.199131	-0.205396	-2.300170

5	1	0	1.199669	-1.346326	-1.355315
6	1	0	-0.598156	-1.444154	-1.275795
7	8	0	-1.126495	1.080680	-0.000000
8	1	0	-0.598156	-1.444154	1.275795
9	1	0	1.199669	-1.346326	1.355315
10	1	0	0.199131	-0.205396	2.300170



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	0.660380	0.000000
2	6	0	-1.401265	-0.513306	0.000000
3	1	0	-2.318575	0.079759	-0.000035
4	1	0	-1.382301	-1.141504	-0.894489
5	1	0	-1.382342	-1.141458	0.894523
6	6	0	1.401265	-0.513306	0.000000
7	1	0	1.382334	-1.141466	-0.894516
8	1	0	2.318575	0.079759	0.000023
9	1	0	1.382308	-1.141496	0.894495

Computed Energies

Table S1. Electronic energies (E_{gas} in Hartree), thermal correction to Gibbs free energy ($\Delta G_{correction}$ in Hartree), Gibbs free energy in gas phase (G_{gas} in Hartree, $G_{gas} = E_{gas} + \Delta G_{correction}$), solvation free energy (G_{uESE} in kcal/mol), Gibbs free energy about molecule converts from the gas-phase standard state to the solution-phase standard state of 1 M ($RTln(RT/p)$ in kcal/mol, which is 1.89 kcal/mol), free energies in solution (ΔG_{solv} in Hartree, $\Delta G_{solv} = G_{gas} + G_{uESE} + RTln(RT/p)$), relative energies ($\Delta G$) at 298 K are reported in kcal/mol.

Structure	E_{gas}	$\Delta G_{correction}$	G_{gas}	G_{uESE}	RTln(RT/p)	ΔG_{solv}	ΔG
DMSO	-553.1889943	0.050841	-553.1381533	-7.155	1.89	-553.1465436	0.0
DMS	-477.9910865	0.048669	-477.9424175	-1.076	1.89	-477.9411204	0.0
1s	-990.9633956	0.148345	-990.8150506	-15.05	1.89	-990.8360224	0.0
2s	-1141.488823	0.157523	-1141.3313	-17.948	1.89	-1141.356891	-69.0
INT1s	-1544.101011	0.2229	-1543.878111	-31.325	1.89	-1543.925019	36.1
INT2s	-1066.176314	0.151818	-1066.024496	-18.075	1.89	-1066.050288	-5.5
INT3s	-1619.390395	0.226765	-1619.16363	-32.269	1.89	-1619.212042	-15.1
TS1s	-1544.104411	0.219693	-1543.884718	-26.136	1.89	-1543.923356	37.2
TS2s	-1544.086074	0.221604	-1543.86447	-30.75	1.89	-1543.910462	45.2
TS3s	-1619.375775	0.224113	-1619.151662	-25.373	1.89	-1619.189085	-0.7
TS4s	-1619.385144	0.226873	-1619.158271	-31.04	1.89	-1619.204724	-10.5

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

N,4-Dimethyl-*N*-(phenylethynyl)benzenesulfonamide (**1a**)

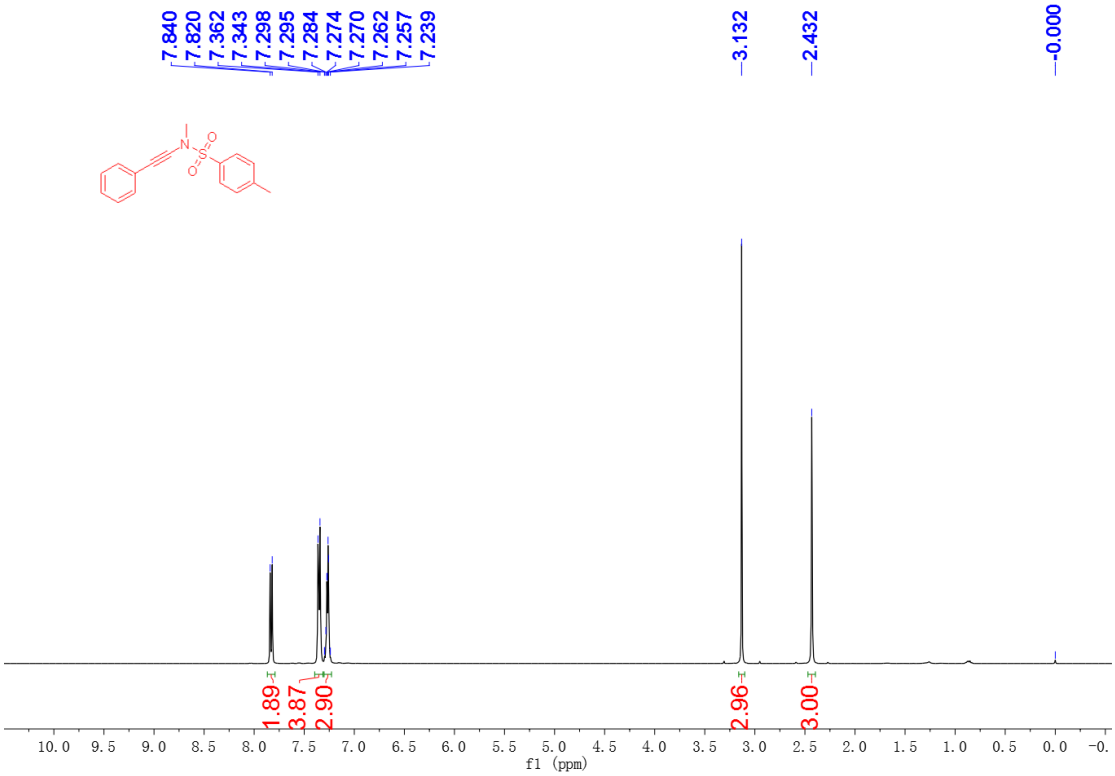


Figure S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*,4-dimethyl-*N*-(phenylethynyl)benzenesulfonamide (**1a**)

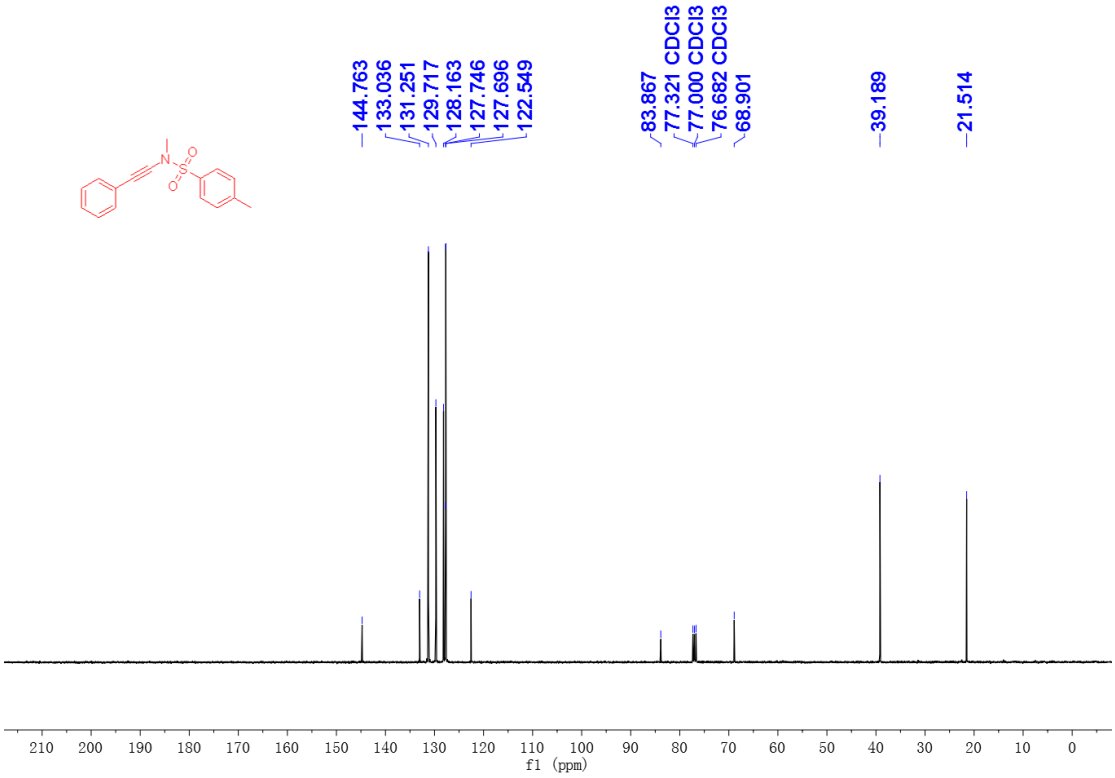


Figure S2. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*,4-dimethyl-*N*-(phenylethynyl)benzenesulfonamide (**1a**)

N-Methyl-*N*-(phenylethynyl)benzenesulfonamide (**1b**)

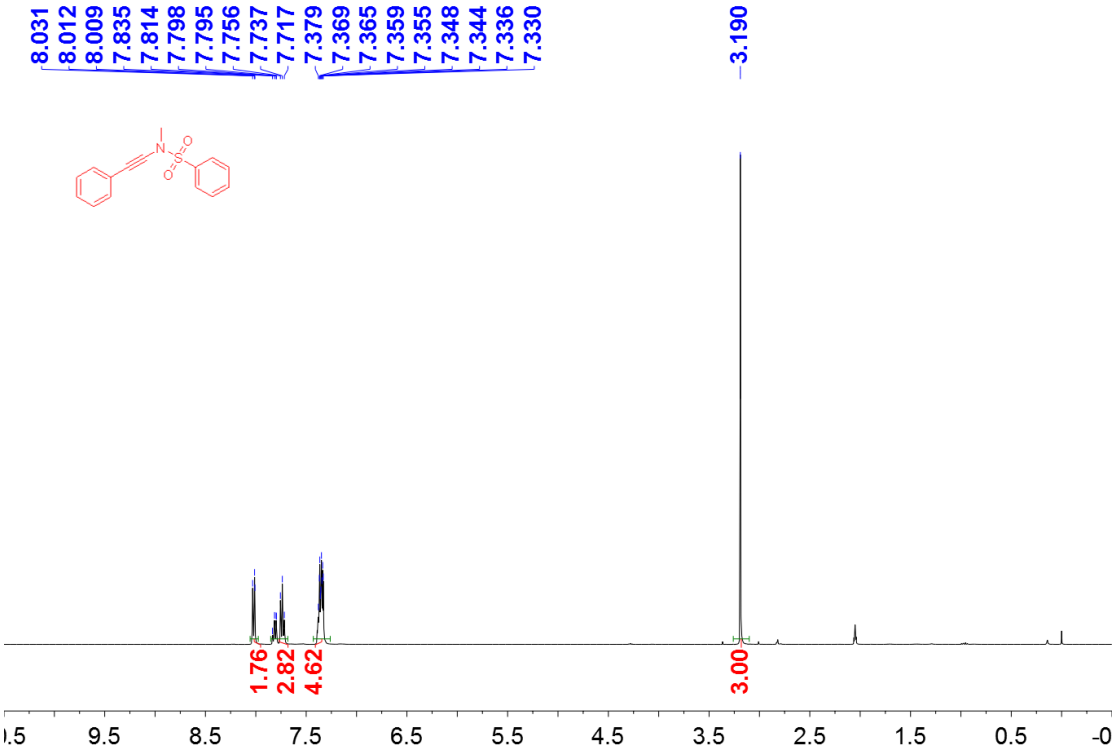


Figure S3. ^{1}H NMR spectrum (400 MHz, CD_3COCD_3) of *N*-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1b**)

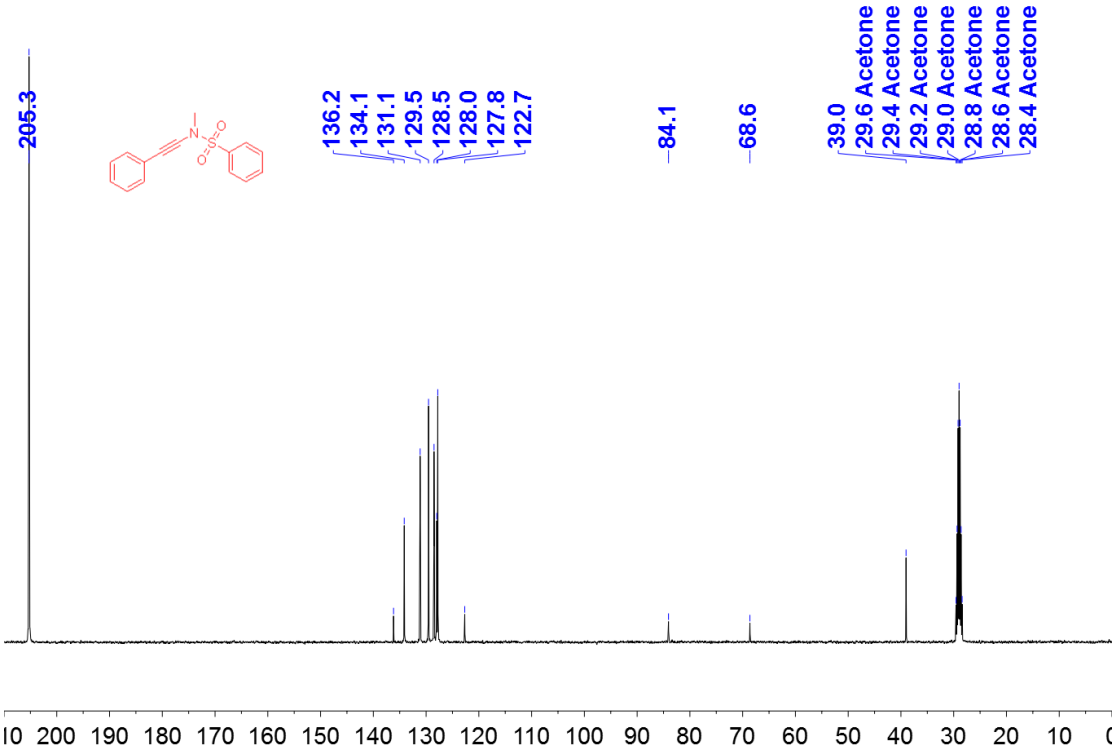


Figure S4. ^{13}C NMR spectrum (101 MHz, CD_3COCD_3) of *N*-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1b**)

4-Bromo-*N*-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1c**)

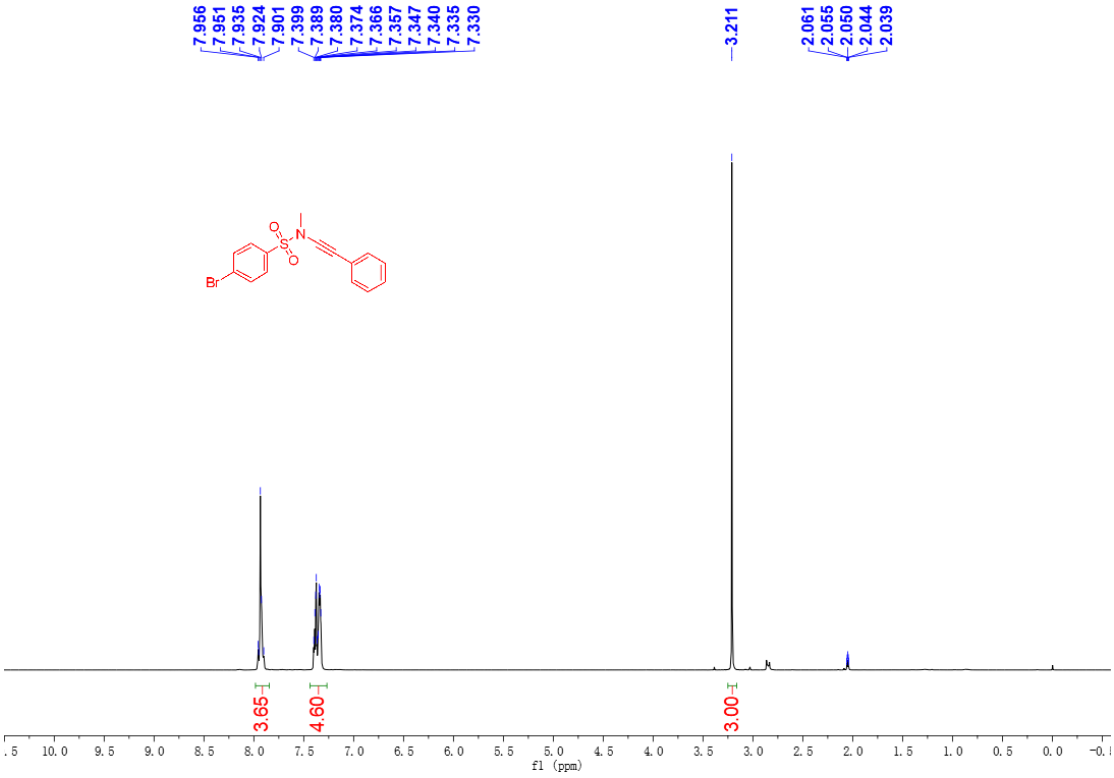


Figure S5. ^{1}H NMR spectrum (400 MHz, CD_3COCD_3) of 4-bromo-*N*-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1c**)

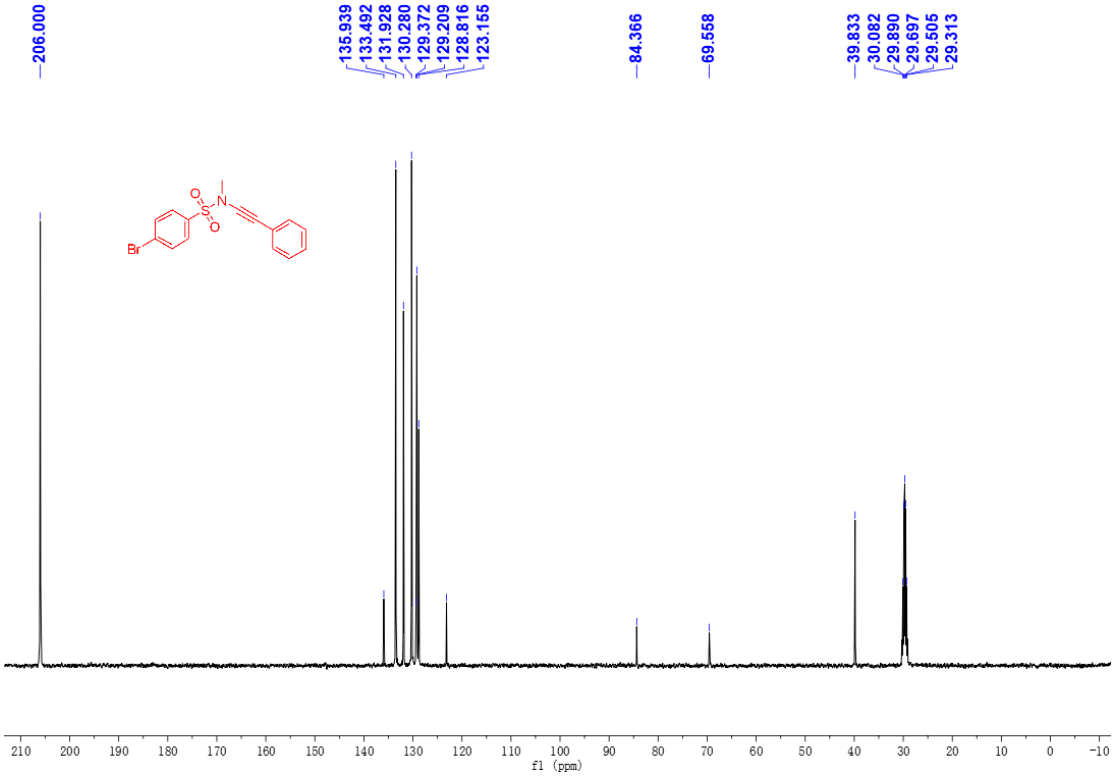


Figure S6. ^{13}C NMR spectrum (101 MHz, CD_3COCD_3) of 4-bromo-*N*-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1c**)

N-Methyl-4-nitro-*N*-(phenylethynyl)benzenesulfonamide (**1d**)

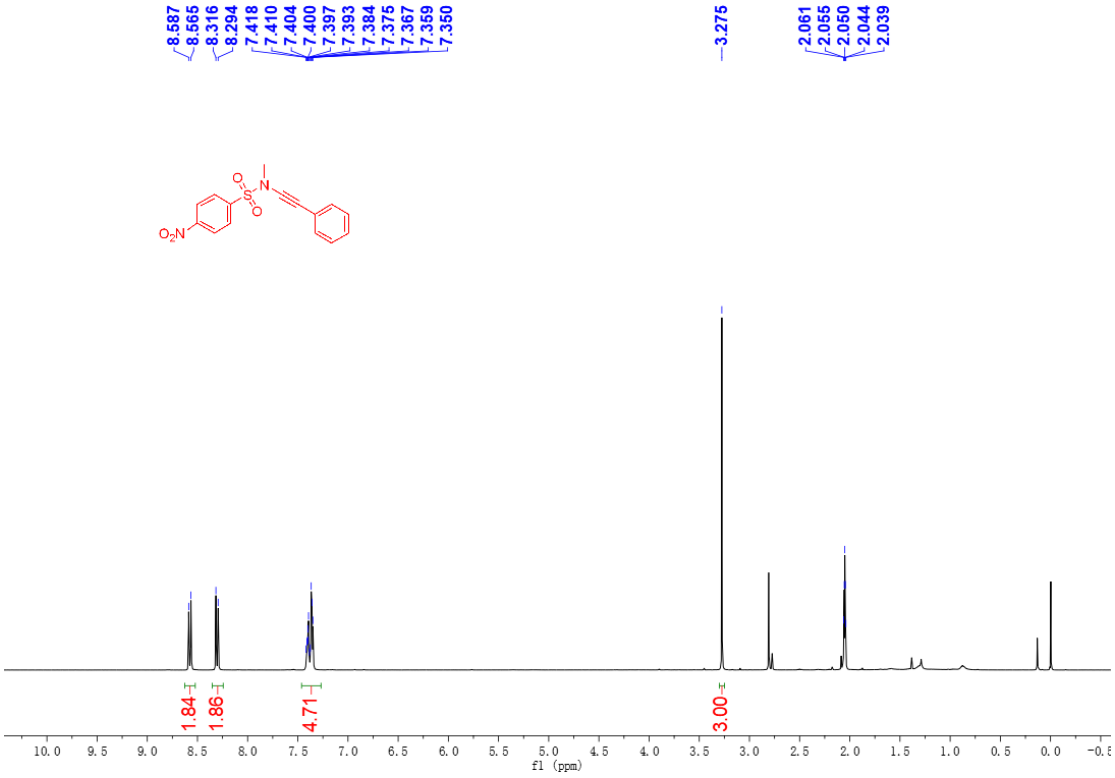


Figure S7. ^{1}H NMR spectrum (400 MHz, CD_3COCD_3) of *N*-methyl-4-nitro-*N*-(phenylethynyl)benzenesulfonamide (**1d**)

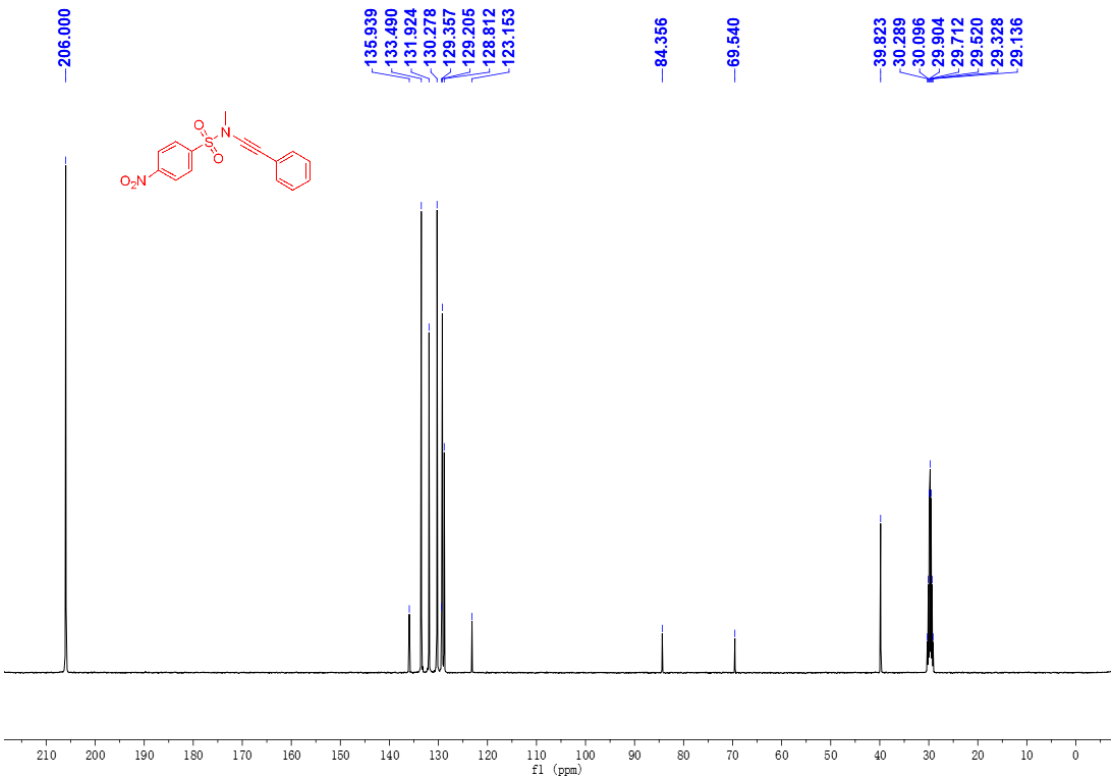


Figure S8. ^{13}C NMR spectrum (101 MHz, CD_3COCD_3) of *N*-methyl-4-nitro-*N*-(phenylethynyl)benzenesulfonamide (**1d**)

N,4-Dimethyl-*N*-(4-methylphenylethynyl)benzenesulfonamide (**1e**)

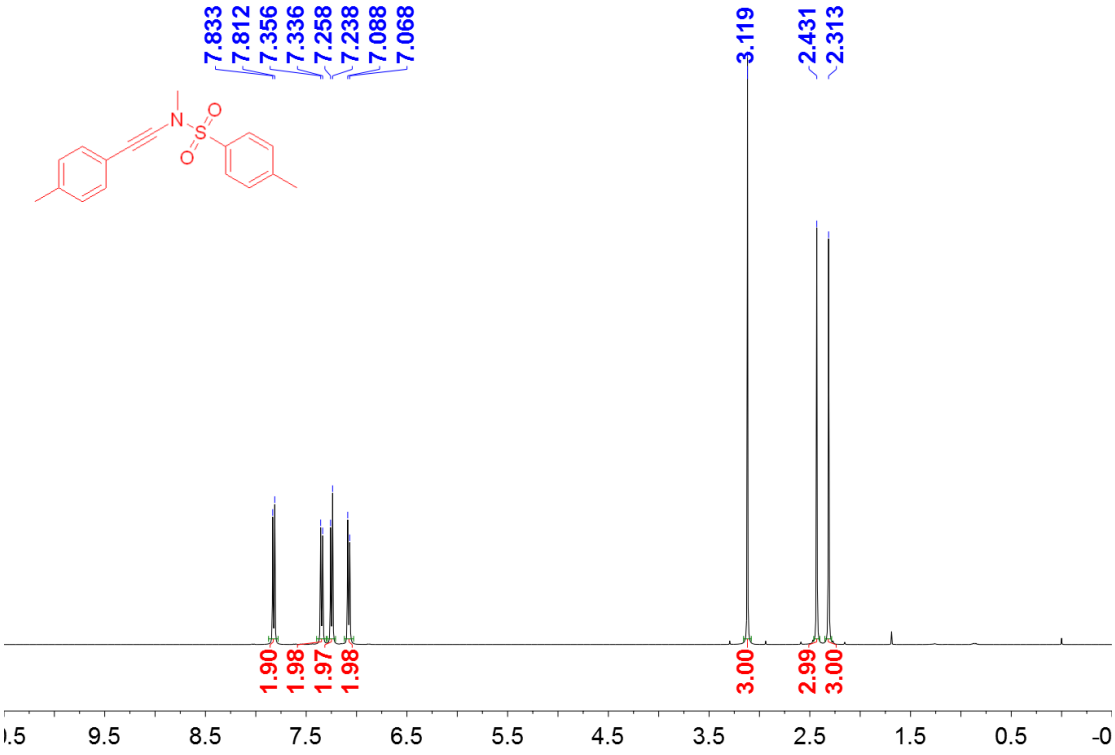


Figure S9. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*,4-dimethyl-*N*-(4-methylphenylethynyl)benzenesulfonamide (**1e**)

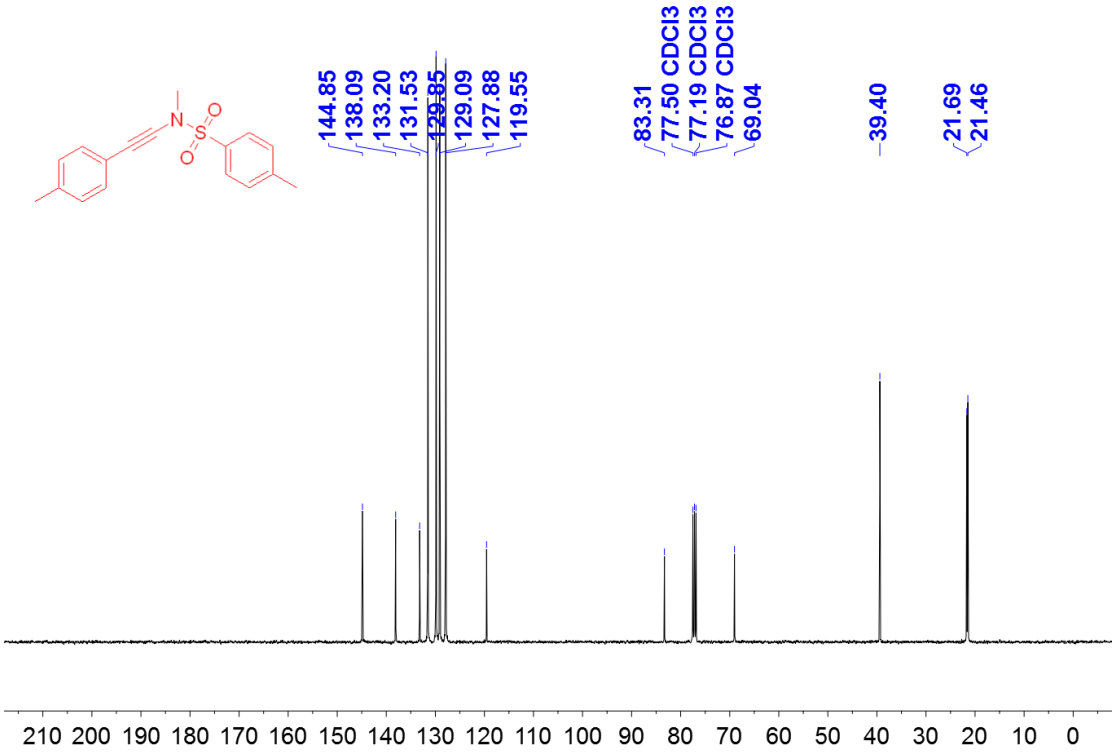


Figure S10. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*,4-dimethyl-*N*-(4-methylphenylethynyl)benzenesulfonamide (**1e**)

N-((4-Fluorophenyl)ethynyl)-*N*,4-dimethylbenzenesulfonamide (**1f**)

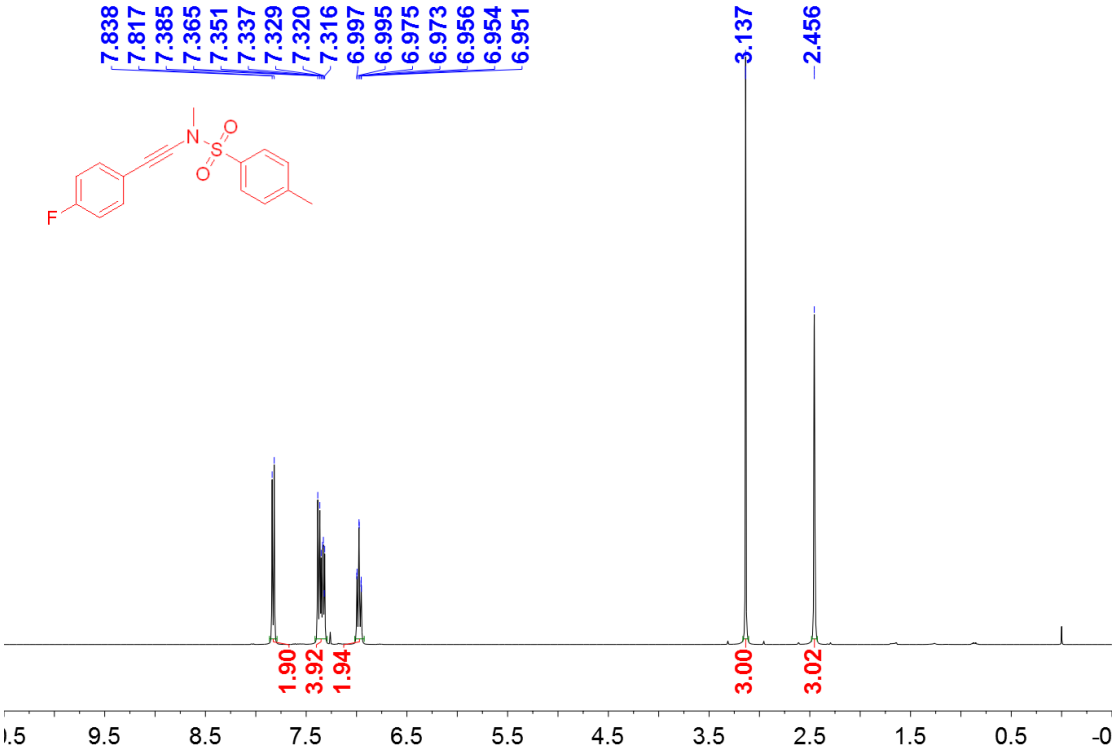


Figure S11. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-((4-fluorophenyl)ethynyl)-*N*,4-dimethylbenzenesulfonamide (**1f**)

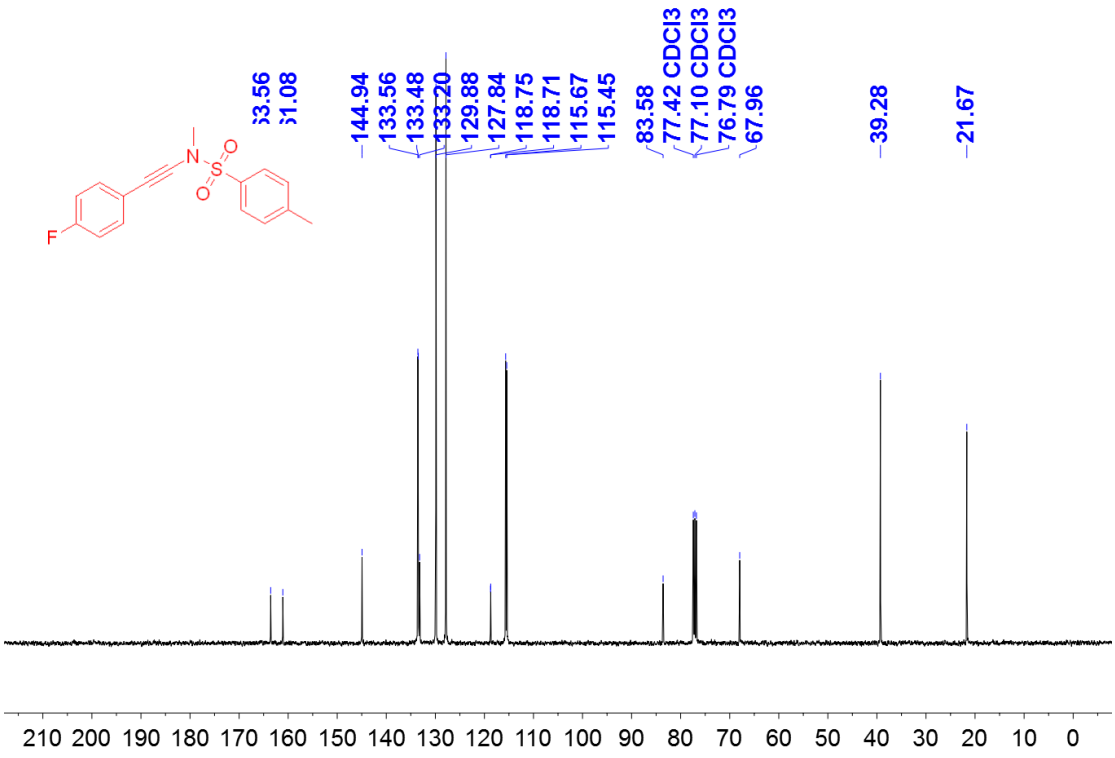


Figure S12. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-((4-fluorophenyl)ethynyl)-*N*,4-dimethylbenzenesulfonamide (**1f**)

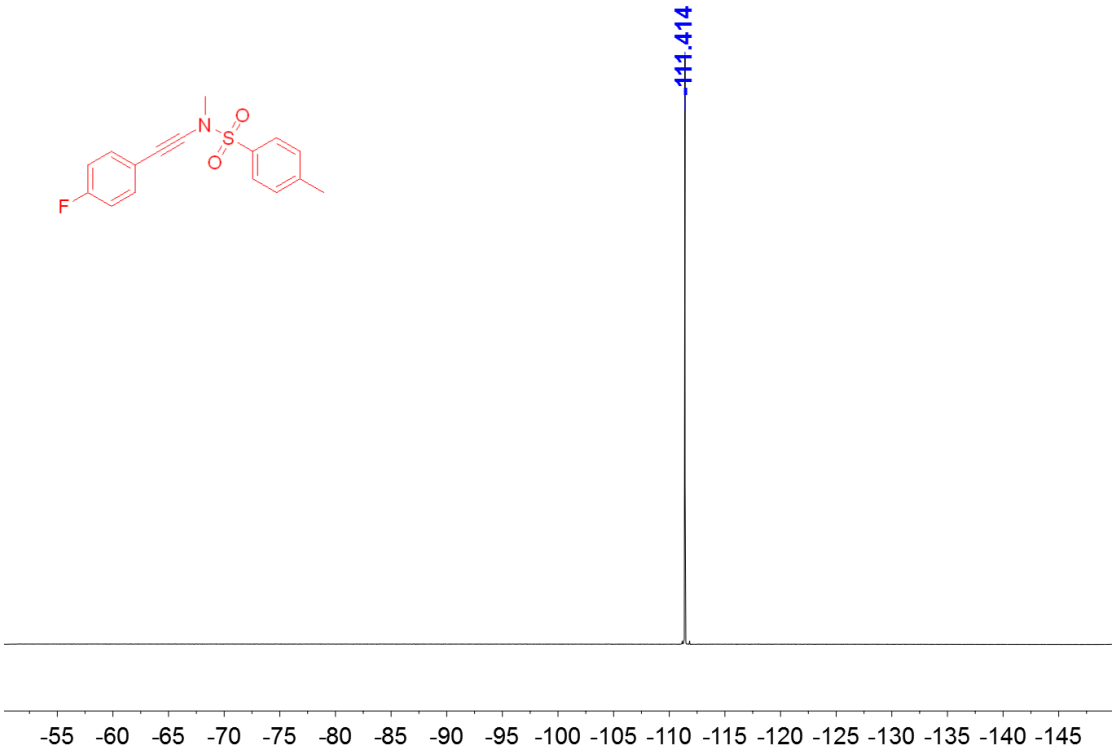


Figure S13. ^{19}F NMR spectrum (377 MHz, $CDCl_3$) of *N*-((4-fluorophenyl)ethynyl)-*N*,4-dimethylbenzenesulfonamide (**1f)**

N-((4-Chlorophenyl)ethynyl)-*N*,4-dimethylbenzenesulfonamide (**1g**)

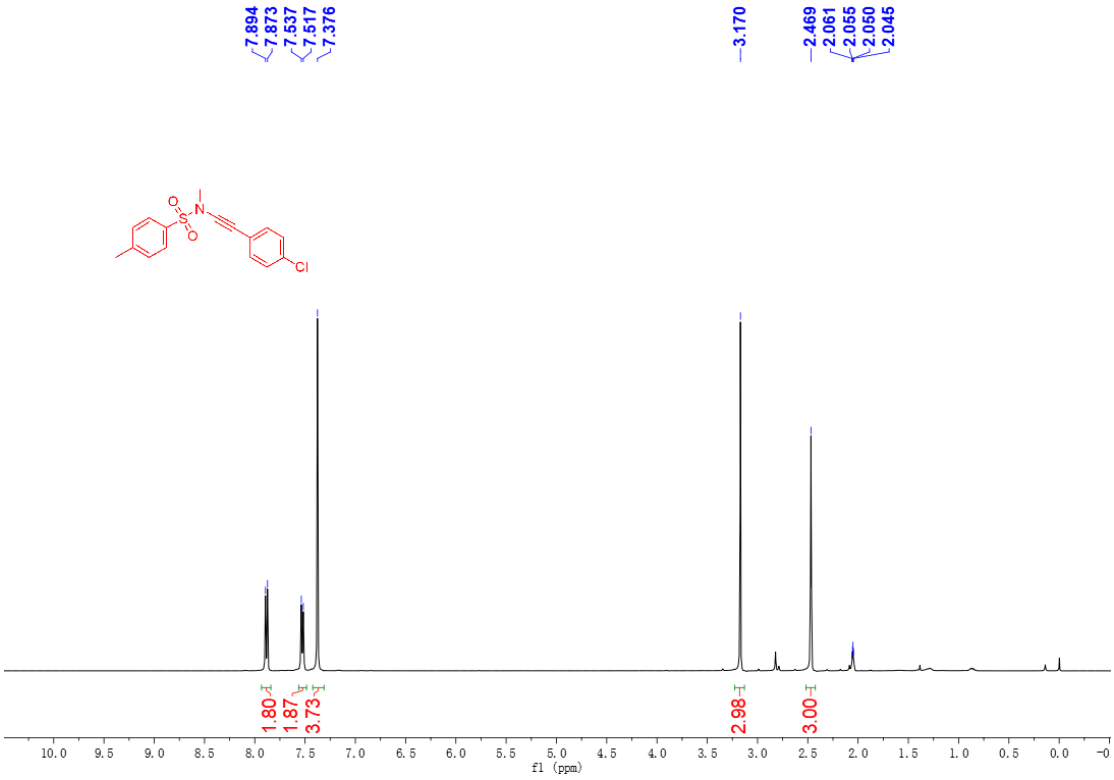


Figure S14. ^{1}H NMR spectrum (400 MHz, CD_3COCD_3) of *N*-((4-chlorophenyl)ethynyl)-*N*,4-dimethylbenzenesulfonamide (**1g**)

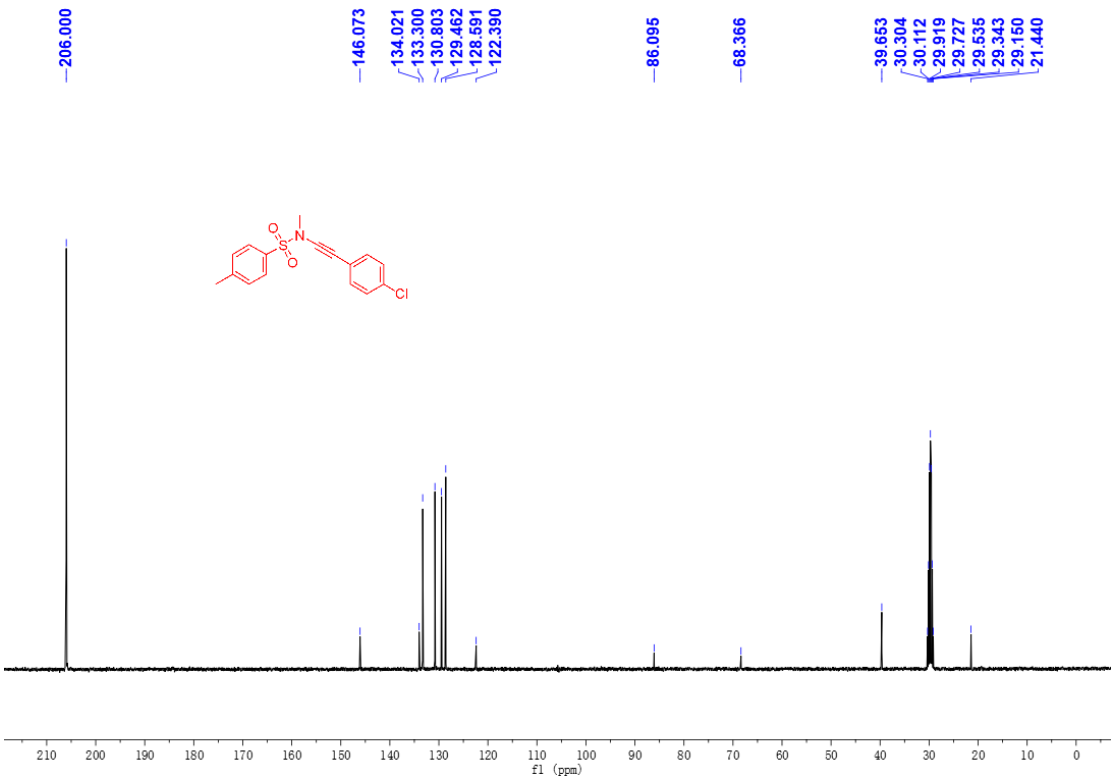


Figure S15. ^{13}C NMR spectrum (101 MHz, CD_3COCD_3) of *N*-((4-chlorophenyl)ethynyl)-*N*,4-dimethylbenzenesulfonamide (**1g**)

N-((4-Bromophenyl)ethynyl)-*N*,4-dimethylbenzenesulfonamide (**1h**)

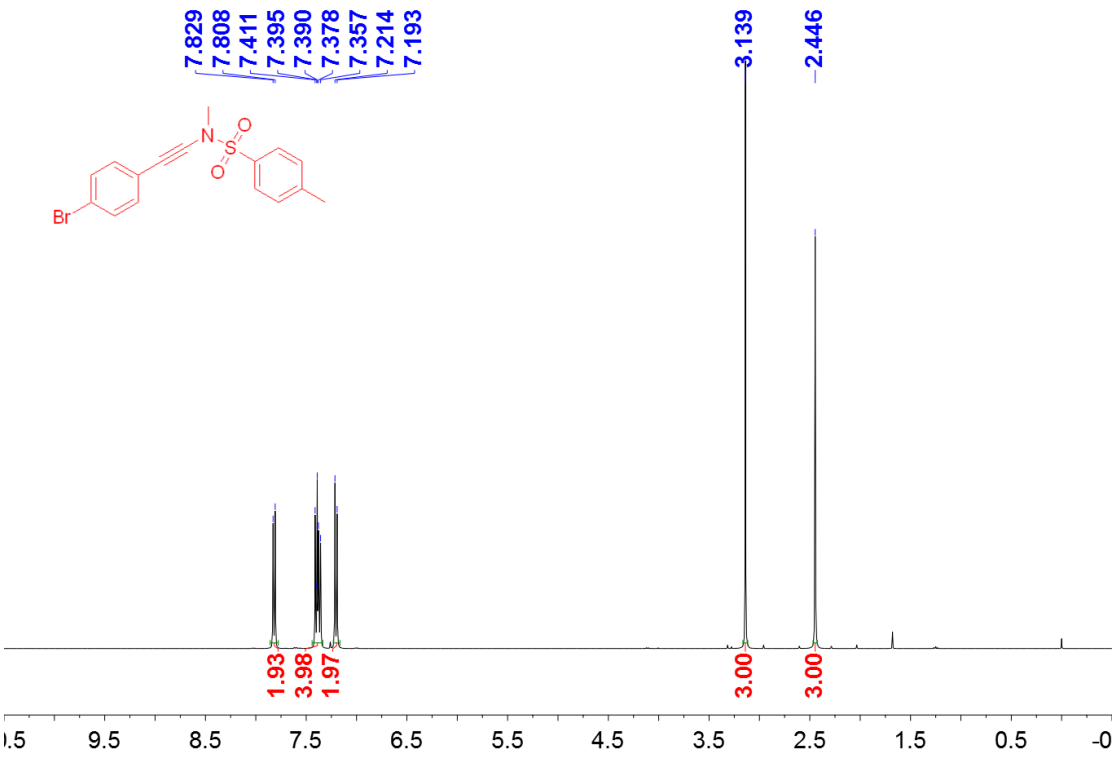


Figure S16. ^{1}H NMR spectrum (400 MHz, CD_3COCD_3) of *N*-((4-bromophenyl)ethynyl)-*N*,4-dimethylbenzenesulfonamide (**1h**)

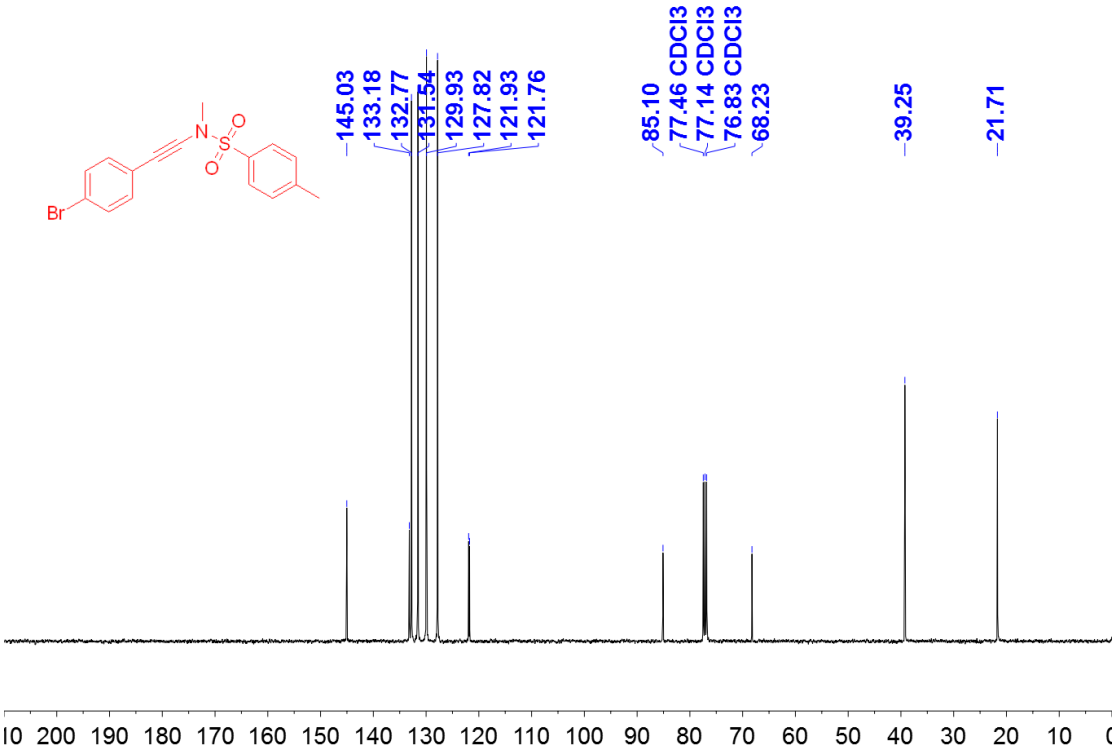


Figure S17. ^{13}C NMR spectrum (101 MHz, CD_3COCD_3) of *N*-((4-bromophenyl)ethynyl)-*N*,4-dimethylbenzenesulfonamide (**1h**)

N,4-Dimethyl-*N*-(thiophen-3-ylethynyl)benzenesulfonamide (**1i**)

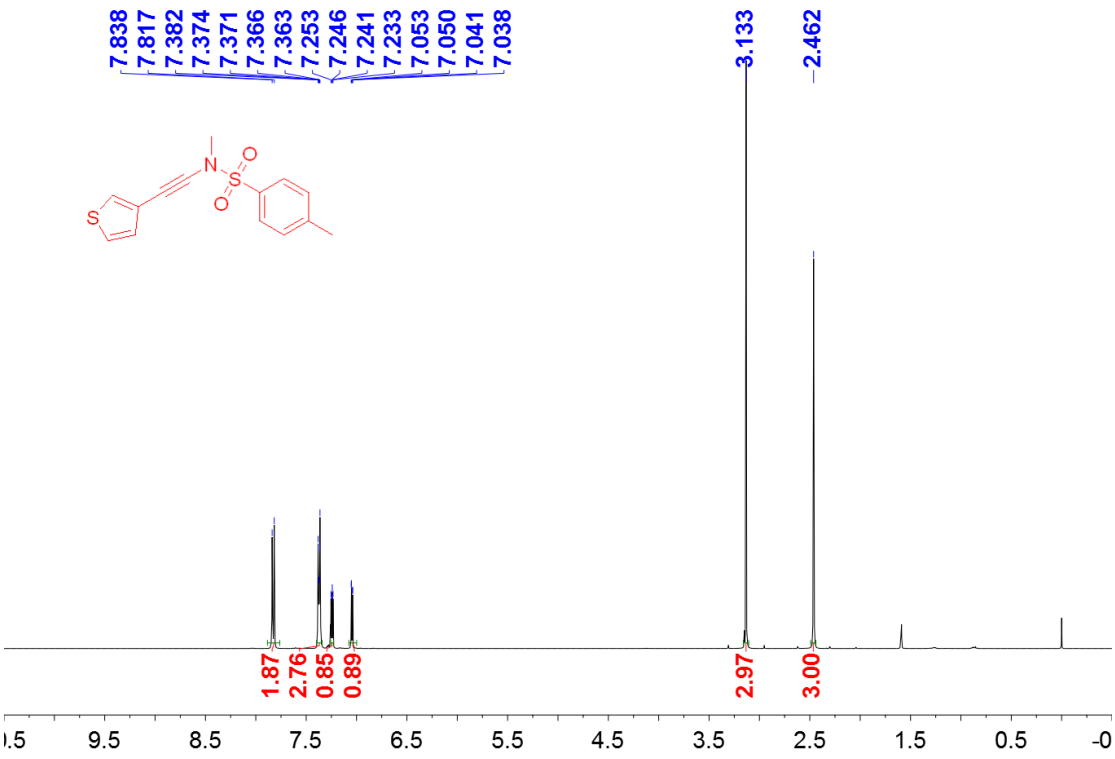


Figure S18. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*,4-dimethyl-*N*-(thiophen-3-ylethynyl)benzenesulfonamide (**1i**)

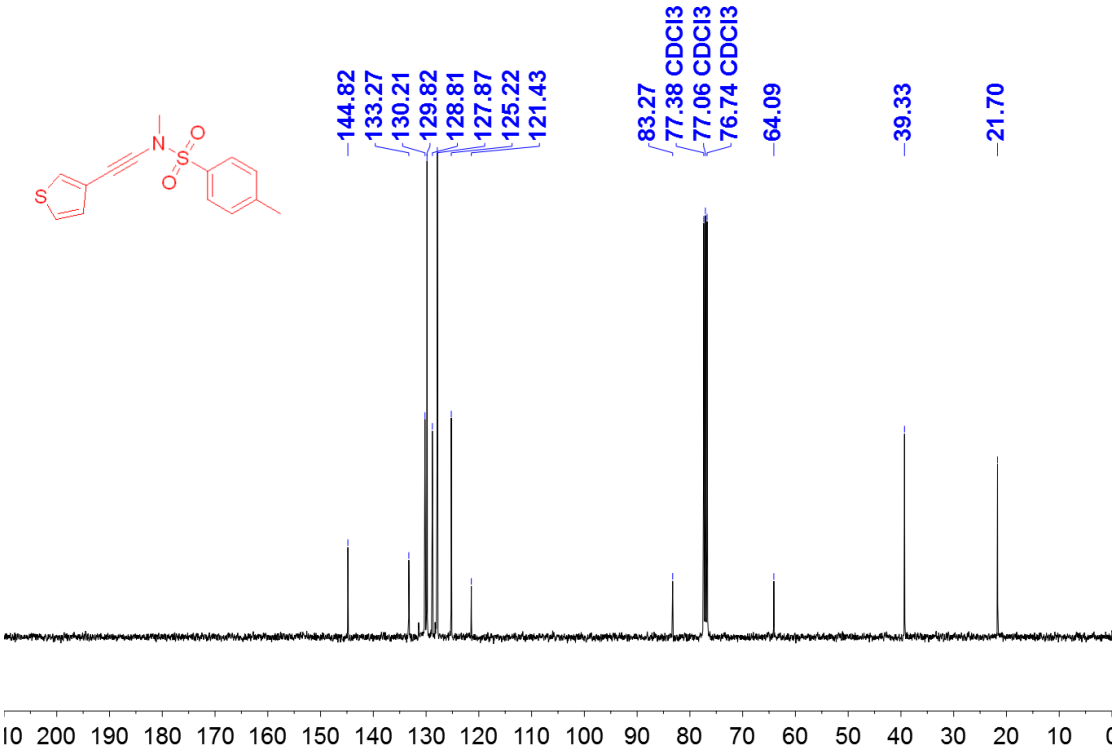


Figure S19. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*,4-dimethyl-*N*-(thiophen-3-ylethynyl)benzenesulfonamide (**1i**)

N-Ethyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1j**)

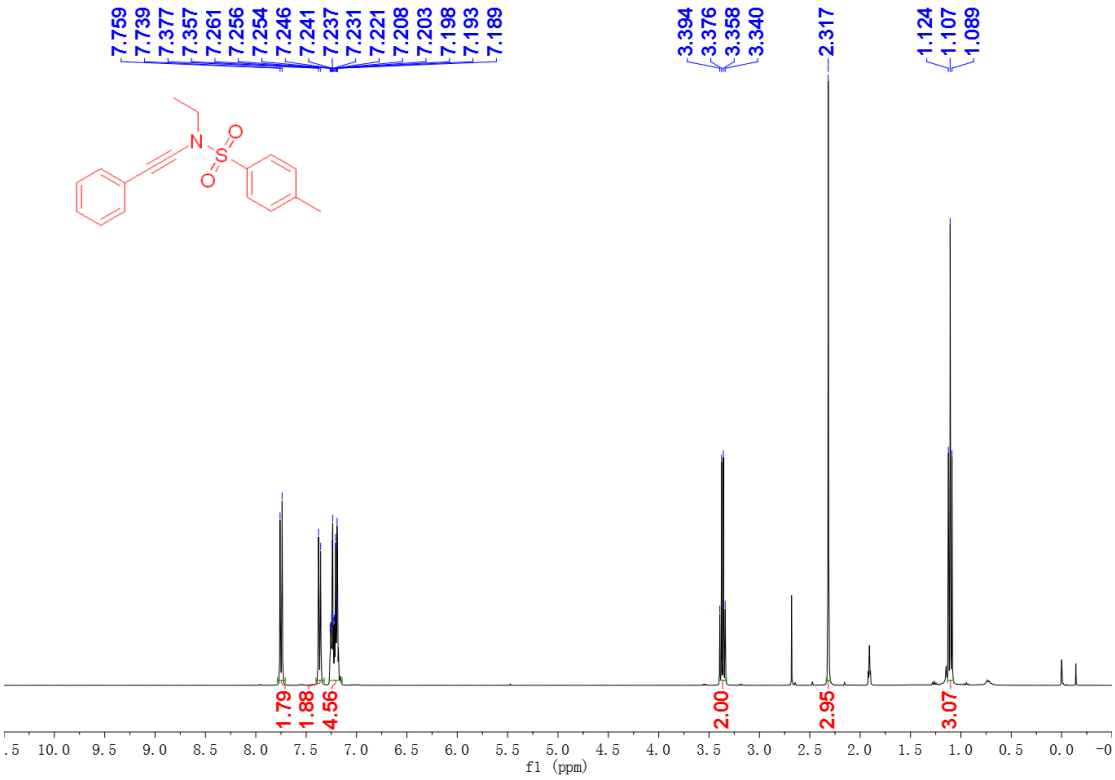


Figure S20. ^{1}H NMR spectrum (400 MHz, CD_3COCD_3) of *N*-ethyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1j**)

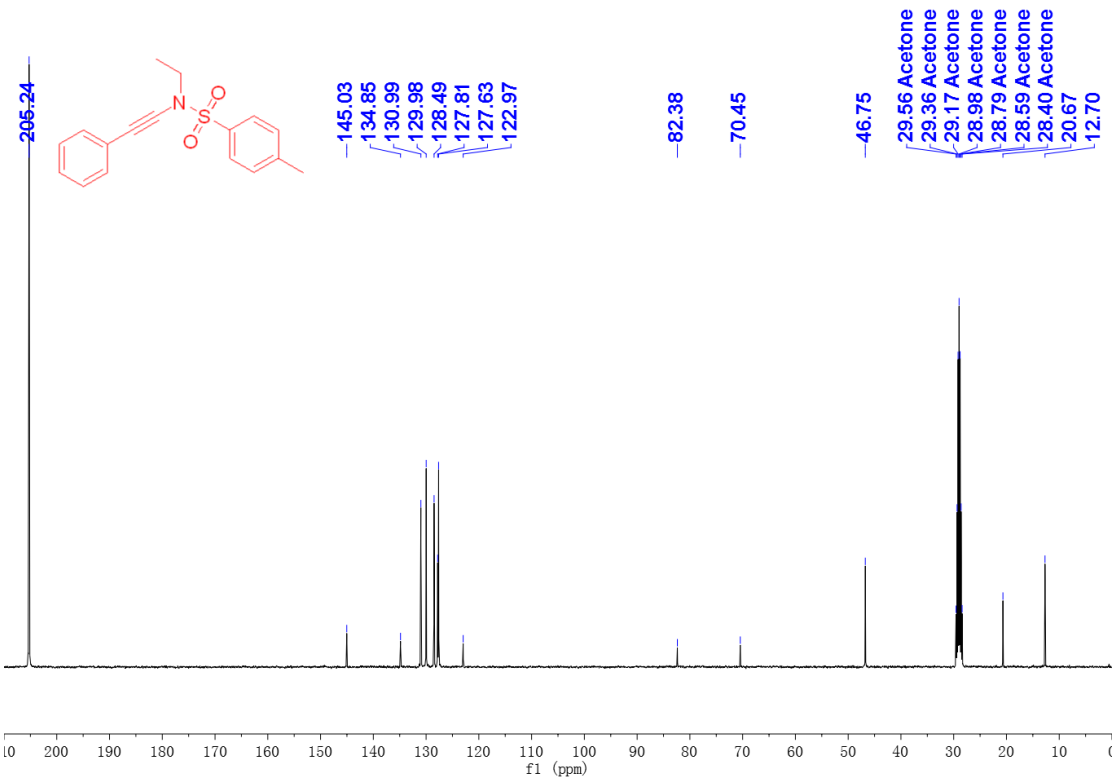


Figure S21. ^{13}C NMR spectrum (101 MHz, CD_3COCD_3) of *N*-ethyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1j**)

N-Butyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1k**)

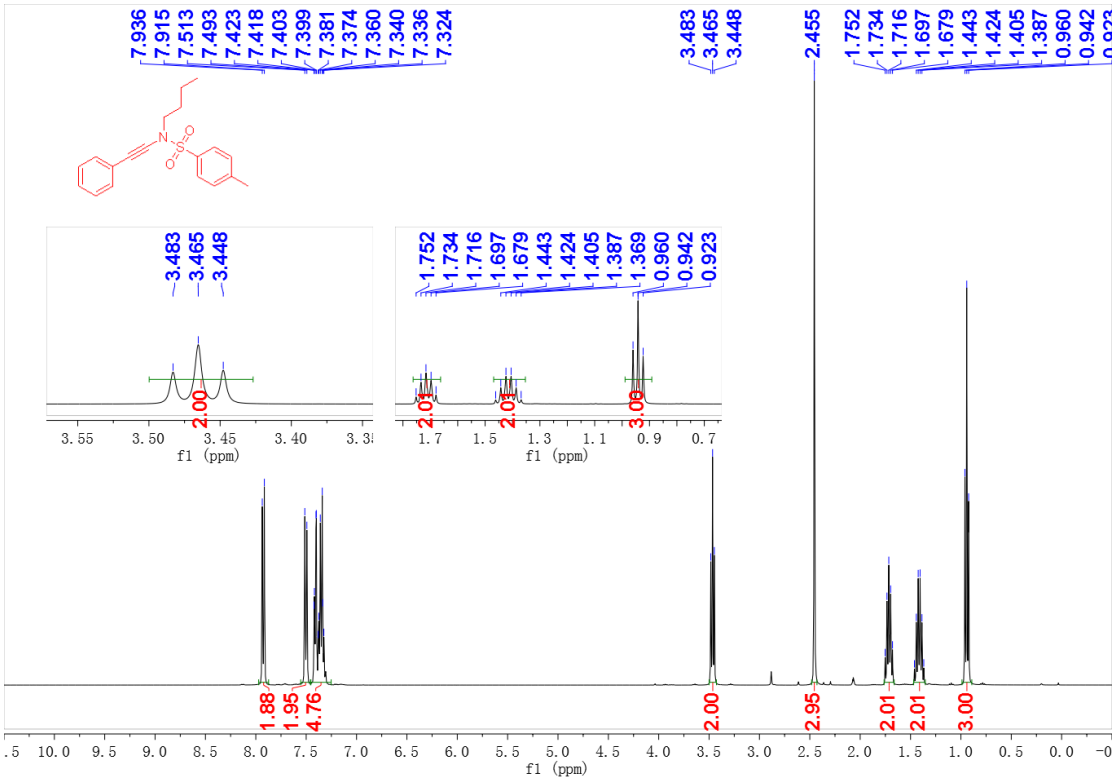


Figure S22. ^{1}H NMR spectrum (400 MHz, CD_3COCD_3) of *N*-butyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1k**)

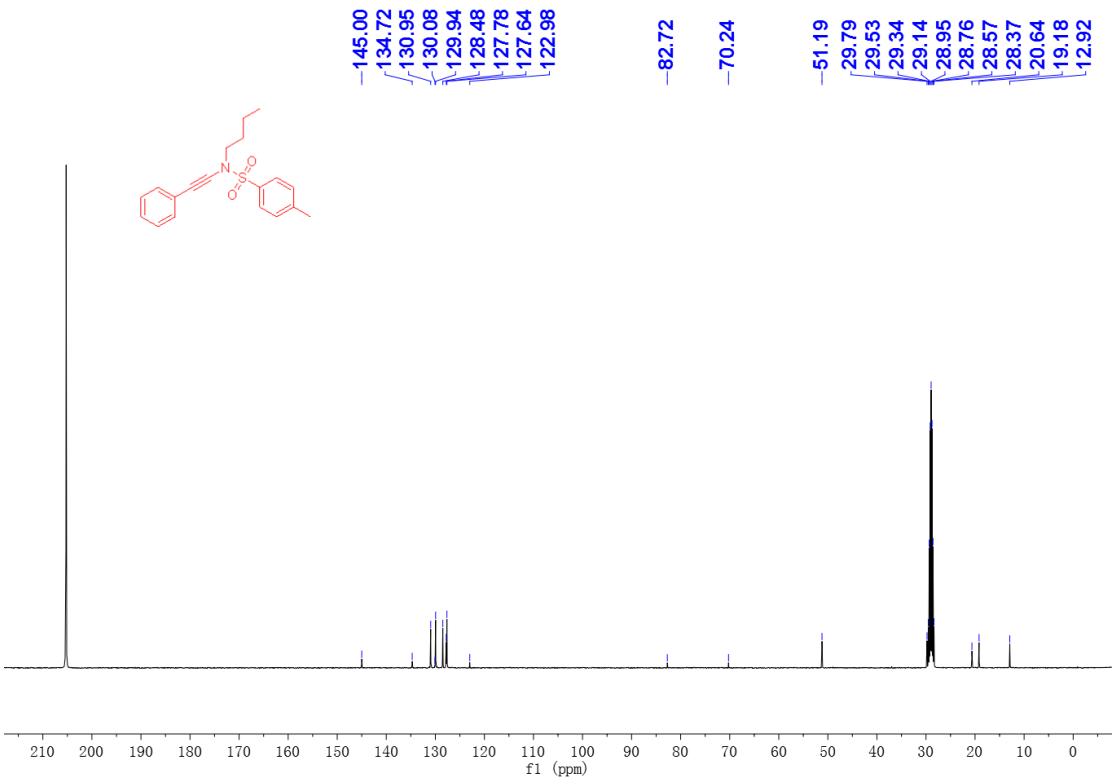


Figure S23. ^{13}C NMR spectrum (101 MHz, CD_3COCD_3) of *N*-butyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1k**)

N-Cyclohexyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1l**)

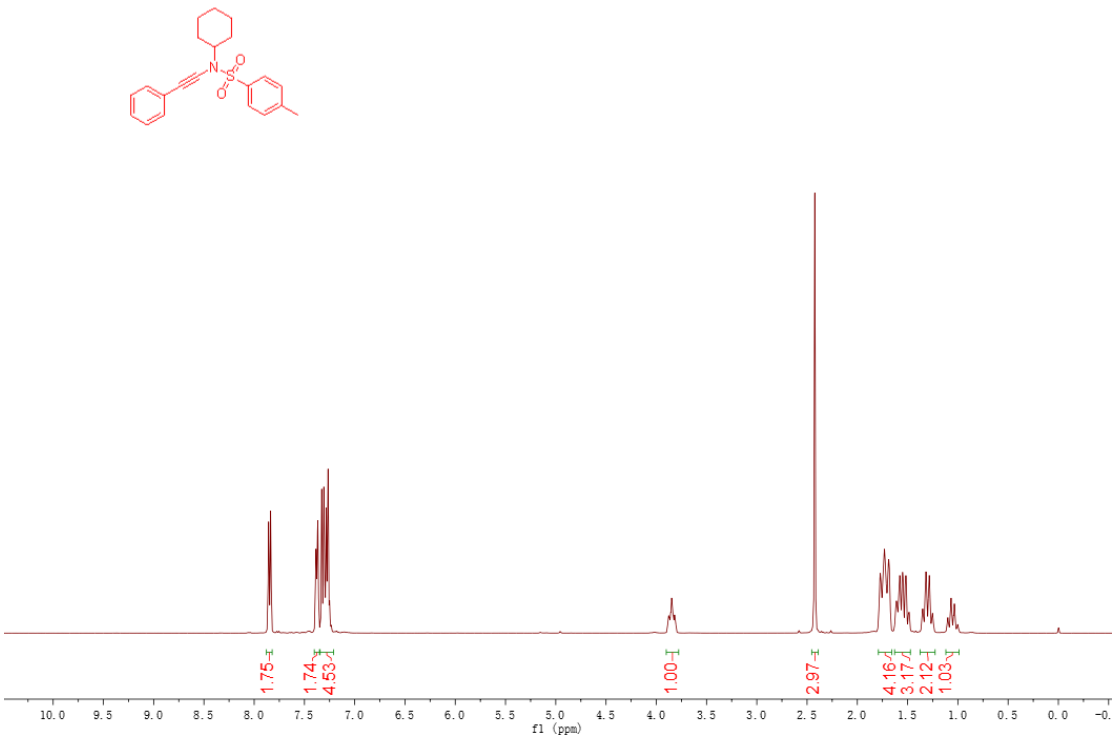


Figure S24 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-cyclohexyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1l**)

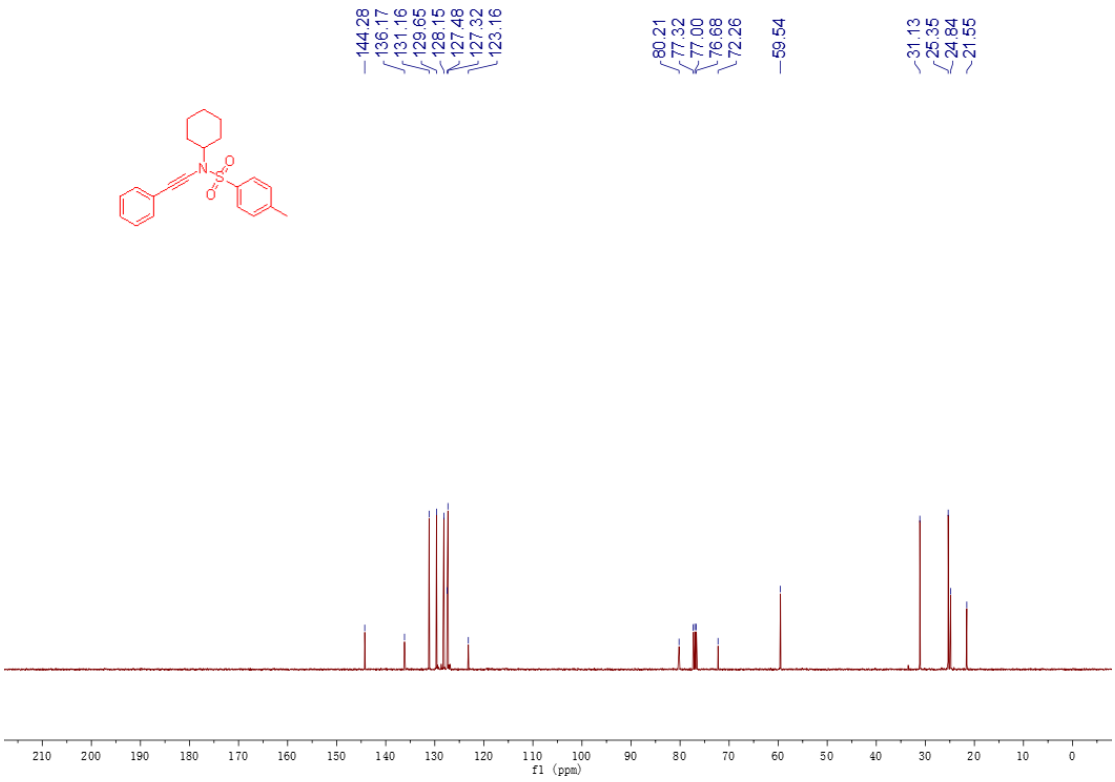


Figure S25. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-cyclohexyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1l**)

N-Cyclopropyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1m**)

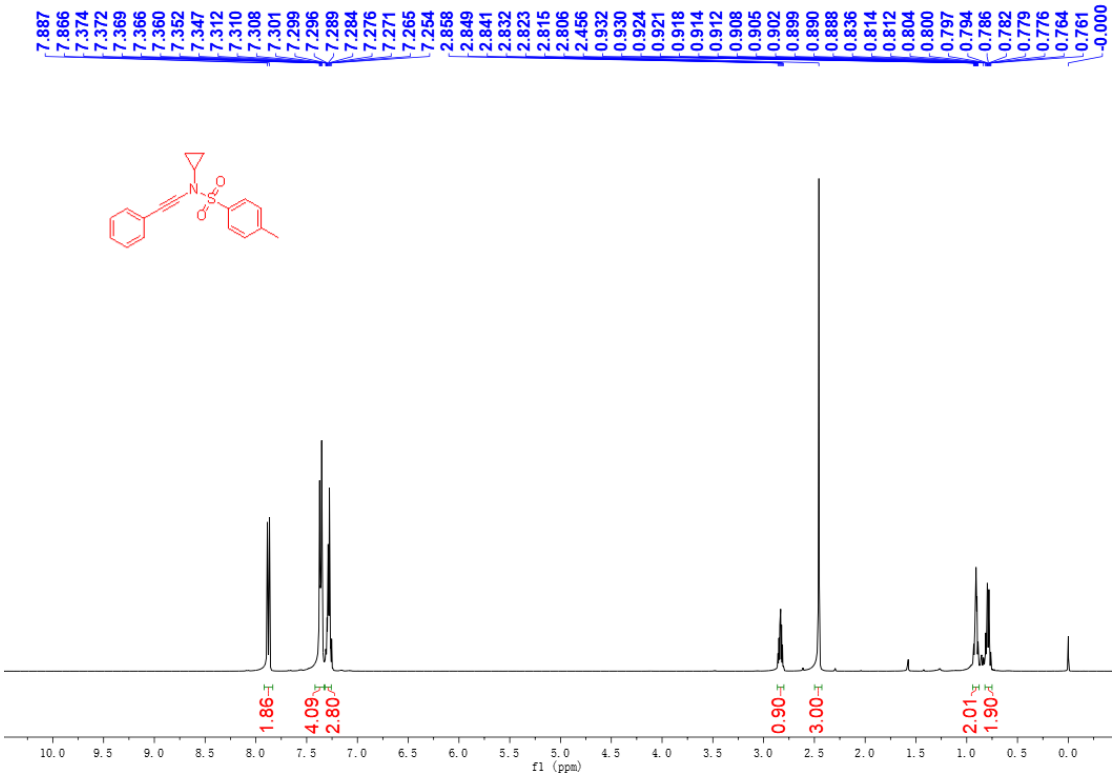


Figure S26. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-cyclopropyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1m**)

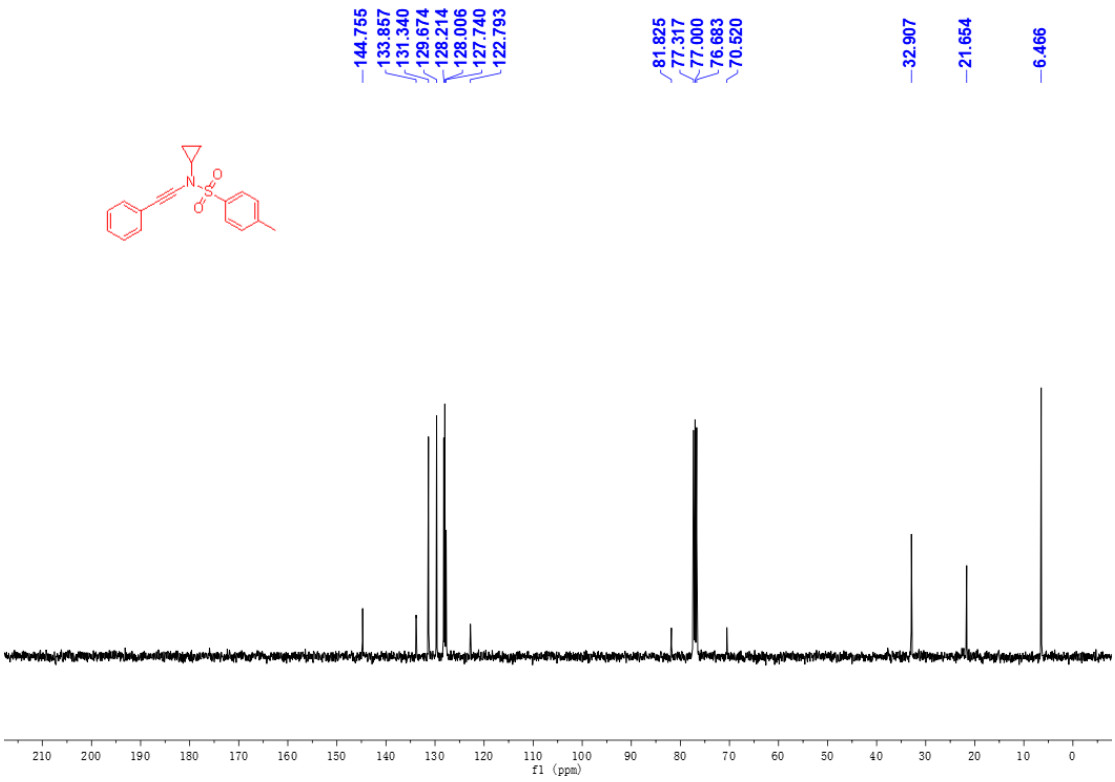


Figure S27. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-cyclopropyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1m**)

N-Benzyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1n**)

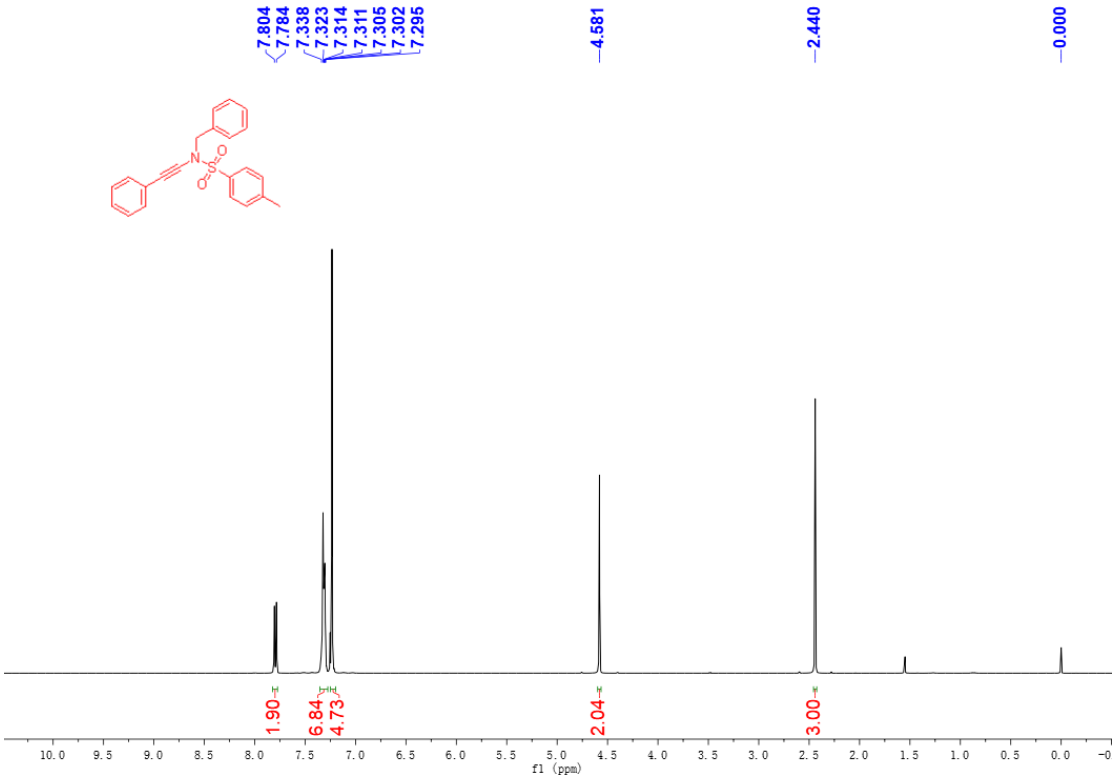


Figure S28. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-benzyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1n**)

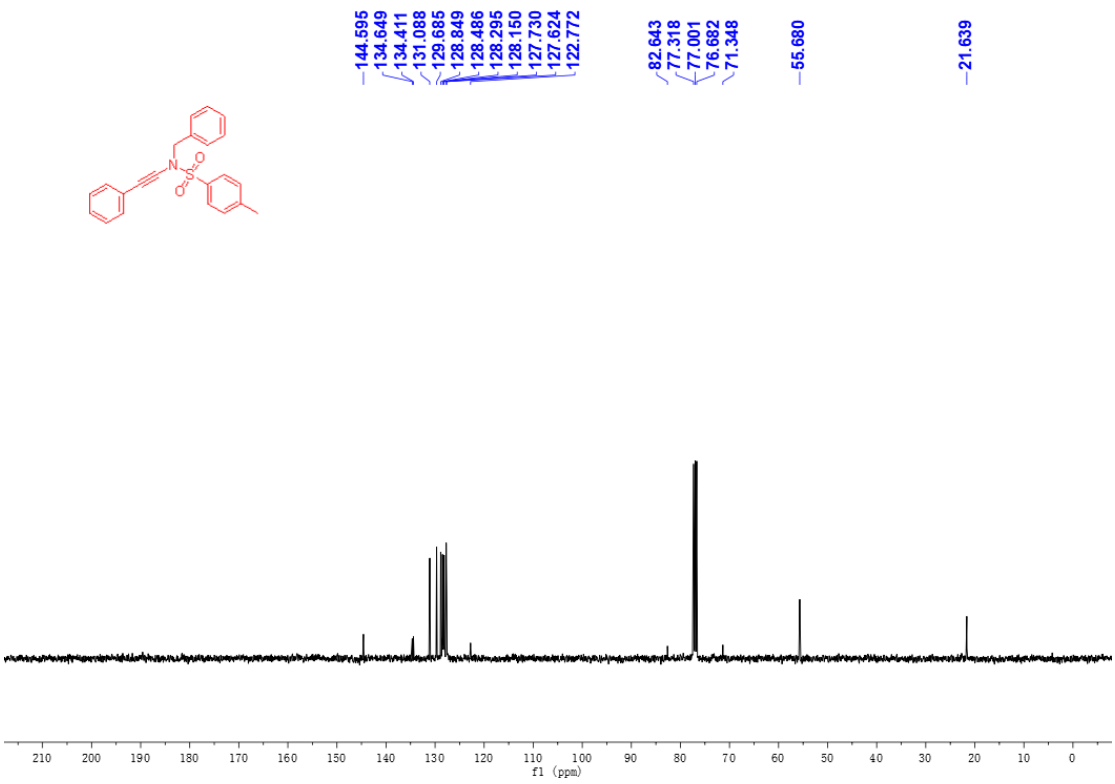


Figure S29. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-benzyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1n**)

4-Methyl-*N*-phenyl-*N*-(phenylethynyl)benzenesulfonamide (**1o**)

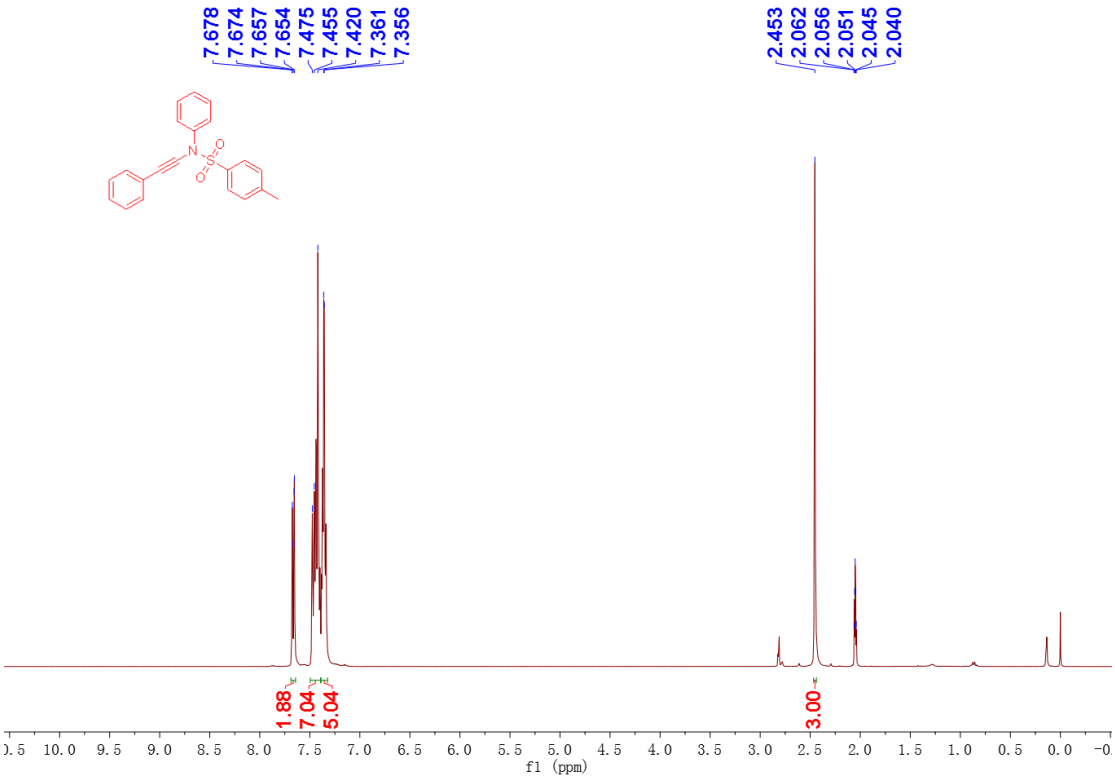


Figure S30. ^{1}H NMR spectrum (400 MHz, CD_3COCD_3) of 4-methyl-*N*-phenyl-*N*-(phenylethynyl)benzenesulfonamide (**1o**)

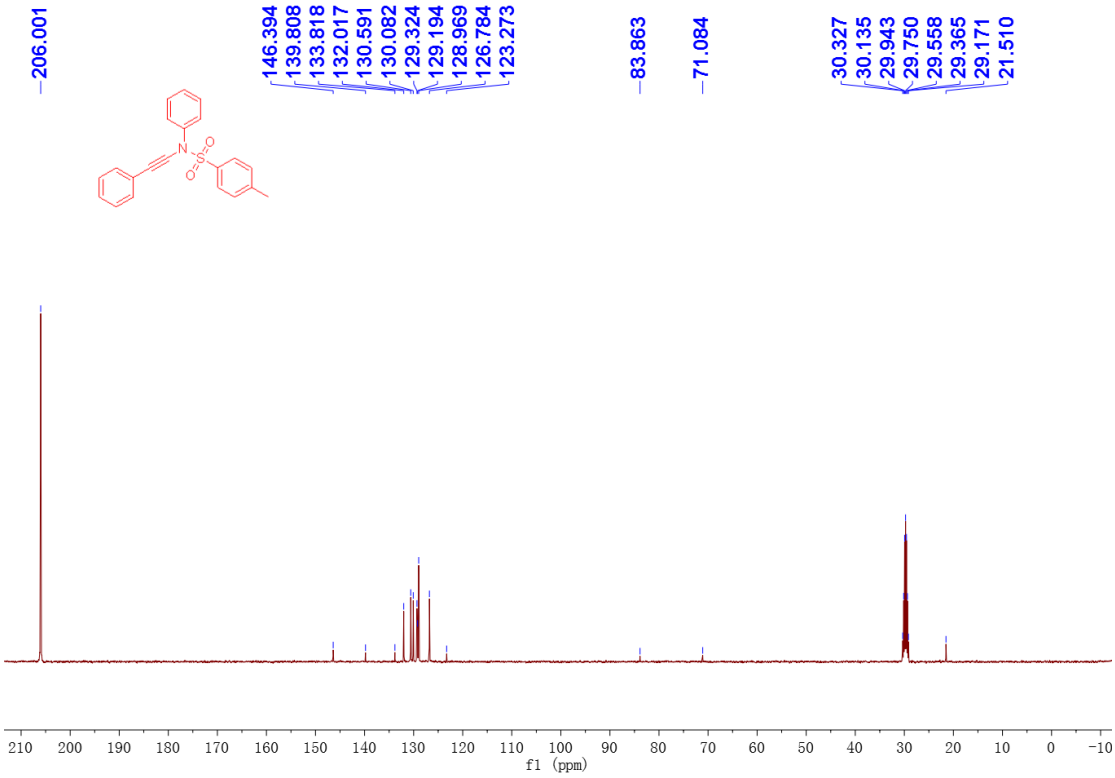


Figure S31. ^{13}C NMR spectrum (101 MHz, CD_3COCD_3) of 4-methyl-*N*-phenyl-*N*-(phenylethynyl)benzenesulfonamide (**1o**)

N-(4-Methoxyphenyl)-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1p**)

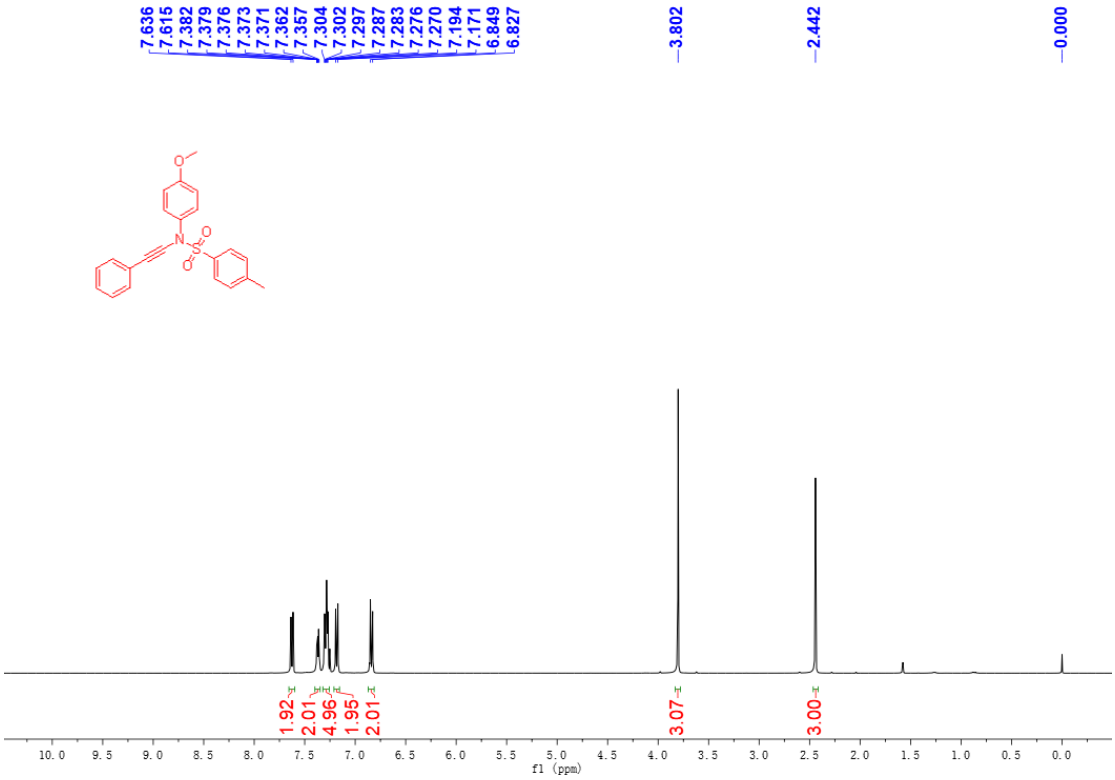


Figure S32. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-(4-methoxyphenyl)-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1p**)

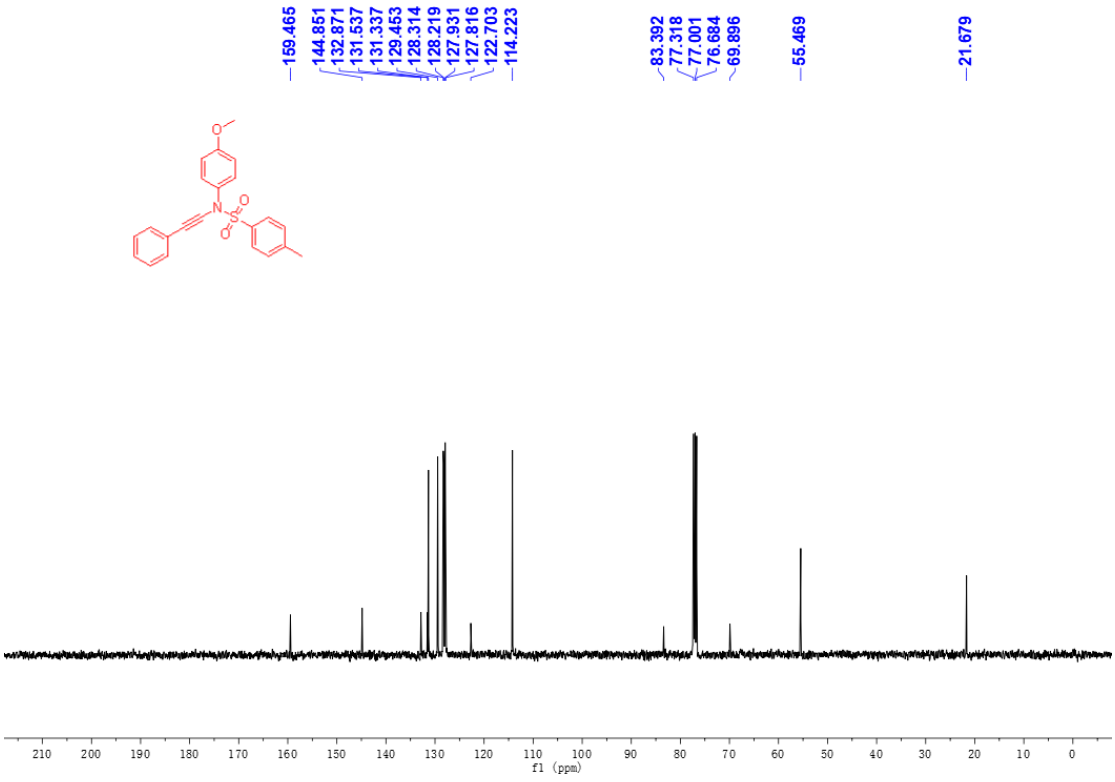


Figure S33. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-(4-methoxyphenyl)-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1p**)

N-Allyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1q**)

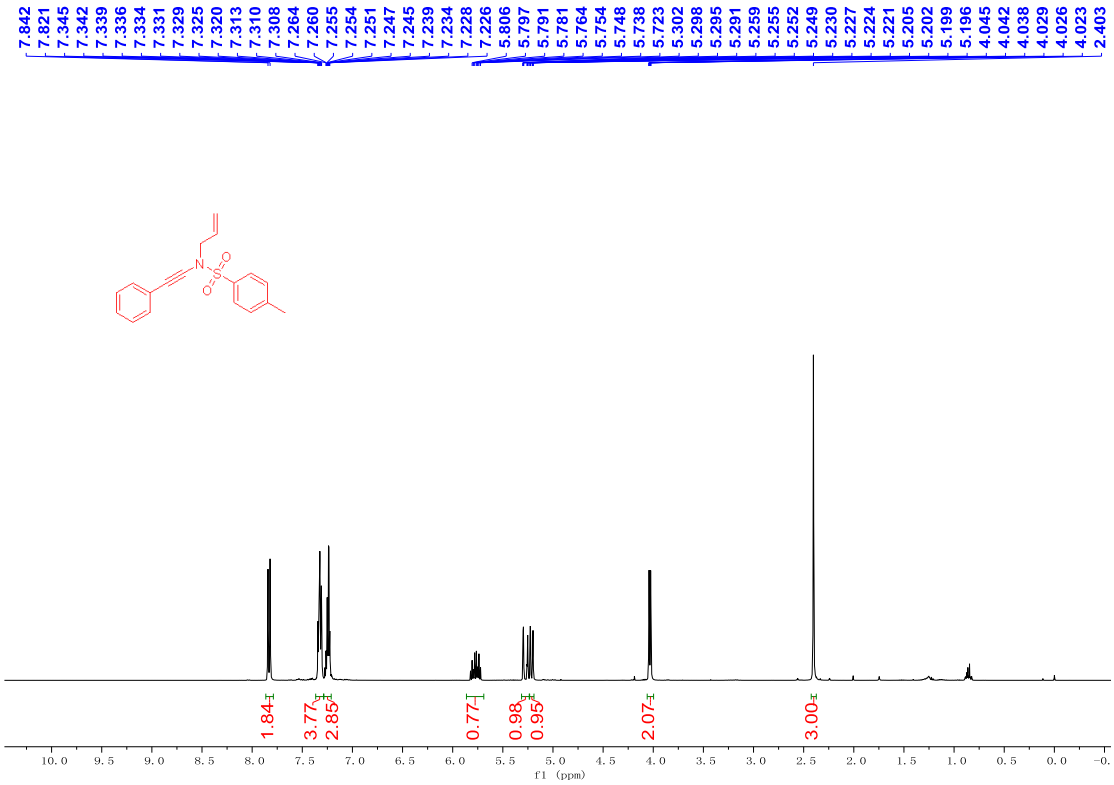


Figure S34. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-allyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1q**)

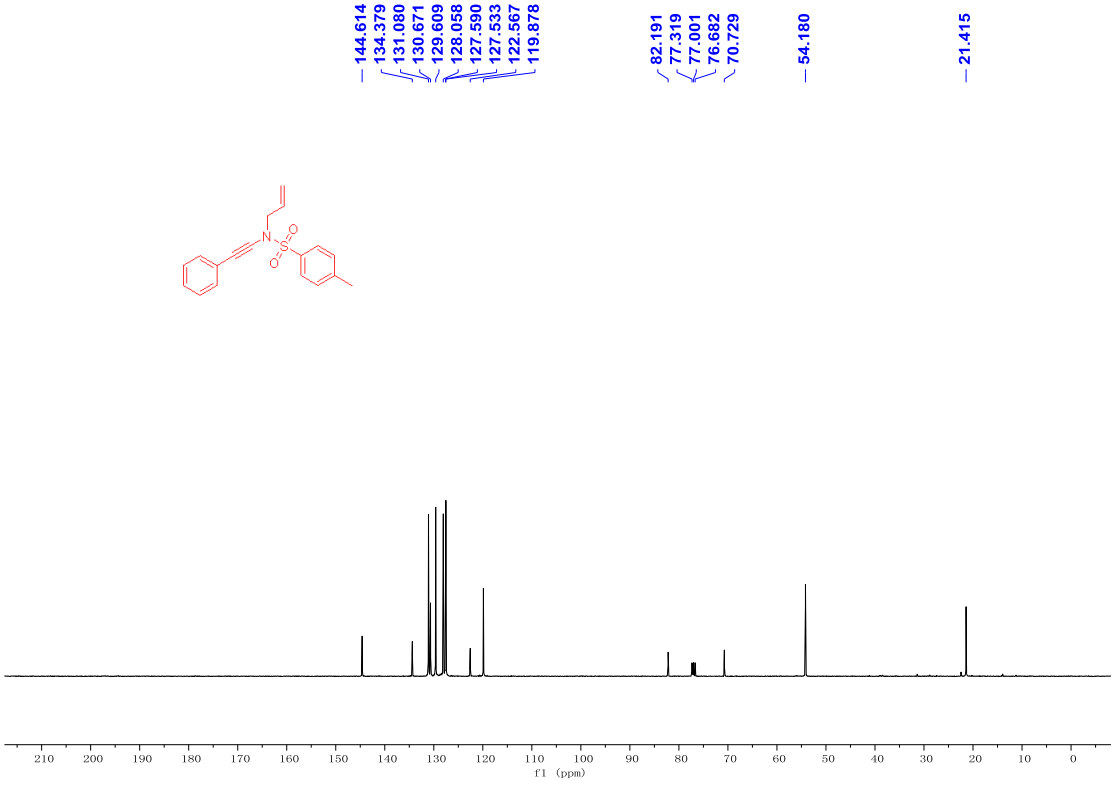


Figure S35. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-allyl-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1q**)

N-(Furan-2-ylmethyl)-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1r**)

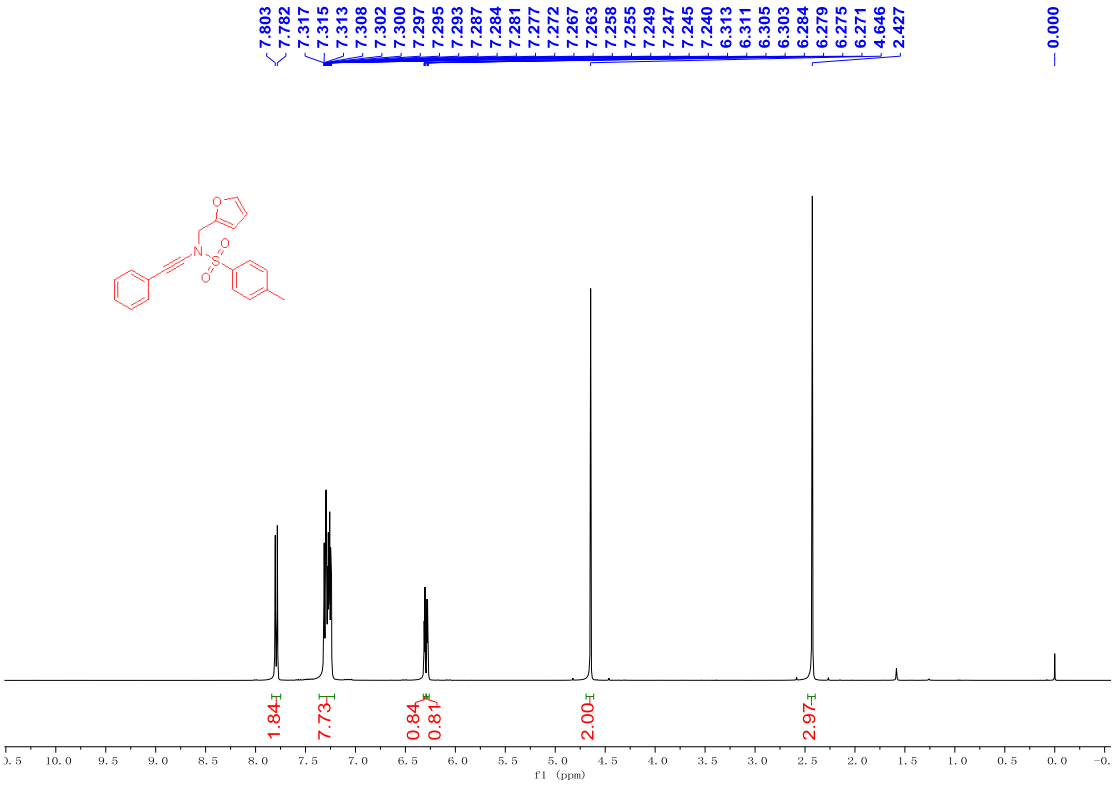


Figure S36. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-(furan-2-ylmethyl)-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1r**)

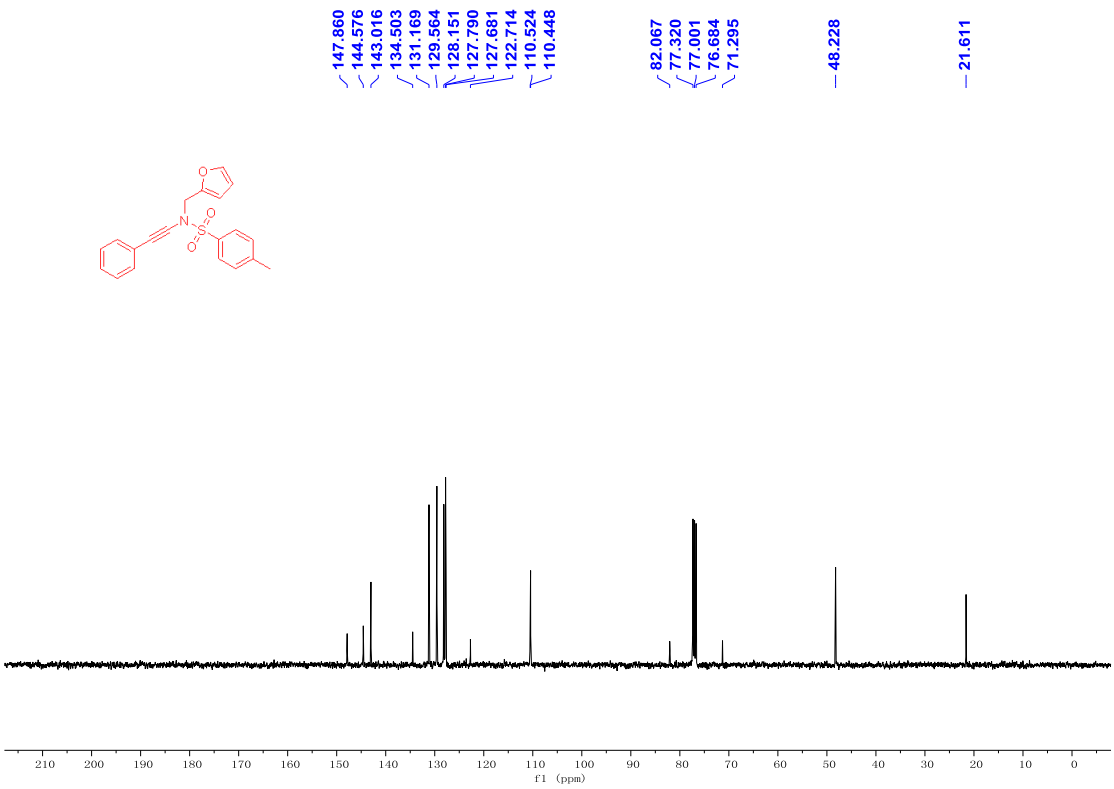


Figure S37. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-(furan-2-ylmethyl)-4-methyl-*N*-(phenylethynyl)benzenesulfonamide (**1r**)

N-Methyl)-*N*-(phenylethynyl)methanesulfonamide (**1s**)

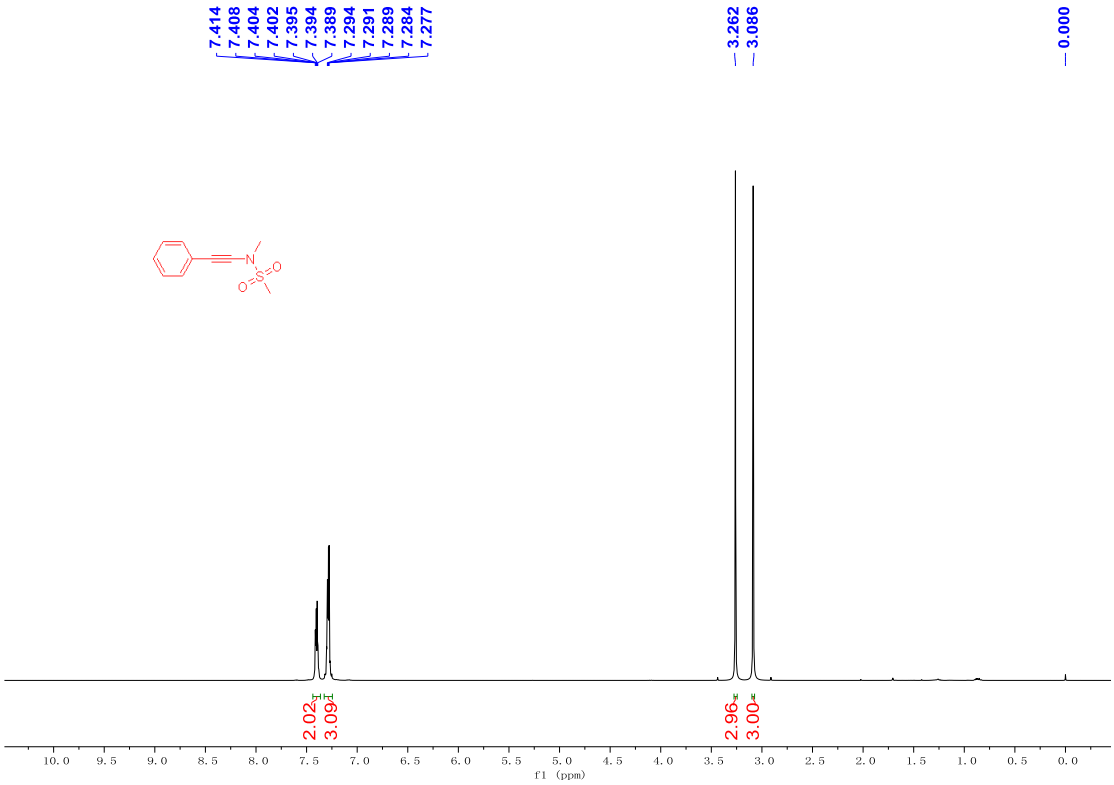


Figure S38. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-methyl-*N*-(phenylethynyl)methanesulfonamide (**1s**)

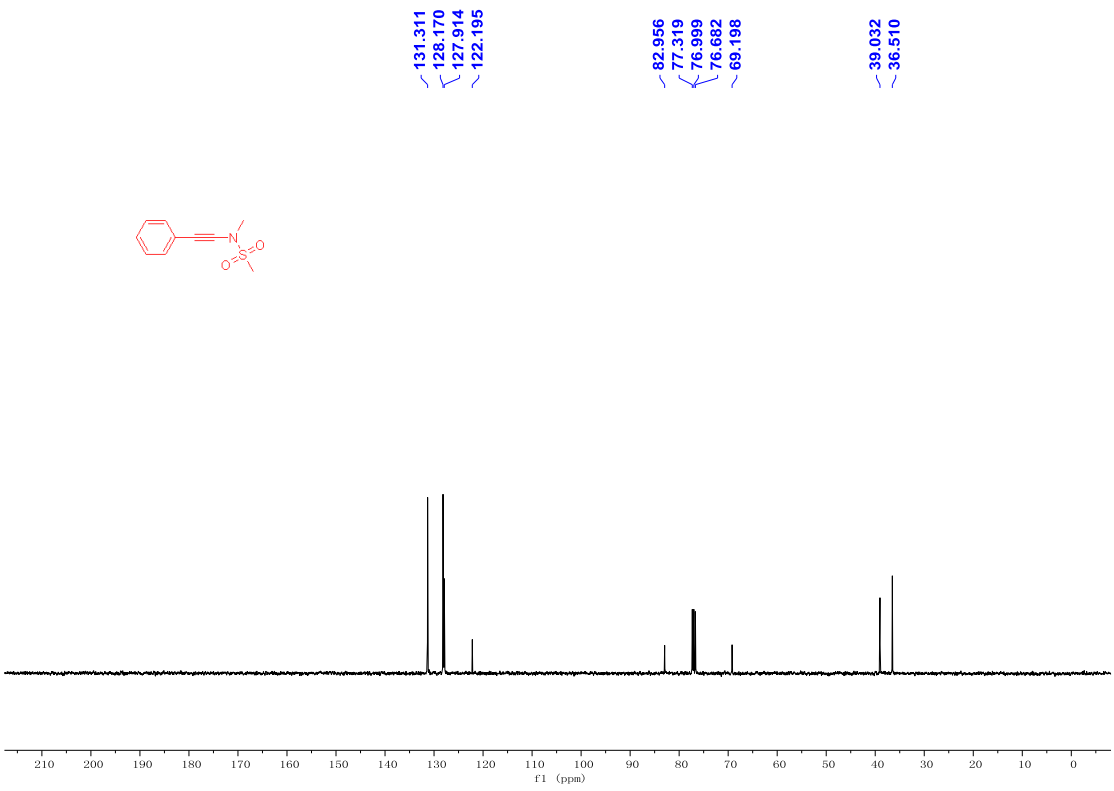


Figure S39. ^{13}C NMR spectrum (101 MHz, $CDCl_3$ of *N*-methyl-*N*-(phenylethynyl)methanesulfonamide (**1s**)

Copies of ^{1}H, ^{13}C, and ^{19}F NMR spectra of compounds **2**.

N-Methyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2a**)

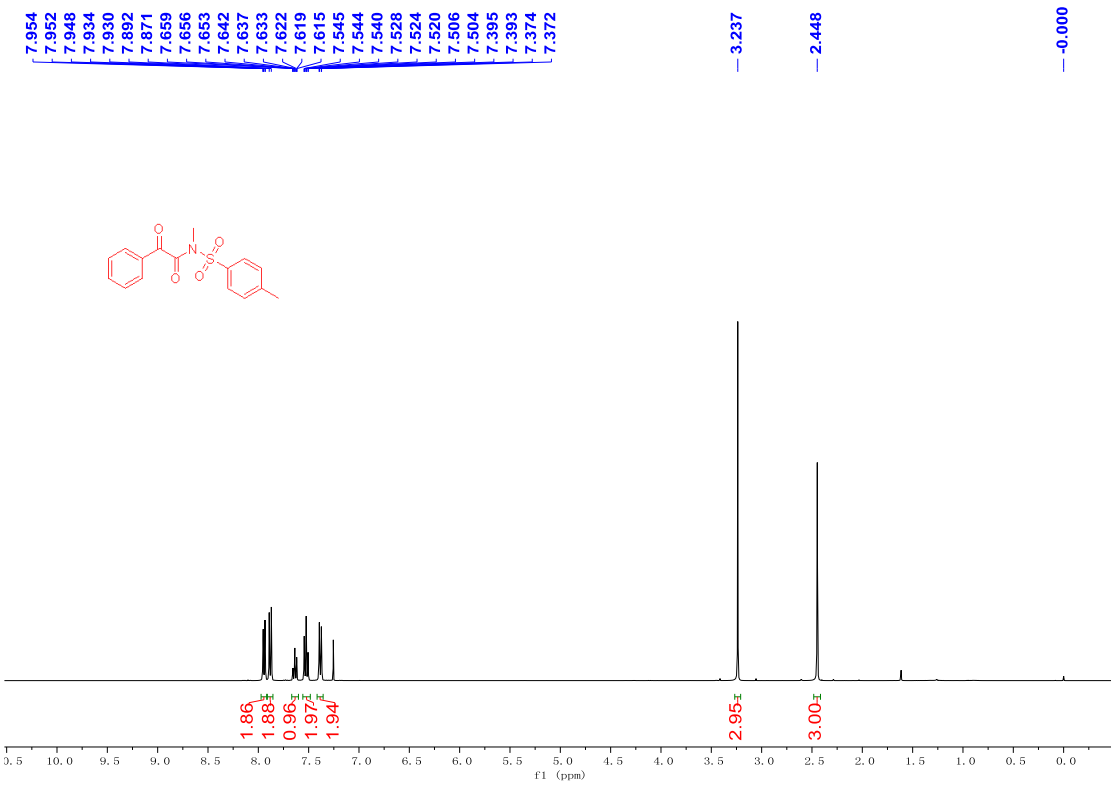


Figure S40. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-methyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2a**)

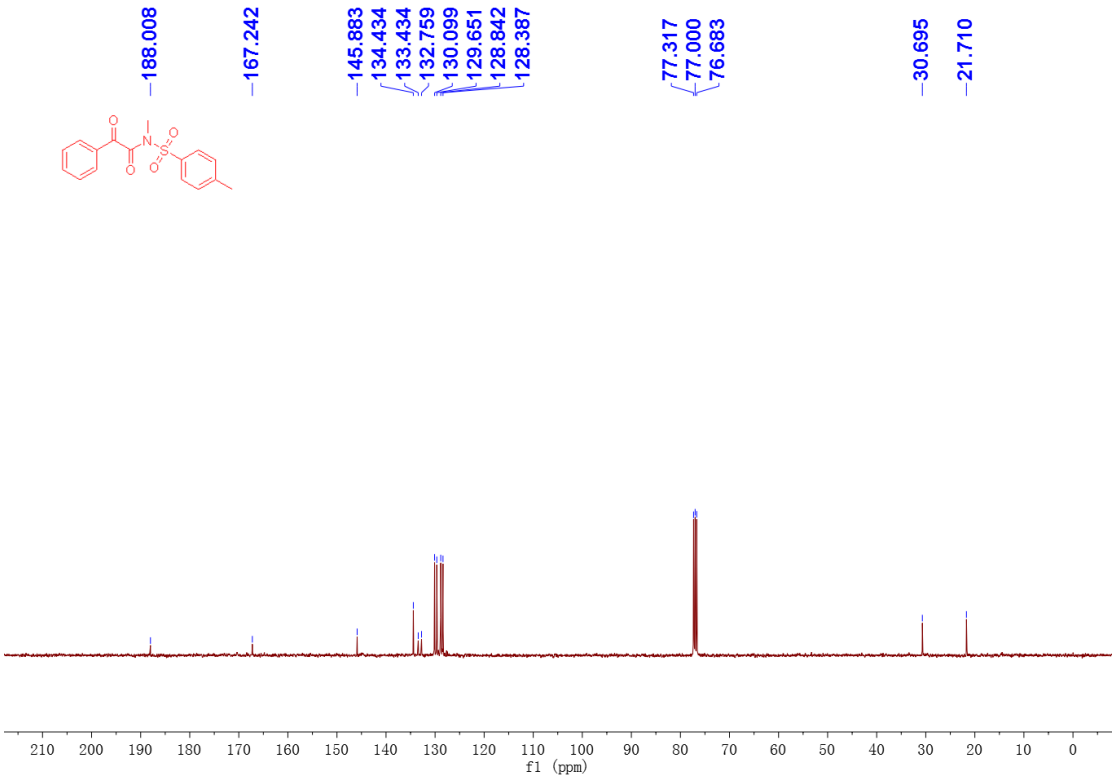


Figure S41. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-methyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2a**)

N-Methyl-2-oxo-2-phenyl-*N*-(phenylsulfonyl)acetamide (**2b**)

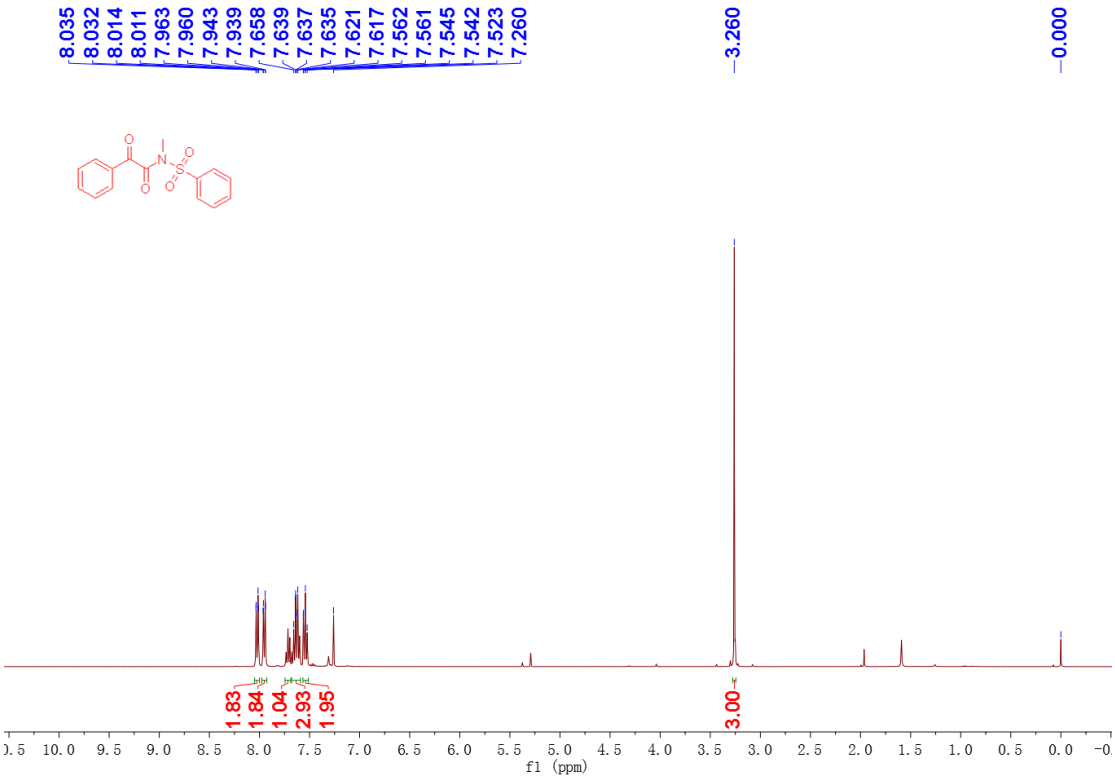


Figure S42. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-methyl-2-oxo-2-phenyl-*N*-(phenylsulfonyl)acetamide (**2b**)

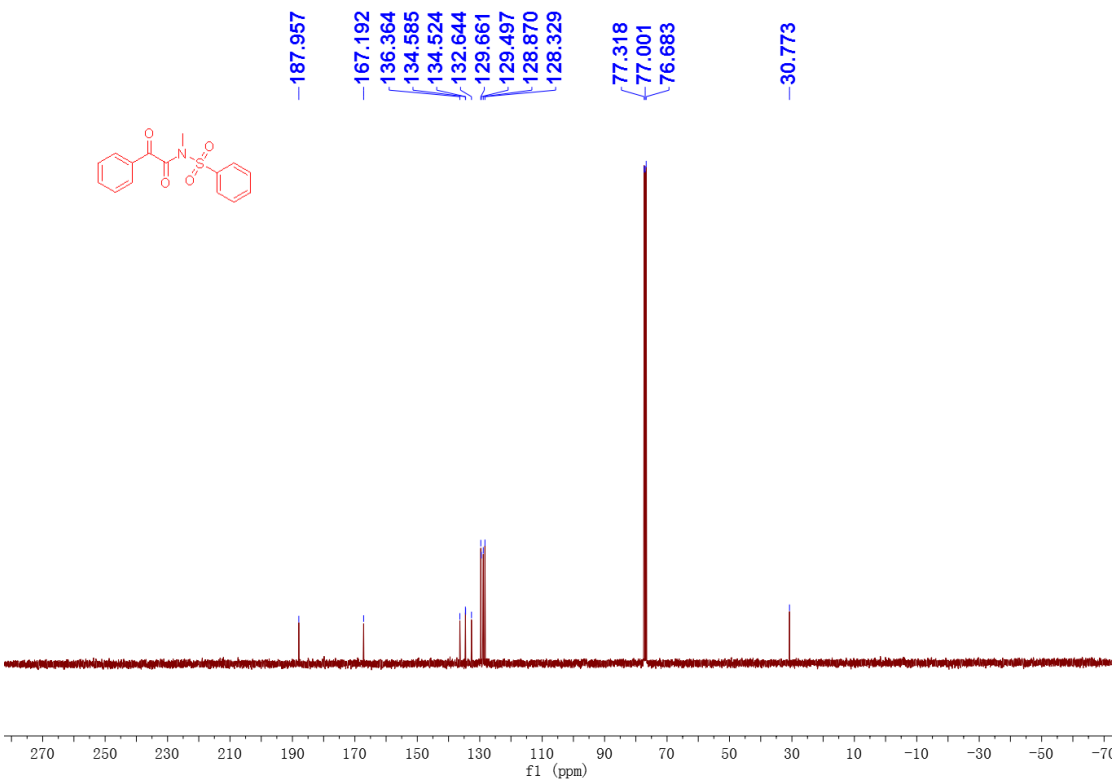


Figure S43. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-methyl-2-oxo-2-phenyl-*N*-(phenylsulfonyl)acetamide (**2b**)

N-((4-Bromophenyl)sulfonyl)-*N*-methyl-2-oxo-2-phenylacetamide (**2c**)

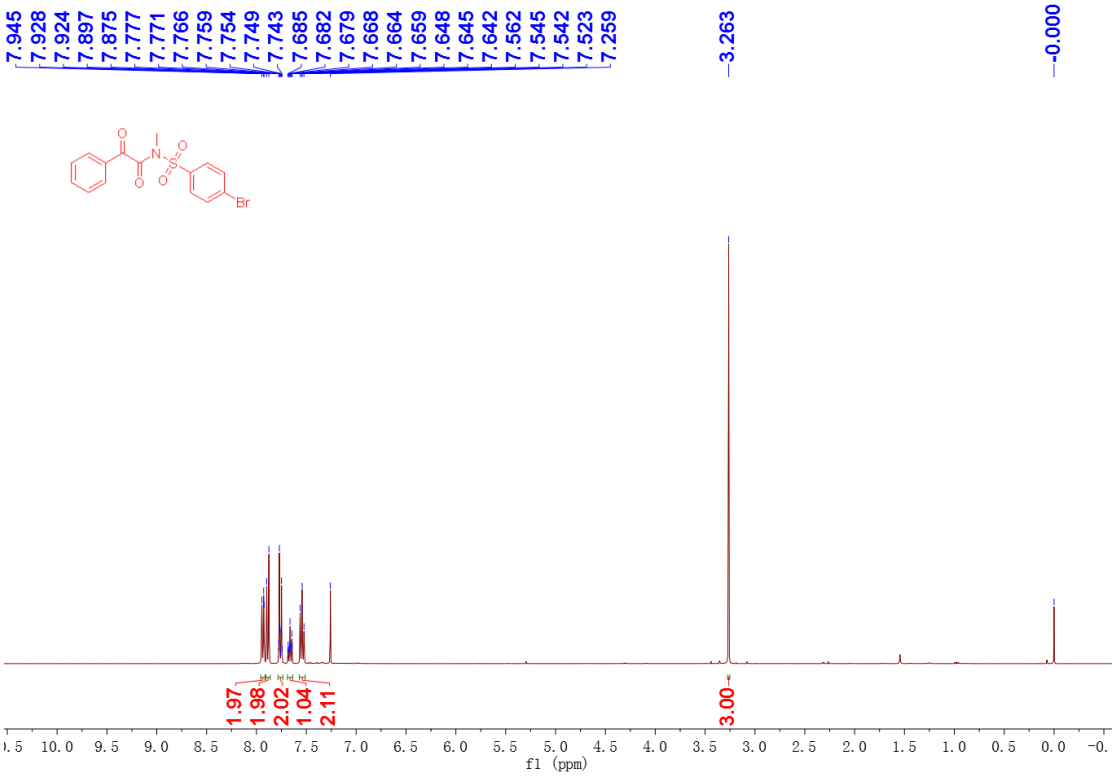


Figure S44. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-((4-bromophenyl)sulfonyl)-*N*-methyl-2-oxo-2-phenylacetamide (**2c)**

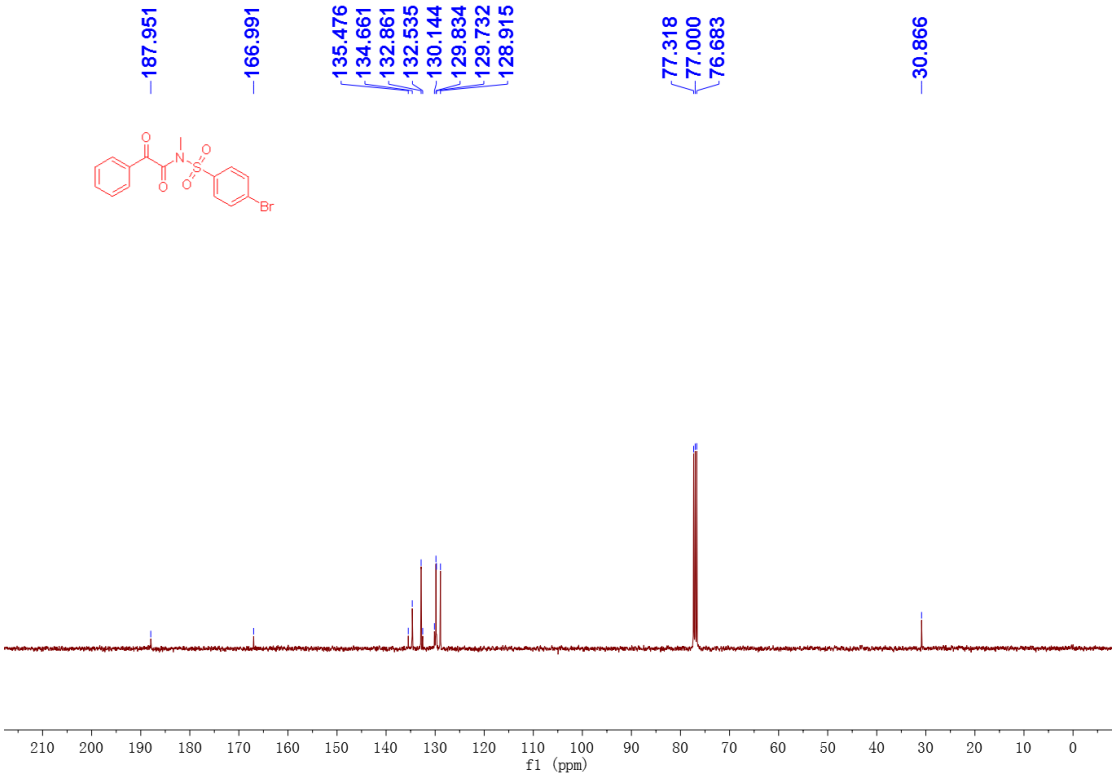


Figure S45. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-((4-bromophenyl)sulfonyl)-*N*-methyl-2-oxo-2-phenylacetamide (**2c)**

N-Methyl-*N*-((4-nitrophenyl)sulfonyl)-2-oxo-2-phenylacetamide (**2d**)

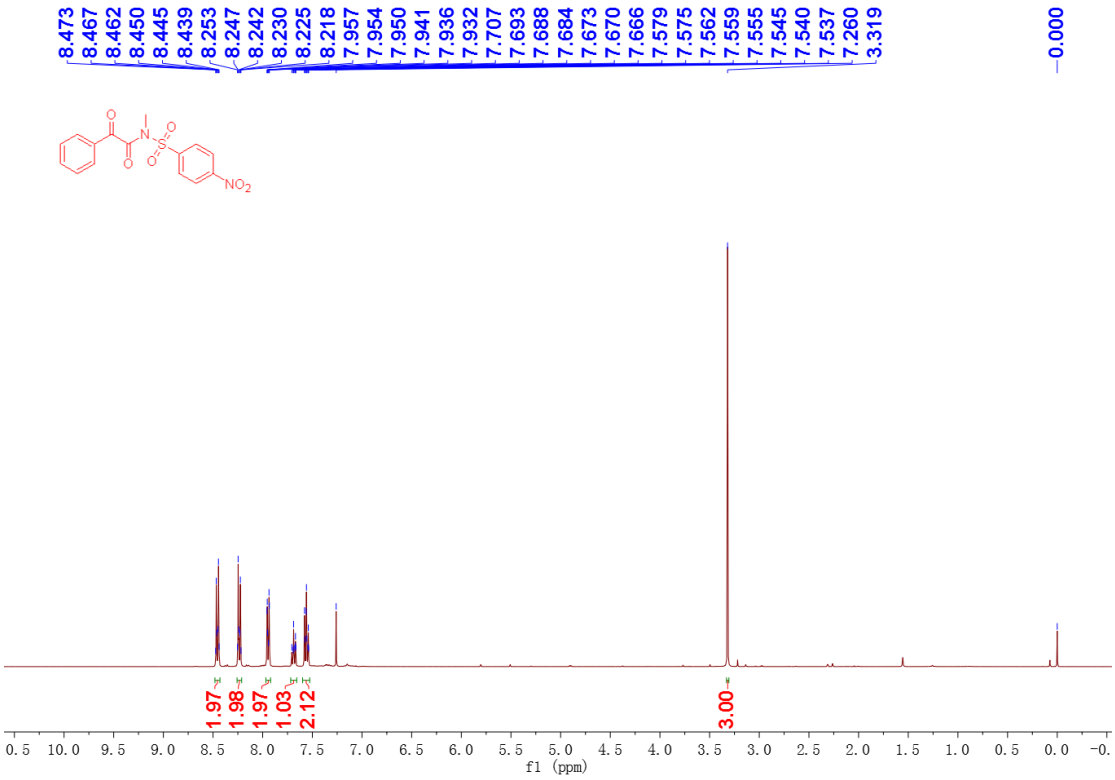


Figure S46. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-methyl-*N*-((4-nitrophenyl)sulfonyl)-2-oxo-2-phenylacetamide (**2d**)

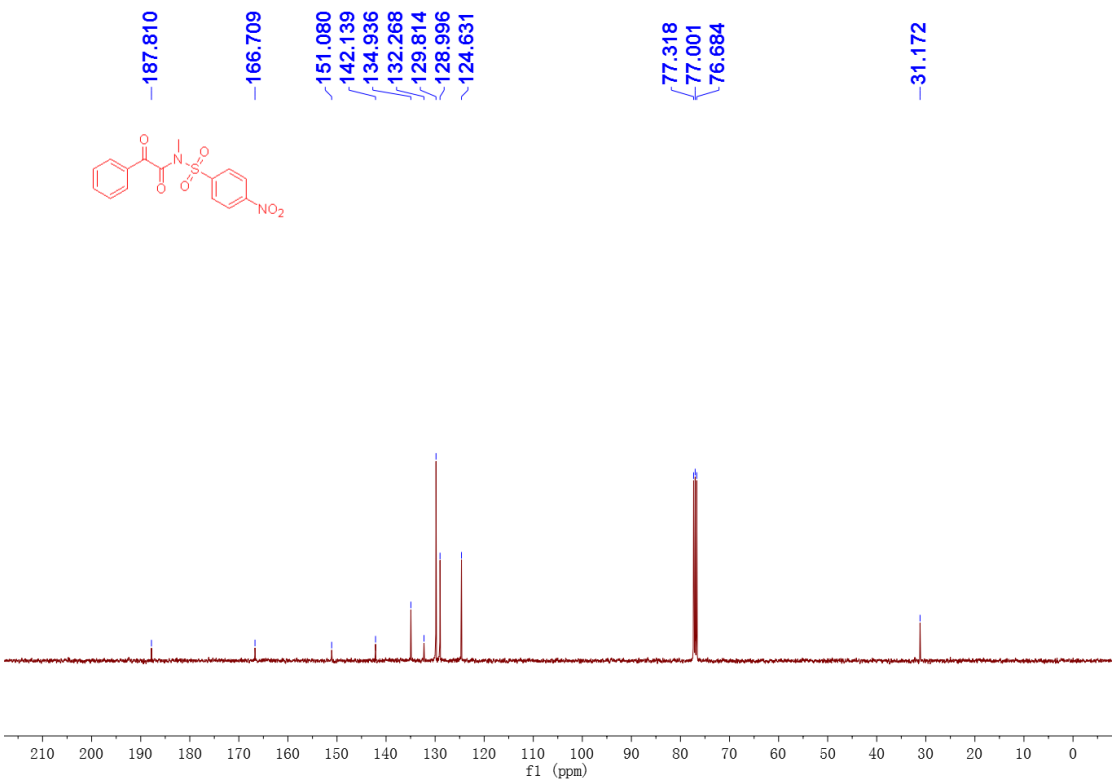


Figure S47. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-methyl-*N*-((4-nitrophenyl)sulfonyl)-2-oxo-2-phenylacetamide (**2d**)

N-Methyl-2-oxo-2-(*p*-tolyl)-*N*-(*p*-tosyl)acetamide (**2e**)

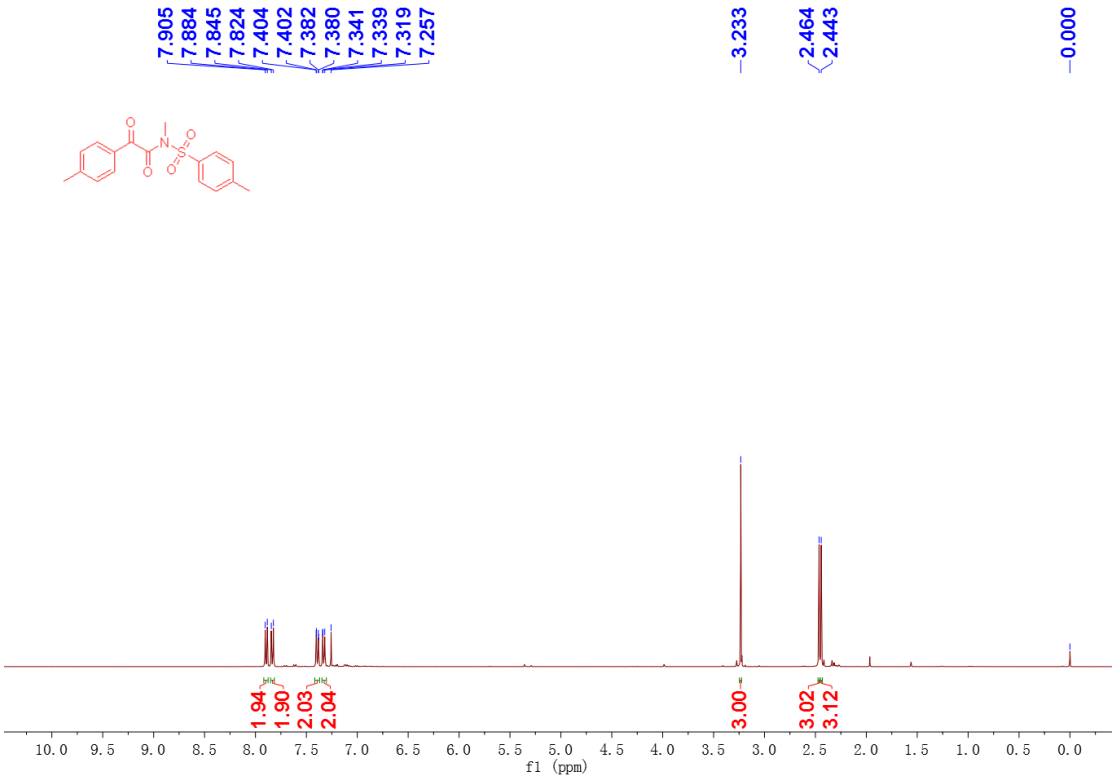


Figure S48. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-methyl-2-oxo-2-(*p*-tolyl)-*N*-(*p*-tosyl)acetamide (**2e**)

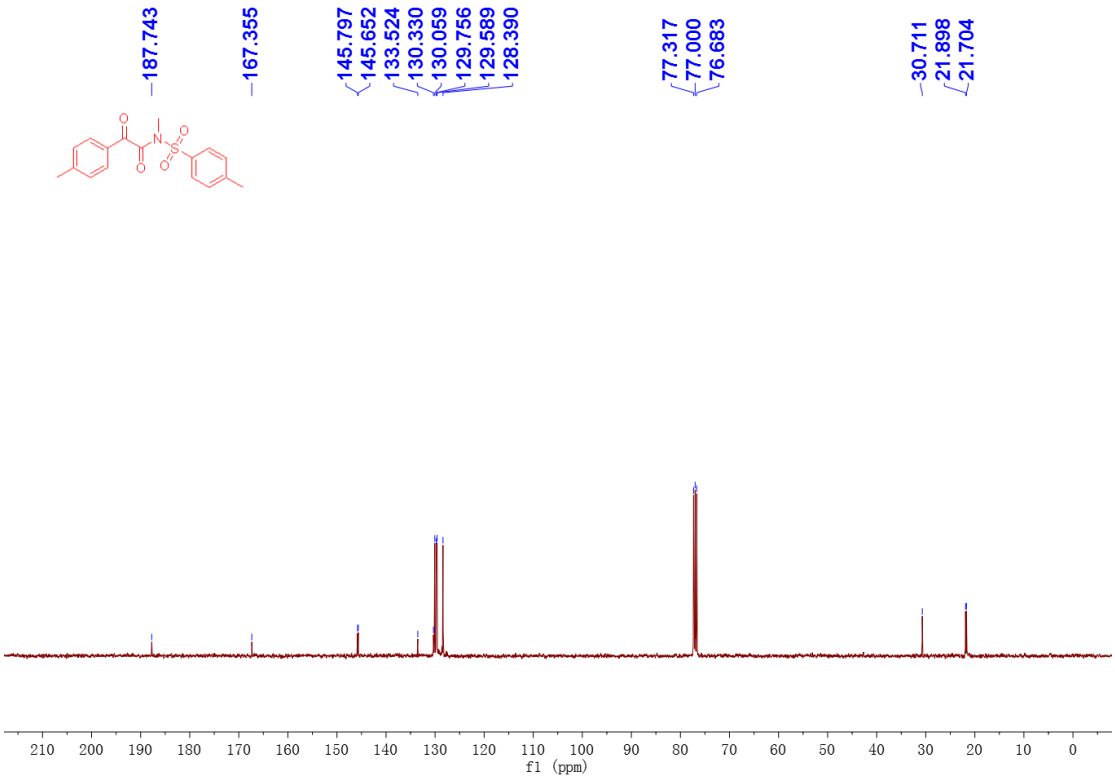


Figure S49. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-methyl-2-oxo-2-(*p*-tolyl)-*N*-(*p*-tosyl)acetamide (**2e**)

2-(4-Fluorophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2f**)

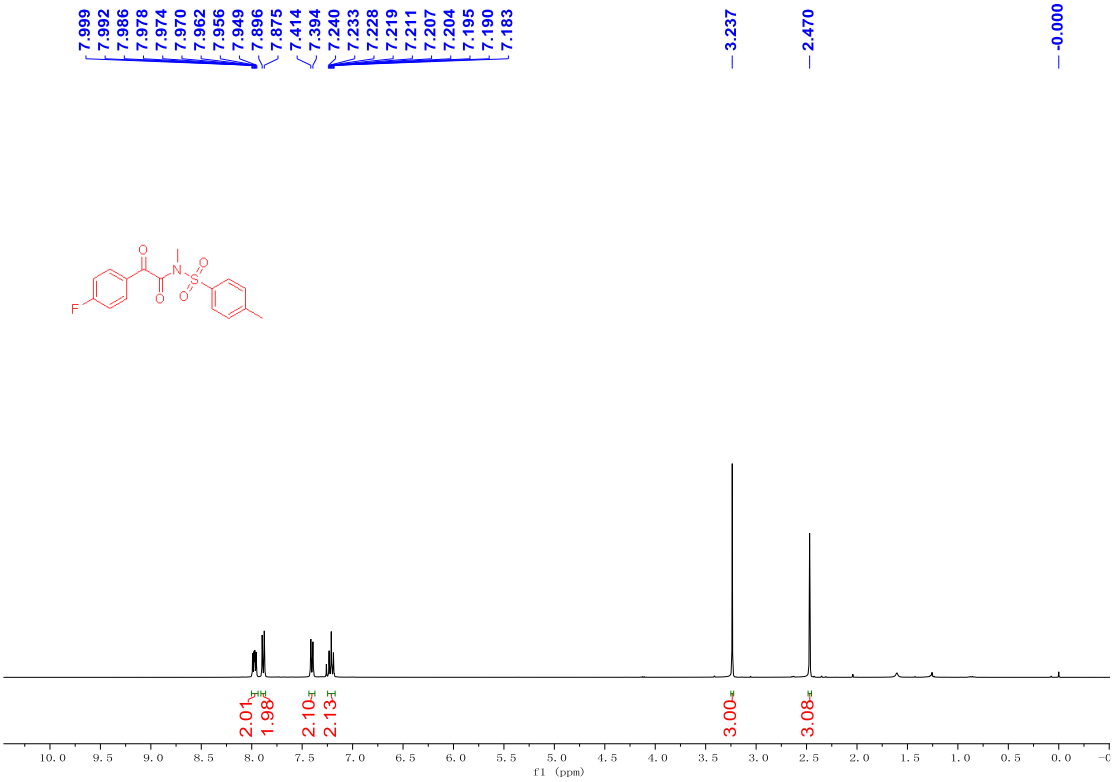


Figure S50. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2-(4-fluorophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2f**)

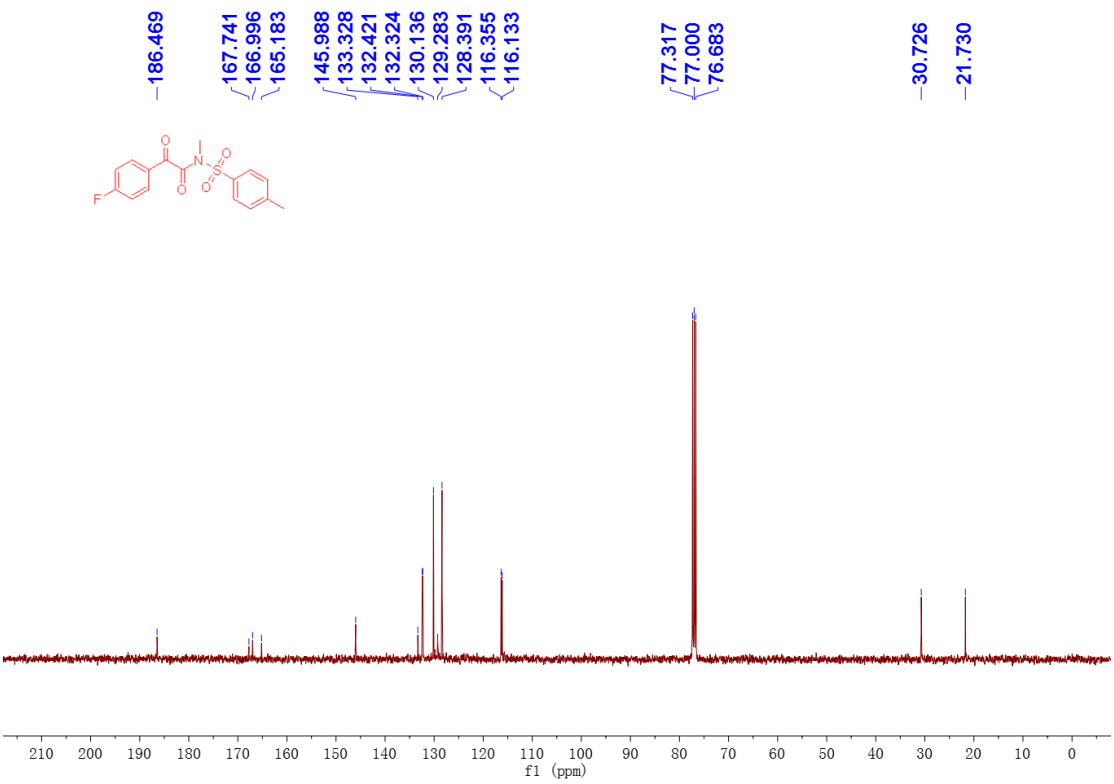


Figure S51. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 2-(4-fluorophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2f**)

^{19}F NMR (377 MHz, $CDCl_3$)

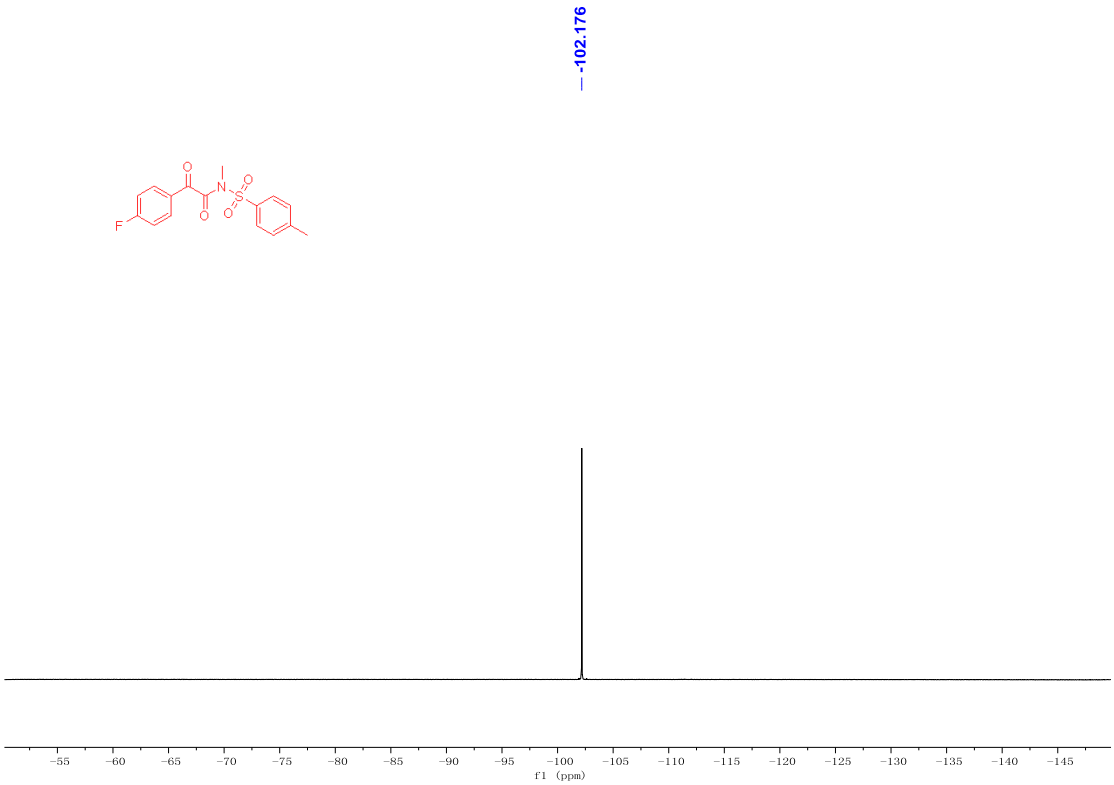


Figure S52. ^{19}F NMR spectrum (377 MHz, $CDCl_3$) of 2-(4-fluorophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2f**)

2-(4-Chlorophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2g**)

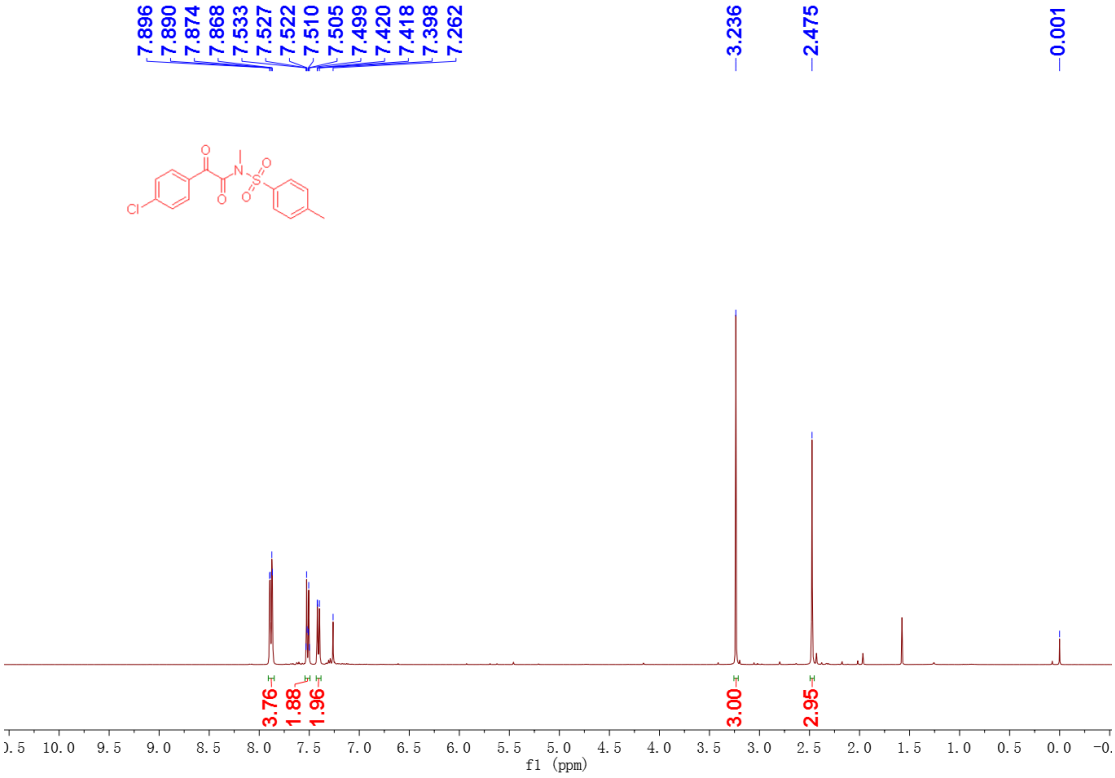


Figure S53. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2-(4-chlorophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2g**)

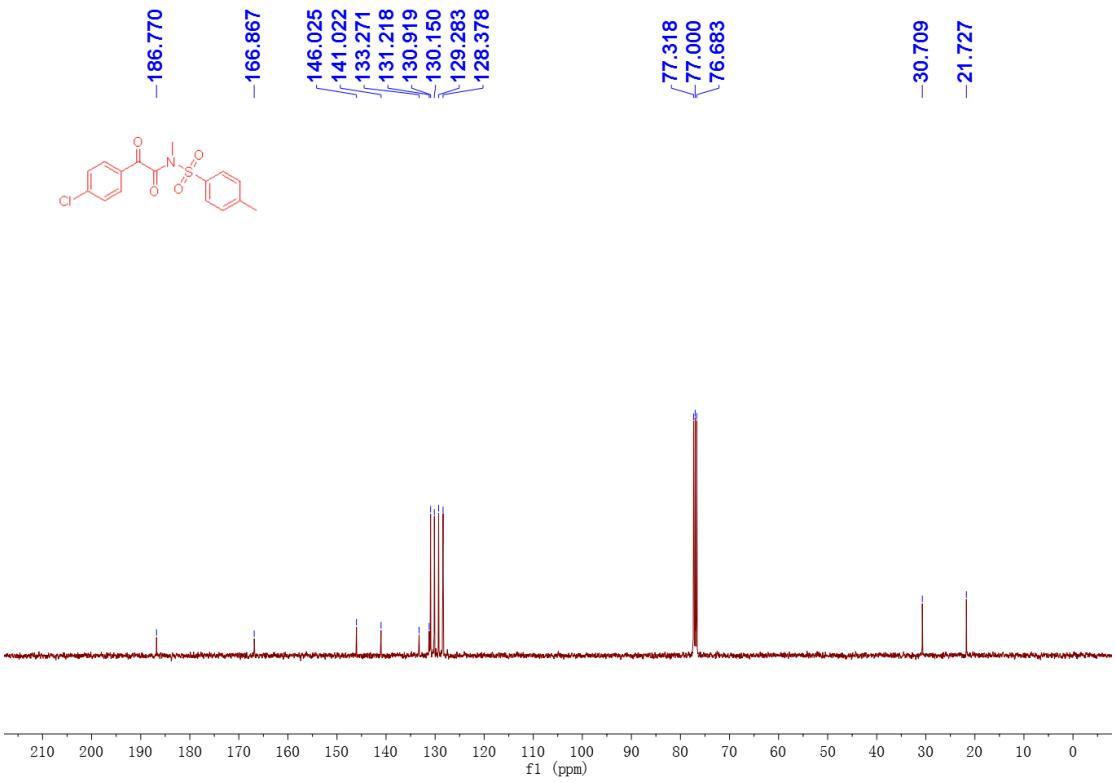


Figure S54. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 2-(4-chlorophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2g**)

2-(4-Bromophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2h**)

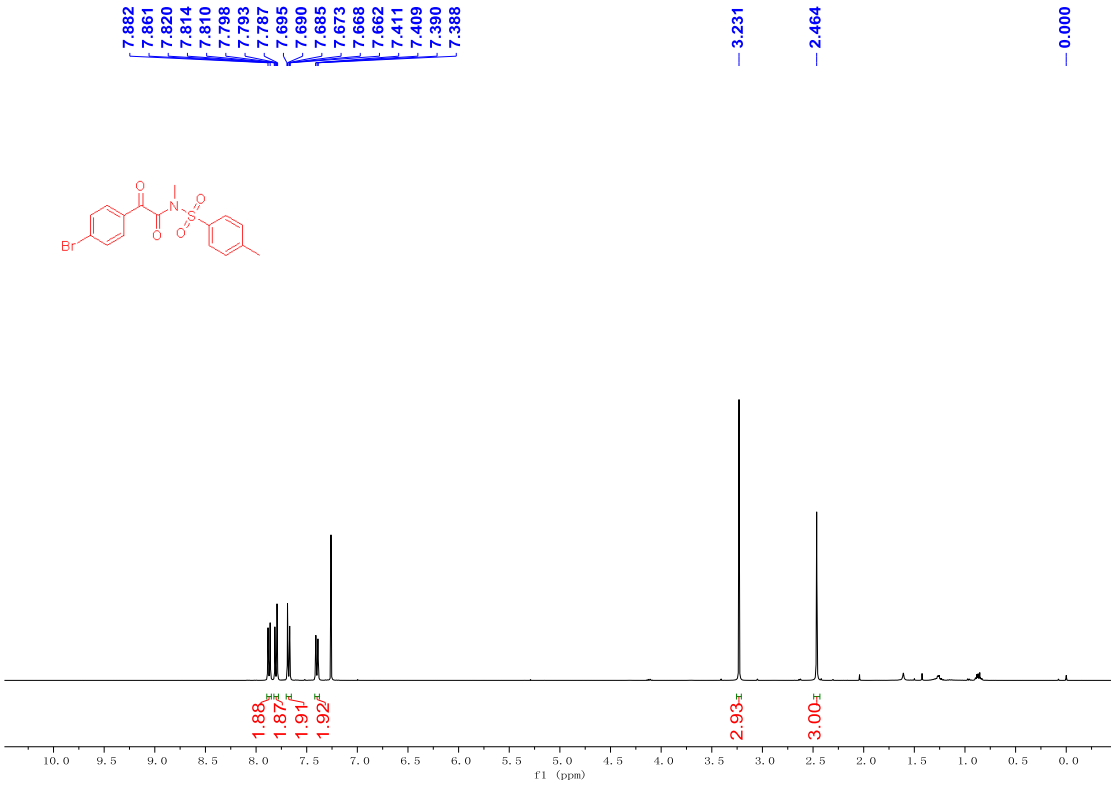


Figure S55. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2-(4-bromophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2h**)

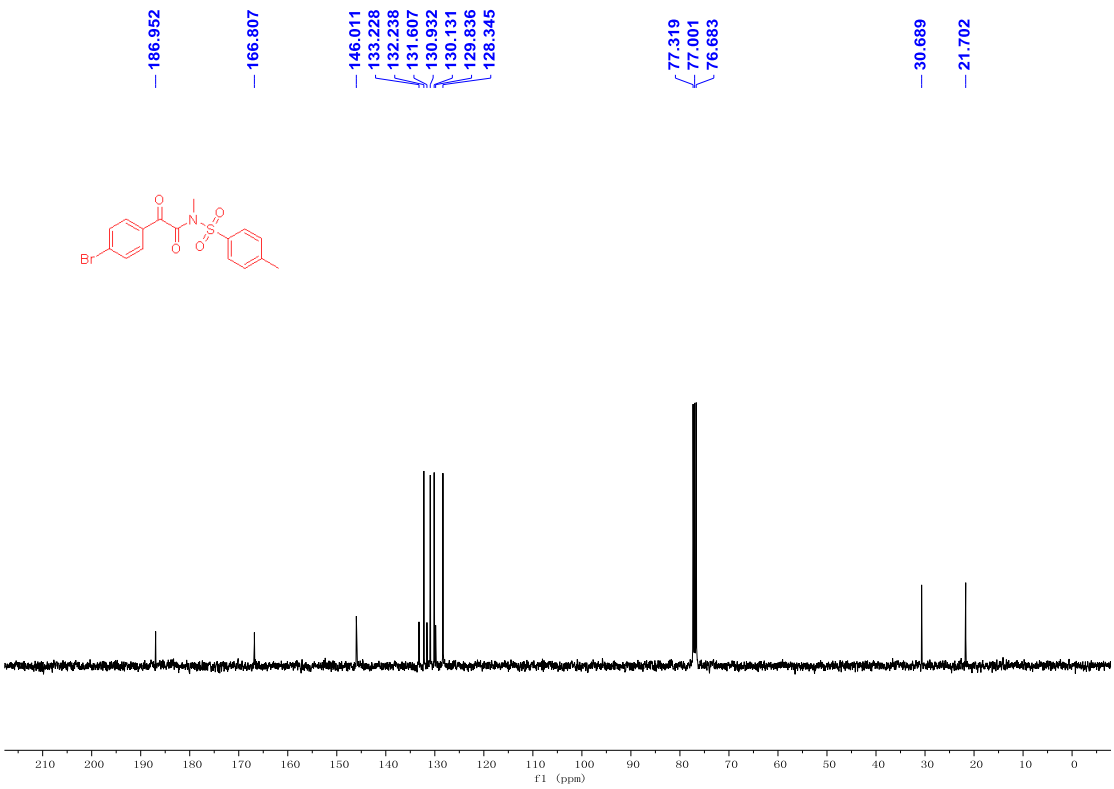


Figure S56. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 2-(4-bromophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2h**)

N-Methyl-2-oxo-2-(thiophen-3-yl)-*N*-tosylacetamide (**2i**)

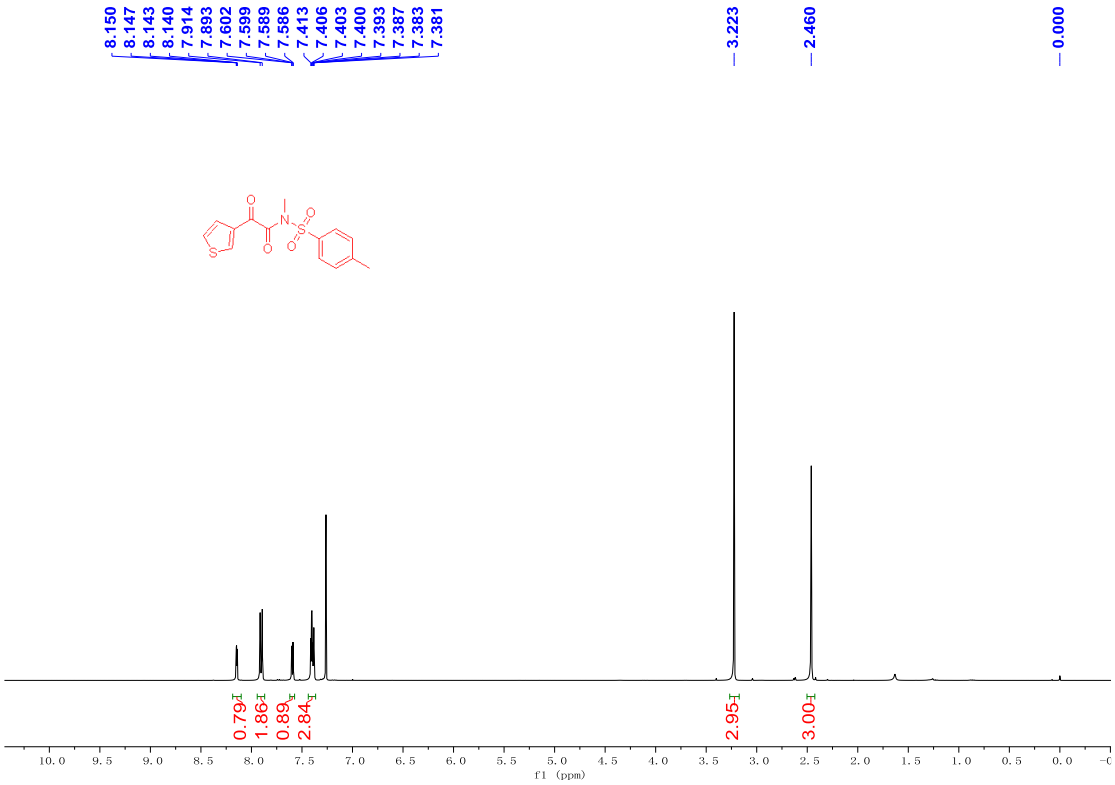


Figure S57. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-methyl-2-oxo-2-(thiophen-3-yl)-*N*-tosylacetamide (**2i**)

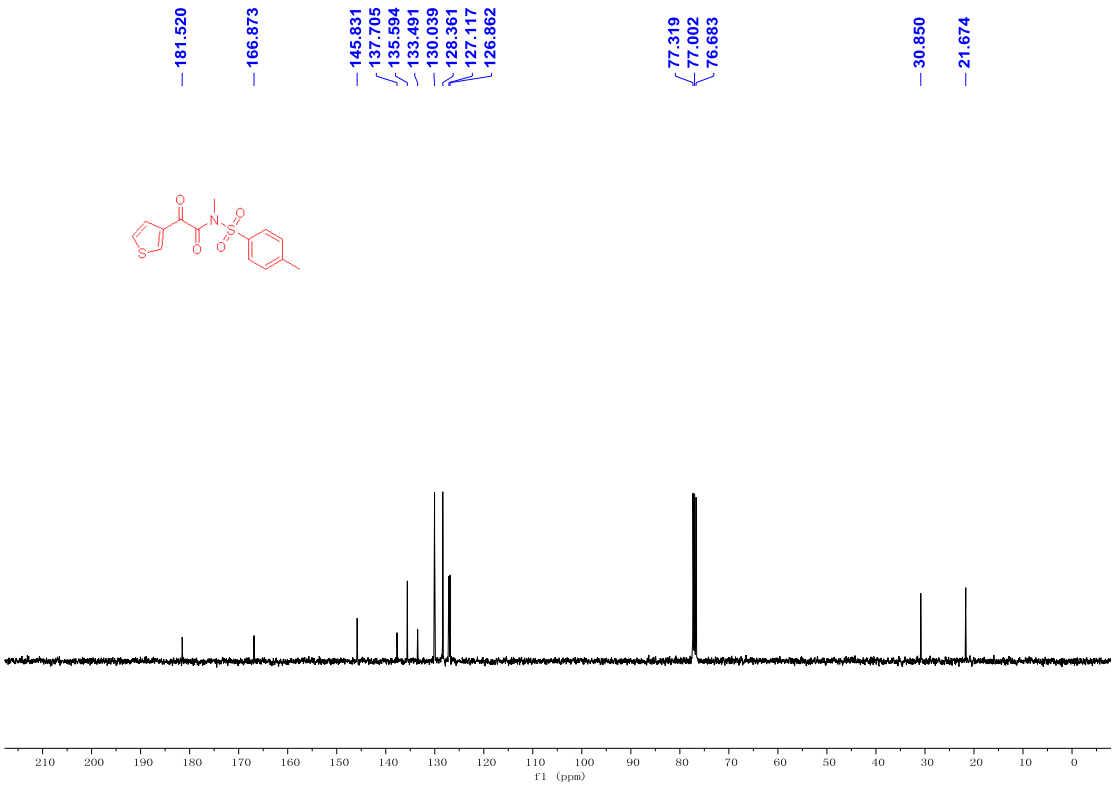


Figure S58. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-methyl-2-oxo-2-(thiophen-3-yl)-*N*-tosylacetamide (**2i**)

N-Ethyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2j**)

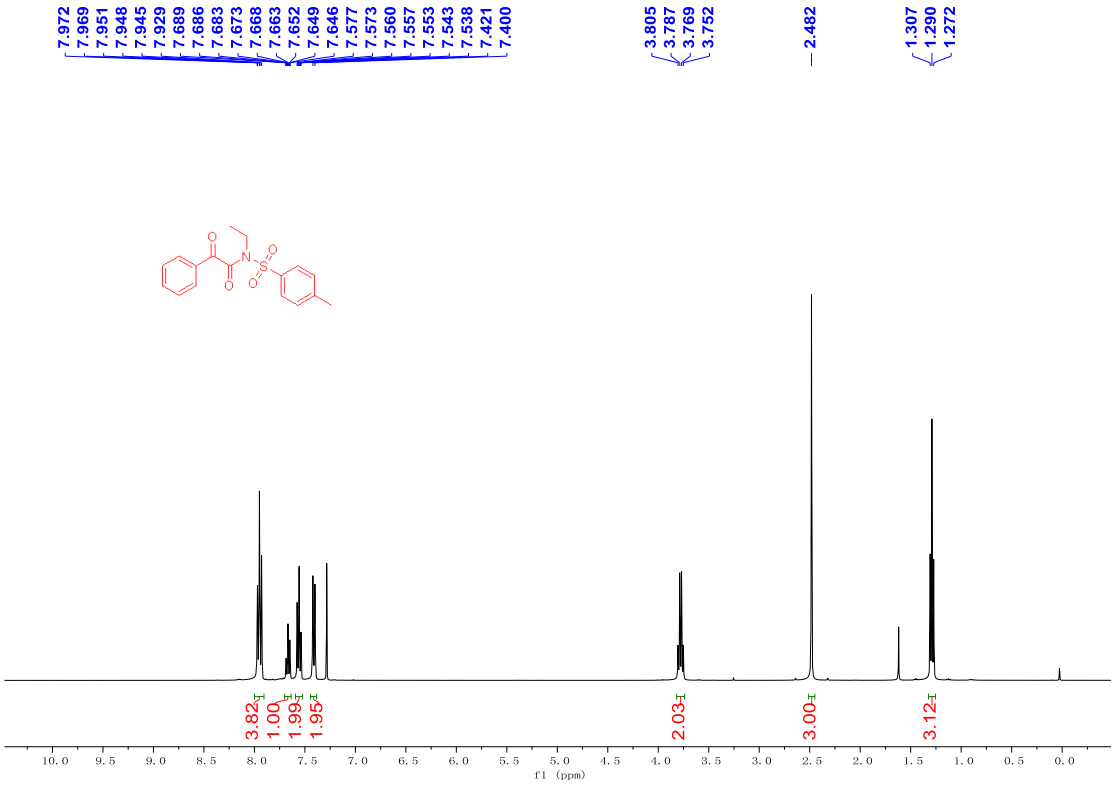


Figure S59. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-ethyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2j**)

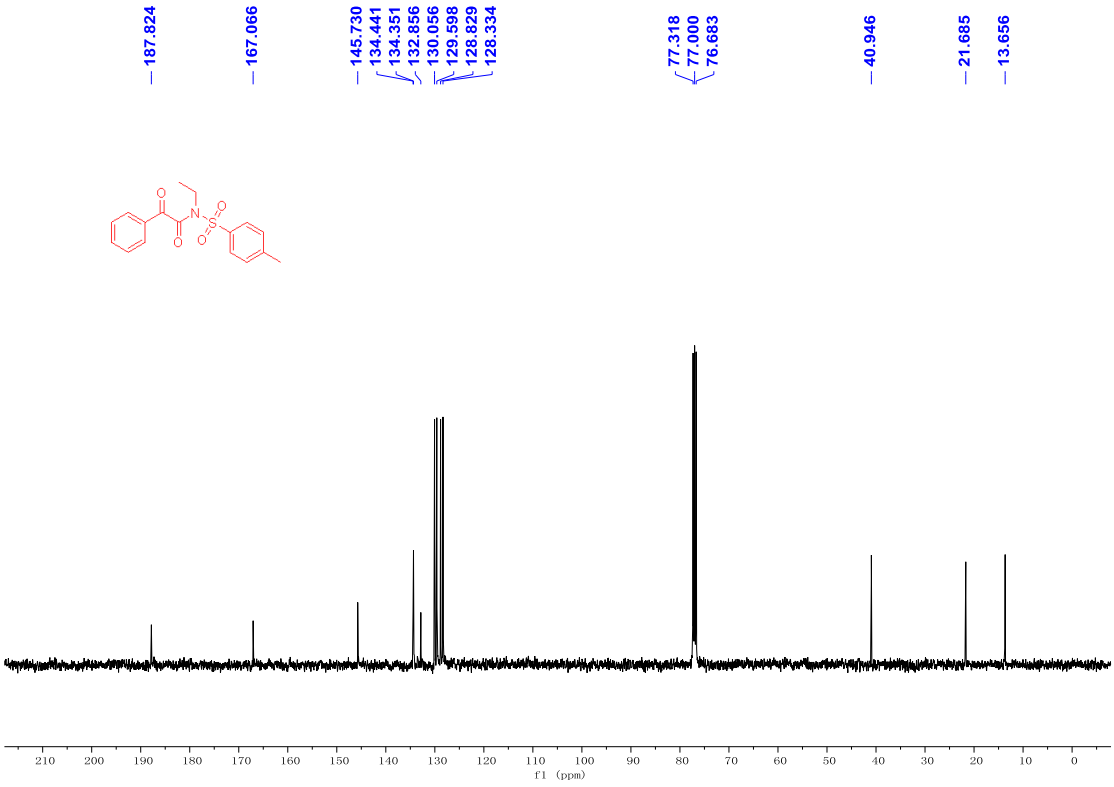


Figure S60. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-ethyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2j**)

N-Butyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2k**)

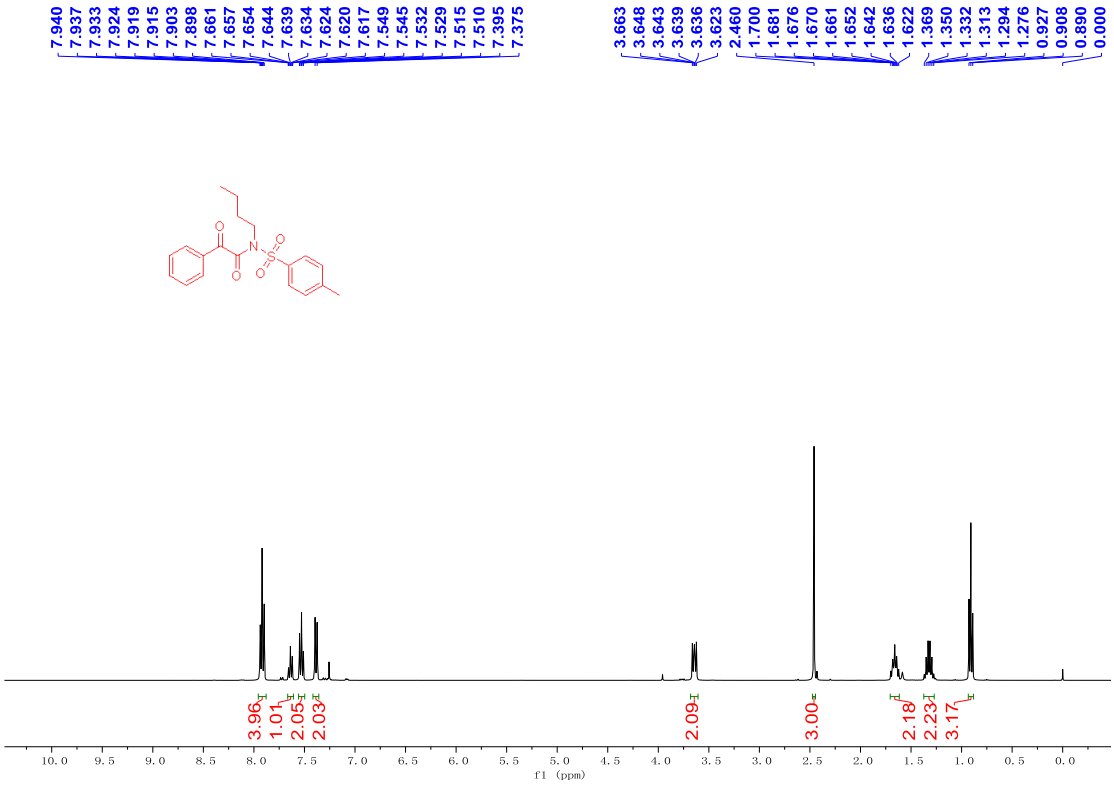


Figure S61. ^{1}H NMR spectrum (101 MHz, $CDCl_3$) of *N*-butyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2k**)

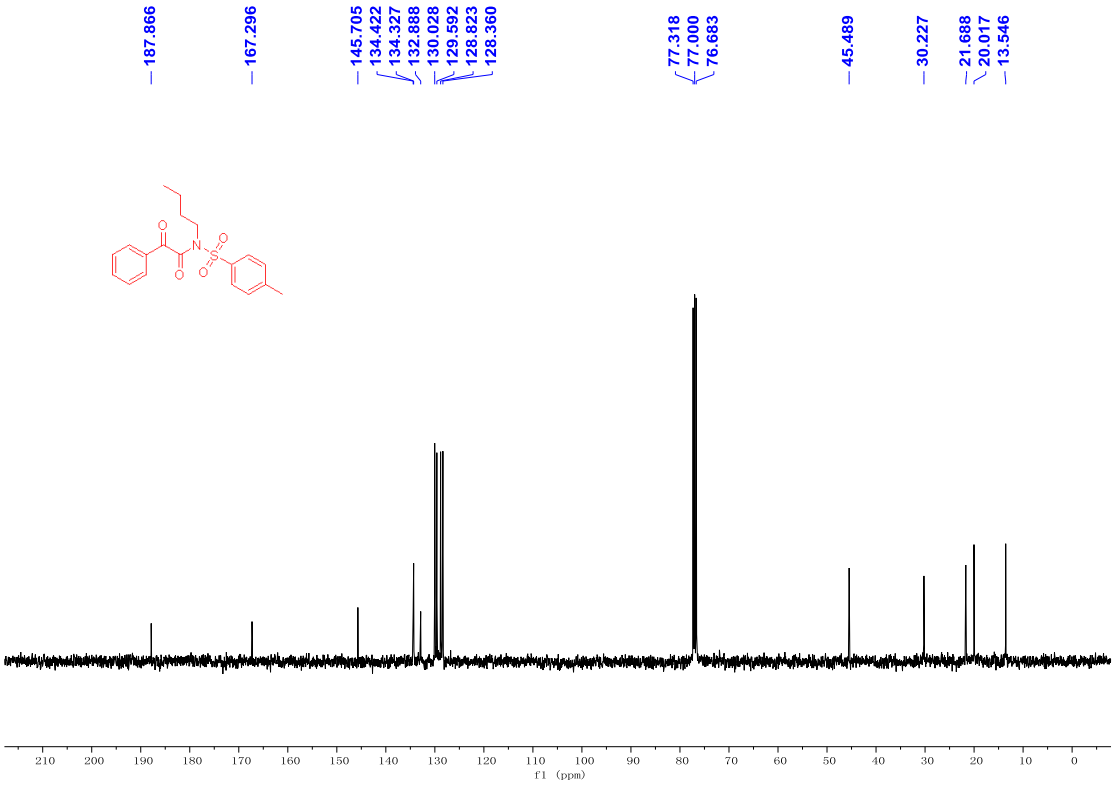


Figure S62. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-butyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2k**)

N-Cyclohexyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2l**)

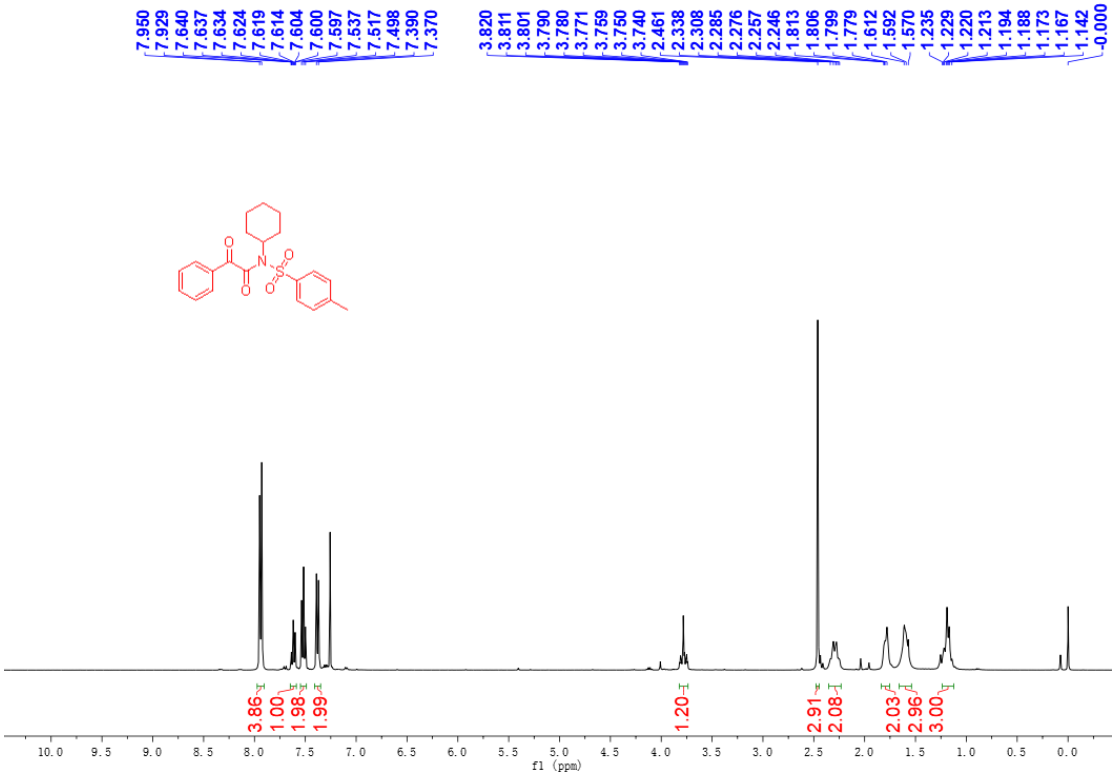


Figure S63. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-cyclohexyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2l**)

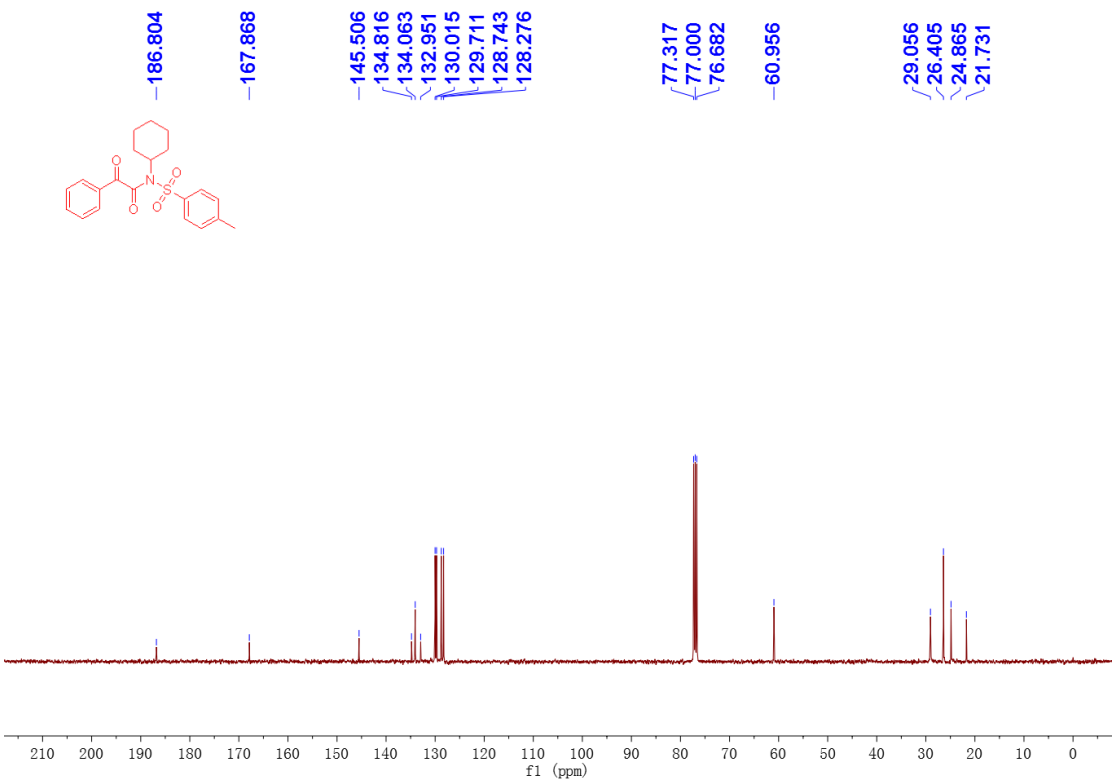


Figure S64. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-cyclohexyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2l**)

N-Cyclopropyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2m**)

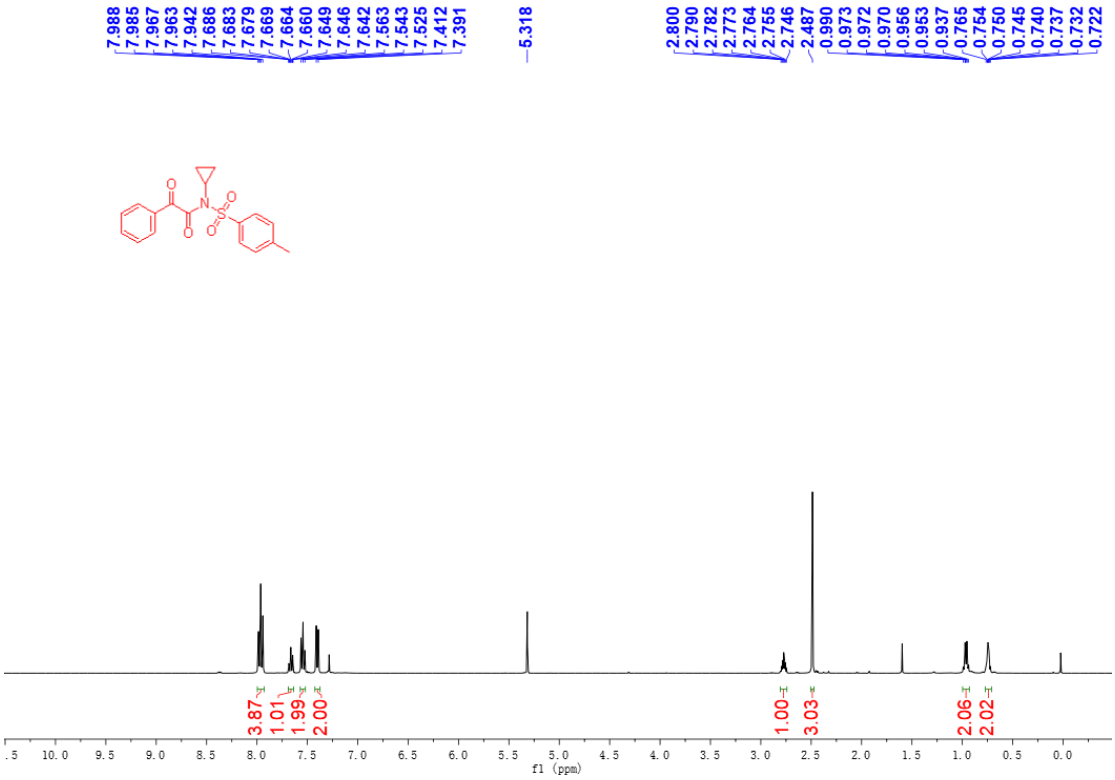


Figure S65. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-cyclopropyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2m**)

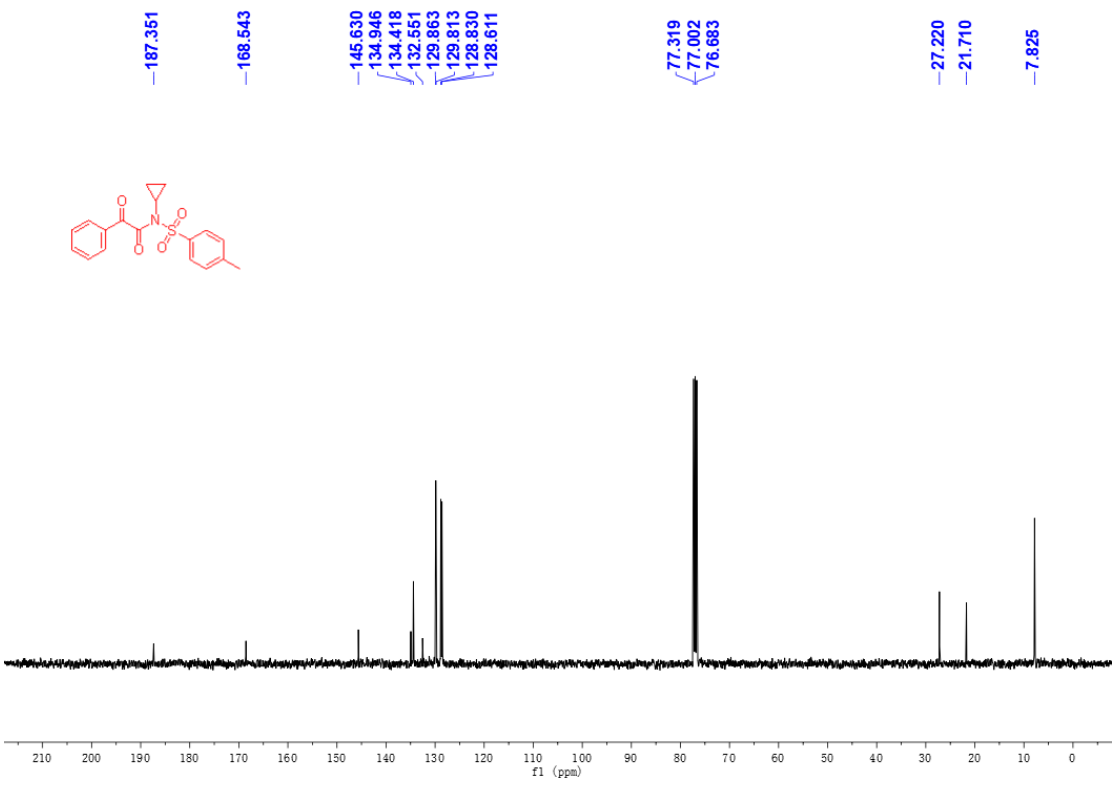


Figure S66. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-cyclopropyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2m**)

N-Benzyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2n**)

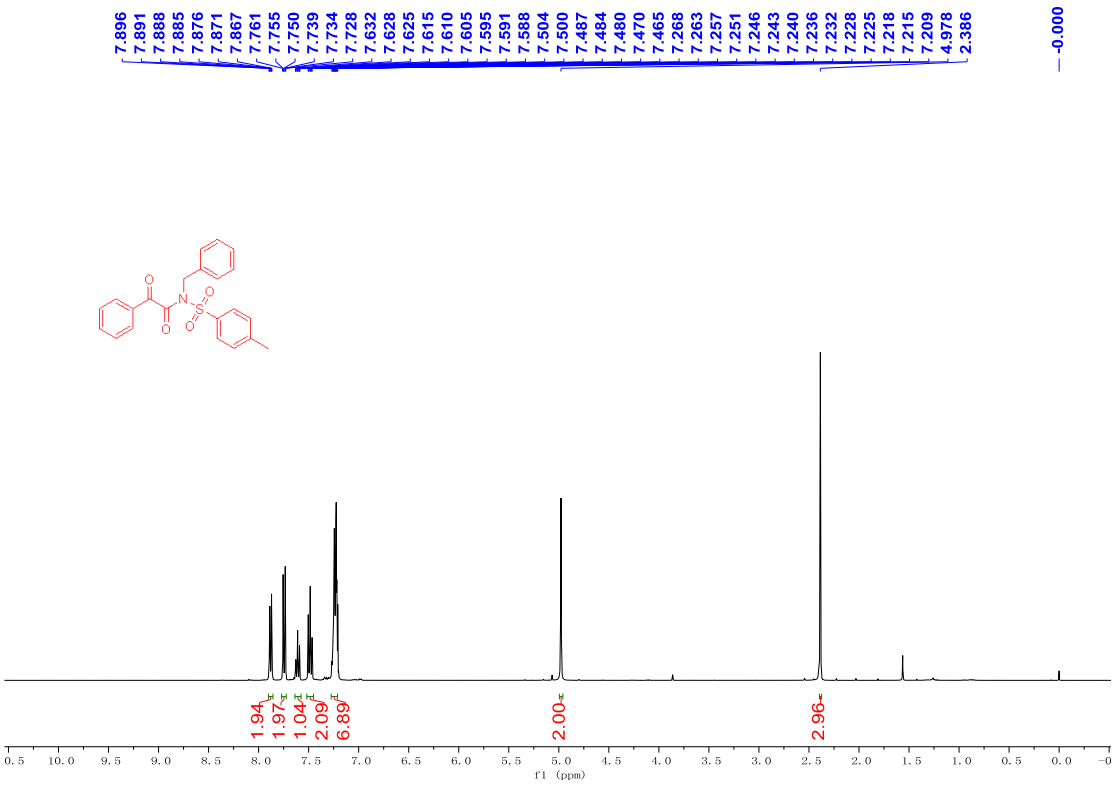


Figure S67. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-benzyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2n**)

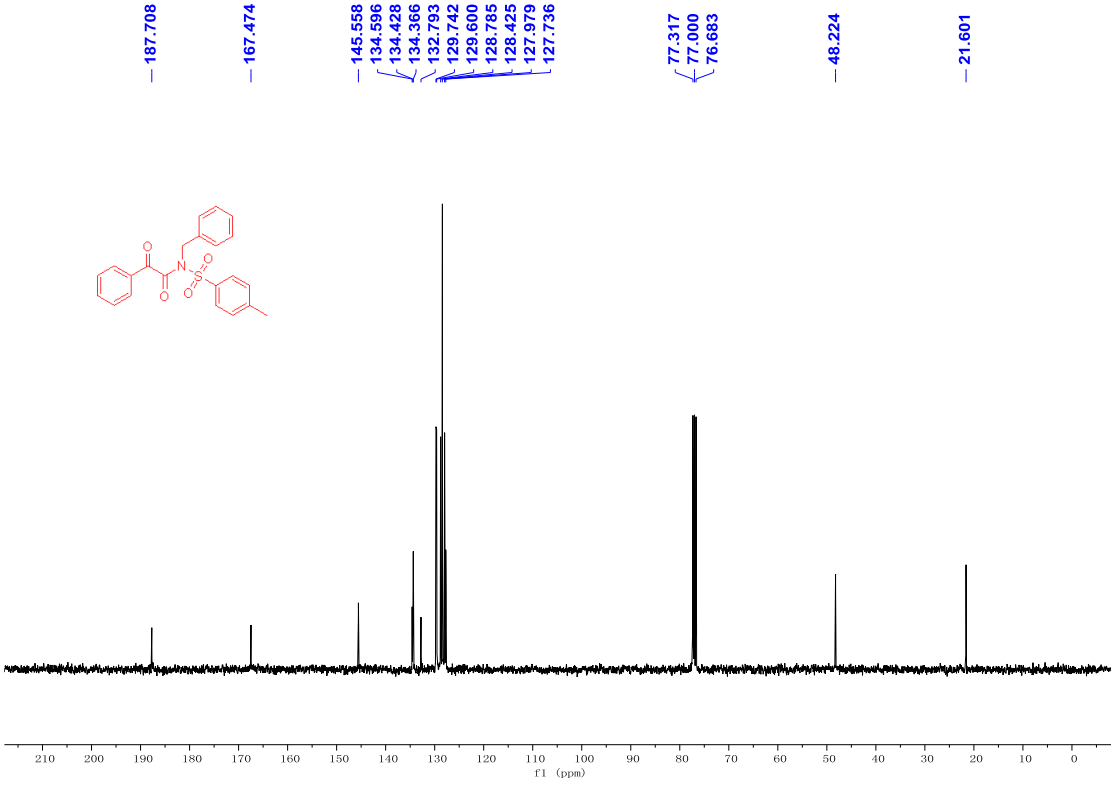


Figure S68. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-benzyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2n**)

2-Oxo-*N*,2-diphenyl-*N*-tosylacetamide (**2o**)

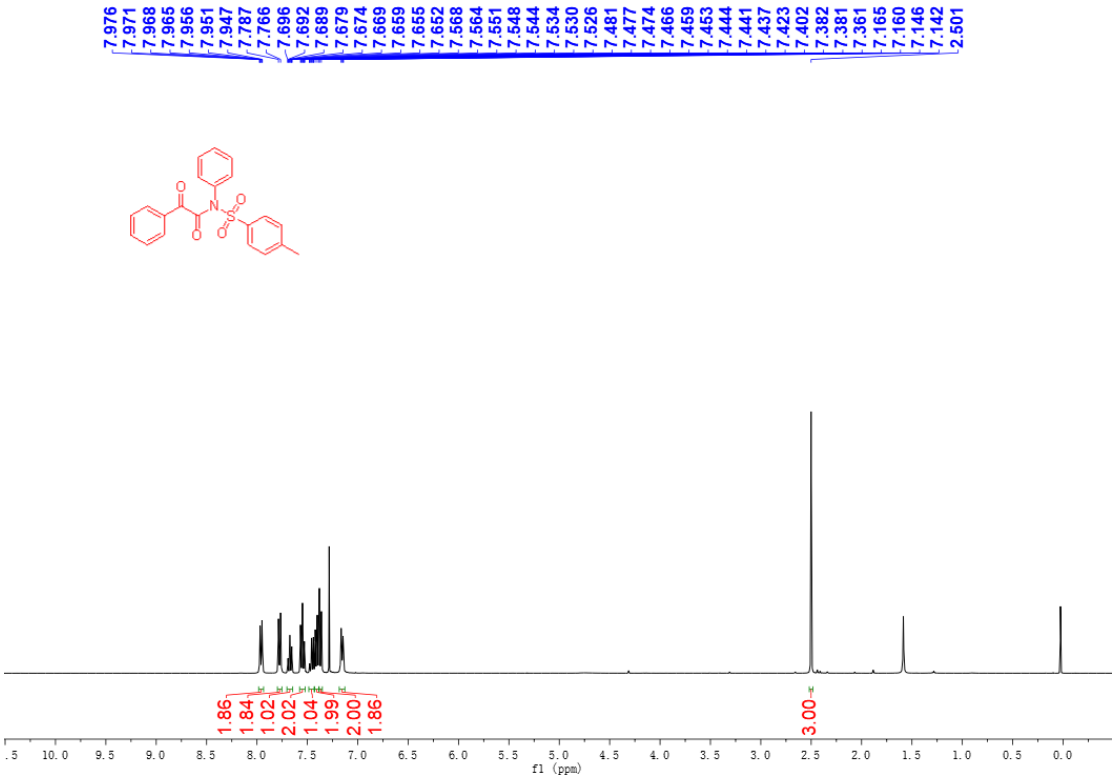


Figure S69. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2-oxo-*N*,2-diphenyl-*N*-tosylacetamide (**2o**)

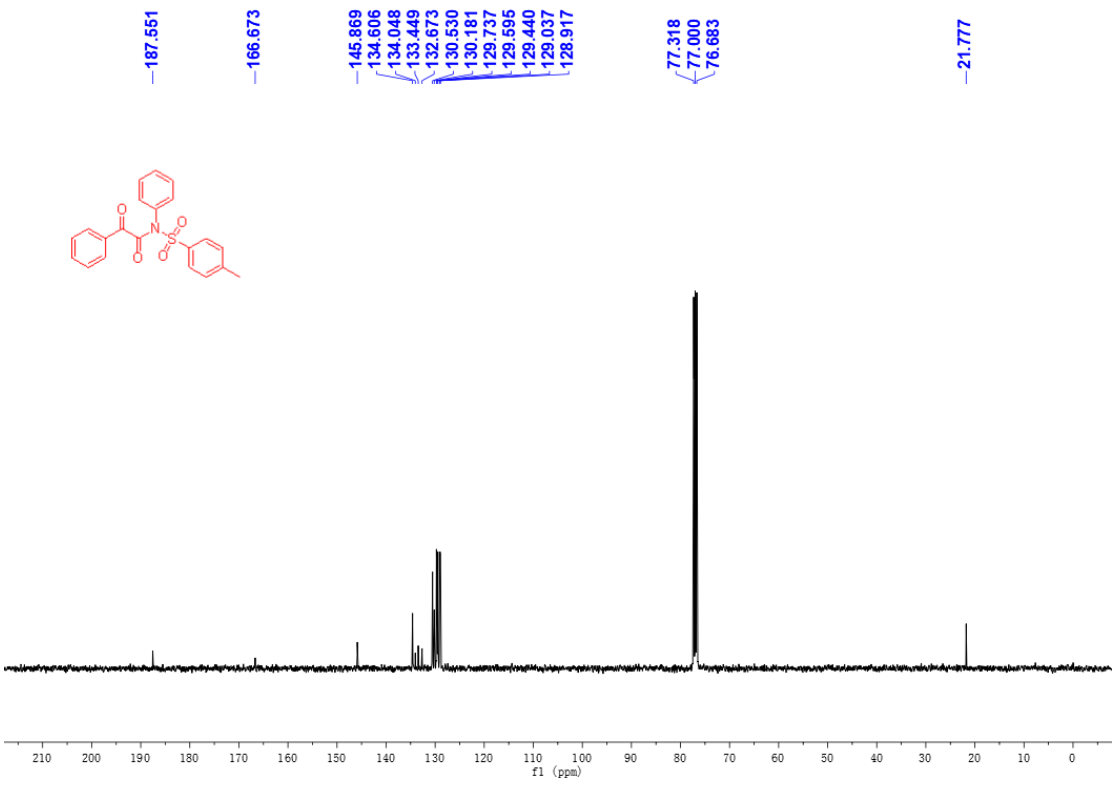


Figure S70. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 2-oxo-*N*,2-diphenyl-*N*-tosylacetamide (**2o**)

N-(4-Methoxyphenyl)-2-oxo-2-phenyl-*N*-tosylacetamide (**2p**)

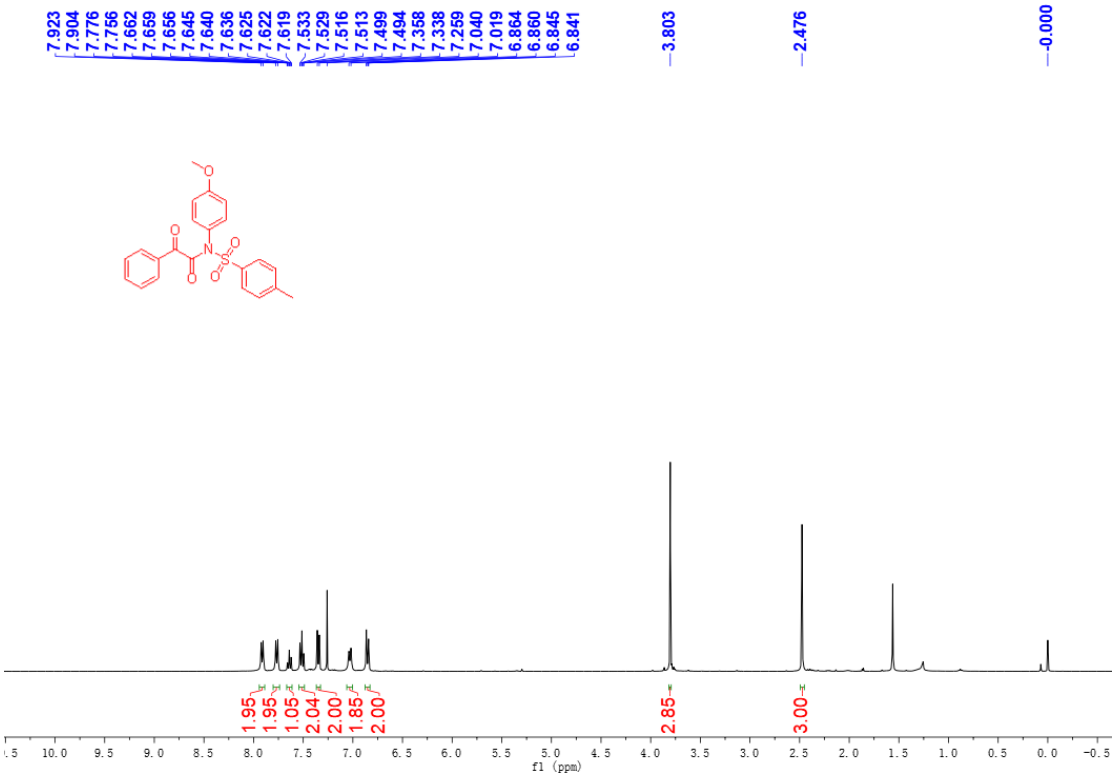


Figure S71. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-(4-methoxyphenyl)-2-oxo-2-phenyl-*N*-tosylacetamide (**2p**)

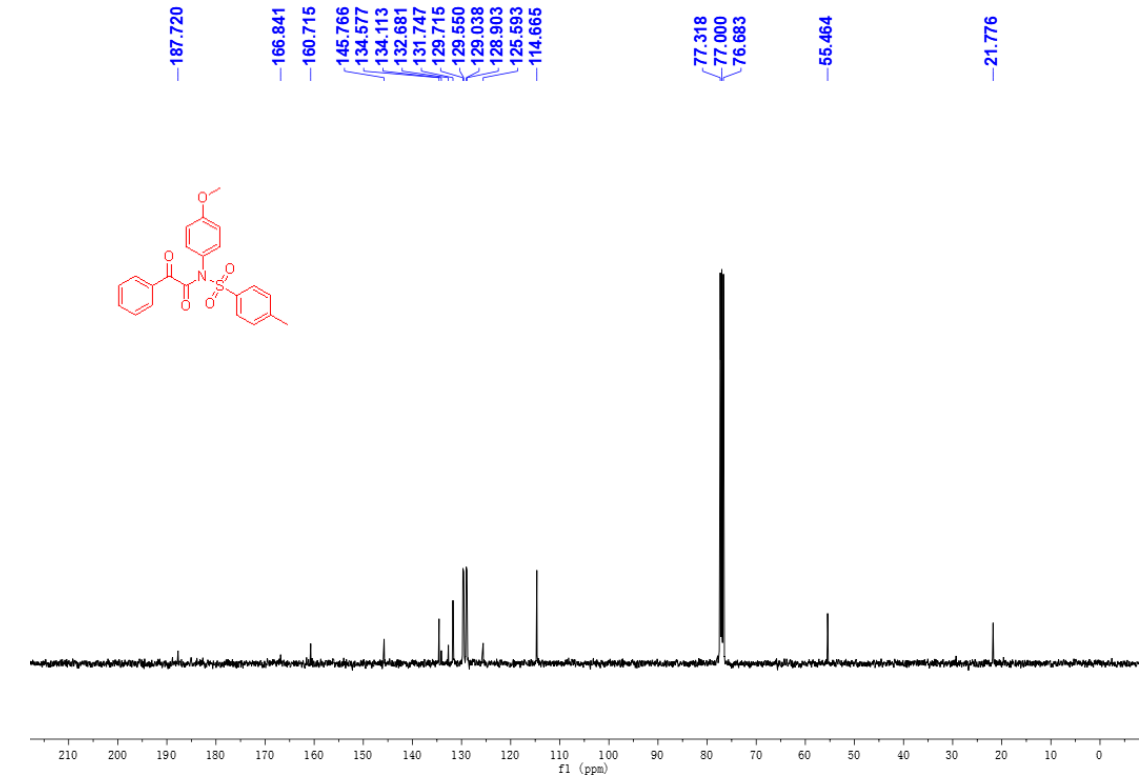


Figure S72. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-(4-methoxyphenyl)-2-oxo-2-phenyl-*N*-tosylacetamide (**2p**)

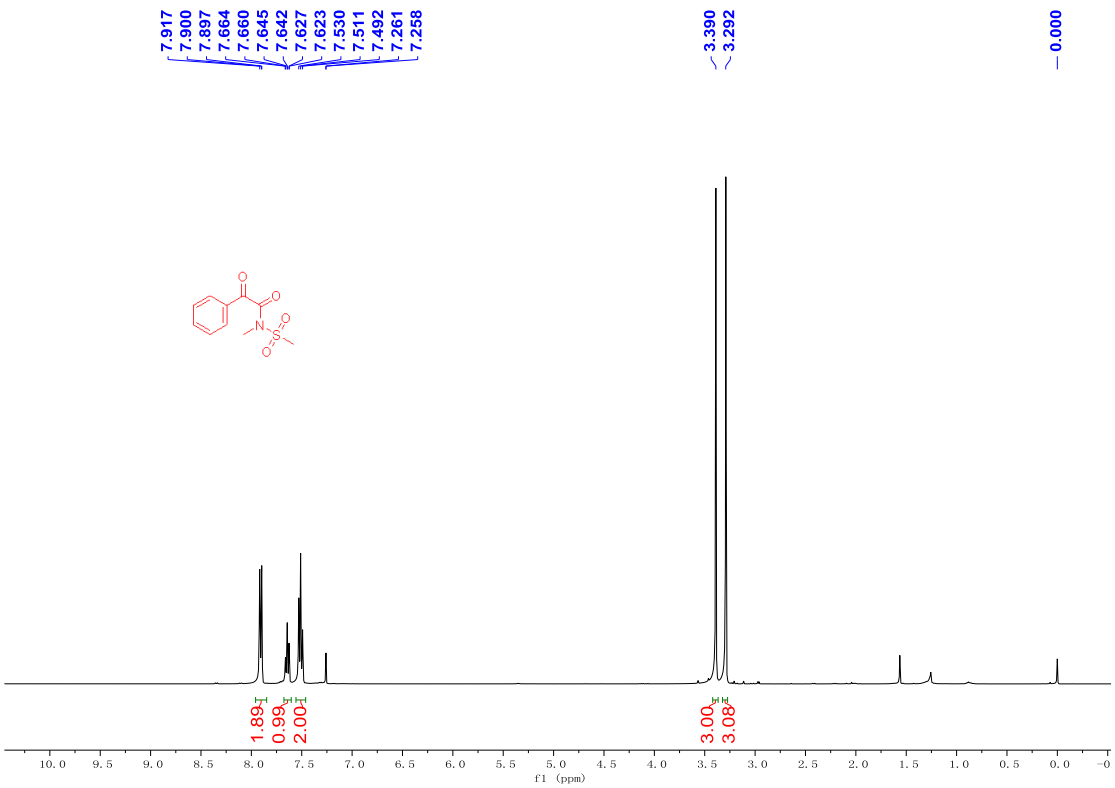


Figure S73. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-methyl-*N*-(methylsulfonyl)-2-oxo-2-phenylacetamide (**2s**)

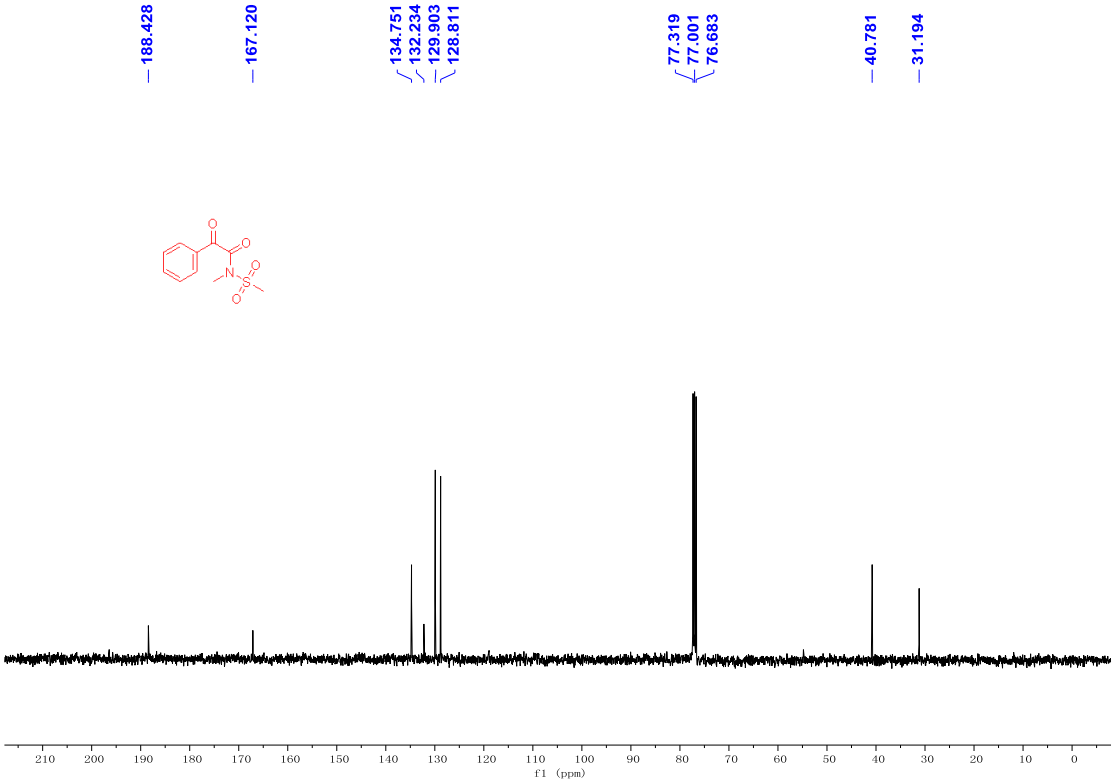


Figure S74. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-methyl-*N*-(methylsulfonyl)-2-oxo-2-phenylacetamide (**2s**)

Copies of NMR spectra of compounds **3** and **4**

N-Cyclohexyl-2-phenyl-*N*-tosylacetamide (**3l**)

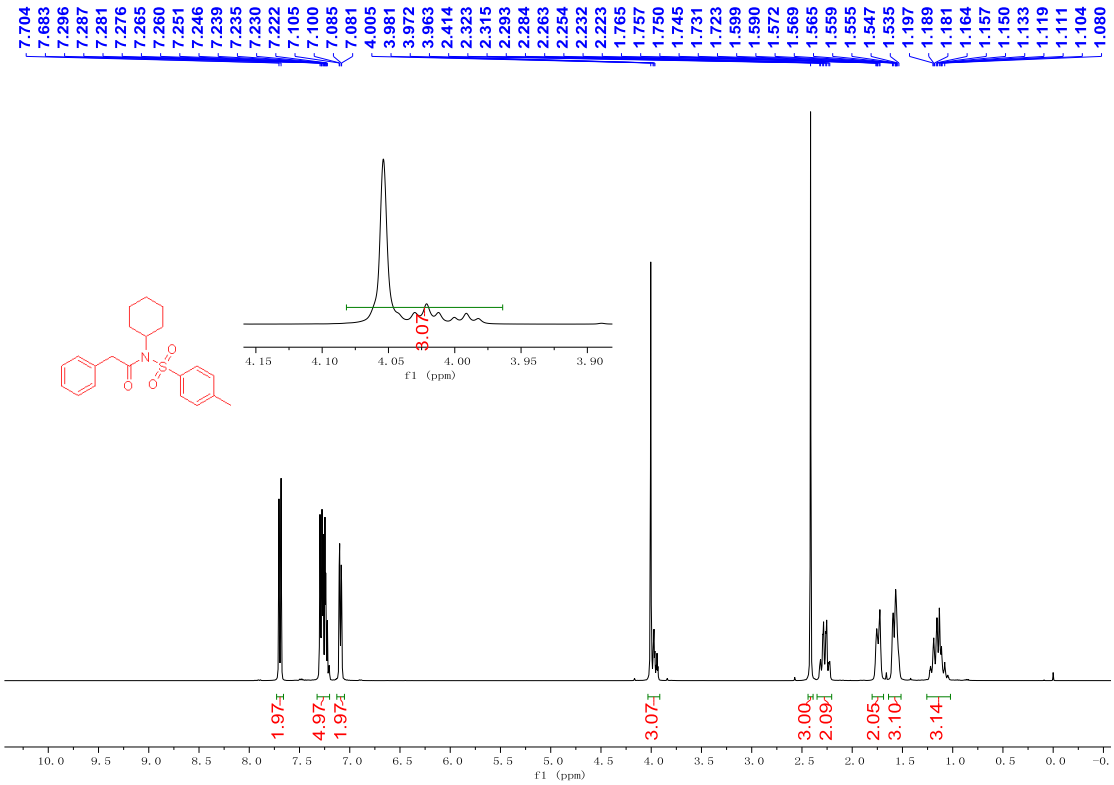


Figure S75. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-cyclohexyl-2-phenyl-*N*-tosylacetamide (**3l**)

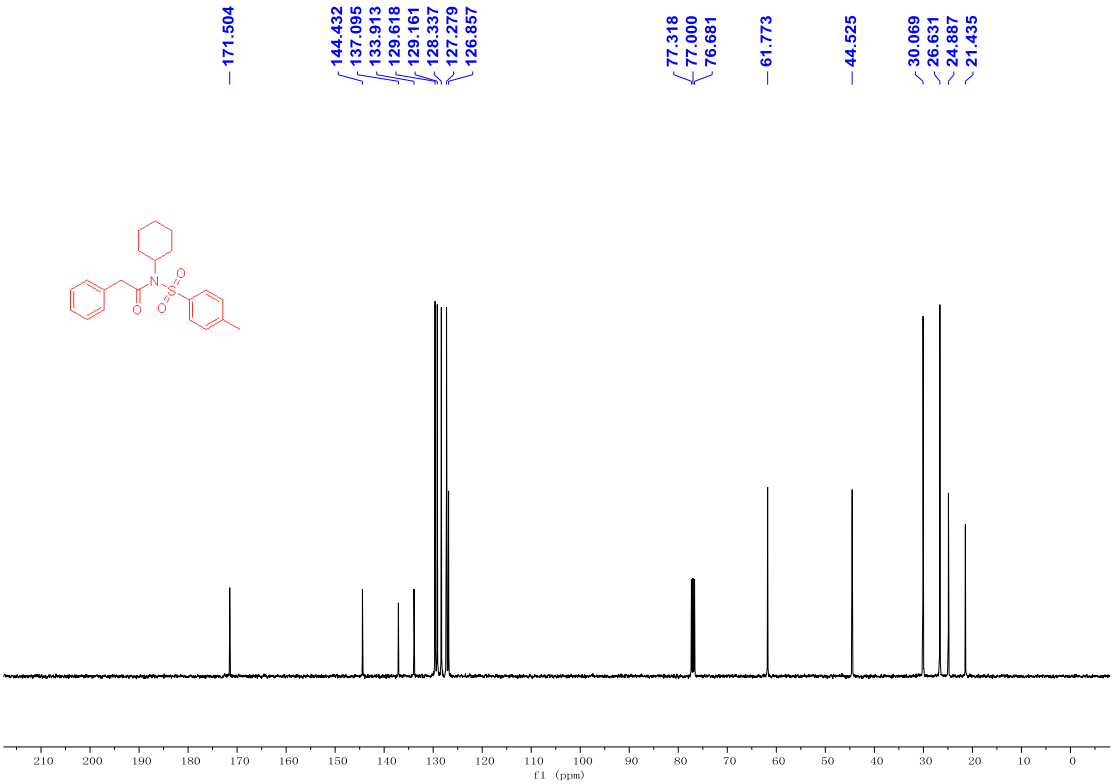


Figure S76. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-cyclohexyl-2-phenyl-*N*-tosylacetamide (**3l**)

2-Hydroxy-*N*-methyl-2-phenyl-*N*-tosylacetamide (**4a**)

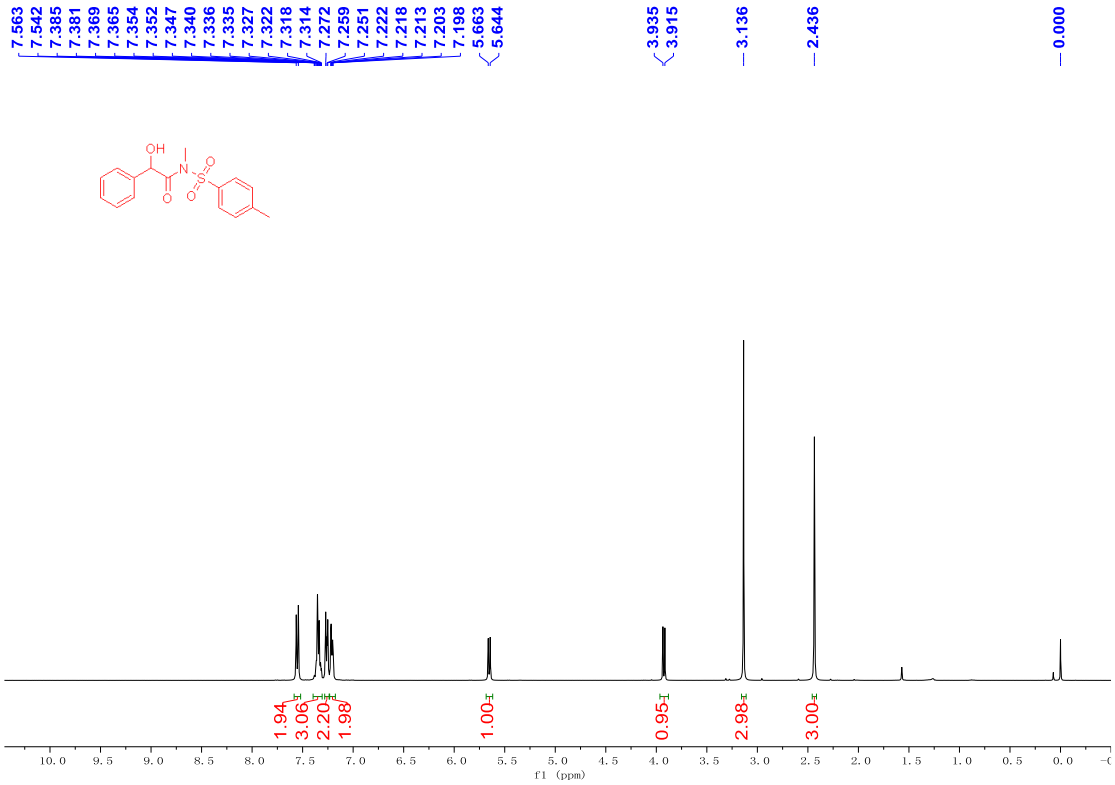


Figure S77. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2-hydroxy-*N*-methyl-2-phenyl-*N*-tosylacetamide (**4a**)

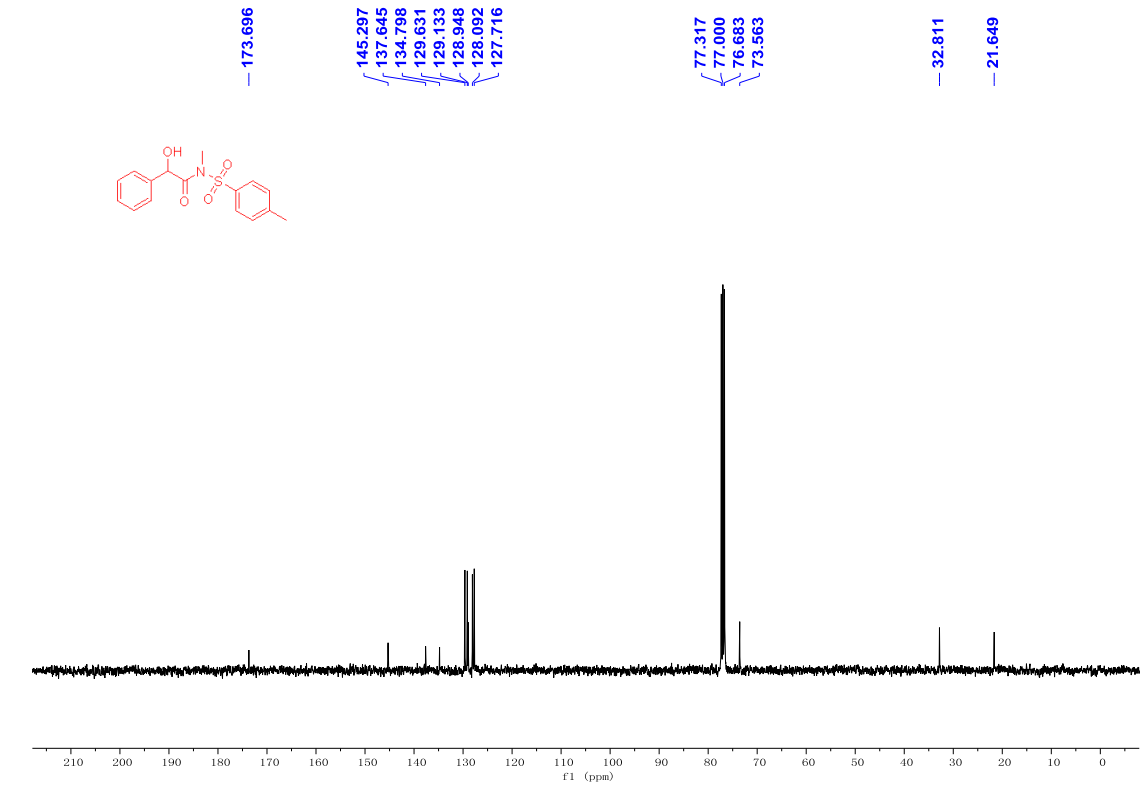


Figure S78. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 2-hydroxy-*N*-methyl-2-phenyl-*N*-tosylacetamide (**4a**)

Copies of HRMS spectra of unknown compounds **2**

N-Methyl-2-oxo-2-phenyl-*N*-(phenylsulfonyl)acetamide (**2b**)
HRMS (ESI-TOF) m/z: [M + Na]+ calcd for $C_{15}H_{13}NNaO_4S^+$ 326.0457, found 326.0451.

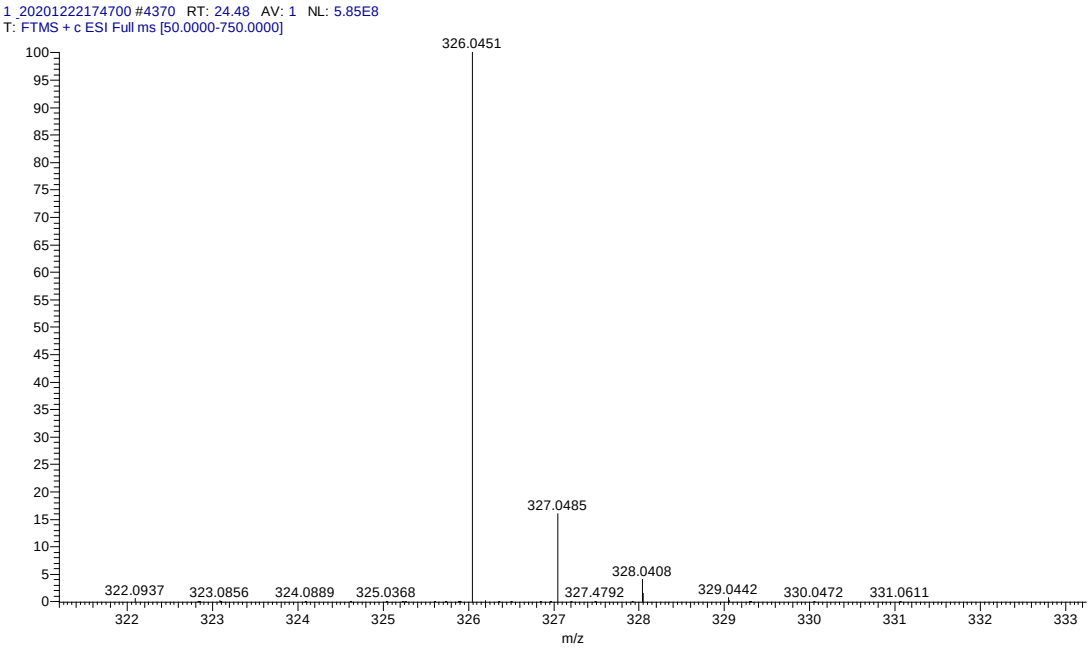


Figure S79. HRMS spectrum of *N*-methyl-2-oxo-2-phenyl-*N*-(phenylsulfonyl)acetamide (**2b**)

N-Methyl-*N*-((4-nitrophenyl)sulfonyl)-2-oxo-2-phenyla-cetamide (**2d**)
HRMS (ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{15}H_{13}N_2O_6S^+$ 349.0489, found 349.0480.

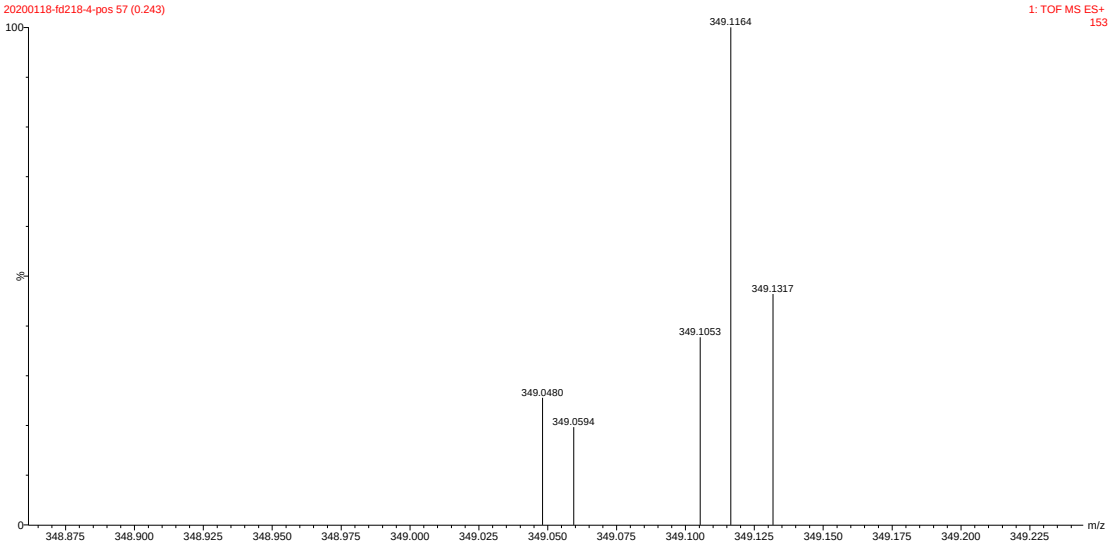


Figure S80. HRMS spectrum of *N*-methyl-*N*-((4-nitrophenyl)sulfonyl)-2-oxo-2-phenyla-cetamide (**2d**)

2-(4-Fluorophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2f**)

HRMS (ESI-TOF) *m*/*z*: $[M + H]^+$ calcd for $C_{16}H_{15}FNO_4S^+$ 336.0700, found 336.0698.

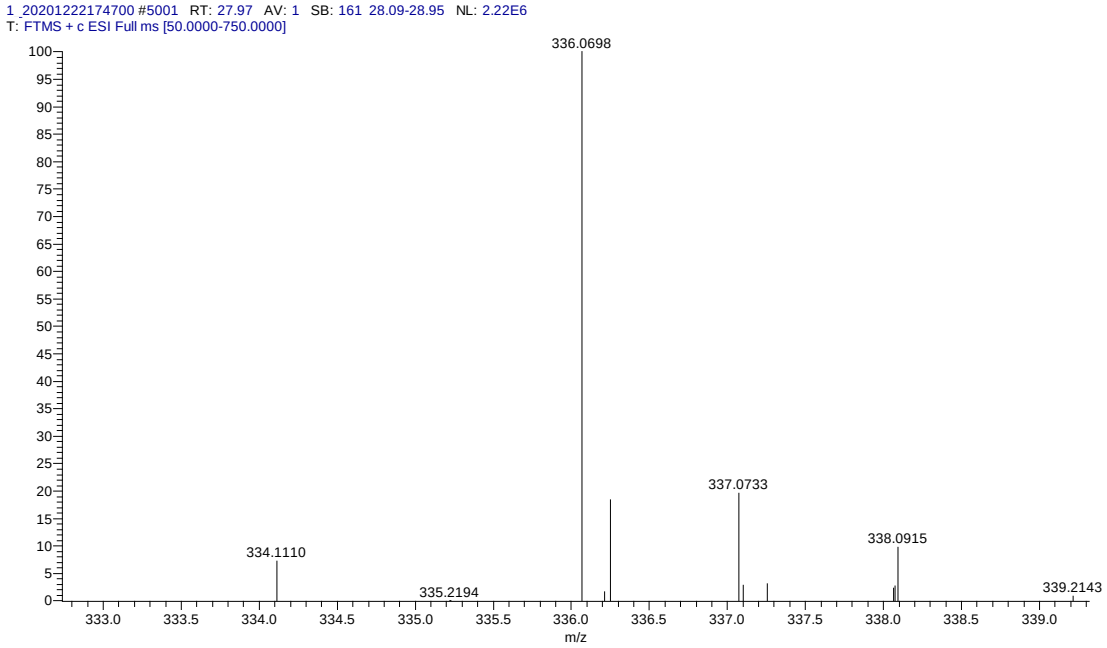


Figure S81. HRMS spectrum of 2-(4-fluorophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2f**)

2-(4-Chlorophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2g**)

HRMS (ESI-TOF) *m*/*z*: $[M + Na]^+$ calcd for $C_{16}H_{14}ClNNaO_4S^+$ 374.0224, found 374.0220.

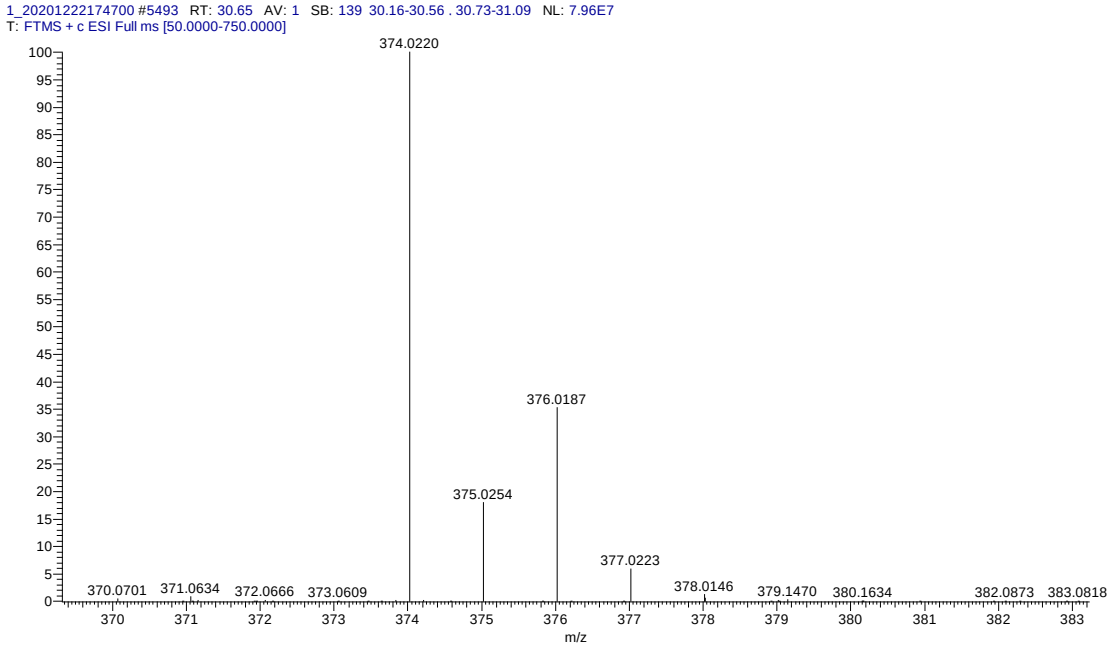


Figure S82. HRMS spectrum of 2-(4-chlorophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2g**)

2-(4-Bromophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2h**)

HRMS (ESI-TOF) *m*/*z*: [M + Na]$^+$ calcd for $C_{16}H_{14}BrNNaO_4S^+$ 417.9719, found 417.9714.

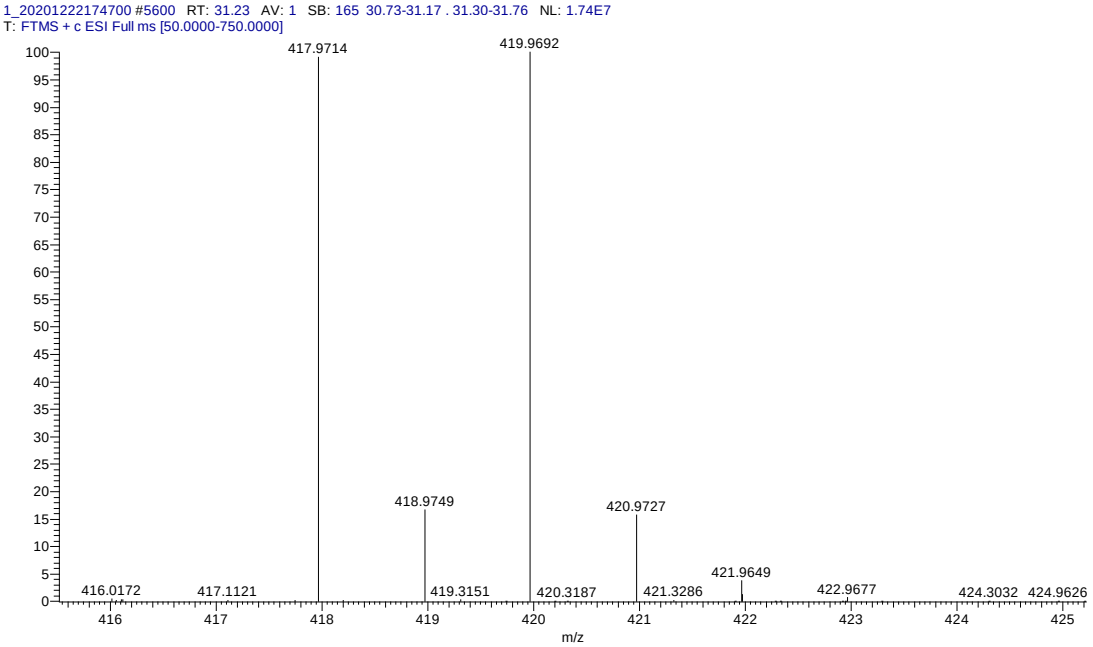


Figure S83. HRMS spectrum of 2-(4-bromophenyl)-*N*-methyl-2-oxo-*N*-tosylacetamide (**2h**)

N-Ethyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2j**)

HRMS (ESI-TOF) *m*/*z*: [M + Na]$^+$ calcd for $C_{17}H_{17}NNaO_4S^+$ 354.0770, found 354.0765.

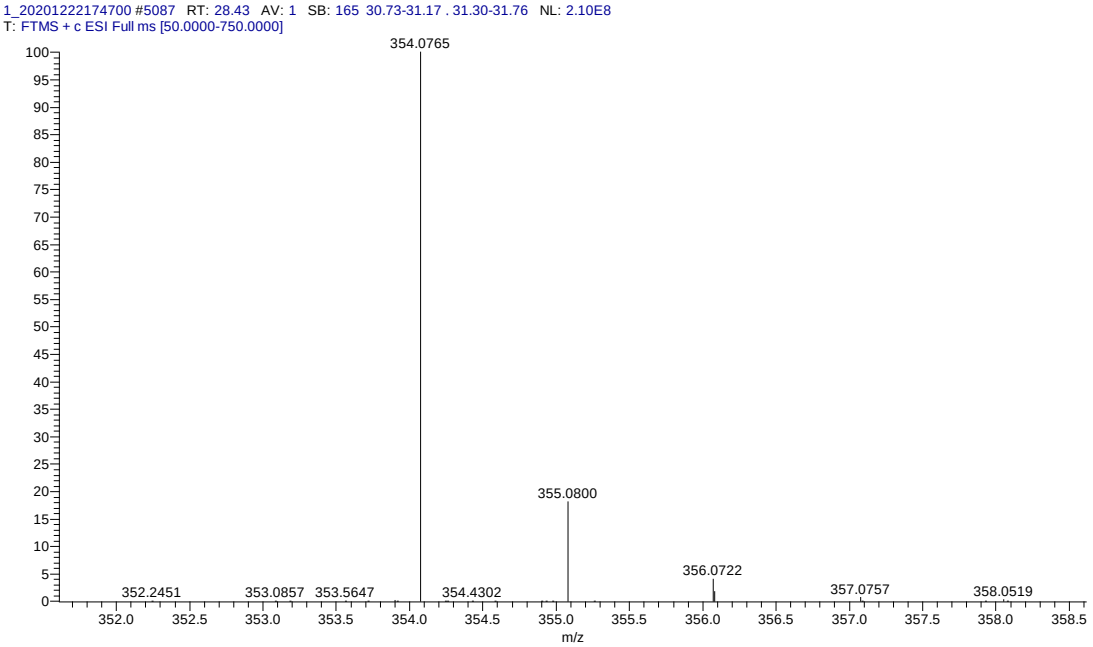


Figure S84. HRMS spectrum of *N*-ethyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2j**)

N-Butyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2k**)

HRMS (ESI-TOF) *m*/*z*: $[M + Na]^+$ calcd for $C_{19}H_{21}NNaO_4S^+$ 382.1083, found 382.1077.

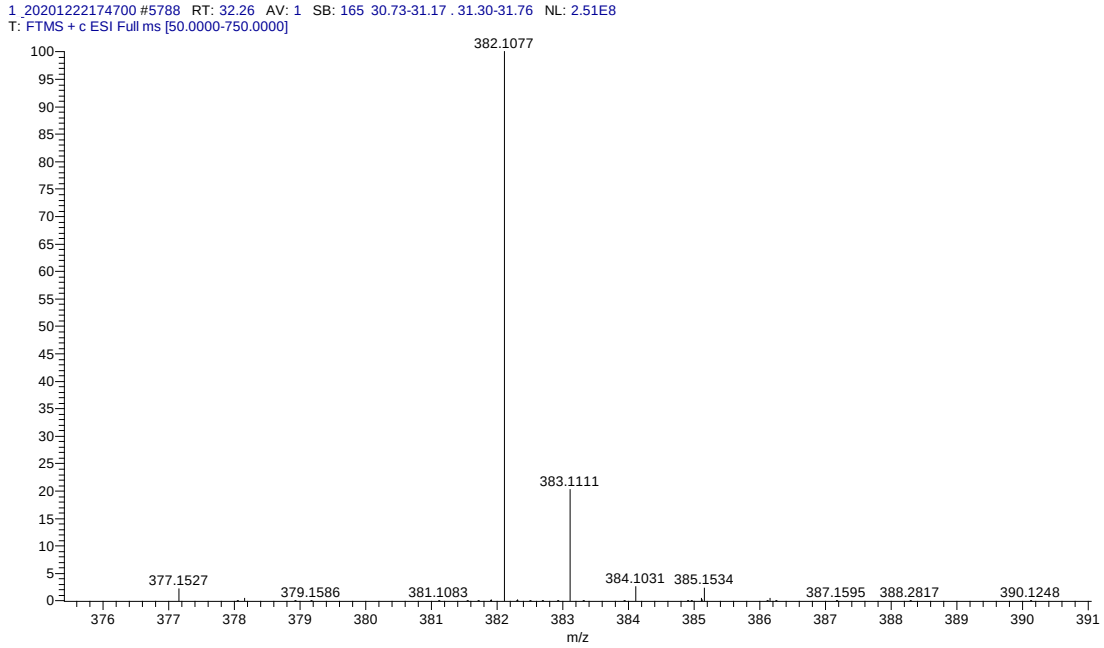


Figure S85. HRMS spectrum of *N*-butyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2k**)

N-Cyclopropyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2m**)

HRMS (ESI-TOF) *m*/*z*: $[M + Na]^+$ calcd for $C_{18}H_{17}NNaO_4S^+$ 366.0770, found 366.0763.

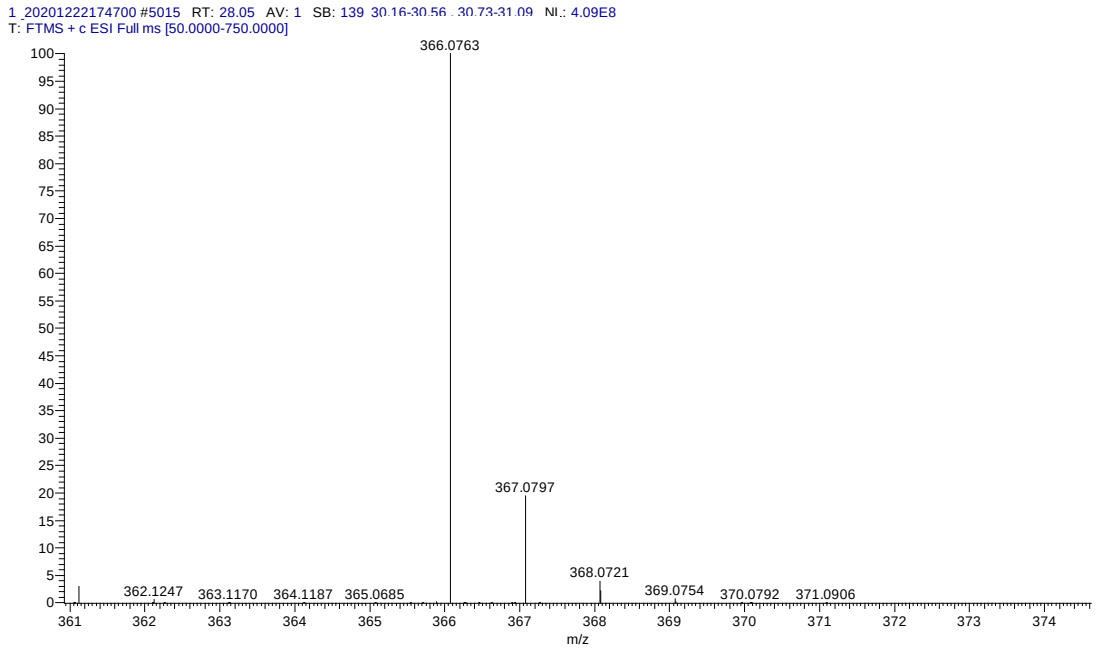


Figure S86. HRMS spectrum of *N*-cyclopropyl-2-oxo-2-phenyl-*N*-tosylacetamide (**2m**)

Copies of HRMS spectra of compounds **3** and **4**

N-Cyclohexyl-2-phenyl-*N*-tosylacetamide (**3l**)
HRMS (ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{26}N0_3S^+$ 372.1628 Found 372.1633.

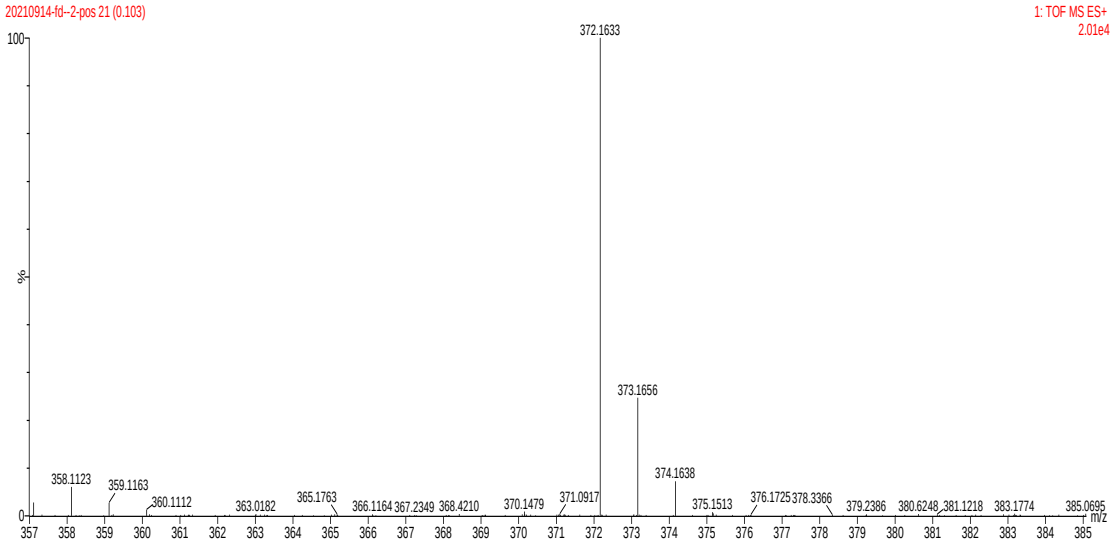


Figure S87. HRMS spectrum of *N*-cyclohexyl-2-phenyl-*N*-tosylacetamide (**3l**)

2-Hydroxy-*N*-methyl-2-phenyl-*N*-tosylacetamide (**4a**)
HRMS (ESI-TOF) *m/z*: [M + Na]+ calcd for $C_{16}H_{17}NaNO_4S^+$ 342.0770, found 342.0778.

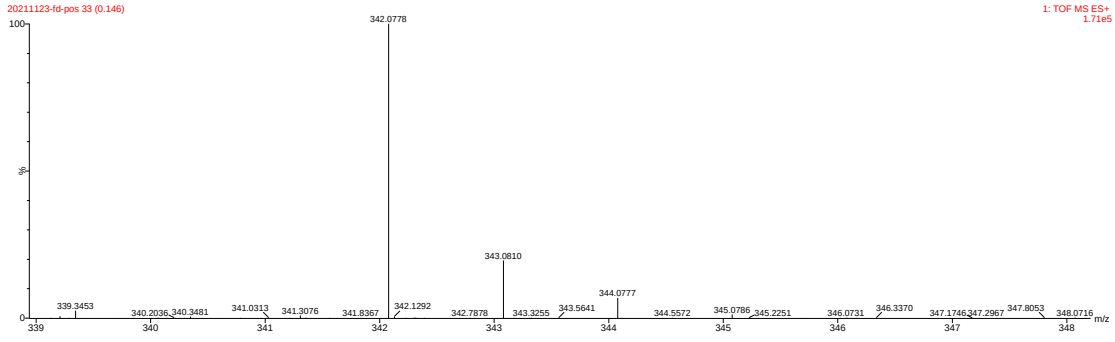


Figure S88. HRMS spectrum of 2-hydroxy-*N*-methyl-2-phenyl-*N*-tosylacetamide (**4a**)