Organic & Biomolecular Chemistry

Benzyl Anion Transfer in the Fragmentation of *N*-(phenylsulfonyl)-benzeneacetamides: A Gas-phase Intramolecular S_NAr Reaction

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Section I Synthesis Procedures

1.1 General procedure for synthesis of compounds **1-7**

A solution of corresponding phenylacetic acids (2 mmol), benzenesulfonamide (2 mmol), 4-dimethyaminopyridine (DMAP, 4 mmol), and 1-[3-(dimethyamino)-propyl]-3-ethylcarbodiimide-hydrochloride (EDCI, 4 mmol) in CH_2Cl_2 (10 mL) was stirred at room temperature for 12 h. Then the resulting mixture was cooled to 5 ℃, and acidified to pH 1 with addition of HCl aqueous solution (10%), which was followed by extraction with CH_2Cl_2 (3 × 10 mL). The combined organic layers were washed with H_2O and brine, dried over Na_2SO_4, and evaporated in *vacuo*. The residue was subjected to silica gel chromatography (PE/EtOAc=3:1) to afford the compounds.

1.1.1 *2-(4-methoxyphenyl)-N-(phenylsulfonyl)acetamide* (**2**)

Pale yellow solid; yield: 73%. ^{1}H NMR (500 MHz, Acetone-d_6): δ (ppm) 8.00 (t, 2H), 7.69 (t, 1H), 7.58 (t, 2H), 7.11 (d, 2H), 6.82 (t, 2H), 3.74 (s, 3H), 3.58 (s, 2H).

1.1.2 *N-(phenylsulfonyl)-2-(p-tolyl)acetamide* (**3**)

White solid; yield: 75%. ^{1}H NMR (400 MHz, Acetone-d_6): δ (ppm) 8.01 (t, 2H), 7.67 (t, 1H), 7.57 (t, 2H), 7.07 (s, 4H), 3.60 (s, 2H), 2.26 (s, 3H).

1.1.3 *2-(4-fluorophenyl)-N-(phenylsulfonyl)acetamide* (**4**)

White solid; yield: 68%. ^{1}H NMR (500 MHz, Acetone-d_6): δ (ppm) 7.96 (t, 2H), 7.63 (t, 1H), 7.54 (t, 2H), 7.25-7.22 (m, 2H), 7.02-6.99 (m, 2H), 3.59 (s, 2H).

1.1.4 *2-(4-chlorophenyl)-N-(phenylsulfonyl)acetamide* (**5**)

White solid; yield: 72%. ^{1}H NMR (500 MHz, Acetone-d_6): δ (ppm) 7.91 (d, 2H), 7.60-7.55 (m, 3H), 7.35 (s, 4H), 3.65 (s, 2H).

1.1.5 *2-(4-bromophenyl)-N-(phenylsulfonyl)acetamide* (**6**)

White solid; yield: 71%. ^{1}H NMR (500 MHz, Acetone-d_6): δ (ppm) 8.00 (d, 2H), 7.69 (t, 1H), 7.58 (t, 2H), 7.44(d, 2H), 7.15(d, 2H), 3.66 (s, 2H).

1.1.6 *methyl 4-(2-oxo-2-(phenylsulfonamido)ethyl)benzoate* (**7**)

White solid; yield: 68%. ^{1}H NMR (500 MHz, Acetone-d_6): δ (ppm) 8.01 (d, 2H), 7.91 (d, 2H), 7.70 (t, 1H), 7.59 (m, 2H), 7.34(d, 2H), 3.86(s, 3H), 3.78 (s, 2H).

1.2 Procedure for synthesis of compound **8**

Further deuteration was achieved by dissolving compound **1** (1 mmol) in 5 mL CD_3OD, then stirring with 40% NaOD in D_2O (0.5 mL) for 1 day at room temperature. More than 99% deutration has been achieved by the repetition of the forgoing precedure. After adding 20 % DCl in D_2O (1 mL), the mixture was stirred for another 30 min, and evaporated in *vacuo* to afford compound **8**.

1.2.1 *N-(phenylsulfonyl)-α,α-d_2-benzeneacetamide* (**8**)

Pale yellow solid. ^{1}H NMR (500 MHz, Acetone-d_6): δ (ppm) 7.98 (d, 2H), 7.64 (t, 1H), 7.54 (t, 2H), 7.23-7.16 (m, 5H).

1.3 General procedure for synthesis of compounds **9-11**

To a round-bottom flask (25 mL) were added NaH (120 mg, 3 mmol, 60%), THF (10 mL) and 2-phenylacetamide (2 mmol). The solution mixture was allowed to stir at room temperature for 1 h. After stirring, the corresponding benzenesulfonyl chlorides (2 mmol) was added into the solution mixture and then heated to 70 ℃ for 1 day. After reacion, the mixture was diluted with EtOAc, extracted by EtOAc/H_2O and then collected the organic layer. The residue was then dried over the Na_2SO_4 and concentrated in *vacuo*. Purification through silica gel chromatography (PE/EtOAc=3:1) afforded the corresponding products.

1.3.1 *2-phenyl-N-tosylacetamide* (**9**)

White solid; yield: 65%. ^{1}H NMR (500 MHz, Acetone-d_6): δ (ppm) 7.88 (d, 2H), 7.38 (d, 1H), 7.28-7.19 (m, 5H), 3.64 (s, 2H), 2.40 (s, 3H).

1.3.2 *N-((2,6-dichlorophenyl)sulfonyl)-2-phenylacetamide* (**10**)

White solid; yield: 61%. ^{1}H NMR (500 MHz, Acetone-d_6): δ (ppm) 7.59-7.54 (m, 3H), 7.32-7.23 (m, 5H), 3.73 (s, 2H).

1.3.3 *N-(mesitylsulfonyl)-2-phenylacetamide* (**11**)

White solid; yield: 68%. ^{1}H NMR (500 MHz, Acetone-d_6): δ (ppm) 7.28-7.19 (m, 5H), 6.99 (s, 2H), 3.66 (s, 2H), 2.62 (s, 6H), 2.26 (s, 3H).

1.4 Procedure for synthesis of compound **12**

To a solution of 2-benzylaniline (500 mg, 2.7 mmol) in H_2O (7.3 mL) at 0 ℃ was added concentrated HCl (0.4 mL). A cold solution of $NaNO_2$ (188 mg, 2.7 mmol) in H_2O (1.5 mL) was added slowly and stirred for 15 min. The cold diazonium solution was added slowly to a solution of potassium ethyl xanthate (525 mg, 3.3 mmol) in H_2O (0.65 mL) at 45 ℃. The reaction mixture was stirred for an additional 30 min at 45 ℃ and then cooled to room temperature. The reaction mixture was extracted with Et_2O (3 × 50 mL). The combined organic extracts were washed with 10% NaOH solution (100 mL), H_2O (3 × 50 mL), brine (50 mL), dried over Na_2SO_4, filtered and evaporated in *vacuo*. The resulting crude crude compound was dissolved in ethanol (8 mL) and heated to reflux. KOH (654 mg, 11.6 mmol) were added and refluxing continued overnight. The solution was cooled to room temperature and the ethanol was evaporated in *vacuo*. The residue was dissolved in water and washed with Et_2O (100 mL). The aqueous layer was acidified with 2 N HCl and extracted with Et_2O (3 × 50 mL). The organic extracts were washed with H_2O (50 mL), brine (50 mL), dried over Na_2SO_4, filtered and evaporated in *vacuo*. The residue was subjected to silica gel

chromatography (PE) to afford the compound (2-benzylbenzenethiol).

The crude 2-benzylbenzenethiol was dissolved in a mixture of 12 mL of 2.5% aqueous NaOH and 12 mL of ethanol. Aqueoius H_2O_2 (30%, 0.6 mL) was added to the solution with stirring at room temperature. The reaction was monitored by TLC. After the reaction was complete, the solvent was evaporated off in *vacuo*. The residue was dissolved in H_2O and acidified by the addition of diluted HCl at 0 ℃. The solution was extracted with Et_2O, and dried over Na_2SO_4. Then the Et_2O was removed to give 2-benzylbenzenesulfinic acid.

1.4.1 *2-benzylbenzenethiol*

White solid; yield: 23%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.28-7.25 (t, 3H), 7.20-7.14 (m, 3H), 7.11-7.05 (m, 3H), 4.03 (s, 2H), 3.25 (s, 1H).

1.4.2 *2-benzylbenzenesulfinic acid*

Pale yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.98 (br, 1H), 7.52 (dd, 1H, J = 7.5, 1.5 Hz), 7.34 (t, 1H), 7.24-7.28 (m, 2H), 7.17-7.21 (m, 2H), 7.12-7.14 (m, 3H), 4.12 (s, 2H).

Table S1. Accurate masses of selected ions derived from deprotonated compounds **1** to **12**

Compound	Nominal *m/z*	Elemental composition	Accurate mass	Observed mass	Relative error (ppm)
1	274	$C_{14}H_{12}NO_3S^-$	274.0543	274.0543	0
	256	$C_{14}H_{10}NO_2S^-$	256.0438	256.0430	-3.1
	231	$C_{13}H_{11}O_2S^-$	231.0485	231.0482	-1.3
	182	$C_7H_4NO_3S^-$	181.9917	181.9915	-1.1
	156	$C_6H_6NO_2S^-$	156.0125	156.0127	1.3
	93	$C_6H_5O^-$	93.0346	93.0345	-1.1
	91	$C_7H_7^-$	91.0553	91.0552	-1.1
2	304	$C_{15}H_{14}NO_4S^-$	304.0649	304.0643	-2.0
3	288	$C_{15}H_{14}NO_3S^-$	288.0700	288.0707	2.4
4	292	$C_{14}H_{11}FNO_3S^-$	292.0449	292.0445	-1.4
5	308	$C_{14}H_{11}ClNO_3S^-$	308.0154	308.0162	2.6
6	352	$C_{14}H_{11}BrNO_3S^-$	351.9649	351.9655	1.7
7	332	$C_{16}H_{14}NO_5S^-$	332.0598	332.0595	-0.9
8	276	$C_{14}H_{10}D_2NO_3S^-$	276.0669	276.0666	-1.1
9	288	$C_{15}H_{14}NO_3S^-$	288.0700	288.0702	0.7
10	342	$C_{14}H_{10}Cl_2NO_3S^-$	341.9764	341.9766	0.6
11	316	$C_{17}H_{18}NO_3S^-$	316.1013	316.1013	0
12	231	$C_{13}H_{11}O_2S^-$	231.0485	231.0482	-1.3

Figure S1. The CID MS spectra of $[M-H]^-$ of compounds **2-7**

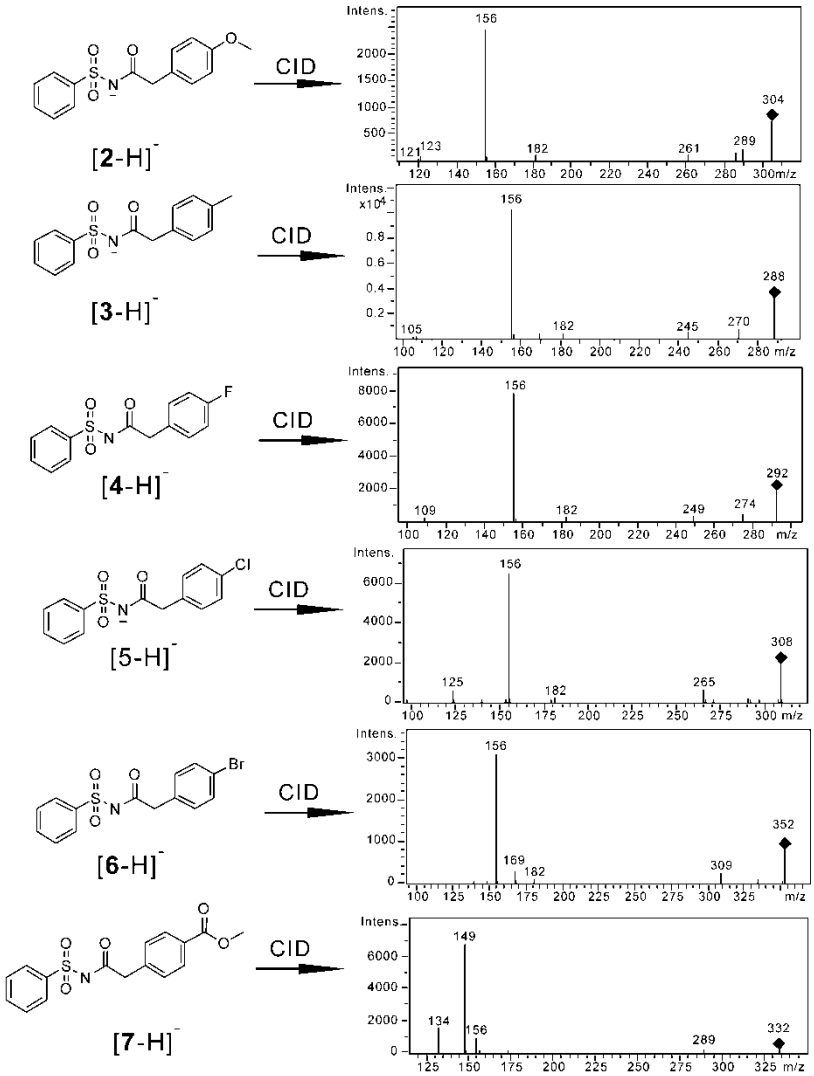
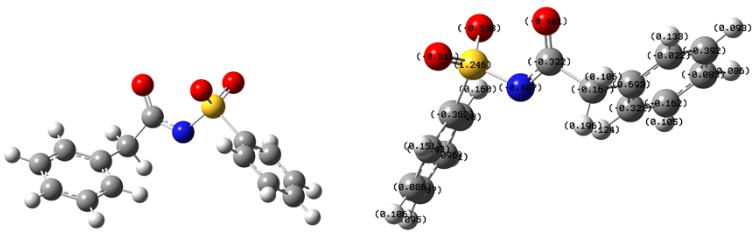


Figure S2. Figures, cartesian coordinates, total energies, zero point energy corrections of all optimized structures discussed in the text and charge distribution of **A-1** at the B3LYP/6-31++G (*d, p*) level

A-1



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4	6	0.000002742	-0.000004584	-0.000001132
5	6	0.000006239	0.000000315	0.000005950
6	6	-0.000000752	0.000000296	-0.000000491
7	1	0.000003724	-0.000002406	-0.000003262
8	1	-0.000000026	-0.000001987	-0.000004554

9	1	0.000000220	0.000001550	0.000003154
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11	1	0.000007595	-0.000000608	-0.000000470
12	16	0.000000978	-0.000000524	0.000001527
13	8	-0.000005499	0.000003081	0.000000262
14	8	-0.000007222	-0.000002431	-0.000003237
15	7	0.000000201	-0.000002995	-0.000000343
16	6	-0.000004667	0.000002102	-0.000003410
17	8	-0.000003775	-0.000001192	-0.000000132
18	6	-0.000002342	-0.000003983	-0.000002136
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21	6	-0.000001635	0.000001493	-0.000002332
22	6	-0.000000119	0.000000022	0.000002288
23	6	-0.000001608	0.000000370	0.000003078
24	6	-0.000003227	0.000002443	0.000002758
25	1	-0.000004342	0.000000043	-0.000000794
26	6	0.000002791	0.000000788	0.000002940
27	1	0.000002316	-0.000000290	-0.000000096
28	6	0.000000678	0.000002013	0.000002261
29	1	-0.000002836	0.000001579	0.000002703
30	1	0.000003255	0.000002100	0.000003763

31	1	0.000000864	0.000002698	0.000004967

Zero-point correction= 0.232579 (Hartree/Particle)

Thermal correction to Energy= 0.249217

Thermal correction to Enthalpy= 0.250161

Thermal correction to Gibbs Free Energy= 0.182523

Sum of electronic and zero-point Energies= -1219.164467

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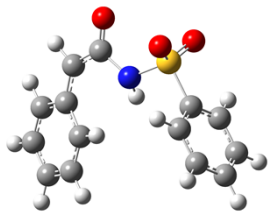
Sum of electronic and thermal Enthalpies= -1219.146884

Sum of electronic and thermal Free Energies= -1219.214523

A-2



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4	6	-0.000002771	-0.000001036	0.000000505
5	6	-0.000005310	0.000001612	-0.000000901
6	6	-0.000003522	0.000001798	0.000000994
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8	1	-0.000002068	0.000000297	0.000003609
9	1	-0.000002302	0.000001157	-0.000000544
10	1	-0.000004962	0.000002388	-0.000001429
11	1	-0.000006622	0.000002194	0.000001860
12	16	0.000003377	-0.000000099	0.000000579
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14	8	-0.000000015	-0.000002692	0.000003923
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16	1	0.000000846	0.000000019	0.000001021
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22	6	-0.000000088	0.000000361	-0.000000191
23	6	0.000004046	-0.000001764	-0.000002571
24	6	0.000000082	-0.000000606	-0.000002701
25	1	0.000000594	0.000000438	-0.000002080

26	6	0.000002373	-0.000000571	-0.000000511
27	1	0.000005071	-0.000001777	-0.000000870
28	6	0.000001540	0.000000195	-0.000003992
29	1	-0.000001144	0.000001153	-0.000002551
30	1	0.000003756	-0.000000898	-0.000002492
31	1	0.000000372	0.000000770	-0.000002385

Cartesian Forces: Max 0.000006622 RMS 0.000002495

Internal Coordinate Forces (Hartree/Bohr or radian)

Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	C							
2	C	1	-0.000012(1)					
3	C	2	0.000014(2)	1	-0.000409(31)			
4	C	3	-0.000012(3)	2	-0.000059(32)	1	0.000020(60)	0
5	C	4	0.000002(4)	3	-0.000035(33)	2	0.000008(61)	0
6	C	1	-0.000010(5)	2	0.000033(34)	3	-0.000010(62)	0
7	H	1	0.000002(6)	6	0.000013(35)	5	-0.000002(63)	0
8	H	2	0.000004(7)	1	0.000004(36)	6	0.000000(64)	0
9	H	4	-0.000002(8)	3	-0.000001(37)	2	-0.000002(65)	0
10	H	5	-0.000004(9)	4	0.000008(38)	3	-0.000004(66)	0

11	H	6	-0.000002(	10)	1	-0.000014(	39)	2	0.000004(	67)	0
12	S	3	-0.000018(	11)	2	0.000275(	40)	1	0.000482(	68)	0
13	O	12	-0.000001(	12)	3	0.000001(	41)	2	0.000001(	69)	0
14	O	12	0.000000(	13)	3	0.000011(	42)	2	0.000007(	70)	0
15	N	12	0.000015(	14)	3	-0.000327(	43)	2	0.000338(	71)	0
16	H	15	-0.000001(	15)	12	0.000001(	44)	3	0.000000(	72)	0
17	C	15	-0.000017(	16)	12	0.000253(	45)	3	-0.000010(	73)	0
18	O	17	-0.000001(	17)	15	0.000003(	46)	12	-0.000009(	74)	0
19	C	17	0.000004(	18)	15	-0.000168(	47)	12	0.000196(	75)	0
20	H	19	-0.000001(	19)	17	0.000004(	48)	15	-0.000010(	76)	0
21	C	19	0.000017(	20)	17	-0.000119(	49)	15	0.000034(	77)	0
22	C	21	0.000014(	21)	19	-0.000045(	50)	17	-0.000008(	78)	0
23	C	21	-0.000001(	22)	19	0.000042(	51)	17	-0.000050(	79)	0
24	C	22	0.000006(	23)	21	0.000047(	52)	19	0.000004(	80)	0
25	H	22	0.000001(	24)	21	0.000004(	53)	19	0.000000(	81)	0
26	C	23	0.000003(	25)	21	-0.000014(	54)	19	0.000012(	82)	0
27	H	23	-0.000002(	26)	21	0.000002(	55)	19	-0.000009(	83)	0
28	C	24	-0.000003(	27)	22	0.000020(	56)	21	-0.000001(	84)	0
29	H	24	0.000002(	28)	22	-0.000001(	57)	21	-0.000003(	85)	0
30	H	26	-0.000001(	29)	23	0.000006(	58)	21	-0.000006(	86)	0
31	H	28	0.000001(	30)	24	-0.000005(	59)	22	0.000000(	87)	0

Zero-point correction= 0.231600 (Hartree/Particle)

Thermal correction to Energy= 0.248266

Thermal correction to Enthalpy= 0.249210

Thermal correction to Gibbs Free Energy= 0.184408

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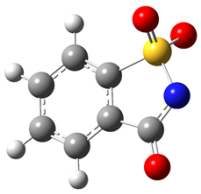
Sum of electronic and thermal Free Energies= -1219.177005

C.*o*



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5	6	0.000070043	-0.000018713	-0.000009390

6	1	0.000008931	0.000003186	-0.000011988
7	1	0.000021848	-0.000016851	0.000001132
8	1	0.000008443	0.000005386	0.000002819
9	16	-0.000051795	-0.000193414	-0.000003903
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11	8	-0.000003268	0.000034918	-0.000008584
12	7	-0.000027963	0.000026315	0.000298624
13	6	0.000002169	0.000028048	-0.000190213
14	8	0.000062711	-0.000019179	-0.000049266
15	6	-0.000005101	-0.000023759	-0.000071804
16	1	0.000006249	0.000014737	0.000008218

Zero-point correction= 0.102646 (Hartree/Particle)

Thermal correction to Energy= 0.111684

Thermal correction to Enthalpy= 0.112628

Thermal correction to Gibbs Free Energy= 0.067923

Sum of electronic and zero-point Energies= -947.710419

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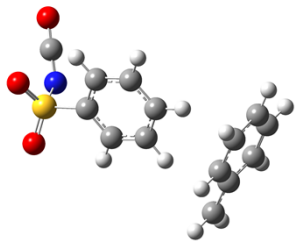
INC-1



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5	6	-0.000004452	0.000010519	-0.000010262
6	6	0.000005512	-0.000001459	0.000000248
7	1	-0.000000736	-0.000001624	-0.000001041
8	1	-0.000000415	-0.000003368	-0.000000345
9	1	-0.000000932	-0.000000064	0.000000405
10	1	0.000001586	-0.000019619	0.000009450
11	1	-0.000001846	-0.000000441	-0.000000785
12	16	0.000018215	-0.000010286	-0.000008140
13	8	0.000000435	0.000001080	0.000002607
14	8	-0.000019094	0.000014299	0.000011858
15	7	-0.000002373	-0.000005646	0.000002330

16	6	0.000003347	-0.000000508	-0.000012138
17	8	-0.000002938	-0.000004068	0.000005772
18	6	0.000002543	0.000001522	-0.000001735
19	6	-0.000000656	0.000003885	0.000012121
20	6	0.000000982	0.000003479	-0.000000250
21	6	-0.000000357	0.000000586	-0.000000743
22	1	0.000001932	0.000001447	-0.000002025
23	6	0.000001550	0.000000889	0.000001068
24	1	-0.000000894	0.000001208	0.000000193
25	6	-0.000000047	-0.000001946	-0.000001017
26	1	0.000002898	0.000000123	-0.000000121
27	1	-0.000001101	0.000000328	-0.000000028
28	1	0.000000738	0.000000981	0.000000337
29	6	0.000001153	0.000011217	-0.000007702
30	1	0.000001952	0.000001659	-0.000000680
31	1	-0.000002157	0.000001332	0.000006320

Zero-point correction= 0.226175 (Hartree/Particle)

Thermal correction to Energy= 0.244911

Thermal correction to Enthalpy= 0.245855

Thermal correction to Gibbs Free Energy= 0.173532

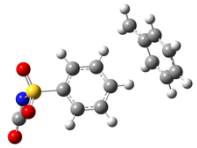
Sum of electronic and zero-point Energies= -1219.089001

Sum of electronic and thermal Energies= -1219.070265

Sum of electronic and thermal Enthalpies= -1219.069321

Sum of electronic and thermal Free Energies= -1219.141644

INC-1(2)



Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000021816	-0.000028811	-0.000010462
2	6	0.000000412	-0.000007238	0.000021190
3	6	-0.000007936	-0.000018993	-0.000015867
4	6	0.000004957	0.000009773	-0.000021436
5	6	0.000032577	0.000022097	0.000031546
6	6	-0.000013388	-0.000101600	-0.000002844
7	1	-0.000001826	-0.000003540	-0.000000069
8	1	0.000006620	0.000000366	0.000001560
9	1	0.000004473	-0.000000680	-0.000001333
10	1	-0.000016635	-0.000058188	-0.000017458
11	1	-0.000021856	0.000156306	0.000009347
12	16	-0.000144046	0.000019180	0.000048512

13	8	0.000059188	0.000027371	-0.000026677
14	8	0.000046411	-0.000006590	0.000002323
15	7	0.000009138	0.000020676	0.000014243
16	6	-0.000026457	-0.000014392	-0.000060358
17	8	0.000017584	-0.000014005	0.000034720
18	6	-0.000014804	0.000009070	-0.000014244
19	6	-0.000003500	0.000001704	-0.000006702
20	6	0.000008354	0.000009049	0.000015734
21	6	0.000017787	-0.000002310	-0.000006454
22	1	0.000007325	0.000009537	0.000012003
23	6	0.000018098	-0.000013588	-0.000004688
24	1	0.000001192	0.000004218	-0.000019442
25	6	-0.000013157	-0.000022729	0.000002751
26	1	-0.000001176	-0.000003800	0.000013744
27	1	-0.000003054	-0.000012794	-0.000010342
28	1	0.000001856	-0.000019254	0.000009302
29	6	0.000011012	0.000032781	0.000006623
30	1	0.000005532	0.000002227	-0.000017544
31	1	-0.000006498	0.000004157	0.000012324

Zero-point correction= 0.226315 (Hartree/Particle)

Thermal correction to Energy= 0.245029

Thermal correction to Enthalpy= 0.245973

Thermal correction to Gibbs Free Energy= 0.173867

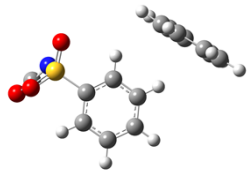
Sum of electronic and zero-point Energies= -1219.088259

Sum of electronic and thermal Energies= -1219.069545

Sum of electronic and thermal Enthalpies= -1219.068601

Sum of electronic and thermal Free Energies= -1219.140707

INC-1(3)



Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000003868	-0.000000289	0.000007207
2	6	-0.000000553	-0.000000126	-0.000001644
3	6	0.000001007	-0.000001037	0.000001501
4	6	-0.000000850	-0.000002149	0.000001098
5	6	0.000001078	-0.000001786	0.000001029
6	1	0.000002465	-0.000002314	-0.000000345
7	1	-0.000001122	-0.000000383	0.000000809
8	1	0.000000568	-0.000002743	0.000001216
9	1	0.000000373	-0.000002844	0.000000626
10	16	-0.000000260	-0.000000221	0.000003617
11	8	-0.000002602	0.000001845	-0.000001179
12	8	-0.000001070	0.000003790	-0.000000152
13	7	-0.000004510	0.000003248	0.000002258
14	6	0.000002119	-0.000000296	-0.000006440
15	8	-0.000006692	0.000002860	0.000006326
16	6	0.000001323	-0.000001220	-0.000001222
17	1	-0.000000795	0.000001979	0.000000247
18	6	0.000001069	0.000000930	-0.000000880
19	1	0.000001195	0.000001677	-0.000002649

20	1	0.000002517	0.000001187	-0.000002277
21	6	-0.000001624	0.000001414	-0.000003748
22	6	-0.000000575	0.000002006	0.000000926
23	6	-0.000000971	-0.000000796	-0.000005215
24	6	0.000000557	-0.000000306	-0.000001003
25	1	-0.000000495	0.000001497	-0.000000971
26	6	0.000001008	-0.000000025	-0.000000709
27	1	0.000002531	-0.000000872	-0.000001379
28	6	0.000000034	-0.000001600	0.000001453
29	1	-0.000001276	0.000000333	0.000000816
30	1	0.000001790	-0.000002179	-0.000000014
31	1	-0.000000103	-0.000001579	0.000000696

Zero-point correction= 0.226047 (Hartree/Particle)

Thermal correction to Energy= 0.244832

Thermal correction to Enthalpy= 0.245776

Thermal correction to Gibbs Free Energy= 0.172614

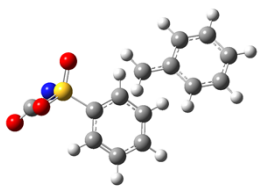
Sum of electronic and zero-point Energies= -1219.086045

Sum of electronic and thermal Energies= -1219.067260

Sum of electronic and thermal Enthalpies= -1219.066316

Sum of electronic and thermal Free Energies= -1219.139478

INC-TS

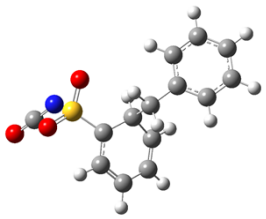


Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000005213	0.000015922	-0.000004820

2	6	0.000014781	0.000002203	0.000027443
3	6	0.000002019	0.000001956	0.000001294
4	6	0.000006909	-0.000002210	0.000009854
5	6	-0.000007633	-0.000000013	-0.000004097
6	1	0.000000632	-0.000004490	-0.000000336
7	1	-0.000000558	0.000002859	0.000001365
8	1	0.000000598	0.000010179	0.000002358
9	1	0.000001952	0.000002369	0.000001131
10	16	0.000000478	0.000010868	-0.000000245
11	8	-0.000000354	0.000001716	0.000000726
12	8	-0.000003751	0.000000198	-0.000001086
13	7	-0.000000458	-0.000016371	-0.000000550
14	6	0.000003045	-0.000002210	-0.000000422
15	8	0.000003201	0.000000692	0.000000176
16	6	-0.000021806	-0.000000548	-0.000024491
17	1	0.000011957	-0.000006795	-0.000001983
18	6	-0.000009577	-0.000005864	-0.000032320
19	1	-0.000004504	0.000000856	-0.000001442
20	1	-0.000000573	0.000007077	0.000001423
21	6	0.000003317	-0.000000665	0.000026594
22	6	0.000001404	-0.000001830	0.000000592
23	6	-0.000002504	-0.000002489	0.000005967
24	6	0.000000045	-0.000003770	-0.000002369
25	1	-0.000000463	-0.000004064	-0.000002370
26	6	-0.000001818	-0.000000807	-0.000002222
27	1	-0.000002296	0.000002076	0.000000922
28	6	0.000000702	-0.000001745	0.000001896
29	1	0.000000223	-0.000004542	-0.000002190
30	1	-0.000000862	0.000001186	0.000000597
31	1	0.000000681	-0.000001743	-0.000001397

Zero-point correction= 0.226468 (Hartree/Particle)
Thermal correction to Energy= 0.244103
Thermal correction to Enthalpy= 0.245047
Thermal correction to Gibbs Free Energy= 0.176931
Sum of electronic and zero-point Energies= -1219.084169
Sum of electronic and thermal Energies= -1219.066534
Sum of electronic and thermal Enthalpies= -1219.065590
Sum of electronic and thermal Free Energies= -1219.133706

E.*o*



Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000006887	0.000003120	-0.000001165
2	6	0.000004947	0.000010952	-0.000003538
3	6	-0.000003449	-0.000002722	0.000005458
4	6	-0.000000125	-0.000001380	-0.000005260
5	6	0.000001673	0.000003070	0.000002235
6	1	0.000001440	-0.000000182	-0.000000120
7	1	0.000001071	0.000000638	-0.000001777
8	1	0.000000490	0.000002325	-0.000000610
9	1	0.000000419	0.000001658	-0.000000273
10	16	-0.000002236	-0.000004208	0.000002634
11	8	0.000001377	0.000000087	-0.000000898
12	8	0.000002188	-0.000000026	-0.000003351
13	7	0.000002066	-0.000005691	0.000002768
14	6	-0.000000772	0.000005513	-0.000003599
15	8	0.000004531	-0.000004320	-0.000000355

16	6	0.000005833	-0.000008639	-0.000001126
17	1	-0.000000452	0.000000934	0.000000107
18	6	-0.000004454	0.000005810	0.000001060
19	1	0.000000201	-0.000001138	-0.000000535
20	1	0.000000183	-0.000000793	0.000000014
21	6	0.000001525	0.000002594	0.000001929
22	6	-0.000002182	-0.000002917	-0.000000921
23	6	-0.000000995	-0.000000264	0.000001524
24	6	0.000000794	-0.000003108	0.000001661
25	1	0.000000228	-0.000001372	0.000000521
26	6	-0.000001978	-0.000001630	-0.000000782
27	1	-0.000001447	0.000000470	0.000000450
28	6	-0.000000537	0.000002875	0.000001015
29	1	-0.000000668	-0.000001246	0.000000729
30	1	-0.000001612	0.000000381	0.000001044
31	1	-0.000001173	-0.000000790	0.000001159

Zero-point correction= 0.230712 (Hartree/Particle)

Thermal correction to Energy= 0.248079

Thermal correction to Enthalpy= 0.249023

Thermal correction to Gibbs Free Energy= 0.181896

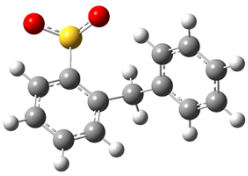
Sum of electronic and zero-point Energies= -1219.114712

Sum of electronic and thermal Energies= -1219.097345

Sum of electronic and thermal Enthalpies= -1219.096401

Sum of electronic and thermal Free Energies= -1219.163528

B.*o*



Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000004139	-0.000009443	0.000021513
2	6	-0.000026726	-0.000001767	-0.000013883
3	6	0.000028310	-0.000005005	-0.000004538
4	1	-0.000000811	-0.000003349	0.000001345
5	1	-0.000001390	0.000000035	0.000000292
6	16	0.000005191	-0.000000684	-0.000006598
7	8	-0.000006299	0.000000245	0.000007633
8	8	-0.000007874	0.000002102	0.000000635
9	6	0.000002065	-0.000002065	-0.000027397
10	6	-0.000008054	0.000004765	-0.000010846
11	6	-0.000014474	-0.000000218	0.000014747

12	1	0.000001841	-0.000004308	0.000000757
13	1	0.000000331	-0.000004933	-0.000001107
14	6	0.000033354	0.000000062	0.000005454
15	1	0.000000836	0.000003522	-0.000004266
16	1	-0.000004223	-0.000001285	-0.000001221
17	6	-0.000041951	0.000017236	0.000010683
18	6	0.000006680	-0.000001867	-0.000001213
19	6	0.000020528	-0.000013350	0.000002192
20	6	0.000003141	0.000001513	0.000002238
21	1	0.000002294	0.000001139	0.000000148
22	6	0.000006818	0.000001183	-0.000003145
23	1	-0.000002851	0.000004918	-0.000001796
24	6	-0.000001902	0.000003607	-0.000001467
25	1	0.000001929	-0.000000877	0.000000002
26	1	-0.000001382	0.000003342	0.000006106
27	1	0.000000481	0.000005482	0.000003732

Zero-point correction= 0.206252 (Hartree/Particle)

Thermal correction to Energy= 0.219834

Thermal correction to Enthalpy= 0.220778

Thermal correction to Gibbs Free Energy= 0.164474

Sum of electronic and zero-point Energies= -1050.504338

Sum of electronic and thermal Energies= -1050.490757

Sum of electronic and thermal Enthalpies= -1050.489813

Sum of electronic and thermal Free Energies= -1050.546117

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Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000083817	-0.000048392	0.000038363
2	7	-0.000033823	-0.000019528	-0.000067027
3	8	0.000116356	0.000067178	-0.000034388
4	1	0.000001285	0.000000742	0.000063052

Zero-point correction= 0.021189 (Hartree/Particle)

Thermal correction to Energy= 0.024458

Thermal correction to Enthalpy= 0.025402

Thermal correction to Gibbs Free Energy= -0.001715

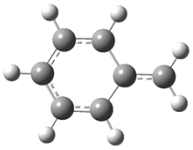
Sum of electronic and zero-point Energies= -168.670134

Sum of electronic and thermal Energies= -168.666865

Sum of electronic and thermal Enthalpies= -168.665920

Sum of electronic and thermal Free Energies= -168.693038

D



Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000066337	-0.000028546	0.000041079
2	6	-0.000008418	0.000007850	-0.000001895
3	6	-0.000011027	0.000006172	-0.000006728
4	6	-0.000012982	0.000007206	0.000002325
5	1	-0.000010065	-0.000002876	-0.000011598
6	6	0.000002375	0.000004406	-0.000013060
7	1	-0.000014678	-0.000001513	-0.000005453
8	6	-0.000006666	-0.000001418	-0.000002218
9	1	0.000017958	-0.000001591	0.000012086
10	1	0.000018704	-0.000000761	0.000012452
11	1	0.000021950	-0.000001690	0.000012972
12	6	-0.000057279	0.000010288	-0.000036898

13	1	0.000001895	0.000001553	-0.000009523
14	1	-0.000008104	0.000000919	0.000006460

Zero-point correction= 0.111927 (Hartree/Particle)

Thermal correction to Energy= 0.117921

Thermal correction to Enthalpy= 0.118866

Thermal correction to Gibbs Free Energy= 0.082666

Sum of electronic and zero-point Energies= -270.855024

Sum of electronic and thermal Energies= -270.849030

Sum of electronic and thermal Enthalpies= -270.848086

Sum of electronic and thermal Free Energies= -270.884285

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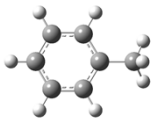


Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000029972	0.000010508	0.000047534
2	6	-0.000004744	0.000009559	-0.000039561
3	6	0.000011286	-0.000028645	0.000012787

4	6	-0.000004112	0.000011692	-0.000025623
5	6	-0.000040952	0.000009424	0.000030823
6	6	0.000010555	-0.000012935	0.000031210
7	1	-0.000029125	0.000002850	0.000005873
8	1	-0.000024791	-0.000003558	0.000009601
9	1	0.000025277	-0.000003899	0.000007523
10	1	0.000030678	0.000002747	0.000007708
11	1	-0.000000917	0.000002262	-0.000006055
12	6	-0.000002620	0.000020370	0.000023472
13	1	-0.000001421	0.000067068	-0.000022447
14	1	-0.000063512	-0.000045143	-0.000041232
15	1	0.000064425	-0.000042298	-0.000041614

Zero-point correction= 0.127729 (Hartree/Particle)

Thermal correction to Energy= 0.133947

Thermal correction to Enthalpy= 0.134891

Thermal correction to Gibbs Free Energy= 0.097143

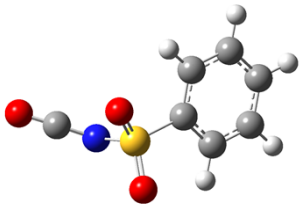
Sum of electronic and zero-point Energies= -271.461622

Sum of electronic and thermal Energies= -271.455405

Sum of electronic and thermal Enthalpies= -271.454461

Sum of electronic and thermal Free Energies= -271.492208

Benzenesulfonylisocyanate



Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000010764	0.000004424	0.000017030
2	6	-0.000005668	-0.000008183	-0.000005465
3	6	-0.000000584	-0.000002159	0.000001527
4	6	-0.000006489	0.000001063	0.000005609
5	6	-0.000011220	-0.000000936	-0.000017952
6	6	0.000011060	0.000000251	0.000000204
7	1	-0.000004005	0.000002642	0.000002988
8	1	0.000002430	0.000006571	0.000003346
9	1	0.000001324	-0.000006860	-0.000004265
10	1	-0.000003635	-0.000001781	-0.000002561
11	1	-0.000010141	0.000000212	-0.000000191
12	16	0.000002395	-0.000009619	-0.000030608
13	8	0.000003639	-0.000003848	-0.000016998
14	8	0.000003569	0.000005941	0.000020811

15	7	-0.000096237	-0.000020280	-0.000084771
16	6	0.000290040	0.000070662	0.000283826
17	8	-0.000165712	-0.000038100	-0.000172532

Zero-point correction= 0.113780 (Hartree/Particle)

Thermal correction to Energy= 0.124316

Thermal correction to Enthalpy= 0.125260

Thermal correction to Gibbs Free Energy= 0.074068

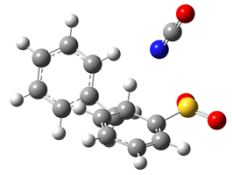
Sum of electronic and zero-point Energies= -948.208470

Sum of electronic and thermal Energies= -948.197933

Sum of electronic and thermal Enthalpies= -948.196989

Sum of electronic and thermal Free Energies= -948.248182

TS.*o*

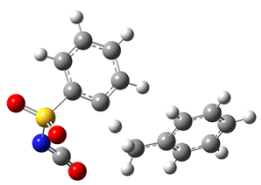


Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000000456	0.000000804	0.000000867
2	6	-0.000001078	-0.000002561	0.000005440
3	6	-0.000001737	-0.000002470	0.000002513
4	6	0.000000706	-0.000000680	0.000003582
5	6	0.000000257	0.000000440	0.000002618
6	1	0.000001489	0.000001537	0.000001075
7	1	-0.000001982	-0.000003041	0.000002600

8	1	-0.000000583	-0.000001009	0.000004016
9	1	0.000001404	0.000001284	0.000002935
10	16	-0.000018192	0.000003601	-0.000006176
11	8	-0.000002260	-0.000004562	0.000003400
12	8	0.000011856	-0.000009301	0.000000308
13	7	-0.000001279	-0.000000711	-0.000001942
14	6	-0.000001170	-0.000004466	-0.000002708
15	8	-0.000002812	-0.000000108	-0.000005177
16	6	-0.000000649	-0.000001195	-0.000000274
17	1	-0.000001453	0.000001676	0.000000636
18	6	0.000000274	-0.000000715	0.000001154
19	1	-0.000000761	-0.000000978	-0.000000356
20	1	0.000000510	-0.000000154	0.000001822
21	6	0.000001165	0.000001323	-0.000000491
22	6	0.000000135	0.000000445	-0.000001646
23	6	0.000001814	0.000001667	0.000000573
24	6	0.000000363	0.000001533	-0.000003618
25	1	0.000000675	-0.000000100	-0.000002748
26	6	0.000002311	0.000003376	-0.000000717
27	1	0.000001660	0.000001668	0.000001772
28	6	0.000002164	0.000002430	-0.000001842
29	1	0.000001308	0.000002556	-0.000004228
30	1	0.000002922	0.000003907	-0.000000154
31	1	0.000002485	0.000003803	-0.000003232

Zero-point correction= 0.229008 (Hartree/Particle)
Thermal correction to Energy= 0.246297
Thermal correction to Enthalpy= 0.247242
Thermal correction to Gibbs Free Energy= 0.180661
Sum of electronic and zero-point Energies= -1219.101362
Sum of electronic and thermal Energies= -1219.084072
Sum of electronic and thermal Enthalpies= -1219.083128
Sum of electronic and thermal Free Energies= -1219.149709

PT-TS.*o*

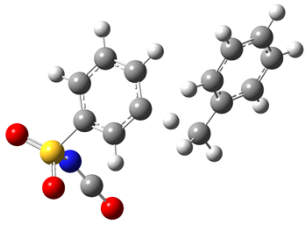


Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000694	-0.000000326	0.000000327
2	6	0.000000051	-0.000000339	-0.000002058
3	6	0.000005589	0.000002203	-0.000004446
4	6	-0.000005417	-0.000004253	0.000004754
5	6	0.000000102	0.000000150	0.000001997
6	6	-0.000000020	-0.000000604	-0.000000350
7	1	0.000000178	-0.000000508	0.000001360
8	1	0.000000829	0.000002155	0.000000315
9	1	-0.000000628	0.000005789	-0.000000185
10	1	0.000000275	-0.000000816	0.000000128
11	1	-0.000000577	-0.000001272	0.000000990
12	16	0.000002684	-0.000007708	0.000004519
13	8	0.000000227	0.000002492	-0.000002597
14	8	0.000002698	-0.000000705	0.000007492
15	7	-0.000005971	0.000009697	-0.000000639
16	6	-0.000001699	0.000001918	0.000000738
17	8	0.000003334	-0.000000767	0.000000793
18	6	0.000000103	-0.000001870	-0.000000686
19	6	0.000000805	-0.000000167	-0.000000152

20	6	-0.000001706	-0.000002175	-0.000000688
21	6	-0.000000220	-0.000001538	-0.000000759
22	1	-0.000000001	0.000000233	-0.000000072
23	6	0.000000285	-0.000001090	-0.000002204
24	1	0.000000706	0.000001131	-0.000000343
25	6	-0.000001049	-0.000000171	-0.000000838
26	1	-0.000000411	-0.000001174	-0.000000460
27	1	-0.000000428	-0.000001116	-0.000001752
28	1	-0.000000364	-0.000001471	-0.000001688
29	6	0.000000325	0.000000554	-0.000002458
30	1	0.000000898	0.000000943	-0.000000295
31	1	0.000000094	0.000000804	-0.000000745

Zero-point correction= 0.222112 (Hartree/Particle)
Thermal correction to Energy= 0.239963
Thermal correction to Enthalpy= 0.240907
Thermal correction to Gibbs Free Energy= 0.171937
Sum of electronic and zero-point Energies= -1219.074116
Sum of electronic and thermal Energies= -1219.056265
Sum of electronic and thermal Enthalpies= -1219.055321
Sum of electronic and thermal Free Energies= -1219.124290

PT-TS.*m*



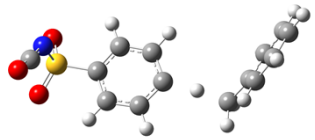
Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000201	0.000000909	0.000000718
2	6	0.000000138	-0.000001397	0.000000309
3	6	0.000000522	-0.000002030	0.000000554
4	6	0.000000693	0.000001299	0.000000521
5	6	0.000000045	0.000001017	-0.000000067
6	1	0.000000433	0.000002939	0.000000954
7	1	0.000000472	-0.000000269	0.000000686
8	1	-0.000000037	0.000002303	0.000000676
9	16	0.000003041	-0.000008510	0.000002800
10	8	-0.000001405	-0.000007922	-0.000000263
11	8	0.000001207	-0.000004552	0.000001466
12	7	0.000001329	-0.000000216	-0.000004633
13	6	-0.000001771	-0.000007009	-0.000002496
14	8	-0.000002185	-0.000006429	-0.000004119
15	6	-0.000000395	0.000002100	0.000000102
16	6	-0.000000459	0.000001861	-0.000000841
17	6	0.000000645	0.000002110	0.000001343
18	6	-0.000001626	0.000005059	-0.000002294
19	1	-0.000001933	0.000001957	-0.000002899
20	6	0.000000565	0.000004781	0.000002332
21	1	0.000001637	0.000001760	0.000002966
22	6	-0.000000262	0.000005288	0.000000810
23	1	-0.000002164	0.000005183	-0.000002613
24	1	0.000001334	0.000005497	0.000003048
25	1	-0.000000700	0.000007238	0.000000090
26	6	0.000000563	-0.000001063	0.000000064
27	1	-0.000000324	-0.000001408	0.000000346
28	1	-0.000000537	-0.000001526	-0.000001050
29	1	0.000000741	-0.000001617	0.000000899
30	6	-0.000000249	-0.000004249	0.000000277
31	1	0.000000886	-0.000003104	0.000000314

Zero-point correction= 0.221547 (Hartree/Particle)

Thermal correction to Energy= 0.239703

Thermal correction to Enthalpy=	0.240648
Thermal correction to Gibbs Free Energy=	0.169127
Sum of electronic and zero-point Energies=	-1219.070445
Sum of electronic and thermal Energies=	-1219.052289
Sum of electronic and thermal Enthalpies=	-1219.051345
Sum of electronic and thermal Free Energies=	-1219.122866

PT-TS.*p*

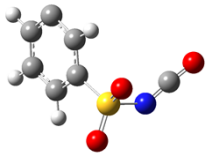


Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000201	0.000000909	0.000000718
2	6	0.000000138	-0.000001397	0.000000309
3	6	0.000000522	-0.000002030	0.000000554
4	6	0.000000693	0.000001299	0.000000521
5	6	0.000000045	0.000001017	-0.000000067
6	1	0.000000433	0.000002939	0.000000954
7	1	0.000000472	-0.000000269	0.000000686
8	1	-0.000000037	0.000002303	0.000000676
9	16	0.000003041	-0.000008510	0.000002800
10	8	-0.000001405	-0.000007922	-0.000000263
11	8	0.000001207	-0.000004552	0.000001466
12	7	0.000001329	-0.000000216	-0.000004633
13	6	-0.000001771	-0.000007009	-0.000002496
14	8	-0.000002185	-0.000006429	-0.000004119
15	6	-0.000000395	0.000002100	0.000000102
16	6	-0.000000459	0.000001861	-0.000000841
17	6	0.000000645	0.000002110	0.000001343
18	6	-0.000001626	0.000005059	-0.000002294
19	1	-0.000001933	0.000001957	-0.000002899
20	6	0.000000565	0.000004781	0.000002332
21	1	0.000001637	0.000001760	0.000002966
22	6	-0.000000262	0.000005288	0.000000810
23	1	-0.000002164	0.000005183	-0.000002613
24	1	0.000001334	0.000005497	0.000003048
25	1	-0.000000700	0.000007238	0.000000090
26	6	0.000000563	-0.000001063	0.000000064

27	1	-0.000000324	-0.000001408	0.000000346
28	1	-0.000000537	-0.000001526	-0.000001050
29	1	0.000000741	-0.000001617	0.000000899
30	6	-0.000000249	-0.000004249	0.000000277
31	1	0.000000886	-0.000003104	0.000000314

Zero-point correction= 0.221547 (Hartree/Particle)
Thermal correction to Energy= 0.239703
Thermal correction to Enthalpy= 0.240648
Thermal correction to Gibbs Free Energy= 0.169127
Sum of electronic and zero-point Energies= -1219.070445
Sum of electronic and thermal Energies= -1219.052289
Sum of electronic and thermal Enthalpies= -1219.051345
Sum of electronic and thermal Free Energies= -1219.122866

C.*m*



Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000002485	-0.000016162	0.000006823
2	6	-0.000010124	0.000038200	-0.000005553
3	6	-0.000012700	-0.000030691	0.000031972
4	6	0.000000597	-0.000005308	0.000010071
5	6	0.000009257	-0.000004042	0.000007185
6	6	0.000007196	-0.000015013	-0.000004895
7	1	0.000005102	0.000004993	-0.000005055
8	1	0.000000545	-0.000006838	-0.000008605
9	1	0.000000609	-0.000005290	-0.000002707
10	16	-0.000022417	-0.000086795	-0.000049438
11	8	0.000064647	0.000014961	-0.000006684
12	8	-0.000033775	0.000027294	0.000010635
13	7	-0.000055260	0.000058438	0.000002701
14	6	0.000071370	0.000004040	-0.000018896
15	8	-0.000020160	0.000001676	0.000017554

16	1	-0.000007372	0.000020537	0.000014892

Zero-point correction= 0.098339 (Hartree/Particle)
Thermal correction to Energy= 0.109140
Thermal correction to Enthalpy= 0.110084
Thermal correction to Gibbs Free Energy= 0.059489
Sum of electronic and zero-point Energies= -947.609878
Sum of electronic and thermal Energies= -947.599077
Sum of electronic and thermal Enthalpies= -947.598133
Sum of electronic and thermal Free Energies= -947.648728

C.*p*

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000001693	-0.000001075	-0.000002843
2	6	0.000003257	0.000002561	0.000001349
3	6	0.000000437	0.000006654	-0.000002282
4	6	0.000002853	-0.000011599	-0.000000034
5	6	0.000002244	-0.000004467	0.000001800
6	6	-0.000000320	-0.000005544	-0.000000200
7	1	0.000001983	0.000003646	-0.000001144
8	1	0.000001221	0.000005950	-0.000001637
9	16	-0.000008111	0.000003653	-0.000011165
10	8	0.000006139	0.000004572	0.000009196
11	8	0.000004327	0.000004077	-0.000008486
12	7	0.000002055	0.000015079	0.000064807
13	6	-0.000012803	-0.000022160	-0.000096812
14	8	-0.000006484	0.000012556	0.000047512
15	1	0.000000730	-0.000004081	0.000000336
16	1	0.000000781	-0.000009824	-0.000000398

Zero-point correction= 0.098787 (Hartree/Particle)
Thermal correction to Energy= 0.109407
Thermal correction to Enthalpy= 0.110351
Thermal correction to Gibbs Free Energy= 0.060442

Sum of electronic and zero-point Energies=	-947.609063
Sum of electronic and thermal Energies=	-947.598443
Sum of electronic and thermal Enthalpies=	-947.597499
Sum of electronic and thermal Free Energies=	-947.647408

Figure S3. DFT potential energy surfaces for PT of different sites (compound **1** as the model). All structures were optimized at the B3LYP/6-31++G(d,p) level of theory in kcal mol^{-1} (in parentheses). The inset shows the optimized structure of **C.*o***. The most energy-favorable channels are indicated by solid line, while others by dashed line

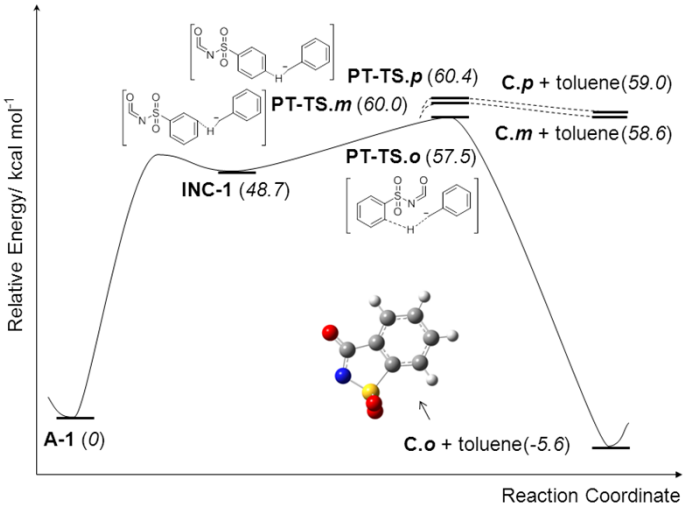
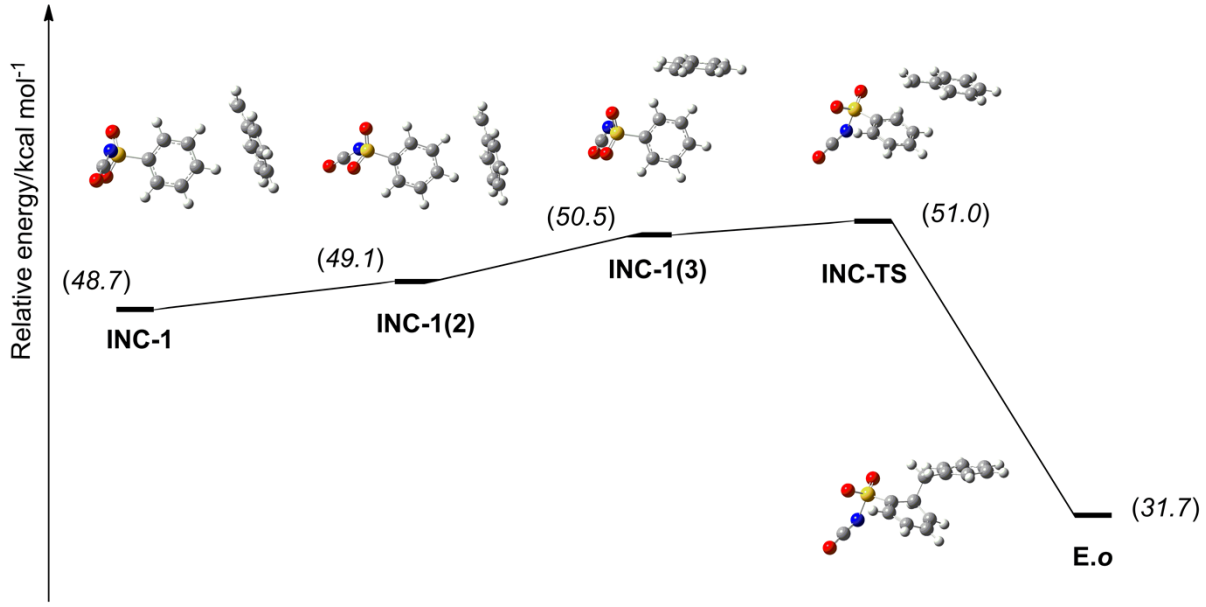
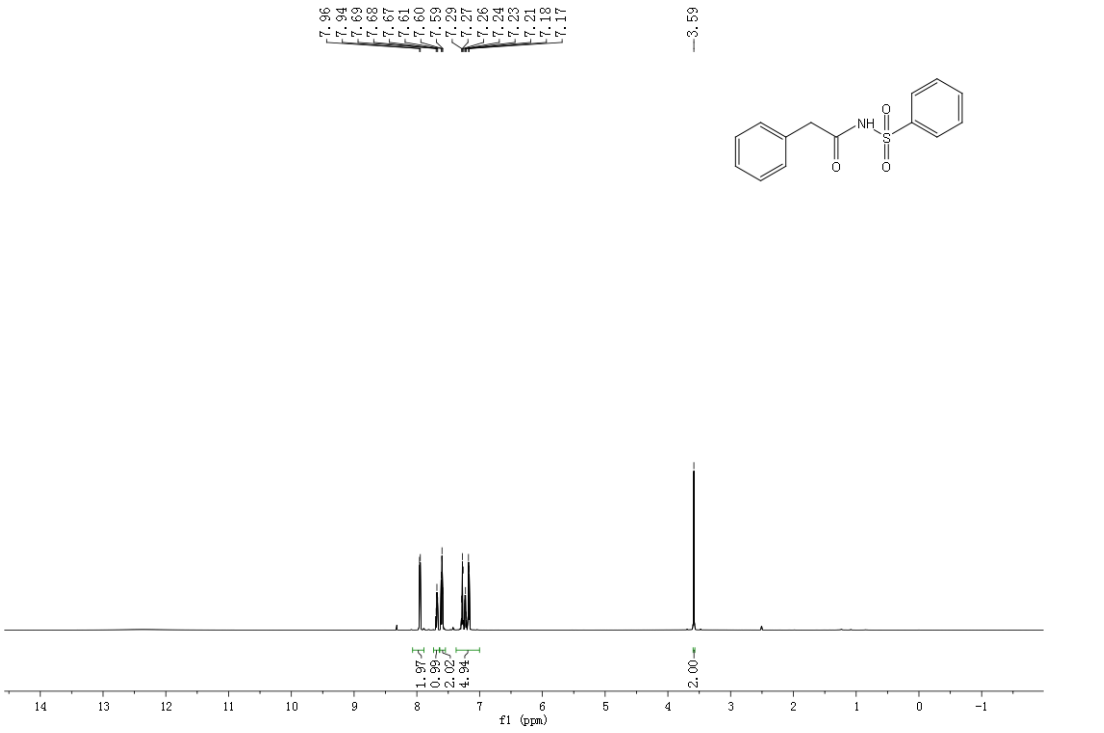


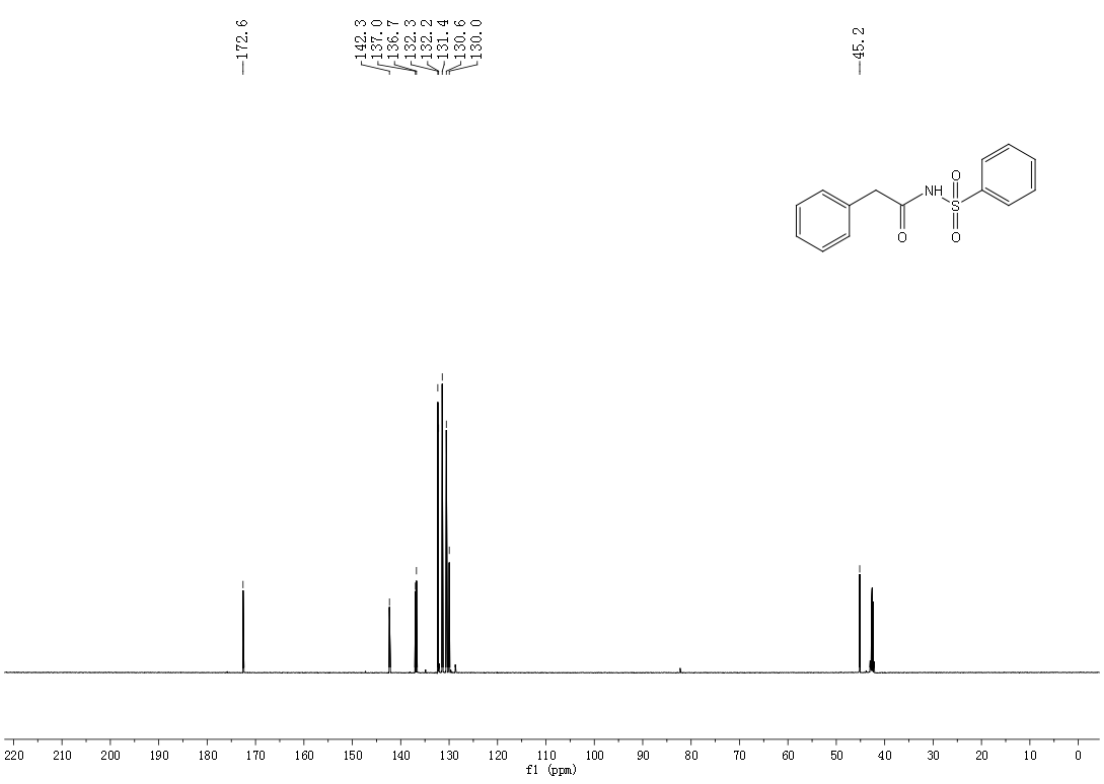
Figure S4 Calculated potential energy diagram for the conversion of **INC-1** to **E.*o*** at the B3LYP/6-31++G(d,p) level. The relative energy of [**1** - H]$^-$ is zero

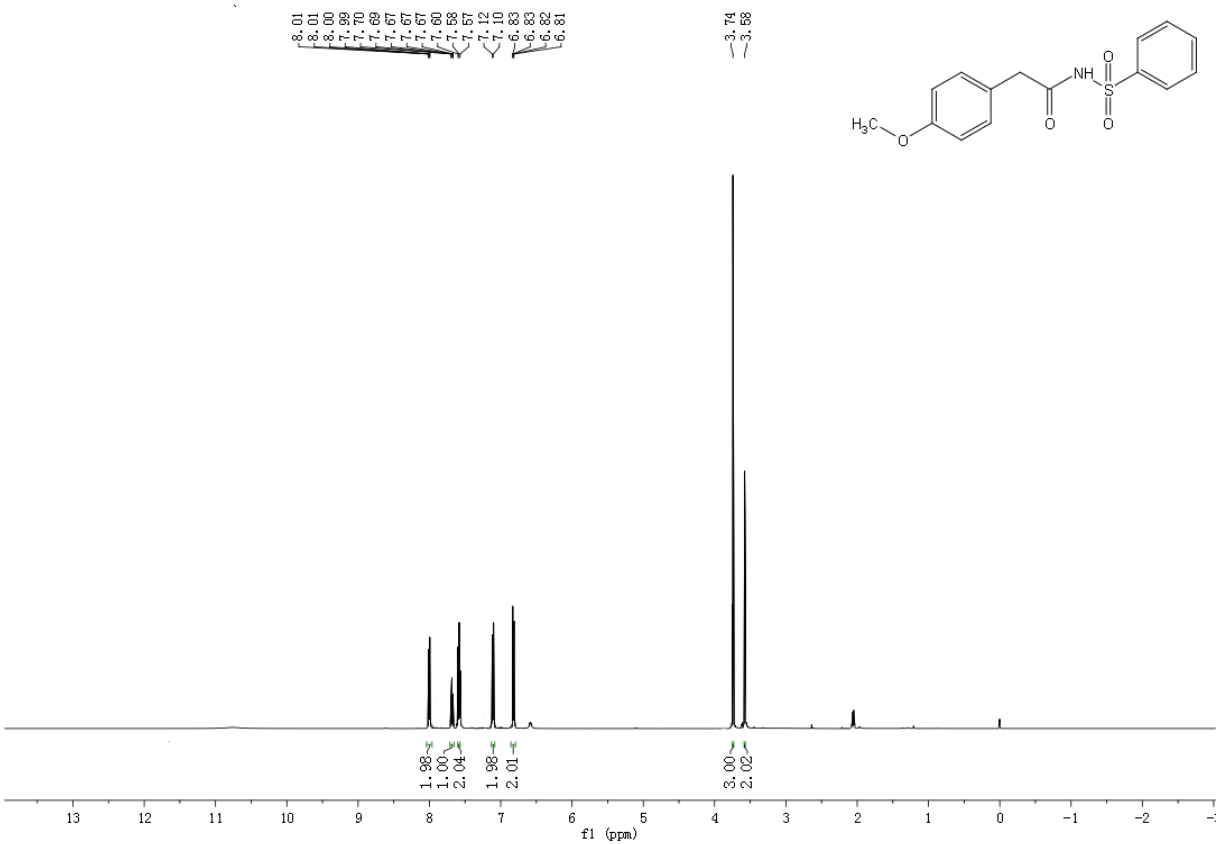


Statement: Within the ion/neutral complex, the ionic and neutral species can rotate with respect to each other. For the occurrence of the S_NAr reaction, benzyl anion must migrate to approach the *ortho* carbon. No significant energy barrier exists in the rotation process and the subsequent nucleophilic addition. Therefore formation of the σ-complex from the ion/neutral complex is favorable in terms of energy.

Figure S5. ^{1}H NMR, ^{13}C NMR spectra of *N*-(phenylsulfonyl)-benzeneacetamide (solvent: d_6-DMSO), ^{1}H NMR spectra of other compounds



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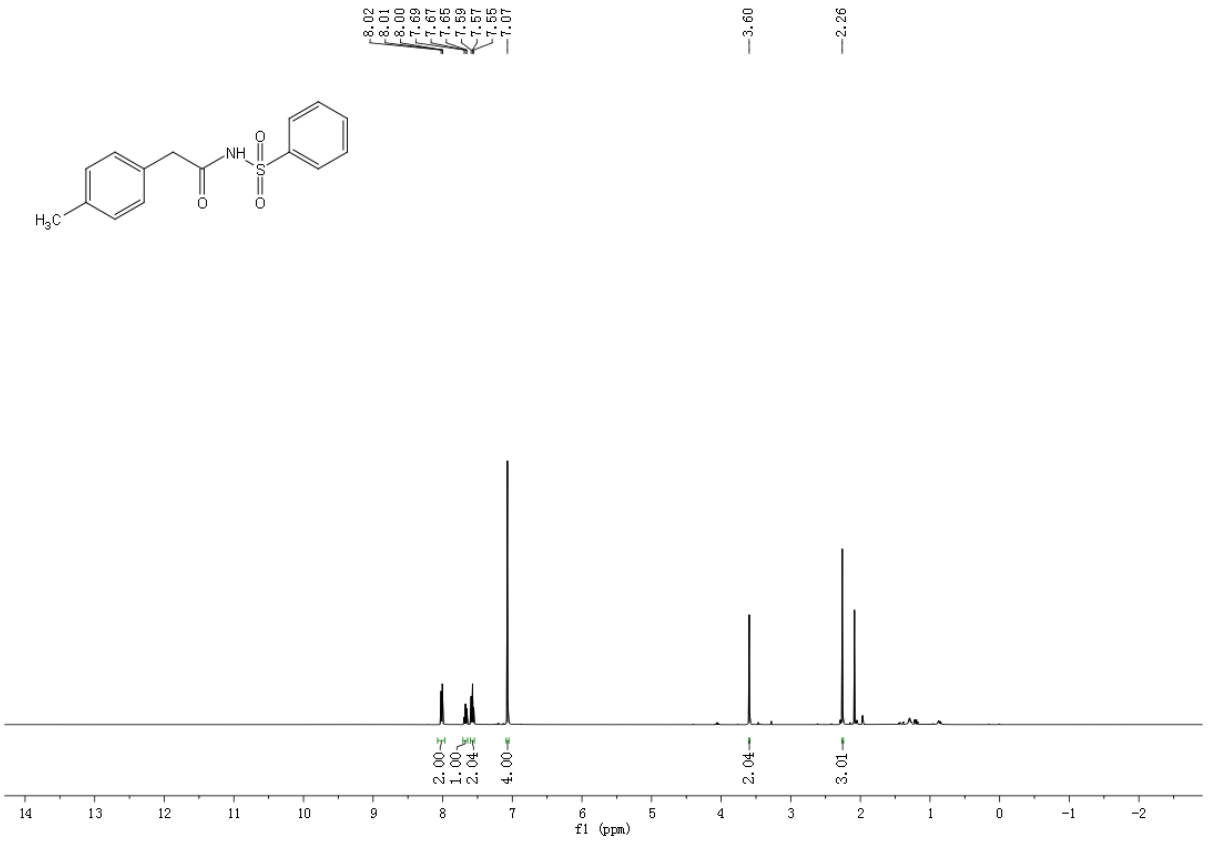
7.67
7.67
7.60
7.58
7.57
7.12
7.10
6.83
6.83
6.82
6.81
3.74
3.58
NH
O
S
O
O
H_3C
O
1.98
1.00
2.04
1.98
2.01
3.00
2.02
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
f1 (ppm)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H_3C
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1.00
2.04
4.00
2.04
3.01
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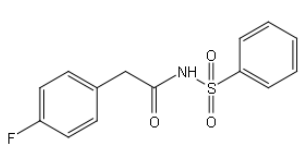
10
9
8
7
6
5
4
3
2
1
0
−1
−2
f1 (ppm)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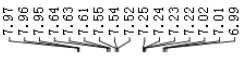
S
O
O
F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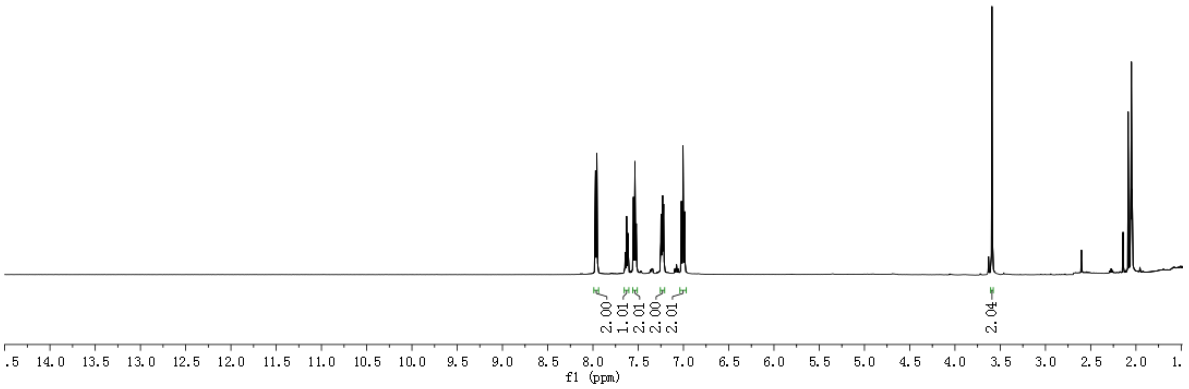
7.02
7.01
6.99


3.59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2.00
2.01
2.04
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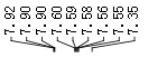
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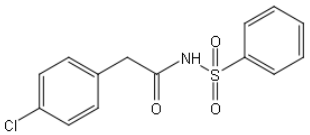
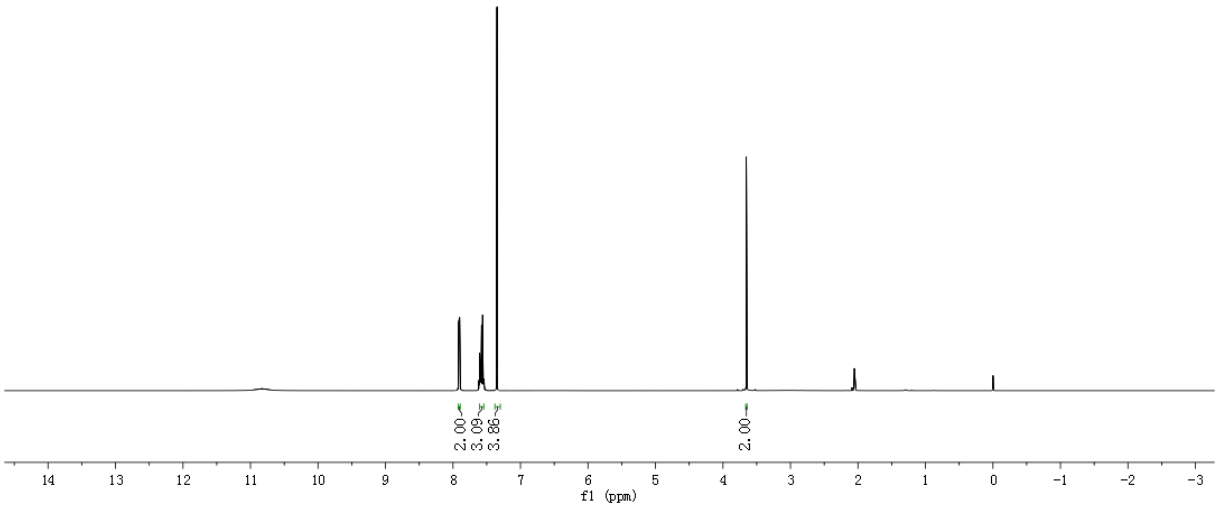
7.55
7.35


3.65


NH
O
S
O
O
Cl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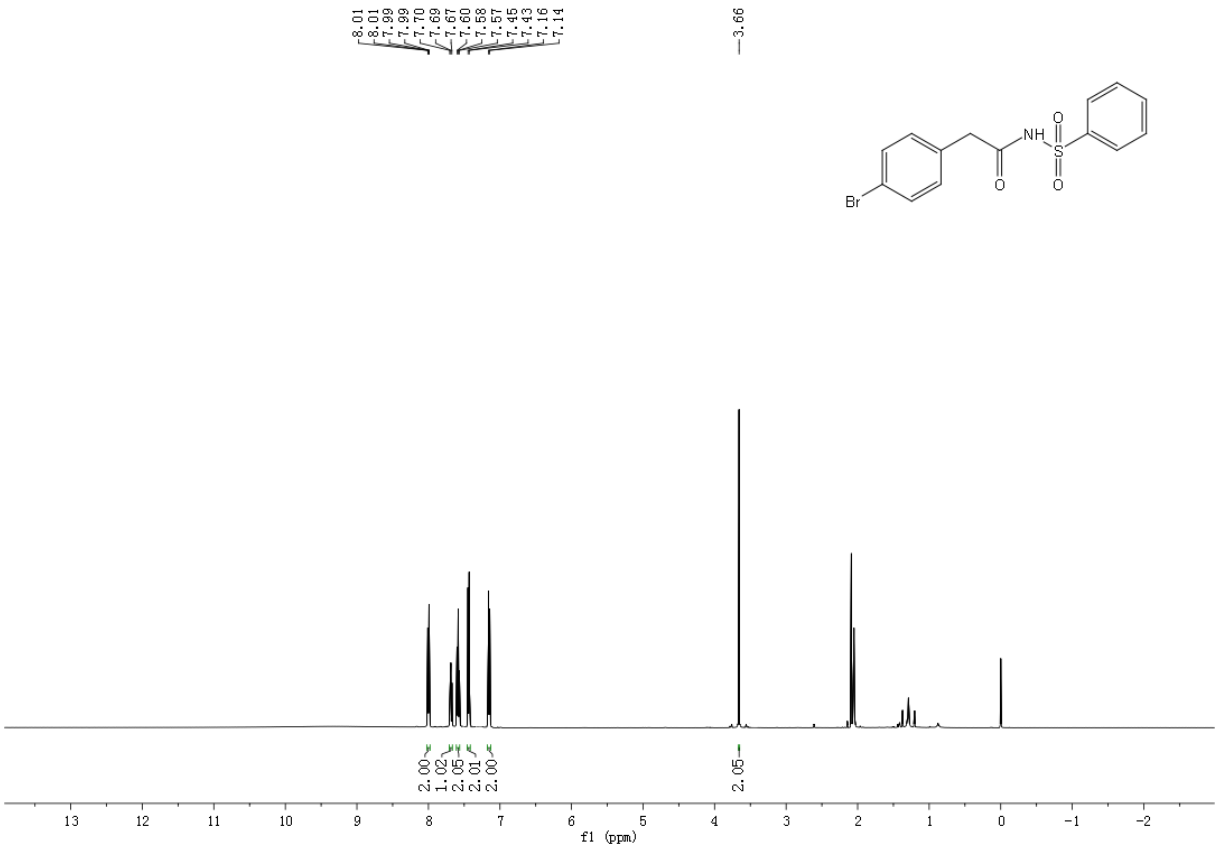
f1 (ppm)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2.05
2.01
2.00
2.05
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11
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9
8
7
6
5
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3
2
1
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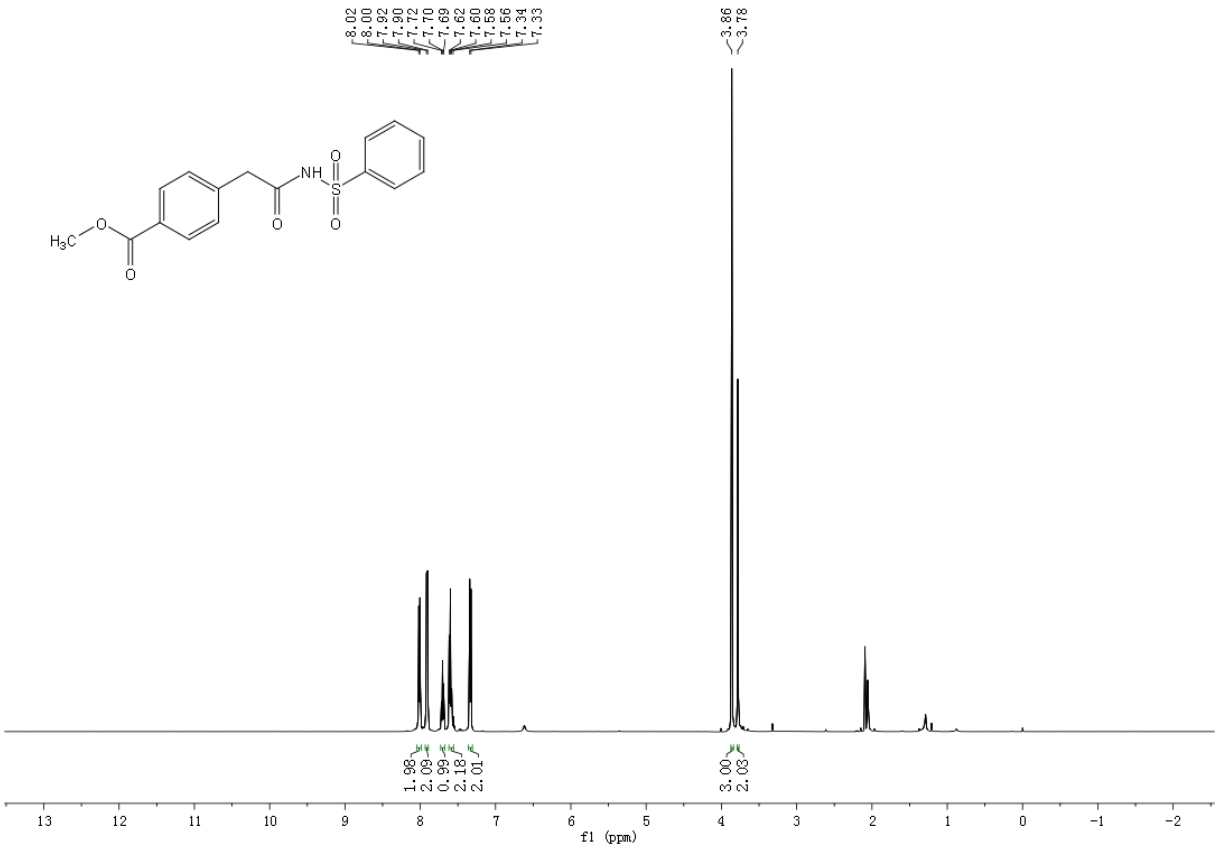
−1
−2
f1 (ppm)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3.78
NH
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S
O
O
O
H3C
O
O
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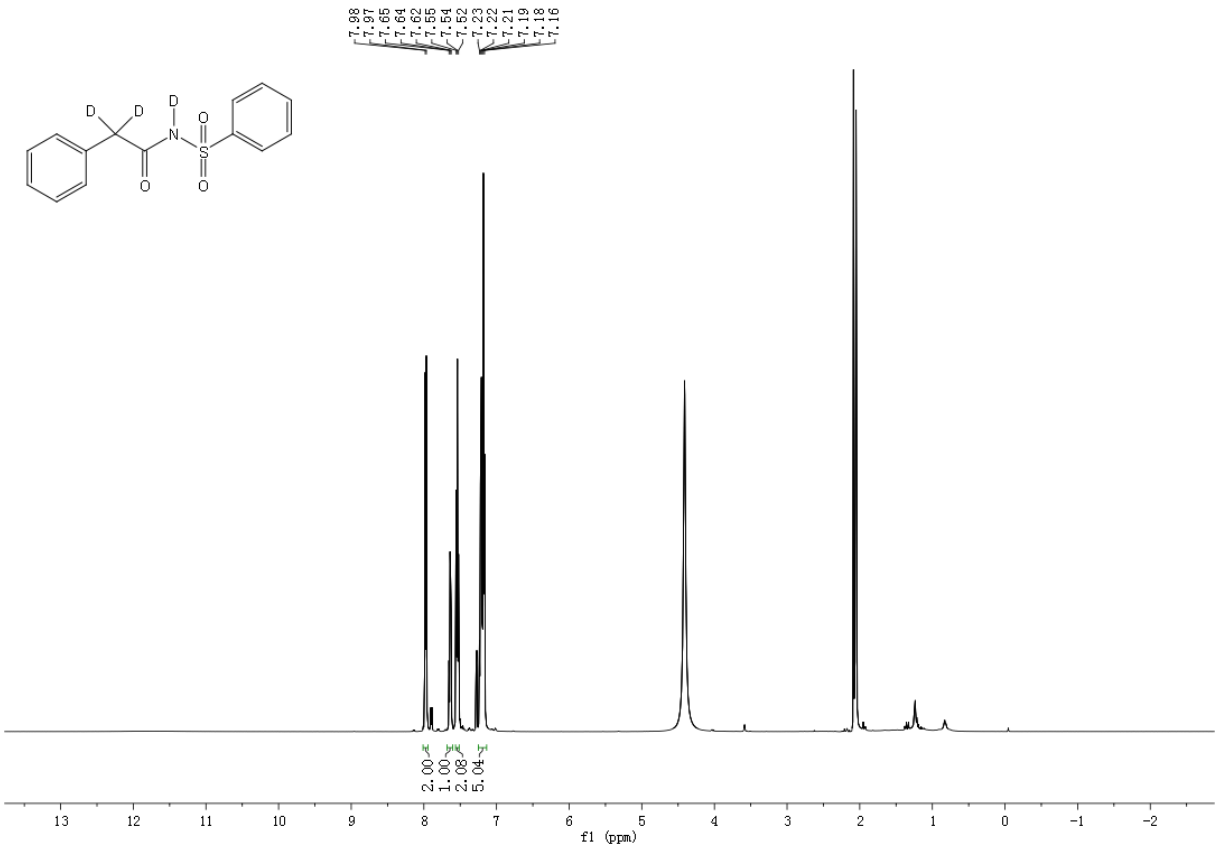
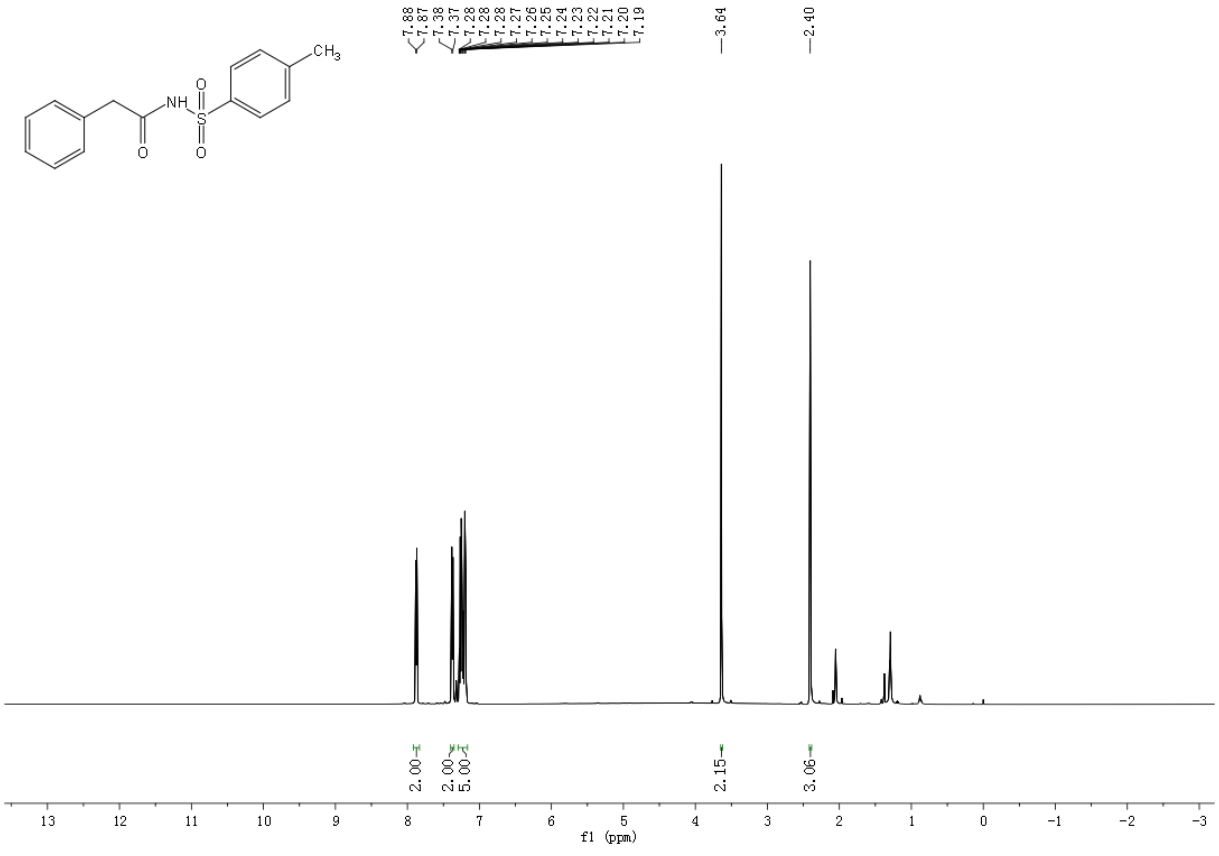
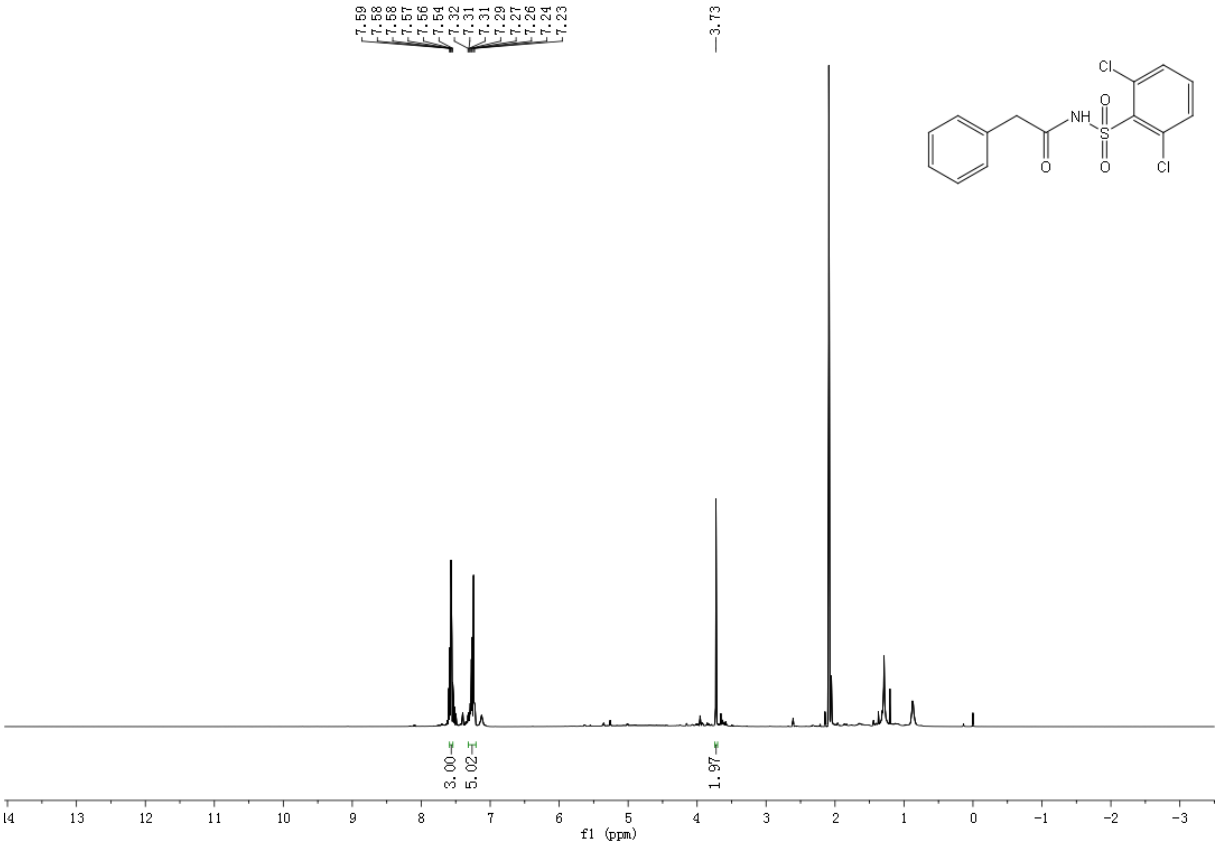
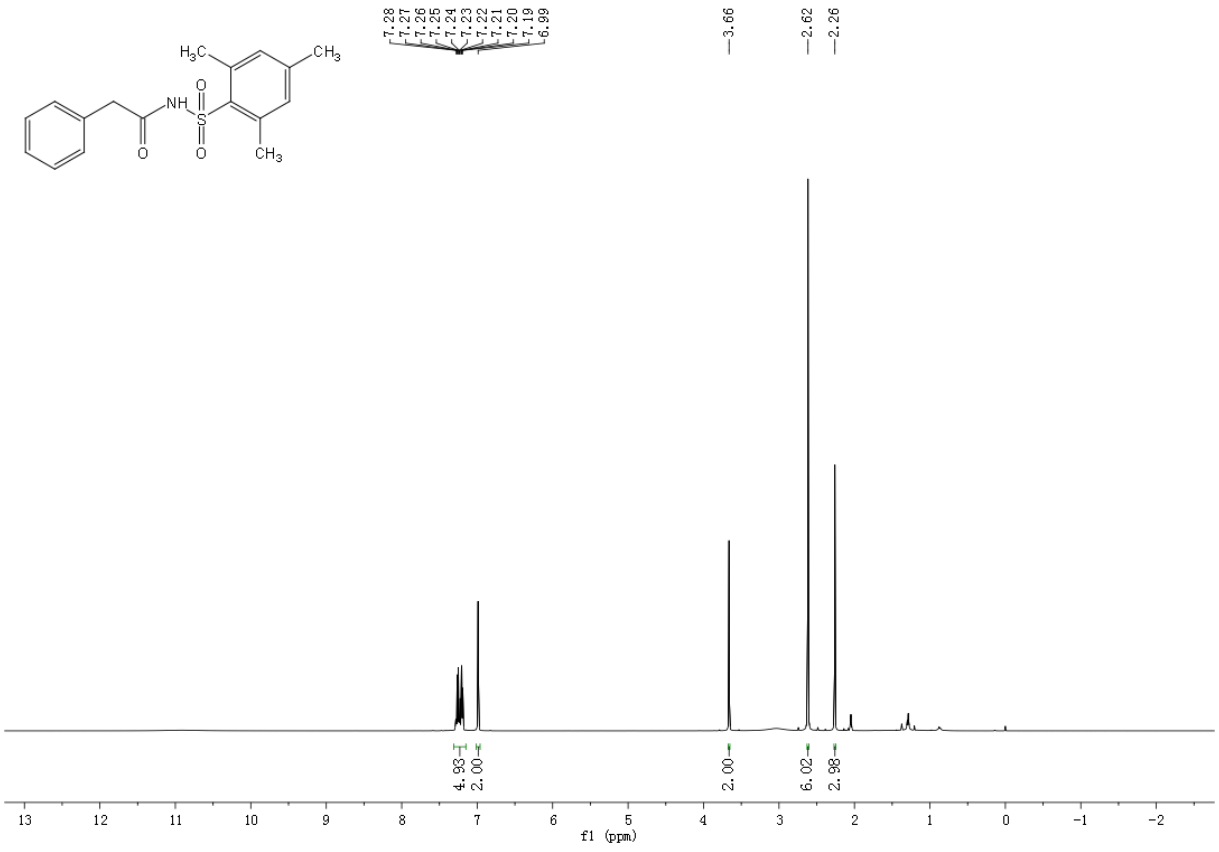
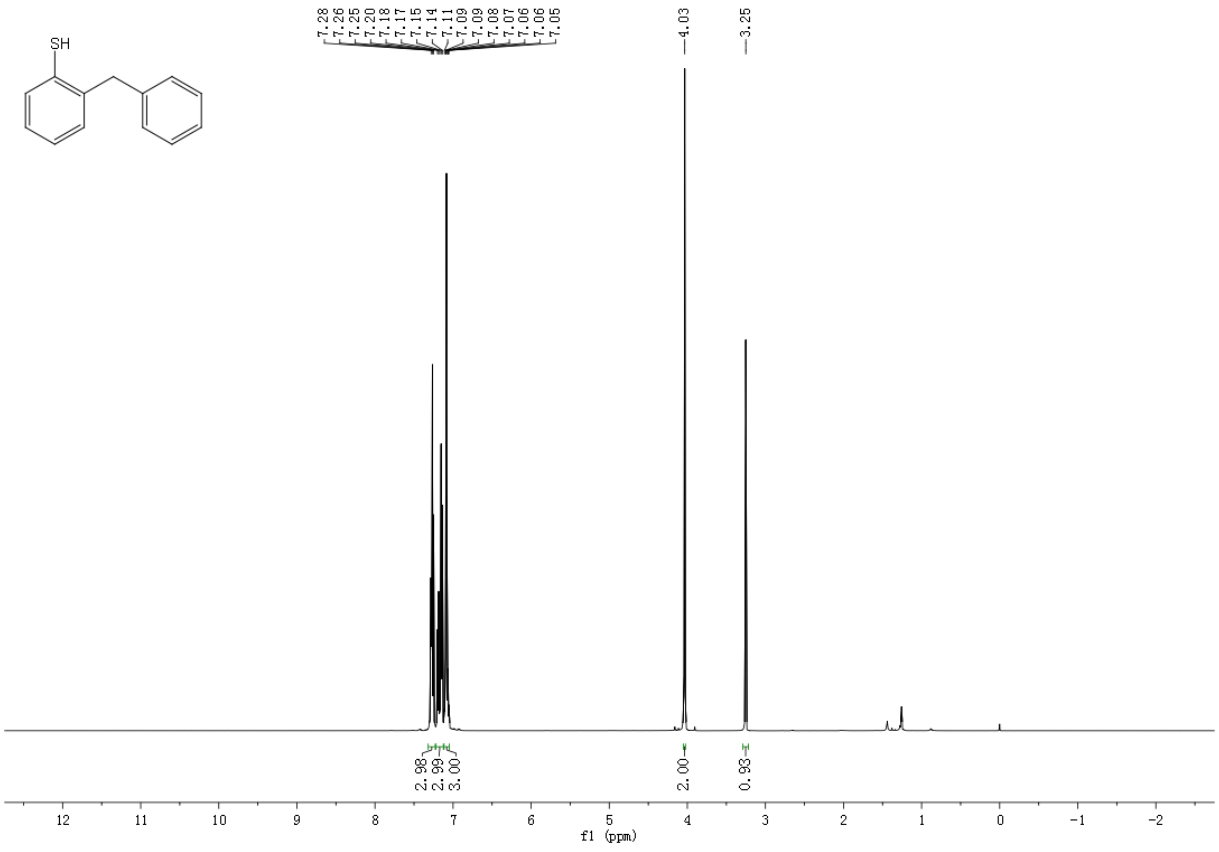
2.09
0.99
2.18
2.01
3.00
2.03
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
f1 (ppm)


7.98
7.97
7.65
7.64
7.62
7.55
7.54
7.52
7.23
7.22
7.21
7.19
7.18
7.16
D
D
D
N
O
S
O
O
O
2.00
1.00
2.08
5.04
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


7.88
7.87
7.38
7.37
7.28
7.28
7.28
7.27
7.26
7.25
7.24
7.23
7.22
7.21
7.20
7.19
3.64
2.40
CH3
NH
O
S
O
O
2.00
2.00
5.00
2.15
3.06
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


7.59
7.58
7.58
7.57
7.56
7.54
7.32
7.31
7.31
7.29
7.27
7.26
7.24
7.23
3.73
Cl
NH
O
S
O
O
Cl
3.00
5.02
1.97
f1 (ppm)


7.28
7.27
7.26
7.25
7.24
7.23
7.22
7.21
7.20
7.19
6.99
3.66
2.62
2.26
H3C
CH3
NH
O
S
O
O
O
CH3
4.93
2.00
2.00
6.02
2.98
f1 (ppm)


SH
7.28
7.26
7.25
7.20
7.18
7.17
7.15
7.14
7.11
7.09
7.09
7.08
7.07
7.06
7.06
7.05
4.03
3.25
2.98
2.99
3.00
2.00
0.93
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)