

**Supporting Information:**

**On the Understanding of  $\text{BF}_3 \cdot \text{Et}_2\text{O}$ -Promoted Intra- and Intermolecular Amination and Oxygenation of Unfunctionalized Olefins**

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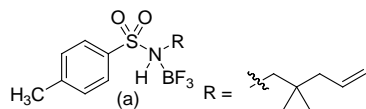
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# 1. Cartesian coordinates and energies for calculated intermediates

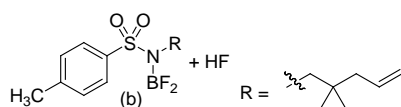


Zero-point correction=	0.347060 (Hartree/Particle)
Thermal correction to Energy=	0.370100
Thermal correction to Enthalpy=	0.371044
Thermal correction to Gibbs Free Energy=	0.294598
Sum of electronic and zero-point Energies=	-1473.692730
Sum of electronic and thermal Energies=	-1473.669690
Sum of electronic and thermal Enthalpies=	-1473.668745
Sum of electronic and thermal Free Energies=	-1473.745192

## Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.834681	0.386915	-0.501573
2	1	0	-1.353111	-0.555357	-0.339630
3	1	0	-0.255749	0.480264	-1.415217
4	6	0	-0.907977	1.381367	0.377694
5	1	0	-0.371718	2.305452	0.170098
6	6	0	-1.694601	1.338266	1.653370
7	1	0	-2.048994	0.316846	1.833722
8	1	0	-1.034824	1.600674	2.488054
9	6	0	-2.914448	2.301669	1.719525
10	6	0	-2.469323	3.737533	1.426871
11	1	0	-2.104319	3.870233	0.402897
12	1	0	-3.277501	4.454215	1.606737
13	1	0	-1.649900	4.008223	2.098157
14	6	0	-3.466893	2.222162	3.148336
15	1	0	-4.342646	2.857774	3.273832
16	1	0	-3.748774	1.193602	3.396747
17	1	0	-2.702678	2.541265	3.863412
18	6	0	-3.955347	1.770678	0.692627
19	1	0	-3.452848	1.112407	-0.012624
20	1	0	-4.722217	1.172429	1.184830
21	7	0	-4.661313	2.776820	-0.185517
22	1	0	-4.088558	3.626285	-0.254858
23	6	0	-7.374517	2.146991	0.153879

24	6	0	-8.102737	2.170627	-1.031016
25	6	0	-7.552874	1.150048	1.109734
26	6	0	-9.024413	1.162023	-1.258646
27	1	0	-7.946907	2.954799	-1.760358
28	6	0	-8.475832	0.149646	0.856102
29	1	0	-6.992579	1.161064	2.036735
30	6	0	-9.221794	0.139803	-0.326321
31	1	0	-9.597379	1.166525	-2.179348
32	1	0	-8.623088	-0.634220	1.590979
33	16	0	-6.207802	3.421190	0.473826
34	8	0	-6.001242	3.540808	1.899242
35	8	0	-6.467145	4.596757	-0.321635
36	6	0	-10.239398	-0.936303	-0.572702
37	1	0	-10.424657	-1.071192	-1.639815
38	1	0	-9.915767	-1.888951	-0.148235
39	1	0	-11.190134	-0.670236	-0.099116
40	5	0	-4.708425	2.214779	-1.750881
41	9	0	-3.381465	2.265744	-2.159323
42	9	0	-5.195790	0.920018	-1.710094
43	9	0	-5.505447	3.053780	-2.503201



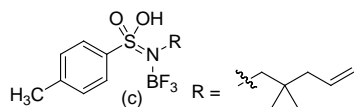
Zero-point correction=	0.344422 (Hartree/Particle)
Thermal correction to Energy=	0.368431
Thermal correction to Enthalpy=	0.369375
Thermal correction to Gibbs Free Energy=	0.289922
Sum of electronic and zero-point Energies=	-1473.672788
Sum of electronic and thermal Energies=	-1473.648780
Sum of electronic and thermal Enthalpies=	-1473.647836
Sum of electronic and thermal Free Energies=	-1473.727289

#### Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.566801	3.536057	1.630361
2	1	0	0.740240	3.901436	2.235519
3	1	0	2.515879	3.378793	2.133895
4	6	0	1.423308	3.297478	0.330043

5	1	0	2.280674	2.932648	-0.232416
6	6	0	0.149753	3.489143	-0.441956
7	1	0	-0.560543	4.069727	0.157925
8	1	0	0.367797	4.078090	-1.339948
9	6	0	-0.543517	2.179550	-0.911202
10	6	0	0.439638	1.297218	-1.682745
11	1	0	1.298925	1.000841	-1.079512
12	1	0	-0.051151	0.388766	-2.041092
13	1	0	0.812398	1.840995	-2.556215
14	6	0	-1.687083	2.571683	-1.853015
15	1	0	-2.182736	1.694733	-2.277808
16	1	0	-2.440432	3.178133	-1.341978
17	1	0	-1.290823	3.153505	-2.690662
18	6	0	-1.070063	1.502704	0.374561
19	1	0	-0.274546	1.500826	1.120177
20	1	0	-1.883555	2.098067	0.794663
21	7	0	-1.546883	0.099455	0.237440
22	6	0	0.902106	-1.117874	0.546507
23	6	0	1.139084	-1.834362	-0.623057
24	6	0	1.917462	-0.436573	1.203820
25	6	0	2.421690	-1.854378	-1.139937
26	1	0	0.337884	-2.355207	-1.133688
27	6	0	3.198004	-0.470352	0.668092
28	1	0	1.712675	0.115210	2.112958
29	6	0	3.467542	-1.171575	-0.506894
30	1	0	2.617898	-2.404323	-2.054225
31	1	0	3.997568	0.061984	1.171694
32	16	0	-0.738409	-1.026636	1.190605
33	8	0	-0.675423	-0.508838	2.541106
34	8	0	-1.412374	-2.307226	0.994152
35	6	0	4.852855	-1.212198	-1.085113
36	1	0	4.831830	-1.017796	-2.160452
37	1	0	5.504856	-0.477021	-0.610328
38	1	0	5.296942	-2.202109	-0.940901
39	5	0	-2.833077	-0.178627	-0.318037
40	9	0	-3.691175	0.822210	-0.507821
41	9	0	-1.691099	-4.146946	-0.786397
42	9	0	-3.245881	-1.383111	-0.686027
43	1	0	-1.603843	-3.455387	-0.149924

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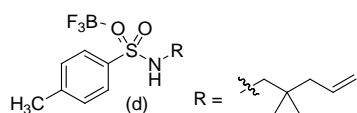


Zero-point correction= 0.344886 (Hartree/Particle)  
 Thermal correction to Energy= 0.368123  
 Thermal correction to Enthalpy= 0.369068  
 Thermal correction to Gibbs Free Energy= 0.292086  
 Sum of electronic and zero-point Energies= -1473.679191  
 Sum of electronic and thermal Energies= -1473.655954  
 Sum of electronic and thermal Enthalpies= -1473.655009  
 Sum of electronic and thermal Free Energies= -1473.731991

#### Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.642066	1.633860	2.667643
2	1	0	-5.544033	1.050248	2.497919
3	1	0	-4.463410	1.985661	3.679223
4	6	0	-3.798200	1.908584	1.677297
5	1	0	-2.908304	2.496952	1.894293
6	6	0	-3.985275	1.468415	0.254529
7	1	0	-4.957425	0.972809	0.153865
8	1	0	-4.010083	2.355631	-0.389938
9	6	0	-2.887322	0.529336	-0.307894
10	6	0	-1.523916	1.226849	-0.293432
11	1	0	-1.188664	1.454881	0.720802
12	1	0	-0.757615	0.602563	-0.760678
13	1	0	-1.573811	2.163142	-0.858171
14	6	0	-3.260589	0.180199	-1.751117
15	1	0	-2.506561	-0.460784	-2.213522
16	1	0	-4.223113	-0.337239	-1.802726
17	1	0	-3.335376	1.093538	-2.349302
18	6	0	-2.880854	-0.727566	0.578592
19	1	0	-2.572471	-0.460215	1.589970
20	1	0	-3.887293	-1.138303	0.647793
21	7	0	-2.012928	-1.827899	0.070991
22	6	0	0.499127	-2.752331	-0.278850
23	6	0	0.623117	-2.120092	-1.512153
24	6	0	1.329858	-3.803122	0.098303
25	6	0	1.595009	-2.570479	-2.389381
26	1	0	-0.039593	-1.312549	-1.795542

27	6	0	2.293124	-4.234794	-0.798066
28	1	0	1.224778	-4.285039	1.061850
29	6	0	2.439717	-3.630652	-2.049780
30	1	0	1.691943	-2.096085	-3.359556
31	1	0	2.937449	-5.062201	-0.522124
32	16	0	-0.671071	-2.110491	0.866297
33	8	0	-0.183955	-1.000408	1.644099
34	8	0	-0.887301	-3.297686	1.915508
35	6	0	3.498901	-4.101034	-3.003571
36	1	0	3.685023	-5.170796	-2.889942
37	1	0	3.218896	-3.899311	-4.039186
38	1	0	4.440783	-3.578329	-2.806502
39	5	0	-2.635954	-3.011728	-0.792911
40	9	0	-2.214980	-2.952839	-2.116821
41	9	0	-4.018930	-2.942984	-0.706630
42	9	0	-2.180784	-4.241726	-0.219672
43	1	0	-1.401442	-4.012321	1.487882



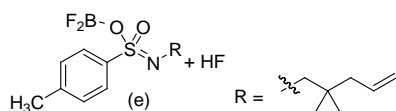
Zero-point correction=	0.344695 (Hartree/Particle)
Thermal correction to Energy=	0.368323
Thermal correction to Enthalpy=	0.369267
Thermal correction to Gibbs Free Energy=	0.290363
Sum of electronic and zero-point Energies=	-1473.700146
Sum of electronic and thermal Energies=	-1473.676518
Sum of electronic and thermal Enthalpies=	-1473.675574
Sum of electronic and thermal Free Energies=	-1473.754479

#### Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.395811	-2.684705	1.873171
2	1	0	3.185027	-2.146883	2.393743
3	1	0	1.770972	-3.342567	2.469630
4	6	0	2.207503	-2.544420	0.564336
5	1	0	1.404605	-3.103465	0.086963
6	6	0	3.027612	-1.655770	-0.326086
7	1	0	3.899462	-1.287490	0.226503
8	1	0	3.406477	-2.247532	-1.167593

9	6	0	2.264703	-0.445858	-0.922175
10	6	0	1.020303	-0.907060	-1.687659
11	1	0	0.273320	-1.350566	-1.023033
12	1	0	0.549200	-0.067472	-2.204625
13	1	0	1.295598	-1.653589	-2.438865
14	6	0	3.205202	0.304219	-1.869925
15	1	0	2.720903	1.189695	-2.294122
16	1	0	4.114565	0.626273	-1.352064
17	1	0	3.500339	-0.339275	-2.704210
18	6	0	1.871334	0.462405	0.251055
19	1	0	1.267029	-0.105052	0.960295
20	1	0	2.758778	0.808448	0.787536
21	7	0	1.096542	1.636358	-0.189895
22	1	0	1.629883	2.447669	-0.490669
23	6	0	-1.341820	0.711254	0.438402
24	6	0	-2.057933	0.598558	-0.748686
25	6	0	-1.427256	-0.243989	1.444732
26	6	0	-2.882586	-0.500197	-0.920549
27	1	0	-1.974407	1.349493	-1.525585
28	6	0	-2.257218	-1.335946	1.247921
29	1	0	-0.863391	-0.142663	2.363542
30	6	0	-2.996090	-1.479412	0.071036
31	1	0	-3.446845	-0.599962	-1.841100
32	1	0	-2.333128	-2.088347	2.025298
33	16	0	-0.245874	2.078710	0.588212
34	8	0	0.112363	2.177222	2.065732
35	8	0	-0.763001	3.285655	-0.010233
36	6	0	-3.919933	-2.649313	-0.106577
37	1	0	-4.119467	-2.842803	-1.162006
38	1	0	-3.504032	-3.552118	0.345873
39	1	0	-4.877619	-2.446382	0.383876
40	5	0	-0.775542	2.755914	3.228212
41	9	0	-0.427448	4.085162	3.369980
42	9	0	-2.107147	2.598435	2.872043
43	9	0	-0.428297	1.997482	4.328843

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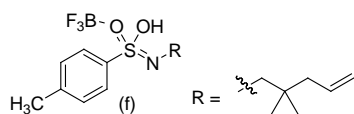
Zero-point correction= 0.341928 (Hartree/Particle)  
 Thermal correction to Energy= 0.366905  
 Thermal correction to Enthalpy= 0.367849  
 Thermal correction to Gibbs Free Energy= 0.284327  
 Sum of electronic and zero-point Energies= -1473.639328  
 Sum of electronic and thermal Energies= -1473.614351  
 Sum of electronic and thermal Enthalpies= -1473.613406  
 Sum of electronic and thermal Free Energies= -1473.696929

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.021760	-3.467763	1.561606
2	1	0	3.857380	-3.018945	2.093919
3	1	0	2.424268	-4.195469	2.102551
4	6	0	2.748249	-3.141465	0.301709
5	1	0	1.901341	-3.616426	-0.190916
6	6	0	3.529662	-2.151052	-0.512222
7	1	0	4.433628	-1.862372	0.036072
8	1	0	3.858157	-2.635944	-1.439391
9	6	0	2.758690	-0.867995	-0.911981
10	6	0	1.489388	-1.218775	-1.695558
11	1	0	0.766890	-1.764484	-1.081782
12	1	0	0.998987	-0.314229	-2.065303
13	1	0	1.737215	-1.840201	-2.562084
14	6	0	3.676462	-0.005293	-1.782457
15	1	0	3.183302	0.928474	-2.065277
16	1	0	4.601070	0.246129	-1.252224
17	1	0	3.946181	-0.537668	-2.700001
18	6	0	2.407632	-0.117380	0.383433
19	1	0	1.809379	-0.770320	1.024847
20	1	0	3.328959	0.110281	0.927876
21	7	0	1.739160	1.162912	0.115317
22	1	0	-0.141065	4.269370	0.551648
23	6	0	-0.844657	0.199543	0.502280
24	6	0	-1.692390	0.204294	-0.601326
25	6	0	-0.850353	-0.840042	1.424314



26	6	0	-2.569178	-0.853810	-0.767722
27	1	0	-1.674735	1.021416	-1.312505
28	6	0	-1.736643	-1.892002	1.233461
29	1	0	-0.188367	-0.838275	2.281724
30	6	0	-2.603522	-1.917011	0.140732
31	1	0	-3.243599	-0.853804	-1.617555
32	1	0	-1.752836	-2.703530	1.952733
33	16	0	0.364193	1.495271	0.590488
34	8	0	0.419895	1.734738	2.257870
35	8	0	-0.198688	2.722957	0.030853
36	6	0	-3.570207	-3.049221	-0.058359
37	1	0	-3.426061	-3.515870	-1.036879
38	1	0	-3.450930	-3.814874	0.710048
39	1	0	-4.600484	-2.683484	-0.020326
40	5	0	-0.592456	2.190795	3.043860
41	9	0	-0.133446	5.156522	0.873737
42	9	0	-1.802478	2.467844	2.583163
43	9	0	-0.353485	2.347993	4.335503



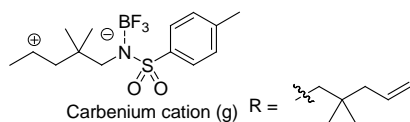
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Thermal correction to Energy=	0.366752
Thermal correction to Enthalpy=	0.367696
Thermal correction to Gibbs Free Energy=	0.284826
Sum of electronic and zero-point Energies=	-1473.658587
Sum of electronic and thermal Energies=	-1473.634223
Sum of electronic and thermal Enthalpies=	-1473.633279
Sum of electronic and thermal Free Energies=	-1473.716148

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.805528	0.258881	2.517350
2	1	0	-5.654513	-0.368467	2.254808
3	1	0	-4.624788	0.430229	3.574078
4	6	0	-4.021446	0.789972	1.584035
5	1	0	-3.180770	1.408401	1.893594
6	6	0	-4.210085	0.602625	0.106577

7	1	0	-5.146440	0.061979	-0.073079
8	1	0	-4.313794	1.587418	-0.365365
9	6	0	-3.060901	-0.134856	-0.623379
10	6	0	-1.730020	0.602109	-0.443080
11	1	0	-1.396315	0.589163	0.598139
12	1	0	-0.945806	0.136827	-1.046957
13	1	0	-1.823762	1.645584	-0.759917
14	6	0	-3.410942	-0.213843	-2.111826
15	1	0	-2.639992	-0.753181	-2.669080
16	1	0	-4.365107	-0.728707	-2.265806
17	1	0	-3.495754	0.790005	-2.539703
18	6	0	-2.961734	-1.547804	-0.030331
19	1	0	-2.755555	-1.475041	1.040448
20	1	0	-3.916291	-2.068691	-0.154646
21	7	0	-1.926301	-2.322622	-0.726515
22	6	0	0.276827	-3.678468	-1.275145
23	6	0	0.288613	-3.035135	-2.503841
24	6	0	1.221277	-4.641441	-0.928058
25	6	0	1.275492	-3.380645	-3.416230
26	1	0	-0.458274	-2.288105	-2.740187
27	6	0	2.194077	-4.965751	-1.855662
28	1	0	1.197213	-5.129468	0.038560
29	6	0	2.236939	-4.344018	-3.109652
30	1	0	1.295212	-2.889166	-4.382399
31	1	0	2.935731	-5.715858	-1.603598
32	16	0	-0.932606	-3.221562	-0.093829
33	8	0	-0.140567	-2.728798	1.136020
34	8	0	-1.439555	-4.682383	0.383806
35	6	0	3.307803	-4.713966	-4.094500
36	1	0	3.304824	-5.791532	-4.280149
37	1	0	3.171737	-4.198098	-5.046112
38	1	0	4.294817	-4.454767	-3.700301
39	5	0	-0.627699	-2.620899	2.602280
40	9	0	-0.832862	-1.287916	2.883296
41	9	0	0.361062	-3.183842	3.378030
42	9	0	-1.834295	-3.352047	2.691655
43	1	0	-1.840586	-4.618082	1.272649

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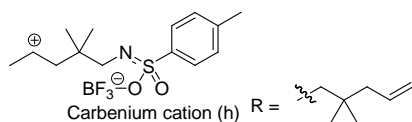
Zero-point correction=	0.340864 (Hartree/Particle)
Thermal correction to Energy=	0.364903
Thermal correction to Enthalpy=	0.365847
Thermal correction to Gibbs Free Energy=	0.285197
Sum of electronic and zero-point Energies=	-1473.659760
Sum of electronic and thermal Energies=	-1473.635721
Sum of electronic and thermal Enthalpies=	-1473.634777
Sum of electronic and thermal Free Energies=	-1473.715426

### Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.604888	-0.744623	5.092831
2	1	0	-5.100347	-1.433188	4.410719
3	1	0	-3.824004	-1.199979	5.704836
4	6	0	-4.190476	0.495238	4.495124
5	1	0	-3.516745	1.125278	5.076444
6	6	0	-4.574989	0.936923	3.194806
7	1	0	-3.666246	0.486235	2.697408
8	1	0	-5.418636	0.366831	2.794974
9	6	0	-4.618573	2.446334	2.876020
10	6	0	-3.341756	3.151941	3.328954
11	1	0	-2.449066	2.685070	2.904171
12	1	0	-3.365124	4.191203	2.999370
13	1	0	-3.249746	3.157584	4.418966
14	6	0	-5.822396	3.040932	3.614262
15	1	0	-5.910674	4.109023	3.403035
16	1	0	-6.756763	2.560168	3.317988
17	1	0	-5.692845	2.925632	4.696032
18	6	0	-4.783087	2.513713	1.335454
19	1	0	-3.905791	2.047405	0.878408
20	1	0	-5.652195	1.913882	1.054554
21	7	0	-4.898349	3.860203	0.773966
22	6	0	-6.602336	4.593290	-1.272779
23	6	0	-6.541722	5.834639	-1.886939
24	6	0	-6.803443	3.434940	-2.015626
25	6	0	-6.687214	5.913927	-3.266512

26	1	0	-6.375301	6.725442	-1.295021
27	6	0	-6.945475	3.529862	-3.391073
28	1	0	-6.844515	2.468684	-1.526301
29	6	0	-6.890749	4.768762	-4.036878
30	1	0	-6.635855	6.883374	-3.751214
31	1	0	-7.099806	2.627720	-3.974412
32	16	0	-6.411145	4.453076	0.497306
33	8	0	-7.377781	3.451668	0.948123
34	8	0	-6.530099	5.795161	1.052645
35	6	0	-7.074447	4.863430	-5.526218
36	1	0	-6.596759	5.758853	-5.929307
37	1	0	-6.658184	3.989078	-6.031834
38	1	0	-8.139516	4.913394	-5.776451
39	5	0	-3.708316	4.370625	-0.074134
40	9	0	-2.502115	4.187240	0.639031
41	9	0	-3.592064	3.630582	-1.285664
42	9	0	-3.862939	5.732555	-0.386686
43	1	0	-5.357912	-0.377773	5.825270

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Zero-point correction= 0.341243 (Hartree/Particle)  
 Thermal correction to Energy= 0.365354  
 Thermal correction to Enthalpy= 0.366298  
 Thermal correction to Gibbs Free Energy= 0.285894  
 Sum of electronic and zero-point Energies= -1473.636150  
 Sum of electronic and thermal Energies= -1473.612039  
 Sum of electronic and thermal Enthalpies= -1473.611094  
 Sum of electronic and thermal Free Energies= -1473.691499

Input orientation:

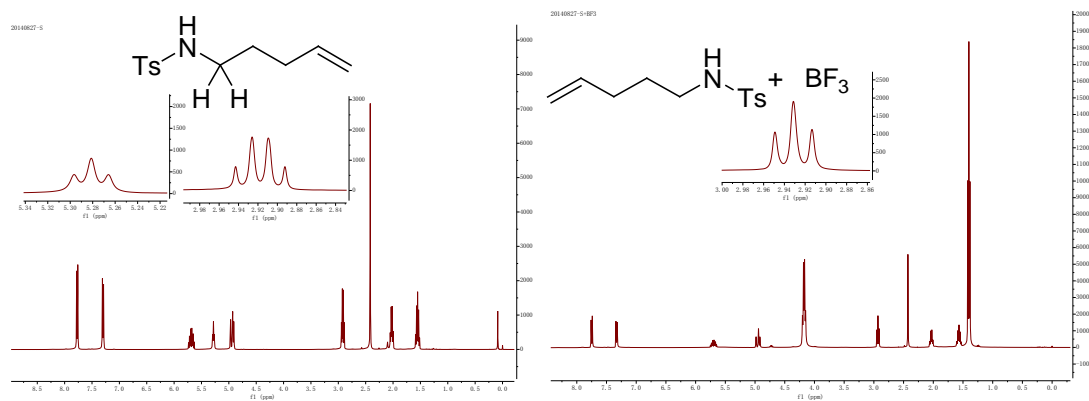
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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3	1	0	1.757554	-2.598273	2.608752
4	6	0	2.386994	-2.420049	0.606538
5	1	0	1.533655	-2.986936	0.233824
6	6	0	3.143963	-1.659941	-0.344461
7	1	0	4.063232	-1.260456	0.083123
8	1	0	3.340619	-2.293582	-1.218218
9	6	0	2.258322	-0.454060	-0.918222
10	6	0	1.046028	-0.979064	-1.685349
11	1	0	0.320132	-1.473527	-1.033407
12	1	0	0.538295	-0.140453	-2.165721
13	1	0	1.351833	-1.682654	-2.464780
14	6	0	3.179053	0.331423	-1.849736
15	1	0	2.643398	1.201661	-2.234208
16	1	0	4.070407	0.684882	-1.324198
17	1	0	3.493581	-0.283412	-2.697486
18	6	0	1.831119	0.399635	0.291718
19	1	0	1.208575	-0.229055	0.947454
20	1	0	2.724097	0.663035	0.872606
21	7	0	1.150934	1.609415	-0.138379
22	6	0	-1.372327	0.694689	0.423526
23	6	0	-2.101575	0.608032	-0.757120
24	6	0	-1.498864	-0.275999	1.409899

25	6	0	-2.972443	-0.455938	-0.941100
26	1	0	-1.994968	1.365014	-1.525839
27	6	0	-2.373085	-1.336840	1.208838
28	1	0	-0.939415	-0.199055	2.333907
29	6	0	-3.123317	-1.442695	0.036763
30	1	0	-3.546880	-0.519273	-1.859593
31	1	0	-2.479646	-2.089958	1.983273
32	16	0	-0.157462	2.003813	0.546198
33	8	0	0.085464	2.081614	2.094184
34	8	0	-0.727406	3.229722	0.011397
35	6	0	-4.096905	-2.573187	-0.150442
36	1	0	-4.291904	-2.759158	-1.208607
37	1	0	-3.725531	-3.495017	0.303313
38	1	0	-5.052876	-2.334454	0.326951
39	5	0	-0.794388	2.684413	3.155227
40	9	0	-0.477438	4.038759	3.304653
41	9	0	-2.148913	2.535555	2.831429
42	9	0	-0.493052	1.984426	4.332937
43	1	0	3.120752	-3.532786	2.079453

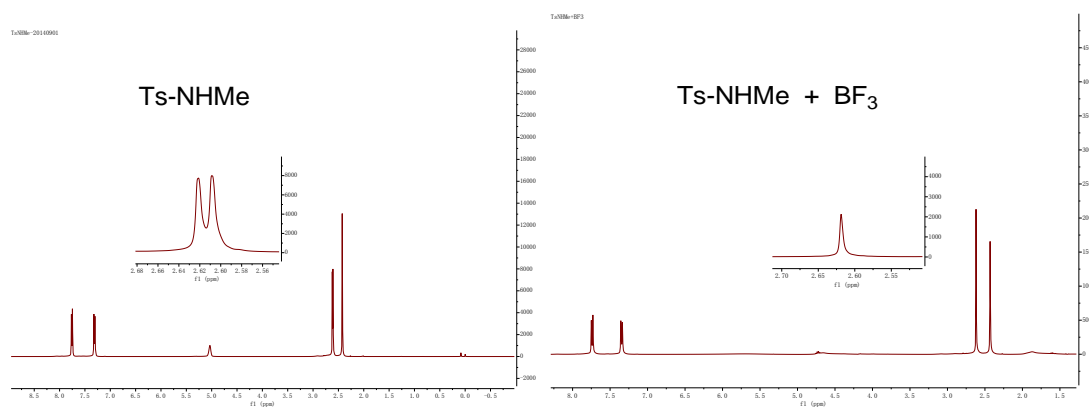
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## 2. Mechanism Studies

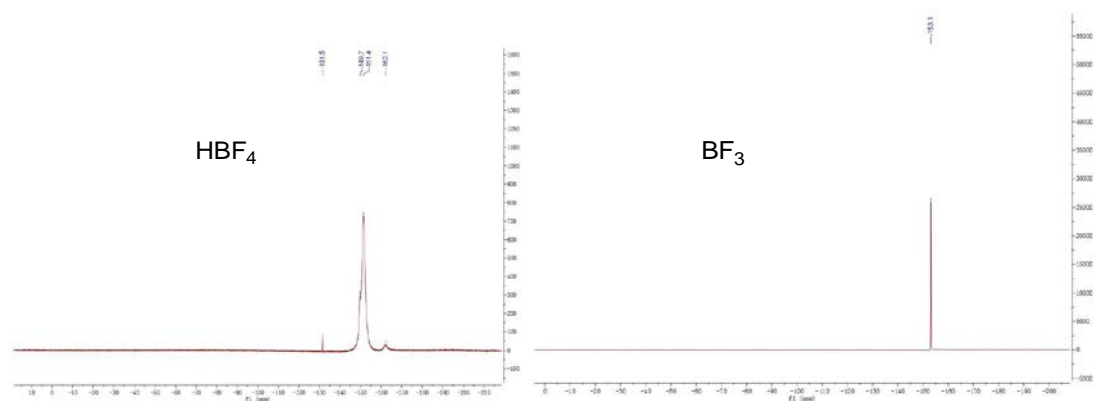
NMR spectra of substrate **1e** before and after the addition of  $\text{BF}_3$ .

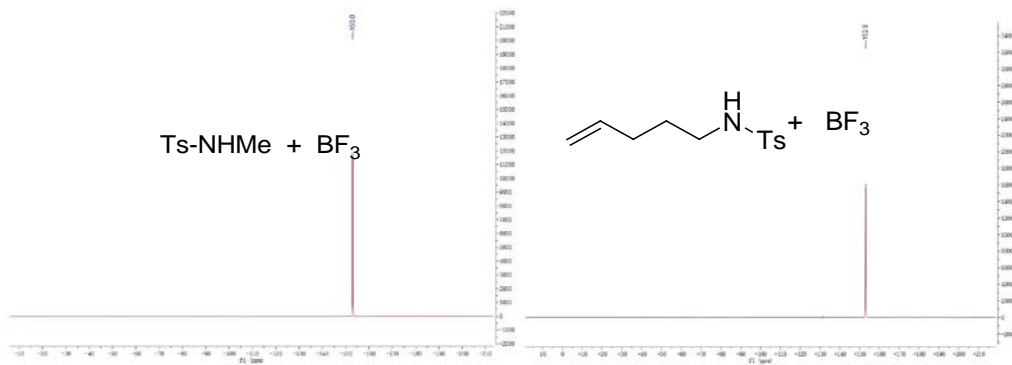


NMR spectra of substrate N-methyl p-toluenesulfonamide before and after the addition of  $\text{BF}_3$ .

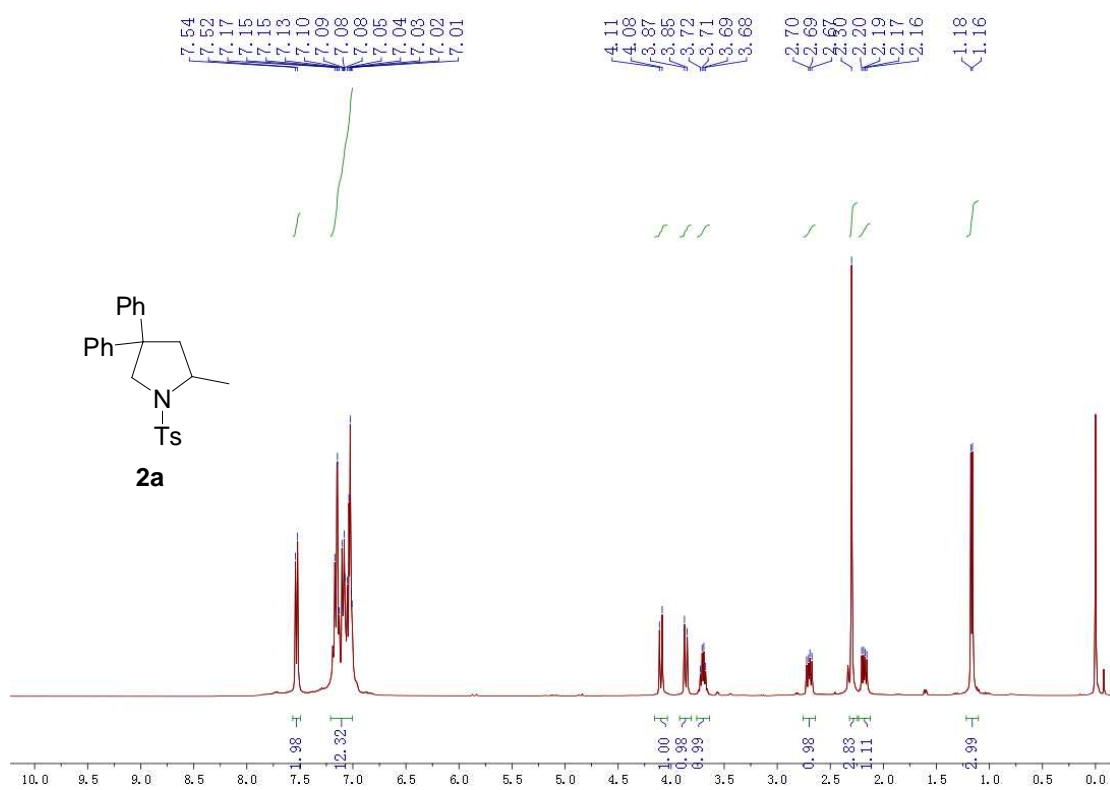


$^{19}\text{F}$  NMR spectra of  $\text{HBF}_4$  and a mixture N-methyl p-toluenesulfonamide  $\text{BF}_3$ .

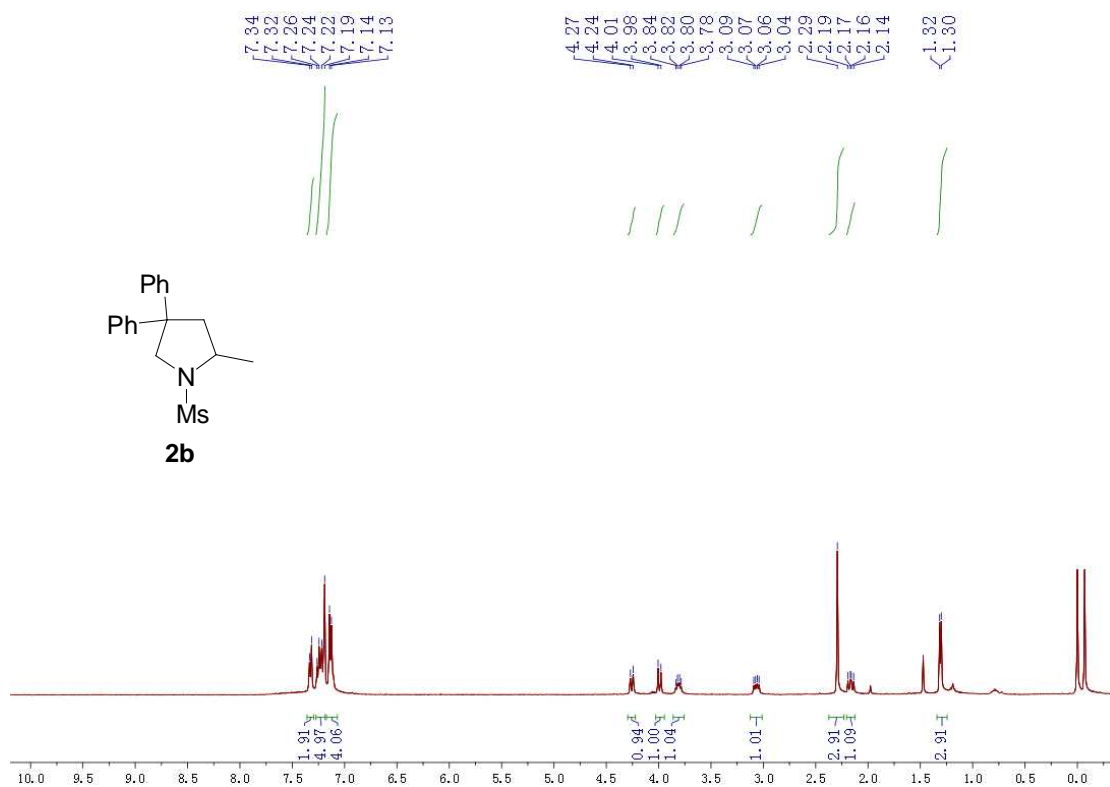
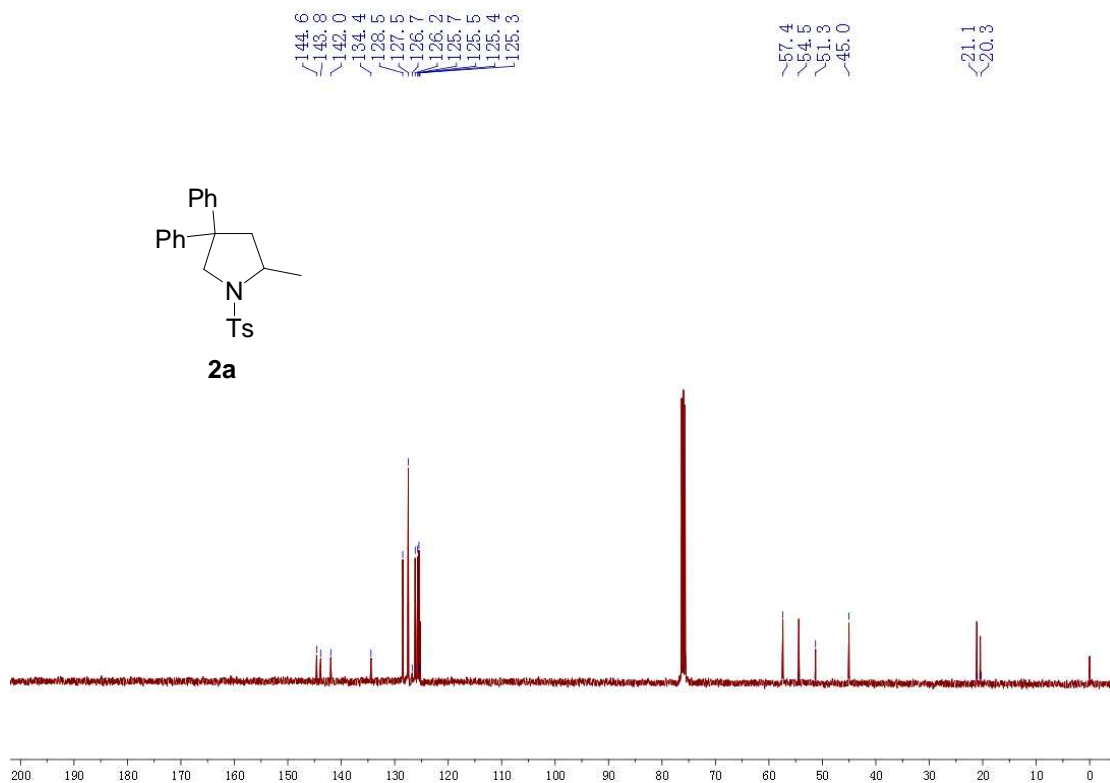


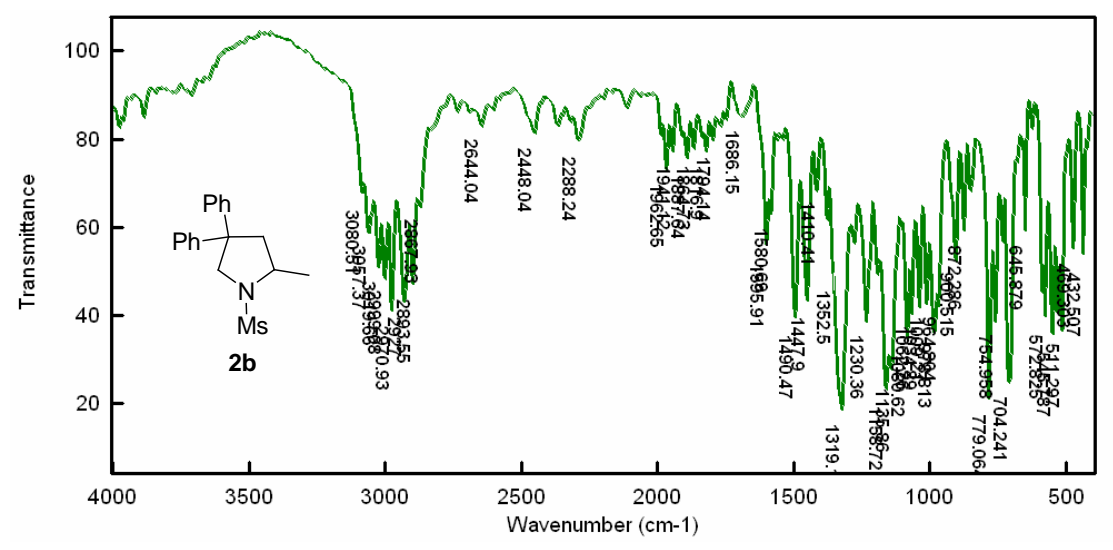
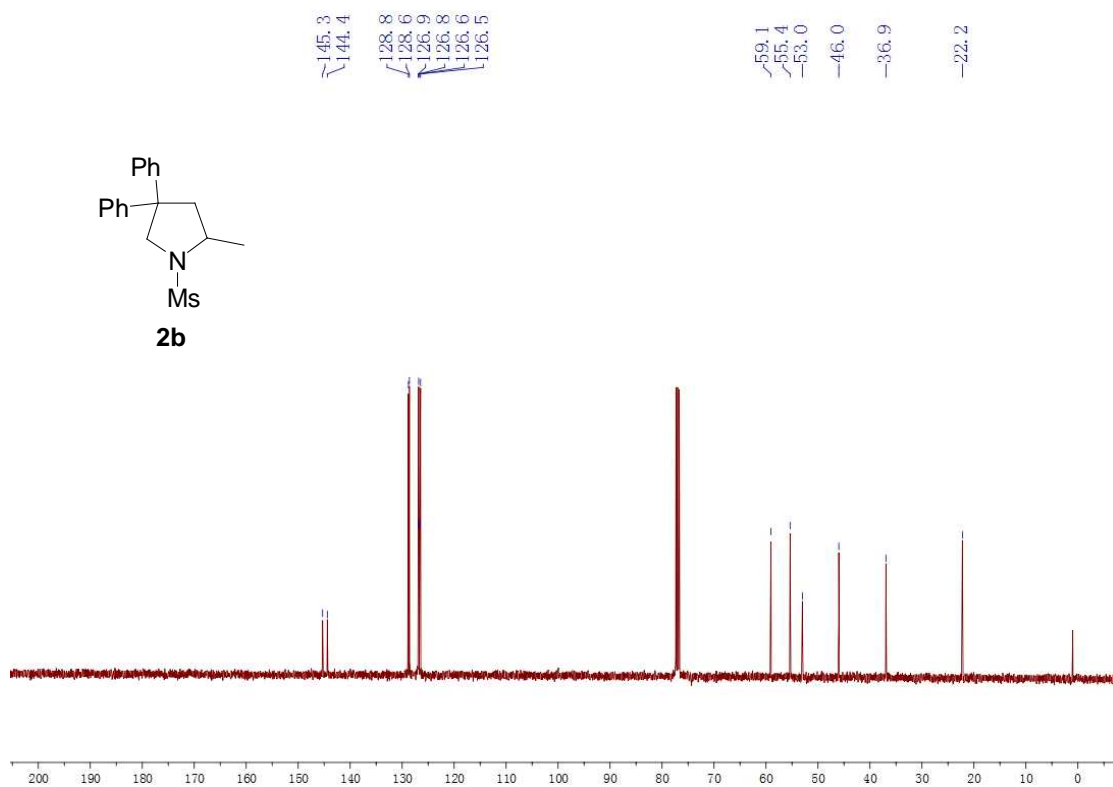


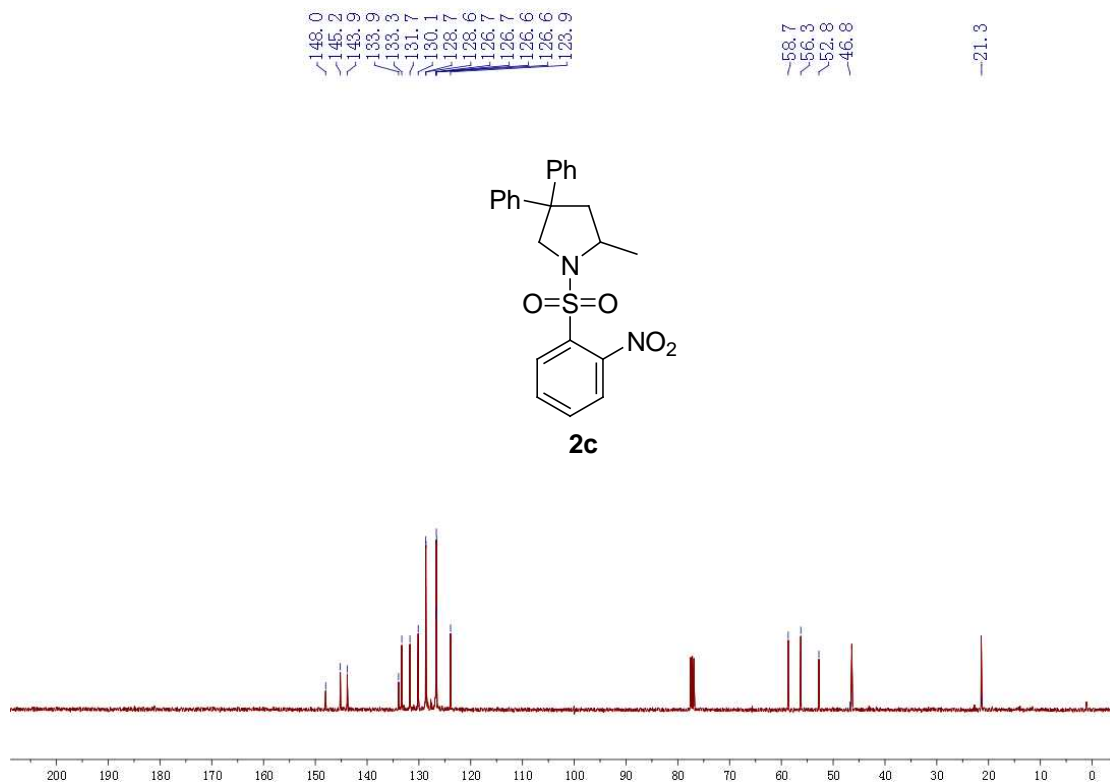
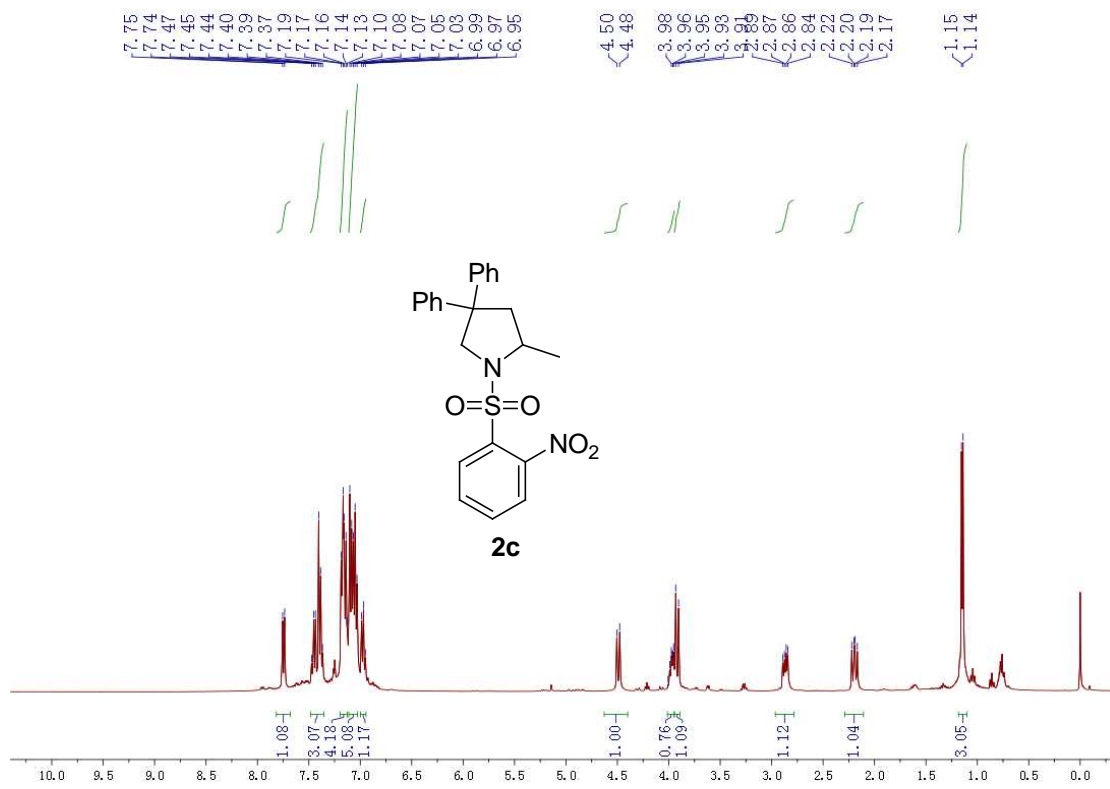
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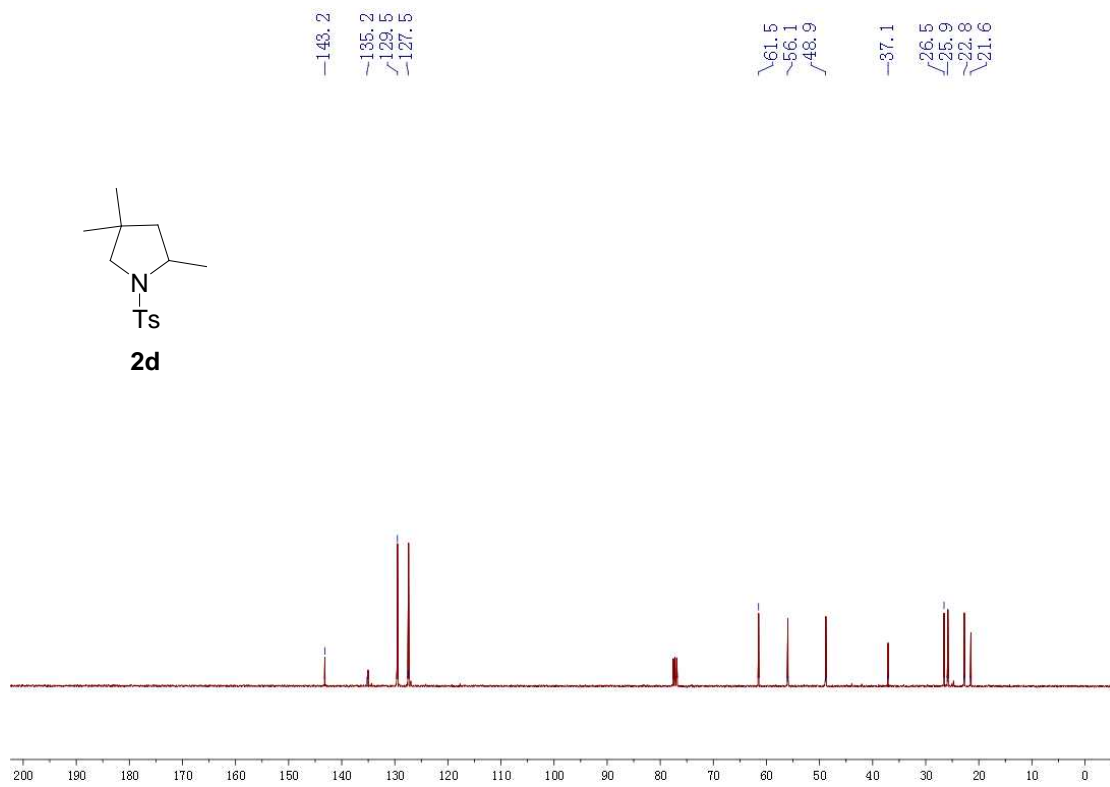
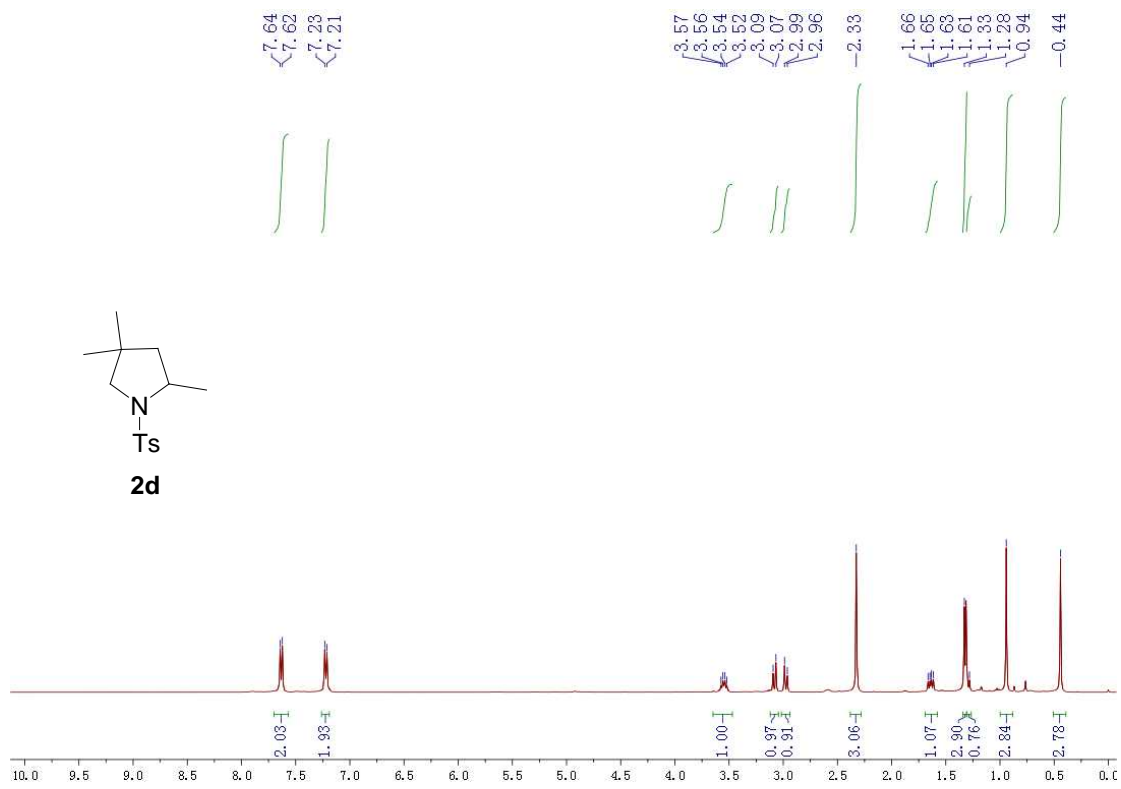


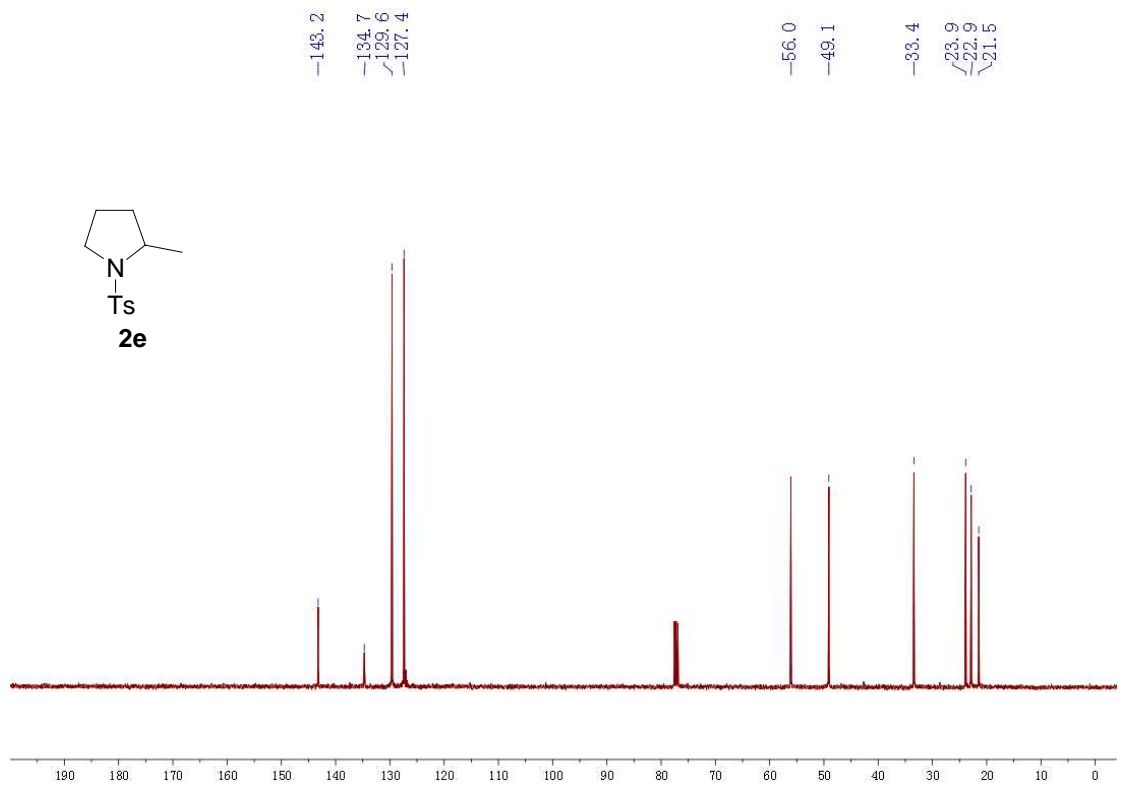
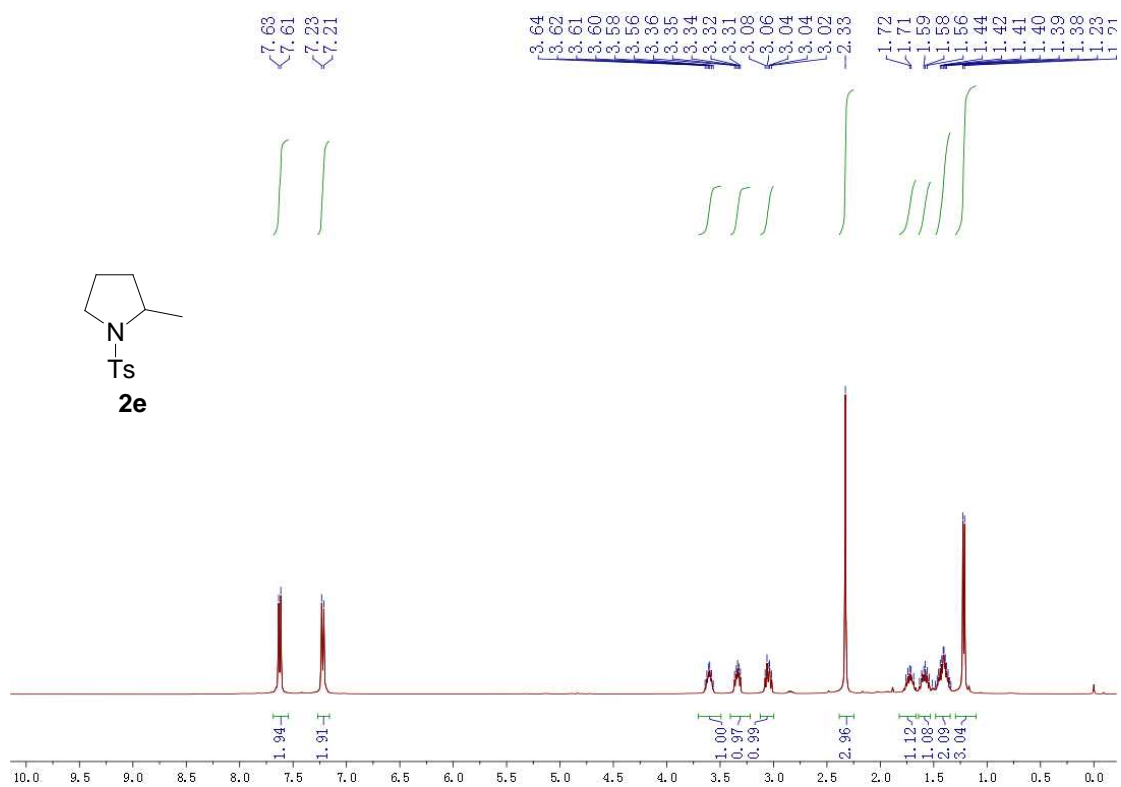


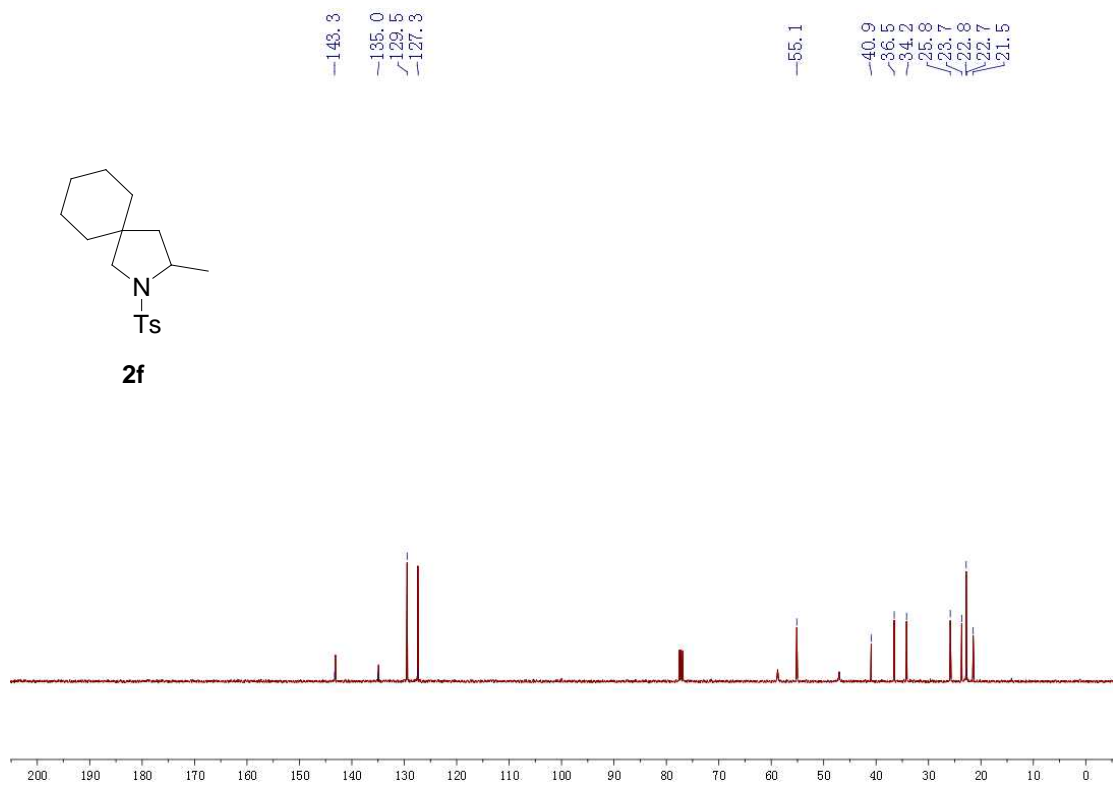
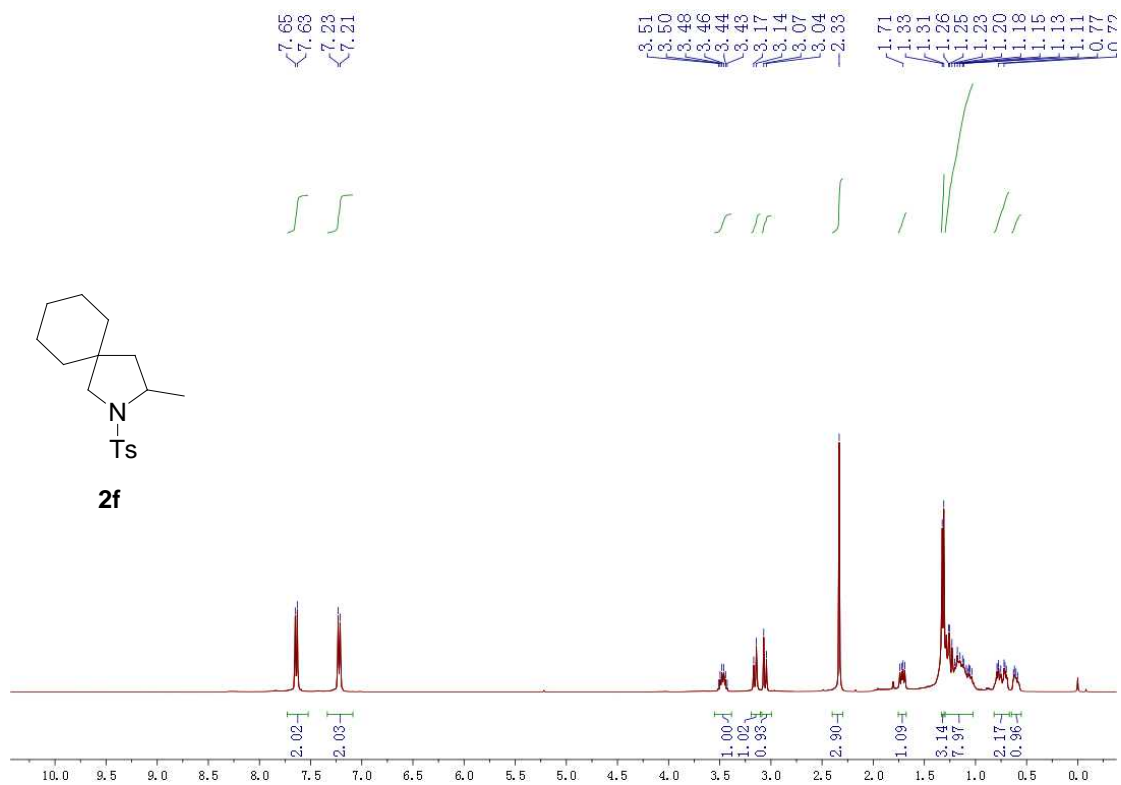


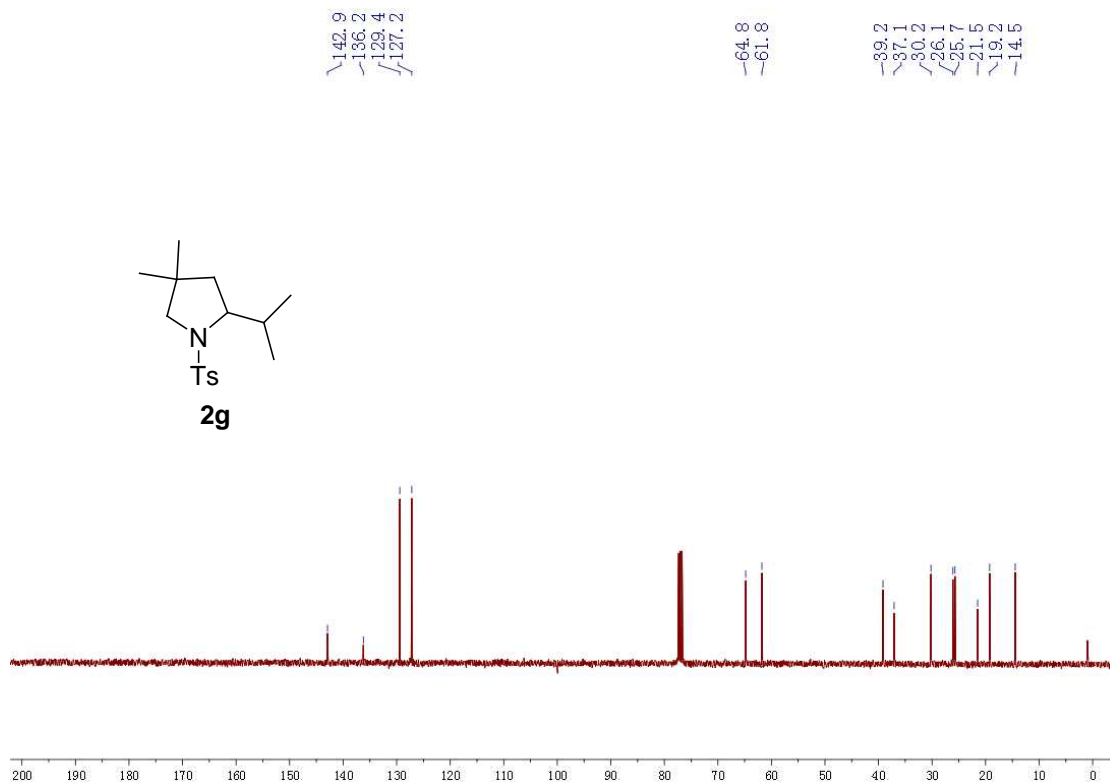
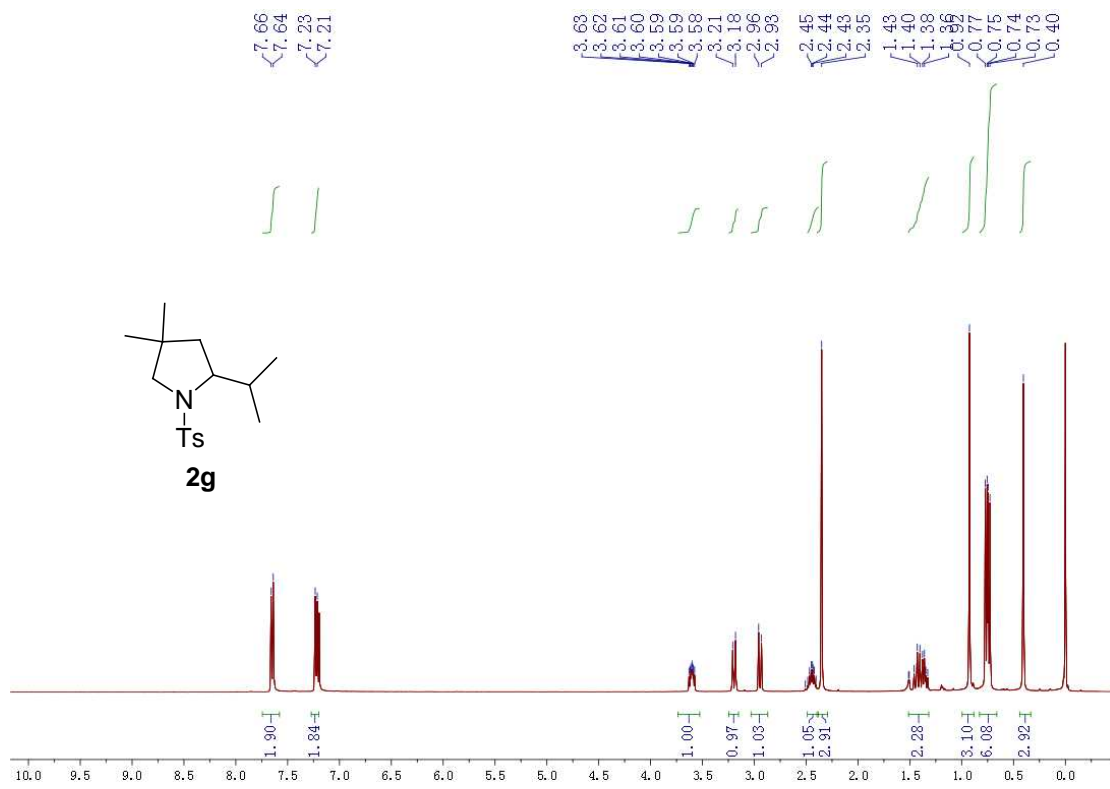


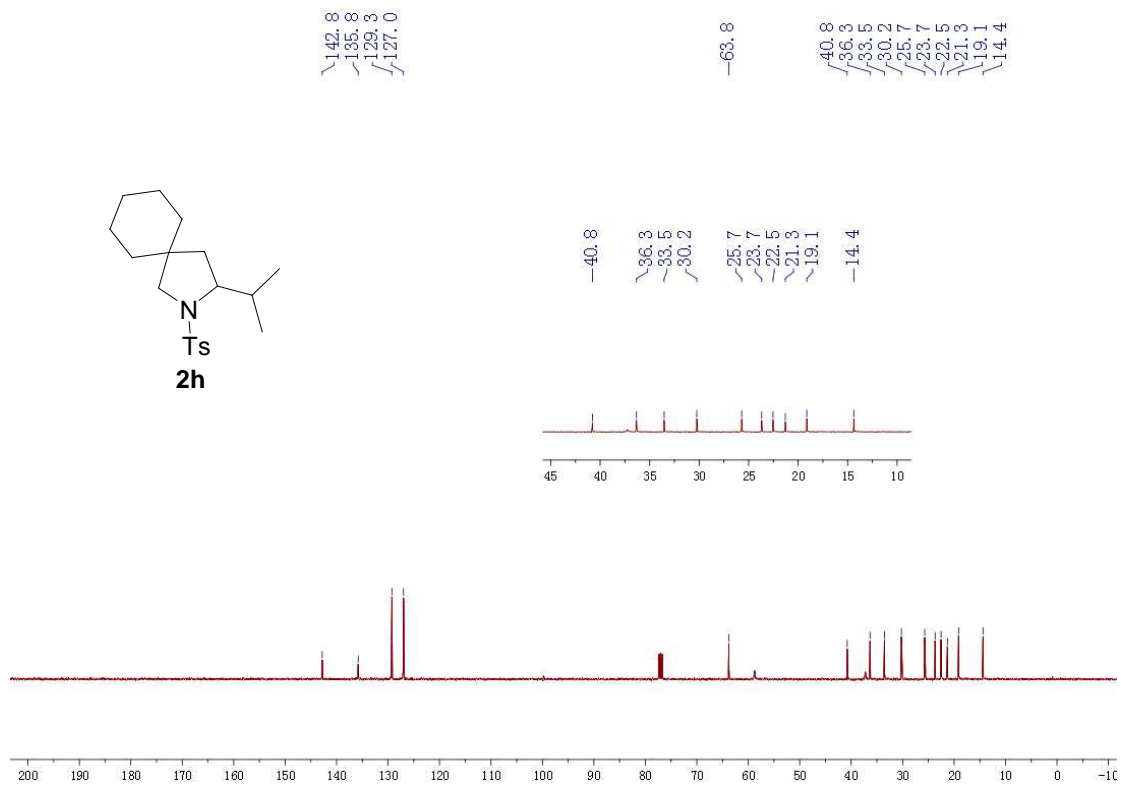
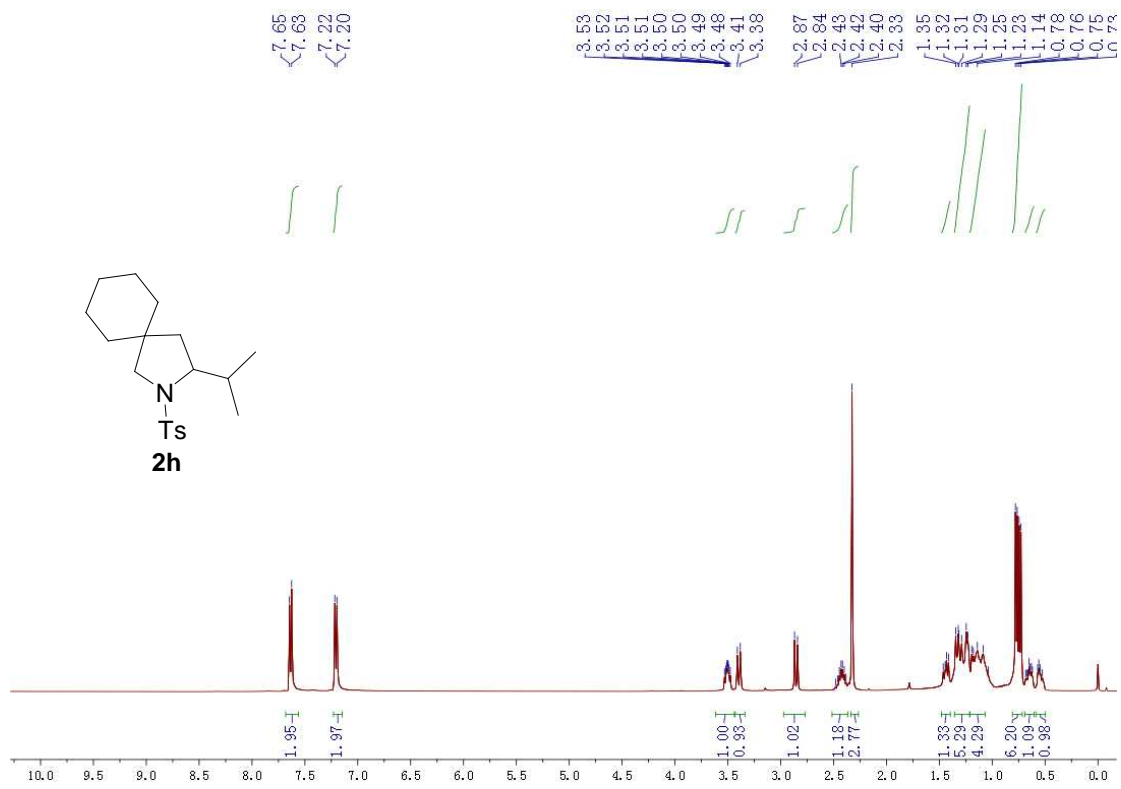






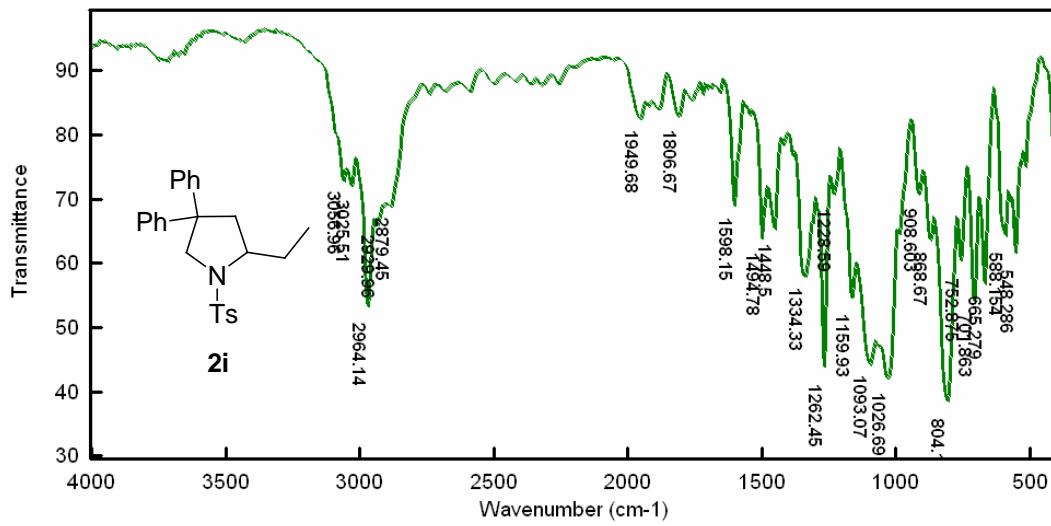
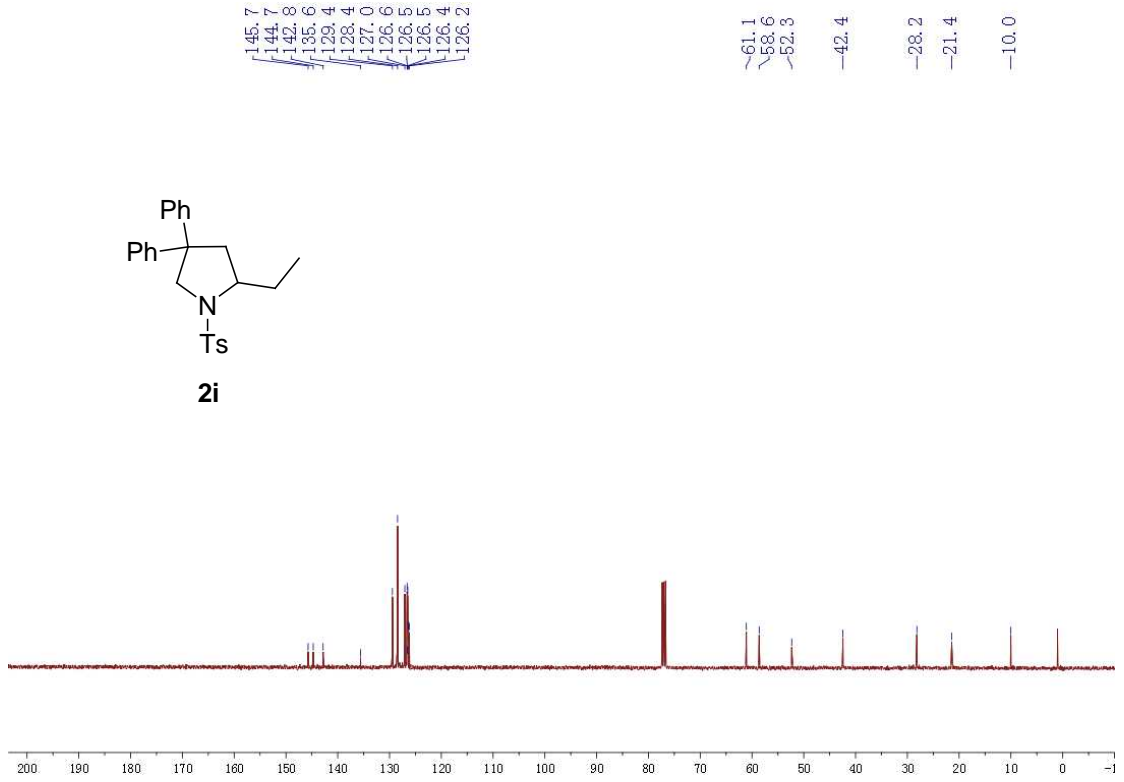
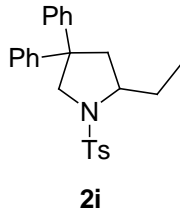


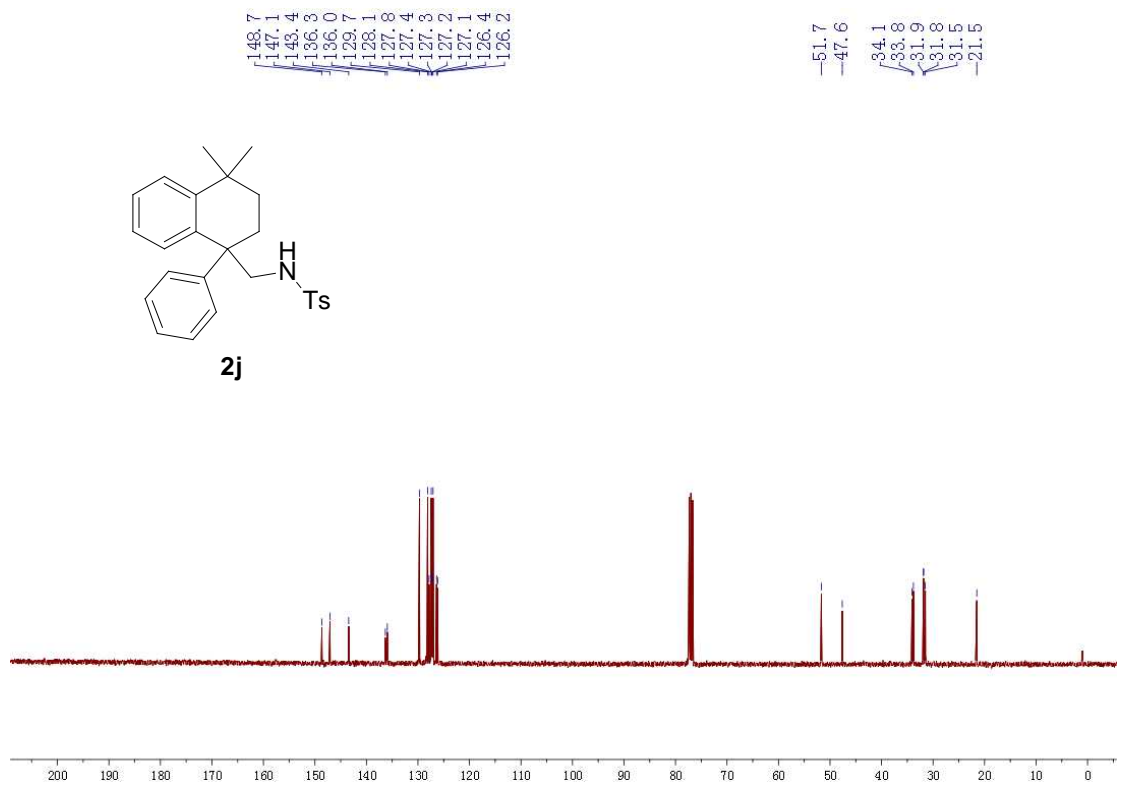
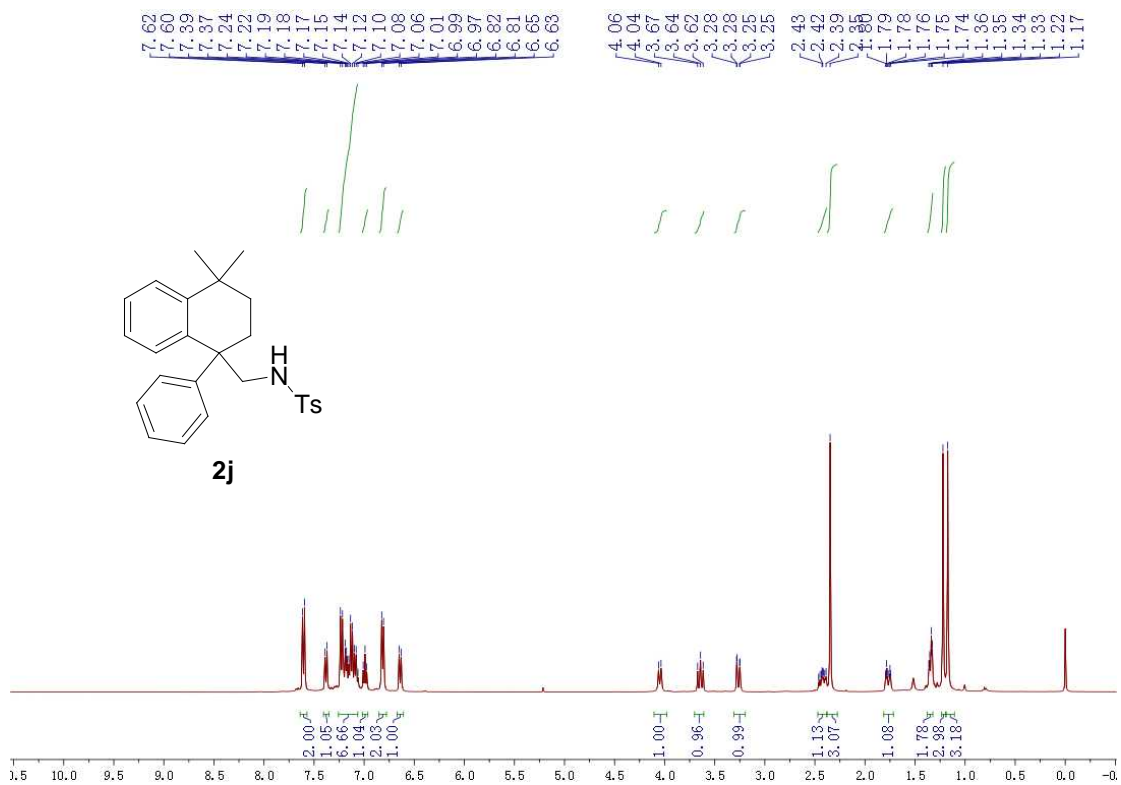




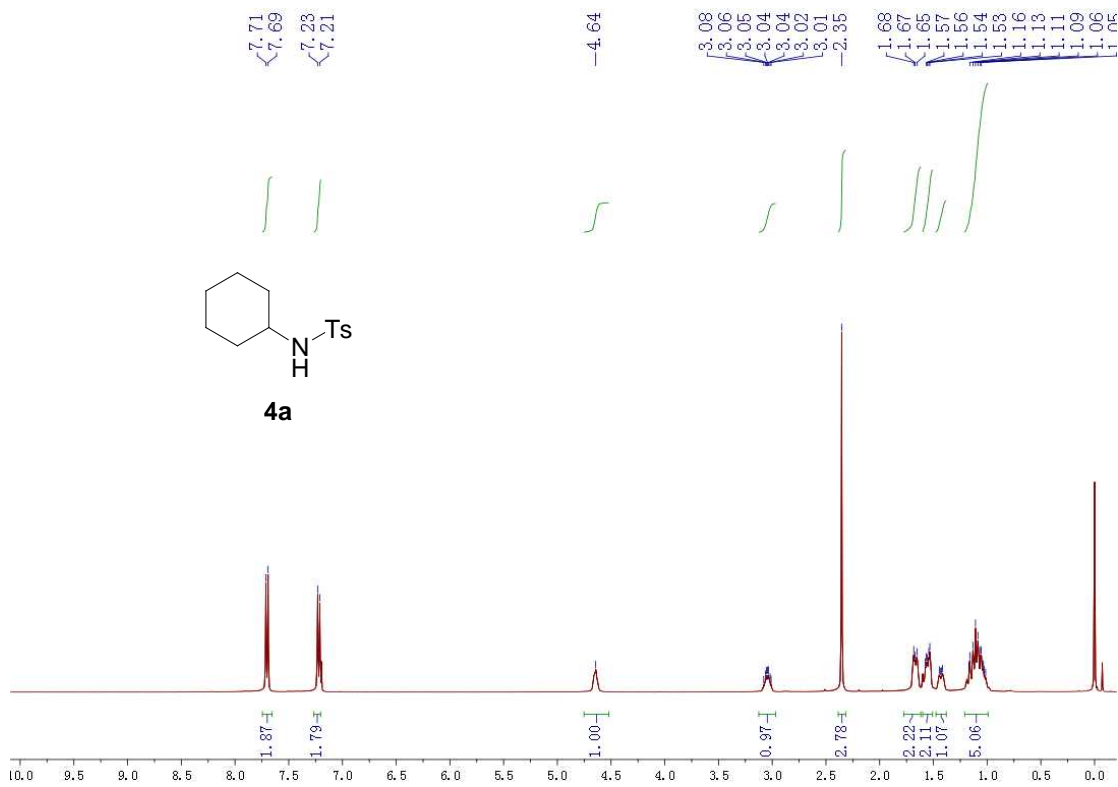
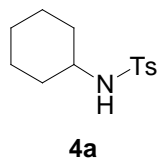
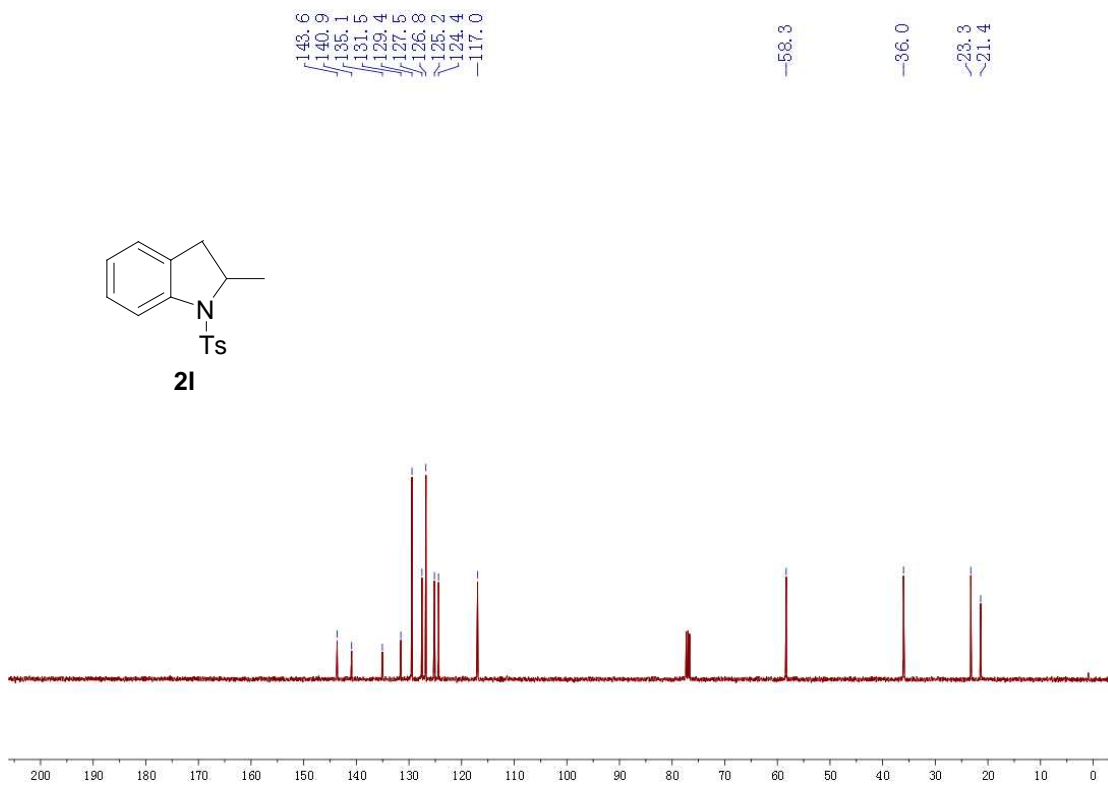
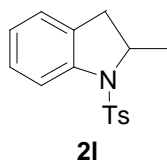


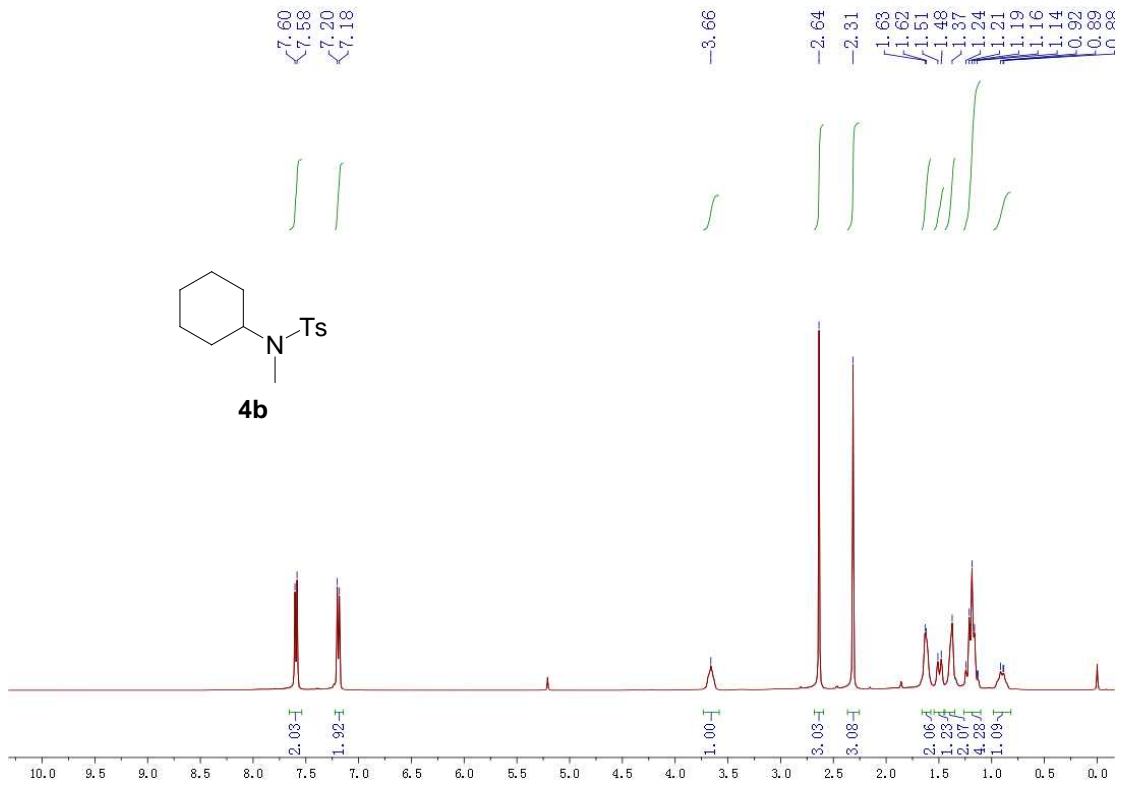
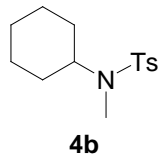
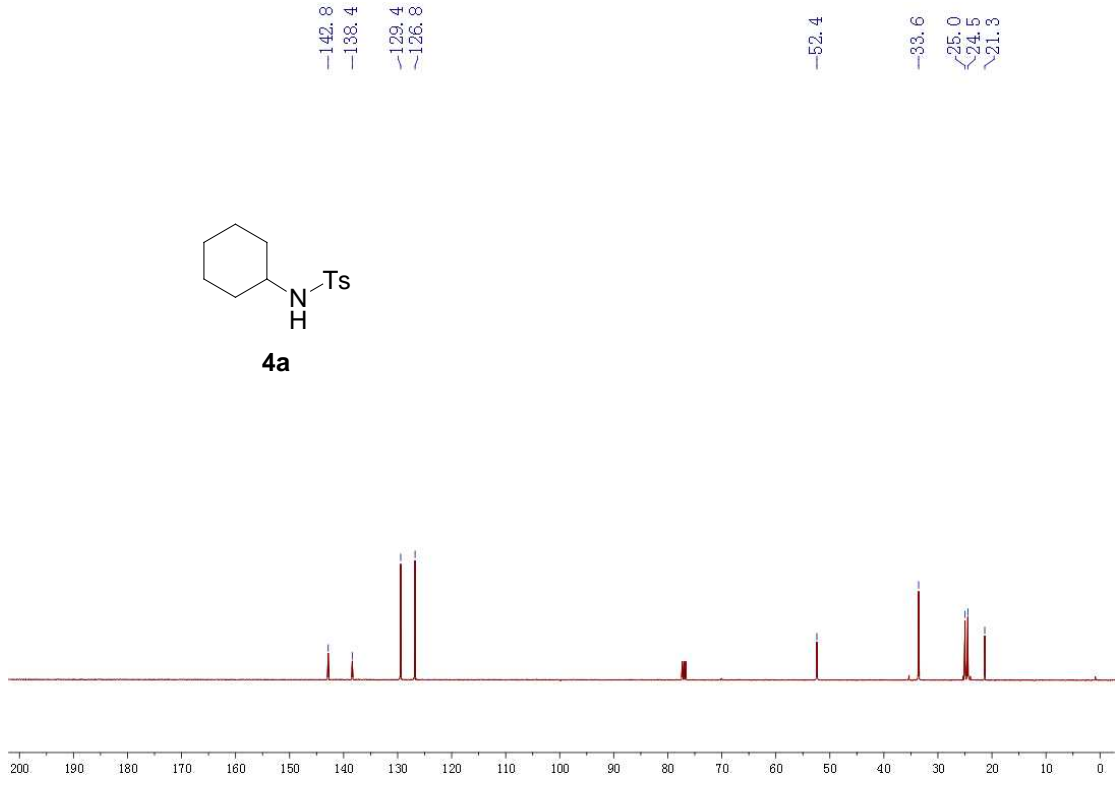
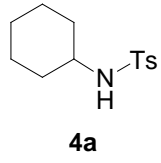


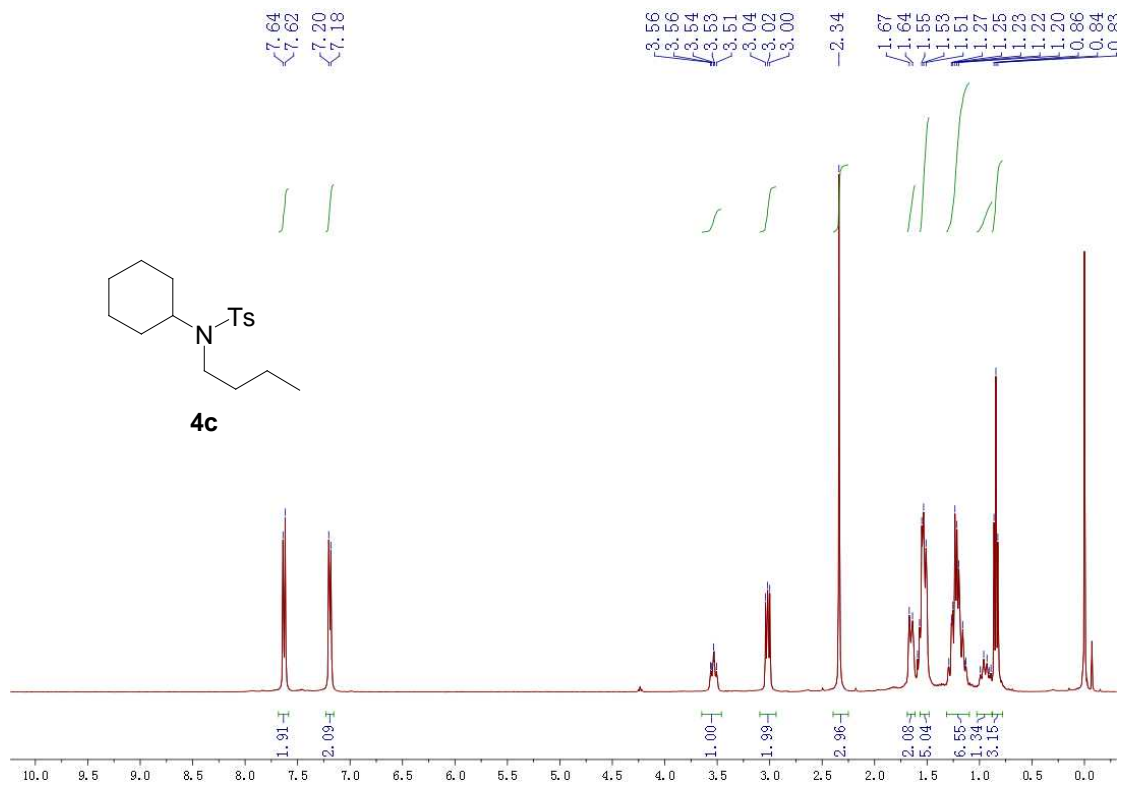
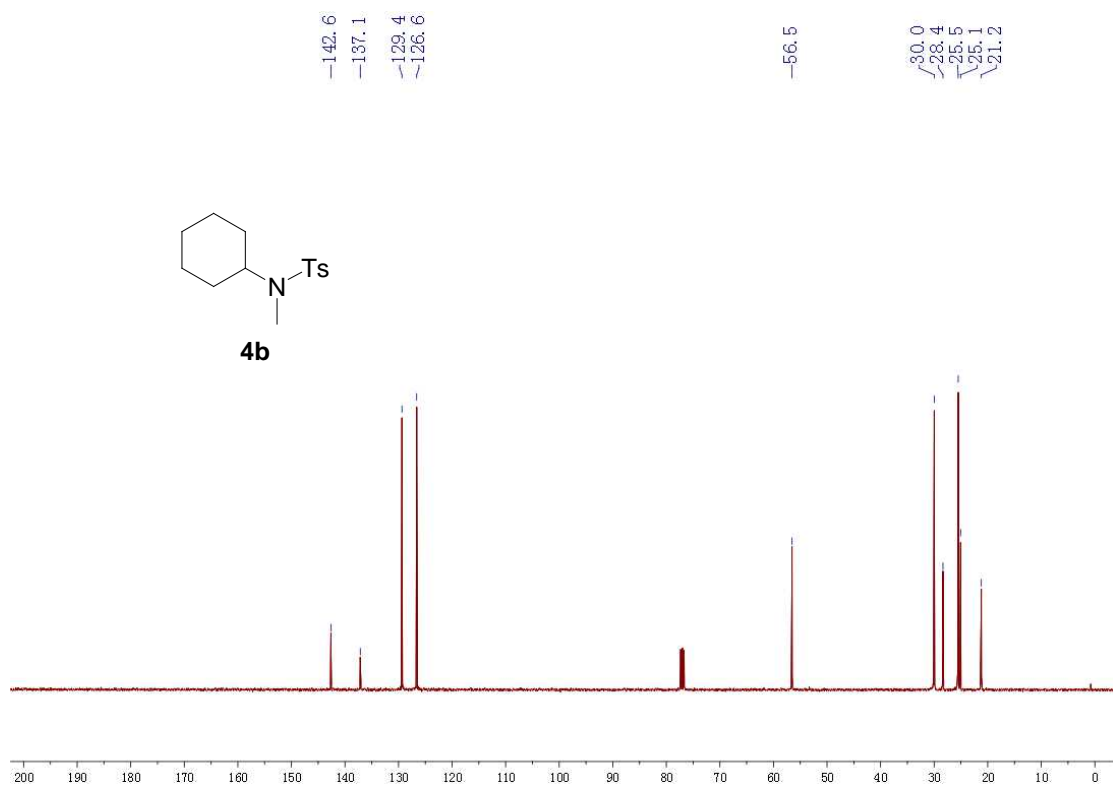


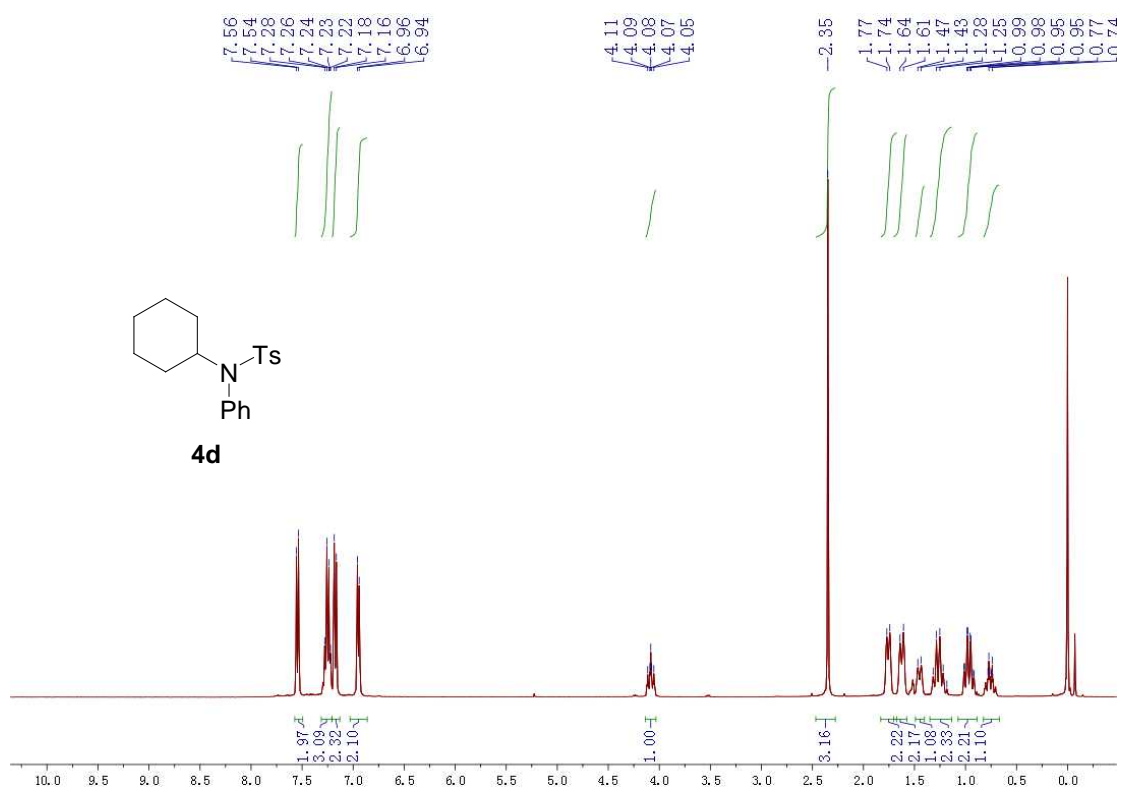
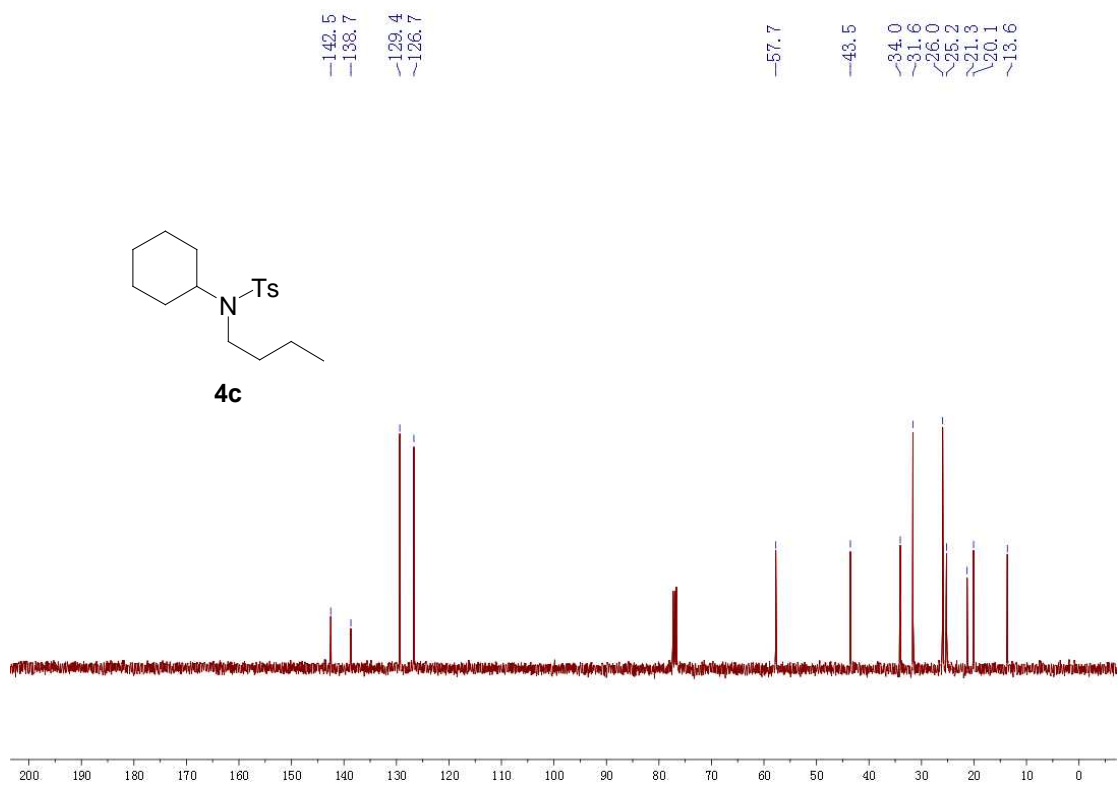




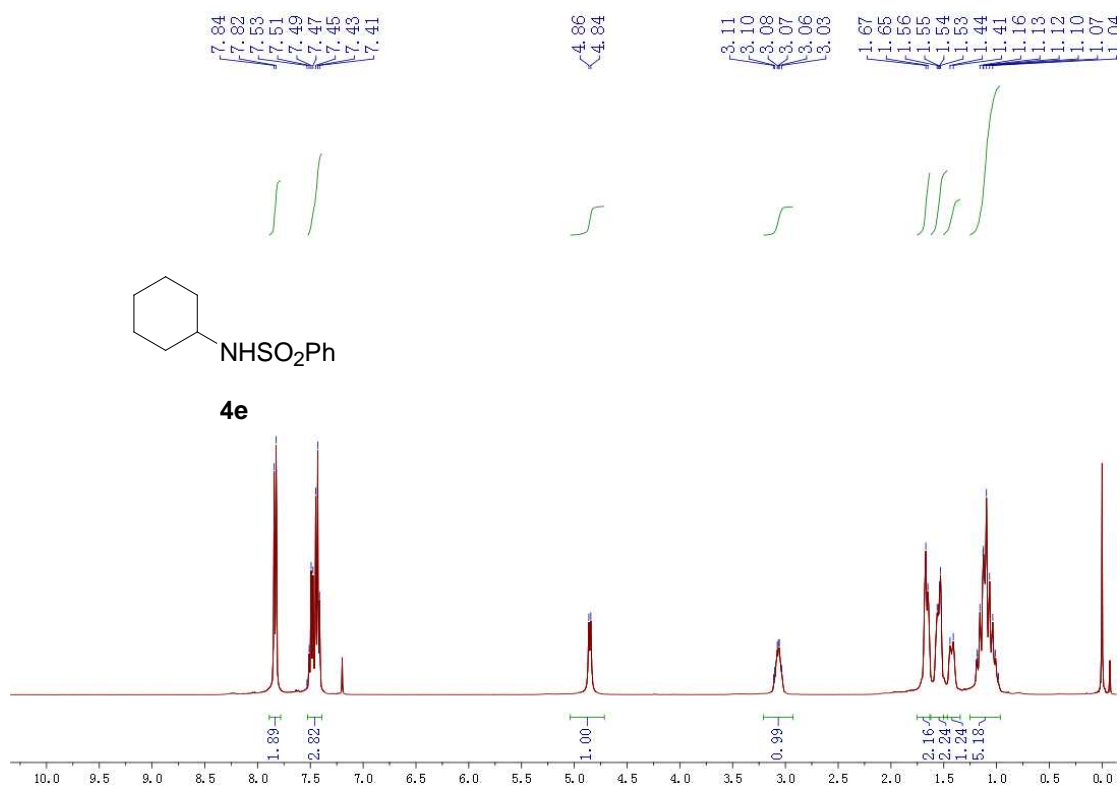
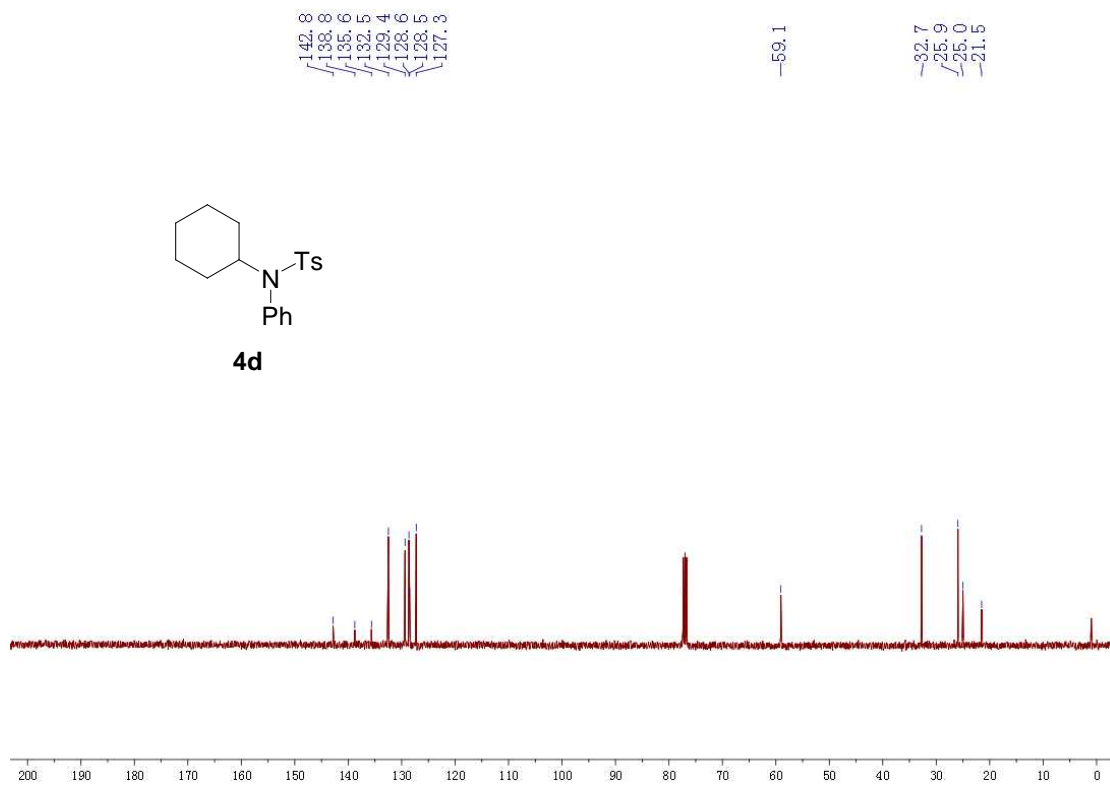


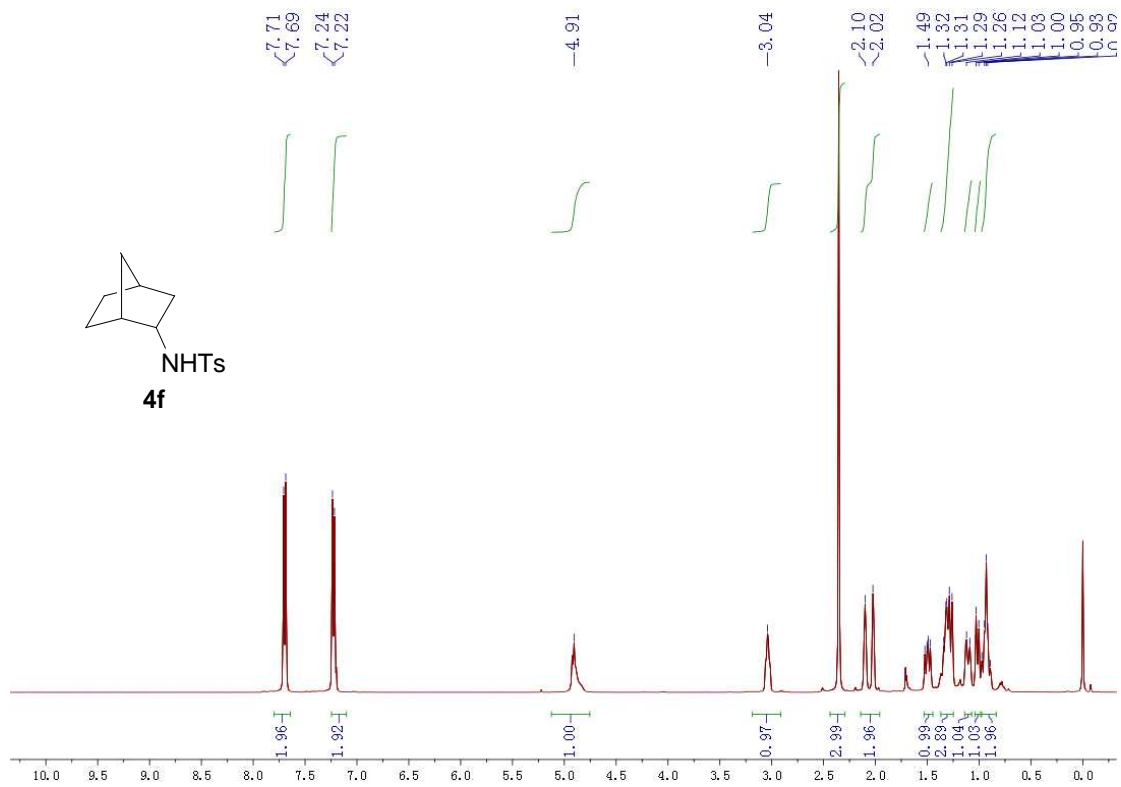
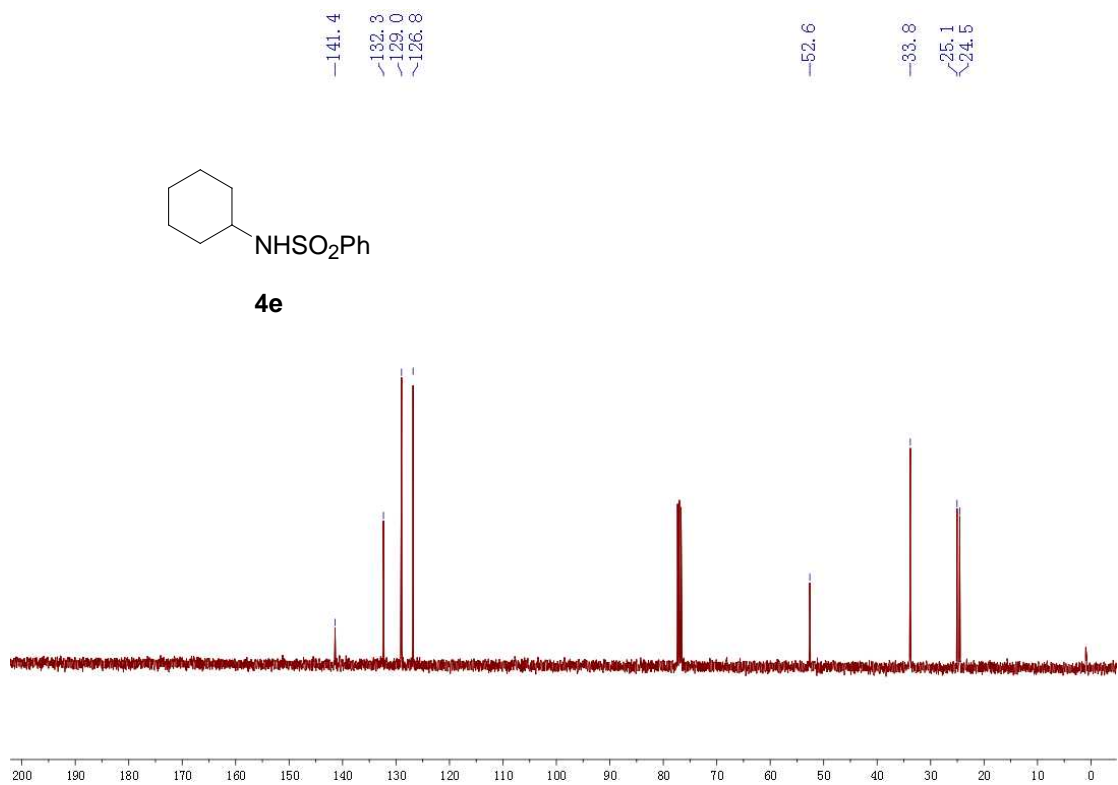


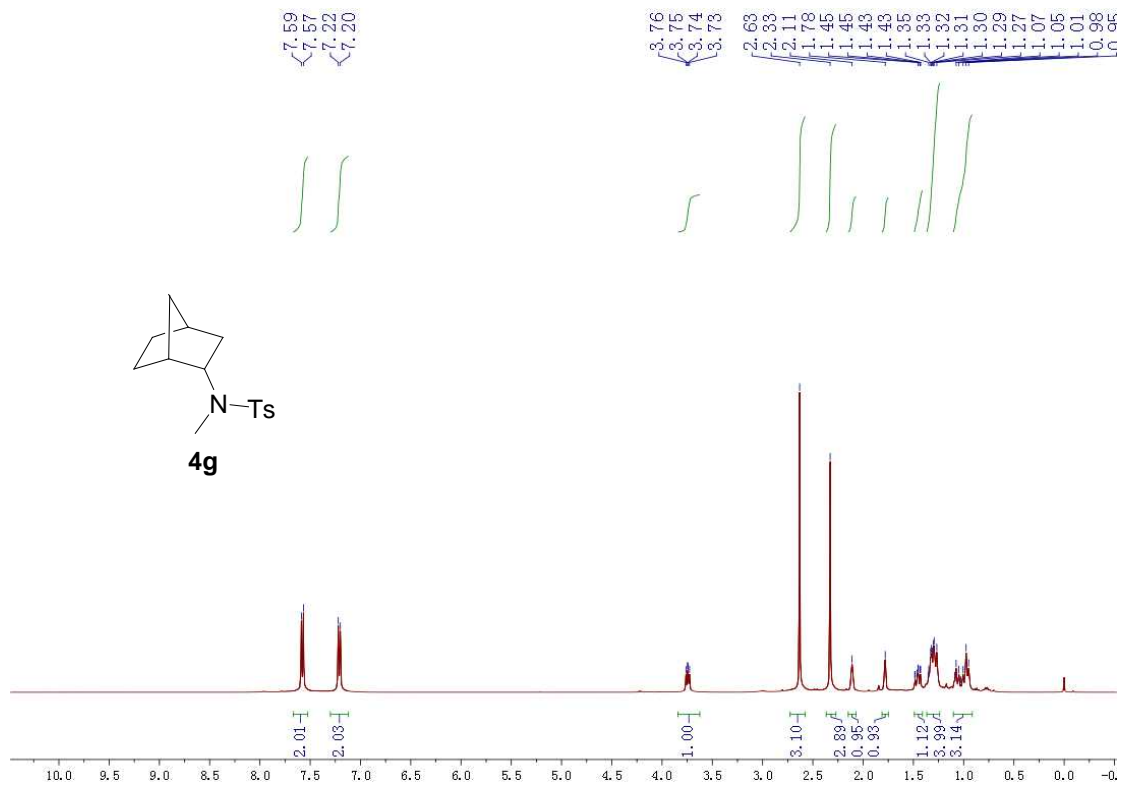
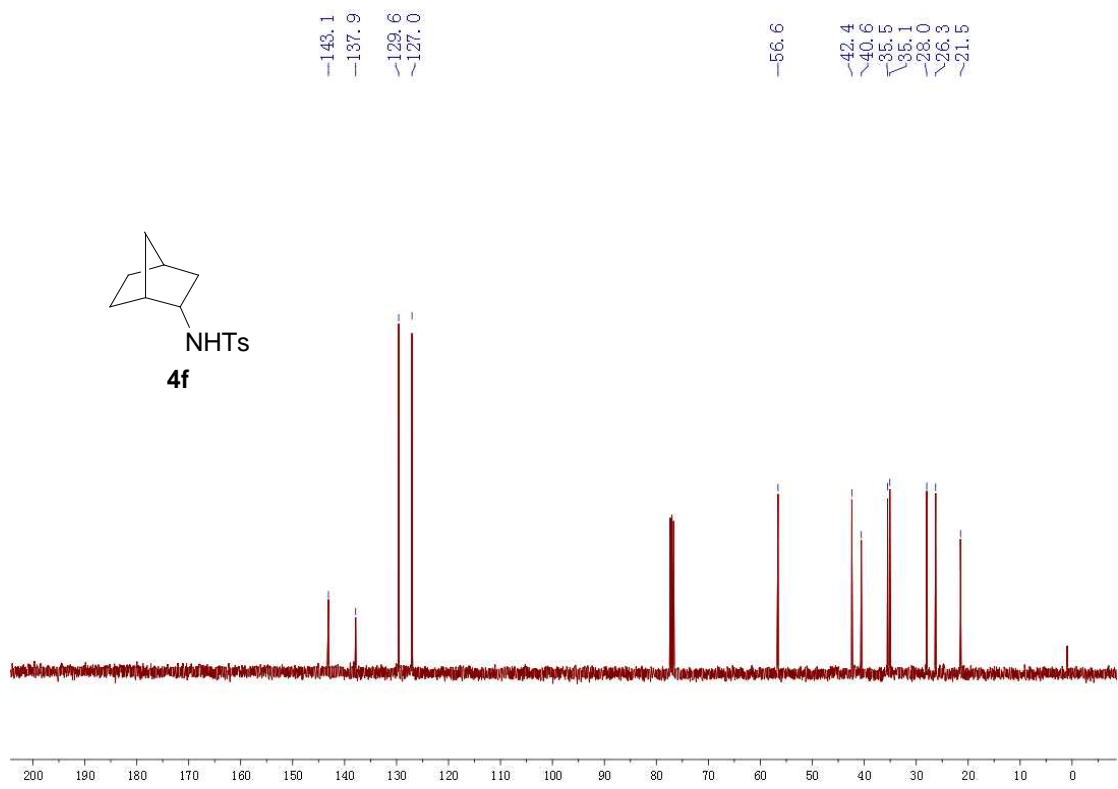


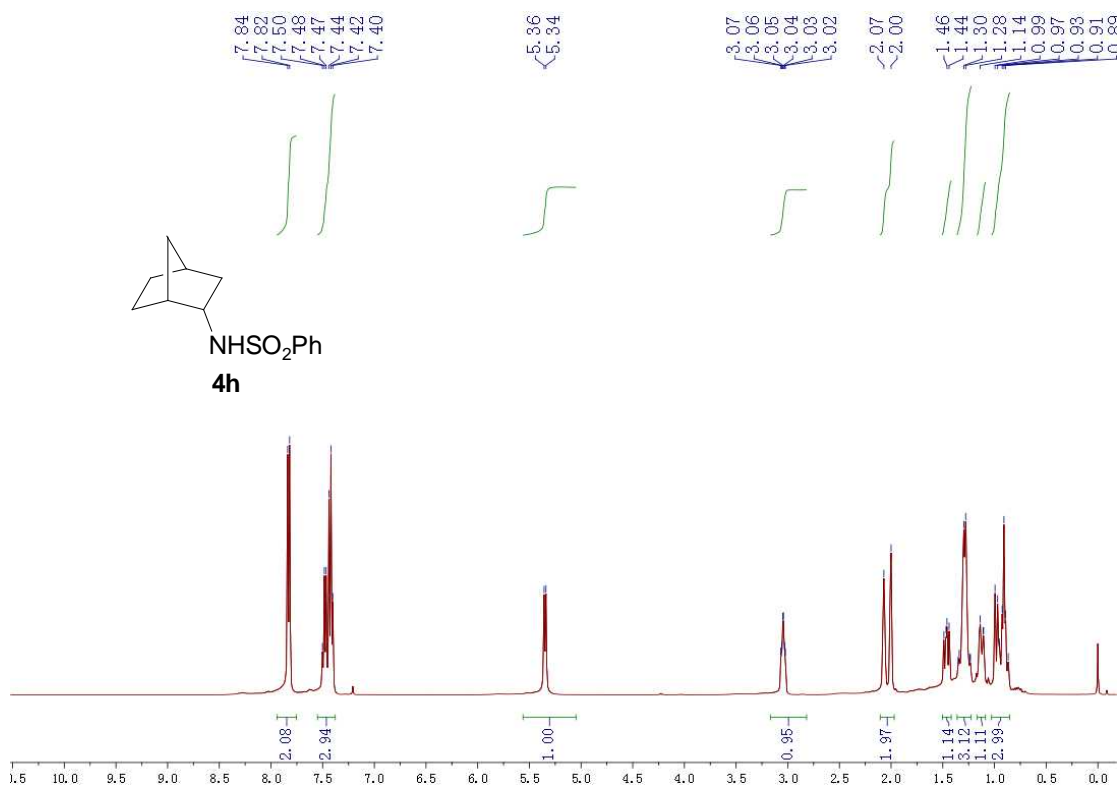
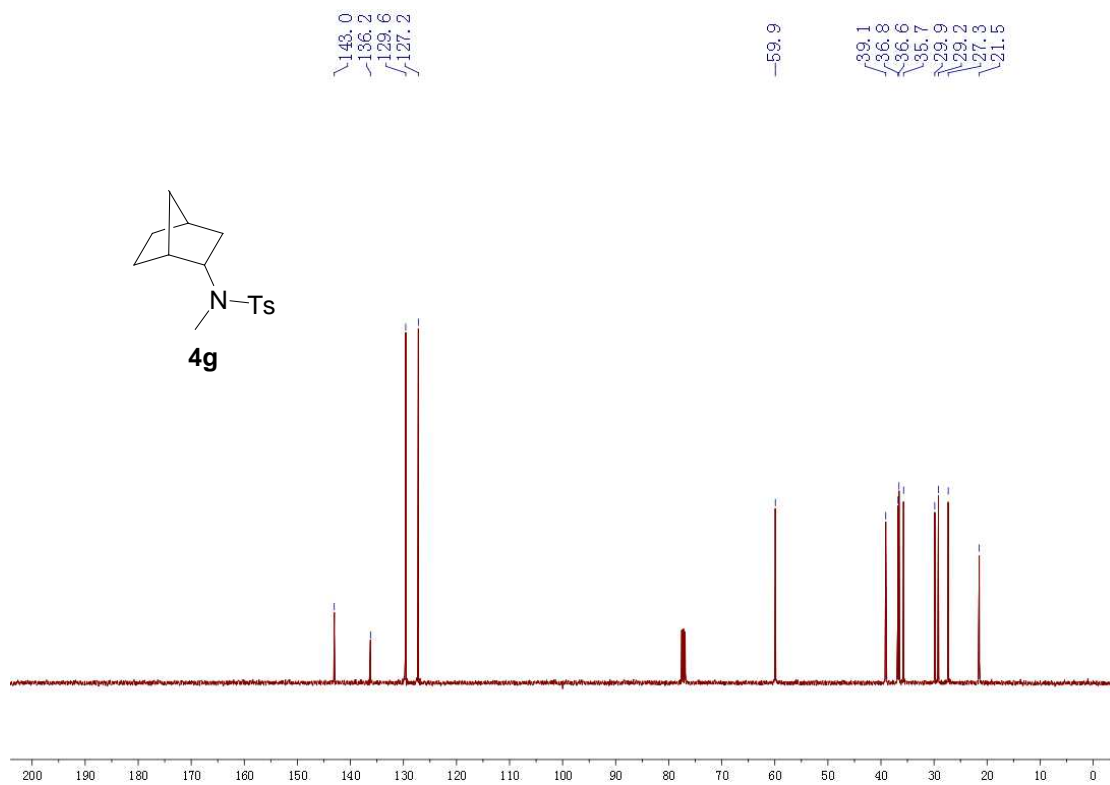


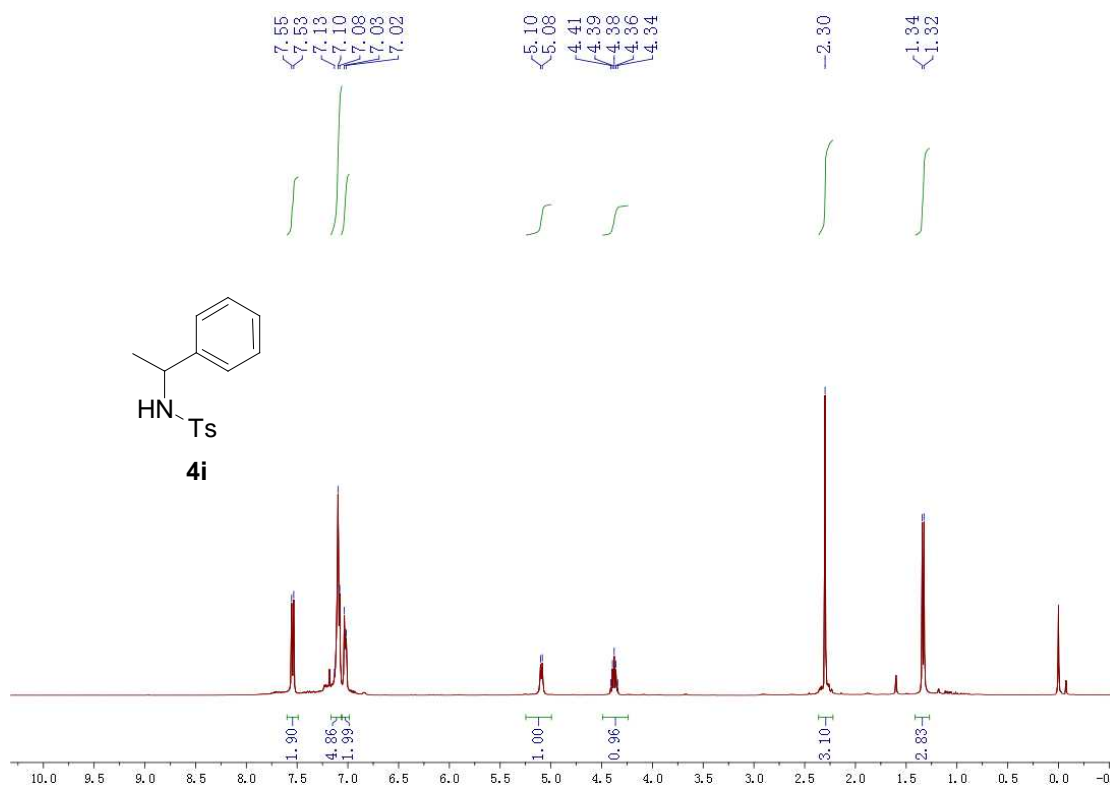
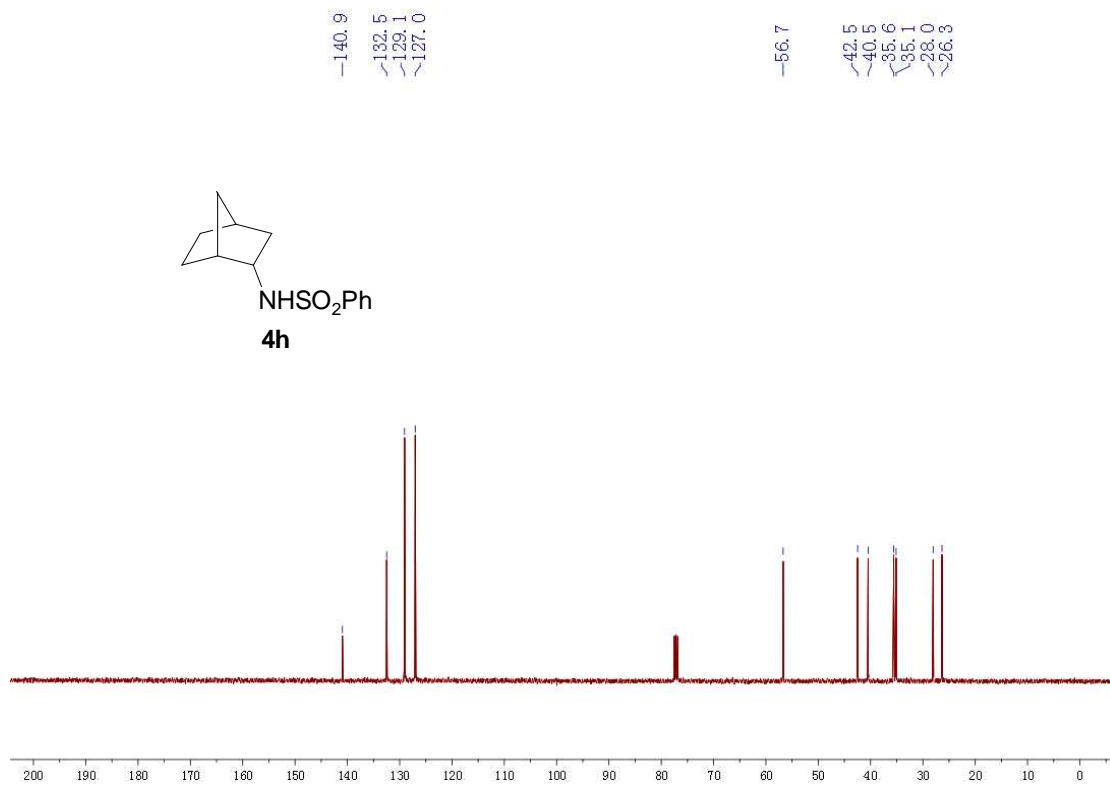


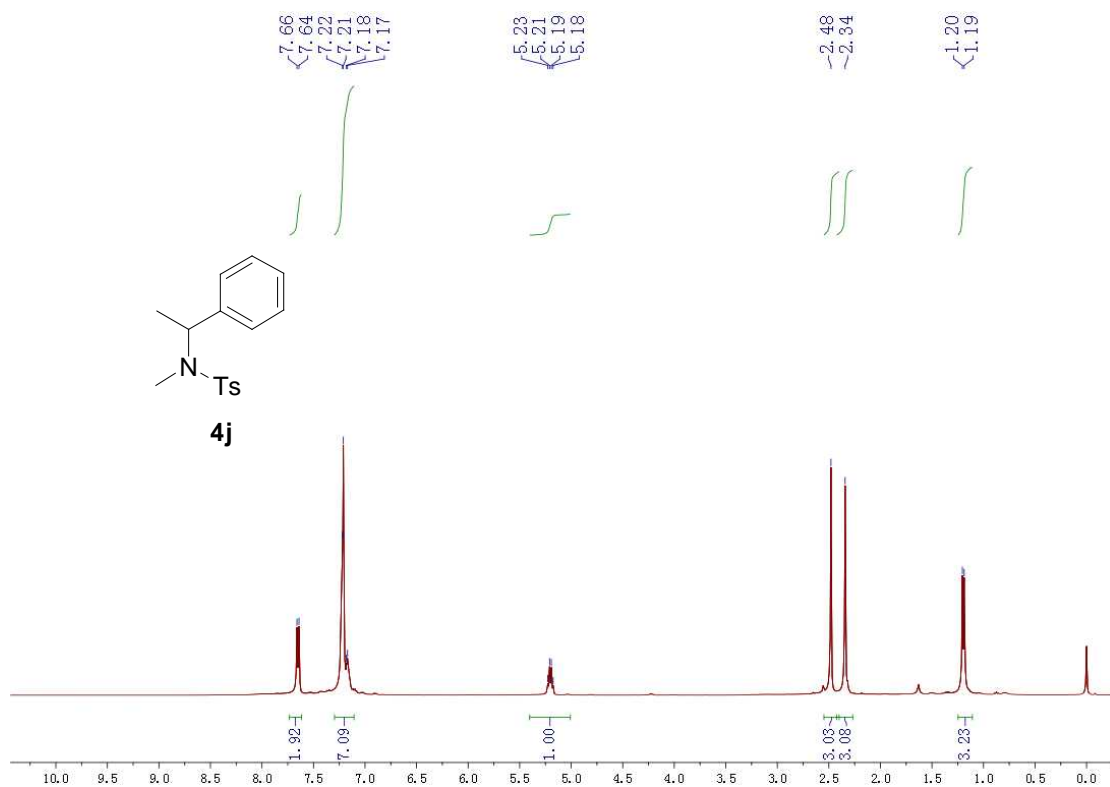
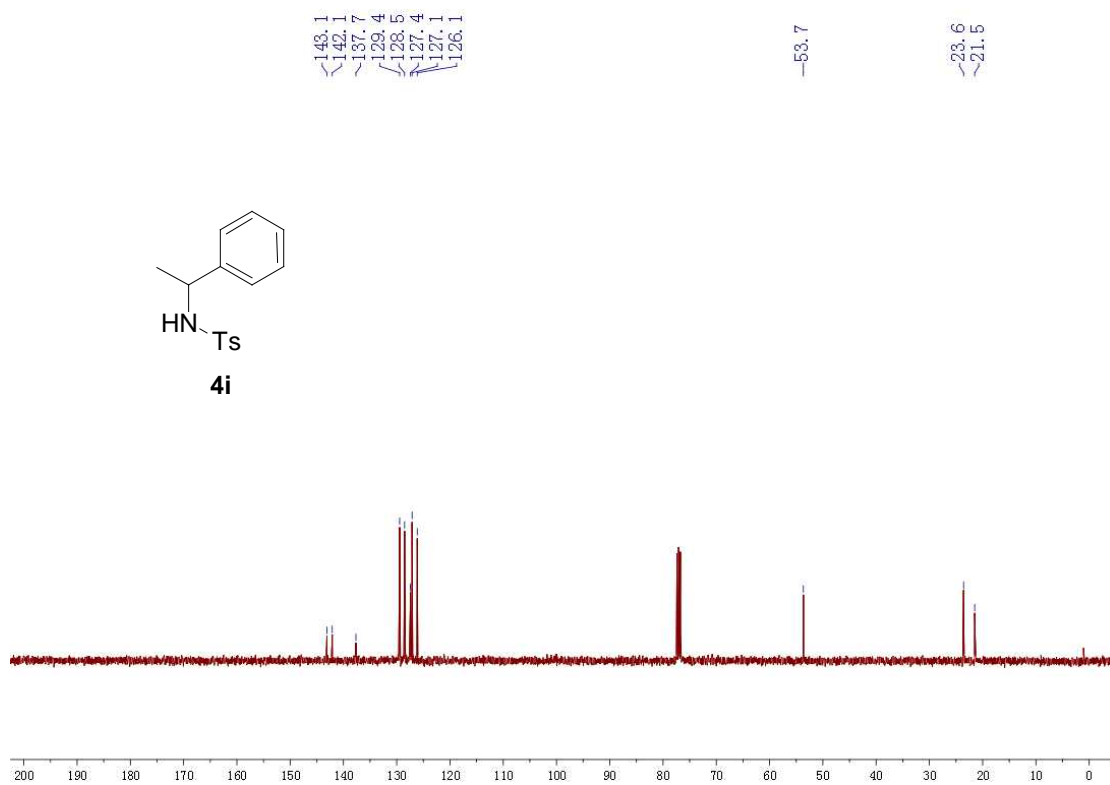


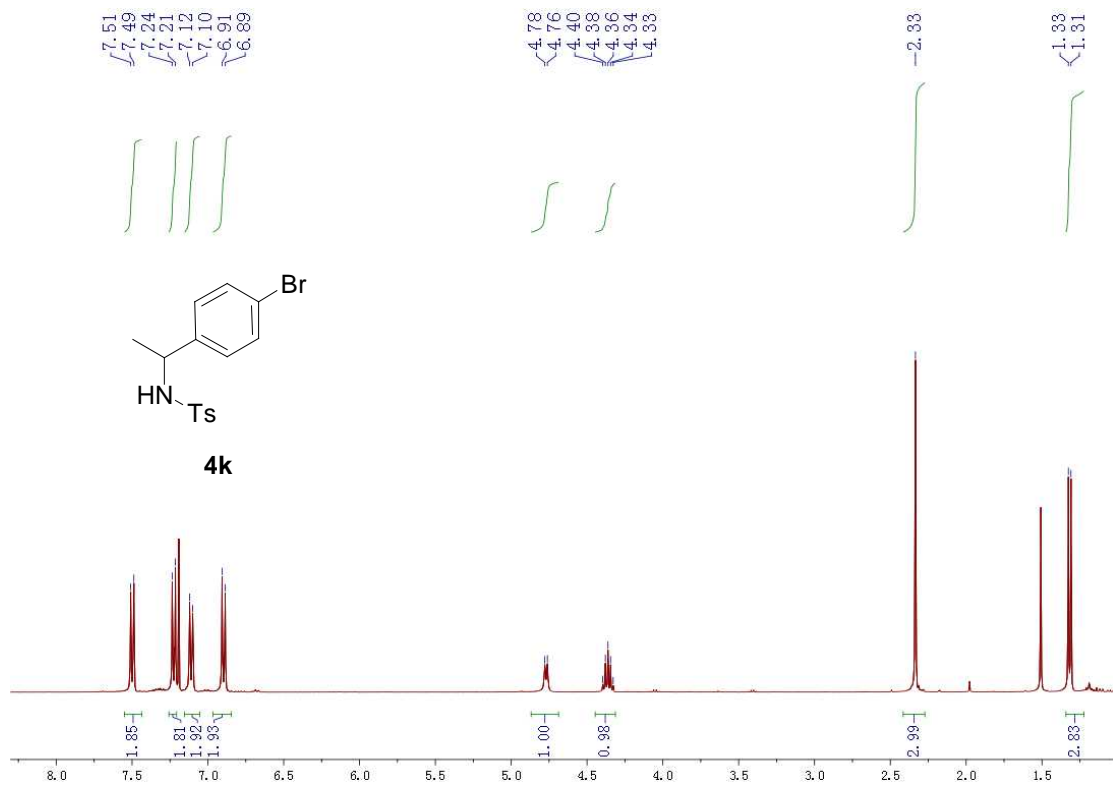
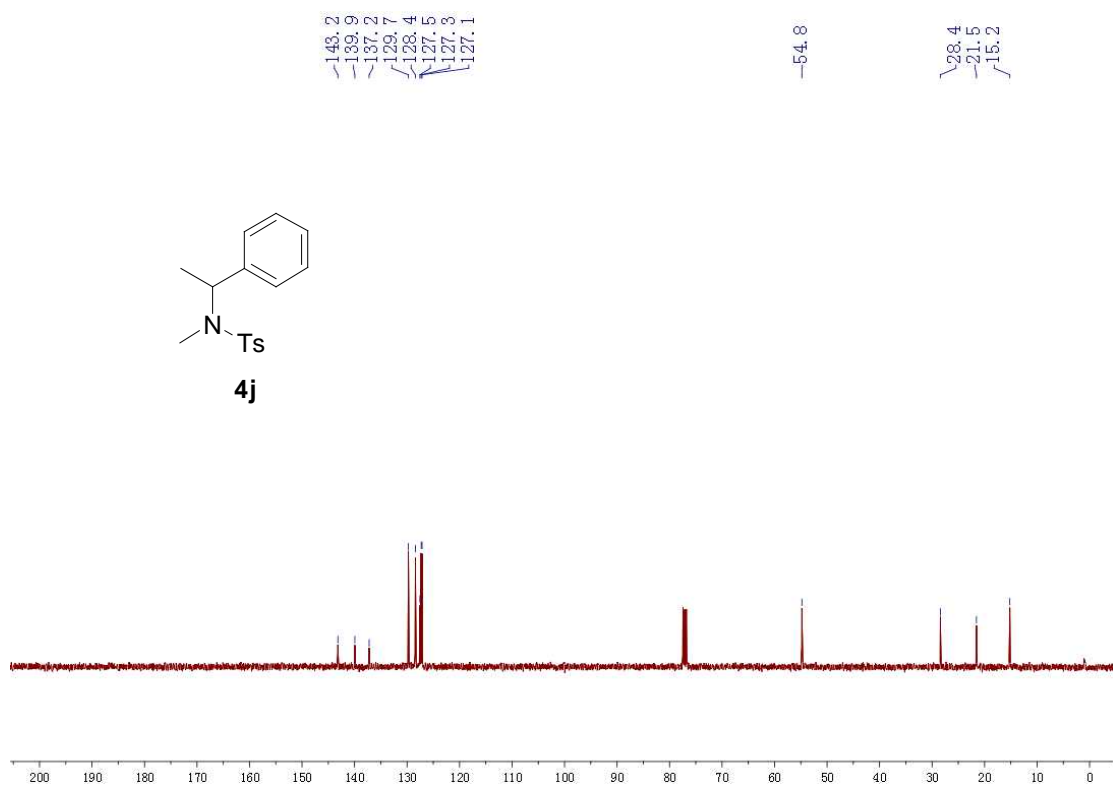


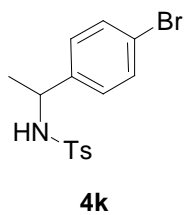








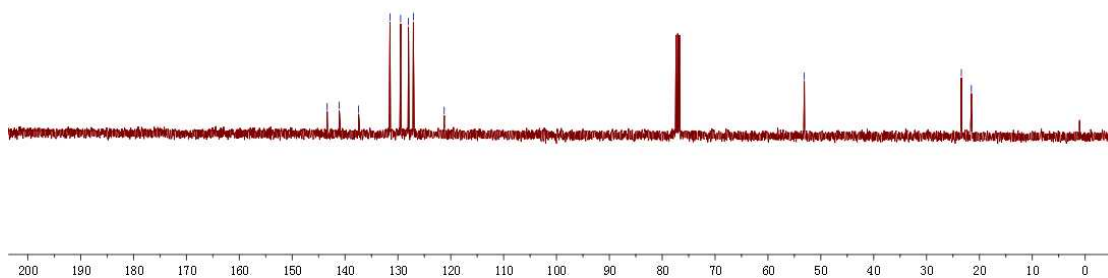




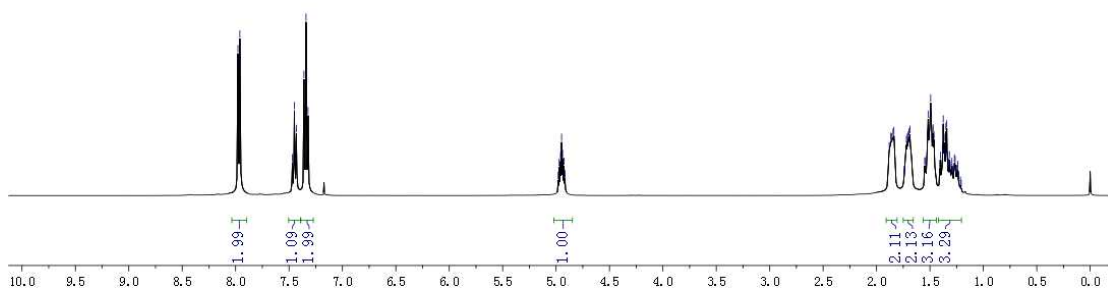
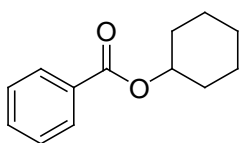
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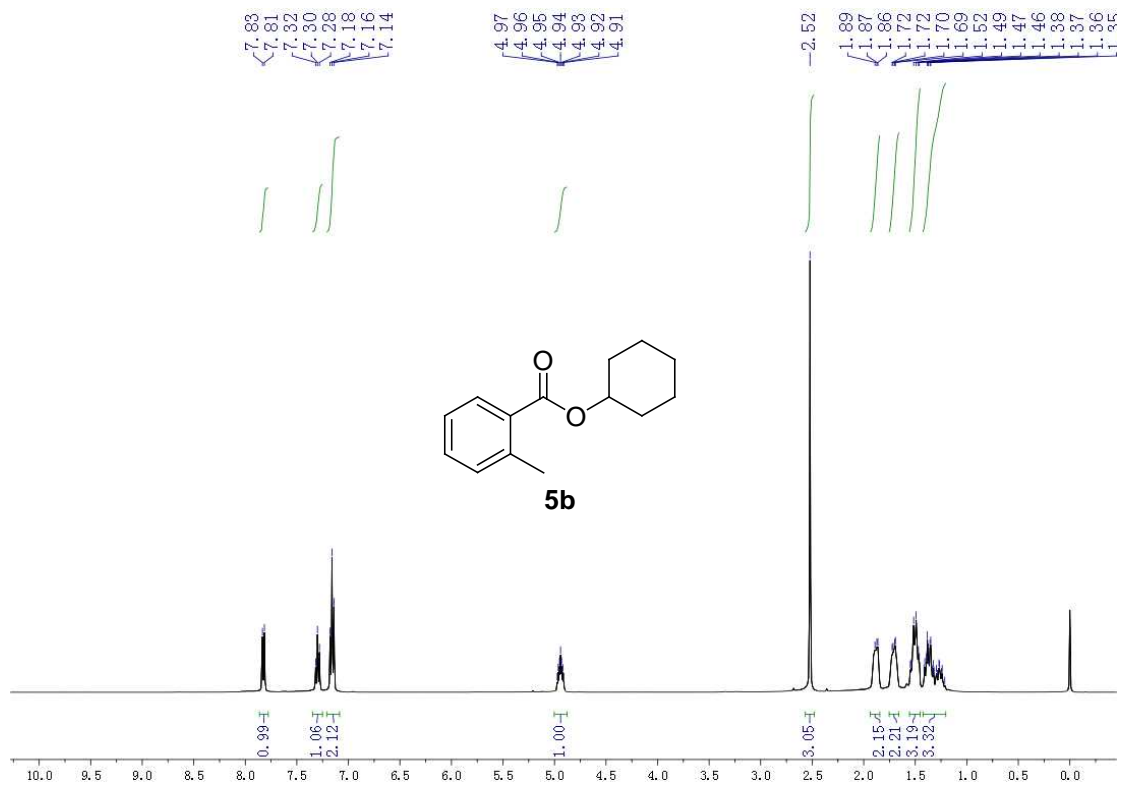
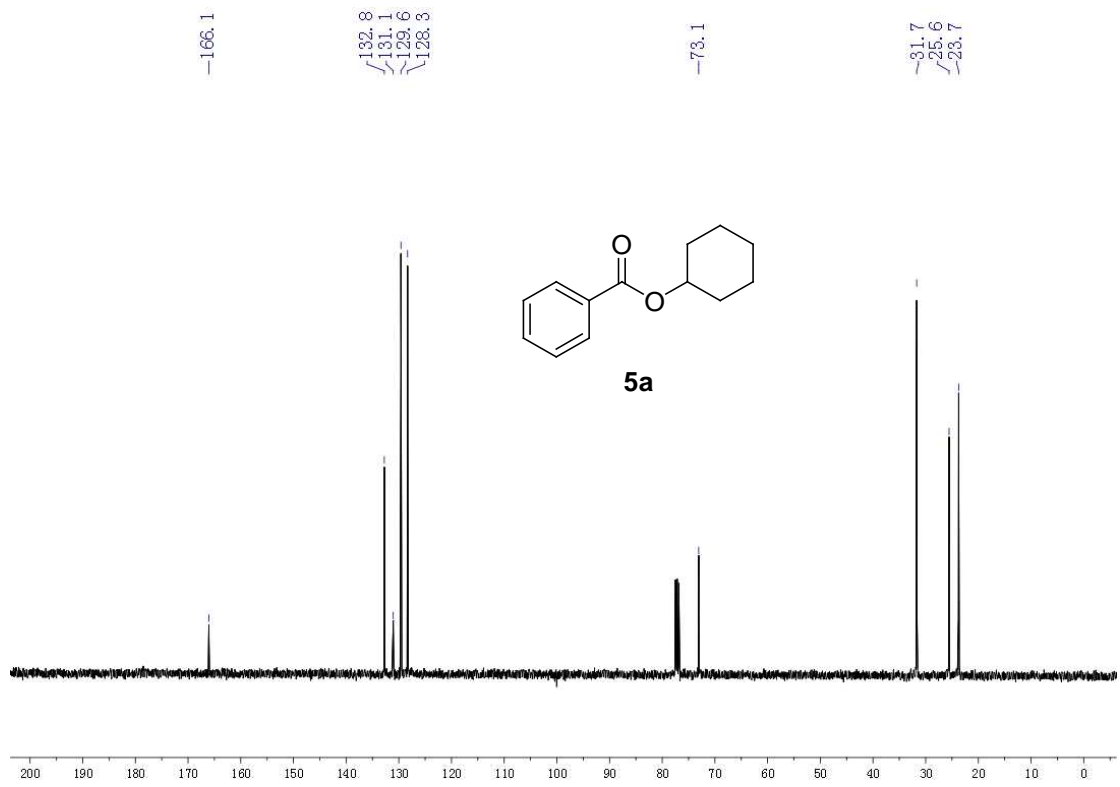
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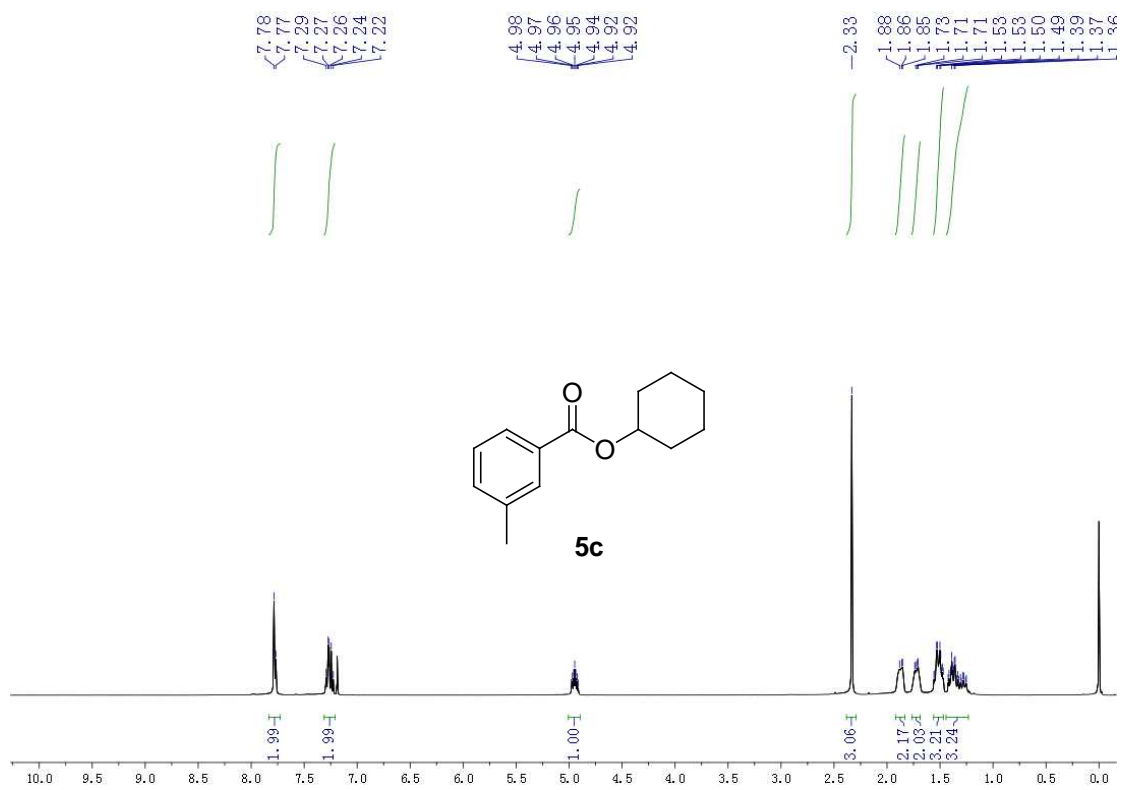
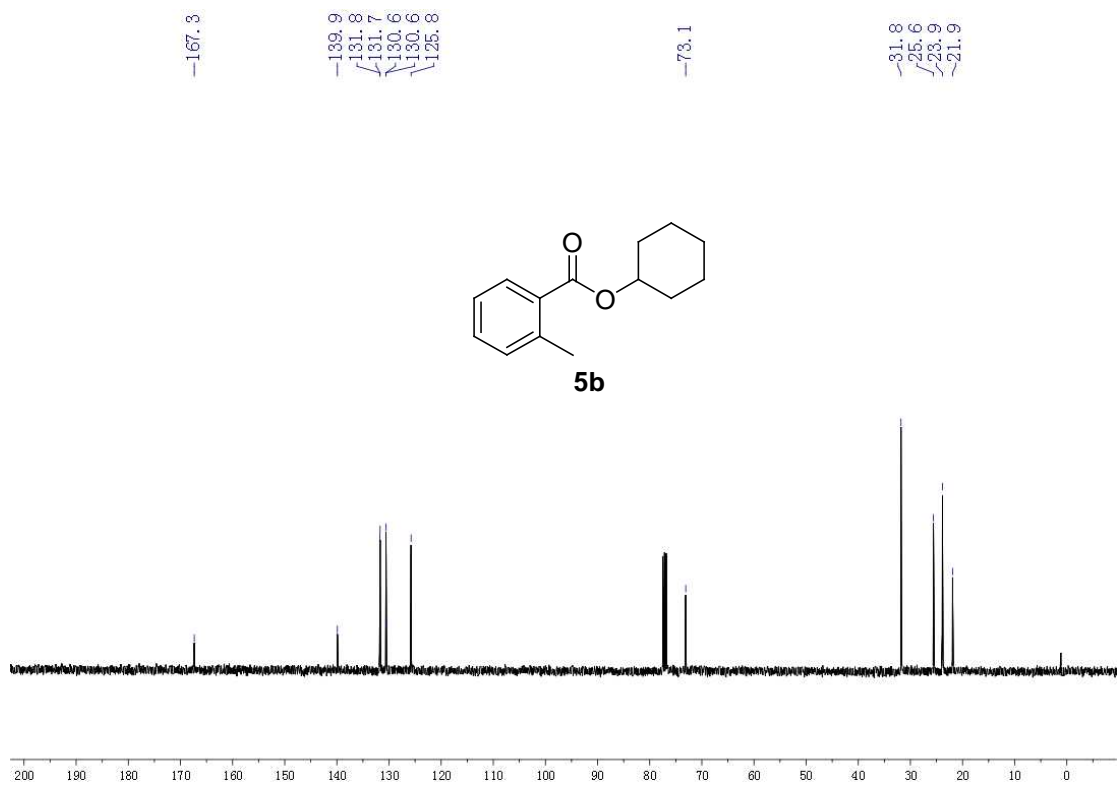


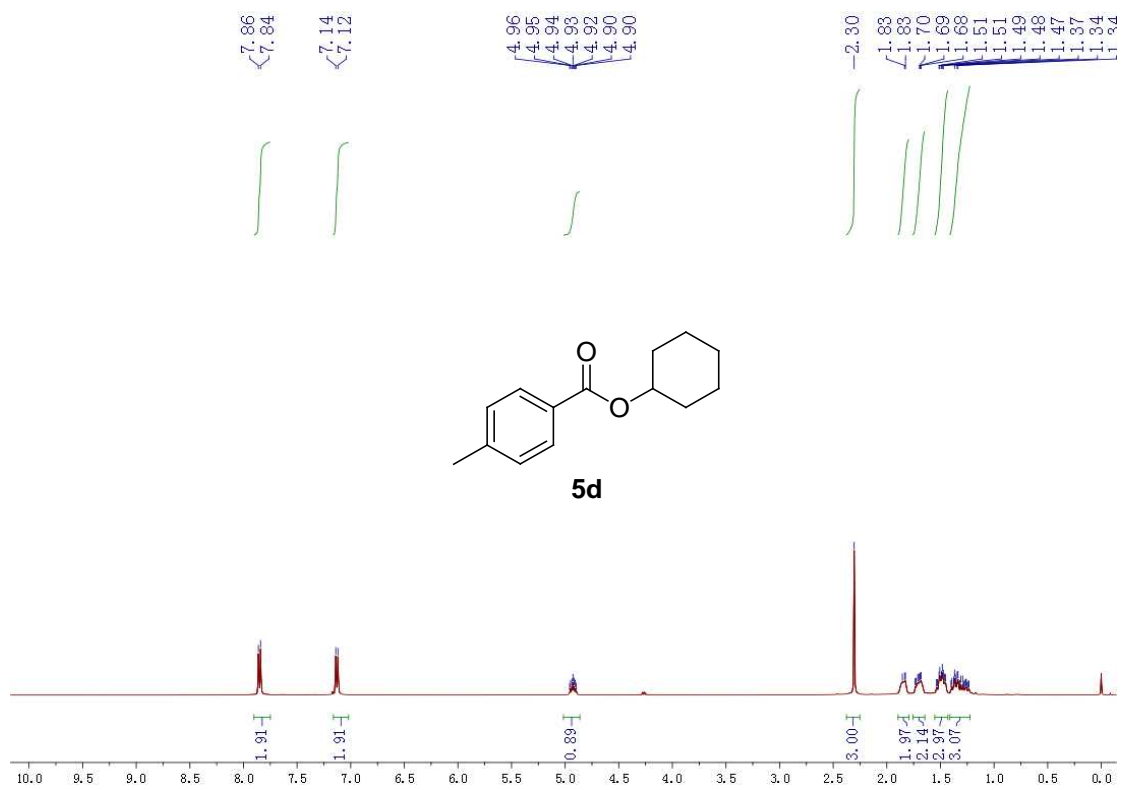
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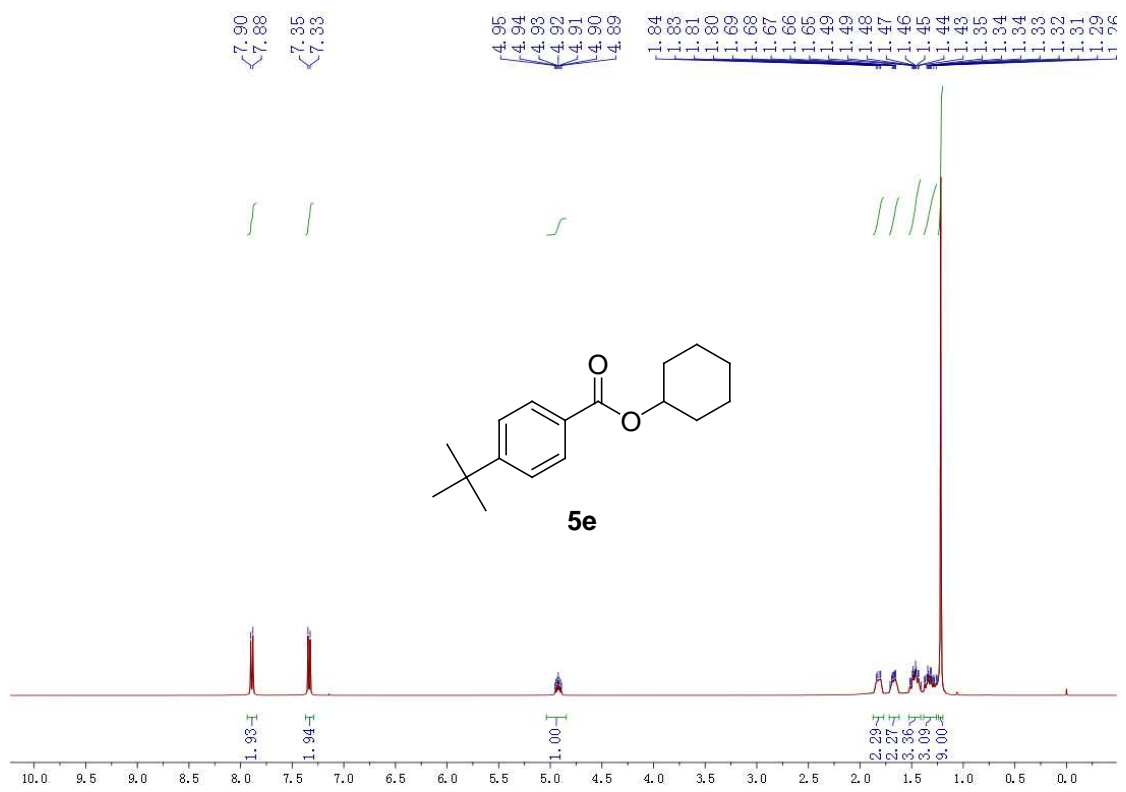
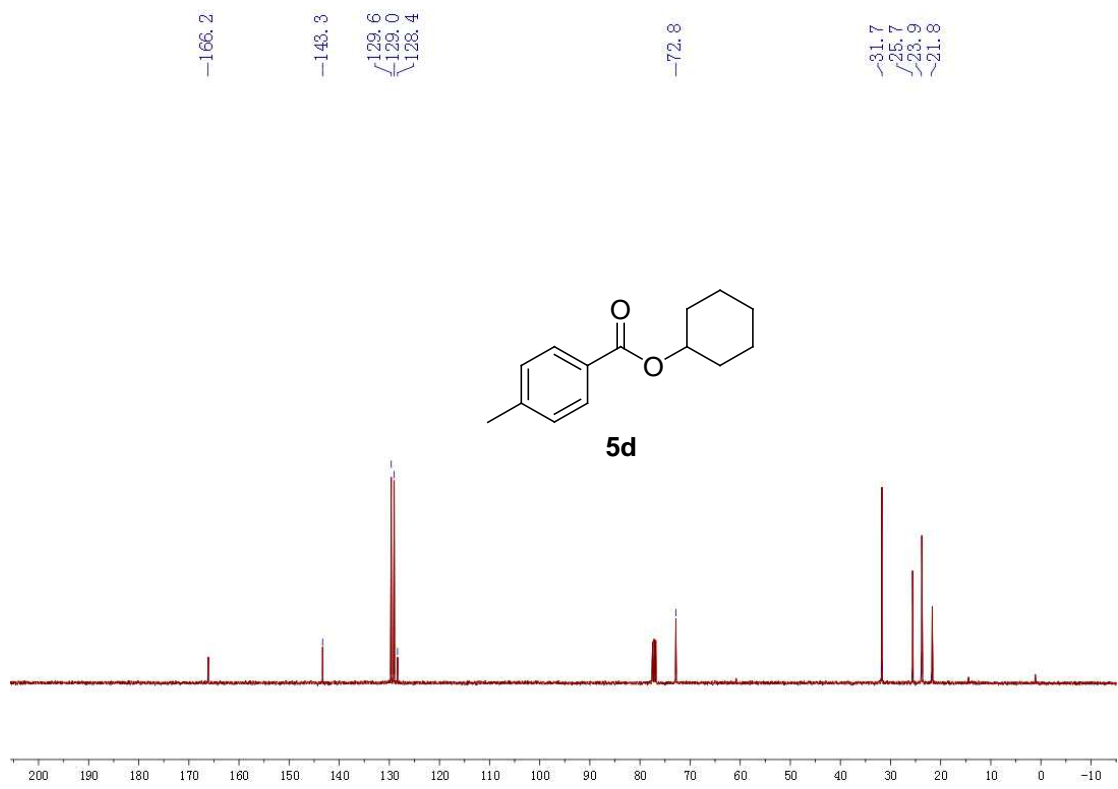


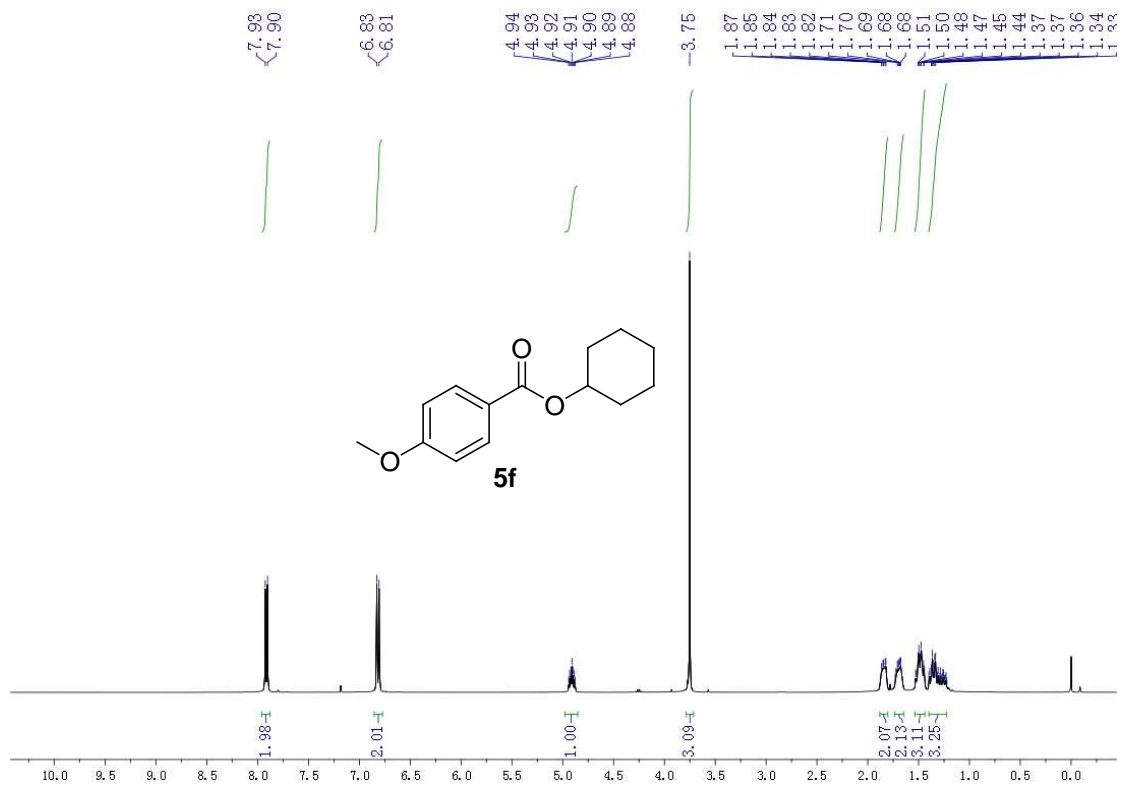
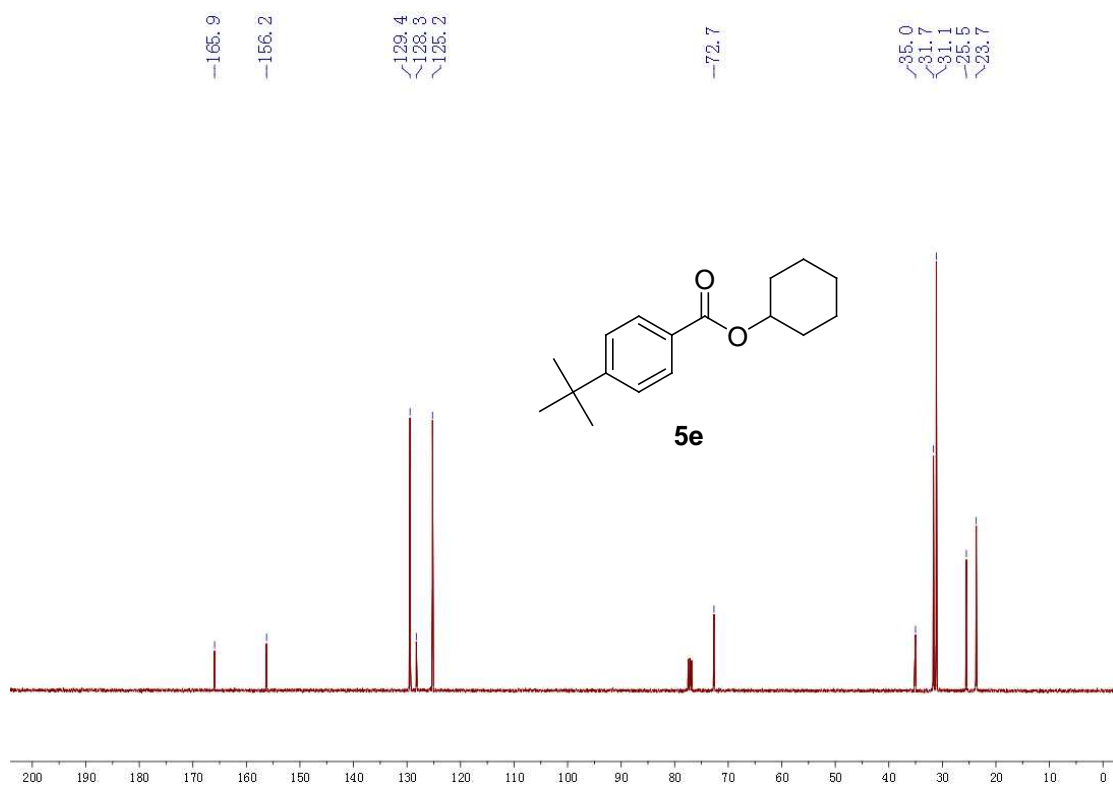


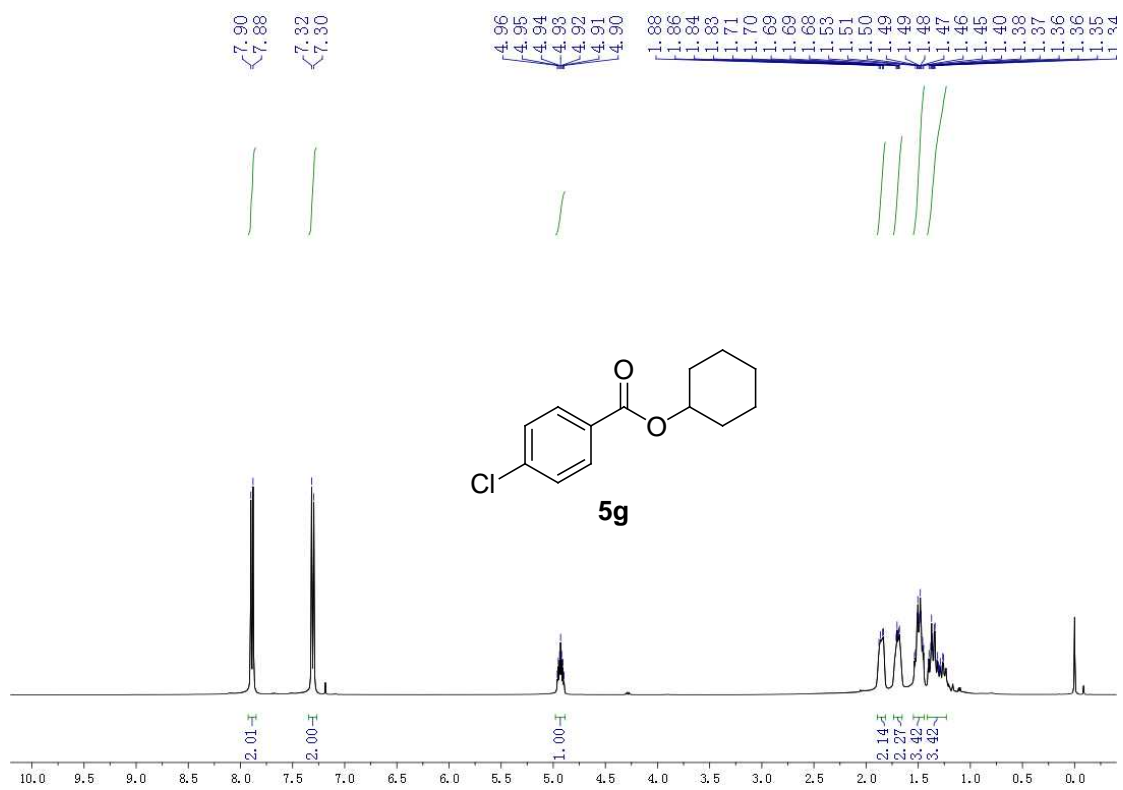
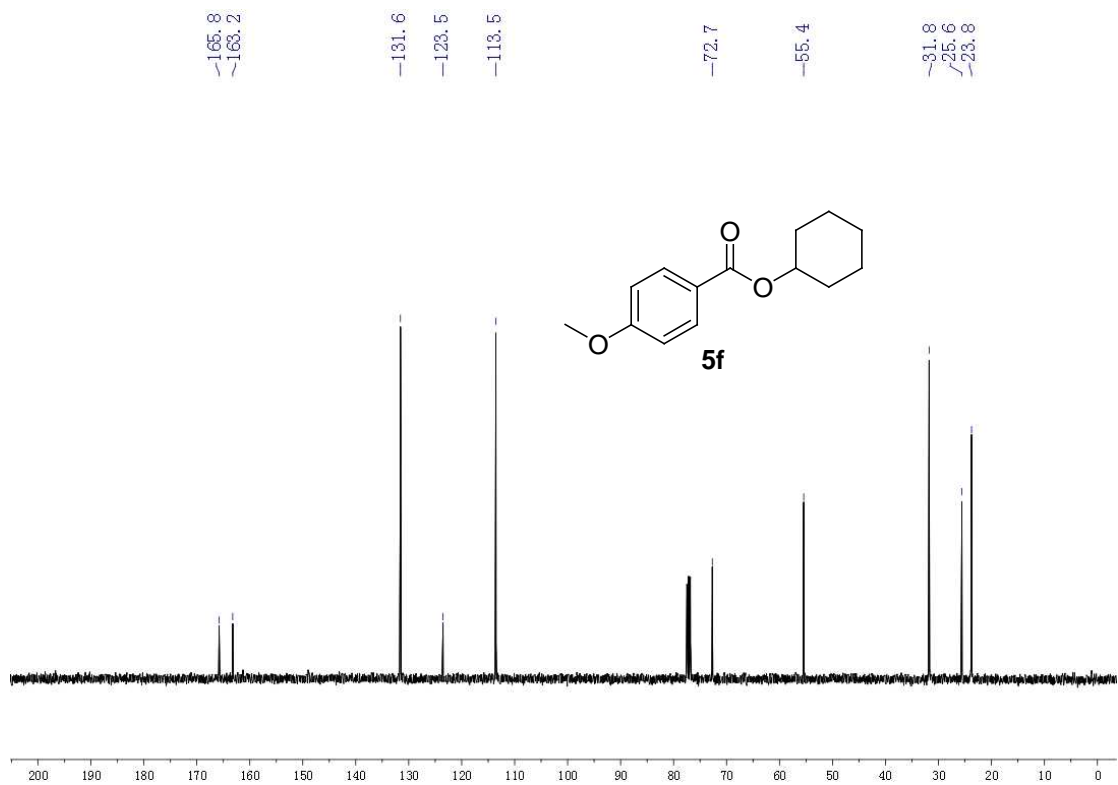


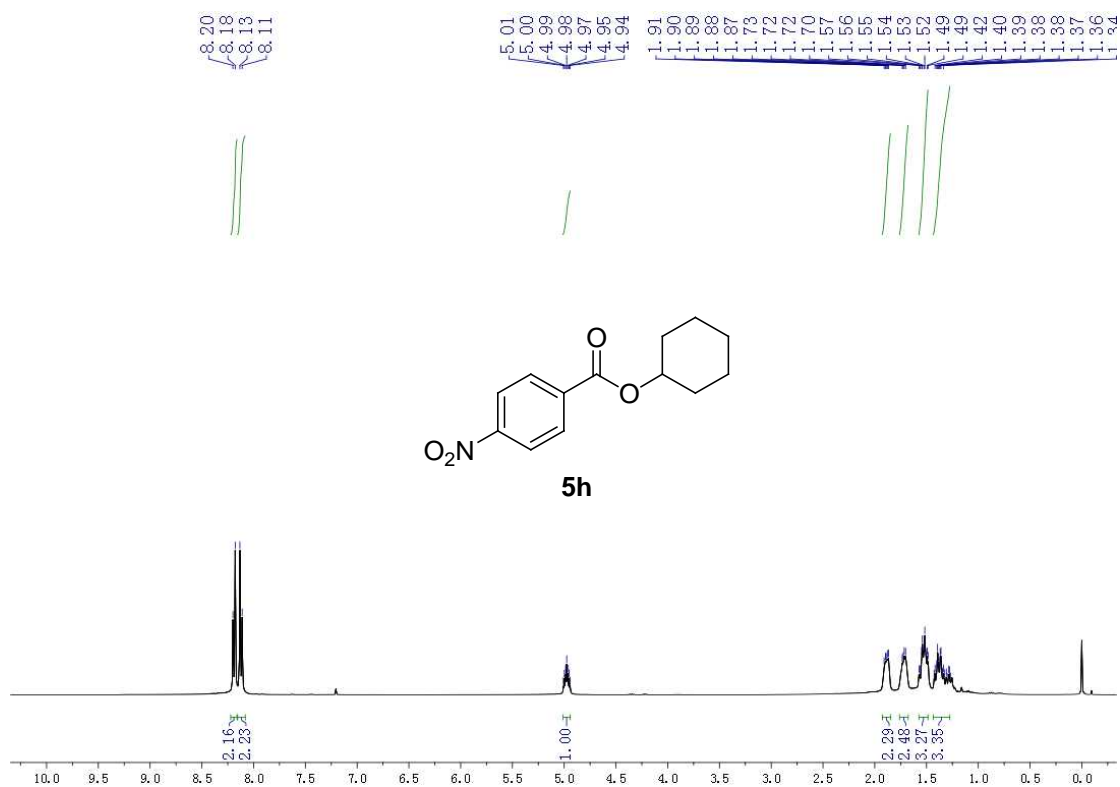
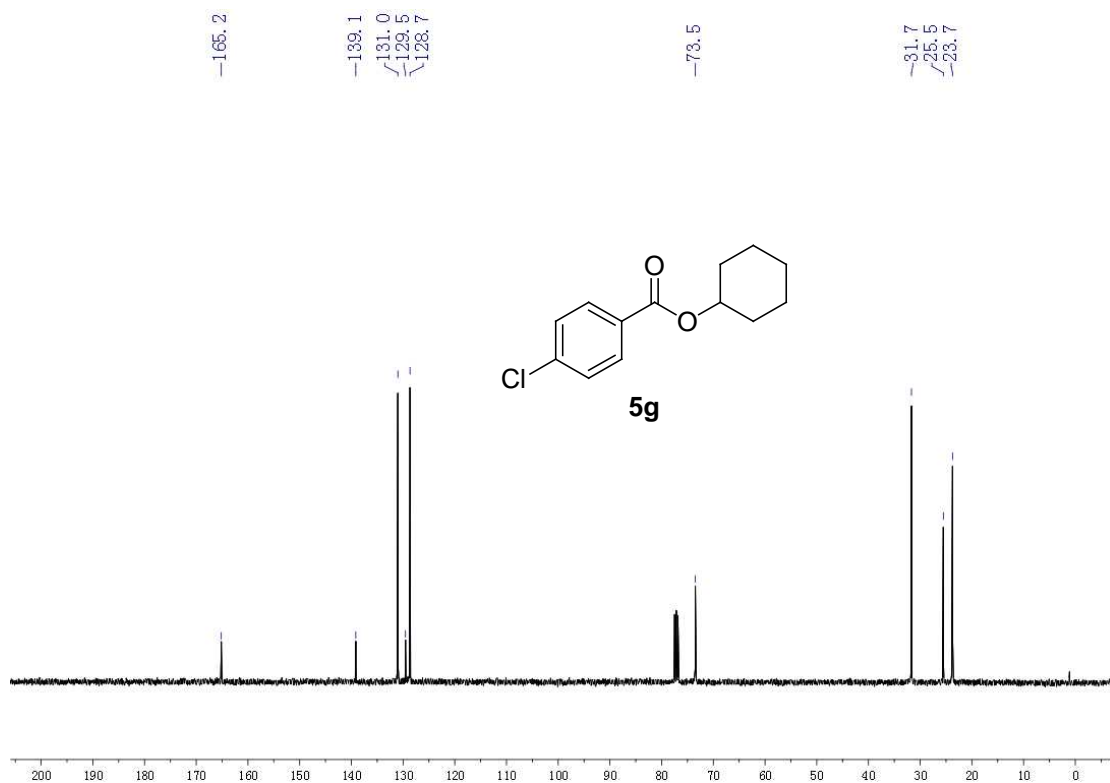


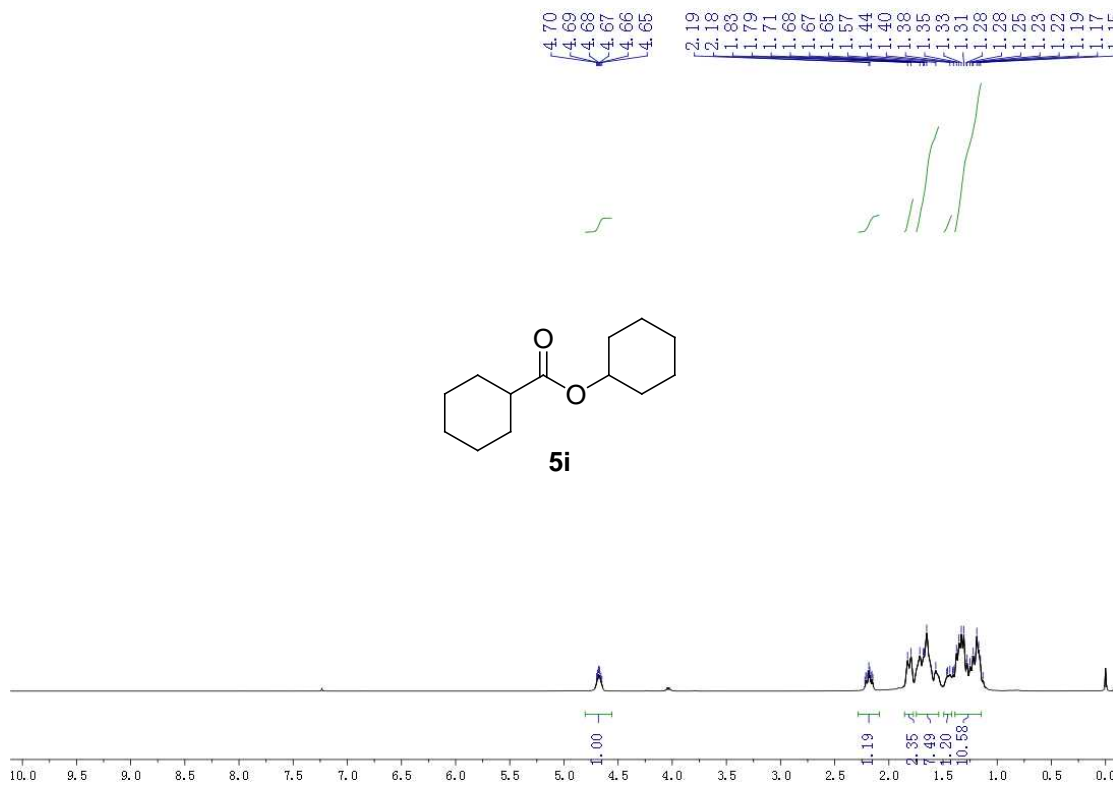
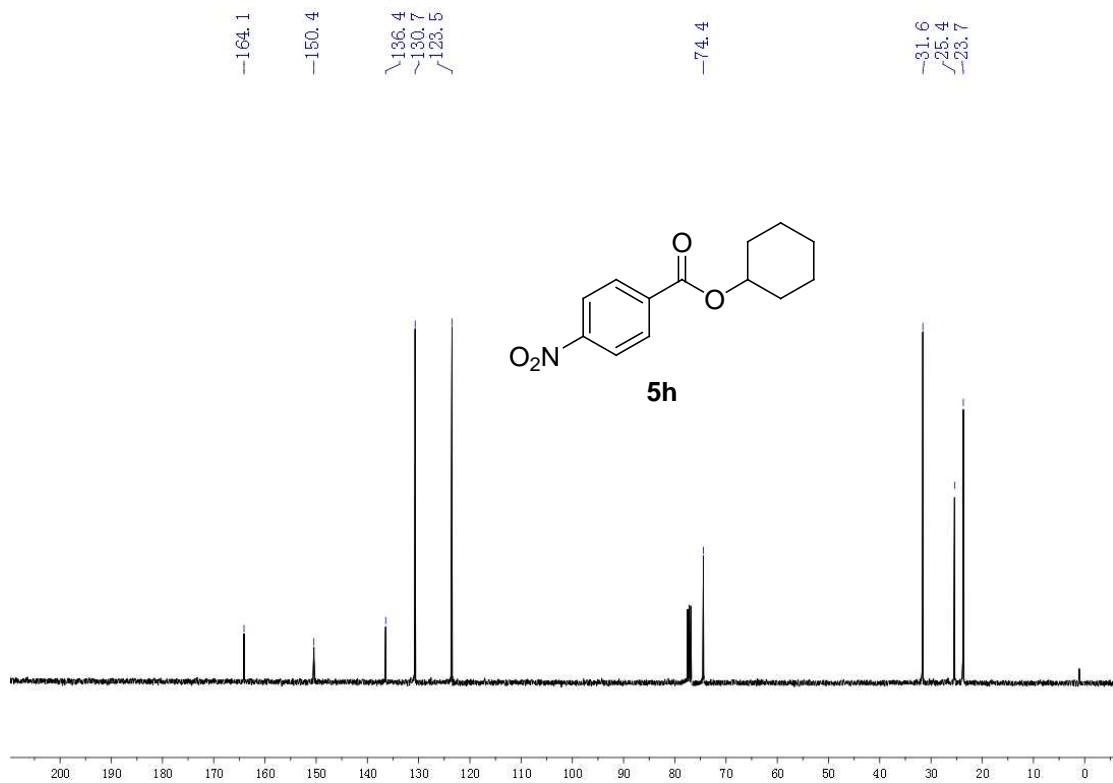




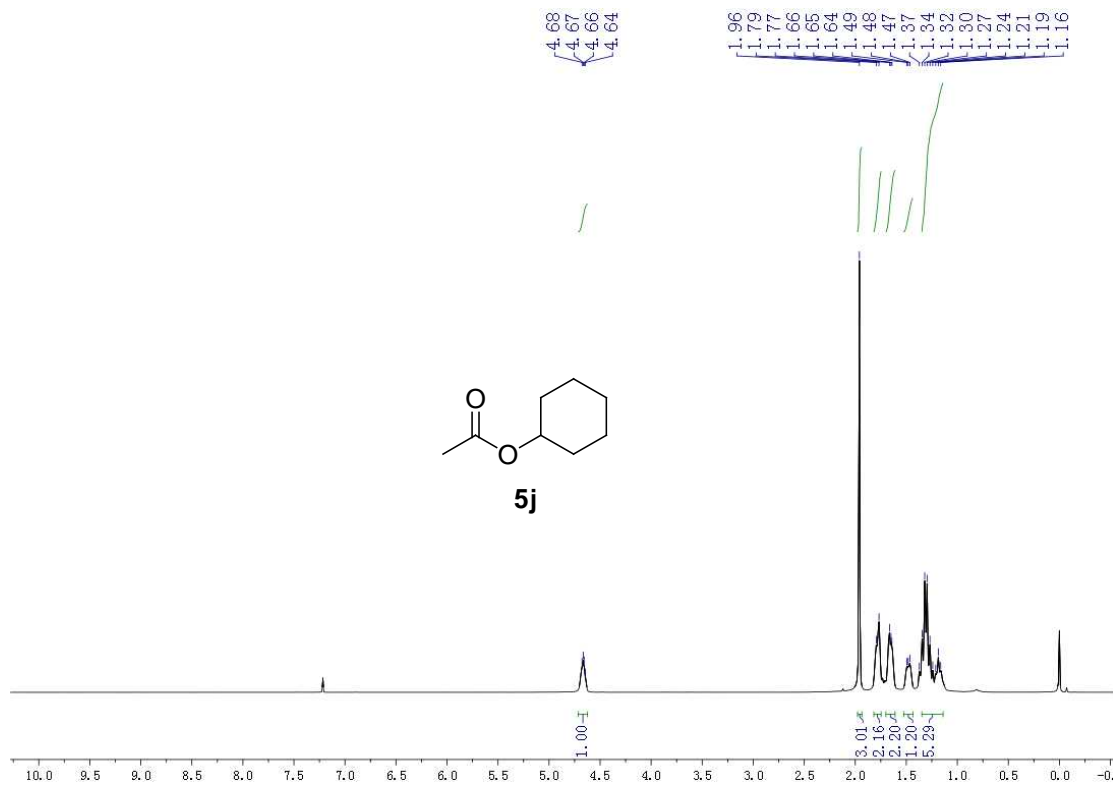
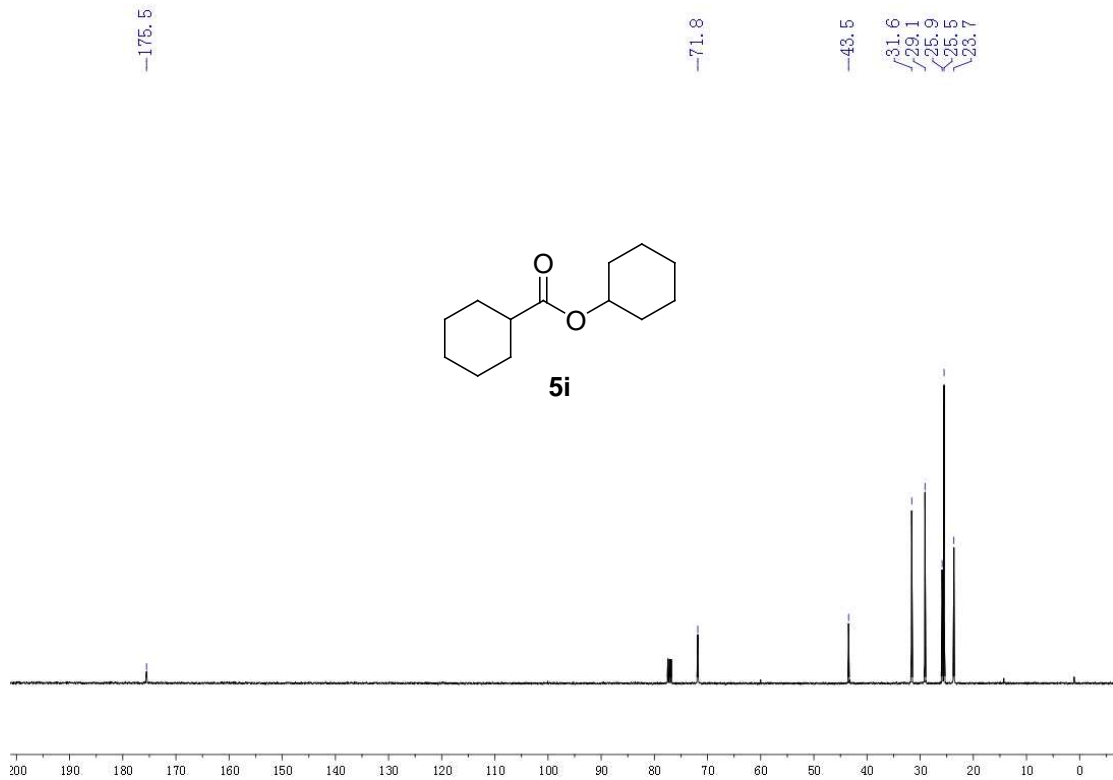


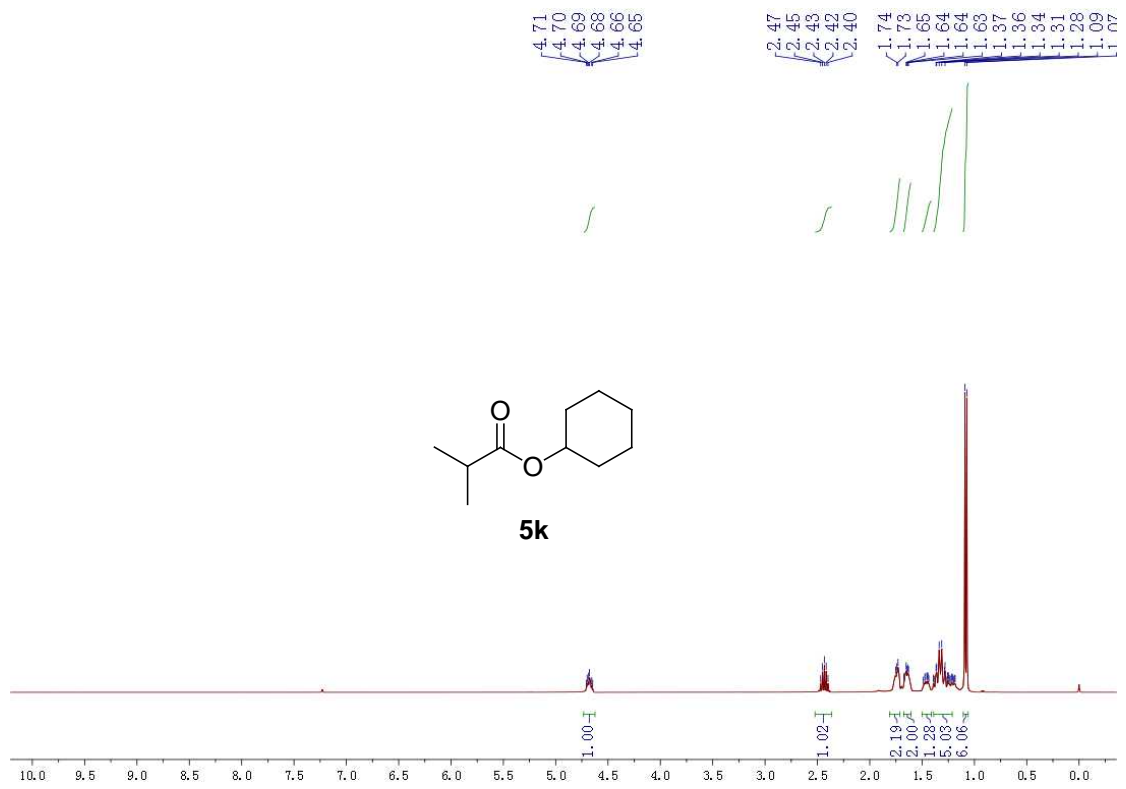
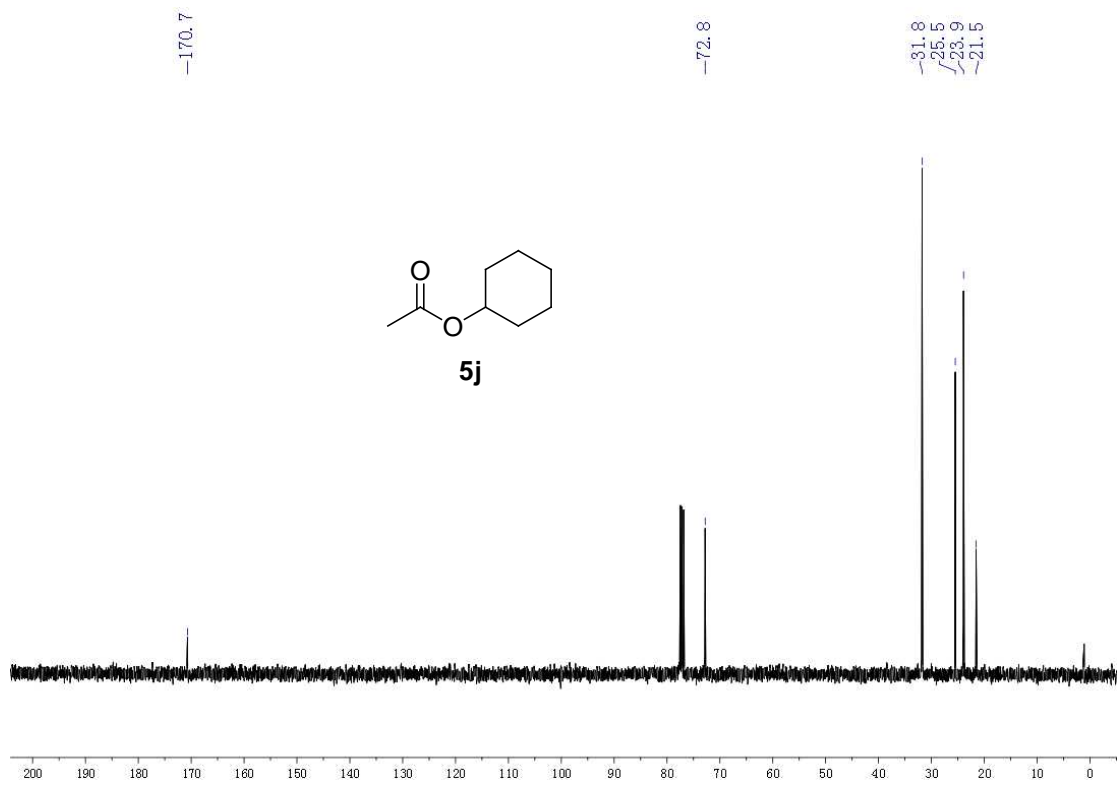


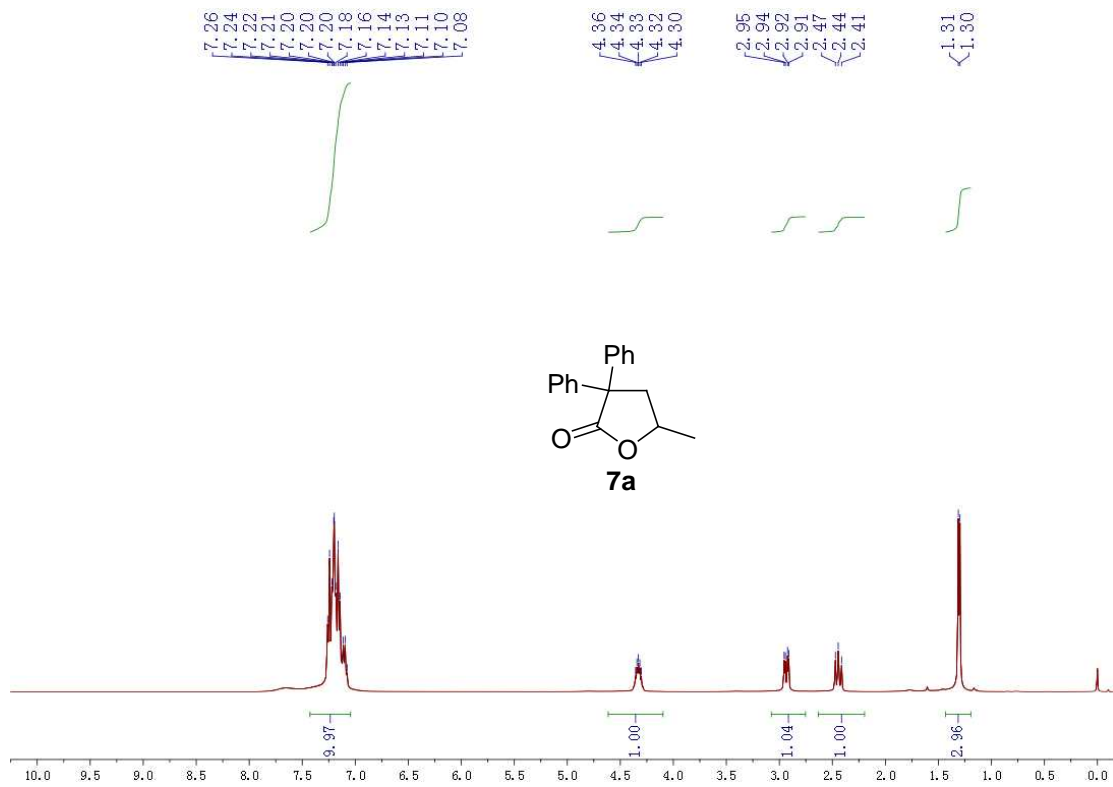
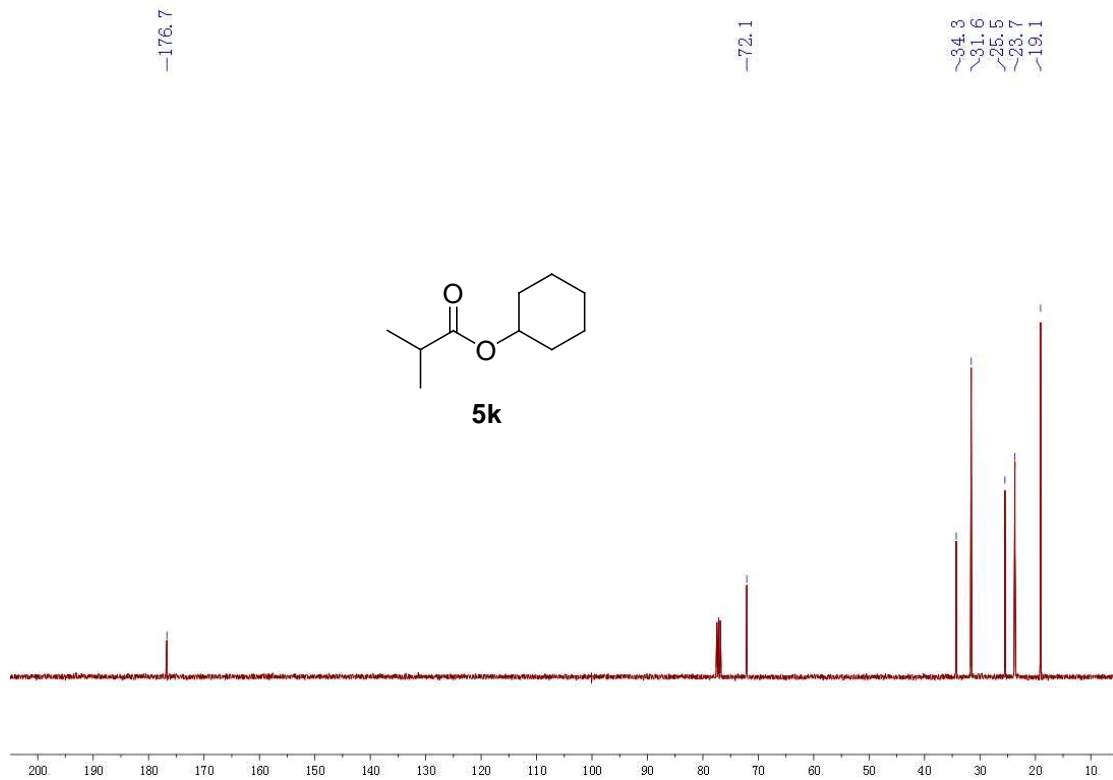


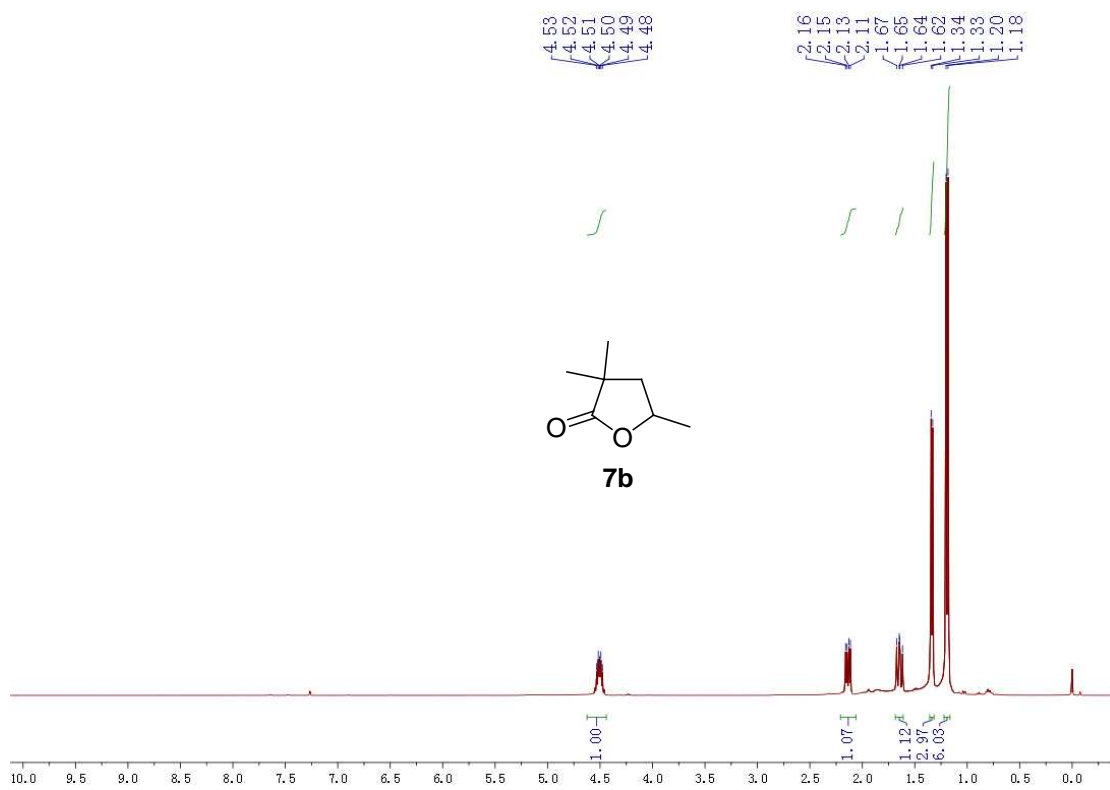
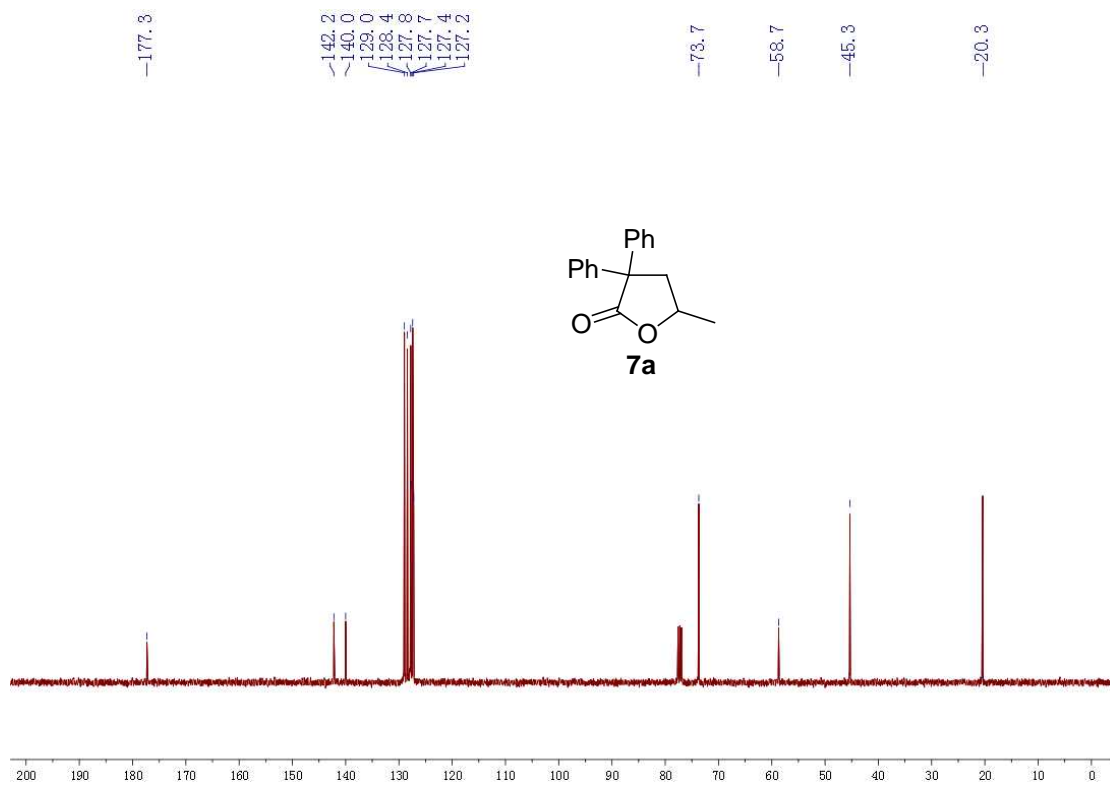


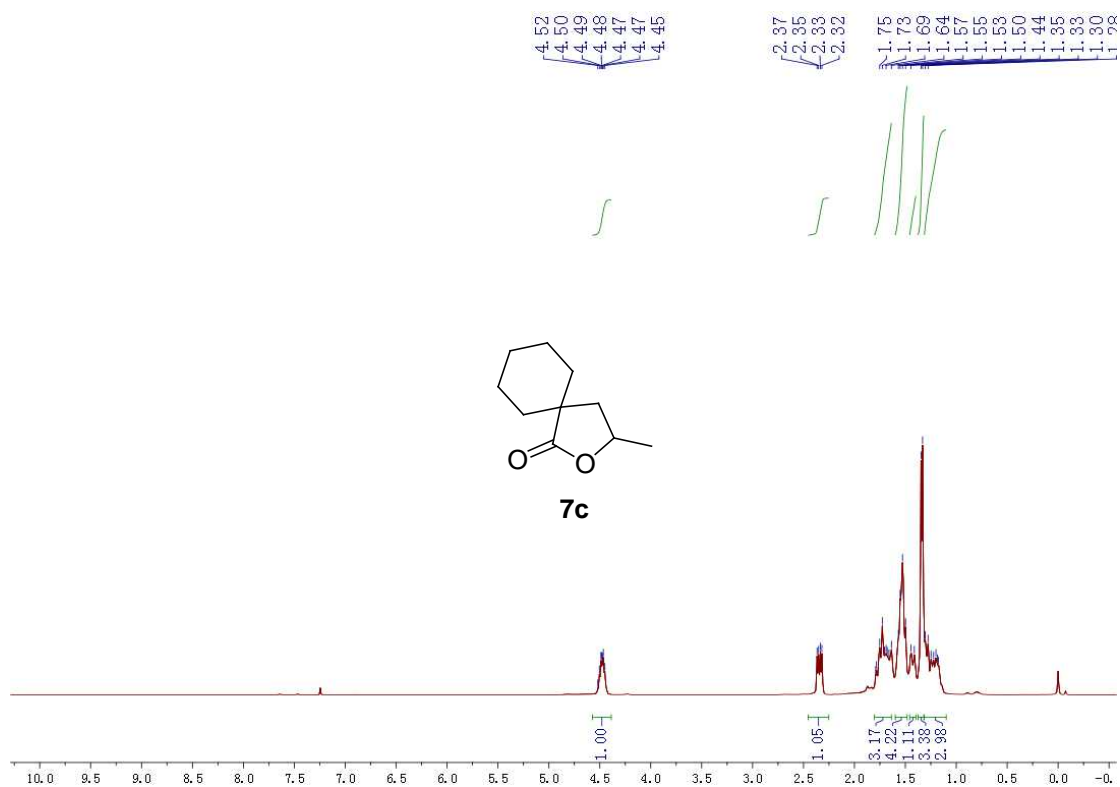
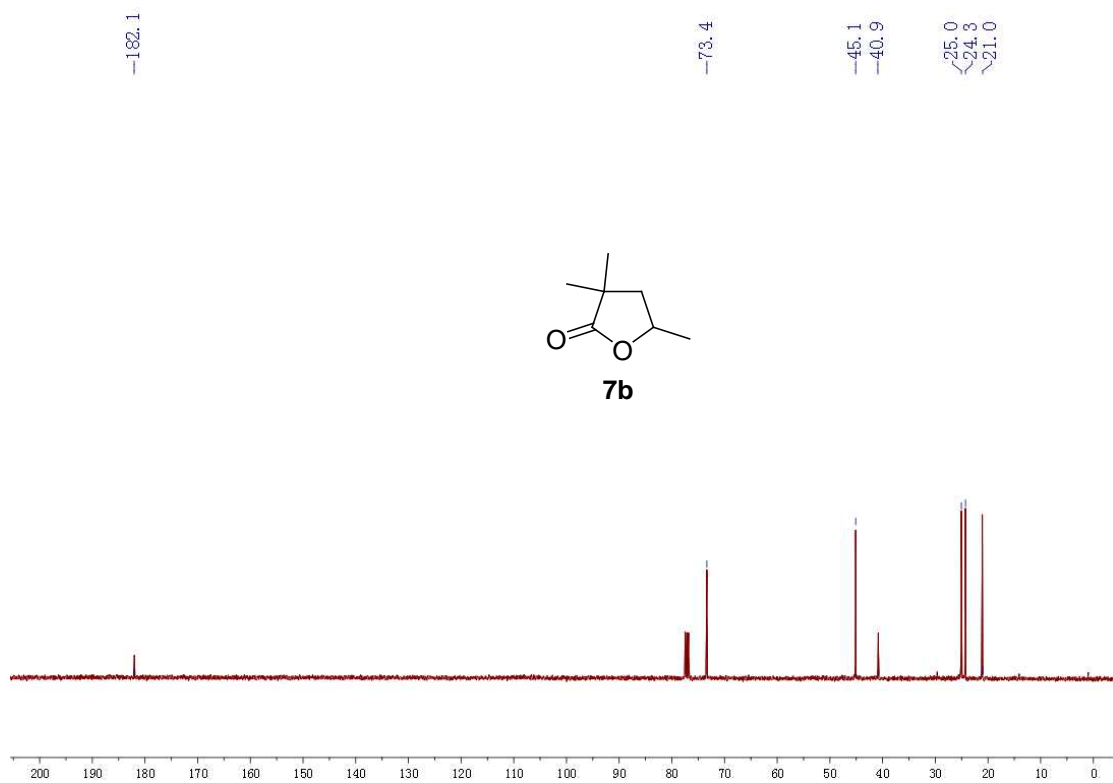








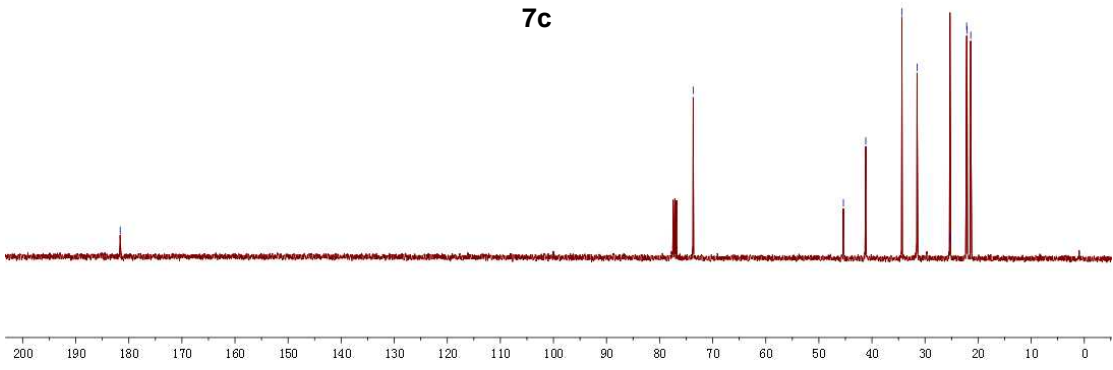
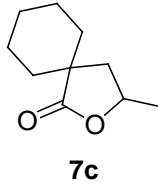




-181.6

-73.7

45.4  
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34.4  
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25.4  
22.2  
22.1  
21.4

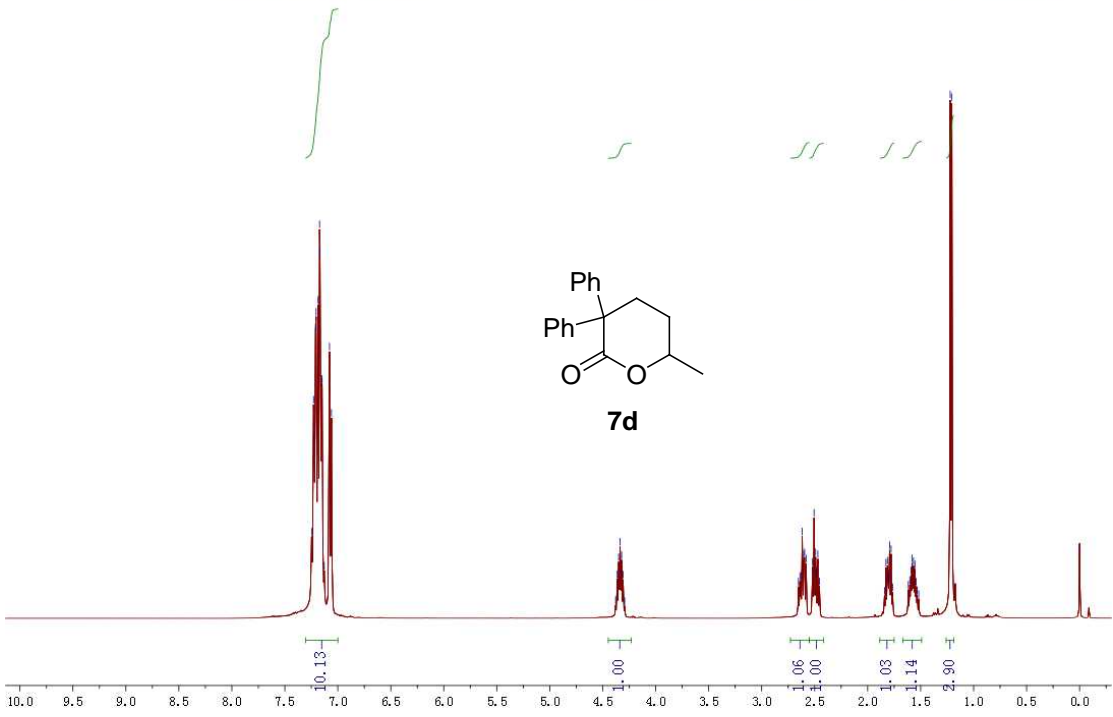
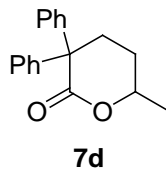


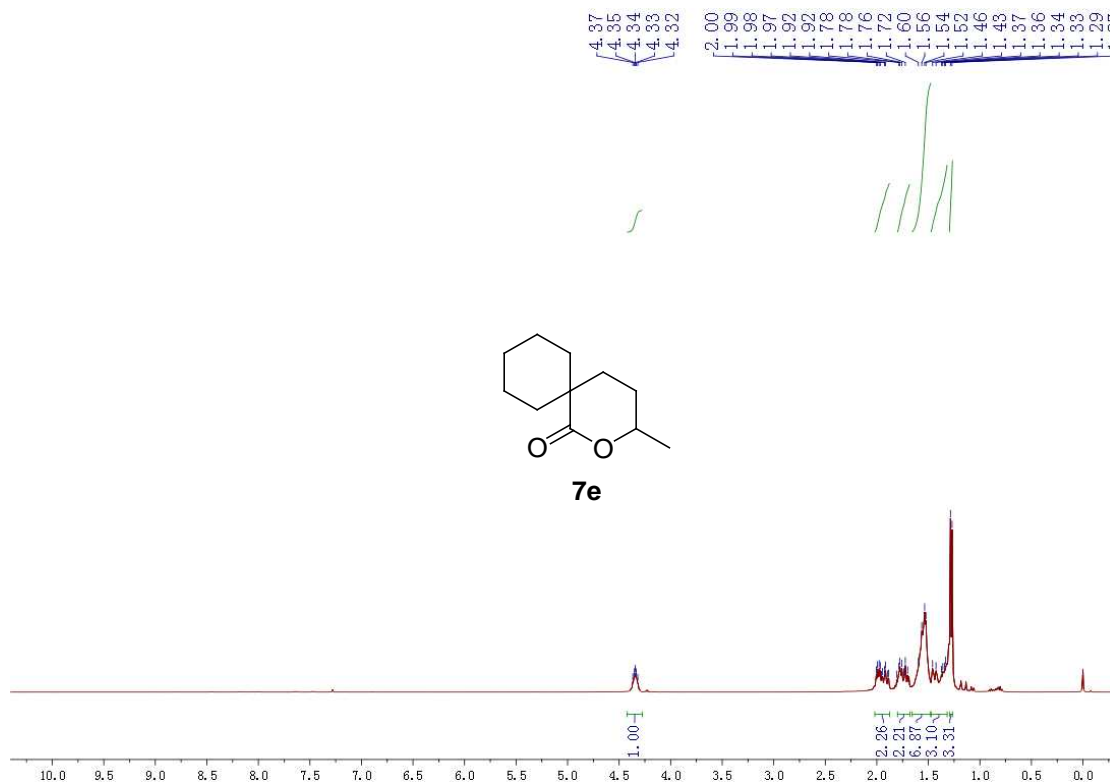
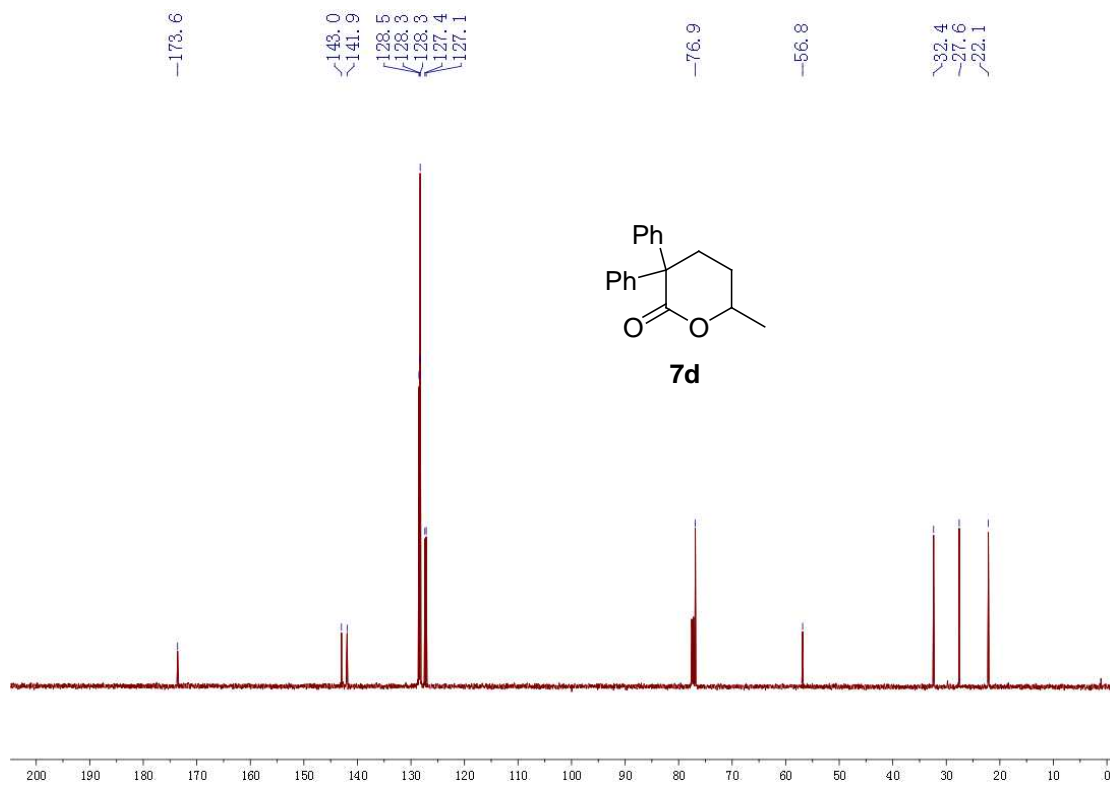
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7.06

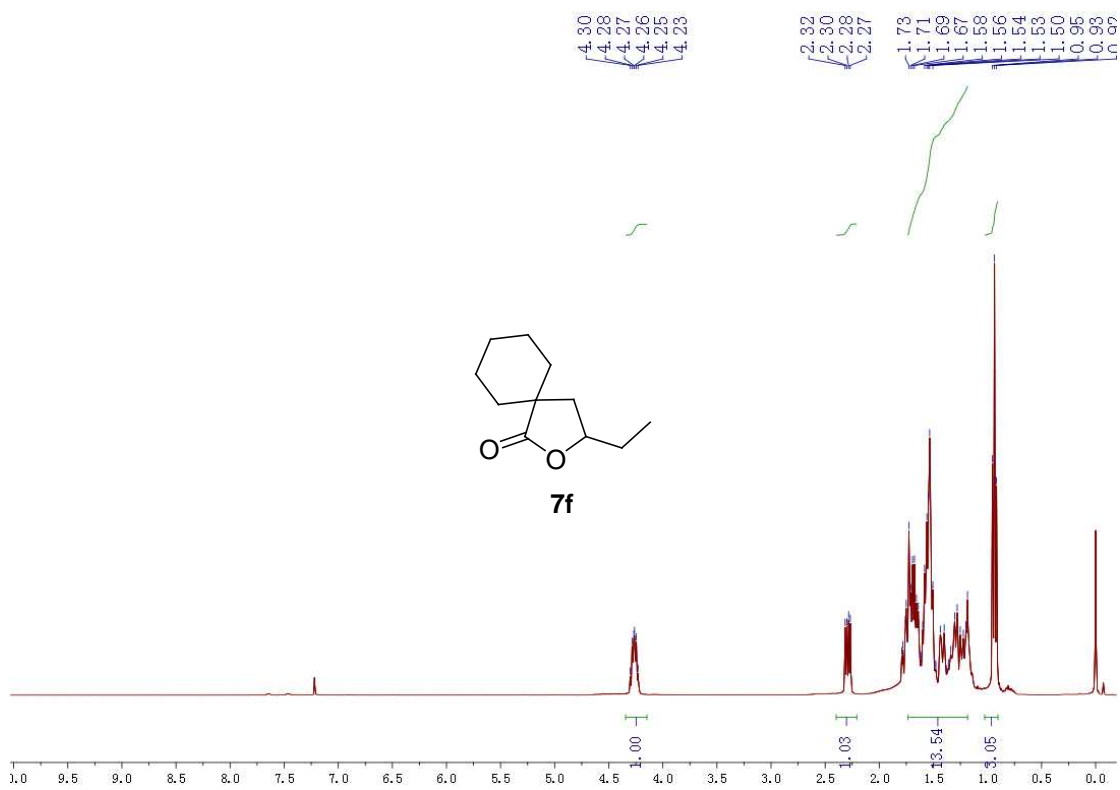
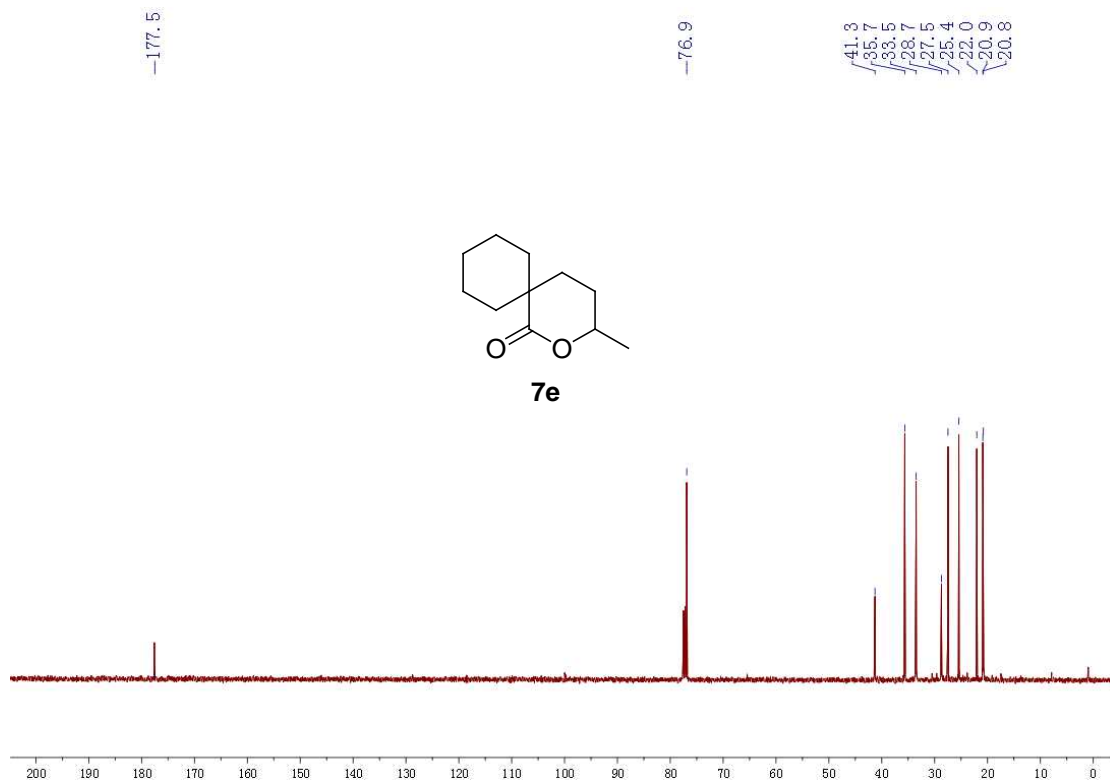
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2.49  
2.47

1.83  
1.81  
1.81  
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1.59  
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1.55  
1.51







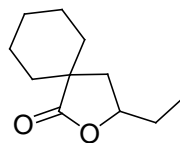


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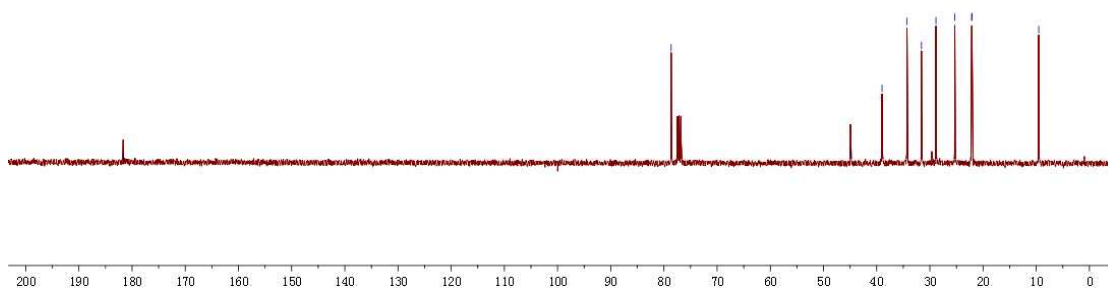
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31.6  
28.9  
25.3  
22.1  
22.1

-9.5



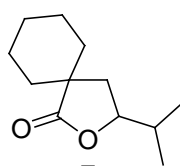
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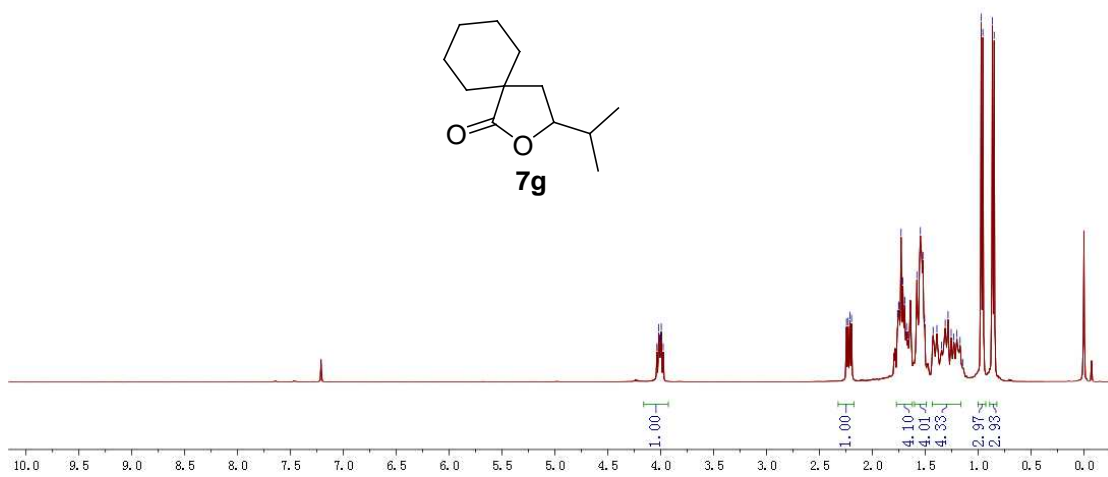
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4.01  
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3.98

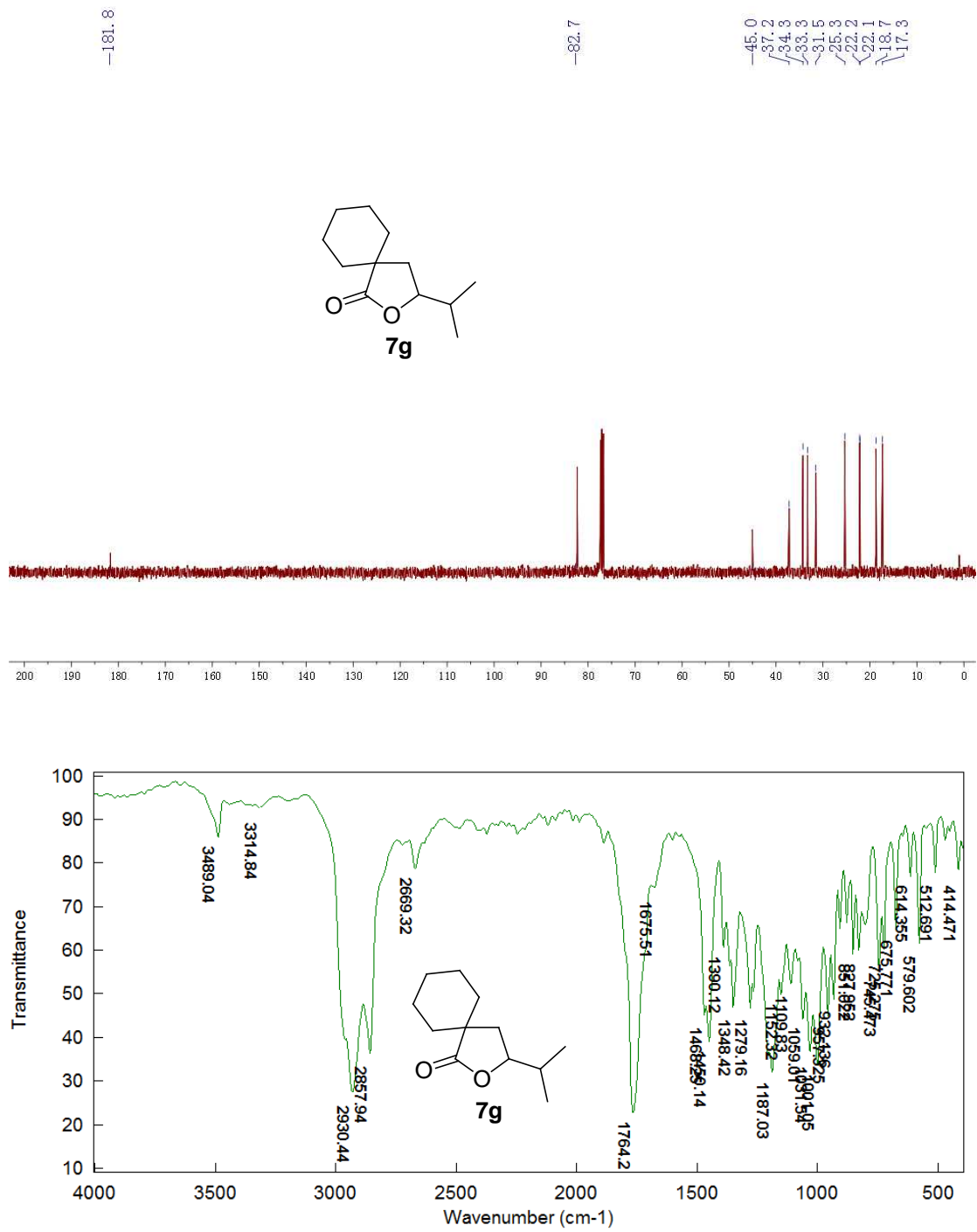
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0.96  
0.87



7g





#### 4. X-ray crystal structure and data of compound **2h**

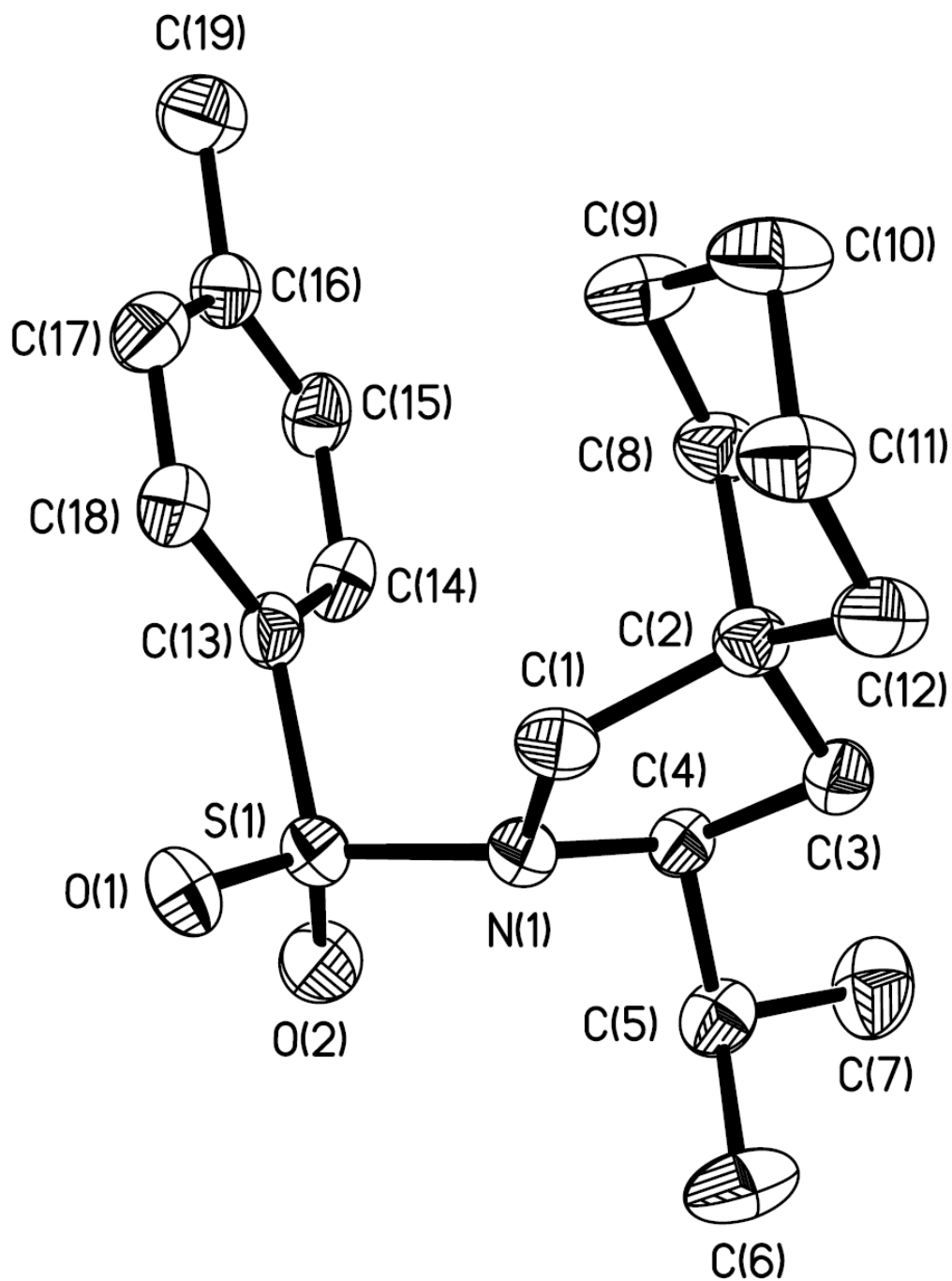


Figure 1. ORTEP drawing of **2h** Hydrogen atoms were omitted for clarity.

Table 1. Crystal data and structure refinement for **2h**.

Identification code	r141014a1
Empirical formula	C <sub>19</sub> H <sub>29</sub> N O <sub>2</sub> S
Formula weight	335.49
	58

Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pna2(1)
Unit cell dimensions	a = 9.2889(19) Å    alpha = 90 deg. b = 17.158(3) Å    beta = 90 deg. c = 11.652(2) Å    gamma = 90 deg.
Volume	1857.1(6) Å <sup>3</sup>
Z, Calculated density	4, 1.200 Mg/m <sup>3</sup>
Absorption coefficient	0.184 mm <sup>-1</sup>
F(000)	728
Crystal size	0.20 x 0.18 x 0.12 mm
Theta range for data collection	2.11 to 27.88 deg.
Limiting indices	-12 ≤ h ≤ 11, -15 ≤ k ≤ 22, -15 ≤ l ≤ 15
Reflections collected / unique	17703 / 4426 [R(int) = 0.0518]
Completeness to theta = 27.88	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9783 and 0.9642
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	4426 / 1 / 212
Goodness-of-fit on F <sup>2</sup>	0.979
Final R indices [I > 2σ(I)]	R1 = 0.0441, wR2 = 0.0986
R indices (all data)	R1 = 0.0585, wR2 = 0.1084
Absolute structure parameter	0.00(7)
Extinction coefficient	0.074(3)
Largest diff. peak and hole	0.164 and -0.184 e.Å <sup>-3</sup>

Table 2. Atomic coordinates ( x 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup> x 10<sup>3</sup>) for **2h**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	-815(1)	1098(1)	7108(1)	54(1)
O(1)	-1340(2)	358(1)	7503(2)	74(1)
O(2)	-1800(2)	1681(1)	6731(1)	74(1)
N(1)	273(2)	920(1)	6047(1)	46(1)
C(1)	1348(2)	291(1)	6218(2)	47(1)
C(2)	2751(2)	597(1)	5682(2)	45(1)
C(3)	2167(2)	1159(1)	4784(2)	50(1)
C(4)	861(2)	1555(1)	5320(2)	44(1)
C(5)	-232(3)	1891(1)	4457(2)	56(1)
C(6)	-934(3)	1278(2)	3716(3)	85(1)
C(7)	510(4)	2521(2)	3753(3)	85(1)
C(8)	3669(2)	1024(1)	6576(2)	55(1)
C(9)	4373(3)	485(1)	7445(2)	67(1)
C(10)	5231(3)	-157(2)	6857(3)	77(1)
C(11)	4284(3)	-600(1)	6021(2)	69(1)
C(12)	3632(2)	-54(1)	5142(2)	60(1)
C(13)	225(2)	1494(1)	8227(2)	48(1)
C(14)	613(2)	2278(1)	8207(2)	57(1)
C(15)	1507(3)	2569(1)	9058(2)	60(1)
C(16)	2021(2)	2103(1)	9926(2)	57(1)
C(17)	1613(3)	1328(1)	9944(2)	60(1)
C(18)	730(2)	1025(1)	9100(2)	55(1)
C(19)	2991(3)	2423(2)	10838(2)	80(1)

Table 3. Bond lengths [Å] and angles [deg] for **2h**.

S(1)-O(2)	1.4250(16)
S(1)-O(1)	1.4366(17)
S(1)-N(1)	1.6249(17)
S(1)-C(13)	1.760(2)
N(1)-C(1)	1.483(3)
N(1)-C(4)	1.486(3)
C(1)-C(2)	1.538(3)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(12)	1.520(3)
C(2)-C(3)	1.522(3)
C(2)-C(8)	1.533(3)
C(3)-C(4)	1.525(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.540(3)
C(4)-H(4)	0.9800
C(5)-C(6)	1.509(3)
C(5)-C(7)	1.523(4)
C(5)-H(5)	0.9800
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-C(9)	1.519(3)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700

C(9)-C(10)	1.523(3)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-C(11)	1.516(3)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(12)	1.514(3)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(18)	1.379(3)
C(13)-C(14)	1.392(3)
C(14)-C(15)	1.387(3)
C(14)-H(14)	0.9300
C(15)-C(16)	1.375(3)
C(15)-H(15)	0.9300
C(16)-C(17)	1.384(3)
C(16)-C(19)	1.498(4)
C(17)-C(18)	1.382(3)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
O(2)-S(1)-O(1)	120.10(10)
O(2)-S(1)-N(1)	107.27(10)
O(1)-S(1)-N(1)	106.75(10)
O(2)-S(1)-C(13)	108.03(11)

O(1)-S(1)-C(13)	106.87(11)
N(1)-S(1)-C(13)	107.20(8)
C(1)-N(1)-C(4)	111.27(15)
C(1)-N(1)-S(1)	116.98(14)
C(4)-N(1)-S(1)	121.59(14)
N(1)-C(1)-C(2)	105.57(15)
N(1)-C(1)-H(1A)	110.6
C(2)-C(1)-H(1A)	110.6
N(1)-C(1)-H(1B)	110.6
C(2)-C(1)-H(1B)	110.6
H(1A)-C(1)-H(1B)	108.8
C(12)-C(2)-C(3)	111.89(18)
C(12)-C(2)-C(8)	109.41(16)
C(3)-C(2)-C(8)	111.31(17)
C(12)-C(2)-C(1)	111.93(17)
C(3)-C(2)-C(1)	101.13(16)
C(8)-C(2)-C(1)	111.00(18)
C(2)-C(3)-C(4)	106.54(17)
C(2)-C(3)-H(3A)	110.4
C(4)-C(3)-H(3A)	110.4
C(2)-C(3)-H(3B)	110.4
C(4)-C(3)-H(3B)	110.4
H(3A)-C(3)-H(3B)	108.6
N(1)-C(4)-C(3)	101.44(16)
N(1)-C(4)-C(5)	113.86(16)
C(3)-C(4)-C(5)	115.09(17)
N(1)-C(4)-H(4)	108.7
C(3)-C(4)-H(4)	108.7
C(5)-C(4)-H(4)	108.7



C(6)-C(5)-C(7)	112.4(2)
C(6)-C(5)-C(4)	113.47(18)
C(7)-C(5)-C(4)	108.6(2)
C(6)-C(5)-H(5)	107.3
C(7)-C(5)-H(5)	107.3
C(4)-C(5)-H(5)	107.3
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(9)-C(8)-C(2)	113.72(18)
C(9)-C(8)-H(8A)	108.8
C(2)-C(8)-H(8A)	108.8
C(9)-C(8)-H(8B)	108.8
C(2)-C(8)-H(8B)	108.8
H(8A)-C(8)-H(8B)	107.7
C(8)-C(9)-C(10)	111.4(2)
C(8)-C(9)-H(9A)	109.3
C(10)-C(9)-H(9A)	109.3
C(8)-C(9)-H(9B)	109.3
C(10)-C(9)-H(9B)	109.3

H(9A)-C(9)-H(9B)	108.0
C(11)-C(10)-C(9)	110.40(19)
C(11)-C(10)-H(10A)	109.6
C(9)-C(10)-H(10A)	109.6
C(11)-C(10)-H(10B)	109.6
C(9)-C(10)-H(10B)	109.6
H(10A)-C(10)-H(10B)	108.1
C(12)-C(11)-C(10)	110.8(2)
C(12)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	108.1
C(11)-C(12)-C(2)	113.0(2)
C(11)-C(12)-H(12A)	109.0
C(2)-C(12)-H(12A)	109.0
C(11)-C(12)-H(12B)	109.0
C(2)-C(12)-H(12B)	109.0
H(12A)-C(12)-H(12B)	107.8
C(18)-C(13)-C(14)	119.2(2)
C(18)-C(13)-S(1)	120.50(17)
C(14)-C(13)-S(1)	120.16(17)
C(15)-C(14)-C(13)	119.4(2)
C(15)-C(14)-H(14)	120.3
C(13)-C(14)-H(14)	120.3
C(16)-C(15)-C(14)	121.7(2)
C(16)-C(15)-H(15)	119.2
C(14)-C(15)-H(15)	119.2
C(15)-C(16)-C(17)	118.4(2)

C(15)-C(16)-C(19)	121.2(2)
C(17)-C(16)-C(19)	120.4(2)
C(18)-C(17)-C(16)	120.8(2)
C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(13)-C(18)-C(17)	120.5(2)
C(13)-C(18)-H(18)	119.7
C(17)-C(18)-H(18)	119.7
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

---

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) for **2h**.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$$

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	U11	U22	U33	U23	U13	U12
S(1)	40(1)	74(1)	50(1)	3(1)	3(1)	1(1)
O(1)	59(1)	90(1)	73(1)	10(1)	9(1)	-29(1)
O(2)	49(1)	107(1)	66(1)	0(1)	2(1)	32(1)
N(1)	41(1)	51(1)	45(1)	2(1)	0(1)	1(1)
C(1)	45(1)	43(1)	54(1)	-3(1)	-7(1)	2(1)
C(2)	43(1)	46(1)	45(1)	-6(1)	-3(1)	1(1)
C(3)	50(1)	59(1)	43(1)	-1(1)	3(1)	3(1)

C(4)	47(1)	47(1)	38(1)	-1(1)	0(1)	1(1)
C(5)	63(1)	53(1)	52(1)	4(1)	-3(1)	13(1)
C(6)	93(2)	87(2)	73(2)	-13(2)	-40(2)	20(2)
C(7)	95(2)	83(2)	77(2)	29(2)	12(2)	18(2)
C(8)	51(1)	54(1)	59(1)	-11(1)	-10(1)	-5(1)
C(9)	70(1)	66(1)	65(2)	-12(1)	-29(1)	7(1)
C(10)	67(2)	73(2)	91(2)	-15(2)	-34(2)	18(1)
C(11)	65(1)	58(1)	85(2)	-20(1)	-19(1)	17(1)
C(12)	52(1)	67(2)	62(1)	-21(1)	-8(1)	13(1)
C(13)	47(1)	54(1)	44(1)	3(1)	10(1)	6(1)
C(14)	73(1)	53(1)	45(1)	4(1)	9(1)	11(1)
C(15)	73(2)	55(1)	50(1)	-7(1)	11(1)	-4(1)
C(16)	51(1)	71(2)	48(1)	-12(1)	8(1)	7(1)
C(17)	68(1)	64(1)	49(1)	2(1)	-1(1)	11(1)
C(18)	61(1)	53(1)	50(1)	4(1)	6(1)	1(1)
C(19)	67(1)	101(2)	70(2)	-27(2)	-2(1)	8(2)

---

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **2h**.

	x	y	z	U(eq)
H(1A)	1040	-184	5840	57
H(1B)	1480	185	7029	57
H(3A)	1890	878	4095	61
H(3B)	2892	1542	4581	61
H(4)	1195	1978	5820	53
H(5)	-996	2144	4902	67
H(6A)	-1624	1521	3217	127
H(6B)	-1412	904	4195	127
H(6C)	-213	1021	3264	127
H(7A)	1204	2285	3250	127
H(7B)	988	2880	4258	127
H(7C)	-193	2796	3305	127
H(8A)	4415	1316	6183	65
H(8B)	3066	1394	6982	65
H(9A)	3636	253	7925	80
H(9B)	5009	786	7935	80
H(10A)	6038	70	6448	93
H(10B)	5608	-513	7429	93
H(11A)	4853	-994	5632	83
H(11B)	3521	-861	6439	83
H(12A)	3020	-351	4630	72
H(12B)	4399	174	4687	72
H(14)	276	2603	7627	68
H(15)	1767	3092	9040	71

H(17)	1937	1006	10532	72
H(18)	474	501	9120	66
H(19A)	3352	2003	11301	119
H(19B)	2462	2780	11312	119
H(19C)	3783	2691	10485	119

---

Table 6. Torsion angles [deg] for **2h**.

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O(2)-S(1)-N(1)-C(1)	-176.40(14)
O(1)-S(1)-N(1)-C(1)	-46.45(16)
C(13)-S(1)-N(1)-C(1)	67.78(16)
O(2)-S(1)-N(1)-C(4)	41.33(17)
O(1)-S(1)-N(1)-C(4)	171.28(15)
C(13)-S(1)-N(1)-C(4)	-74.49(17)
C(4)-N(1)-C(1)-C(2)	6.8(2)
S(1)-N(1)-C(1)-C(2)	-139.17(14)
N(1)-C(1)-C(2)-C(12)	-146.01(17)
N(1)-C(1)-C(2)-C(3)	-26.8(2)
N(1)-C(1)-C(2)-C(8)	91.43(19)
C(12)-C(2)-C(3)-C(4)	157.07(17)
C(8)-C(2)-C(3)-C(4)	-80.2(2)
C(1)-C(2)-C(3)-C(4)	37.8(2)
C(1)-N(1)-C(4)-C(3)	16.1(2)
S(1)-N(1)-C(4)-C(3)	160.32(14)
C(1)-N(1)-C(4)-C(5)	140.36(17)
S(1)-N(1)-C(4)-C(5)	-75.5(2)
C(2)-C(3)-C(4)-N(1)	-33.6(2)
C(2)-C(3)-C(4)-C(5)	-157.03(17)
N(1)-C(4)-C(5)-C(6)	-53.0(3)

C(3)-C(4)-C(5)-C(6)	63.5(3)
N(1)-C(4)-C(5)-C(7)	-178.80(19)
C(3)-C(4)-C(5)-C(7)	-62.3(2)
C(12)-C(2)-C(8)-C(9)	-51.6(3)
C(3)-C(2)-C(8)-C(9)	-175.74(19)
C(1)-C(2)-C(8)-C(9)	72.4(2)
C(2)-C(8)-C(9)-C(10)	53.4(3)
C(8)-C(9)-C(10)-C(11)	-55.0(3)
C(9)-C(10)-C(11)-C(12)	57.0(3)
C(10)-C(11)-C(12)-C(2)	-57.7(3)
C(3)-C(2)-C(12)-C(11)	177.35(19)
C(8)-C(2)-C(12)-C(11)	53.5(2)
C(1)-C(2)-C(12)-C(11)	-70.0(2)
O(2)-S(1)-C(13)-C(18)	148.48(17)
O(1)-S(1)-C(13)-C(18)	17.9(2)
N(1)-S(1)-C(13)-C(18)	-96.21(18)
O(2)-S(1)-C(13)-C(14)	-35.14(19)
O(1)-S(1)-C(13)-C(14)	-165.67(17)
N(1)-S(1)-C(13)-C(14)	80.17(18)
C(18)-C(13)-C(14)-C(15)	0.5(3)
S(1)-C(13)-C(14)-C(15)	-175.94(16)
C(13)-C(14)-C(15)-C(16)	-0.2(3)
C(14)-C(15)-C(16)-C(17)	-0.6(3)
C(14)-C(15)-C(16)-C(19)	179.7(2)
C(15)-C(16)-C(17)-C(18)	1.0(3)
C(19)-C(16)-C(17)-C(18)	-179.3(2)
C(14)-C(13)-C(18)-C(17)	-0.1(3)
S(1)-C(13)-C(18)-C(17)	176.35(17)
C(16)-C(17)-C(18)-C(13)	-0.7(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **2h** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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## 5. X-ray crystal structure and data of compound **2j**

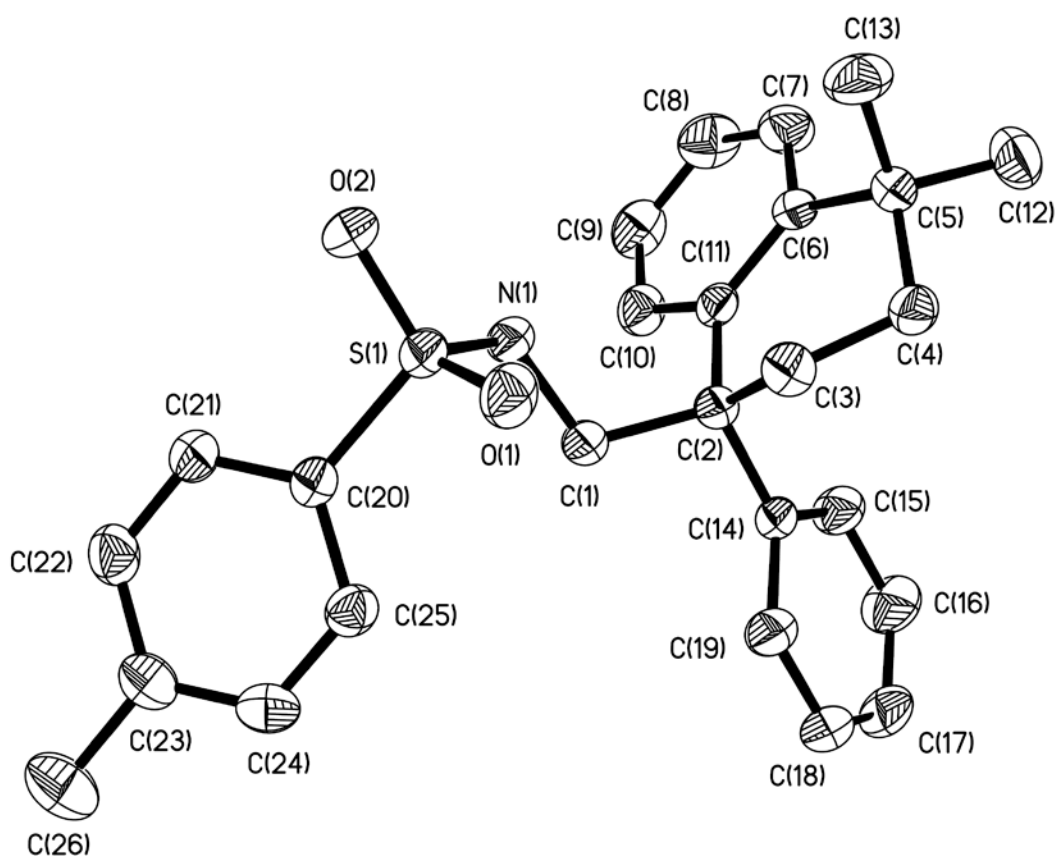


Figure 1. ORTEP drawing of **2j**. Hydrogen atoms were omitted for clarity.

Table 1. Crystal data and structure refinement for **2j**.

Identification code	shelxl
Empirical formula	C <sub>26</sub> H <sub>29</sub> NO <sub>2</sub> S
Formula weight	419.56



Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.089(2) Å    alpha = 80.22(3) deg. b = 13.375(3) Å    beta = 77.60(3) deg. c = 16.281(3) Å    gamma = 77.15(3) deg.
Volume	2280.3(8) Å <sup>3</sup>
Z, Calculated density	4, 1.222 Mg/m <sup>3</sup>
Absorption coefficient	0.164 mm <sup>-1</sup>
F(000)	896
Crystal size	0.20 x 0.18 x 0.12 mm
Theta range for data collection	1.57 to 27.88 deg.
Limiting indices	-14 ≤ h ≤ 14, -17 ≤ k ≤ 17, -19 ≤ l ≤ 21
Reflections collected / unique	28896 / 10801 [R(int) = 0.0359]
Completeness to theta = 27.88	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9806 and 0.9680
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	10801 / 2 / 556
Goodness-of-fit on F <sup>2</sup>	1.018
Final R indices [I > 2σ(I)]	R1 = 0.0540, wR2 = 0.1309
R indices (all data)	R1 = 0.0868, wR2 = 0.1512
Extinction coefficient	0.033(2)
Largest diff. peak and hole	0.235 and -0.317 e.Å <sup>-3</sup>

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for shelxl.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	7952(1)	-231(1)	4837(1)	49(1)
S(2)	500(1)	4894(1)	1297(1)	46(1)
O(1)	7008(1)	208(1)	4334(1)	64(1)
O(2)	9233(1)	-547(1)	4438(1)	63(1)
O(3)	-545(1)	5532(1)	948(1)	54(1)
O(4)	427(1)	4728(1)	2194(1)	64(1)
N(1)	7966(2)	607(1)	5436(1)	53(1)
N(2)	691(2)	3796(1)	961(1)	49(1)
C(1)	6805(2)	1042(2)	5989(1)	55(1)
C(2)	6533(2)	2230(1)	5900(1)	46(1)
C(3)	6304(2)	2640(2)	4987(1)	55(1)
C(4)	6267(2)	3786(2)	4790(1)	53(1)
C(5)	7538(2)	4064(2)	4781(1)	52(1)
C(6)	8088(2)	3473(1)	5545(1)	45(1)
C(7)	9094(2)	3784(2)	5757(2)	69(1)
C(8)	9650(2)	3297(2)	6426(2)	81(1)
C(9)	9205(2)	2481(2)	6928(2)	73(1)
C(10)	8202(2)	2162(2)	6751(1)	61(1)
C(11)	7634(2)	2635(1)	6058(1)	45(1)
C(12)	7317(2)	5236(2)	4782(2)	85(1)
C(13)	8451(2)	3789(2)	3969(1)	82(1)
C(14)	5314(2)	2573(1)	6531(1)	46(1)
C(15)	5195(2)	3324(2)	7038(1)	64(1)

C(16)	4061(2)	3650(2)	7576(2)	85(1)
C(17)	3037(2)	3226(2)	7613(2)	82(1)
C(18)	3129(2)	2487(2)	7113(2)	80(1)
C(19)	4247(2)	2163(2)	6571(2)	67(1)
C(20)	7436(2)	-1307(1)	5496(1)	44(1)
C(21)	8292(2)	-2155(2)	5751(1)	55(1)
C(22)	7874(2)	-2983(2)	6275(1)	64(1)
C(23)	6606(2)	-2984(2)	6556(1)	59(1)
C(24)	5763(2)	-2124(2)	6290(1)	59(1)
C(25)	6158(2)	-1295(2)	5761(1)	52(1)
C(26)	6153(3)	-3885(2)	7129(2)	95(1)
C(27)	1728(2)	2949(1)	1149(1)	50(1)
C(28)	1297(2)	1897(1)	1397(1)	42(1)
C(29)	522(2)	1764(1)	764(1)	42(1)
C(30)	974(2)	1994(2)	-97(1)	54(1)
C(31)	312(2)	1933(2)	-705(1)	66(1)
C(32)	-816(2)	1621(2)	-465(2)	67(1)
C(33)	-1279(2)	1377(2)	381(1)	60(1)
C(34)	-631(2)	1436(1)	1014(1)	45(1)
C(35)	-1223(2)	1167(2)	1947(1)	52(1)
C(36)	-250(2)	1037(2)	2506(1)	57(1)
C(37)	485(2)	1901(2)	2295(1)	52(1)
C(38)	-2332(2)	2028(2)	2209(2)	82(1)
C(39)	-1699(3)	141(2)	2081(2)	86(1)
C(40)	2487(2)	1049(2)	1409(1)	49(1)
C(41)	2719(2)	208(2)	970(2)	76(1)
C(42)	3805(3)	-547(2)	996(2)	107(1)
C(43)	4673(3)	-466(2)	1456(2)	95(1)
C(44)	4456(2)	356(2)	1896(2)	79(1)

C(45)	3379(2)	1100(2)	1876(1)	62(1)
C(46)	1852(2)	5432(1)	849(1)	45(1)
C(47)	2381(2)	5879(2)	1355(1)	57(1)
C(48)	3406(2)	6340(2)	987(2)	67(1)
C(49)	3909(2)	6362(2)	137(2)	64(1)
C(50)	3366(2)	5902(2)	-353(2)	69(1)
C(51)	2337(2)	5444(2)	-4(1)	59(1)
C(52)	5019(2)	6878(2)	-255(2)	100(1)

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Table 3. Bond lengths [Å] and angles [deg] for shelxl.

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S(1)-O(1)	1.4289(15)
S(1)-O(2)	1.4315(14)
S(1)-N(1)	1.6105(18)
S(1)-C(20)	1.769(2)
S(2)-O(4)	1.4259(14)
S(2)-O(3)	1.4391(14)
S(2)-N(2)	1.6092(17)
S(2)-C(46)	1.7684(19)
N(1)-C(1)	1.467(2)
N(1)-H(1)	0.886(10)
N(2)-C(27)	1.467(2)
N(2)-H(2)	0.886(9)
C(1)-C(2)	1.539(3)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(11)	1.525(3)

C(2)-C(14)	1.543(3)
C(2)-C(3)	1.548(3)
C(3)-C(4)	1.505(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.532(3)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.525(3)
C(5)-C(13)	1.527(3)
C(5)-C(12)	1.532(3)
C(6)-C(7)	1.399(3)
C(6)-C(11)	1.399(3)
C(7)-C(8)	1.364(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.366(3)
C(8)-H(8)	0.9300
C(9)-C(10)	1.376(3)
C(9)-H(9)	0.9300
C(10)-C(11)	1.397(3)
C(10)-H(10)	0.9300
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-C(15)	1.372(3)
C(14)-C(19)	1.396(3)

C(15)-C(16)	1.396(3)
C(15)-H(15)	0.9300
C(16)-C(17)	1.364(4)
C(16)-H(16)	0.9300
C(17)-C(18)	1.357(4)
C(17)-H(17)	0.9300
C(18)-C(19)	1.387(3)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-C(21)	1.375(3)
C(20)-C(25)	1.387(2)
C(21)-C(22)	1.381(3)
C(21)-H(21)	0.9300
C(22)-C(23)	1.382(3)
C(22)-H(22)	0.9300
C(23)-C(24)	1.383(3)
C(23)-C(26)	1.504(3)
C(24)-C(25)	1.375(3)
C(24)-H(24)	0.9300
C(25)-H(25)	0.9300
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-C(28)	1.548(3)
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(28)-C(29)	1.530(2)
C(28)-C(40)	1.538(3)
C(28)-C(37)	1.544(3)

C(29)-C(30)	1.390(3)
C(29)-C(34)	1.399(2)
C(30)-C(31)	1.375(3)
C(30)-H(30)	0.9300
C(31)-C(32)	1.363(3)
C(31)-H(31)	0.9300
C(32)-C(33)	1.372(3)
C(32)-H(32)	0.9300
C(33)-C(34)	1.399(3)
C(33)-H(33)	0.9300
C(34)-C(35)	1.536(3)
C(35)-C(36)	1.519(3)
C(35)-C(38)	1.527(3)
C(35)-C(39)	1.543(3)
C(36)-C(37)	1.510(3)
C(36)-H(36A)	0.9700
C(36)-H(36B)	0.9700
C(37)-H(37A)	0.9700
C(37)-H(37B)	0.9700
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
C(39)-H(39A)	0.9600
C(39)-H(39B)	0.9600
C(39)-H(39C)	0.9600
C(40)-C(41)	1.381(3)
C(40)-C(45)	1.391(3)
C(41)-C(42)	1.392(3)
C(41)-H(41)	0.9300

C(42)-C(43)	1.372(4)
C(42)-H(42)	0.9300
C(43)-C(44)	1.363(4)
C(43)-H(43)	0.9300
C(44)-C(45)	1.376(3)
C(44)-H(44)	0.9300
C(45)-H(45)	0.9300
C(46)-C(51)	1.376(3)
C(46)-C(47)	1.383(3)
C(47)-C(48)	1.388(3)
C(47)-H(47)	0.9300
C(48)-C(49)	1.374(3)
C(48)-H(48)	0.9300
C(49)-C(50)	1.384(3)
C(49)-C(52)	1.513(3)
C(50)-C(51)	1.384(3)
C(50)-H(50)	0.9300
C(51)-H(51)	0.9300
C(52)-H(52A)	0.9600
C(52)-H(52B)	0.9600
C(52)-H(52C)	0.9600
O(1)-S(1)-O(2)	120.20(9)
O(1)-S(1)-N(1)	107.70(10)
O(2)-S(1)-N(1)	105.88(9)
O(1)-S(1)-C(20)	106.00(9)
O(2)-S(1)-C(20)	108.72(9)
N(1)-S(1)-C(20)	107.83(9)
O(4)-S(2)-O(3)	119.26(9)
O(4)-S(2)-N(2)	108.84(9)



O(3)-S(2)-N(2)	104.89(9)
O(4)-S(2)-C(46)	107.18(9)
O(3)-S(2)-C(46)	108.03(8)
N(2)-S(2)-C(46)	108.23(9)
C(1)-N(1)-S(1)	120.28(14)
C(1)-N(1)-H(1)	121.3(18)
S(1)-N(1)-H(1)	112.1(18)
C(27)-N(2)-S(2)	121.07(14)
C(27)-N(2)-H(2)	110.8(14)
S(2)-N(2)-H(2)	117.4(14)
N(1)-C(1)-C(2)	113.48(15)
N(1)-C(1)-H(1A)	108.9
C(2)-C(1)-H(1A)	108.9
N(1)-C(1)-H(1B)	108.9
C(2)-C(1)-H(1B)	108.9
H(1A)-C(1)-H(1B)	107.7
C(11)-C(2)-C(1)	111.29(16)
C(11)-C(2)-C(14)	111.63(15)
C(1)-C(2)-C(14)	107.68(15)
C(11)-C(2)-C(3)	109.65(15)
C(1)-C(2)-C(3)	107.75(16)
C(14)-C(2)-C(3)	108.73(16)
C(4)-C(3)-C(2)	111.44(17)
C(4)-C(3)-H(3A)	109.3
C(2)-C(3)-H(3A)	109.3
C(4)-C(3)-H(3B)	109.3
C(2)-C(3)-H(3B)	109.3
H(3A)-C(3)-H(3B)	108.0
C(3)-C(4)-C(5)	112.21(17)

C(3)-C(4)-H(4A)	109.2
C(5)-C(4)-H(4A)	109.2
C(3)-C(4)-H(4B)	109.2
C(5)-C(4)-H(4B)	109.2
H(4A)-C(4)-H(4B)	107.9
C(6)-C(5)-C(13)	109.21(17)
C(6)-C(5)-C(12)	111.76(19)
C(13)-C(5)-C(12)	108.34(19)
C(6)-C(5)-C(4)	110.20(16)
C(13)-C(5)-C(4)	109.8(2)
C(12)-C(5)-C(4)	107.51(17)
C(7)-C(6)-C(11)	117.69(18)
C(7)-C(6)-C(5)	118.72(18)
C(11)-C(6)-C(5)	123.59(17)
C(8)-C(7)-C(6)	122.7(2)
C(8)-C(7)-H(7)	118.7
C(6)-C(7)-H(7)	118.7
C(7)-C(8)-C(9)	119.6(2)
C(7)-C(8)-H(8)	120.2
C(9)-C(8)-H(8)	120.2
C(8)-C(9)-C(10)	119.5(2)
C(8)-C(9)-H(9)	120.3
C(10)-C(9)-H(9)	120.3
C(9)-C(10)-C(11)	122.0(2)
C(9)-C(10)-H(10)	119.0
C(11)-C(10)-H(10)	119.0
C(10)-C(11)-C(6)	118.52(18)
C(10)-C(11)-C(2)	118.80(17)
C(6)-C(11)-C(2)	122.67(17)

C(5)-C(12)-H(12A)	109.5
C(5)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(5)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(5)-C(13)-H(13A)	109.5
C(5)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(5)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(19)	116.85(19)
C(15)-C(14)-C(2)	122.67(18)
C(19)-C(14)-C(2)	120.38(18)
C(14)-C(15)-C(16)	121.3(2)
C(14)-C(15)-H(15)	119.3
C(16)-C(15)-H(15)	119.3
C(17)-C(16)-C(15)	120.7(2)
C(17)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(18)-C(17)-C(16)	119.1(2)
C(18)-C(17)-H(17)	120.5
C(16)-C(17)-H(17)	120.5
C(17)-C(18)-C(19)	120.8(2)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.6
C(18)-C(19)-C(14)	121.3(2)
C(18)-C(19)-H(19)	119.4

C(14)-C(19)-H(19)	119.4
C(21)-C(20)-C(25)	119.63(18)
C(21)-C(20)-S(1)	120.55(15)
C(25)-C(20)-S(1)	119.82(15)
C(20)-C(21)-C(22)	119.82(19)
C(20)-C(21)-H(21)	120.1
C(22)-C(21)-H(21)	120.1
C(21)-C(22)-C(23)	121.6(2)
C(21)-C(22)-H(22)	119.2
C(23)-C(22)-H(22)	119.2
C(22)-C(23)-C(24)	117.6(2)
C(22)-C(23)-C(26)	121.5(2)
C(24)-C(23)-C(26)	120.9(2)
C(25)-C(24)-C(23)	121.8(2)
C(25)-C(24)-H(24)	119.1
C(23)-C(24)-H(24)	119.1
C(24)-C(25)-C(20)	119.59(19)
C(24)-C(25)-H(25)	120.2
C(20)-C(25)-H(25)	120.2
C(23)-C(26)-H(26A)	109.5
C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
N(2)-C(27)-C(28)	111.86(15)
N(2)-C(27)-H(27A)	109.2
C(28)-C(27)-H(27A)	109.2
N(2)-C(27)-H(27B)	109.2

C(28)-C(27)-H(27B)	109.2
H(27A)-C(27)-H(27B)	107.9
C(29)-C(28)-C(40)	112.10(15)
C(29)-C(28)-C(37)	110.15(15)
C(40)-C(28)-C(37)	109.89(16)
C(29)-C(28)-C(27)	109.71(15)
C(40)-C(28)-C(27)	107.37(15)
C(37)-C(28)-C(27)	107.47(16)
C(30)-C(29)-C(34)	118.50(18)
C(30)-C(29)-C(28)	118.55(16)
C(34)-C(29)-C(28)	122.95(16)
C(31)-C(30)-C(29)	122.2(2)
C(31)-C(30)-H(30)	118.9
C(29)-C(30)-H(30)	118.9
C(32)-C(31)-C(30)	119.5(2)
C(32)-C(31)-H(31)	120.2
C(30)-C(31)-H(31)	120.2
C(31)-C(32)-C(33)	119.6(2)
C(31)-C(32)-H(32)	120.2
C(33)-C(32)-H(32)	120.2
C(32)-C(33)-C(34)	122.2(2)
C(32)-C(33)-H(33)	118.9
C(34)-C(33)-H(33)	118.9
C(29)-C(34)-C(33)	117.99(18)
C(29)-C(34)-C(35)	122.98(17)
C(33)-C(34)-C(35)	119.01(17)
C(36)-C(35)-C(38)	109.89(19)
C(36)-C(35)-C(34)	110.01(16)
C(38)-C(35)-C(34)	109.50(18)

C(36)-C(35)-C(39)	107.70(19)
C(38)-C(35)-C(39)	108.8(2)
C(34)-C(35)-C(39)	110.90(18)
C(37)-C(36)-C(35)	112.54(17)
C(37)-C(36)-H(36A)	109.1
C(35)-C(36)-H(36A)	109.1
C(37)-C(36)-H(36B)	109.1
C(35)-C(36)-H(36B)	109.1
H(36A)-C(36)-H(36B)	107.8
C(36)-C(37)-C(28)	111.44(16)
C(36)-C(37)-H(37A)	109.3
C(28)-C(37)-H(37A)	109.3
C(36)-C(37)-H(37B)	109.3
C(28)-C(37)-H(37B)	109.3
H(37A)-C(37)-H(37B)	108.0
C(35)-C(38)-H(38A)	109.5
C(35)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(35)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(35)-C(39)-H(39A)	109.5
C(35)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(35)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(41)-C(40)-C(45)	117.0(2)
C(41)-C(40)-C(28)	122.41(19)

C(45)-C(40)-C(28)	120.55(18)
C(40)-C(41)-C(42)	121.0(3)
C(40)-C(41)-H(41)	119.5
C(42)-C(41)-H(41)	119.5
C(43)-C(42)-C(41)	120.4(3)
C(43)-C(42)-H(42)	119.8
C(41)-C(42)-H(42)	119.8
C(44)-C(43)-C(42)	119.4(3)
C(44)-C(43)-H(43)	120.3
C(42)-C(43)-H(43)	120.3
C(43)-C(44)-C(45)	120.3(3)
C(43)-C(44)-H(44)	119.9
C(45)-C(44)-H(44)	119.9
C(44)-C(45)-C(40)	121.9(2)
C(44)-C(45)-H(45)	119.1
C(40)-C(45)-H(45)	119.1
C(51)-C(46)-C(47)	120.45(18)
C(51)-C(46)-S(2)	120.05(15)
C(47)-C(46)-S(2)	119.43(15)
C(46)-C(47)-C(48)	118.8(2)
C(46)-C(47)-H(47)	120.6
C(48)-C(47)-H(47)	120.6
C(49)-C(48)-C(47)	121.9(2)
C(49)-C(48)-H(48)	119.1
C(47)-C(48)-H(48)	119.1
C(48)-C(49)-C(50)	118.06(19)
C(48)-C(49)-C(52)	121.2(2)
C(50)-C(49)-C(52)	120.8(2)
C(51)-C(50)-C(49)	121.3(2)

C(51)-C(50)-H(50)	119.4
C(49)-C(50)-H(50)	119.4
C(46)-C(51)-C(50)	119.5(2)
C(46)-C(51)-H(51)	120.3
C(50)-C(51)-H(51)	120.3
C(49)-C(52)-H(52A)	109.5
C(49)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(49)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for shelxl.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$$

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	U11	U22	U33	U23	U13	U12
S(1)	44(1)	46(1)	50(1)	-6(1)	0(1)	-3(1)
S(2)	46(1)	42(1)	49(1)	-6(1)	-3(1)	-11(1)
O(1)	63(1)	65(1)	58(1)	4(1)	-18(1)	1(1)
O(2)	47(1)	62(1)	66(1)	-12(1)	12(1)	-3(1)
O(3)	44(1)	48(1)	68(1)	-7(1)	-7(1)	-4(1)
O(4)	80(1)	68(1)	45(1)	-6(1)	-2(1)	-29(1)
N(1)	41(1)	46(1)	68(1)	-16(1)	4(1)	-7(1)
N(2)	52(1)	40(1)	58(1)	-6(1)	-15(1)	-10(1)



C(1)	48(1)	43(1)	63(1)	-9(1)	9(1)	-7(1)
C(2)	42(1)	41(1)	51(1)	-6(1)	-1(1)	-8(1)
C(3)	56(1)	58(1)	54(1)	-8(1)	-13(1)	-13(1)
C(4)	45(1)	57(1)	51(1)	1(1)	-11(1)	-6(1)
C(5)	46(1)	49(1)	55(1)	5(1)	-5(1)	-8(1)
C(6)	35(1)	49(1)	47(1)	-5(1)	-4(1)	-8(1)
C(7)	54(1)	78(2)	80(2)	-2(1)	-17(1)	-23(1)
C(8)	62(2)	108(2)	84(2)	-11(2)	-29(1)	-23(2)
C(9)	69(2)	90(2)	61(1)	-11(1)	-29(1)	0(1)
C(10)	61(1)	64(1)	51(1)	2(1)	-14(1)	-3(1)
C(11)	39(1)	44(1)	47(1)	-9(1)	-4(1)	-1(1)
C(12)	82(2)	57(2)	115(2)	14(1)	-28(2)	-21(1)
C(13)	56(1)	118(2)	54(1)	9(1)	4(1)	-8(1)
C(14)	40(1)	42(1)	49(1)	-2(1)	-1(1)	-3(1)
C(15)	53(1)	63(1)	69(1)	-21(1)	3(1)	-7(1)
C(16)	73(2)	87(2)	85(2)	-37(2)	13(1)	0(2)
C(17)	52(1)	82(2)	87(2)	-7(2)	19(1)	7(1)
C(18)	42(1)	69(2)	113(2)	-2(2)	9(1)	-6(1)
C(19)	46(1)	57(1)	92(2)	-16(1)	2(1)	-9(1)
C(20)	42(1)	44(1)	45(1)	-10(1)	-10(1)	-4(1)
C(21)	44(1)	50(1)	69(1)	-6(1)	-13(1)	-4(1)
C(22)	66(2)	51(1)	74(2)	1(1)	-24(1)	-5(1)
C(23)	72(2)	60(1)	52(1)	-4(1)	-17(1)	-24(1)
C(24)	52(1)	74(2)	57(1)	-9(1)	-9(1)	-24(1)
C(25)	43(1)	55(1)	59(1)	-9(1)	-15(1)	-7(1)
C(26)	118(2)	86(2)	84(2)	17(2)	-21(2)	-47(2)
C(27)	44(1)	43(1)	63(1)	-4(1)	-10(1)	-11(1)
C(28)	41(1)	39(1)	46(1)	-6(1)	-4(1)	-11(1)
C(29)	45(1)	35(1)	44(1)	-4(1)	-2(1)	-11(1)

C(30)	65(1)	53(1)	45(1)	-3(1)	-3(1)	-24(1)
C(31)	99(2)	56(1)	46(1)	-5(1)	-10(1)	-26(1)
C(32)	85(2)	65(2)	60(1)	-9(1)	-29(1)	-16(1)
C(33)	52(1)	63(1)	70(2)	-12(1)	-16(1)	-18(1)
C(34)	44(1)	40(1)	53(1)	-8(1)	-6(1)	-10(1)
C(35)	46(1)	56(1)	54(1)	-8(1)	3(1)	-19(1)
C(36)	61(1)	60(1)	46(1)	3(1)	0(1)	-19(1)
C(37)	54(1)	60(1)	46(1)	-9(1)	-7(1)	-16(1)
C(38)	52(1)	103(2)	83(2)	-29(2)	4(1)	-3(1)
C(39)	102(2)	90(2)	74(2)	-9(1)	9(1)	-62(2)
C(40)	47(1)	45(1)	52(1)	0(1)	-4(1)	-10(1)
C(41)	75(2)	60(1)	93(2)	-25(1)	-22(1)	5(1)
C(42)	108(2)	79(2)	124(3)	-39(2)	-31(2)	28(2)
C(43)	72(2)	90(2)	101(2)	-3(2)	-18(2)	24(2)
C(44)	59(2)	83(2)	87(2)	6(2)	-21(1)	-2(1)
C(45)	57(1)	59(1)	71(1)	-3(1)	-20(1)	-8(1)
C(46)	44(1)	38(1)	51(1)	-4(1)	-9(1)	-6(1)
C(47)	57(1)	56(1)	61(1)	-6(1)	-14(1)	-16(1)
C(48)	59(1)	63(1)	88(2)	-8(1)	-26(1)	-20(1)
C(49)	43(1)	54(1)	93(2)	-3(1)	-6(1)	-12(1)
C(50)	58(1)	73(2)	67(2)	-6(1)	8(1)	-18(1)
C(51)	56(1)	66(1)	59(1)	-13(1)	-4(1)	-21(1)
C(52)	60(2)	91(2)	143(3)	-2(2)	1(2)	-35(2)

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Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for shelxl.

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	x	y	z	U(eq)
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H(1A)	6866	771	6574	65
H(1B)	6104	815	5857	65
H(3A)	6971	2284	4586	66
H(3B)	5513	2493	4924	66
H(4A)	5631	4137	5210	63
H(4B)	6027	4029	4240	63
H(7)	9397	4347	5427	83
H(8)	10327	3519	6540	98
H(9)	9578	2142	7385	88
H(10)	7892	1616	7102	73
H(12A)	6759	5421	5294	128
H(12B)	6948	5582	4302	128
H(12C)	8106	5439	4749	128
H(13A)	9239	3980	3960	123
H(13B)	8104	4155	3486	123
H(13C)	8584	3058	3951	123
H(15)	5882	3622	7023	76
H(16)	4003	4162	7912	102
H(17)	2285	3440	7976	99
H(18)	2435	2194	7134	96
H(19)	4286	1663	6228	80
H(21)	9150	-2171	5572	66
H(22)	8460	-3554	6443	77
H(24)	4905	-2104	6473	70
H(25)	5573	-731	5582	62
H(26A)	6562	-4514	6897	142
H(26B)	5259	-3800	7176	142
H(26C)	6349	-3916	7680	142

H(27A)	2063	3094	1610	60
H(27B)	2397	2909	655	60
H(30)	1750	2195	-268	65
H(31)	632	2103	-1277	79
H(32)	-1270	1574	-871	81
H(33)	-2049	1165	538	72
H(36A)	-671	1014	3094	68
H(36B)	330	383	2440	68
H(37A)	1025	1824	2707	63
H(37B)	-95	2559	2330	63
H(38A)	-2054	2676	2099	123
H(38B)	-2660	1886	2804	123
H(38C)	-2978	2062	1891	123
H(39A)	-2352	215	1759	128
H(39B)	-2026	-29	2672	128
H(39C)	-1016	-400	1895	128
H(41)	2141	145	653	91
H(42)	3943	-1110	699	128
H(43)	5402	-968	1467	114
H(44)	5038	415	2211	95
H(45)	3245	1653	2184	74
H(47)	2055	5872	1932	68
H(48)	3763	6643	1325	80
H(50)	3700	5900	-928	82
H(51)	1976	5146	-344	71
H(52A)	4738	7521	-585	149
H(52B)	5628	6433	-614	149
H(52C)	5396	7007	185	149
H(2)	549(19)	3801(17)	445(8)	63(7)

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H(1)	8712(14)	530(20)	5578(16)	90(9)
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Table 6. Torsion angles [deg] for shelxl.

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O(1)-S(1)-N(1)-C(1)	54.45(17)
O(2)-S(1)-N(1)-C(1)	-175.78(15)
C(20)-S(1)-N(1)-C(1)	-59.54(18)
O(4)-S(2)-N(2)-C(27)	-54.72(17)
O(3)-S(2)-N(2)-C(27)	176.59(14)
C(46)-S(2)-N(2)-C(27)	61.45(16)
S(1)-N(1)-C(1)-C(2)	-129.16(17)
N(1)-C(1)-C(2)-C(11)	-55.9(2)
N(1)-C(1)-C(2)-C(14)	-178.49(16)
N(1)-C(1)-C(2)-C(3)	64.4(2)
C(11)-C(2)-C(3)-C(4)	-48.2(2)
C(1)-C(2)-C(3)-C(4)	-169.50(16)
C(14)-C(2)-C(3)-C(4)	74.1(2)
C(2)-C(3)-C(4)-C(5)	65.3(2)
C(3)-C(4)-C(5)-C(6)	-45.0(2)
C(3)-C(4)-C(5)-C(13)	75.3(2)
C(3)-C(4)-C(5)-C(12)	-167.07(19)
C(13)-C(5)-C(6)-C(7)	73.4(3)
C(12)-C(5)-C(6)-C(7)	-46.4(3)
C(4)-C(5)-C(6)-C(7)	-165.91(19)
C(13)-C(5)-C(6)-C(11)	-107.3(2)
C(12)-C(5)-C(6)-C(11)	132.9(2)
C(4)-C(5)-C(6)-C(11)	13.4(3)
C(11)-C(6)-C(7)-C(8)	1.0(3)

C(5)-C(6)-C(7)-C(8)	-179.6(2)
C(6)-C(7)-C(8)-C(9)	-1.2(4)
C(7)-C(8)-C(9)-C(10)	-0.1(4)
C(8)-C(9)-C(10)-C(11)	1.5(4)
C(9)-C(10)-C(11)-C(6)	-1.6(3)
C(9)-C(10)-C(11)-C(2)	179.4(2)
C(7)-C(6)-C(11)-C(10)	0.3(3)
C(5)-C(6)-C(11)-C(10)	-179.00(19)
C(7)-C(6)-C(11)-C(2)	179.26(18)
C(5)-C(6)-C(11)-C(2)	-0.1(3)
C(1)-C(2)-C(11)-C(10)	-45.0(2)
C(14)-C(2)-C(11)-C(10)	75.4(2)
C(3)-C(2)-C(11)-C(10)	-164.09(18)
C(1)-C(2)-C(11)-C(6)	136.09(18)
C(14)-C(2)-C(11)-C(6)	-103.6(2)
C(3)-C(2)-C(11)-C(6)	17.0(2)
C(11)-C(2)-C(14)-C(15)	13.0(3)
C(1)-C(2)-C(14)-C(15)	135.4(2)
C(3)-C(2)-C(14)-C(15)	-108.1(2)
C(11)-C(2)-C(14)-C(19)	-170.80(18)
C(1)-C(2)-C(14)-C(19)	-48.4(2)
C(3)-C(2)-C(14)-C(19)	68.1(2)
C(19)-C(14)-C(15)-C(16)	0.8(3)
C(2)-C(14)-C(15)-C(16)	177.1(2)
C(14)-C(15)-C(16)-C(17)	0.2(4)
C(15)-C(16)-C(17)-C(18)	-0.6(4)
C(16)-C(17)-C(18)-C(19)	0.1(4)
C(17)-C(18)-C(19)-C(14)	0.9(4)
C(15)-C(14)-C(19)-C(18)	-1.3(3)

C(2)-C(14)-C(19)-C(18)	-177.8(2)
O(1)-S(1)-C(20)-C(21)	149.19(16)
O(2)-S(1)-C(20)-C(21)	18.67(19)
N(1)-S(1)-C(20)-C(21)	-95.70(17)
O(1)-S(1)-C(20)-C(25)	-31.11(18)
O(2)-S(1)-C(20)-C(25)	-161.62(15)
N(1)-S(1)-C(20)-C(25)	84.01(17)
C(25)-C(20)-C(21)-C(22)	-0.6(3)
S(1)-C(20)-C(21)-C(22)	179.13(16)
C(20)-C(21)-C(22)-C(23)	-0.2(3)
C(21)-C(22)-C(23)-C(24)	0.3(3)
C(21)-C(22)-C(23)-C(26)	-179.7(2)
C(22)-C(23)-C(24)-C(25)	0.4(3)
C(26)-C(23)-C(24)-C(25)	-179.6(2)
C(23)-C(24)-C(25)-C(20)	-1.2(3)
C(21)-C(20)-C(25)-C(24)	1.3(3)
S(1)-C(20)-C(25)-C(24)	-178.44(15)
S(2)-N(2)-C(27)-C(28)	137.63(15)
N(2)-C(27)-C(28)-C(29)	47.1(2)
N(2)-C(27)-C(28)-C(40)	169.18(16)
N(2)-C(27)-C(28)-C(37)	-72.6(2)
C(40)-C(28)-C(29)-C(30)	-73.0(2)
C(37)-C(28)-C(29)-C(30)	164.32(17)
C(27)-C(28)-C(29)-C(30)	46.2(2)
C(40)-C(28)-C(29)-C(34)	108.05(19)
C(37)-C(28)-C(29)-C(34)	-14.6(2)
C(27)-C(28)-C(29)-C(34)	-132.75(18)
C(34)-C(29)-C(30)-C(31)	1.6(3)
C(28)-C(29)-C(30)-C(31)	-177.45(19)

C(29)-C(30)-C(31)-C(32)	-1.1(3)
C(30)-C(31)-C(32)-C(33)	0.3(4)
C(31)-C(32)-C(33)-C(34)	0.0(4)
C(30)-C(29)-C(34)-C(33)	-1.2(3)
C(28)-C(29)-C(34)-C(33)	177.77(18)
C(30)-C(29)-C(34)-C(35)	-179.67(18)
C(28)-C(29)-C(34)-C(35)	-0.7(3)
C(32)-C(33)-C(34)-C(29)	0.4(3)
C(32)-C(33)-C(34)-C(35)	179.0(2)
C(29)-C(34)-C(35)-C(36)	-14.8(3)
C(33)-C(34)-C(35)-C(36)	166.77(18)
C(29)-C(34)-C(35)-C(38)	106.1(2)
C(33)-C(34)-C(35)-C(38)	-72.4(2)
C(29)-C(34)-C(35)-C(39)	-133.8(2)
C(33)-C(34)-C(35)-C(39)	47.7(3)
C(38)-C(35)-C(36)-C(37)	-73.9(2)
C(34)-C(35)-C(36)-C(37)	46.8(2)
C(39)-C(35)-C(36)-C(37)	167.76(18)
C(35)-C(36)-C(37)-C(28)	-65.3(2)
C(29)-C(28)-C(37)-C(36)	45.9(2)
C(40)-C(28)-C(37)-C(36)	-78.1(2)
C(27)-C(28)-C(37)-C(36)	165.39(16)
C(29)-C(28)-C(40)-C(41)	-7.4(3)
C(37)-C(28)-C(40)-C(41)	115.5(2)
C(27)-C(28)-C(40)-C(41)	-127.9(2)
C(29)-C(28)-C(40)-C(45)	173.14(17)
C(37)-C(28)-C(40)-C(45)	-64.0(2)
C(27)-C(28)-C(40)-C(45)	52.6(2)
C(45)-C(40)-C(41)-C(42)	-0.4(4)



C(28)-C(40)-C(41)-C(42)	-179.9(2)
C(40)-C(41)-C(42)-C(43)	-0.3(5)
C(41)-C(42)-C(43)-C(44)	0.7(5)
C(42)-C(43)-C(44)-C(45)	-0.3(4)
C(43)-C(44)-C(45)-C(40)	-0.5(4)
C(41)-C(40)-C(45)-C(44)	0.8(3)
C(28)-C(40)-C(45)-C(44)	-179.69(19)
O(4)-S(2)-C(46)-C(51)	164.27(16)
O(3)-S(2)-C(46)-C(51)	-66.04(18)
N(2)-S(2)-C(46)-C(51)	47.03(19)
O(4)-S(2)-C(46)-C(47)	-18.62(18)
O(3)-S(2)-C(46)-C(47)	111.07(16)
N(2)-S(2)-C(46)-C(47)	-135.86(16)
C(51)-C(46)-C(47)-C(48)	0.0(3)
S(2)-C(46)-C(47)-C(48)	-177.06(16)
C(46)-C(47)-C(48)-C(49)	-0.1(3)
C(47)-C(48)-C(49)-C(50)	-0.4(3)
C(47)-C(48)-C(49)-C(52)	179.4(2)
C(48)-C(49)-C(50)-C(51)	0.9(3)
C(52)-C(49)-C(50)-C(51)	-178.9(2)
C(47)-C(46)-C(51)-C(50)	0.5(3)
S(2)-C(46)-C(51)-C(50)	177.54(17)
C(49)-C(50)-C(51)-C(46)	-0.9(3)

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Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for shelxl [A and deg.].

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D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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N(2)-H(2)...O(3)#1	0.886(9)	2.293(13)	3.114(2)	154.2(19)
N(1)-H(1)...O(2)#2	0.886(10)	2.277(12)	3.139(2)	164(2)

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Symmetry transformations used to generate equivalent atoms:

#1  $-x, -y+1, -z$     #2  $-x+2, -y, -z+1$