

Supplementary Material
**Novel synthesis of quinazolino[3,2-*a*][1,5]benzodiazepines:
an experimental and computational study**

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Gytis Vektaris,^b and Kazimieras Algirdas Klimavicius^a**

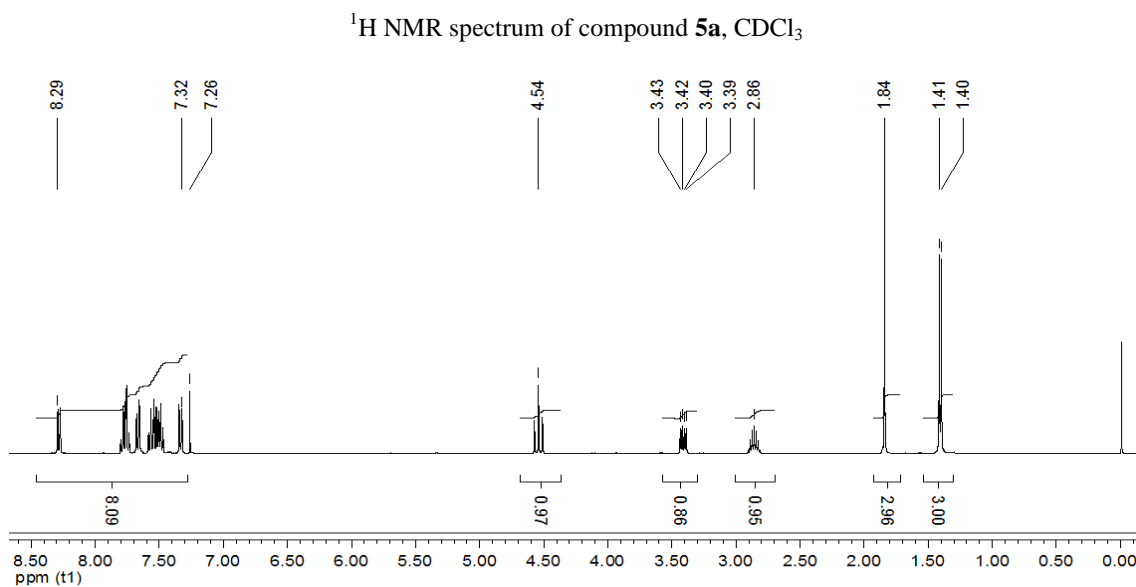
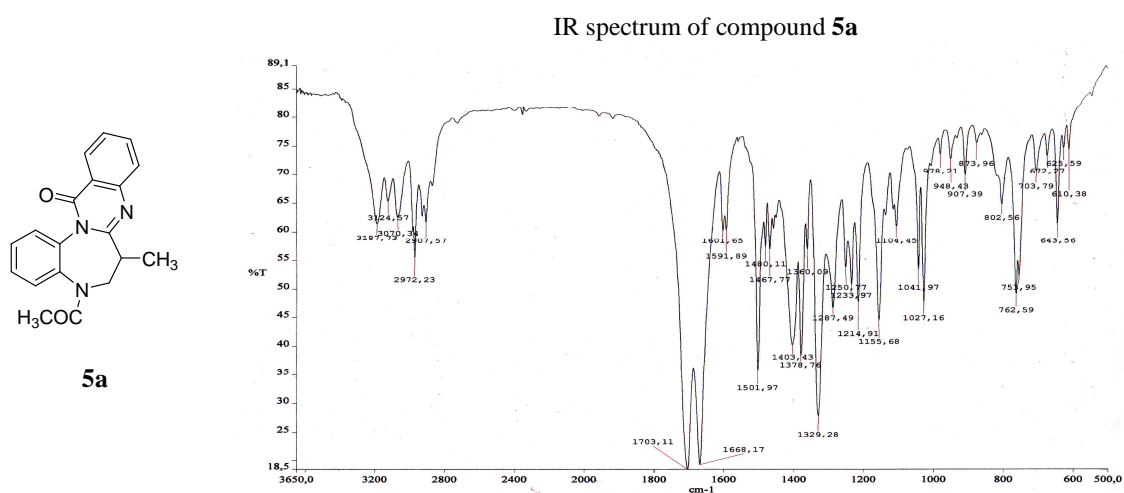
^a *Vilnius University Institute of Biochemistry, Mokslininku 12, LT-08662 Vilnius, Lithuania*

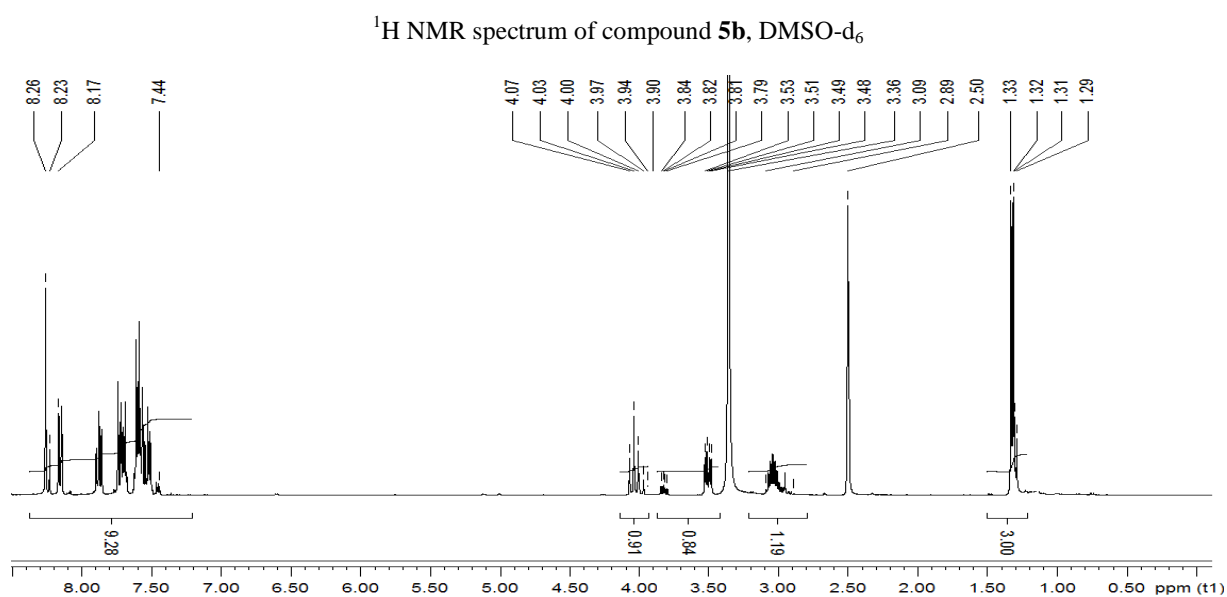
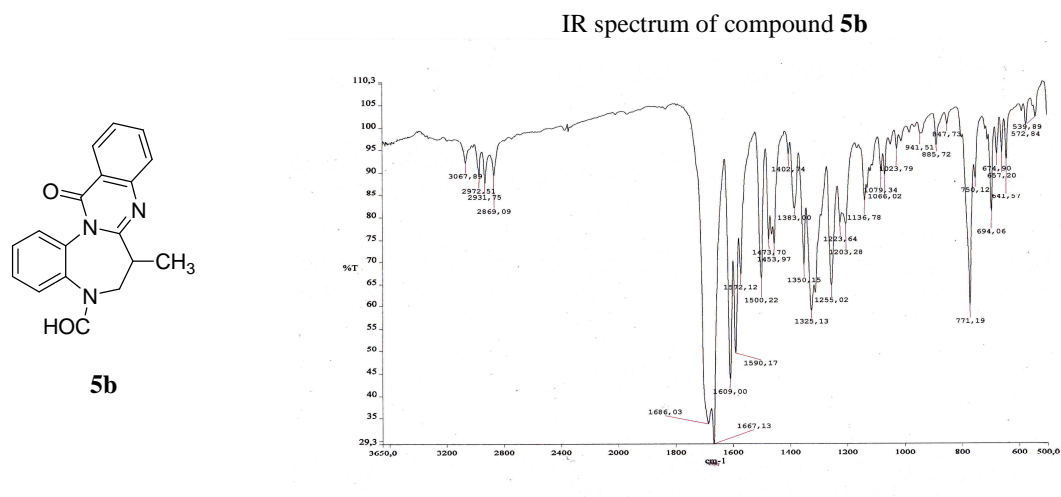
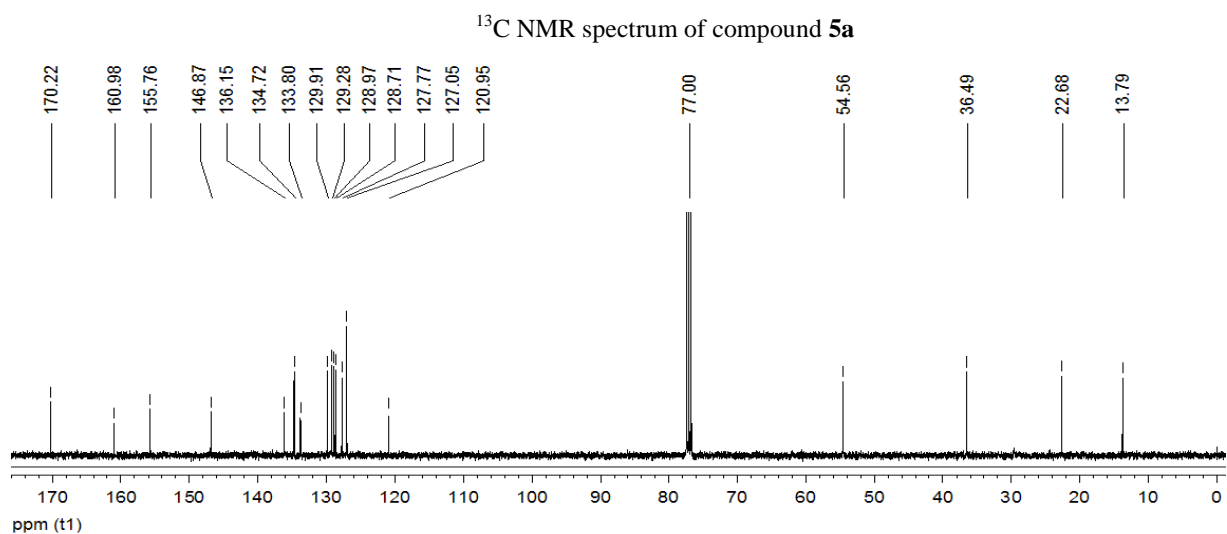
^b *Vilnius University Institute of Theoretical Physics and Astronomy, A. Gostauto 12,
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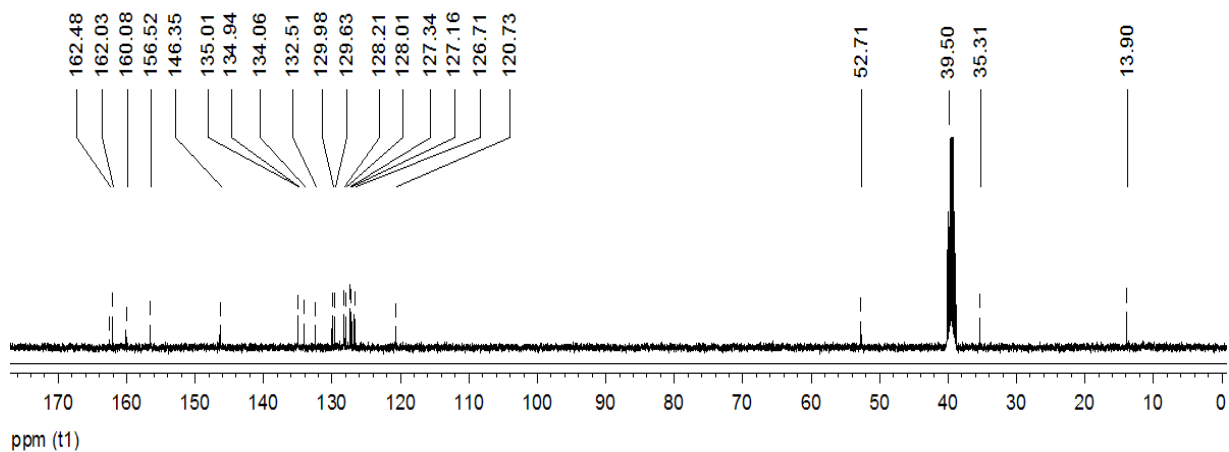
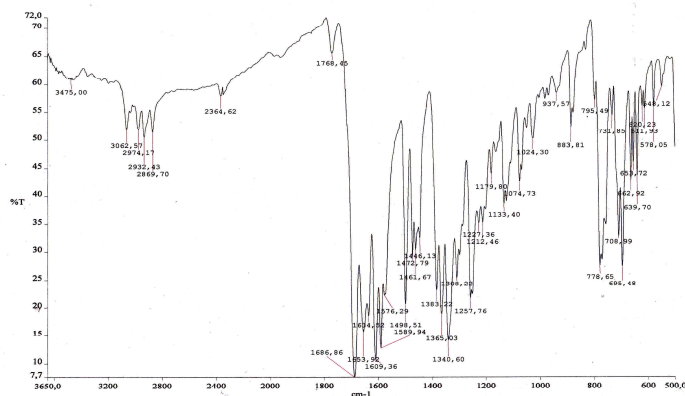
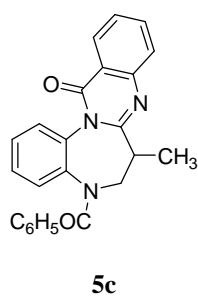
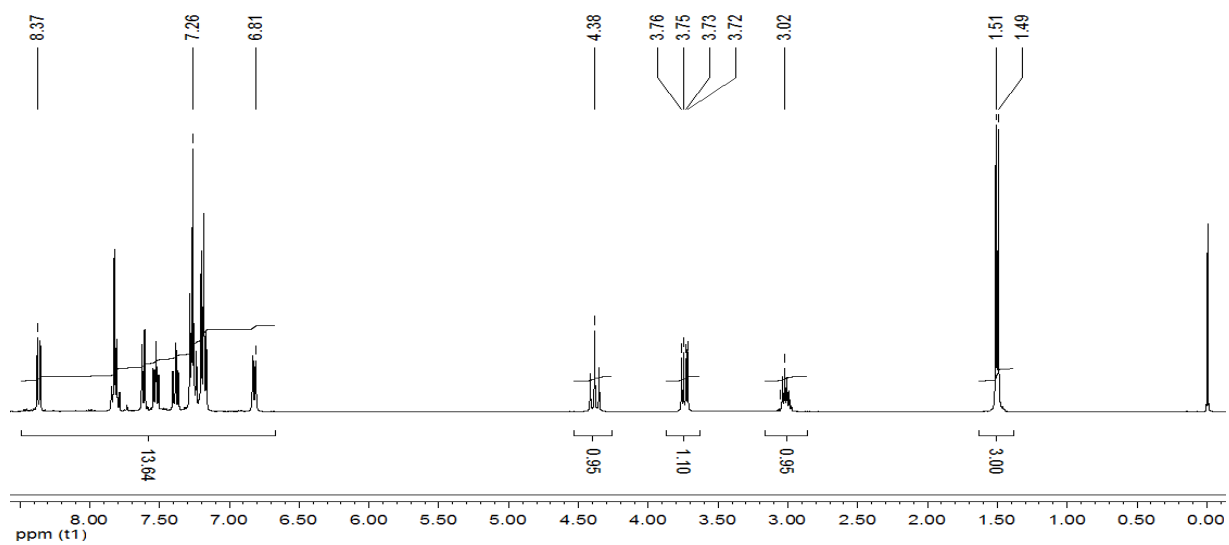
E-mail: gema.mikulskiene@bchi.vu.lt

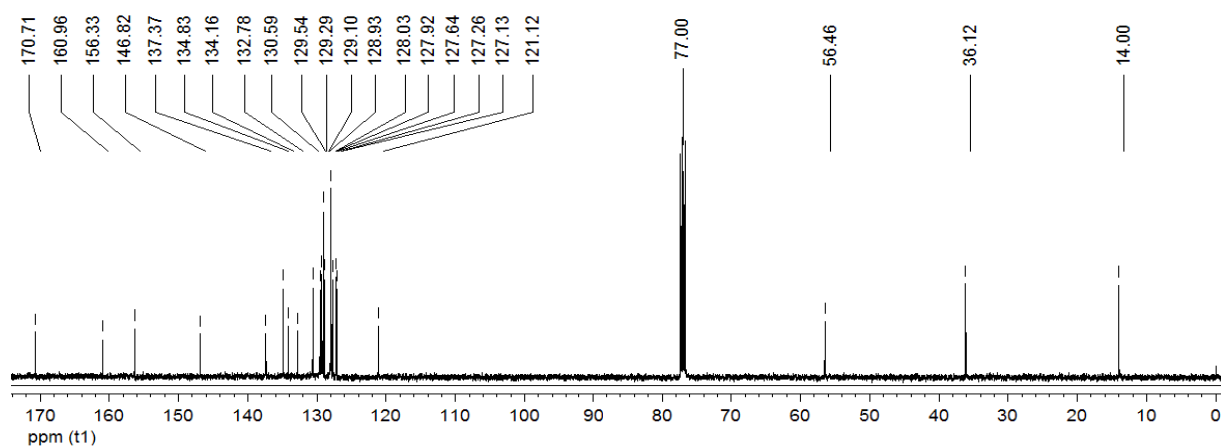
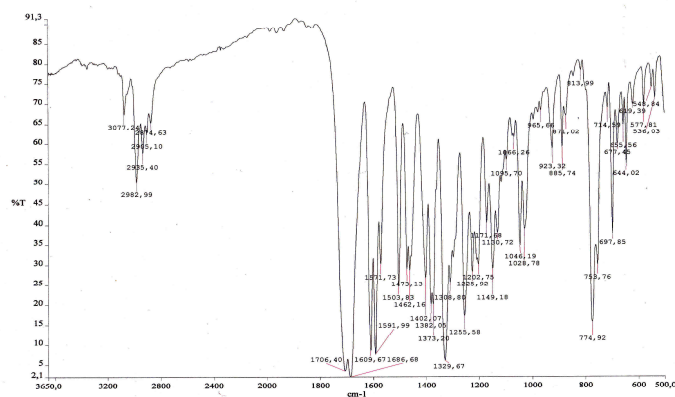
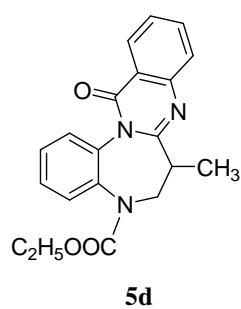
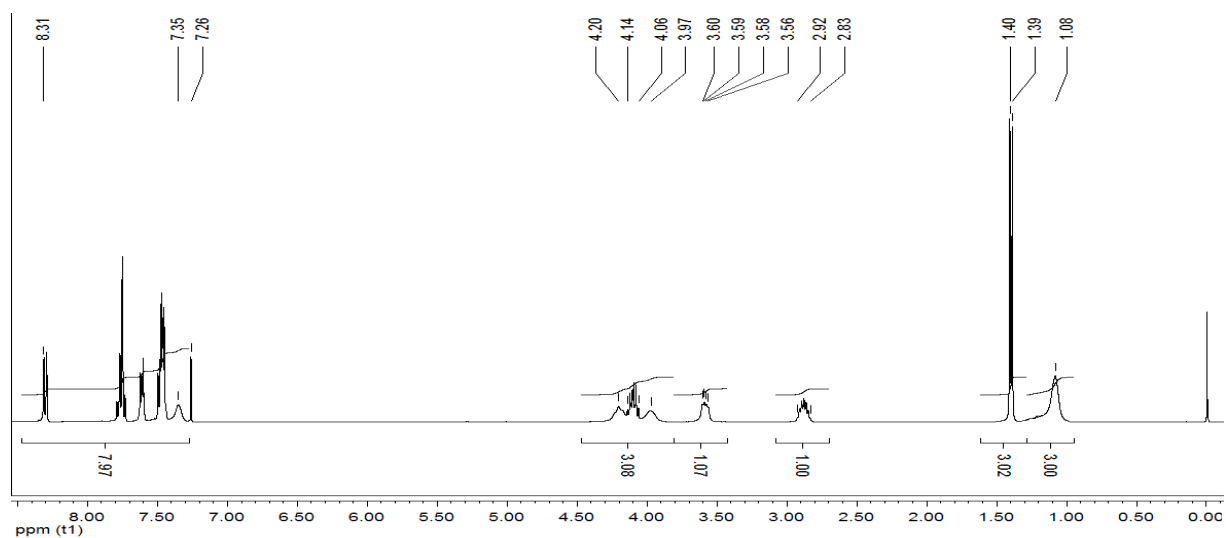
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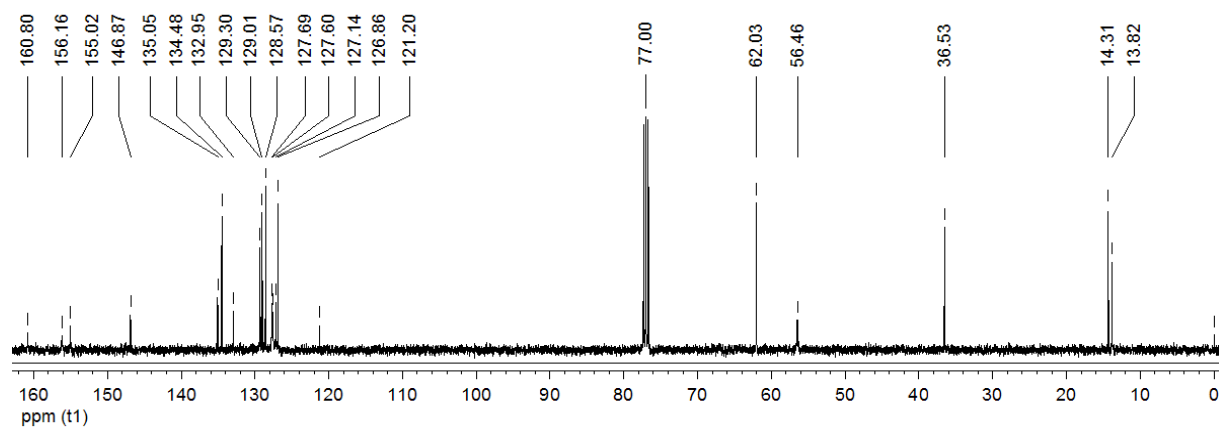
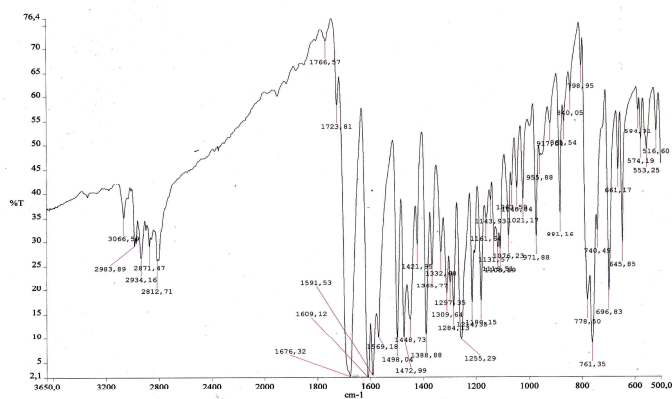
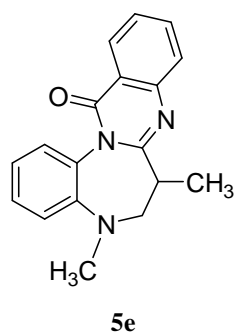
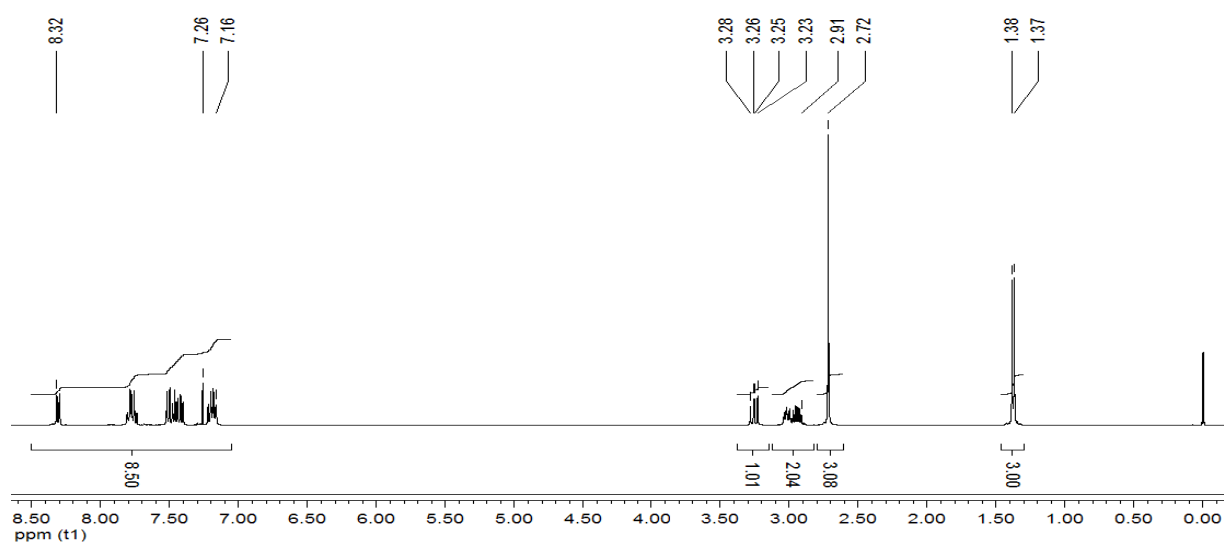
Copies of IR, ¹ H, ¹³ C NMR spectra	S2-S10 pages
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Cartesian coordinates	S13-S20 pages

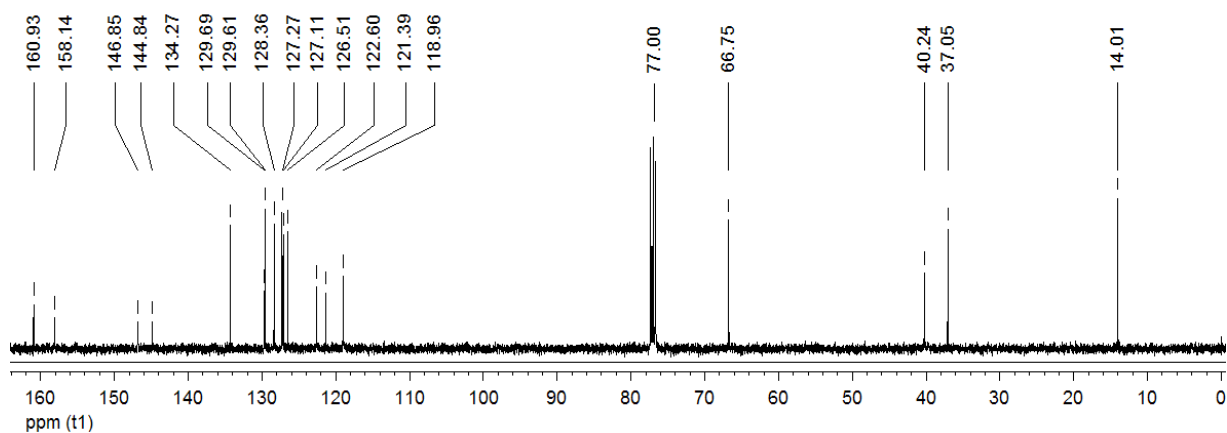
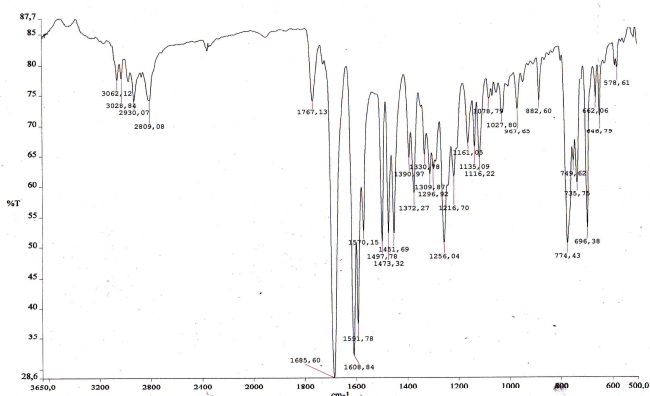
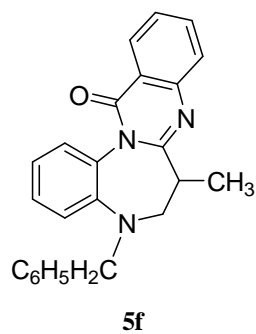
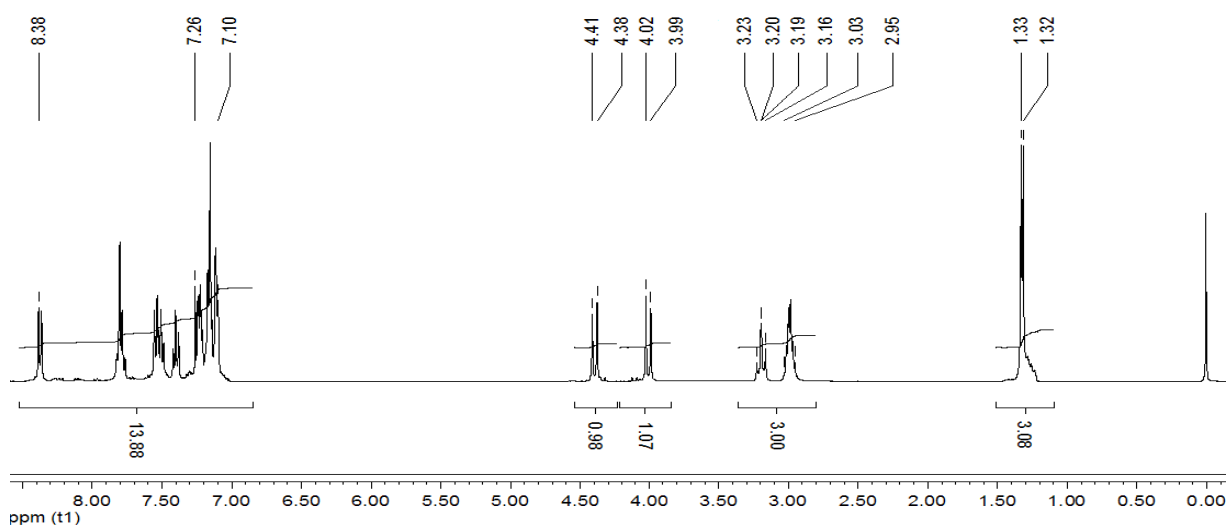
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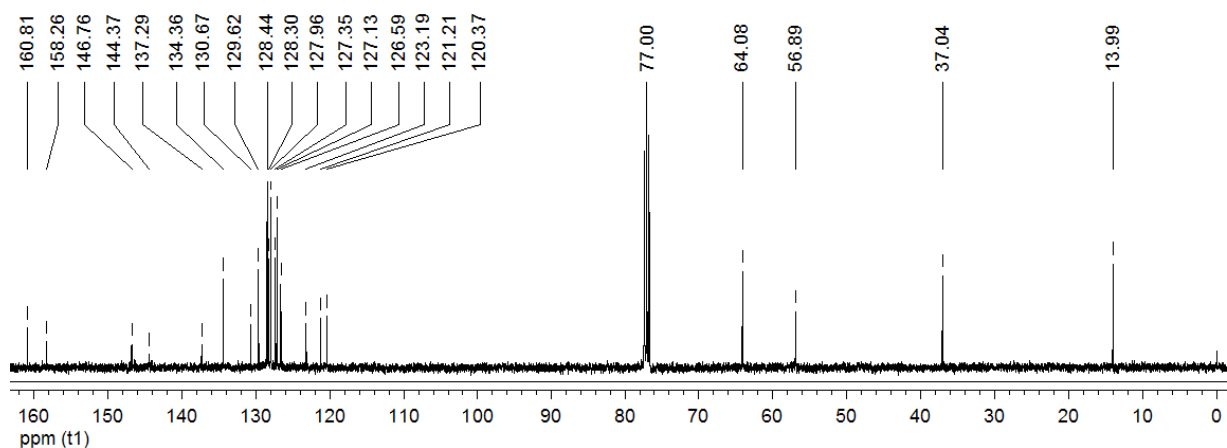
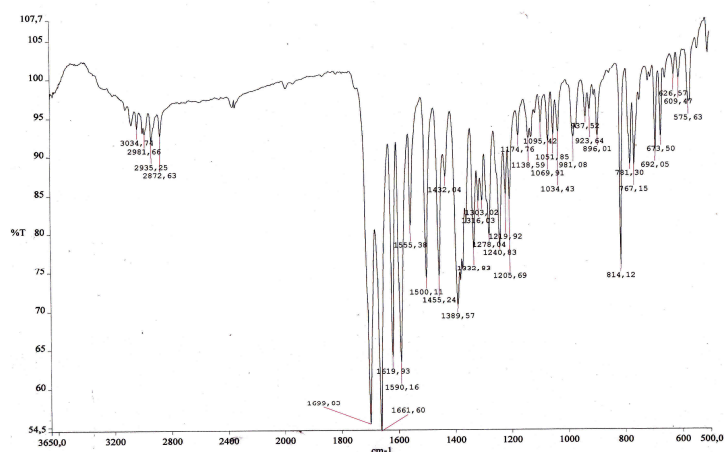
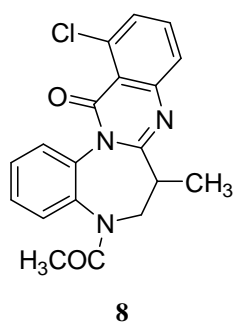
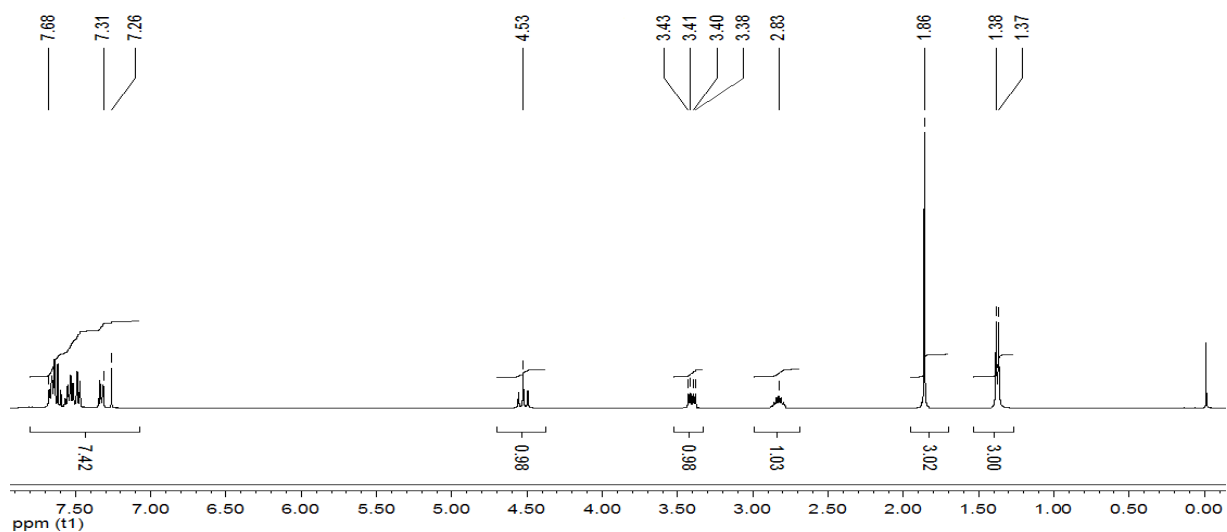


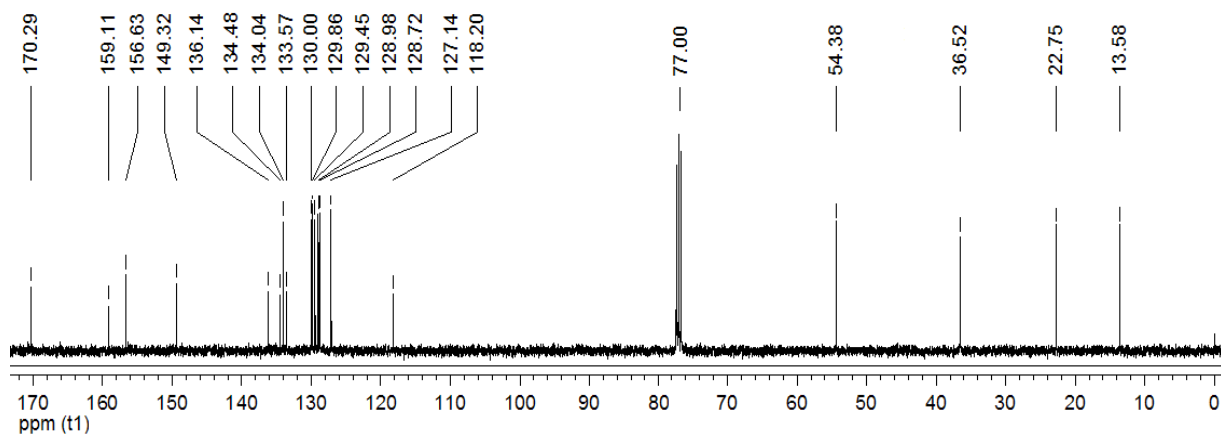
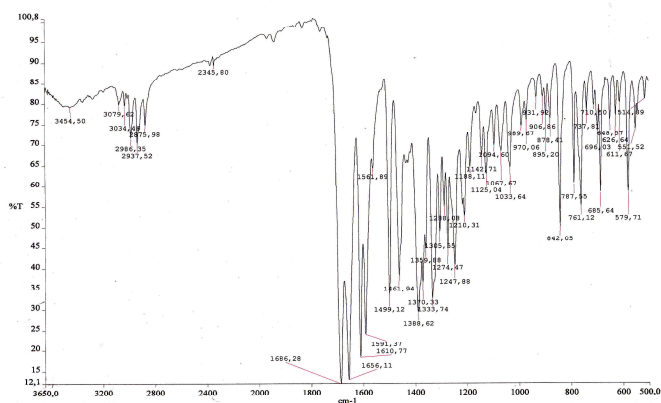
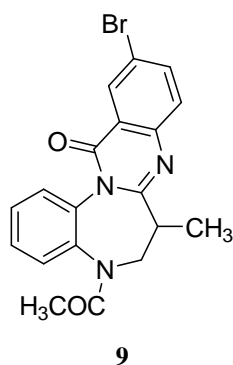
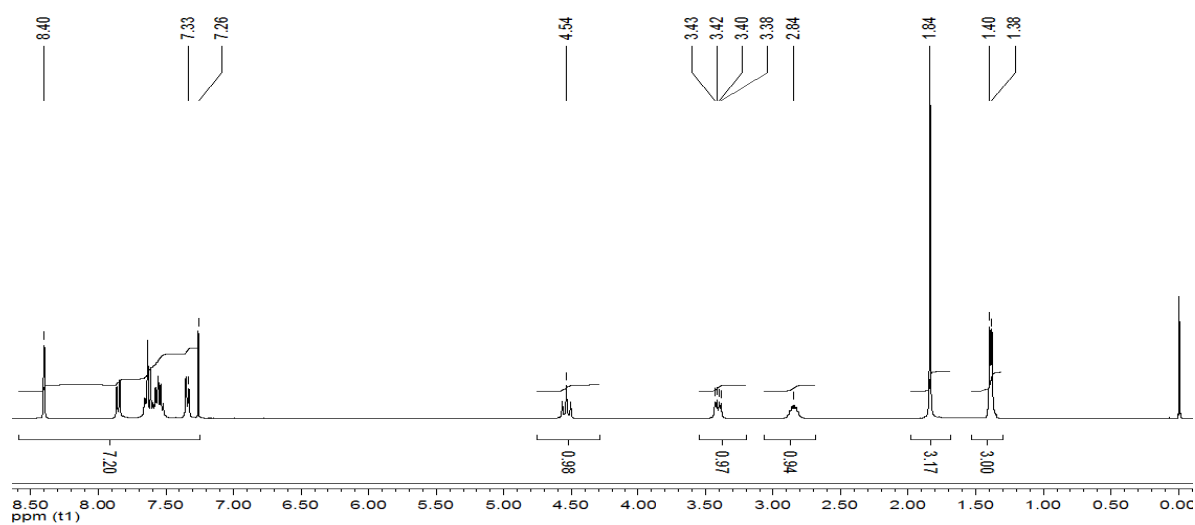
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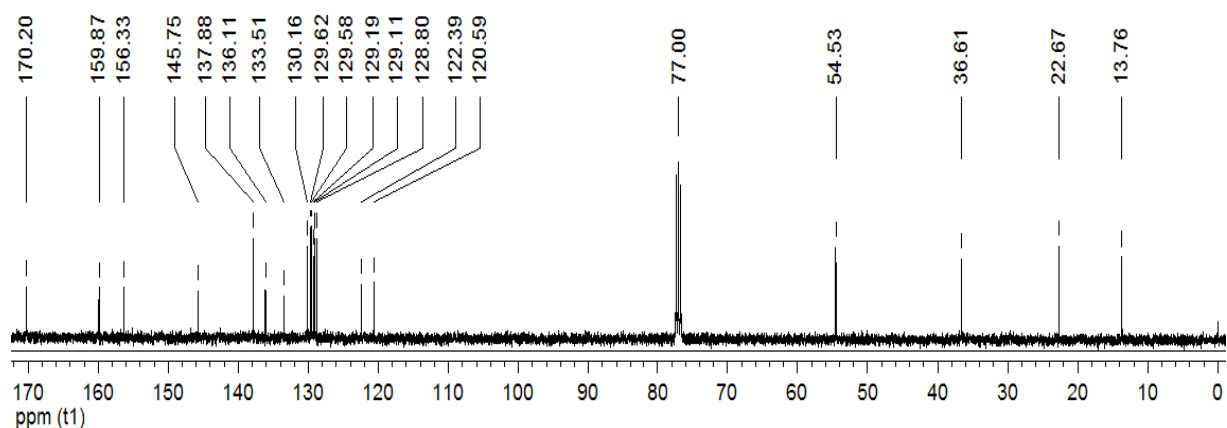
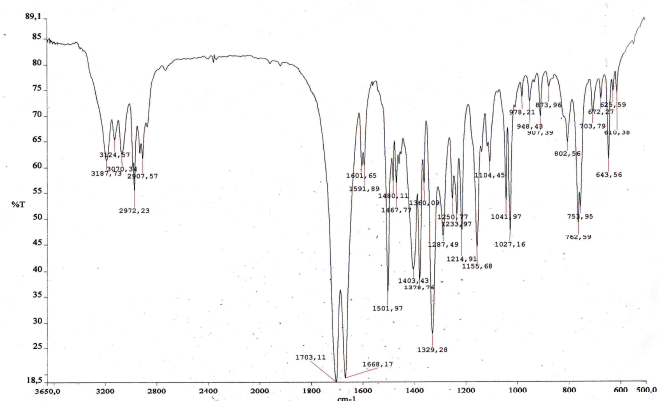
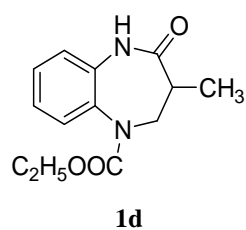
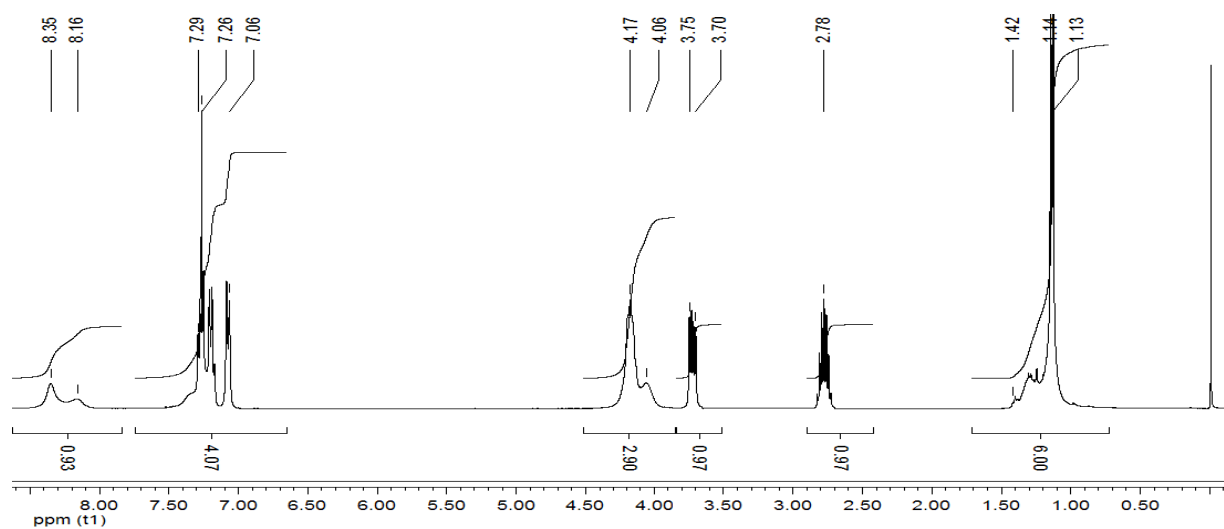
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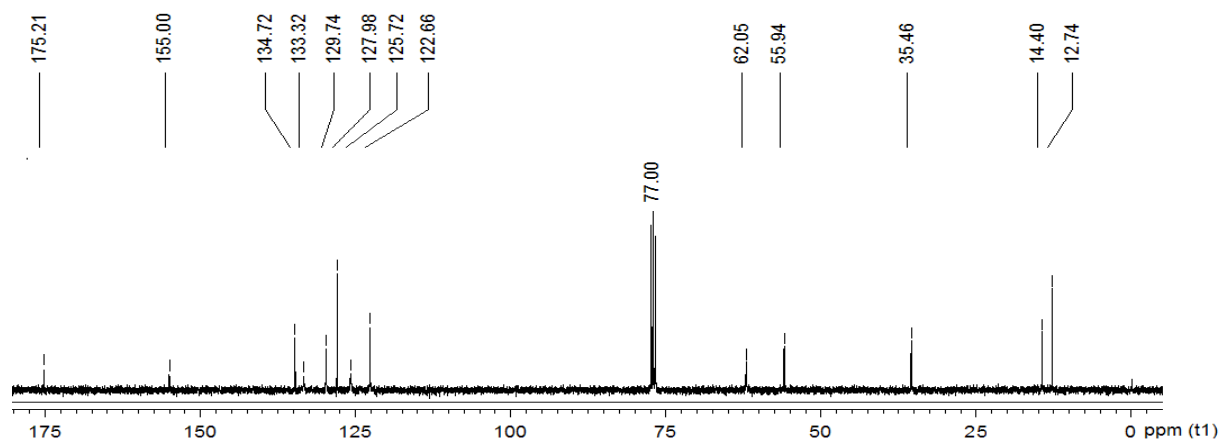
^{13}C NMR spectrum of compound **5d**IR spectrum of compound **5e** ^1H NMR spectrum of compound **5e**, CDCl_3 

^{13}C NMR spectrum of compound **5e**IR spectrum of compound **5f** ^1H NMR spectrum of compound **5f**, CDCl_3 

^{13}C NMR spectrum of compound **5f**IR spectrum of compound **8** ^1H NMR spectrum of compound **8**, CDCl_3 

^{13}C NMR spectrum of compound **8**IR spectrum of compound **9** ^1H NMR spectrum of compound **9**, CDCl_3 

^{13}C NMR spectrum of compound **9**IR spectrum of compound **1d** ^1H NMR spectrum of compound **1d**, CDCl₃

^{13}C NMR spectrum of compound **1d**

Tabulations of computational data

Table S1. B3LYP/6-31+G(d,p) calculated ΔG_{rel} for **T**, **I**, and **P** for acylation-cyclization reaction of **1e** with **4**

Structure	ΔG_{rel} (gas phase), kcal/mol	ΔG_{rel} (solvent), kcal/mol
R	0	0
T1	41.13	32.17
I1	-1.63	0.32
T2	43.84	38.50
I2	17.33	15.20
T3	24.75	23.88
P	-18.24	-14.06
T1'	61.49	42.09
I1'	39.76	32.25
T1''	47.94	39.67
I1''	38.88	32.35

Table S2. B3LYP/6-31+G(d,p) calculated total energies (E) with Zero-point energy corrections, Gibbs free energies (G) and imaginary frequencies (ν_i) of **T**, **R**, **I**, and **P** for acylation-cyclization reaction of **1e** with **4**

Structure	E (gas phase), a.u.	G (gas phase), a.u.	G (solvent), a.u.	ν_i , cm^{-1}
R	-1944.7519	-1944.8285	-1945.1024	
T1	-1944.7069	-1944.7630	-1945.0511	i-172.77
T1'	-1944.6813	-1944.7305	-1945.0353	i-52.53
T1''	-1944.6990	-1944.7521	-1945.0392	i-263.2
I1	-1944.7729	-1944.8311	-1945.1016	
I1'	-1944.7129	-1944.7652	-1945.0510	
I1''	-1944.7132	-1944.7666	-1945.0508	
T2	-1944.6925	-1944.7586	-1945.0410	i-502.74
I2	-1944.7347	-1944.8009	-1945.0781	
T3	-1944.7225	-1944.7891	-1945.0643	i-459.39
P	-1944.7863	-1944.8576	-1945.1248	

Table S3. B3LYP/6-31+G(d,p) calculated NPA charges on selected atoms of reaction stationary points for acylation-cyclization reaction of **1e** with **4**

Structure	Unit 4					N(1)	Unit 1e	
	C(1')=O(1')		N(2')=S(2')=O(2')				C(2)=O(2')	
	C(1')	O(1')	N(2')	S(2')	O(2')		C(2)	O(2')
R	+0.55	-0.49	-0.70	+1.38	-0.81	-0.60	+0.70	-0.63
T1	+0.80	-0.40	-0.87	+1.44	-0.87	-0.65	+0.74	-0.50
I1	+0.74	-0.58	-0.74	+1.35	-0.86	-0.51	+0.74	-0.58
T2	+0.72	-0.53	-0.83	+1.58	-0.85	-0.49	+0.69	-0.74
I2	+0.69	-0.60	-0.69	+1.61	-0.85	-0.53	+0.68	-0.69
T3	+0.71	-0.56	-0.67	+1.61	-0.86	-0.48	+0.61	-0.84
P	+0.68	-0.60	-0.53	+1.62	-0.83	-0.46	+0.52	-0.84

Table S4. B3LYP/6-31+G(d,p) calculated selected BD (Å) of reaction stationary points for acylation-cyclization reaction of **1e** with **4**

	Unit 4			Bonds between 4 and 1e			Unit 1e	
	C(1)=O(1')	N(2')=S(2')	S(2')=O(2')	C(1')-N(1)	C(2)-N(2')	S(2')-O(2')	N(1)-C(2)	C(2)=O(2')
R	1.20	1.56	1.48	-	-	-	1.37	1.23
T1	1.17	1.60	1.49	1.95	3.76	4.50	1.47	1.21
I1	1.23	1.80	1.47	1.39	1.46	1.73	1.47	1.44
T2	1.21	1.66	1.48	1.46	2.03	1.93	1.36	1.35
I2	1.23	1.79	1.47	1.39	1.46	1.73	1.47	1.73
T3	1.22	1.95	1.48	1.44	1.42	1.60	1.37	1.82
P	1.22	2.84	1.47	1.43	1.30	1.47	1.39	3.77

Table S5. B3LYP/6-31+G(d,p) calculated Wiberg BI for selected bonds of reaction stationary points for acylation-cyclization reaction of **1e** with **4**

	Unit 4			Bonds between 4 and 1e			Unit 1e	
	C(1)=O(1')	N(2')=S(2')	S(2')=O(2')	C(1')-N(1)	C(2)-N(2')	S(2')-O(2')	N(1)-C(2)	C(2)=O(2')
R	1.86	1.47	1.42	-	-	-	1.01	1.13
T1	2.05	1.20	1.35	0.41	0.00	0.00	0.92	1.86
I1	1.68	1.50	1.34	1.05	0.00	0.00	1.03	1.75
T2	1.17	0.81	0.98	0.84	0.36	0.33	1.05	0.90
I2	1.66	0.74	1.45	1.10	0.96	0.72	0.92	0.90
T3	1.73	0.55	1.43	0.96	1.08	0.94	1.18	0.47
P	1.68	0.07	1.48	1.00	1.59	1.46	1.14	0.00

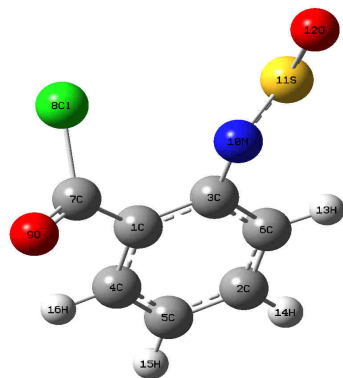
Cartesian coordinates, optimized geometries, total energies (a.u) of stationary points from Gaussian03 output file for acylation-cyclization reaction of **1e** with **4**

HCl

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Reactant 4

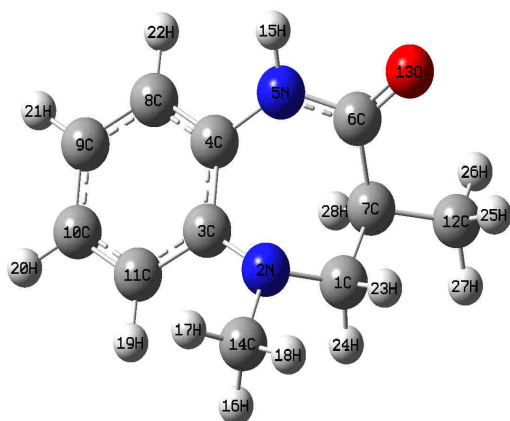


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3	6	0	-0.082133	-0.748083	0.188236
4	6	0	-2.481435	-0.411072	-0.081224
5	6	0	-2.670250	-1.780532	-0.263274
6	6	0	-0.294982	-2.131762	0.033950
7	6	0	-1.134402	1.600037	0.284452
8	17	0	0.185750	2.424845	-0.635825
9	8	0	-1.931007	2.258264	0.885945
10	7	0	1.172574	-0.224929	0.532450
11	16	0	2.454349	-0.735480	-0.190297
12	8	0	3.697698	-0.196987	0.401986
13	1	0	0.542661	-2.810940	0.157170
14	1	0	-1.705479	-3.710336	-0.319301
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Reactant 1e

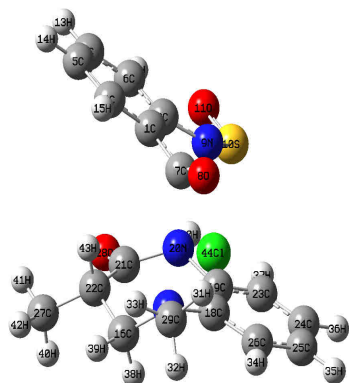


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4	6	0	-0.782363	-0.904190	-0.251729
5	7	0	0.440444	-1.424193	-0.736382
6	6	0	1.709312	-1.027030	-0.390710
7	6	0	1.781080	-0.001044	0.740071
8	6	0	-1.831486	-1.787556	0.022035
9	6	0	-3.084073	-1.315992	0.418045
10	6	0	-3.280368	0.057270	0.566388
11	6	0	-2.233550	0.946260	0.312027
12	6	0	3.190575	0.079002	1.333513
13	8	0	2.695796	-1.509709	-0.937674
14	6	0	-0.329873	2.729860	-0.883356
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20	1	0	-4.244532	0.442835	0.884385
21	1	0	-3.890205	-2.015769	0.614629
22	1	0	-1.657022	-2.854226	-0.091739
23	1	0	2.092763	1.803993	-0.399844
24	1	0	1.240445	2.046275	1.135038
25	1	0	3.922419	0.345674	0.566553
26	1	0	3.491616	-0.884424	1.752642
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Transition state T1

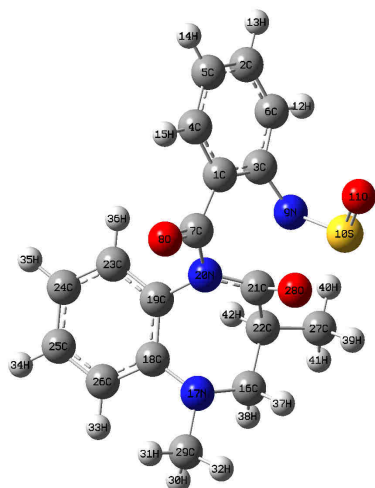


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4	6	0	1.418225	-2.798416	-1.307737
5	6	0	2.627187	-3.400605	-0.996869
6	6	0	3.588708	-1.229128	-0.398621
7	6	0	0.012529	-0.793545	-1.391345
8	8	0	-0.832111	-0.732917	-2.195376
9	7	0	2.121066	0.770244	-0.794683
10	16	0	3.038962	1.989795	-0.323134
11	8	0	4.408798	1.614967	0.128446
12	1	0	4.426718	-0.636961	-0.056497
13	1	0	4.636219	-3.084350	-0.277676
14	1	0	2.746899	-4.472987	-1.108200
15	1	0	0.573255	-3.382792	-1.659137
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19	6	0	-1.672782	0.989280	-0.077647
20	7	0	-0.546389	0.130337	0.237118
21	6	0	-0.520583	-0.852482	1.335848
22	6	0	-1.623279	-1.890462	1.444438
23	6	0	-1.384980	2.353254	-0.212163
24	6	0	-2.353766	3.238138	-0.678011
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38	1	0	-3.298330	-0.587899	1.926326
39	1	0	-3.728806	-2.195915	1.356562
40	1	0	-1.757630	-1.947320	3.621086
41	1	0	-0.528545	-3.021003	2.953327
42	1	0	-2.246740	-3.449943	2.812964
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44	17	0	1.727246	2.594653	1.723687

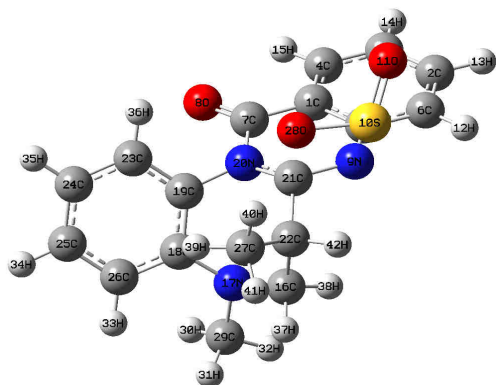
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Number of imaginary frequencies = 1

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			X	Y	Z
1	6	0	1.916411	1.106812	0.478633
2	6	0	4.299843	1.639019	-0.898023
3	6	0	2.342710	0.230548	-0.555509
4	6	0	2.717363	2.211645	0.827670
5	6	0	3.903152	2.474603	0.154980
6	6	0	3.526534	0.536743	-1.248309
7	6	0	0.579864	1.044617	1.111714
8	8	0	0.223013	1.714770	2.055101
9	7	0	1.666918	-0.967002	-0.881002
10	16	0	2.005057	-2.271149	0.086538
11	8	0	3.126574	-2.056814	1.023471
12	1	0	3.835069	-0.131032	-2.045944
13	1	0	5.220299	1.842501	-1.437800
14	1	0	4.510452	3.329183	0.436482
15	1	0	2.370053	2.860645	1.624660
16	6	0	-2.416629	-1.983065	-0.166232
17	7	0	-2.963927	-0.857321	0.600147
18	6	0	-2.847712	0.428989	0.040959
19	6	0	-1.561002	0.995854	-0.121629
20	7	0	-0.407117	0.284654	0.345837
21	6	0	-0.142581	-1.013074	0.042687
22	6	0	-1.113671	-1.671669	-0.930016
23	6	0	-1.407580	2.273965	-0.664581
24	6	0	-2.522772	3.032961	-1.016740
25	6	0	-3.799644	2.499267	-0.833799
26	6	0	-3.958199	1.210425	-0.322702
27	6	0	-0.611915	-2.957827	-1.596830
28	8	0	0.411756	-1.743441	1.032553
29	6	0	-4.220880	-1.202209	1.249243

30	1	0	-5.034777	-1.427158	0.537233
31	1	0	-4.538497	-0.387630	1.903869
32	1	0	-4.060684	-2.092048	1.865698
33	1	0	-4.956206	0.803918	-0.203919
34	1	0	-4.677879	3.079568	-1.101020
35	1	0	-2.392183	4.030012	-1.424415
36	1	0	-0.409888	2.682840	-0.787716
37	1	0	-2.226473	-2.800944	0.538188
38	1	0	-3.156030	-2.346326	-0.904650
39	1	0	-0.350072	-3.722888	-0.860122
40	1	0	0.255516	-2.759131	-2.228832
41	0	0	-1.406007	-3.364803	-2.231079
42	1	0	-1.325225	-0.942377	-1.718216

Transition state T3

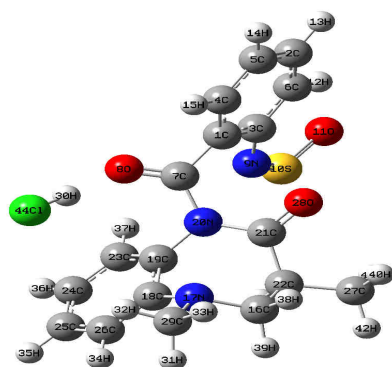
Energy = -1484.2517931 a.u.

Number of imaginary frequencies = 1

Center number	Atomic number	Atomic type	Coordinates, Å		
			X	Y	Z
1	6	0	1.822579	-1.430815	-0.123719
2	6	0	4.371897	-1.371524	0.995950
3	6	0	2.273257	-0.268369	0.524437
4	6	0	2.645560	-2.566306	-0.194340
5	6	0	3.920170	-2.537425	0.356312
6	6	0	3.559079	-0.247482	1.089150
7	6	0	0.461491	-1.479996	-0.669612
8	8	0	-0.015849	-2.441315	-1.243322
9	7	0	1.473371	0.874262	0.590859
10	16	0	2.036799	2.304240	-0.604737
11	8	0	3.212276	1.834682	-1.363747
12	1	0	3.904824	0.650574	1.590255
13	1	0	5.366817	-1.345160	1.430766
14	1	0	4.560806	-3.411322	0.297692
15	1	0	2.257997	-3.452671	-0.685168
16	6	0	-1.388771	1.053459	2.015527
17	7	0	-2.110277	-0.202726	1.747439
18	6	0	-2.639530	-0.440709	0.467602
19	6	0	-1.770135	-0.458481	-0.643921
20	7	0	-0.351819	-0.321540	-0.410267
21	6	0	0.158098	0.861867	0.051606
22	6	0	-0.805998	1.799398	0.794268
23	6	0	-2.243697	-0.664509	-1.936193
24	6	0	-3.602450	-0.900244	-2.152730
25	6	0	-4.473303	-0.927310	-1.061875
26	6	0	-4.003247	-0.690259	0.231295
27	6	0	-1.845125	2.583174	-0.030664
28	8	0	0.667305	1.920631	-1.331774

29	6	0	-2.879651	-0.643254	2.900646
30	1	0	-3.250891	-1.657768	2.738039
31	1	0	-3.733910	0.016460	3.134490
32	1	0	-2.221708	-0.658779	3.775625
33	1	0	-4.702075	-0.683987	1.060045
34	1	0	-5.531656	-1.118049	-1.215161
35	1	0	-3.969736	-1.074285	-3.158665
36	1	0	-1.540297	-0.667342	-2.760816
37	1	0	-2.062703	1.766847	2.521605
38	1	0	-0.576433	0.828061	2.717527
39	1	0	-2.627688	1.964426	-0.467786
40	1	0	-1.346056	3.122817	-0.836584
41	1	0	-2.324485	3.312269	0.631686
42	1	0	-0.141712	2.550820	1.234314

Intermediate II



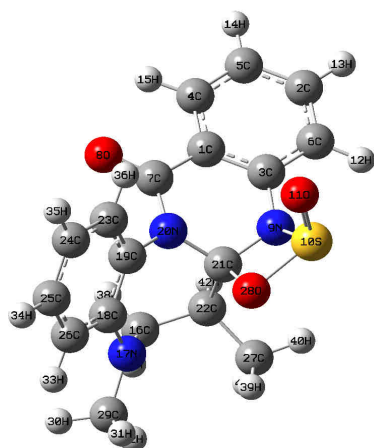
Energy = -1945.1071451 a.u.

Number of imaginary frequencies = 0

Center number	Atomic number	Atomic type	Coordinates, Å		
			X	Y	Z
1	6	0	-1.757248	1.311492	-0.330843
2	6	0	-4.392650	1.884900	-1.097067
3	6	0	-2.821909	0.489193	0.121941
4	6	0	-2.034562	2.429680	-1.117601
5	6	0	-3.342586	2.707947	-1.516135
6	6	0	-4.143826	0.790511	-0.274117
7	6	0	-0.340859	1.117887	0.117538
8	8	0	0.234553	2.048398	0.673925
9	7	0	-2.482778	-0.559364	0.969402
10	16	0	-3.339970	-1.648235	1.663163
11	8	0	-4.821530	-1.673921	1.456725
12	1	0	-4.955898	0.166240	0.076433
13	1	0	-5.411616	2.103661	-1.401124
14	1	0	-3.541453	3.569182	-2.146421
15	1	0	-1.217027	3.071813	-1.427151
16	6	0	2.168306	-1.874241	-1.886008
17	7	0	2.789527	-0.691303	-1.274150
18	6	0	2.717750	-0.637067	0.139589
19	6	0	1.466391	-0.387796	0.740444
20	7	0	0.308824	-0.115122	-0.078436
21	6	0	-0.031036	-0.964976	-1.157314
22	6	0	0.801806	-2.237615	-1.268135
23	6	0	1.331960	-0.363617	2.129777
24	6	0	2.447408	-0.539233	2.947687
25	6	0	3.699251	-0.750968	2.366372
26	6	0	3.830052	-0.812720	0.978550
27	6	0	0.088729	-3.301740	-2.107954

28	8	0	-0.897776	-0.673289	-1.961084
29	6	0	4.071568	-0.361795	-1.885990
30	1	0	1.959509	2.753441	0.565645
31	1	0	4.827635	-1.159433	-1.777920
32	1	0	4.460130	0.561086	-1.450155
33	1	0	3.913612	-0.195024	-2.956100
34	1	0	4.805257	-0.994591	0.541007
35	1	0	4.577092	-0.879465	2.992653
36	1	0	2.338951	-0.501013	4.026779
37	1	0	0.354504	-0.177401	2.561937
38	1	0	2.028809	-1.658813	-2.952008
39	1	0	2.830333	-2.757328	-1.810432
40	1	0	-0.148979	-2.922056	-3.104603
41	1	0	-0.848766	-3.608508	-1.636209
42	1	0	0.725204	-4.186848	-2.208155
43	1	0	0.970550	-2.629566	-0.259035
44	17	0	3.105260	3.339316	0.333859

Intermediate I2

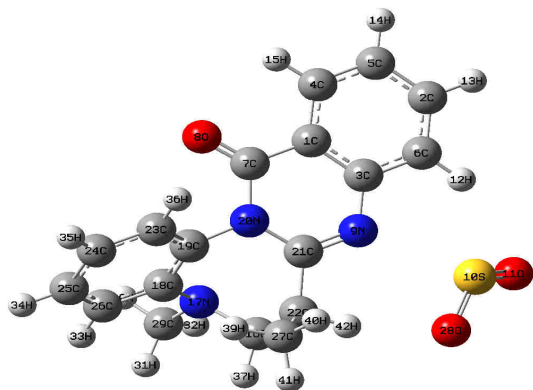


Energy = -1484.265907 a.u.

Number of imaginary frequencies = 0

Center number	Atomic number	Atomic type	Coordinates, Å		
			X	Y	Z
1	6	0	-2.162934	-0.893327	-0.765997
2	6	0	-4.859370	-0.210246	-0.454422
3	6	0	-2.527925	0.254383	-0.042930
4	6	0	-3.161011	-1.672028	-1.366091
5	6	0	-4.503553	-1.335103	-1.210967
6	6	0	-3.876465	0.593626	0.119810
7	6	0	-0.741572	-1.353213	-0.830513
8	8	0	-0.443487	-2.427905	-1.341295
9	7	0	-1.511267	1.081144	0.468454
10	16	0	-1.040908	1.210200	2.196039
11	8	0	-1.208711	-0.062350	2.920458
12	1	0	-4.140347	1.488954	0.674637
13	1	0	-5.905782	0.051386	-0.328532
14	1	0	-5.273424	-1.947715	-1.669431
15	1	0	-2.856234	-2.550785	-1.924181
16	6	0	1.511238	1.231898	-1.847105
17	7	0	2.631800	0.972797	-0.944026
18	6	0	2.696246	-0.266189	-0.296650
19	6	0	1.531878	-1.002359	0.052257
20	7	0	0.197271	-0.526841	-0.221321

21	6	0	-0.123618	0.878312	0.061176
22	6	0	0.277040	1.792621	-1.117215
23	6	0	1.645227	-2.210468	0.746165
24	6	0	2.884065	-2.737064	1.098329
25	6	0	4.035948	-2.025411	0.762676
26	6	0	3.942120	-0.814673	0.082291
27	6	0	0.436838	3.257159	-0.698342
28	8	0	0.448014	1.264830	1.325241
29	6	0	3.862130	1.708880	-1.190914
30	1	0	4.521468	1.220082	-1.927971
31	1	0	4.423332	1.841320	-0.261144
32	1	0	3.608380	2.702257	-1.565671
33	1	0	4.855019	-0.292970	-0.174175
34	1	0	5.017261	-2.410138	1.025315
35	1	0	2.943309	-3.677923	1.635327
36	1	0	0.736258	-2.736207	1.013346
37	1	0	1.832974	1.960332	-2.596590
38	1	0	1.246011	0.318028	-2.393238
39	1	0	1.317879	3.386777	-0.064393
40	1	0	-0.437980	3.607811	-0.143316
41	1	0	0.545245	3.890907	-1.584815
42	1	0	-0.567691	1.717595	-1.818113

Product**P (5e+SO₂)**

Energy = -1484.3160278 a.u.

Number of imaginary frequencies = 0

Center number	Atomic number	Atomic type	Coordinates, Å		
			X	Y	Z
1	6	0	-1.214300	2.156043	0.038690
2	6	0	-3.925036	2.407799	0.635685
3	6	0	-1.989997	0.999751	0.259418
4	6	0	-1.799423	3.432803	0.110014
5	6	0	-3.149458	3.558962	0.401622
6	6	0	-3.358929	1.142388	0.568436
7	6	0	0.216857	2.026657	-0.236687
8	8	0	0.972975	2.969766	-0.421864
9	7	0	-1.429725	-0.269939	0.202274
10	16	0	-3.286769	-2.177802	-0.778240
11	8	0	-4.187767	-2.322276	0.373516
12	1	0	-3.950491	0.256689	0.771357
13	1	0	-4.978948	2.508758	0.878476
14	1	0	-3.605856	4.542321	0.457460
15	1	0	-1.169569	4.298888	-0.062875
16	6	0	1.320986	-1.964202	1.274780
17	7	0	2.181679	-0.815466	1.594896
18	6	0	2.858736	-0.223895	0.503371

19	6	0	2.111156	0.488983	-0.456539
20	7	0	0.692406	0.678720	-0.266714
21	6	0	-0.151771	-0.395796	-0.025428
22	6	0	0.431752	-1.795712	0.018766
23	6	0	2.732367	1.055348	-1.570071
24	6	0	4.113902	0.956122	-1.732614
25	6	0	4.873056	0.286441	-0.771518
26	6	0	4.250493	-0.306196	0.327588
27	6	0	1.059611	-2.297018	-1.300506
28	8	0	-2.356019	-3.285698	-1.042141
29	6	0	2.956253	-1.045128	2.808160
30	1	0	3.525515	-0.147425	3.060411
31	1	0	3.653045	-1.898507	2.731516
32	1	0	2.264014	-1.254220	3.629667
33	1	0	4.848485	-0.846992	1.052419
34	1	0	5.950917	0.210140	-0.881497
35	1	0	4.590275	1.411134	-2.594917
36	1	0	2.134554	1.598900	-2.291463
37	1	0	1.922109	-2.884029	1.149438
38	1	0	0.671258	-2.118651	2.143158
39	1	0	1.988376	-1.794489	-1.571504
40	1	0	0.347839	-2.182578	-2.123478
41	1	0	1.268992	-3.366648	-1.198758
42	1	0	-0.433770	-2.436088	0.194163