Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

STEREOSELECTIVE DOMINO AZIDATION AND [3+2] CYCLOADDITION: A FACILE ROUTE TO CHIRAL HETEROCYCLIC SCAFFOLDS FROM CARBOHYDRATE DERIVED SYNTHONS

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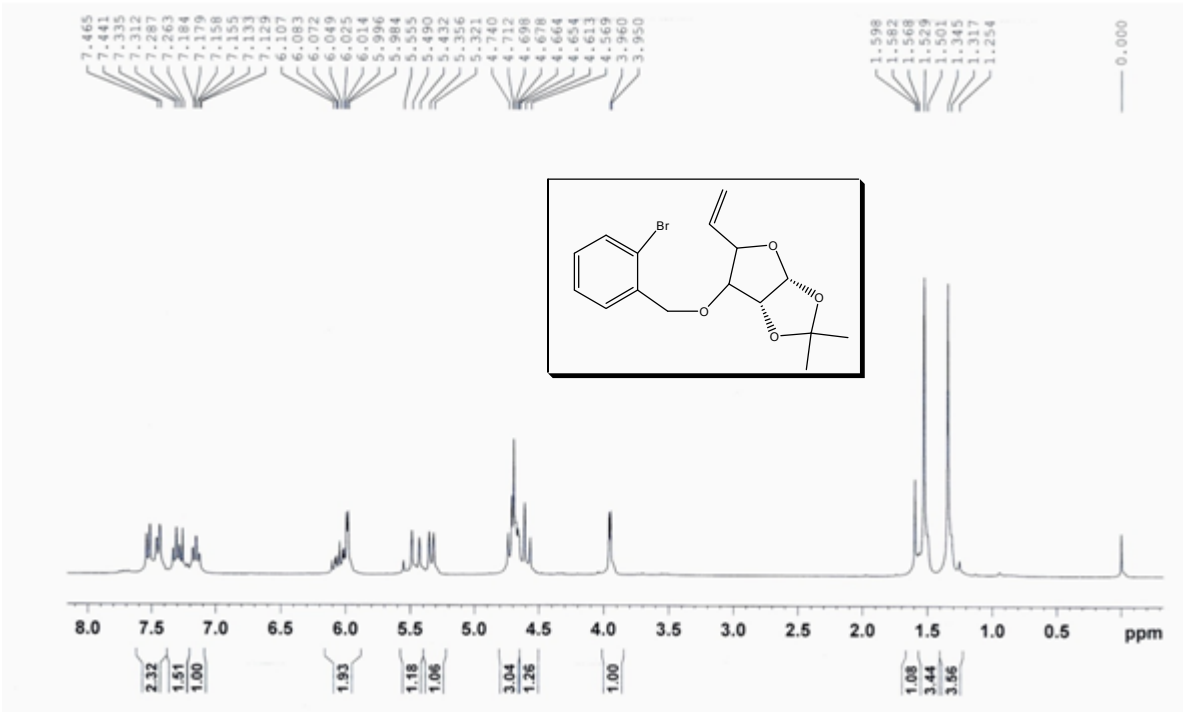
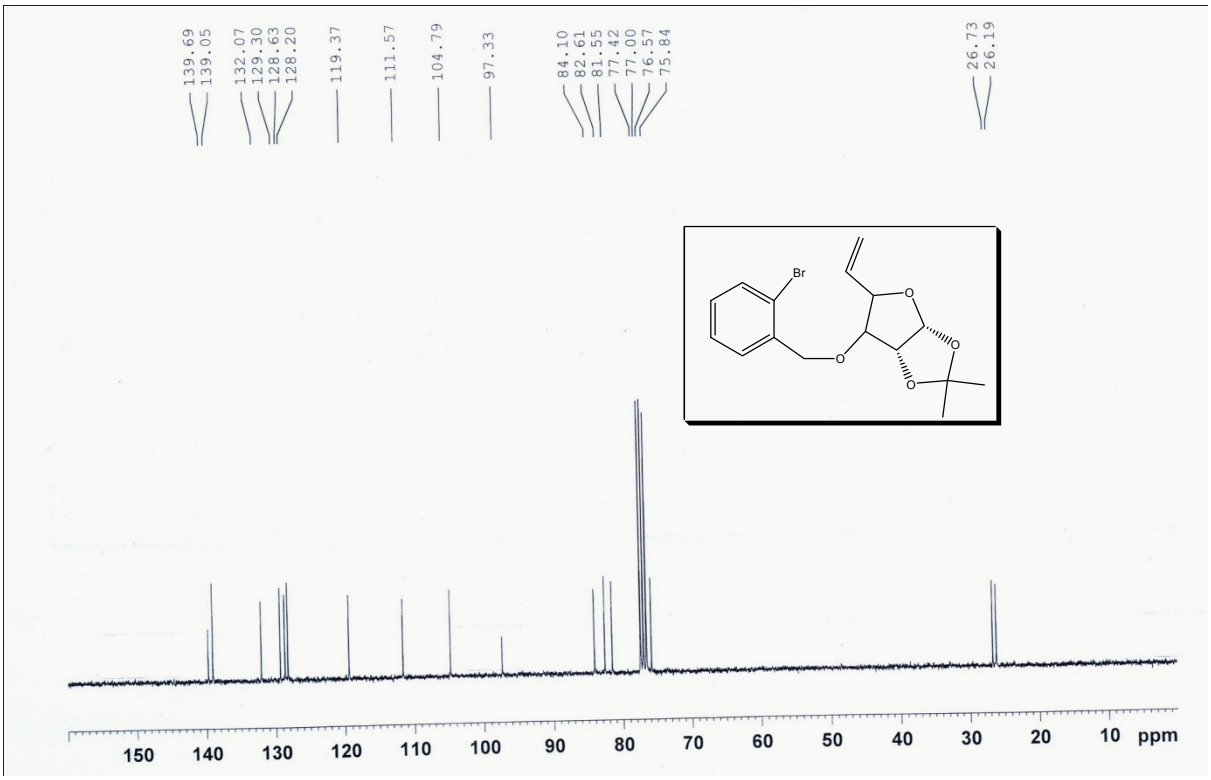
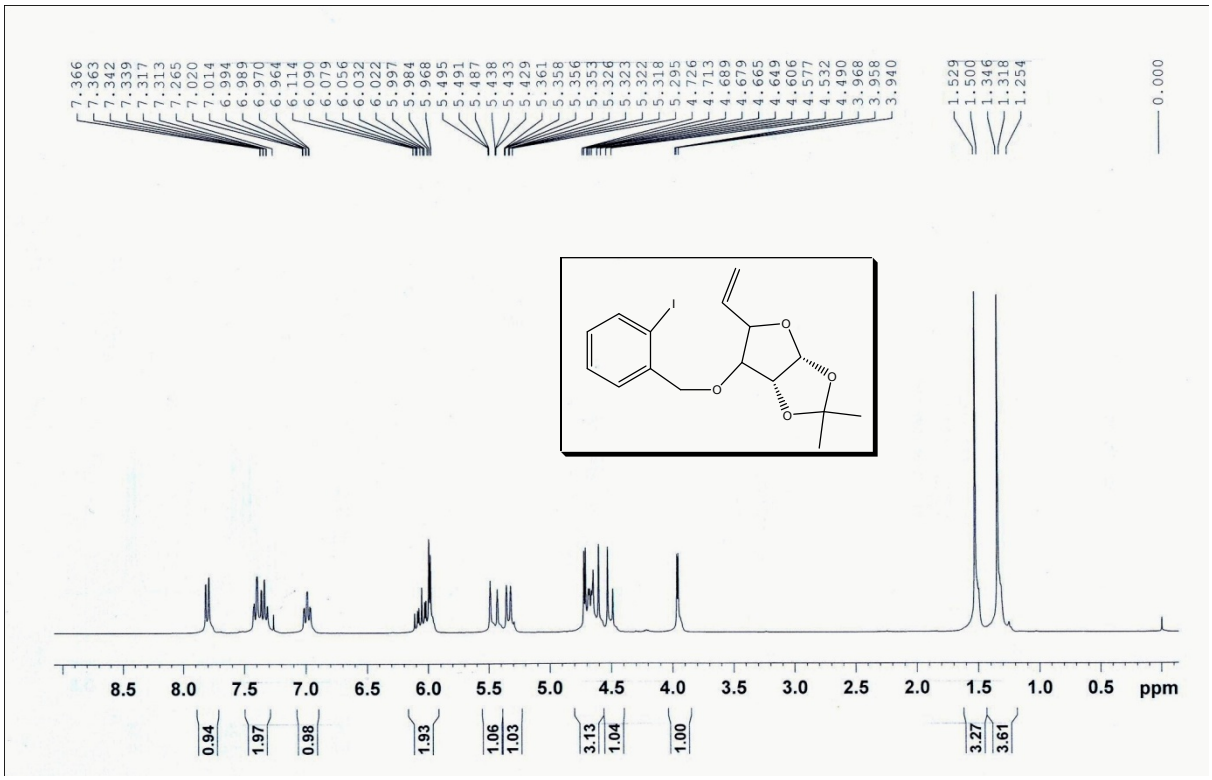
^{1}H NMR spectrum of compound 3a:



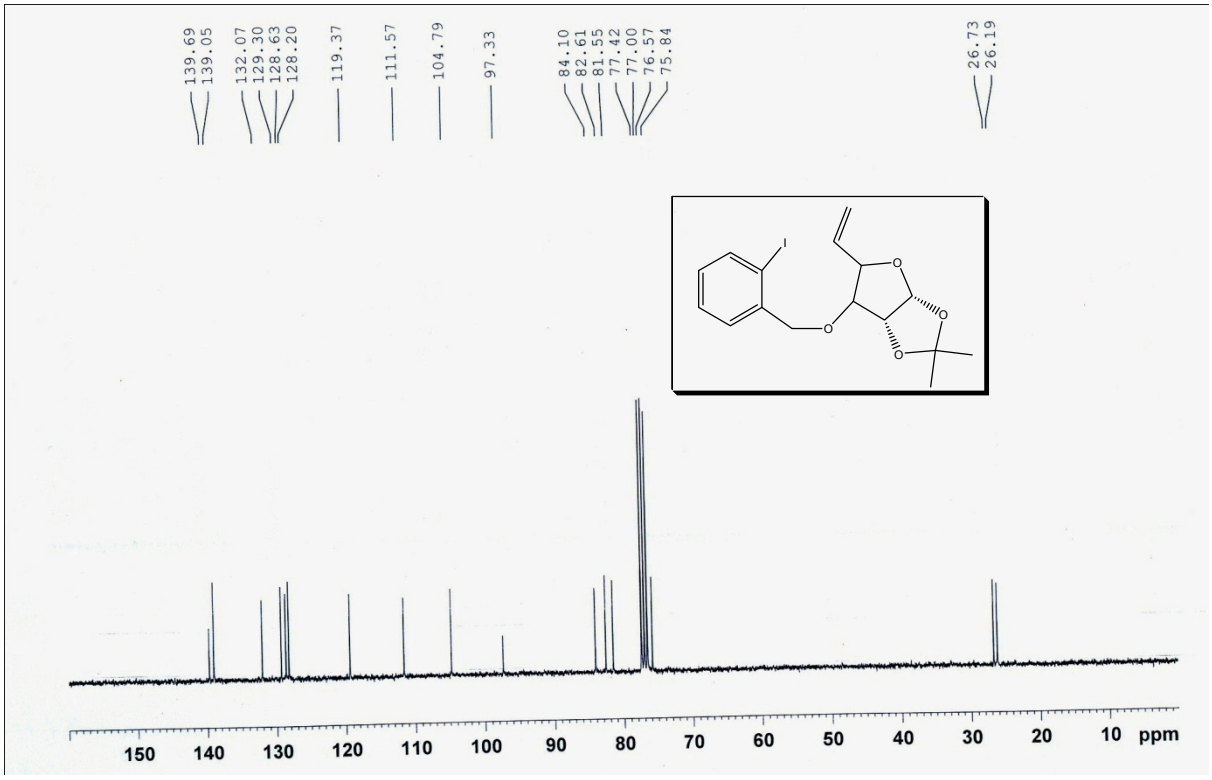
^{13}C NMR spectrum of compound 3a:



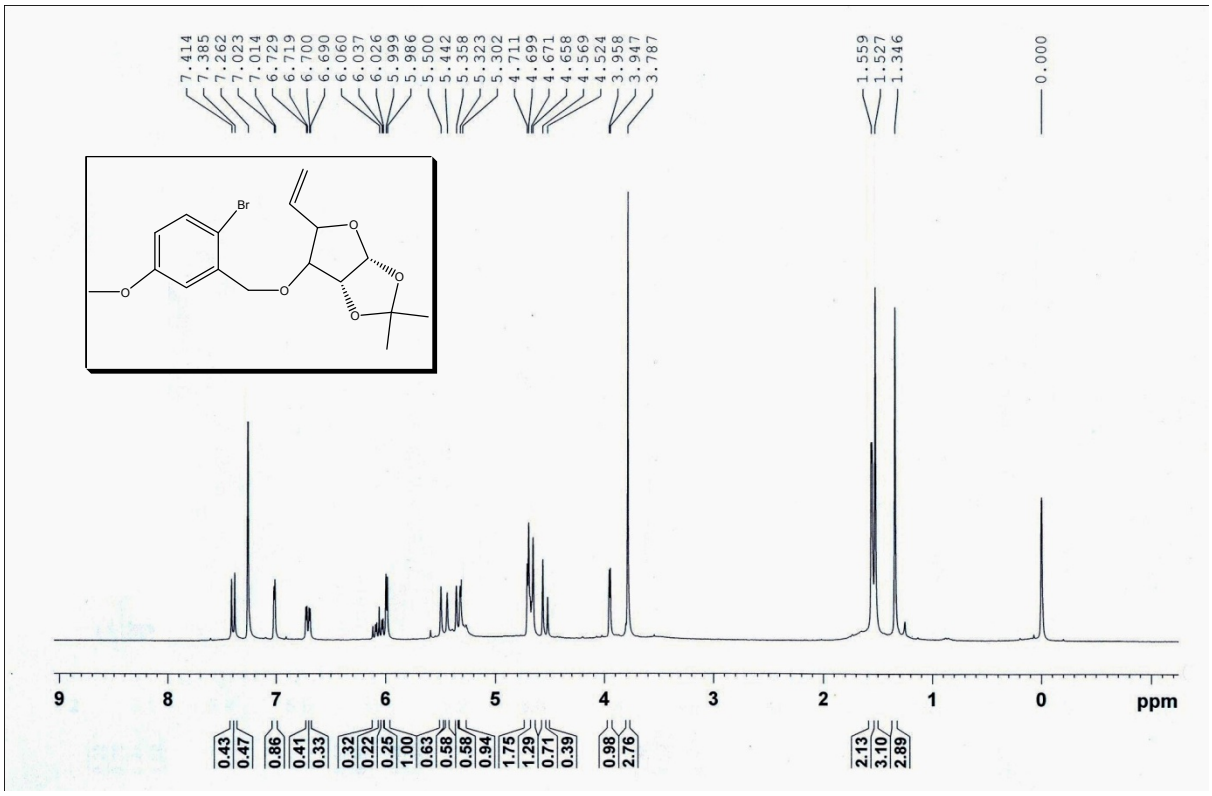
^{1}H NMR spectrum of compound 3b:



^{13}C NMR spectrum of compound 3b:

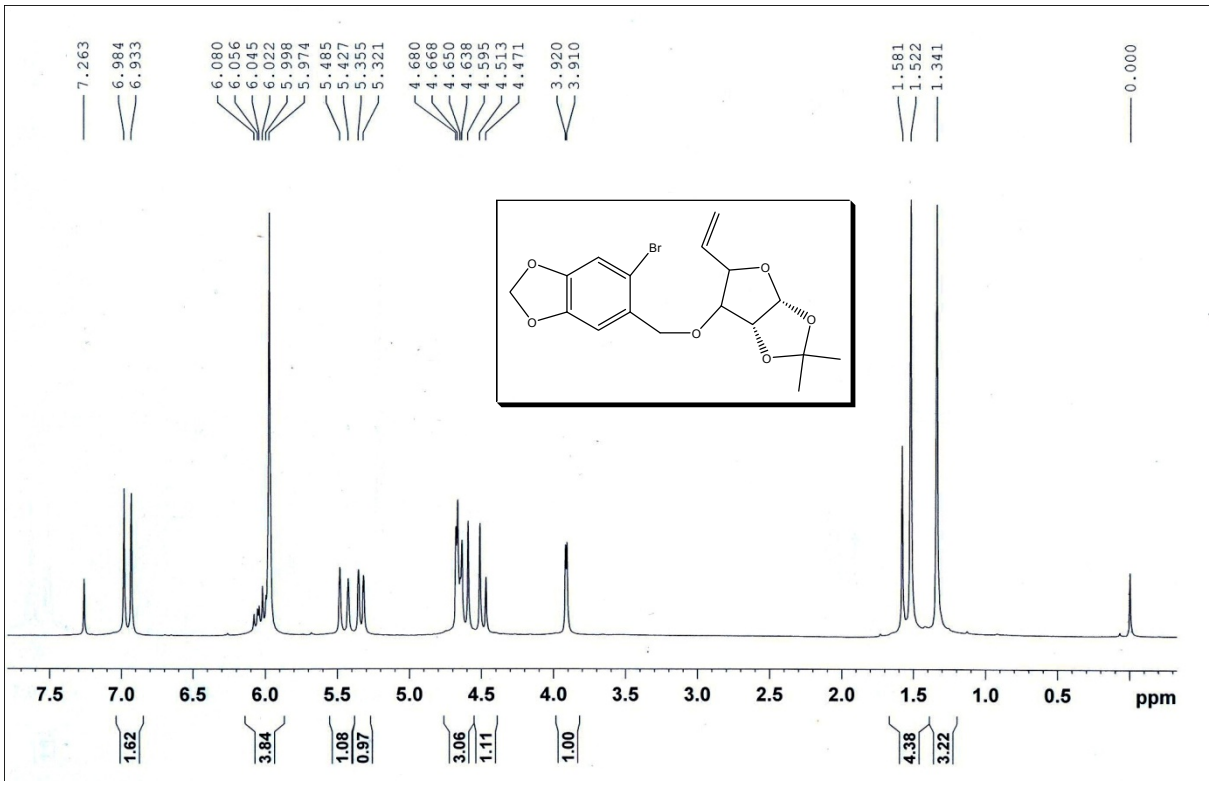


^{1}HNMR spectrum of compound 3c:

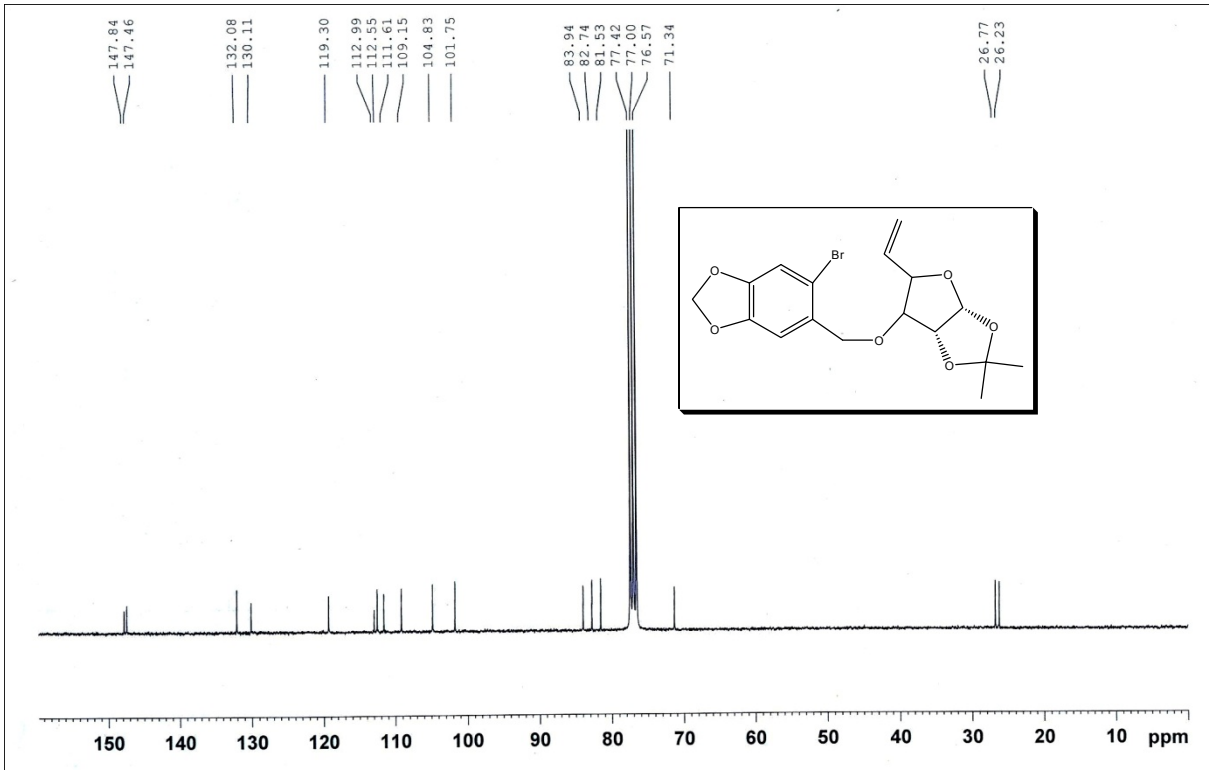


^{13}C NMR spectrum of compound 3c:

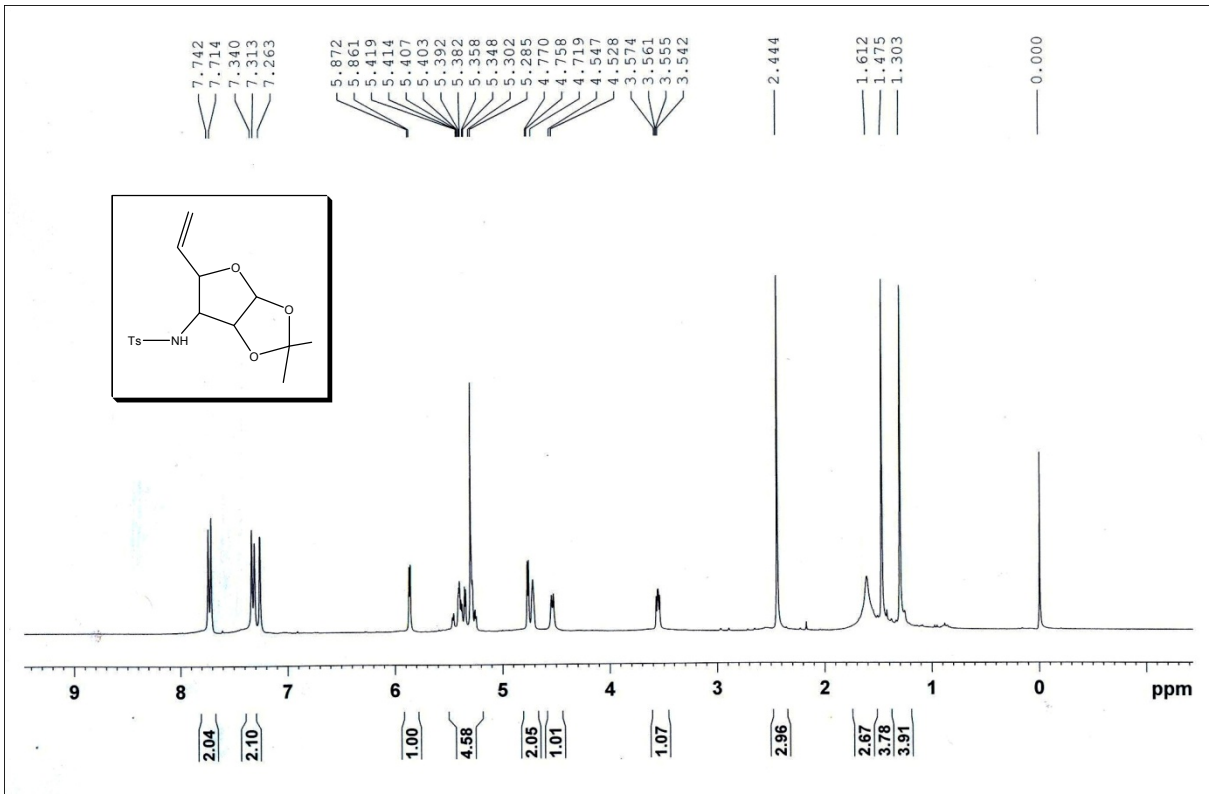
^{1}H NMR spectrum of compound 3d:



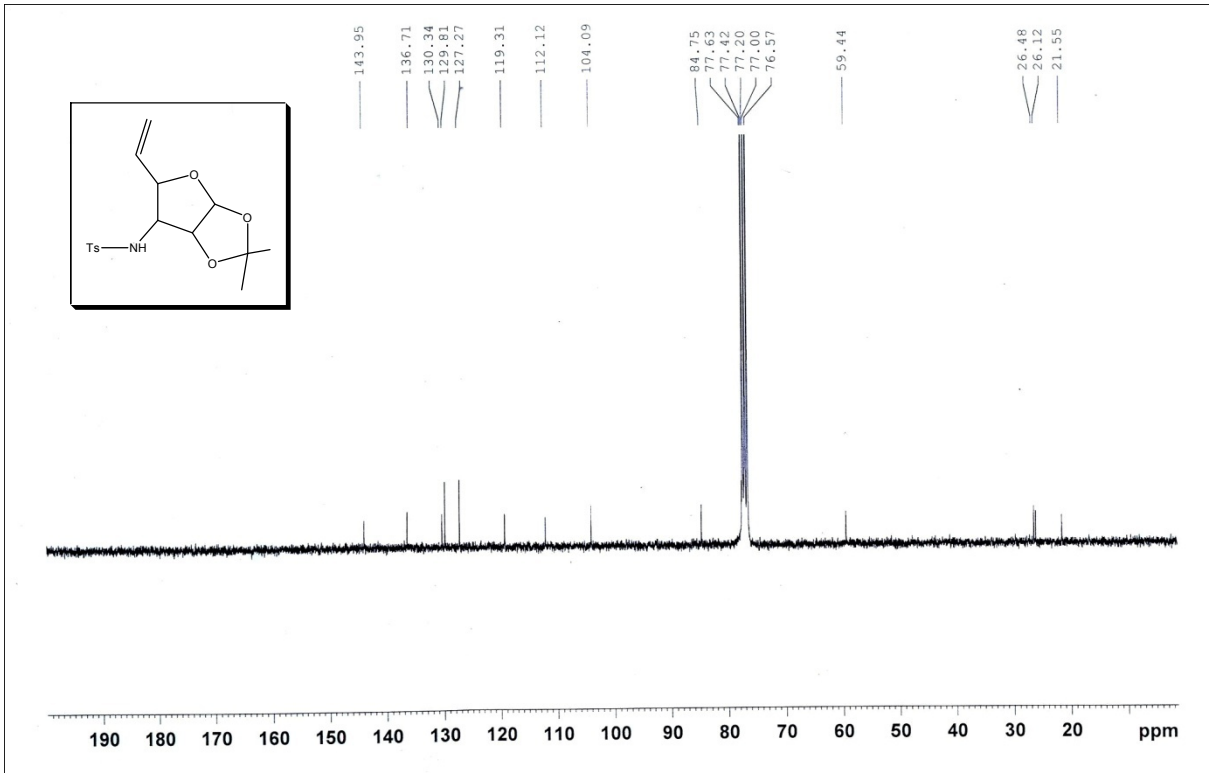
^{13}C NMR spectrum of compound 3d:



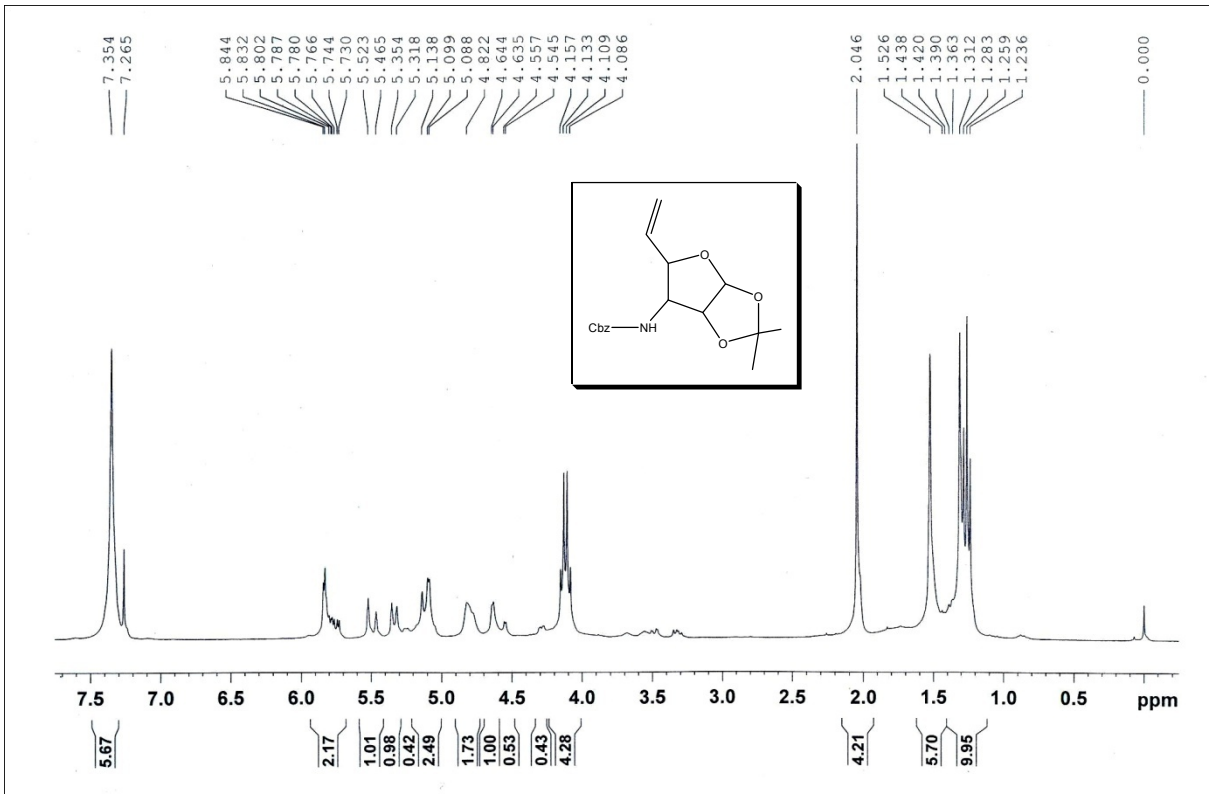
^{1}H NMR spectrum of compound 5a:



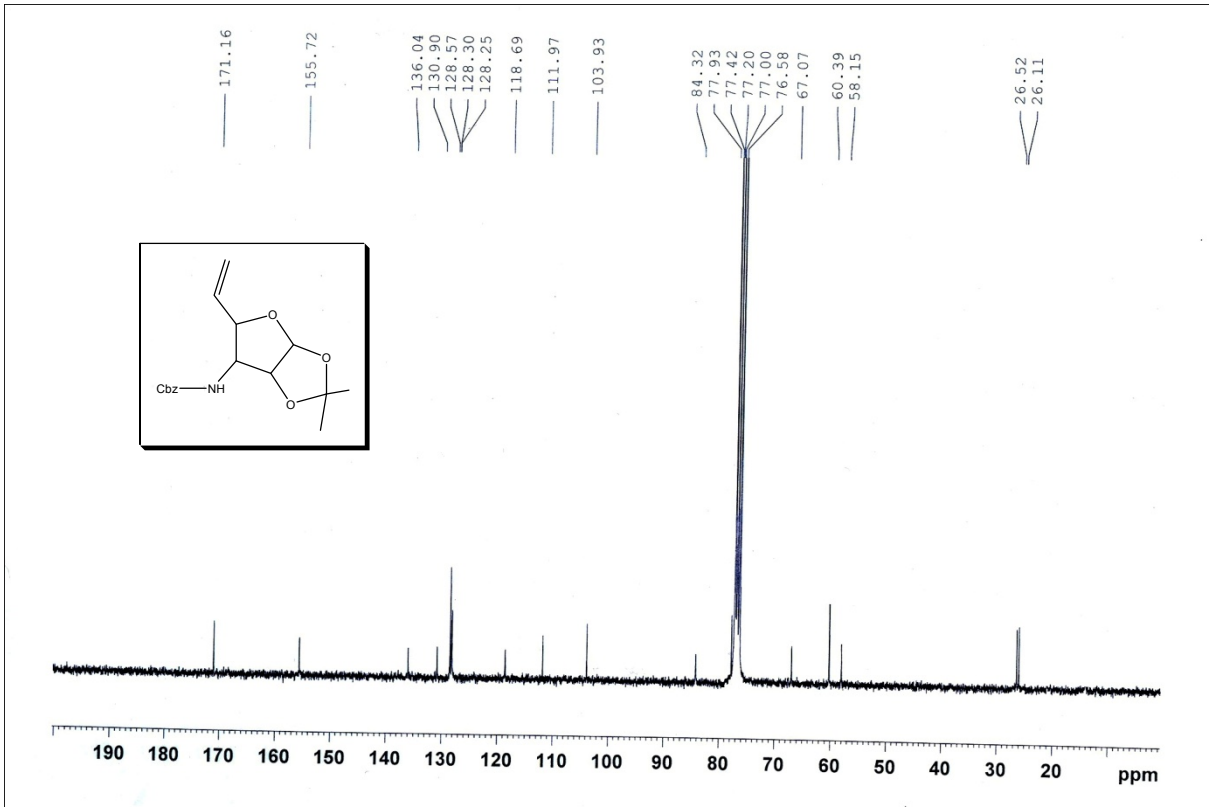
^{13}c NMR spectrum of compound 5a:



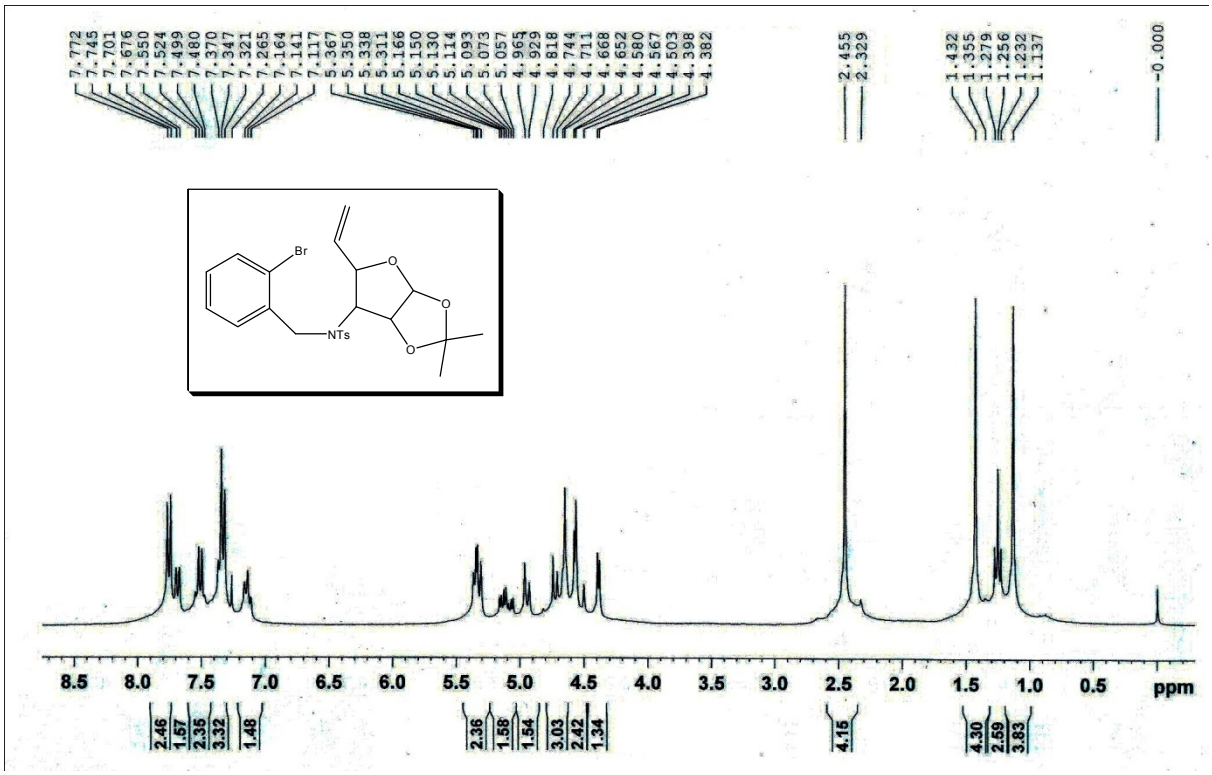
^{1}H NMR spectrum of compound 5b:



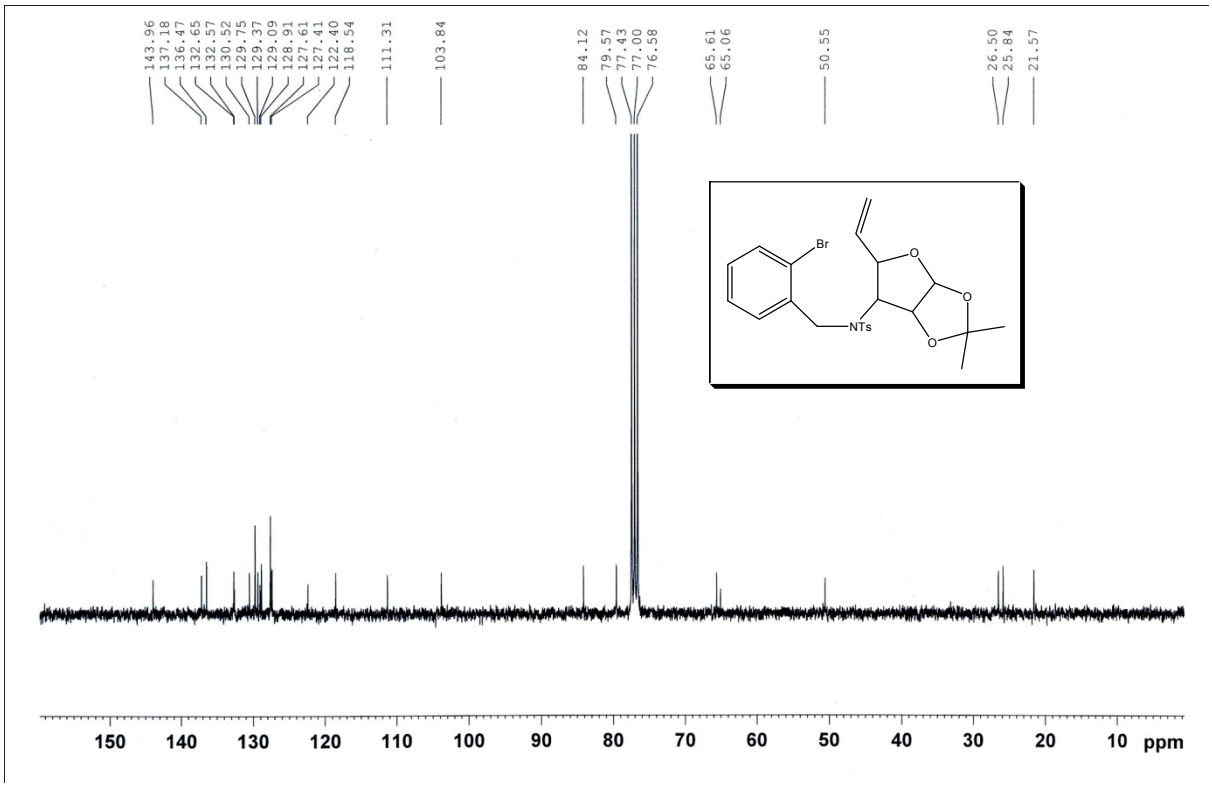
^{13}c NMR spectrum spectra of compound 5b:



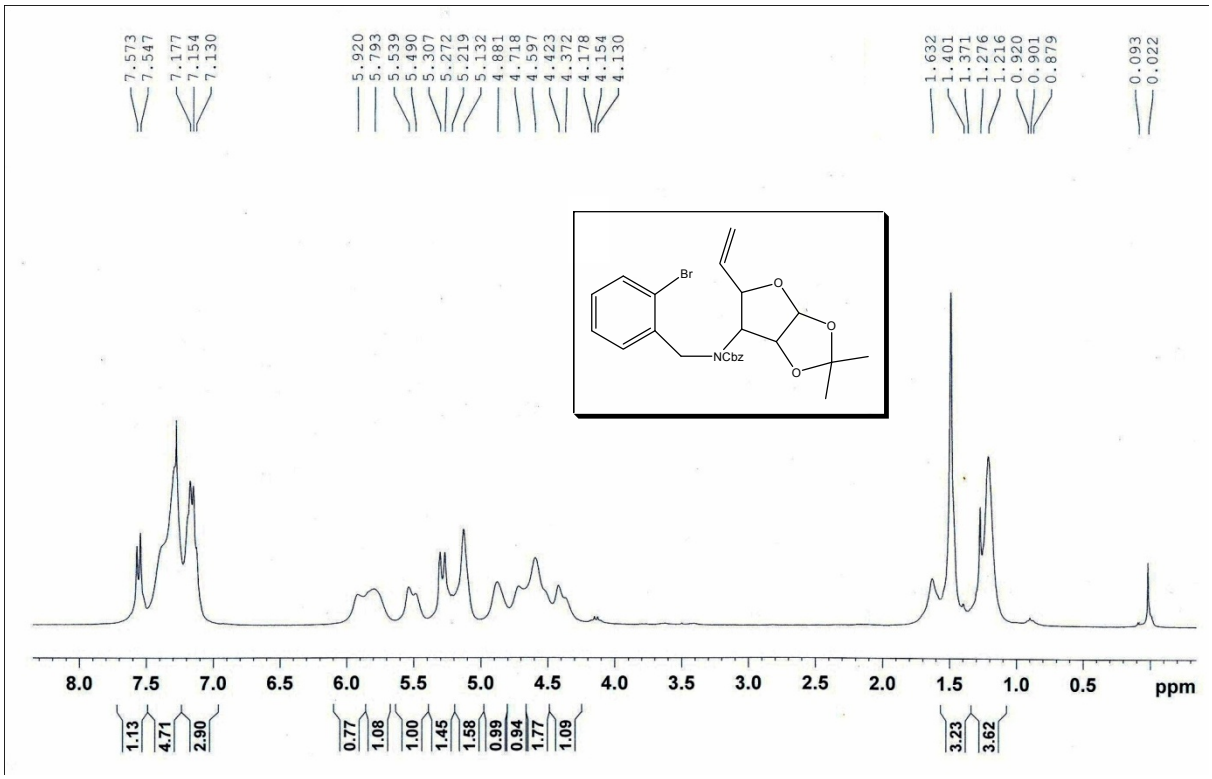
^{1}H NMR spectrum of compound 6a:



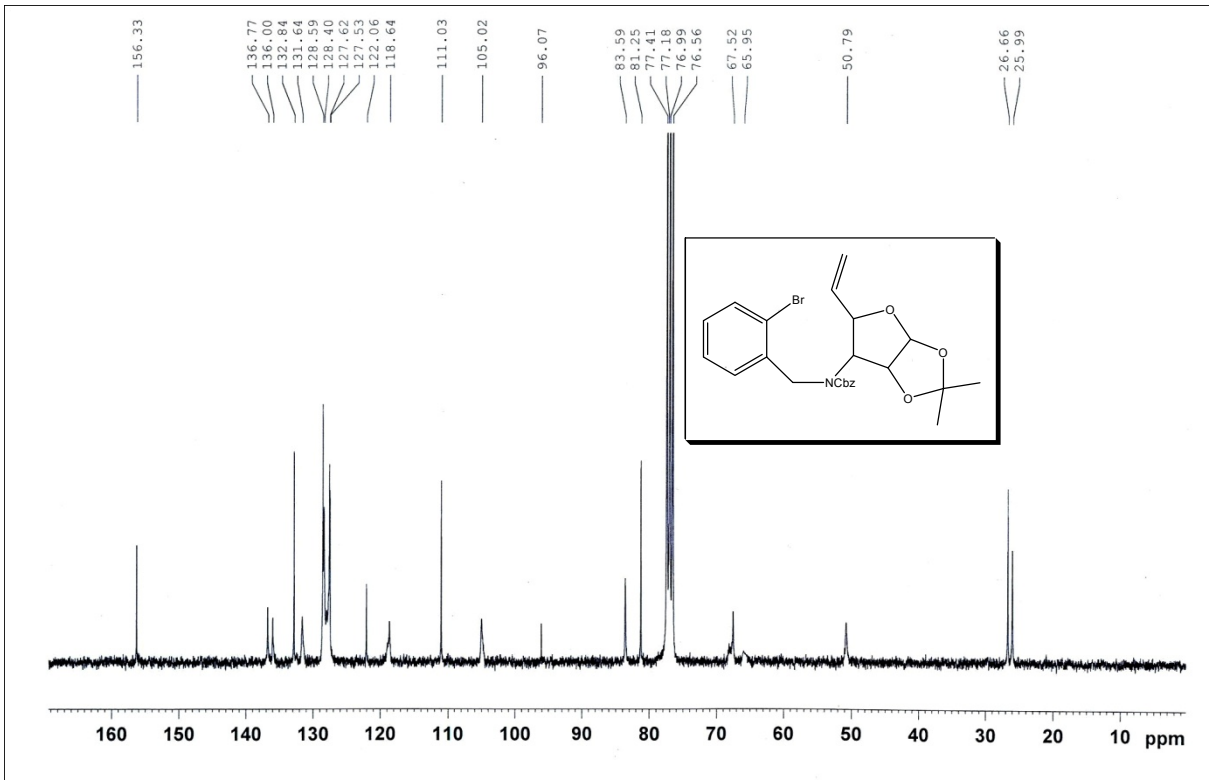
^{13}C NMR spectrum of compound 6b:



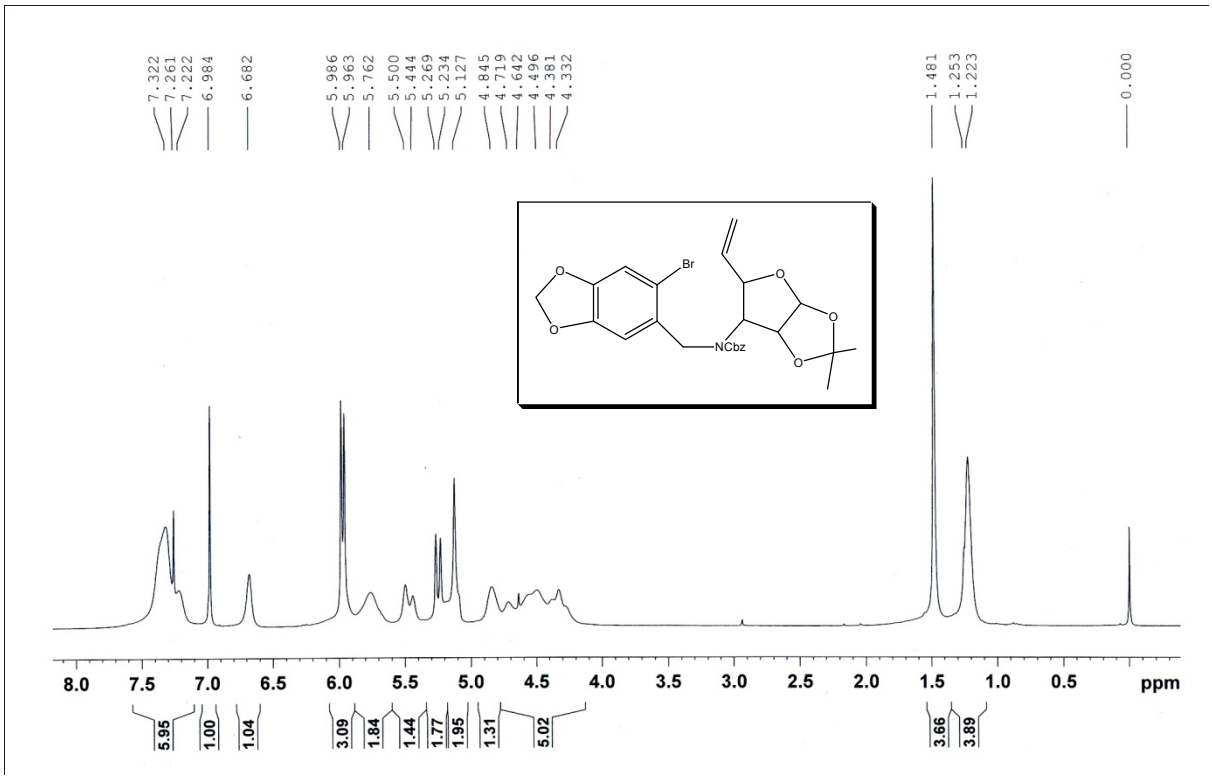
^{1}H NMR spectrum of compound 6b:



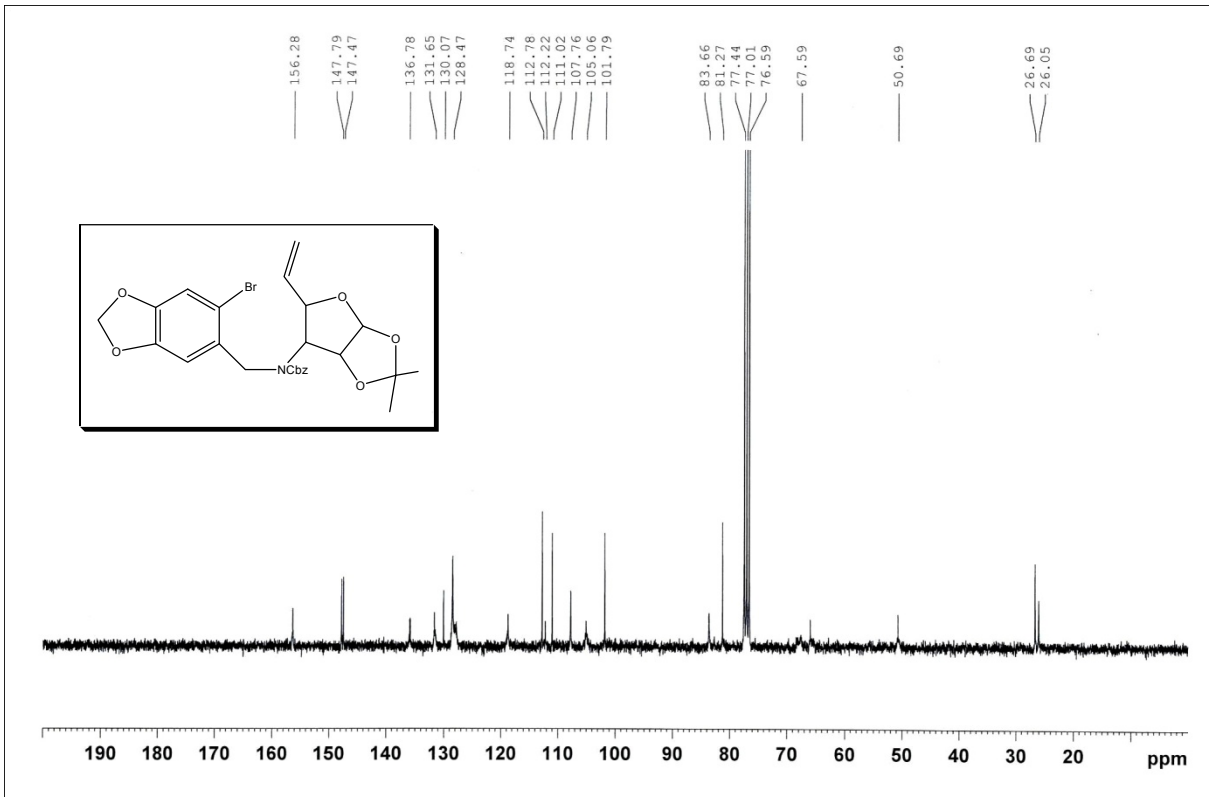
^{13}C NMR spectrum of compound 6b:



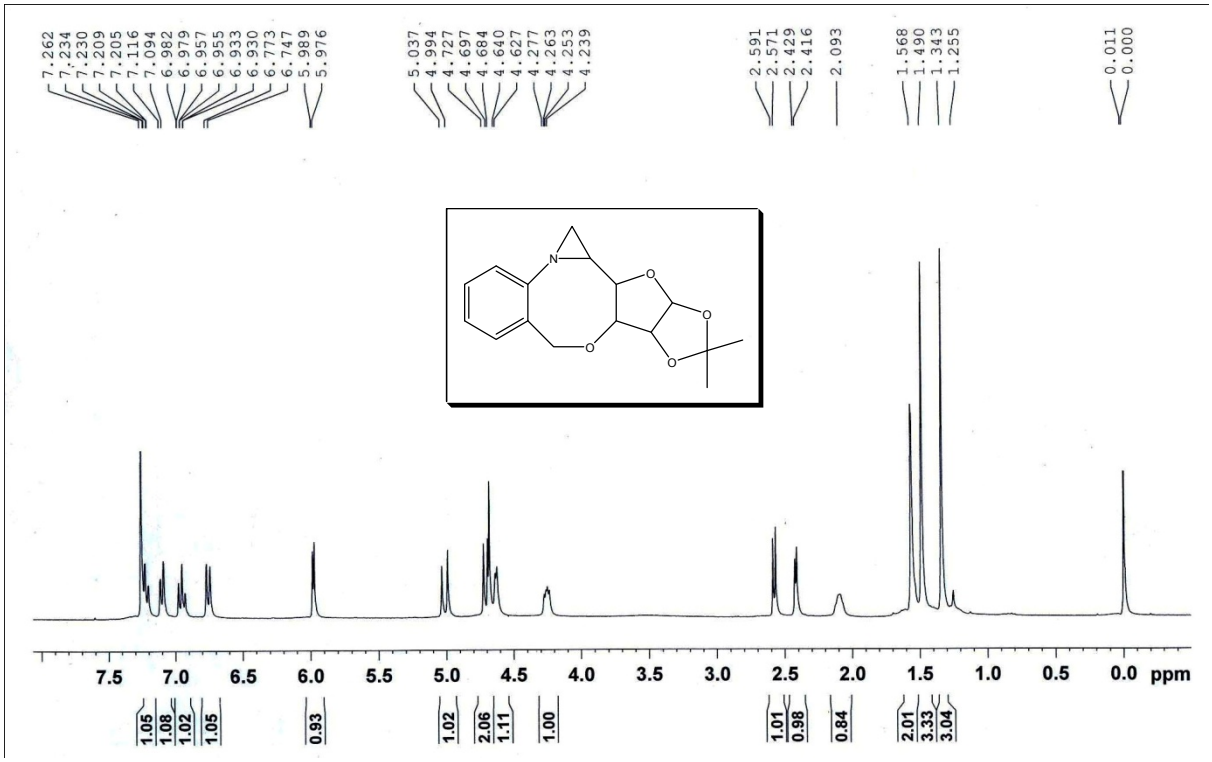
^{1}H NMR spectrum of compound 6c:



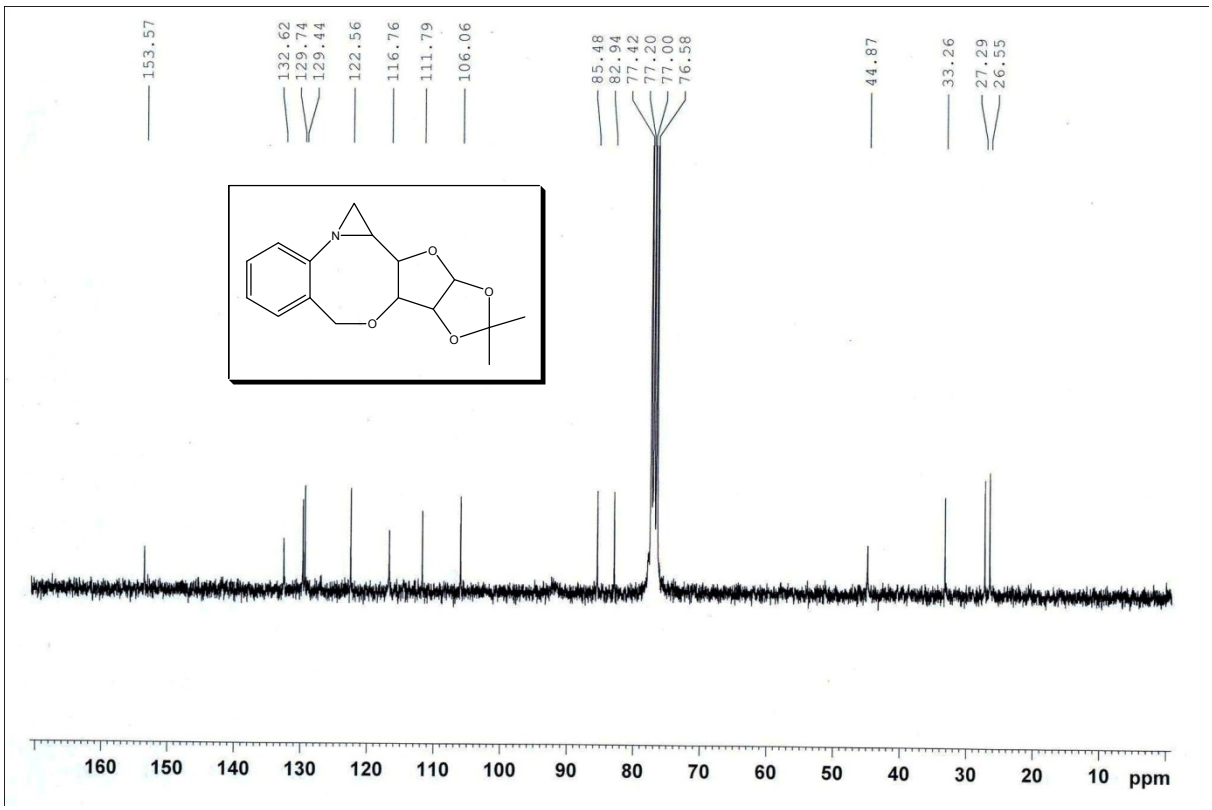
^{13}C NMR spectrum of compound 6c:



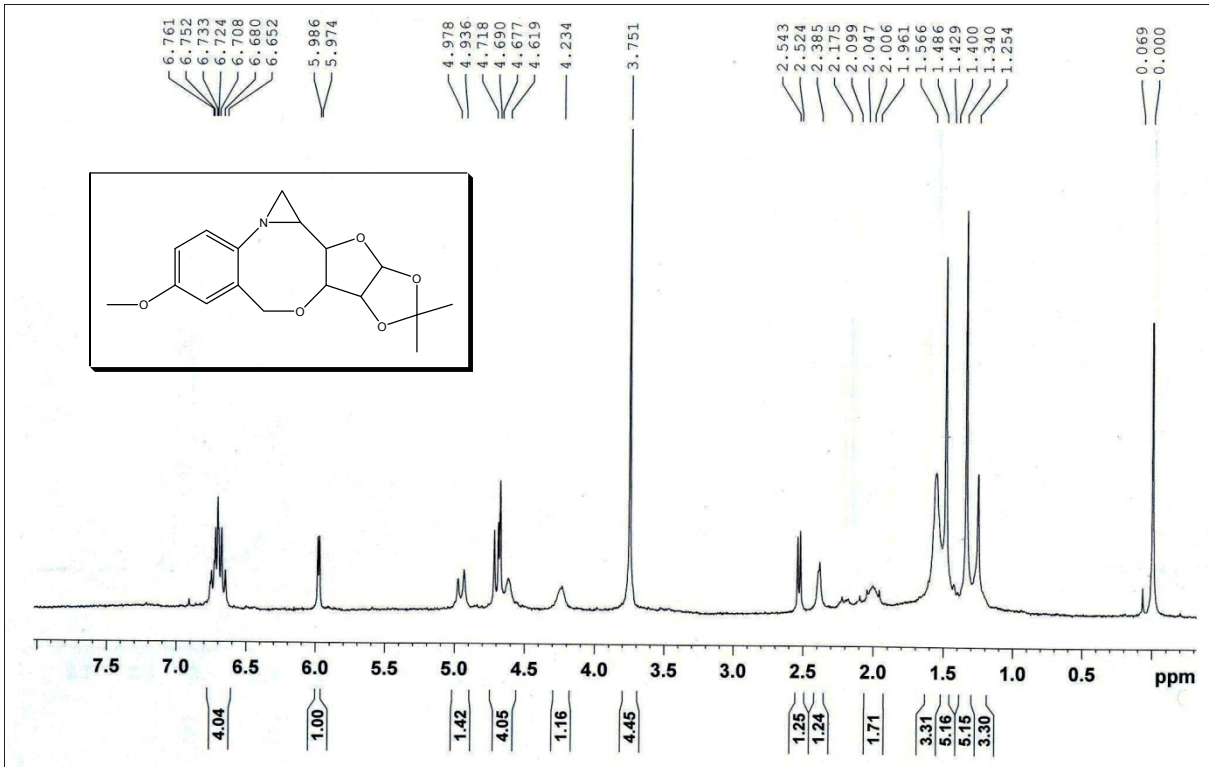
^{1}H NMR spectrum of compound 7a&7b:



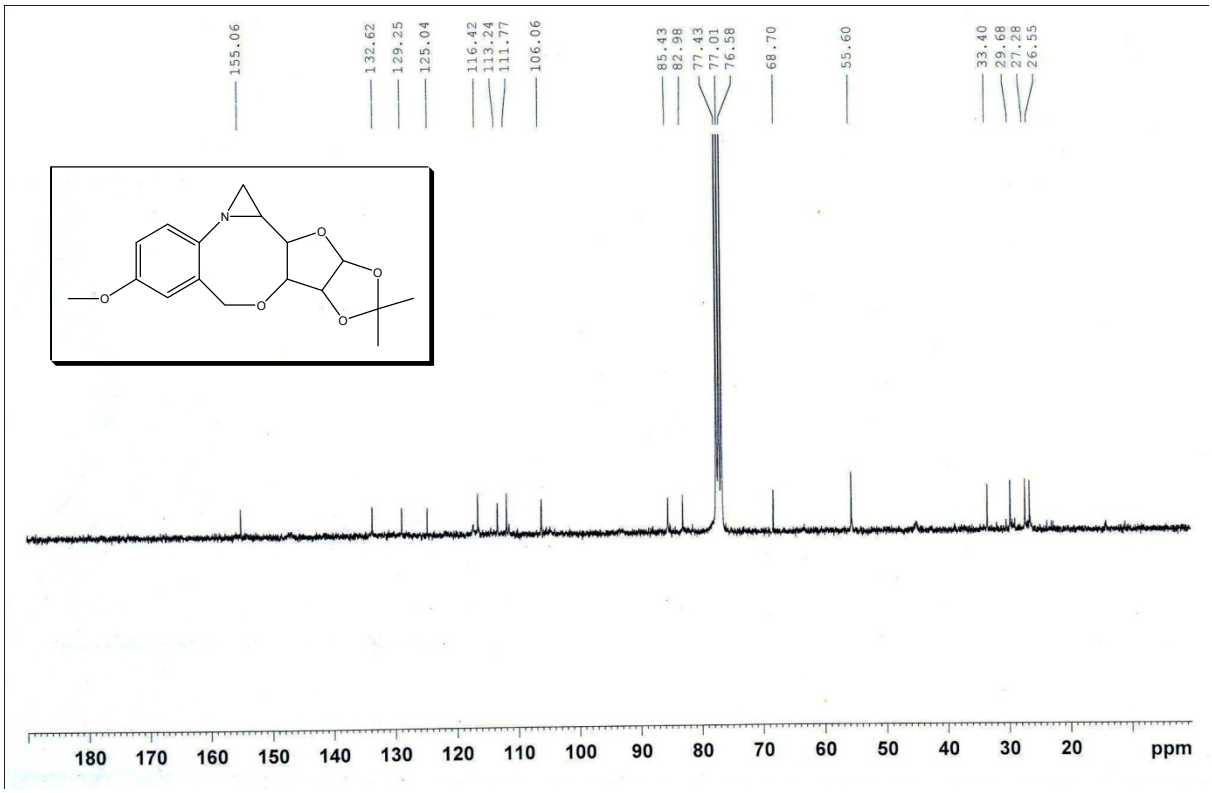
^{13}C NMR spectrum of compound 7a&7b:



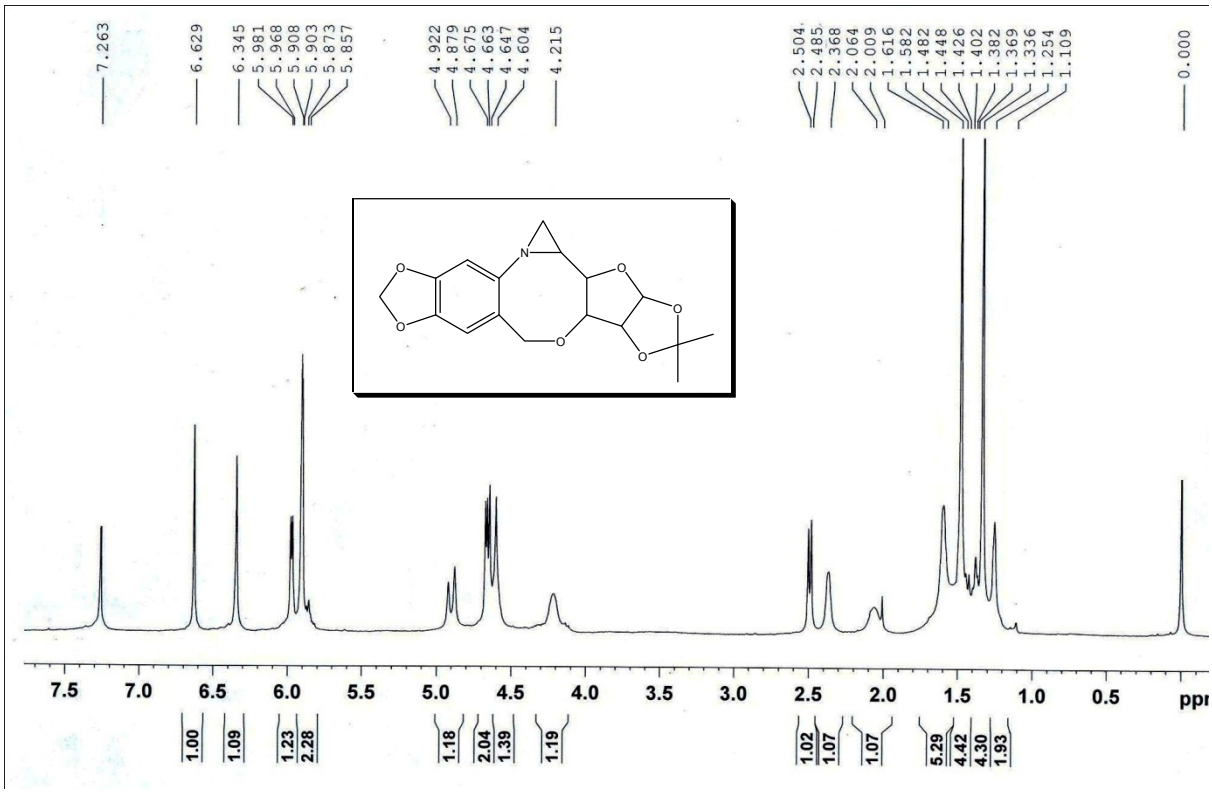
^{1}H NMR spectrum of compound 7c:



^{13}C NMR spectrum of compound 7c:



^{1}H NMR spectrum of compound 7d:



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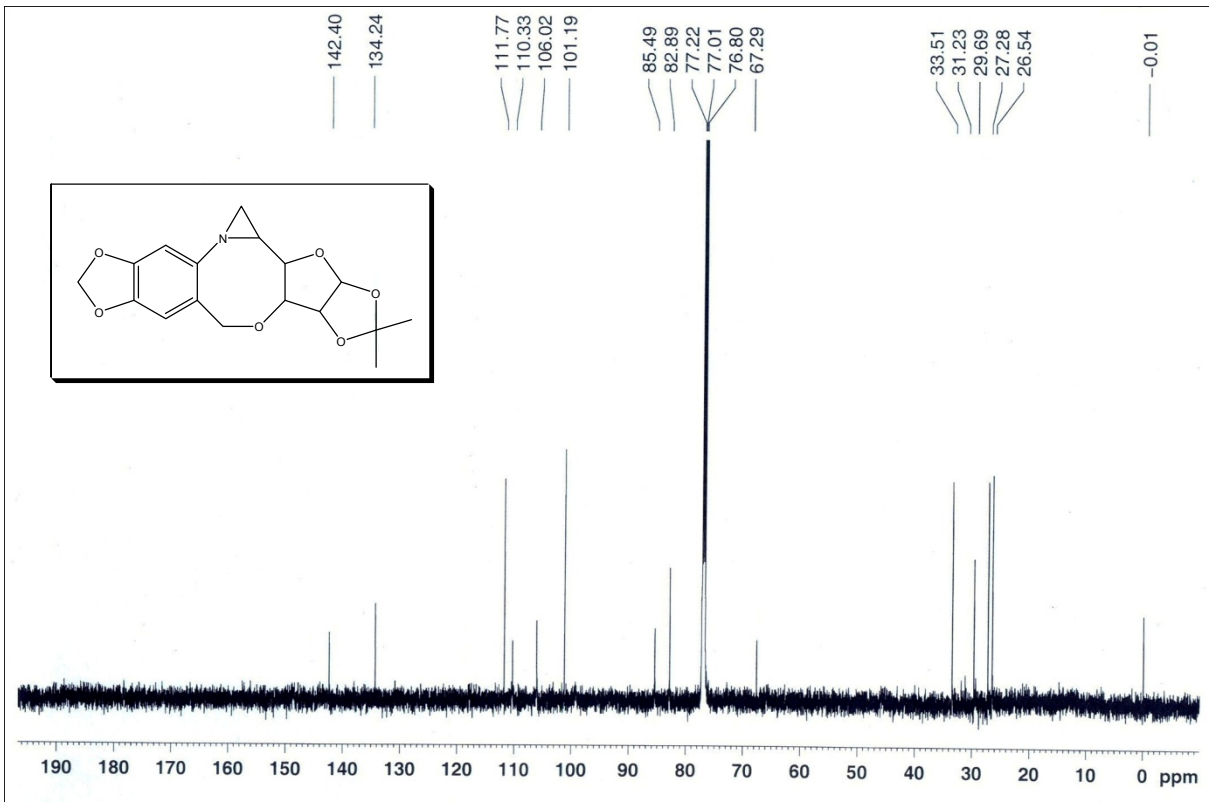
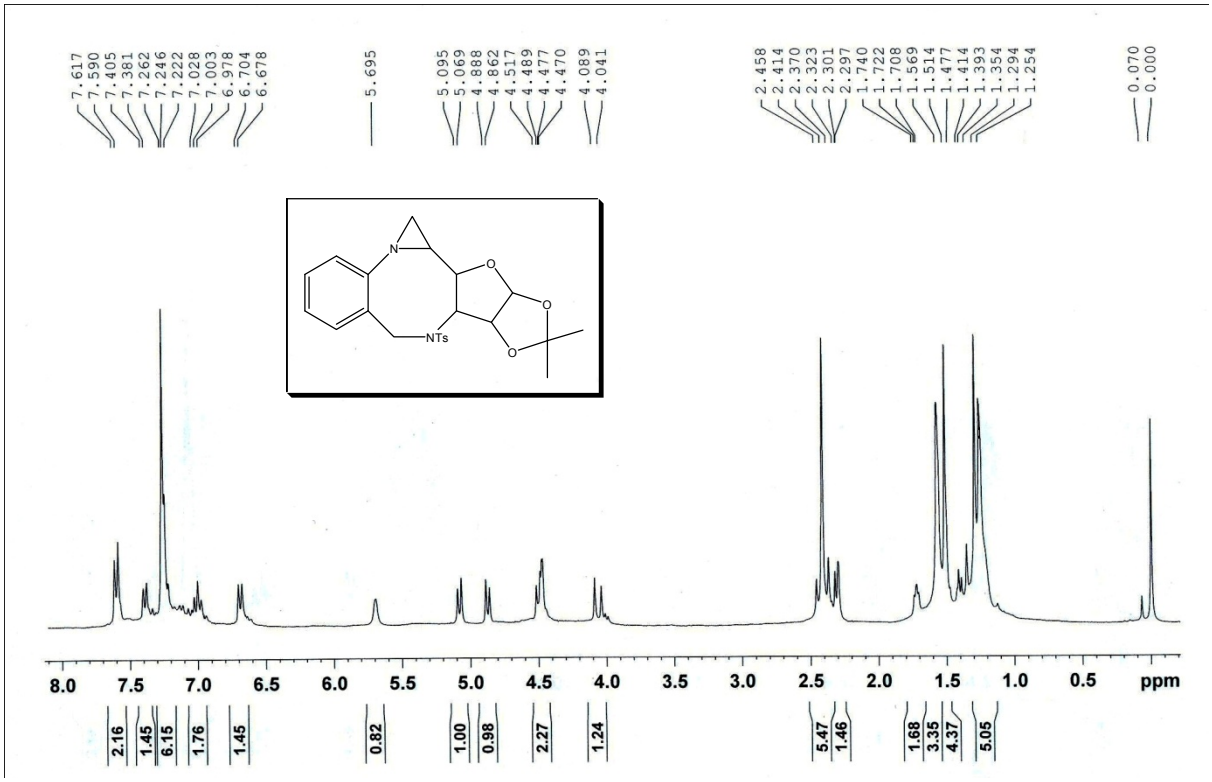
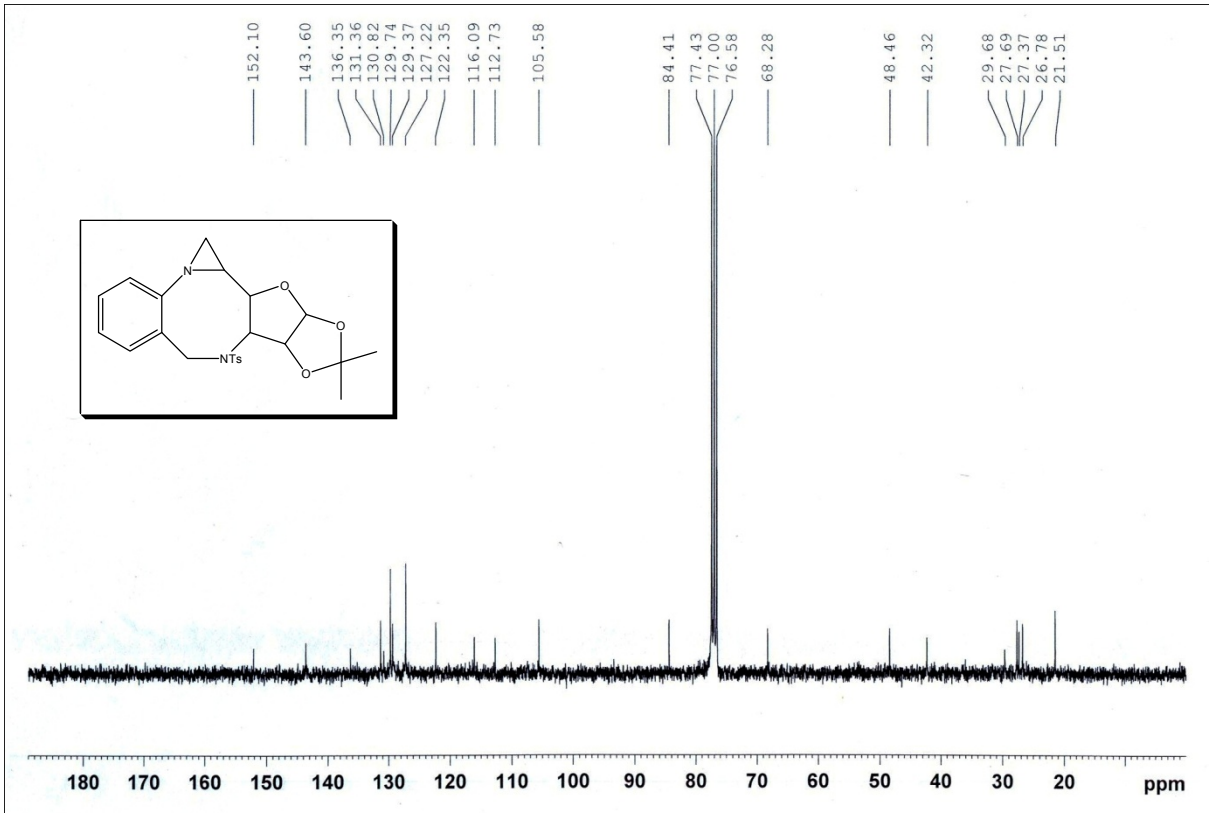


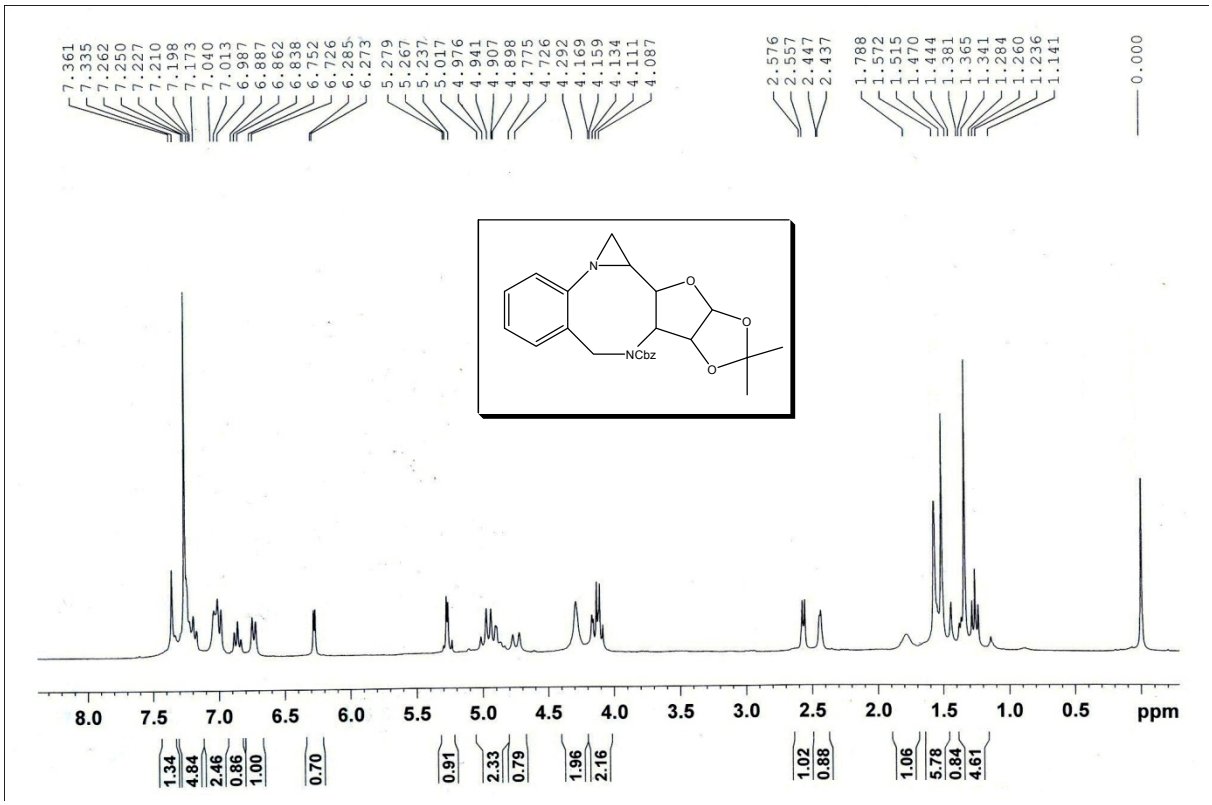
^{1}H NMR spectrum of compound 8a:



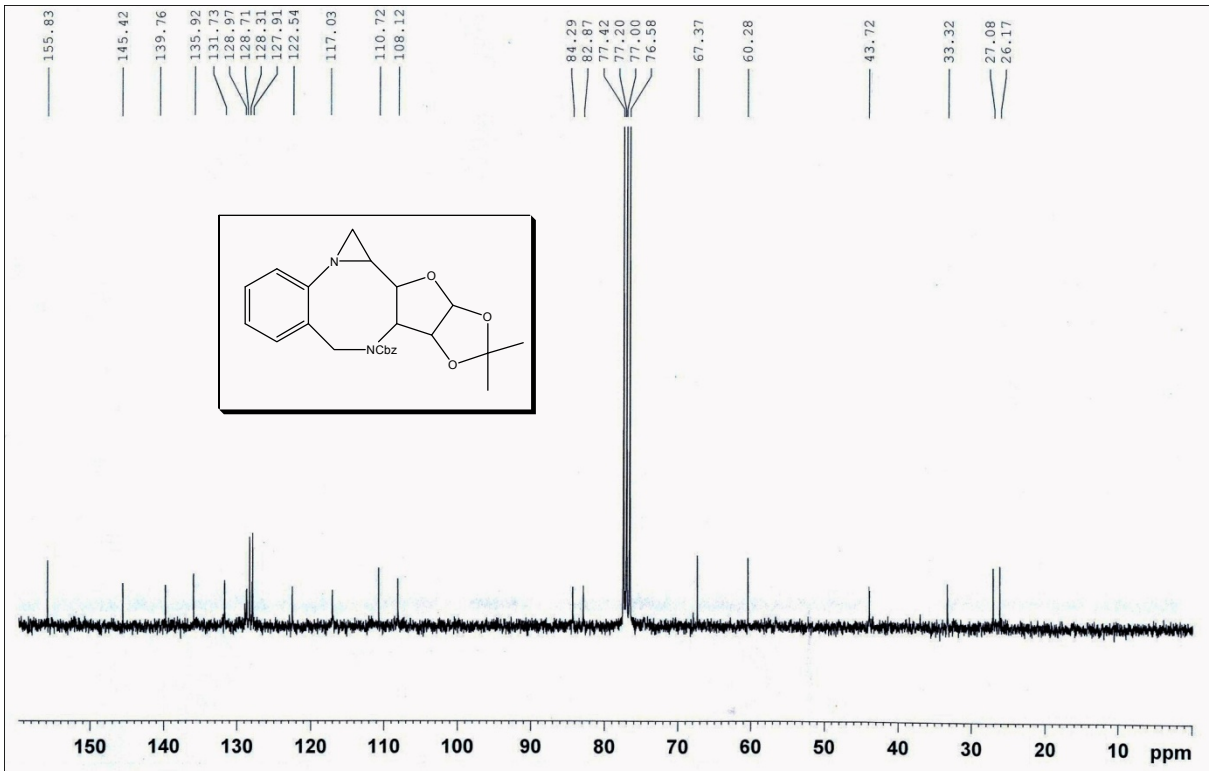
^{13}c NMR spectrum of compound 8a:



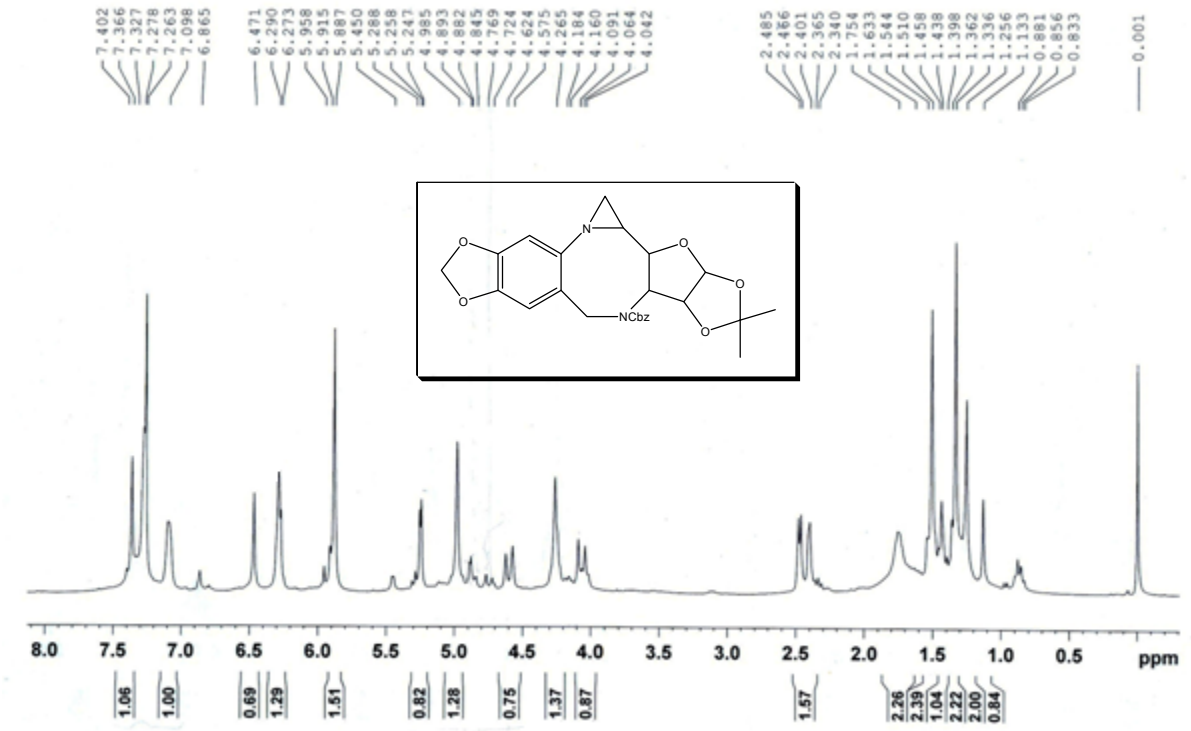
^{1}H NMR spectrum of compound 8b:



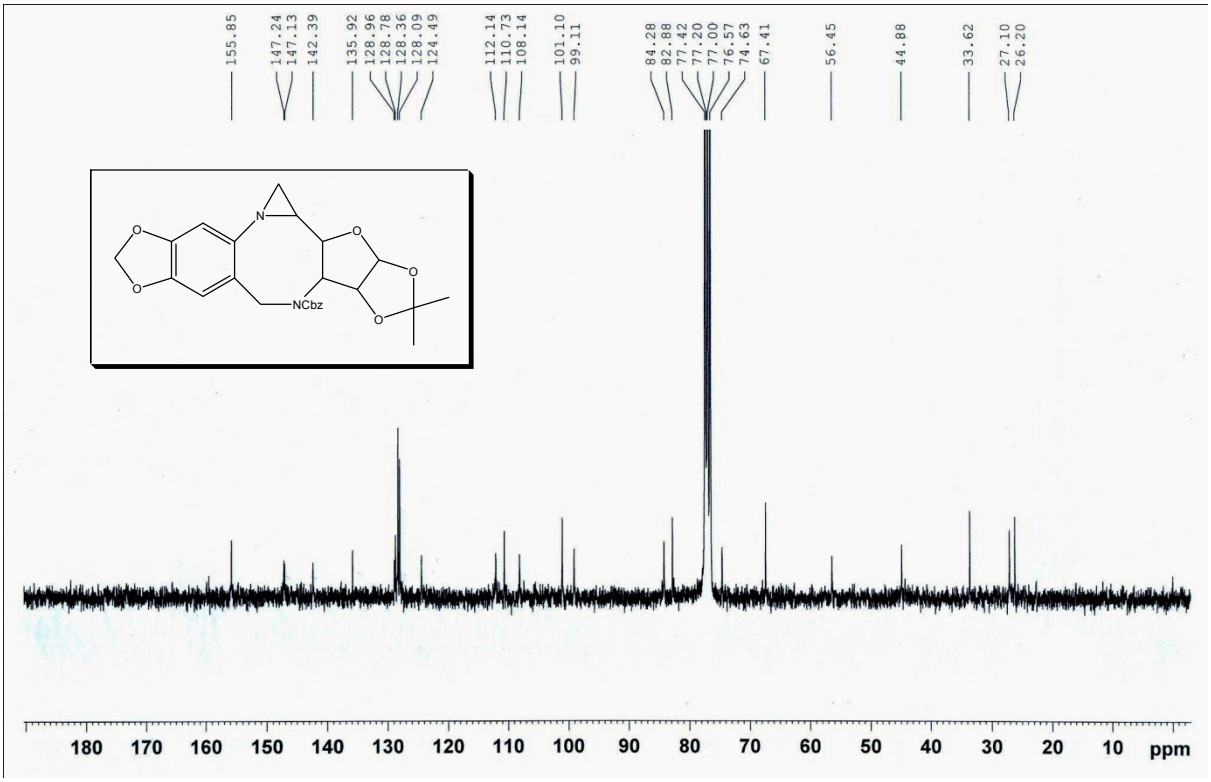
^{13}c NMR spectrum of compound 8b:



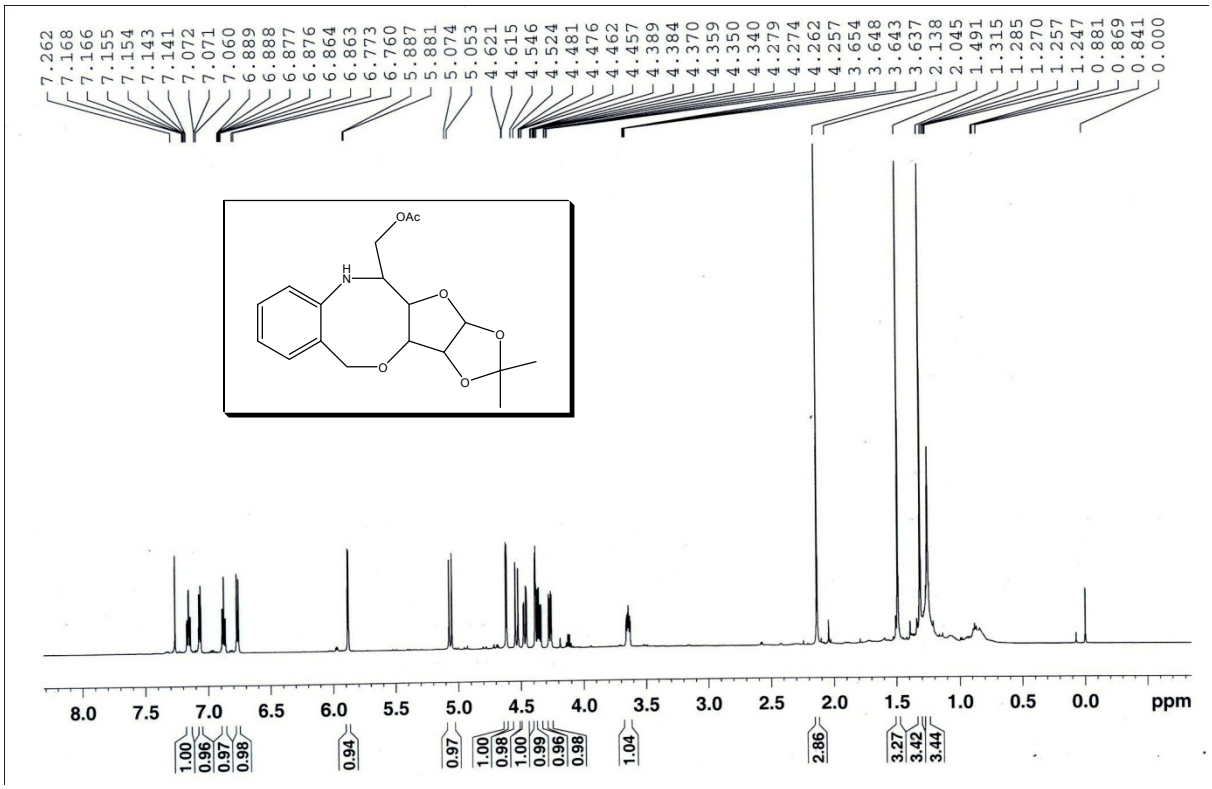
^{1}H spectrum NMR of compound 8c:



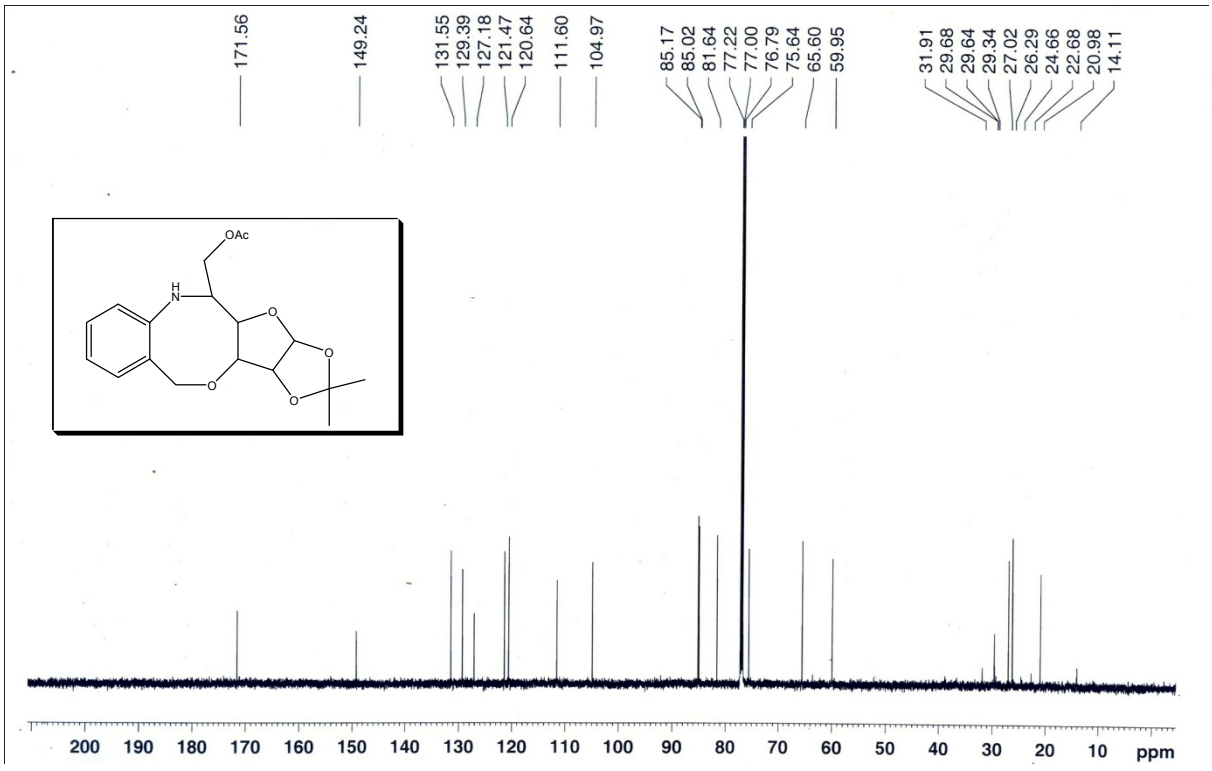
^{13}c NMR spectrum of compound 8c:



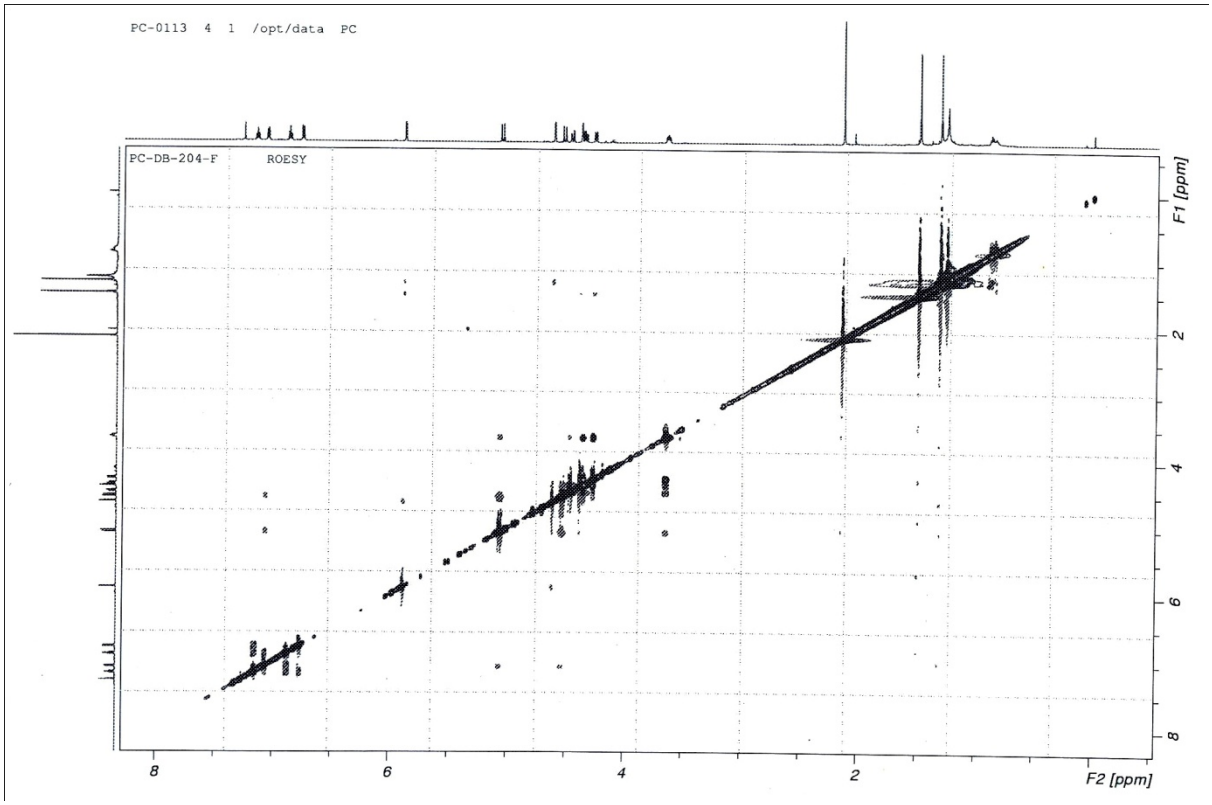
^{1}H NMR spectrum of compound 9b:

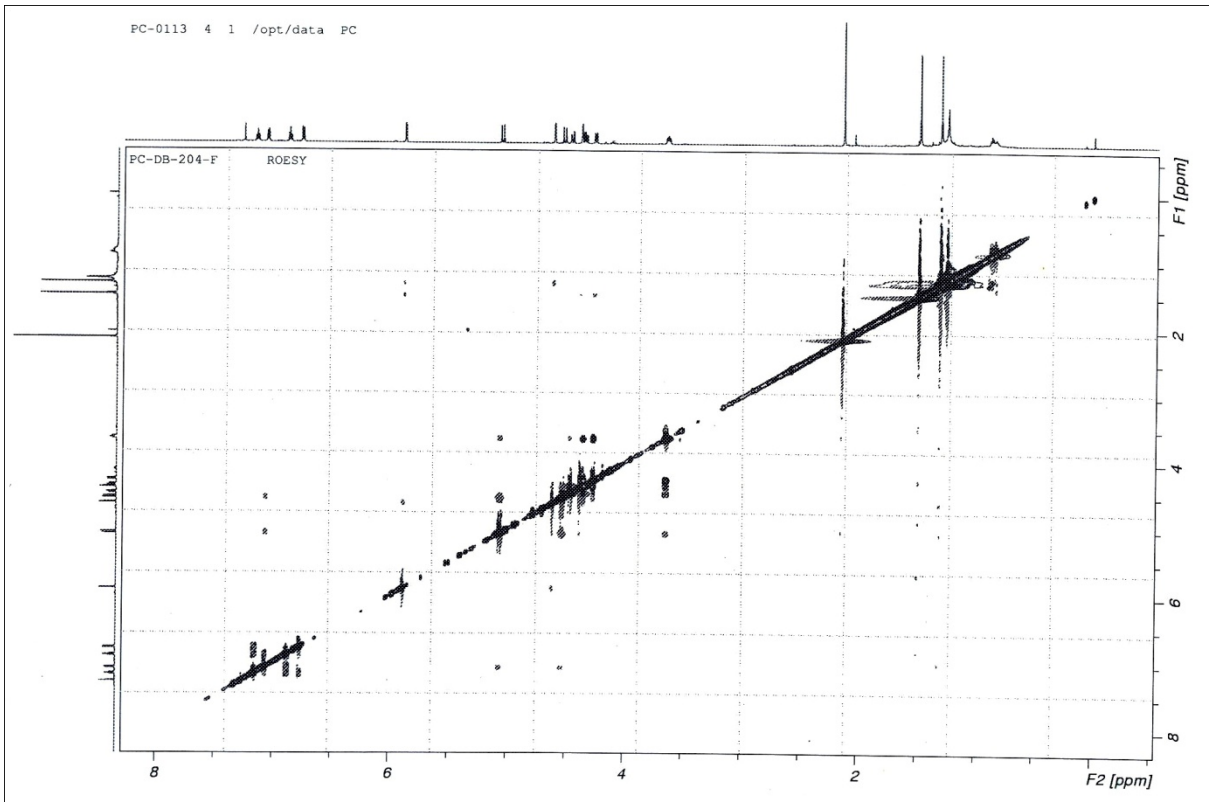


^{13}C NMR spectrum of compound 9b:

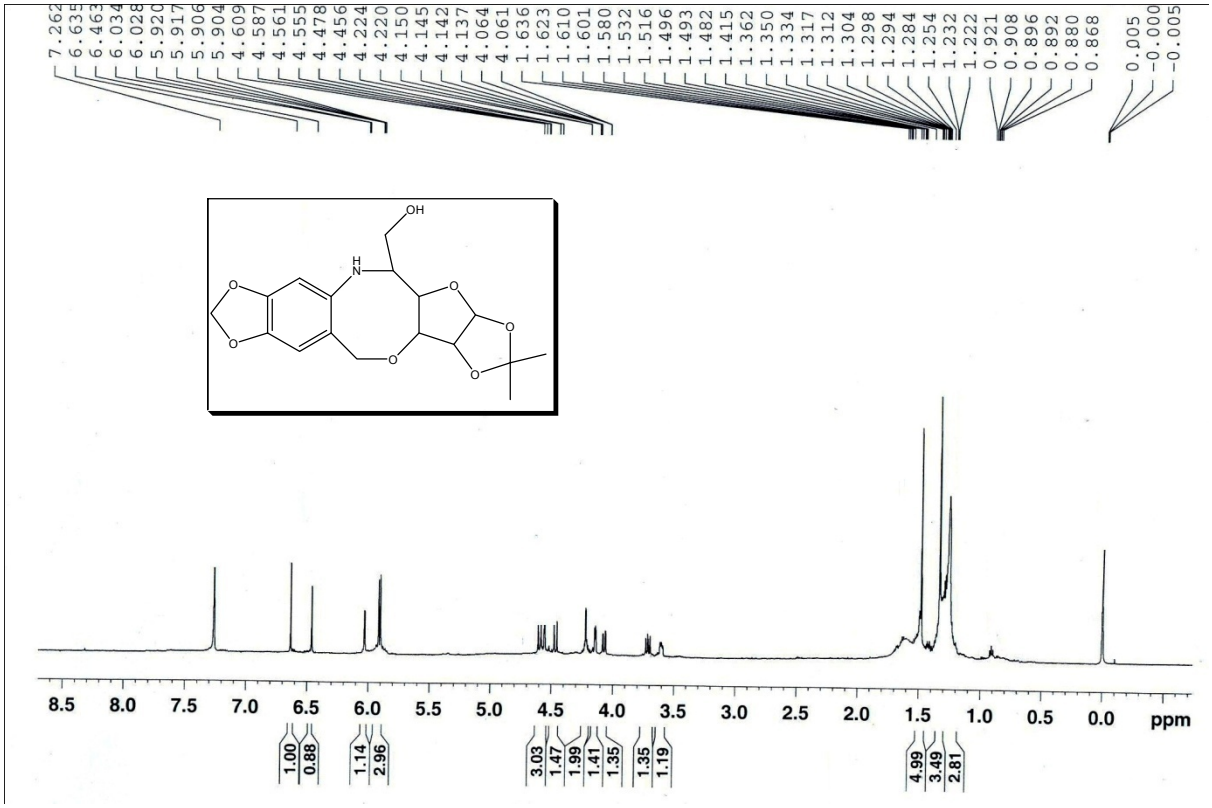


ROESY spectra of compound 9b

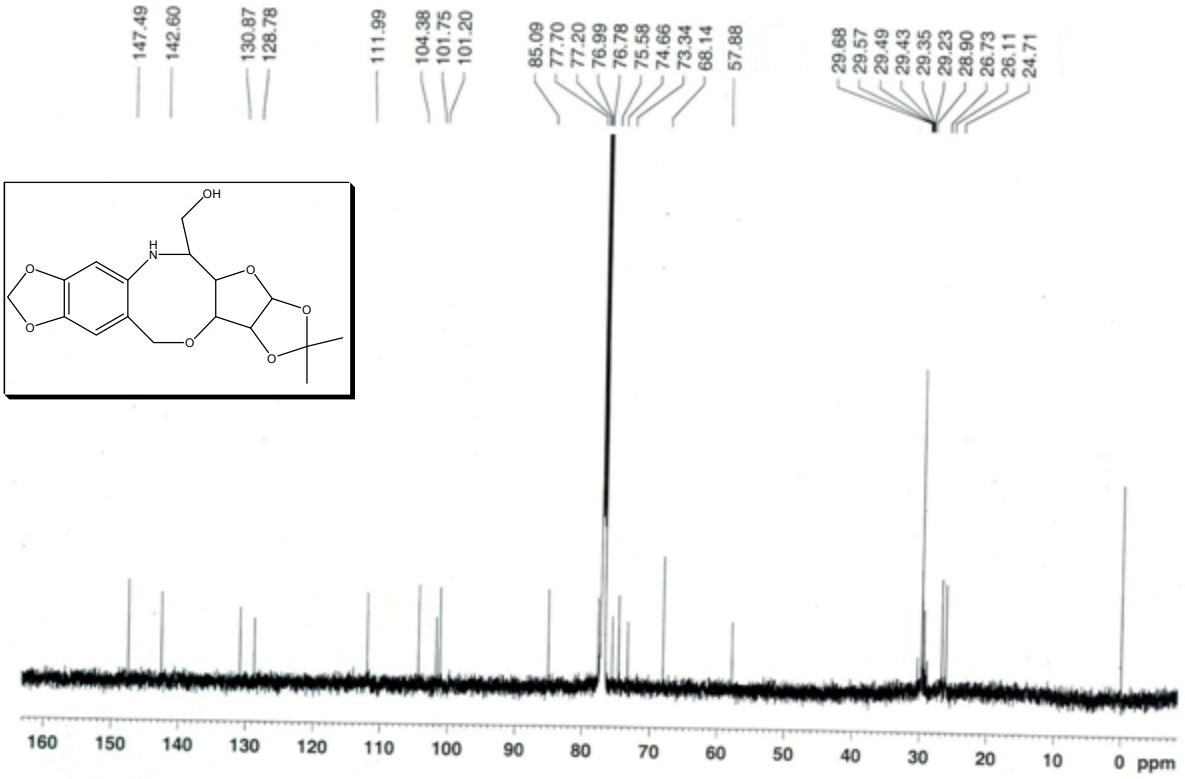




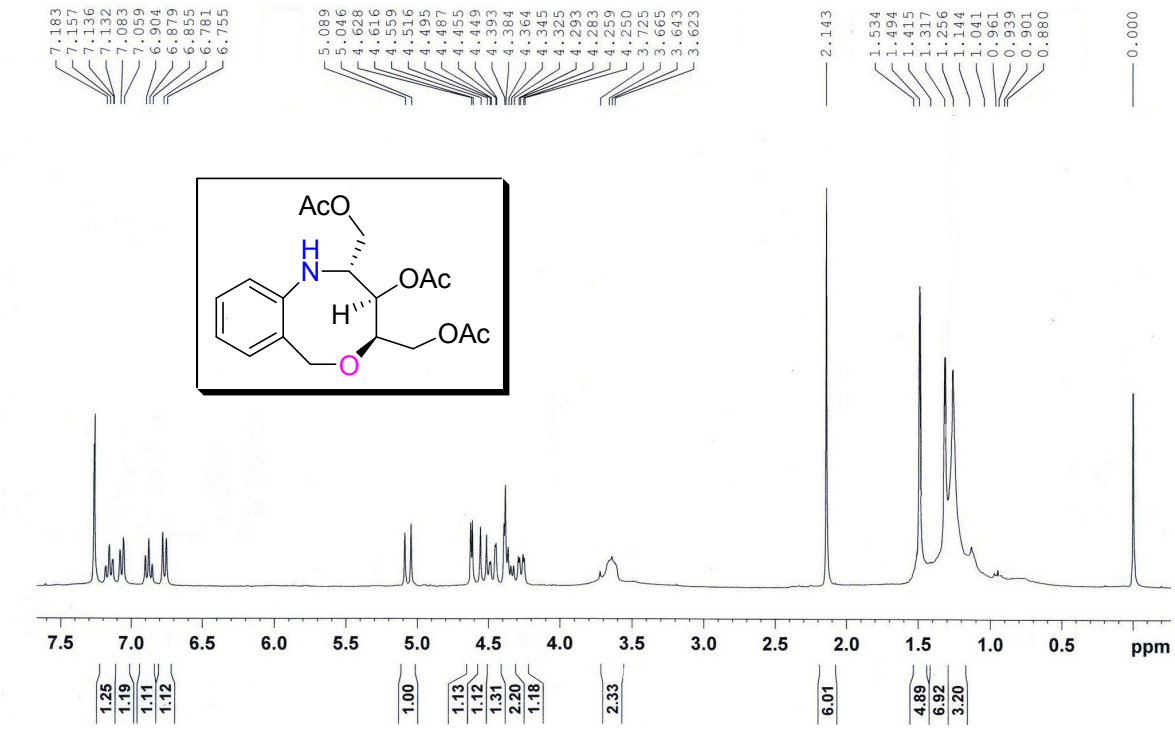
^{1}H NMR spectrum of compound 9d:



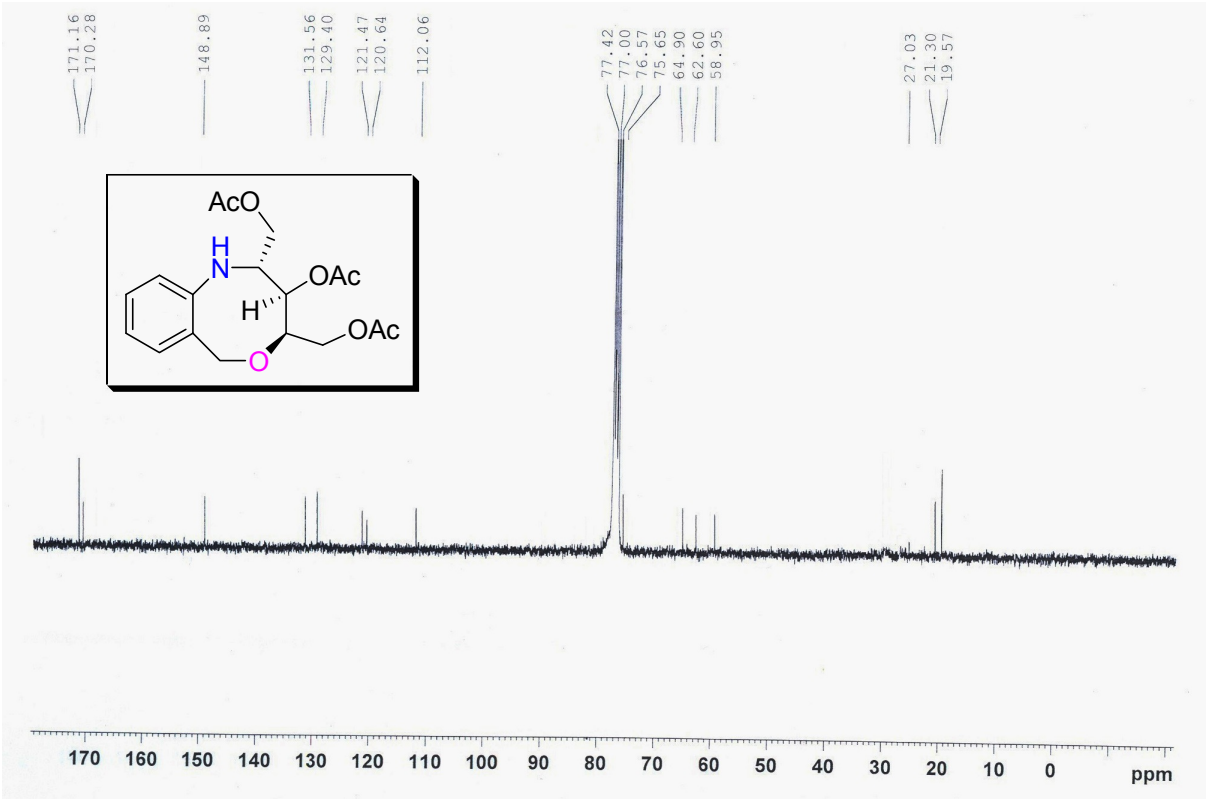
^{13}C NMR spectrum of compound 9d:



^{1}H NMR of compound 10



^{13}CNMR of compound 10



DFT calculation data: Computational details

All geometries and energies were computed using the B3LYP (A. D. Becke, J. Chem. Phys., 1993, 98, 5648. ; C. Lee, W. Yang and R. G. Parr, Phys. Rev. B, 1988, 37, 785.) density functional theory method as implemented in the Gaussian 09 package. The triple-ζ plus polarization basis set 6-311G+(2d,p) was used for all the atoms. The geometry optimization was performed *in vaccuo.* Transition states were determined by potential energy surface scan of the reaction coordinates (Figure S1). The compound 8b contains a freely rotatable side-chain. The orientation of this group in 8b was optimized by applying rotation over the bond that connects it to the eight member ring, followed by geometry optimization to a local minima. The complete 360° scan over that bond was performed in 6 steps. Total energy in each local minima was plotted in the graphs shown in Figure S2. Lowest point in these curves indicate the conformations with optimum side chain orientation. Coordinates for all the optimized geometries are given at the end.

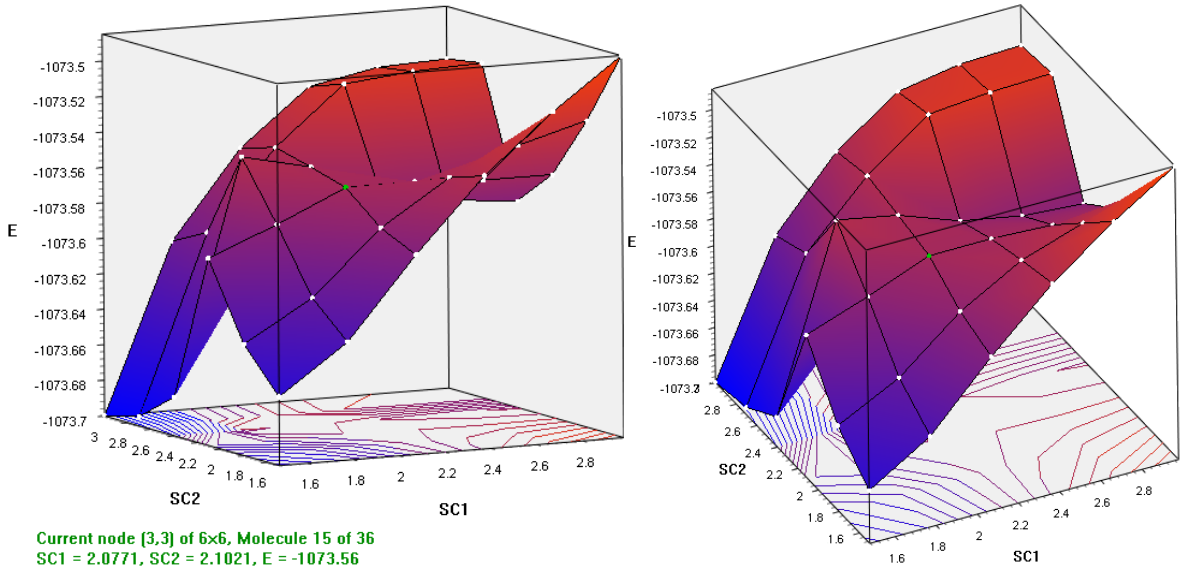
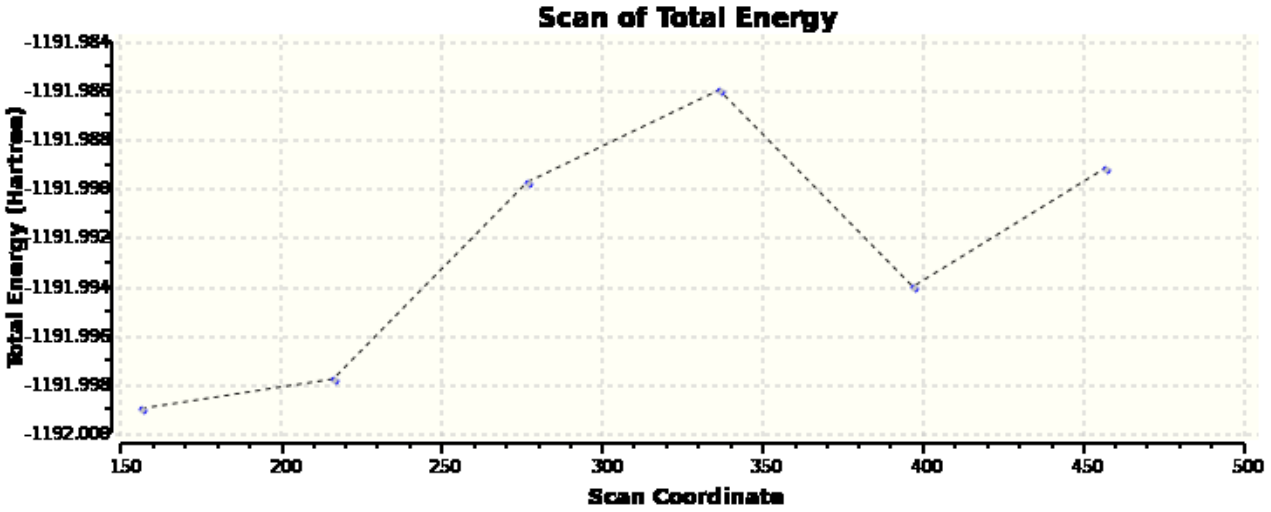


Figure S1 Gaussian scan grid. Potential energy surface generated by perturbing the bond lengths along the reaction coordinate of cycloaddition that results in the trans conformation. The node at (3,3) indicates the transition state. Two different views are shown.

A



B

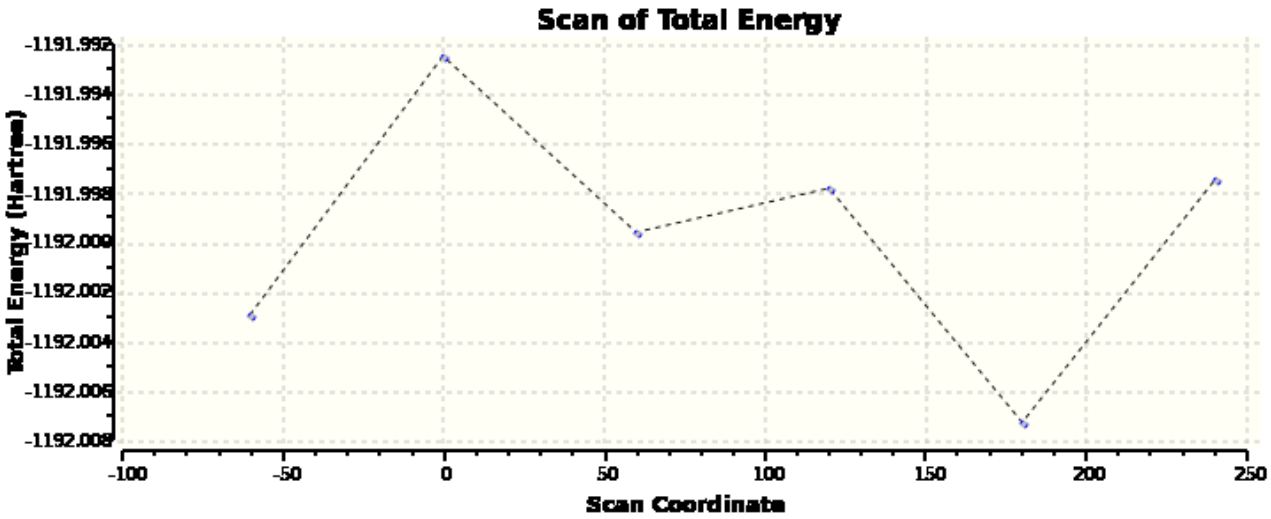
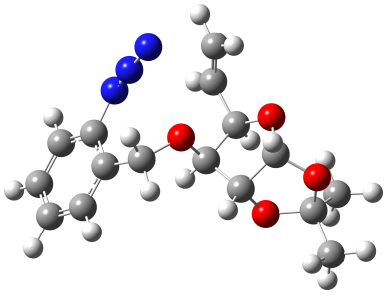


Figure S2 Relaxed z-matrix optimization applying the rotation over the bond connection the acetoxy methyl groups to the eight member ring in cis-9b (A) and in trans-9b (B).

Optimized coordinates of the stable reactant for cis-cycloaddition



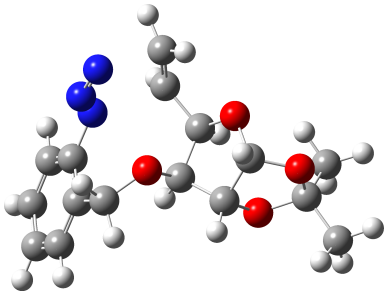
E (Hartree) = -1073.58352375

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.428291	-1.903694	1.108568
2	6	0	3.855496	-2.753949	0.178827
3	6	0	2.892007	-2.261488	-0.677162
4	6	0	2.492635	-0.932441	-0.642383
5	6	0	3.087170	-0.077045	0.283388
6	6	0	4.044290	-0.581988	1.155380
7	6	0	1.412049	-0.476732	-1.599043
8	8	0	0.434747	0.384993	-0.991261
9	6	0	-0.369415	-0.151044	0.070413
10	6	0	-0.972034	1.041053	0.834452
11	6	0	-0.018844	2.151741	1.155201
12	7	0	2.766824	1.294726	0.514970
13	6	0	-1.598203	-0.746074	-0.581665
14	6	0	-2.431763	0.487306	-0.965971
15	8	0	-2.018836	1.511755	-0.066059
16	8	0	-2.412505	-1.350831	0.442699
17	6	0	-3.800129	-0.948439	0.280178
18	8	0	-3.766775	0.064417	-0.748089

19	6	0	0.105111	3.225734	0.406424
20	6	0	-4.298230	-0.359978	1.583453
21	6	0	-4.617905	-2.115929	-0.231089
22	1	0	0.175168	-0.831340	0.703615
23	1	0	-1.426390	0.657317	1.734607
24	1	0	0.564223	2.017373	2.044621
25	1	0	2.427639	-2.921974	-1.384160
26	1	0	4.477490	0.093747	1.862573
27	1	0	1.826308	0.111132	-2.406751
28	1	0	0.937788	-1.349229	-2.032194
29	1	0	-1.405106	-1.424970	-1.395593
30	1	0	-2.342286	0.831006	-1.976344
31	1	0	-0.505616	3.365113	-0.459676
32	1	0	0.750419	4.034088	0.690122
33	1	0	-3.735000	0.533174	1.808050
34	1	0	-4.178599	-1.080540	2.381225
35	1	0	-5.342746	-0.095105	1.487916
36	1	0	-4.185668	-2.484776	-1.151576
37	1	0	-5.631649	-1.793665	-0.425668
38	1	0	-4.623530	-2.911046	0.502268
39	1	0	5.171363	-2.266776	1.789810
40	1	0	4.145015	-3.784058	0.129944
41	7	0	2.396441	2.013341	-0.462215
42	7	0	1.943158	2.811313	-1.074891

Optimized coordinates of transition state for cis-cycloaddition



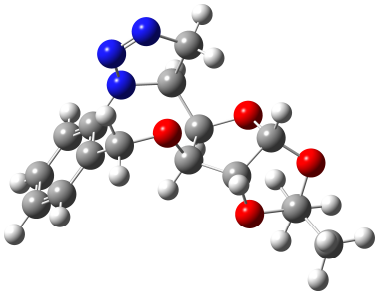
E (Hartree) = -1073.55219857

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.142659	-1.816884	1.338180
2	6	0	3.849608	-2.660776	0.284055
3	6	0	3.018481	-2.222474	-0.732815
4	6	0	2.486574	-0.945654	-0.719820
5	6	0	2.804966	-0.088304	0.330742
6	6	0	3.622091	-0.536396	1.354846
7	6	0	1.536075	-0.507740	-1.811058
8	8	0	0.420639	0.250138	-1.304434
9	6	0	-0.302081	-0.305834	-0.198220
10	6	0	-0.701244	0.822753	0.761006
11	6	0	0.333326	1.864208	1.142869
12	7	0	2.255640	1.226509	0.470526
13	6	0	-1.641320	-0.724166	-0.758723
14	6	0	-2.399841	0.601557	-0.906428
15	8	0	-1.813495	1.467246	0.066018
16	8	0	-2.394027	-1.379965	0.282481
17	6	0	-3.751356	-0.861937	0.319545
18	8	0	-3.737023	0.258247	-0.592502

19	6	0	0.290562	3.101878	0.566769
20	6	0	-4.059802	-0.390624	1.725144
21	6	0	-4.714902	-1.898584	-0.218648
22	1	0	0.228092	-1.100839	0.295852
23	1	0	-1.082212	0.360051	1.657972
24	1	0	0.765208	1.736936	2.112310
25	1	0	2.768978	-2.887664	-1.537088
26	1	0	3.849073	0.140612	2.151934
27	1	0	2.025330	0.155780	-2.509470
28	1	0	1.185777	-1.379736	-2.351422
29	1	0	-1.585070	-1.315629	-1.656868
30	1	0	-2.377254	1.065007	-1.871356
31	1	0	-0.472418	3.322414	-0.145668
32	1	0	0.772627	3.931578	1.047115
33	1	0	-3.400427	0.426272	1.976769
34	1	0	-3.921734	-1.204512	2.424097
35	1	0	-5.081490	-0.038701	1.775891
36	1	0	-4.412559	-2.190354	-1.215408
37	1	0	-5.711582	-1.481474	-0.263808
38	1	0	-4.714155	-2.770083	0.422125
39	1	0	4.776474	-2.147465	2.136277
40	1	0	4.250910	-3.653892	0.257012
41	7	0	2.379061	2.041476	-0.571732
42	7	0	1.828856	2.972049	-0.925000

Optimized coordinates of the intermediate product for cis-cycloaddition



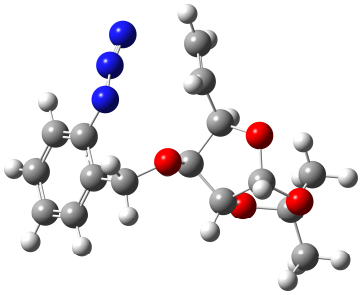
E (Hartree) = -1073.65319993

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.634059	-2.204261	-1.277434
2	6	0	-3.502763	-2.798215	-0.036850
3	6	0	-2.891076	-2.107022	0.994996
4	6	0	-2.414323	-0.821691	0.805154
5	6	0	-2.563569	-0.221036	-0.442702
6	6	0	-3.169777	-0.915938	-1.472528
7	6	0	-1.702913	-0.097130	1.930965
8	8	0	-0.481000	0.548520	1.491688
9	6	0	0.330565	-0.201137	0.584761
10	6	0	0.376391	0.485214	-0.792662
11	6	0	-0.742400	1.494241	-1.091796
12	7	0	-2.115231	1.105928	-0.683046
13	6	0	1.772393	-0.171990	1.042168
14	6	0	2.418346	1.033687	0.350115
15	8	0	1.614570	1.258897	-0.813838
16	8	0	2.435755	-1.272616	0.377847
17	6	0	3.693172	-0.839520	-0.200611
18	8	0	3.714670	0.590730	0.017295

19	6	0	-0.578930	2.833121	-0.333977
20	6	0	3.681171	-1.144520	-1.683792
21	6	0	4.852256	-1.448768	0.558336
22	1	0	-0.000604	-1.220862	0.498700
23	1	0	0.434648	-0.261808	-1.567388
24	1	0	-0.736105	1.679543	-2.154544
25	1	0	-2.772941	-2.577014	1.952248
26	1	0	-3.287627	-0.426306	-2.416913
27	1	0	-2.313076	0.697173	2.327675
28	1	0	-1.472857	-0.800828	2.720987
29	1	0	1.892540	-0.202857	2.110869
30	1	0	2.500025	1.933750	0.927555
31	1	0	0.210760	2.815860	0.390809
32	1	0	-0.450800	3.671535	-0.998489
33	1	0	2.884873	-0.585329	-2.150768
34	1	0	3.527363	-2.203897	-1.838669
35	1	0	4.622195	-0.846215	-2.126090
36	1	0	4.771341	-1.193594	1.606231
37	1	0	5.785133	-1.060090	0.173634
38	1	0	4.835855	-2.525093	0.452470
39	1	0	-4.103443	-2.732242	-2.082931
40	1	0	-3.865008	-3.793223	0.127388
41	7	0	-2.633210	2.076942	0.249543
42	7	0	-1.863150	3.013851	0.413278

Optimized coordinates of the stable reactant for trans-cycloaddition



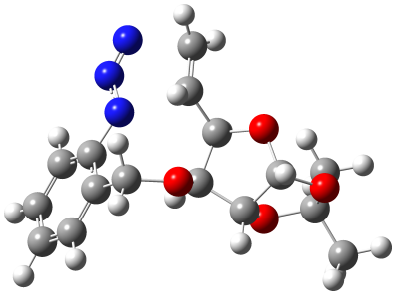
E (Hartree) = -1073.58328259

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.031861	-1.865784	1.331595
2	6	0	3.424846	-2.872059	0.607593
3	6	0	2.567762	-2.538862	-0.427993
4	6	0	2.316396	-1.220950	-0.761212
5	6	0	2.935683	-0.213568	-0.024747
6	6	0	3.786937	-0.541817	1.016556
7	6	0	1.382815	-0.892138	-1.910059
8	8	0	0.299207	0.010139	-1.606699
9	6	0	-0.359058	-0.065967	-0.339678
10	6	0	-0.898088	1.336000	-0.004402
11	6	0	-0.023807	2.468581	-0.438246
12	7	0	2.630438	1.120328	-0.420584
13	6	0	-1.630391	-0.857827	-0.534753
14	6	0	-2.592294	0.137360	-1.197414
15	8	0	-2.137940	1.422074	-0.782231
16	8	0	-2.245214	-1.041622	0.758912
17	6	0	-3.663890	-0.735439	0.686064
18	8	0	-3.852195	-0.201940	-0.641684

19	6	0	0.414535	3.414490	0.368654
20	6	0	-3.994355	0.314014	1.727050
21	6	0	-4.472962	-2.010126	0.803321
22	1	0	0.271418	-0.461471	0.436759
23	1	0	-1.135966	1.383182	1.046419
24	1	0	0.203525	2.468869	-1.482428
25	1	0	2.080820	-3.317193	-0.982697
26	1	0	4.266754	0.236526	1.575233
27	1	0	1.929066	-0.399721	-2.700265
28	1	0	0.981786	-1.820949	-2.297543
29	1	0	-1.510918	-1.788673	-1.063716
30	1	0	-2.667229	0.096571	-2.265327
31	1	0	0.961624	4.257129	-0.004989
32	1	0	0.163545	3.441305	1.412044
33	1	0	-3.463210	1.223222	1.490158
34	1	0	-3.706056	-0.038293	2.708364
35	1	0	-5.056424	0.519766	1.713523
36	1	0	-4.161511	-2.706777	0.036693
37	1	0	-5.523162	-1.789370	0.669770
38	1	0	-4.316278	-2.458051	1.775453
39	1	0	4.695361	-2.103291	2.138827
40	1	0	3.607169	-3.899998	0.846430
41	7	0	2.779945	2.018016	0.456526
42	7	0	2.662884	2.934879	1.065048

Optimized coordinates of transition state for trans-cycloaddition



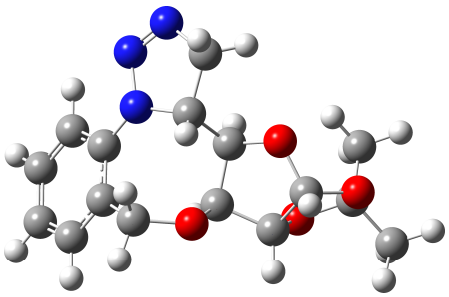
E (Hartree) = -1073.55908695

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.990218	-1.674748	-1.499677
2	6	0	-3.716125	-2.660765	-0.570008
3	6	0	-2.943097	-2.347354	0.532192
4	6	0	-2.449391	-1.068797	0.725947
5	6	0	-2.710306	-0.085496	-0.227635
6	6	0	-3.486234	-0.399957	-1.336455
7	6	0	-1.651690	-0.732877	1.961138
8	8	0	-0.216947	-0.576010	1.767753
9	6	0	0.346026	-0.454796	0.457574
10	6	0	0.649266	1.014295	0.133172
11	6	0	-0.305599	2.012636	0.718515
12	7	0	-2.120665	1.185357	-0.020200
13	6	0	1.726954	-1.050602	0.574718
14	6	0	2.575657	0.062211	1.197271
15	8	0	1.925636	1.273337	0.805711
16	8	0	2.286413	-1.125192	-0.755616
17	6	0	3.652821	-0.633438	-0.751613
18	8	0	3.837825	-0.090740	0.574906

19	6	0	-0.379016	3.289870	0.229886
20	6	0	3.782111	0.461243	-1.790079
21	6	0	4.618952	-1.785460	-0.930140
22	1	0	-0.245232	-0.935075	-0.299442
23	1	0	0.771551	1.144716	-0.928894
24	1	0	-0.590676	1.808688	1.725788
25	1	0	-2.726916	-3.101773	1.263404
26	1	0	-3.694175	0.356948	-2.062995
27	1	0	-2.027569	0.185200	2.386266
28	1	0	-1.764190	-1.521271	2.689432
29	1	0	1.755654	-1.993809	1.090428
30	1	0	2.706412	0.034651	2.260040
31	1	0	-0.734324	4.082817	0.857826
32	1	0	0.222060	3.582025	-0.608975
33	1	0	3.140042	1.283528	-1.513677
34	1	0	3.498061	0.080635	-2.761972
35	1	0	4.804145	0.814421	-1.823604
36	1	0	4.445318	-2.524959	-0.160113
37	1	0	5.635359	-1.425581	-0.847101
38	1	0	4.472798	-2.241617	-1.900037
39	1	0	-4.591253	-1.895745	-2.359158
40	1	0	-4.098357	-3.652776	-0.698906
41	7	0	-2.546985	2.188173	-0.752685
42	7	0	-2.184177	3.253903	-0.941282

Optimized coordinates of the intermediate product for trans-cycloaddition



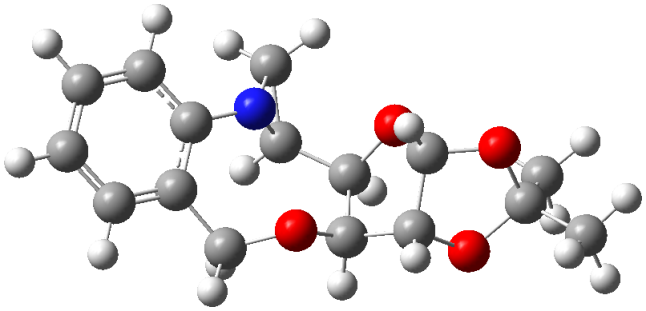
E (Hartree) = -1073.66145233

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.060239	-1.238006	-1.629506
2	6	0	-3.864416	-2.370348	-0.859704
3	6	0	-3.054555	-2.280565	0.251662
4	6	0	-2.440931	-1.090139	0.620615
5	6	0	-2.617940	0.043137	-0.179742
6	6	0	-3.441763	-0.051745	-1.302193
7	6	0	-1.632631	-1.070354	1.898049
8	8	0	-0.184487	-0.980788	1.739709
9	6	0	0.373036	-0.792051	0.434976
10	6	0	0.430909	0.706636	0.096852
11	6	0	-0.679118	1.511281	0.746821
12	7	0	-1.991211	1.262926	0.115512
13	6	0	1.831415	-1.149711	0.581501
14	6	0	2.490668	0.105709	1.163598
15	8	0	1.650287	1.184016	0.736163
16	8	0	2.403973	-1.183351	-0.744080
17	6	0	3.674416	-0.482031	-0.760778
18	8	0	3.757436	0.144635	0.541540

19	6	0	-0.526502	3.022374	0.489168
20	6	0	3.637087	0.570373	-1.848388
21	6	0	4.814213	-1.470823	-0.881599
22	1	0	-0.121985	-1.375095	-0.320510
23	1	0	0.482642	0.868057	-0.967673
24	1	0	-0.683799	1.300248	1.797273
25	1	0	-2.897491	-3.146980	0.864315
26	1	0	-3.589886	0.815670	-1.904750
27	1	0	-1.939644	-0.239193	2.515002
28	1	0	-1.817668	-1.981446	2.445657
29	1	0	2.004829	-2.055912	1.133671
30	1	0	2.620583	0.135541	2.226450
31	1	0	-0.742124	3.612891	1.367342
32	1	0	0.440500	3.288554	0.100075
33	1	0	2.859495	1.283765	-1.621577
34	1	0	3.439067	0.103516	-2.803697
35	1	0	4.585404	1.089291	-1.887902
36	1	0	4.754554	-2.192018	-0.077693
37	1	0	5.758899	-0.948894	-0.814179
38	1	0	4.752162	-1.989291	-1.828834
39	1	0	-4.688822	-1.276512	-2.496869
40	1	0	-4.333360	-3.297887	-1.117546
41	7	0	-2.348967	2.387984	-0.693334
42	7	0	-1.588813	3.335827	-0.525492

Optimized coordinates for cis-7b



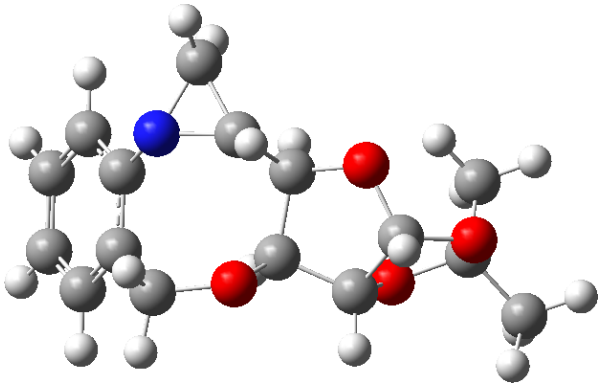
E (Hartree) = -965.39446217

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.048288	0.530260	-0.825869
2	6	0	5.190319	-0.797121	-0.470220
3	6	0	4.095028	-1.482638	0.027011
4	6	0	2.869358	-0.863831	0.189541
5	6	0	2.734358	0.479675	-0.167888
6	6	0	3.828533	1.163297	-0.676897
7	6	0	1.705768	-1.650035	0.762903
8	8	0	0.471413	-1.398594	0.058053
9	6	0	-0.669277	-0.931016	0.782816
10	6	0	-0.675717	0.602951	1.018381
11	6	0	0.703466	1.154589	1.163551
12	7	0	1.486393	1.087014	-0.059031
13	6	0	-1.812457	-1.105216	-0.186078
14	6	0	-1.793777	0.164550	-1.042647
15	8	0	-1.282913	1.173813	-0.164819

16	8	0	-3.049466	-0.932769	0.539929
17	6	0	-3.957220	-0.093800	-0.223196
18	8	0	-3.159948	0.388614	-1.330149
19	6	0	1.141049	2.410185	0.455236
20	6	0	-4.402408	1.060994	0.649268
21	6	0	-5.087264	-0.929054	-0.786704
22	1	0	-0.819216	-1.477958	1.702324
23	1	0	-1.293106	0.827903	1.873985
24	1	0	1.205260	0.939737	2.090201
25	1	0	4.195297	-2.519058	0.288352
26	1	0	3.711461	2.188308	-0.965070
27	1	0	1.916938	-2.707411	0.678411
28	1	0	1.581910	-1.422526	1.816945
29	1	0	-1.775920	-2.028620	-0.735096
30	1	0	-1.231744	0.130700	-1.952990
31	1	0	0.422277	2.941746	-0.128761
32	1	0	1.914826	2.984798	0.930724
33	1	0	-3.538168	1.650584	0.912729
34	1	0	-4.879502	0.682180	1.543273
35	1	0	-5.098567	1.684089	0.103669
36	1	0	-4.679159	-1.737062	-1.378703
37	1	0	-5.714766	-0.315070	-1.418210
38	1	0	-5.677369	-1.342521	0.020145
39	1	0	5.882229	1.075070	-1.222133
40	1	0	6.131594	-1.295239	-0.585918

Optimized coordinates for trans-7b



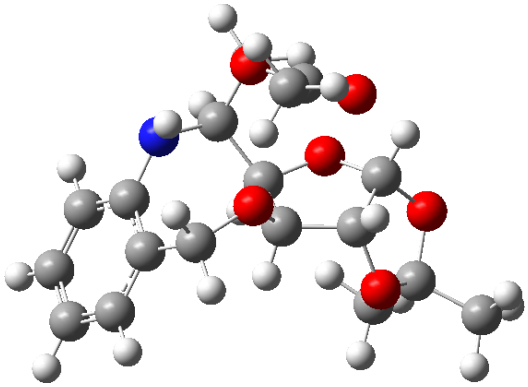
E (Hartree) = -965.39916197

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.030076	-0.992586	1.621883
2	6	0	3.867745	-2.059488	0.759855
3	6	0	3.137063	-1.881933	-0.403386
4	6	0	2.575407	-0.658520	-0.718237
5	6	0	2.725968	0.411198	0.168339
6	6	0	3.459342	0.233719	1.331423
7	6	0	1.824502	-0.461259	-2.015075
8	8	0	0.417429	-0.106397	-1.873649
9	6	0	-0.225924	-0.345241	-0.622577
10	6	0	-0.268684	0.959859	0.207450
11	6	0	0.750122	1.965027	-0.262884
12	7	0	2.181490	1.650714	-0.182221
13	6	0	-1.681335	-0.621509	-0.910620

14	6	0	-2.371418	0.744759	-0.923025
15	8	0	-1.567511	1.560989	-0.064069
16	8	0	-2.248953	-1.213542	0.280831
17	6	0	-3.521198	-0.592253	0.596642
18	8	0	-3.638563	0.492588	-0.353985
19	6	0	1.632671	2.651067	0.741764
20	6	0	-3.463150	-0.050571	2.009621
21	6	0	-4.652625	-1.564946	0.341078
22	1	0	0.219495	-1.156610	-0.075204
23	1	0	-0.195348	0.748221	1.262004
24	1	0	0.453643	2.480741	-1.148670
25	1	0	3.007071	-2.704676	-1.079948
26	1	0	3.593424	1.060869	1.998105
27	1	0	2.268164	0.350106	-2.571292
28	1	0	1.880519	-1.367089	-2.602749
29	1	0	-1.842696	-1.222252	-1.787880
30	1	0	-2.503906	1.211246	-1.879191
31	1	0	1.961662	3.656648	0.579076
32	1	0	1.500682	2.363552	1.768645
33	1	0	-2.695206	0.705532	2.061232
34	1	0	-3.239782	-0.852781	2.700099
35	1	0	-4.413122	0.397308	2.269201
36	1	0	-4.606358	-1.911155	-0.682542
37	1	0	-5.601477	-1.071735	0.501999
38	1	0	-4.566147	-2.412858	1.007144
39	1	0	4.597074	-1.110420	2.524018
40	1	0	4.301283	-3.012692	0.984977

Optimized coordinates for cis-9b



E (Hartree) = -1206.19200639

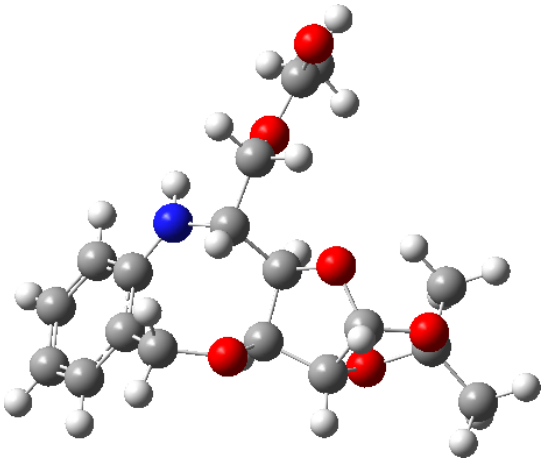
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.383973
3	6	0	1.202770	0.000000	2.065303
4	6	0	2.408176	0.005088	1.380878
5	6	0	2.406806	0.020127	-0.012684
6	6	0	1.197167	0.015800	-0.689432
7	6	0	3.715362	-0.021561	2.148508
8	8	0	4.700790	-0.925570	1.588170
9	6	0	4.207806	-2.238352	1.272161
10	6	0	3.927984	-2.440240	-0.237876
11	6	0	4.173100	-1.253220	-1.203796
12	7	0	3.621705	0.034566	-0.751320
13	6	0	5.210341	-3.328738	1.658558

14	6	0	5.623844	-4.046710	0.354598
15	8	0	4.764697	-3.540702	-0.673681
16	8	0	4.525313	-4.349595	2.420929
17	6	0	4.469599	-5.594062	1.685852
18	8	0	5.402631	-5.419281	0.605567
19	6	0	5.639021	-1.017412	-1.589763
20	6	0	3.069088	-5.816125	1.145062
21	6	0	4.970892	-6.711734	2.574077
22	1	0	3.309224	-2.430207	1.834669
23	1	0	2.900521	-2.748452	-0.356451
24	1	0	3.685898	-1.543758	-2.126739
25	1	0	1.205372	-0.018060	3.138555
26	1	0	1.215247	0.044166	-1.759652
27	1	0	4.191676	0.949567	2.139948
28	1	0	3.522454	-0.298799	3.177482
29	1	0	6.039087	-2.934721	2.213618
30	1	0	6.641617	-3.907186	0.068040
31	1	0	6.164184	-1.951275	-1.657385
32	1	0	5.673120	-0.486120	-2.525814
33	1	0	2.814308	-5.025211	0.455048
34	1	0	2.358652	-5.829272	1.960585
35	1	0	3.029378	-6.756813	0.612525
36	1	0	5.966870	-6.467311	2.915123
37	1	0	5.002922	-7.637606	2.016228
38	1	0	4.318048	-6.823926	3.429242
39	1	0	-0.926916	-0.001649	-0.538186
40	1	0	-0.924279	-0.007307	1.925991
41	8	0	6.303871	-0.122669	-0.649554
42	6	0	7.124724	-0.600192	0.308690
43	8	0	7.421769	-1.765766	0.396407

44	6	0	7.601310	0.502857	1.202389
45	1	0	7.813393	1.387804	0.621409
46	1	0	6.803238	0.723675	1.899882
47	1	0	8.473157	0.178839	1.748593
48	1	0	4.350677	0.564103	-0.313250

Optimized coordinates for trans-9b



E (Hartree) = -1206.19200639

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.384847
3	6	0	1.212621	0.000000	2.038683
4	6	0	2.426597	0.006826	1.360964

5	6	0	2.426137	-0.020708	-0.040452
6	6	0	1.186155	-0.017207	-0.693634
7	6	0	3.693711	0.094864	2.180258
8	8	0	4.558809	-1.077077	2.173440
9	6	0	4.288905	-2.176345	1.295057
10	6	0	4.955310	-1.936040	-0.064301
11	6	0	4.912971	-0.480276	-0.504637
12	7	0	3.557491	-0.053087	-0.840200
13	6	0	5.123901	-3.296914	1.865315
14	6	0	6.545936	-2.993930	1.377186
15	8	0	6.361882	-2.243601	0.173859
16	8	0	4.817648	-4.503465	1.132867
17	6	0	6.041931	-5.190044	0.764074
18	8	0	7.097684	-4.272692	1.130068
19	6	0	5.769127	-0.283080	-1.744622
20	6	0	6.042597	-5.419834	-0.732940
21	6	0	6.201286	-6.448135	1.591277
22	1	0	3.242446	-2.414250	1.225044
23	1	0	4.555350	-2.586477	-0.820572
24	1	0	5.353930	0.101669	0.285353
25	1	0	1.231232	0.005185	3.111563
26	1	0	1.172072	-0.028499	-1.765988
27	1	0	4.288933	0.933546	1.850381
28	1	0	3.430107	0.262430	3.213493
29	1	0	5.021543	-3.419642	2.928590
30	1	0	7.184730	-2.462409	2.052519
31	1	0	5.777506	0.750503	-2.054250
32	1	0	6.769811	-0.634885	-1.570057
33	1	0	6.034929	-4.464020	-1.234522
34	1	0	5.169175	-5.991721	-1.016164

35	1	0	6.936854	-5.956826	-1.019810
36	1	0	6.173819	-6.194782	2.642445
37	1	0	7.151316	-6.914123	1.368166
38	1	0	5.397309	-7.137568	1.371315
39	1	0	-0.925872	0.004552	-0.540703
40	1	0	-0.917969	0.002112	1.935867
41	8	0	5.140369	-1.089143	-2.789565
42	6	0	5.782408	-1.228865	-3.978556
43	8	0	6.820312	-0.671644	-4.213144
44	6	0	5.015252	-2.143553	-4.888139
45	1	0	4.917580	-3.114291	-4.418597
46	1	0	4.019425	-1.747991	-5.042896
47	1	0	5.531189	-2.234991	-5.830284
48	1	0	3.371168	-0.156081	-1.816843