8	4.127910	-2.989026	-0.027970	1	-4.439647	-1.319030	-1.586016
1	4.481736	-0.972911	-0.074024				

TS-C_6, OH-exo-**20**

B3PW91/LanL2DZ, E_t = -768.665819618 a. u.

6	1.139322	-0.627798	-0.899423	8	4.317669	-2.196726	0.457762
6	1.572246	0.716141	-0.930174	1	4.709395	0.317242	0.281204
6	2.591674	0.900507	0.167903	1	4.150009	0.479491	-1.384570
6	1.975519	-1.296201	0.213861	80	-1.126955	-0.178559	-0.136061
6	2.101148	-0.124787	1.222783	8	-2.739403	-1.091215	1.379273
6	3.438404	-1.365084	-0.346026	6	-3.610712	-1.178774	0.426297
6	3.857080	0.142890	-0.385814	8	-3.342777	-0.814168	-0.785636
1	0.870006	-1.158002	-1.814701	1	-4.606917	-1.574005	0.654306
1	1.469763	1.402656	-1.761812	8	-0.138904	1.880010	-0.085999
1	2.757974	1.929036	0.481448	6	-0.177745	3.147744	0.350075
1	1.619183	-2.257248	0.585628	8	0.798182	3.922232	0.341491
1	1.157294	0.167426	1.693896	1	-1.167968	3.462558	0.729231
1	2.838970	-0.298757	2.015069	1	4.410993	-1.835412	1.362185
1	3.467933	-1.839185	-1.329022				

TS-C5, OH-exo-**20**

B3PW91/LanL2DZ, E_t = -768.663906672 a. u.

6	-1.616146	0.357885	-0.927179	1	-1.144213	-0.035854	1.705404
6	-0.987849	-0.906871	-0.858139	1	-2.727337	-0.765100	2.044511
6	-1.725939	-1.660389	0.275665	1	-4.108115	-0.292507	-1.394956
6	-2.661093	0.415676	0.154751	8	-5.032731	-0.391733	0.381372
6	-2.028343	-0.489098	1.245983	1	-3.730146	-2.577016	0.444097
6	-3.807279	-0.543719	-0.376314	1	-3.140324	-2.494196	-1.220888
6	-3.160204	-1.963512	-0.264292	80	1.190442	-0.124880	-0.121487
1	-1.617470	1.023038	-1.782138	8	2.911396	-0.811659	1.402492
1	-0.646415	-1.417451	-1.760664	6	3.789385	-0.763273	0.453567
1	-1.208421	-2.527246	0.689075	8	3.475962	-0.430767	-0.757160
1	-3.012747	1.409797	0.422268	1	4.832884	-1.008360	0.681271

8	-0.099416	1.762885	-0.121674
6	-0.213169	3.056617	0.219831
8	-1.269999	3.710661	0.149558
1	0.730758	3.508050	0.579064
1	-4.881701	-0.567716	1.331984

TS-C6, OH-exo-**21**

B3PW91/LanL2DZ, E_t = -768.668006059 a. u.

6	1.140996	-0.604159	-0.912138
6	1.572628	0.741843	-0.908053
6	2.589262	0.899222	0.195393
6	1.977824	-1.294835	0.187374
6	2.110152	-0.154442	1.226645
6	3.442875	-1.341244	-0.369754
6	3.854827	0.156682	-0.381213
1	0.871543	-1.109009	-1.841904
1	1.470699	1.448194	-1.723066
1	2.762303	1.918605	0.533108
1	1.610706	-2.260260	0.542448
1	1.168857	0.123233	1.713084
1	2.865045	-0.368495	1.988015
1	3.472675	-1.801824	-1.367264
8	4.353575	-2.036019	0.530413
1	4.700204	0.289218	0.300350
1	4.150252	0.516662	-1.370817
80	-1.117805	-0.180238	-0.122548
8	-2.731994	-1.161758	1.339666
6	-3.601282	-1.217516	0.381283
8	-3.333320	-0.806482	-0.814569
1	-4.595301	-1.626727	0.594307
8	-0.154803	1.884550	-0.054168
6	-0.227473	3.159674	0.355104
8	0.721481	3.965323	0.312756
1	-1.221660	3.450184	0.743852
1	4.170739	-2.997009	0.531138

TS-C5, OH-exo-**21**

B3PW91/LanL2DZ, E_t = -768.667286373 a. u.

6	-1.595202	0.337846	-0.949269
6	-0.974893	-0.930411	-0.871676
6	-1.722249	-1.672823	0.263936
6	-2.629358	0.411362	0.142615
6	-2.014069	-0.500256	1.235088
6	-3.790489	-0.538153	-0.366234
6	-3.161101	-1.955718	-0.278483
1	-1.594178	0.994925	-1.810597
1	-0.627819	-1.445688	-1.769447
1	-1.219927	-2.548954	0.676065
1	-2.950372	1.416251	0.414326
1	-1.124456	-0.061458	1.700049
1	-2.741558	-0.757847	2.009323
1	-4.114736	-0.270875	-1.381121
8	-4.923659	-0.500481	0.542633
1	-3.745961	-2.547424	0.432635
1	-3.151379	-2.477240	-1.240164
80	1.185583	-0.133119	-0.109503
8	2.938799	-0.701180	1.409965
6	3.806783	-0.692209	0.448984

8	3.475123	-0.439279	-0.774560	8	-1.351583	3.658037	0.118785
1	4.857178	-0.898888	0.683288	1	0.646521	3.532028	0.588633
8	-0.091957	1.770587	-0.170103	1	-5.365205	0.372171	0.508228
6	-0.267508	3.047205	0.197589				

TS-C6-OH-endo-**20**

B3PW91/LanL2DZ, E_t = -768.666419693 a. u.

6	1.220149	-0.735428	-0.616854	8	3.701822	-2.316466	-0.852761
6	1.701417	0.589737	-0.746149	1	4.693737	0.294179	0.801076
6	2.608423	0.867276	0.425530	1	4.288336	0.207362	-0.914088
6	1.916798	-1.297804	0.642454	80	-1.089609	-0.165349	-0.105721
6	1.989168	-0.030550	1.530615	8	-2.862742	-0.844144	1.344055
6	3.435142	-1.454676	0.280474	6	-3.639707	-1.053875	0.329865
6	3.901116	0.026687	0.095192	8	-3.247923	-0.859454	-0.886979
1	0.996039	-1.353887	-1.487762	1	-4.661276	-1.406709	0.509897
1	1.723031	1.176274	-1.656980	8	-0.036779	1.856894	-0.255463
1	2.778520	1.919300	0.644129	6	-0.082321	3.179572	-0.030381
1	1.480142	-2.197994	1.075680	8	0.906739	3.934124	-0.086406
1	1.016412	0.331347	1.880523	1	-1.092236	3.557067	0.215893
1	2.652794	-0.147296	2.393788	1	3.340732	-1.922824	-1.672759
1	3.962408	-1.942188	1.104228				

TS-C5-OH-endo-**20**

B3PW91/LanL2DZ, E_t = -768.663672815 a. u.

6	-1.733988	0.332712	-0.671624	1	-1.073151	-2.526543	0.912118
6	-1.080171	-0.924667	-0.667454	1	-2.964875	1.376932	0.831295
6	-1.657014	-1.677705	0.553497	1	-0.949468	-0.030374	1.897718
6	-2.640489	0.383999	0.528618	1	-2.481704	-0.779689	2.410332
6	-1.872464	-0.501103	1.543945	1	-4.575216	-0.521529	0.971208
6	-3.825280	-0.612905	0.182208	8	-4.560200	-0.303197	-1.026585
6	-3.139674	-2.017952	0.198297	1	-3.586305	-2.670153	0.956415
1	-1.853003	0.985447	-1.527801	1	-3.231804	-2.525966	-0.769007
1	-0.838951	-1.439832	-1.599947	80	1.152656	-0.118818	-0.169360

8	2.948237	-0.819450	1.272460
6	3.784945	-0.711383	0.293179
8	3.414541	-0.338313	-0.890588
1	4.841674	-0.942245	0.468611
8	-0.167710	1.751120	-0.085786
6	-0.265258	3.041401	0.278840
8	-1.333200	3.676970	0.337163
1	0.706862	3.505200	0.531002
1	-4.043525	-0.537189	-1.823524

TS-C6-OH-endo-**21**

B3PW91/LanL2DZ, E_t =-768.665888538 a. u.

6	0.668780	-0.813978	-0.654530
6	1.058727	0.535143	-0.807307
6	1.926379	0.907848	0.365120
6	1.382276	-1.292323	0.628094
6	1.357445	-0.002534	1.486278
6	2.897973	-1.357401	0.276319
6	3.276054	0.144628	0.062109
1	0.568927	-1.468043	-1.519952
1	1.038544	1.102816	-1.729623
1	2.022417	1.974700	0.555574
1	1.003519	-2.209834	1.078568
1	0.356267	0.297429	1.811982
1	2.013867	-0.050670	2.361719
1	3.454753	-1.785689	1.122507
8	3.068546	-2.191037	-0.901455
1	4.044815	0.482137	0.765846
1	3.639973	0.321827	-0.955883
80	-1.674030	-0.393506	-0.242214
8	-3.405967	-1.205606	1.212868
6	-4.186218	-1.393069	0.198504
8	-3.816680	-1.127788	-1.012936
1	-5.193705	-1.789019	0.369911
8	-0.796695	1.720768	-0.343744
6	-0.935972	3.026218	-0.079978
8	0.004351	3.845182	-0.060511
1	-1.978249	3.335176	0.126543
1	4.016125	-2.348102	-1.082054

TS-C5-OH-endo-**21**

B3PW91/LanL2DZ, E_t =-768.667401447 a. u.

6	-0.185756	1.150037	-0.669876
6	-0.115102	1.085213	0.744091
6	1.395253	1.068445	1.074364
6	1.221349	1.119062	-1.202840
6	1.946671	0.262431	-0.133145
6	1.825152	2.538285	-0.830312
6	1.935442	2.492828	0.728611
1	-1.027158	1.509944	-1.249338
1	-0.835459	1.615155	1.371285
1	1.663603	0.714079	2.070579
1	1.321352	0.851415	-2.252183
1	1.638929	-0.787999	-0.156687
1	3.037474	0.313118	-0.216750
1	2.807736	2.613266	-1.301673
8	1.102897	3.675854	-1.360871
1	2.973366	2.610764	1.057842

1	1.347547	3.288866	1.200783
80	-1.048993	-1.137887	1.006158
8	-0.535094	-3.067914	2.349565
6	-1.776802	-3.165696	2.695035
8	-2.676458	-2.335671	2.271522
1	-2.079510	-3.976241	3.367445
8	-0.910557	-0.833593	-1.259953
6	-0.962508	-1.406441	-2.475041
8	-0.588154	-0.858605	-3.527459
1	-1.375066	-2.432784	-2.463664
1	0.271848	3.827536	-0.867752

TS-C6-OAc-exo-**20**

B3PW91/LanL2DZ, E_t = -921.245758563 a. u.

6	0.554533	-0.087488	-0.954298
6	0.592270	1.323319	-0.889854
6	1.549183	1.710384	0.211218
6	1.566125	-0.567846	0.110860
6	1.395098	0.523776	1.198474
6	2.961176	-0.187834	-0.460444
6	2.959836	1.369515	-0.406200
1	0.422619	-0.609755	-1.903556
1	0.283667	2.006567	-1.671756
1	1.441279	2.723389	0.592880
1	1.497335	-1.610242	0.421201
1	0.420921	0.510110	1.697643
1	2.187914	0.494650	1.950653
1	3.145144	-0.580205	-1.464230
8	3.972544	-0.762274	0.449106
1	3.743213	1.724169	0.270954
1	3.130621	1.826308	-1.384429
80	-1.723899	-0.357180	-0.139230
8	-2.866628	-1.893455	1.304607
6	-3.740867	-2.131462	0.381226
8	-3.688740	-1.559782	-0.778609
1	-4.551399	-2.839389	0.587386
8	-1.357038	1.885527	0.031586
6	-1.768552	3.066730	0.518117
8	-1.073493	4.099840	0.529871
1	-2.799375	3.052057	0.918930
6	5.272253	-0.848755	-0.020663
8	5.602167	-0.454291	-1.147696
6	6.176033	-1.468170	1.010239
1	7.182903	-1.571447	0.603879
1	6.203276	-0.840777	1.907773
1	5.790784	-2.448574	1.308145

TS-C5-OAc-exo-**20**

B3PW91/LanL2DZ, E_t = -921.243442578 a. u.

6	-0.847946	0.474411	-0.993847
6	-0.312578	-0.827919	-0.881872
6	-1.118296	-1.498658	0.257837
6	-1.897272	0.635287	0.082384
6	-1.348443	-0.289378	1.201466
6	-3.086917	-0.242251	-0.437073
6	-2.564258	-1.703973	-0.300588
1	-0.796008	1.112387	-1.867686
1	0.017409	-1.381792	-1.762691
1	-0.677501	-2.395544	0.694965

1	-2.172651	1.658504	0.326688
1	-0.438751	0.105871	1.664924
1	-2.093477	-0.484425	1.977566
1	-3.408991	0.004254	-1.452565
8	-4.214303	0.022227	0.473874
1	-3.184899	-2.255032	0.414096
1	-2.581380	-2.242854	-1.251682
80	1.895617	-0.165890	-0.100860
8	3.528239	-0.889590	1.500554
6	4.423837	-0.969200	0.570669
8	4.158465	-0.691092	-0.665249
1	5.442004	-1.275721	0.835388
8	0.730327	1.799232	-0.212662
6	0.677410	3.102703	0.107228
8	-0.340056	3.811305	-0.004105
1	1.633297	3.507508	0.489043
6	-5.482798	-0.306175	0.022599
8	-5.683600	-0.830021	-1.081489
6	-6.525065	0.066393	1.040881
1	-7.511846	-0.230963	0.683948
1	-6.310214	-0.422426	1.996688
1	-6.504985	1.147492	1.214647

product-Hg-C6, OAc-exo-**20**

B3PW91/LanL2DZ, E_t = -921.277689890 a. u.

6	-0.403585	-0.173898	-0.797886
6	-0.456794	1.323925	-0.429349
6	0.639135	1.468473	0.648062
6	0.697058	-0.745442	0.139710
6	0.526883	0.124438	1.407759
6	2.042600	-0.223026	-0.412581
6	1.996569	1.299428	-0.089196
1	-0.200715	-0.341266	-1.861212
1	-0.318945	2.008210	-1.272019
1	0.564702	2.388049	1.229946
1	0.688999	-1.828108	0.271734
1	-0.437412	-0.014746	1.907689
1	1.332764	-0.024442	2.132096
1	2.191716	-0.432255	-1.475886
8	3.123513	-0.900989	0.336863
1	2.824326	1.561344	0.577243
1	2.084066	1.921934	-0.985032
80	-2.433328	-1.016037	-0.407667
8	-3.980316	-2.217253	1.029355
6	-4.884192	-2.172843	0.107629
8	-4.668625	-1.601595	-1.035010
1	-5.863585	-2.628896	0.294951
8	-1.818922	1.623945	0.138708
6	-2.193796	2.941406	0.267157
8	-1.500990	3.913261	-0.038452
1	-3.210500	2.988858	0.674783
6	4.389934	-0.882773	-0.218079
8	4.643452	-0.320764	-1.293330
6	5.370001	-1.621047	0.653476
1	6.348864	-1.641190	0.172493
1	5.448321	-1.126962	1.628160
1	5.019571	-2.642780	0.831768

product-Hg-C5, OAc-exo-**20**

B3PW91/LanL2DZ, E_t = -921.275978859 a. u.

6	0.192842	0.763764	-0.529103
6	0.724251	-0.639116	-0.893625
6	-0.175049	-1.590033	-0.056431
6	-0.938055	0.478662	0.485882
6	-0.399723	-0.764408	1.233943
6	-2.096808	-0.123510	-0.337451
6	-1.599594	-1.557859	-0.684607
1	-0.138419	1.362661	-1.383574
1	0.681702	-0.840497	-1.969018
1	0.217505	-2.600627	0.071765
1	-1.239596	1.347261	1.071394
1	0.517626	-0.566052	1.798212
1	-1.145630	-1.202344	1.903572
1	-2.359435	0.464005	-1.222712
8	-3.277141	-0.154377	0.548084
1	-2.250759	-2.300131	-0.208921
1	-1.600431	-1.751323	-1.761376
80	2.884864	-0.682287	-0.330482
8	5.211526	-0.190424	-0.785956
6	5.568490	-0.774117	0.310540
8	4.705089	-1.310197	1.113108
1	6.632674	-0.816458	0.571847
8	1.299501	1.539809	0.126416
6	1.160677	2.905100	0.233986
8	0.187960	3.554688	-0.152002
1	2.056853	3.321403	0.708482
6	-4.513722	-0.310740	-0.052336
8	-4.651286	-0.449035	-1.275867
6	-5.615376	-0.279435	0.971970
1	-6.578249	-0.431941	0.482876
1	-5.451684	-1.056938	1.725280
1	-5.613306	0.684872	1.491094

product-Hg-C6, OH-exo-**20**

B3PW91/LanL2DZ, E_t = -768.697750767 a. u.

6	0.333698	-0.518651	-0.843140
6	0.795597	0.910209	-0.488215
6	1.907415	0.680964	0.558979
6	1.230591	-1.426411	0.039623
6	1.385023	-0.563717	1.316696
6	2.667573	-1.366996	-0.557049
6	3.117153	0.091507	-0.217217
1	0.422103	-0.736736	-1.913089
1	1.132577	1.508418	-1.340100
1	2.144566	1.569235	1.146455
1	0.879550	-2.452084	0.165049
1	0.442270	-0.391820	1.846739
1	2.112823	-0.958281	2.036431
1	2.668726	-1.575469	-1.629471
8	3.554114	-2.388072	-0.017185
1	4.010176	0.065878	0.418104
1	3.372441	0.676401	-1.107359
80	-1.844726	-0.645718	-0.372226
8	-3.671351	-1.169291	1.130074
6	-4.531934	-0.890896	0.206550
8	-4.167504	-0.503090	-0.973492
1	-5.601942	-0.985295	0.426987
8	-0.369297	1.650519	0.113108
6	-0.274398	3.016762	0.240675

8	0.693792	3.699423	-0.098469
1	-1.196461	3.401926	0.691792
1	3.647563	-2.286097	0.951477

product-Hg-C5, OH-exo-**20**

B3PW91/LanL2DZ, E_t = -768.695960784 a. u.

6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.543660
6	1.512201	0.000000	1.901453
6	1.498247	0.000000	-0.370913
6	2.107115	-0.863542	0.761690
6	2.039484	1.416802	-0.021965
6	2.074419	1.405908	1.540413
1	-0.551481	0.828641	-0.455692
1	-0.540594	0.853436	1.965427
1	1.741788	-0.314357	2.921582
1	1.697704	-0.278261	-1.406491
1	1.753701	-1.899668	0.756877
1	3.203912	-0.877271	0.760251
1	1.404481	2.206832	-0.430249
8	3.333536	1.684613	-0.628699
1	3.108997	1.521705	1.888822
1	1.488113	2.218034	1.982981
80	-1.088463	-1.833554	2.196859
8	-2.819195	-3.319117	2.682366
6	-2.035316	-4.269174	3.110955
8	-0.759010	-4.138913	3.138622
1	-2.500923	-5.201035	3.454231
8	-0.664564	-1.261847	-0.477059
6	-1.081496	-1.323986	-1.787849
8	-0.957114	-0.423916	-2.619082
1	-1.541253	-2.302011	-1.972222
1	3.995792	1.029090	-0.329953

product-Hg-C6, OH-exo-**21**

B3PW91/LanL2DZ, E_t =-768.699714659 a. u.

6	0.339945	-0.511231	-0.853066
6	0.793355	0.915673	-0.477395
6	1.900748	0.678264	0.572521
6	1.238643	-1.422193	0.024533
6	1.392002	-0.581616	1.313231
6	2.677611	-1.339745	-0.564785
6	3.116244	0.106085	-0.206828
1	0.430578	-0.713626	-1.926528
1	1.130755	1.526514	-1.320233
1	2.133925	1.559353	1.171982
1	0.881689	-2.448771	0.142913
1	0.450251	-0.425324	1.850997
1	2.137264	-0.996001	1.998170
1	2.676029	-1.534992	-1.647455
8	3.605179	-2.249313	0.100302
1	3.995698	0.042267	0.440678
1	3.382939	0.704487	-1.084316
80	-1.837097	-0.644335	-0.377384
8	-3.658857	-1.270869	1.093808
6	-4.522888	-0.910162	0.202908
8	-4.163155	-0.431424	-0.944933
1	-5.592473	-1.011367	0.422756

8	-0.380522	1.641744	0.126185
6	-0.303647	3.008780	0.253995
8	0.654336	3.705192	-0.086102
1	-1.230251	3.381223	0.706693
1	3.400832	-3.177501	-0.131828

product-Hg-C5, OH-exo-**21**

B3PW91/LanL2DZ, E_t = -768.698676235 a.u.

6	-0.811888	0.640523	-0.539926
6	-0.161736	-0.708535	-0.911897
6	-0.960020	-1.737328	-0.062766
6	-1.907036	0.252323	0.475455
6	-1.258043	-0.933700	1.225928
6	-3.021138	-0.464845	-0.338856
6	-2.384549	-1.838385	-0.683257
1	-1.199162	1.207077	-1.393595
1	-0.200249	-0.914154	-1.986690
1	-0.472658	-2.705614	0.066336
1	-2.274894	1.094793	1.065092
1	-0.363398	-0.654271	1.792931
1	-1.966411	-1.438039	1.889333
1	-3.302764	0.115370	-1.230124
8	-4.203433	-0.723818	0.472276
1	-2.977152	-2.619516	-0.195033
1	-2.364861	-2.043033	-1.758715
80	2.001034	-0.559111	-0.378267
8	4.265772	0.155200	-0.777174
6	4.679893	-0.451904	0.288210
8	3.875564	-1.111306	1.055910
1	5.744798	-0.404813	0.546246
8	0.227084	1.516592	0.104803
6	-0.055684	2.853385	0.255384
8	-1.100301	3.405693	-0.096209
1	0.794289	3.350350	0.737348
1	-4.666238	0.113081	0.679565

product-Hg-C6, OH-endo-**20**

B3PW91/LanL2DŻ, E_t =-768.696472786 a.u.

6	0.407913	-0.668396	-0.609456
6	0.926673	0.767180	-0.384938
6	1.924975	0.615208	0.782171
6	1.163126	-1.504603	0.455353
6	1.265668	-0.502988	1.630105
6	2.665964	-1.599865	0.044529
6	3.163637	-0.125206	0.208532
1	0.543260	-1.024845	-1.636505
1	1.373379	1.239473	-1.265844
1	2.158514	1.556747	1.281371
1	0.725164	-2.480750	0.670439
1	0.295822	-0.218468	2.052325
1	1.912401	-0.853746	2.441836
1	3.187435	-2.274956	0.728592
8	2.918745	-2.189085	-1.256161
1	4.005572	-0.063531	0.904991
1	3.505712	0.295901	-0.745679
80	-1.804383	-0.618911	-0.296985
8	-3.754821	-0.973477	1.095545
6	-4.531719	-0.647172	0.115459

8	-4.065067	-0.310520	-1.044350
1	-5.617470	-0.655005	0.268432
8	-0.238237	1.636445	0.009655
6	-0.076941	3.001908	-0.040713
8	0.951656	3.586317	-0.385248
1	-1.008289	3.487096	0.274161
1	2.617111	-1.594811	-1.972084

product-Hg-C5, OH-endo-**20**

B3PW91/LanL2DZ, E_t = -768.693509352 a. u.

6	-0.934140	0.542271	-0.314985
6	-0.251745	-0.771495	-0.754174
6	-0.909843	-1.845526	0.154033
6	-1.909284	0.097124	0.793443
6	-1.126915	-1.054270	1.470088
6	-3.069664	-0.707746	0.128884
6	-2.376551	-2.034402	-0.325477
1	-1.418565	1.109174	-1.115759
1	-0.371207	-0.976933	-1.823902
1	-0.351265	-2.780094	0.236497
1	-2.262125	0.917717	1.419435
1	-0.198323	-0.725567	1.948471
1	-1.726518	-1.602100	2.205381
1	-3.833030	-0.901917	0.886352
8	-3.803641	-0.012451	-0.911408
1	-2.839734	-2.907673	0.147478
1	-2.447827	-2.177284	-1.411289
80	1.940301	-0.512343	-0.406498
8	4.149160	0.187031	-1.055662
6	4.656902	-0.297700	0.031799
8	3.927732	-0.882876	0.924896
1	5.736963	-0.208893	0.199407
8	0.120633	1.454264	0.253318
6	-0.156305	2.799617	0.358830
8	-1.210141	3.340640	0.024443
1	0.713565	3.310309	0.788705
1	-3.290225	0.031288	-1.742131

product-Hg-C6, OH-endo-**21**

B3PW91/LanL2DZ, E_t = -768.698673625 a. u.

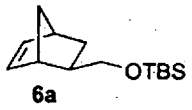
6	0.386128	-0.645323	-0.615089
6	0.953420	0.768605	-0.384686
6	1.944351	0.583581	0.784030
6	1.107230	-1.504949	0.455057
6	1.247771	-0.510949	1.632344
6	2.589645	-1.647242	0.019816
6	3.156321	-0.202116	0.213364
1	0.560004	-1.011560	-1.628682
1	1.419374	1.217456	-1.267006
1	2.211613	1.517405	1.280957
1	0.638049	-2.466681	0.668515
1	0.286213	-0.196626	2.051824
1	1.881156	-0.882977	2.445543
1	3.102198	-2.362387	0.680457
8	2.641082	-2.130691	-1.351974
1	3.989854	-0.186212	0.924273
1	3.512969	0.212974	-0.736852
80	-1.820659	-0.556017	-0.332390

8	-3.766359	-1.066246	1.088723
6	-4.543039	-0.654075	0.146278
8	-4.080108	-0.198901	-0.978838
1	-5.630213	-0.682420	0.289452
8	-0.174920	1.685512	0.009326
6	0.046457	3.040588	-0.033078
8	1.105778	3.583660	-0.354529
1	-0.870234	3.566057	0.260060
1	3.558888	-2.348749	-1.606675

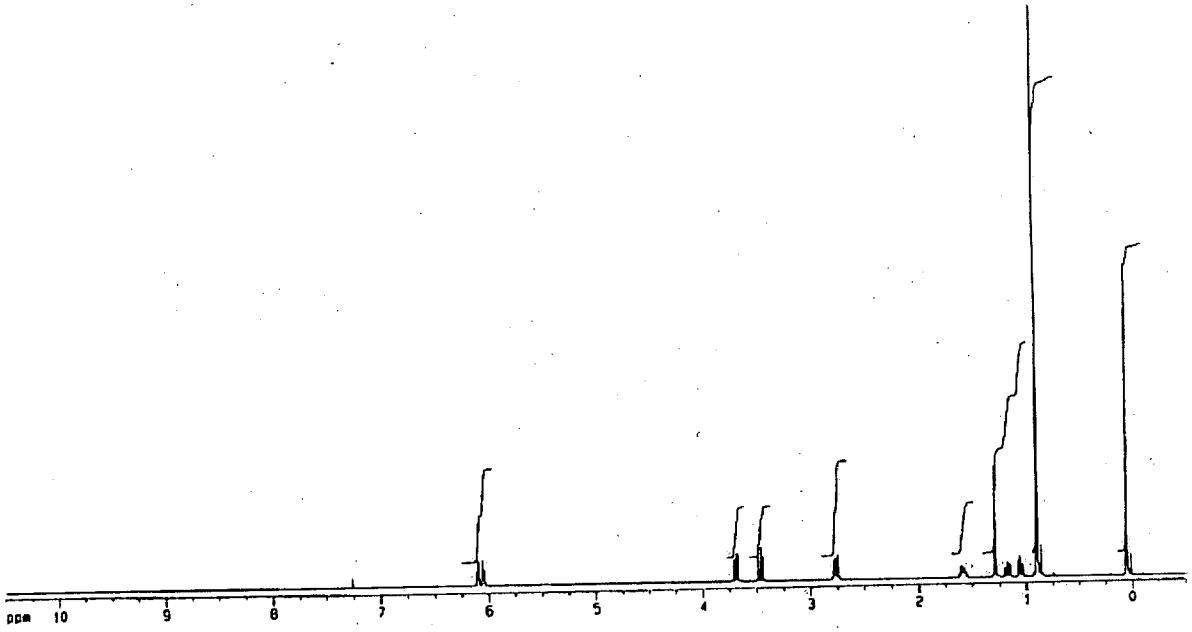
product-Hg-C6, OH-endo-**21**

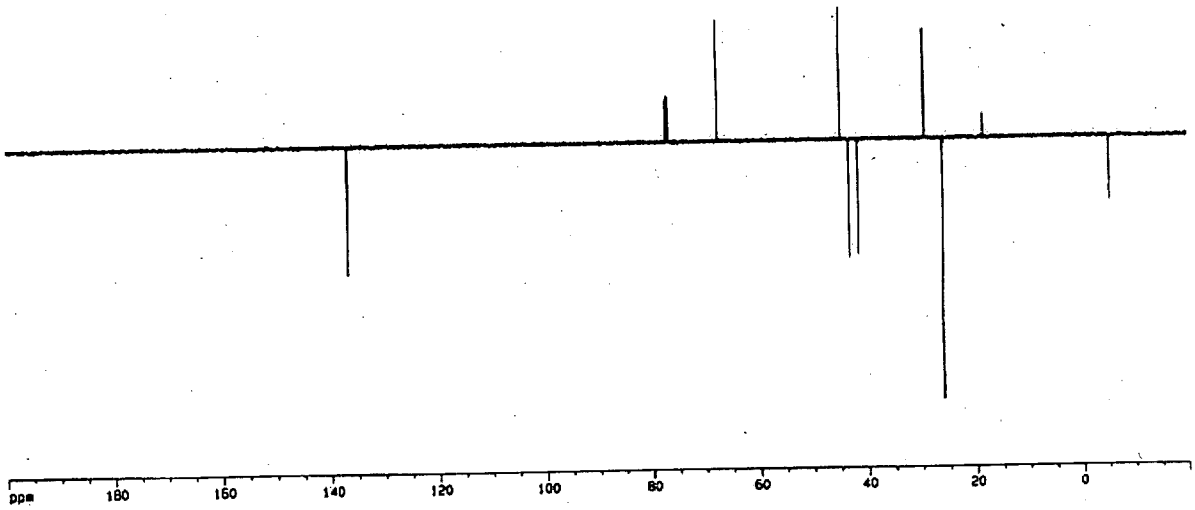
B3PW91/LanL2DZ, E_t =-768.696591056 a.u.

6	-0.944096	0.520104	-0.351887
6	-0.252002	-0.805947	-0.732371
6	-0.901604	-1.846441	0.220532
6	-1.916283	0.112787	0.774423
6	-1.130346	-1.004236	1.502472
6	-3.052777	-0.705518	0.109417
6	-2.367542	-2.065859	-0.248368
1	-1.446571	1.031282	-1.174150
1	-0.380794	-1.054442	-1.790493
1	-0.336164	-2.773056	0.340977
1	-2.281298	0.955043	1.362991
1	-0.206849	-0.645272	1.968464
1	-1.726015	-1.526971	2.259319
1	-3.863892	-0.853092	0.836590
8	-3.554274	0.021962	-1.046592
1	-2.828785	-2.904468	0.288030
1	-2.434249	-2.267567	-1.323658
80	1.937423	-0.514000	-0.409177
8	3.928060	-0.777912	0.968342
6	4.656850	-0.270306	0.029961
8	4.151199	0.121714	-1.095905
1	5.737218	-0.167295	0.189625
8	0.109932	1.457368	0.181101
6	-0.196332	2.788566	0.340224
8	-1.279750	3.314545	0.084012
1	0.684293	3.310945	0.734481
1	-4.382509	-0.377417	-1.376116



6a





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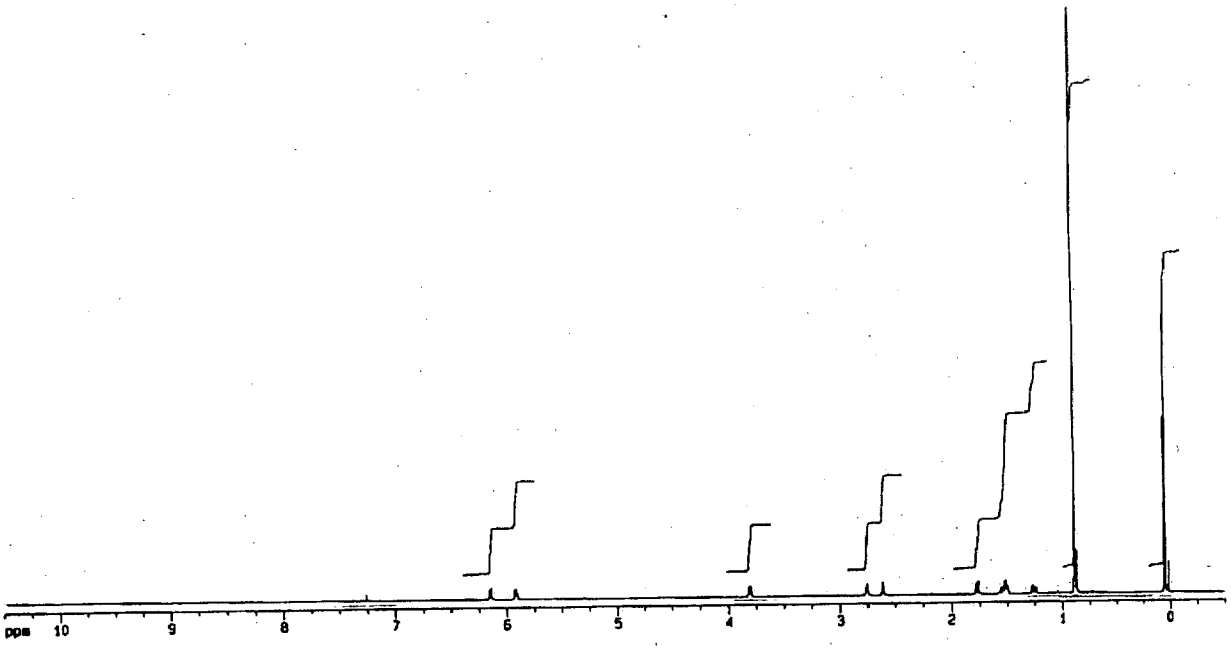

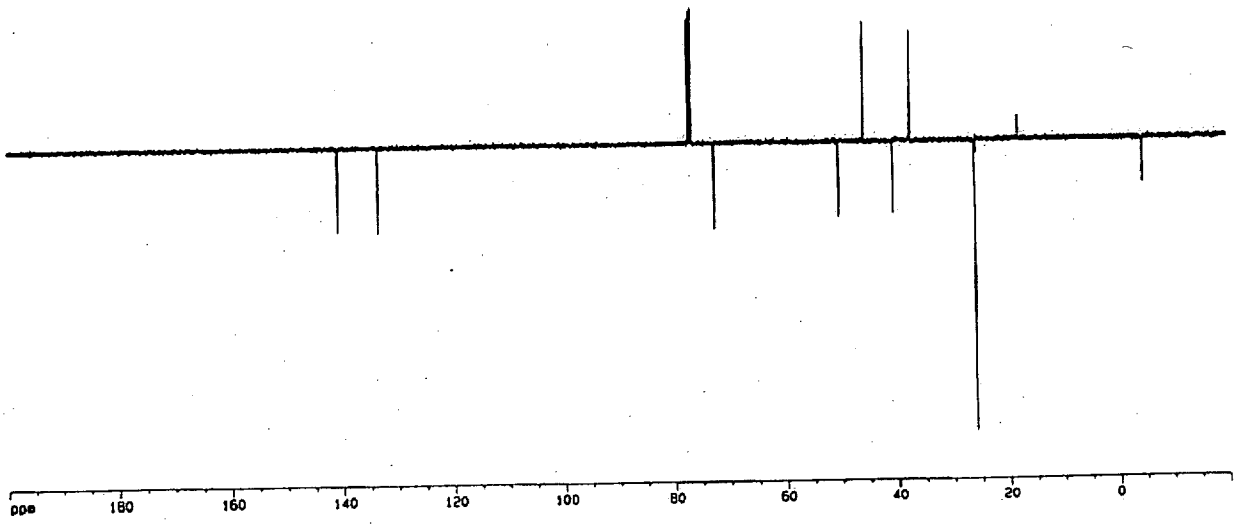

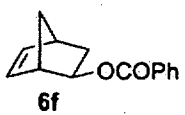

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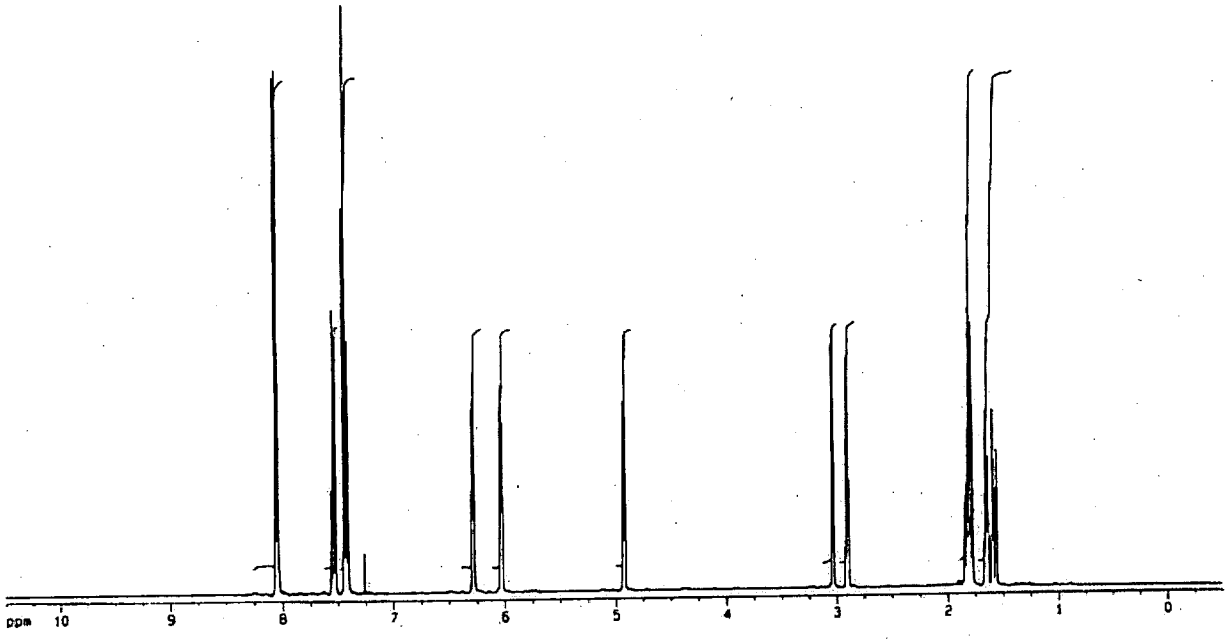
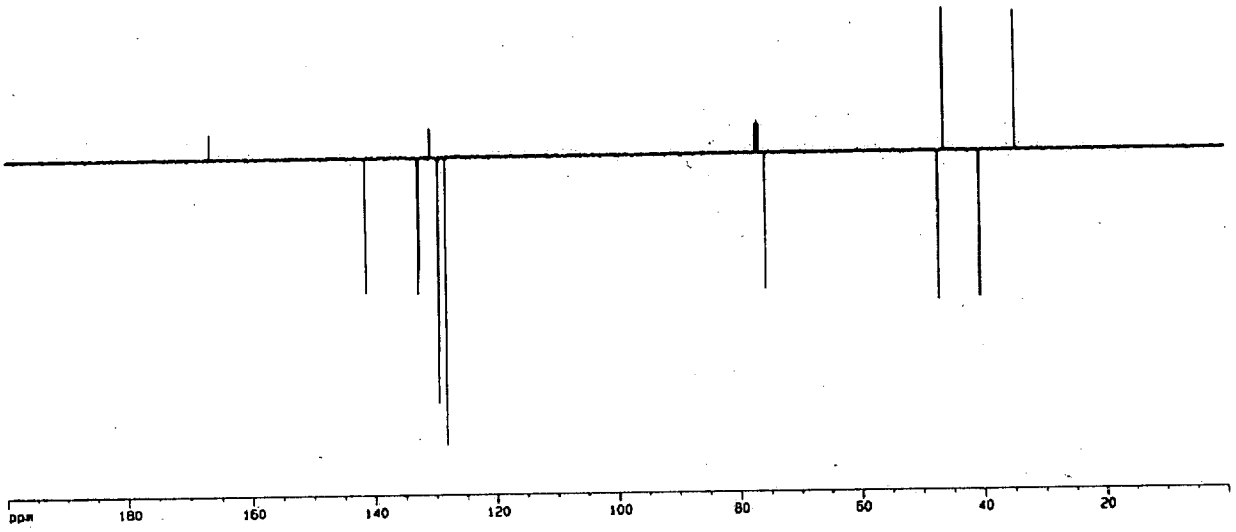
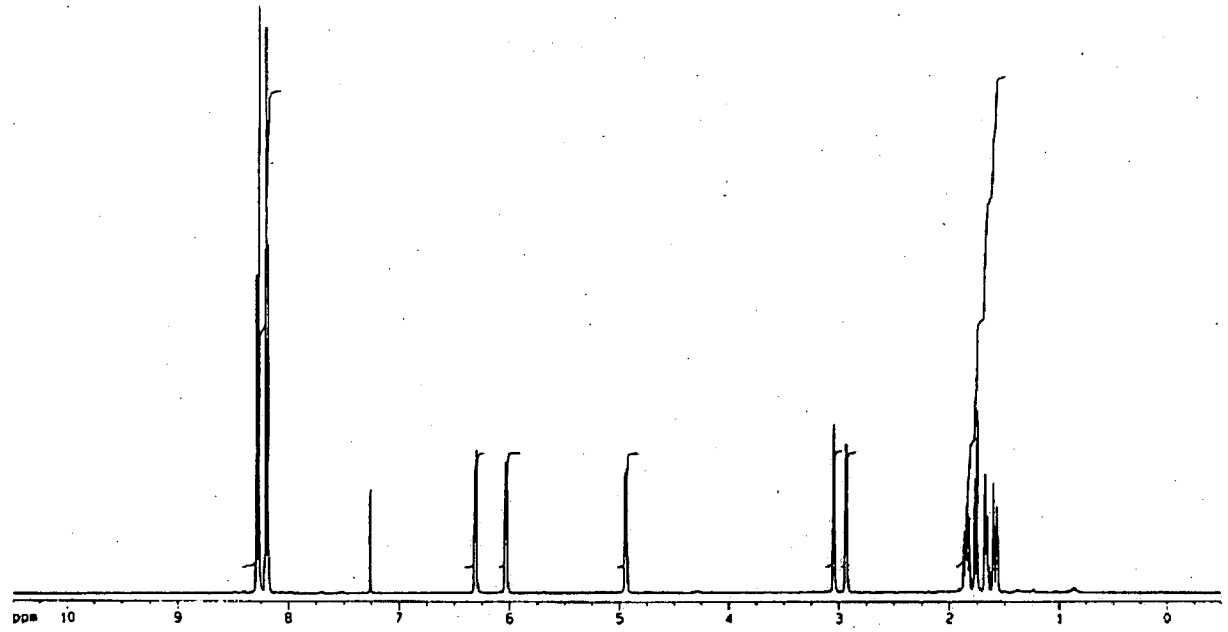
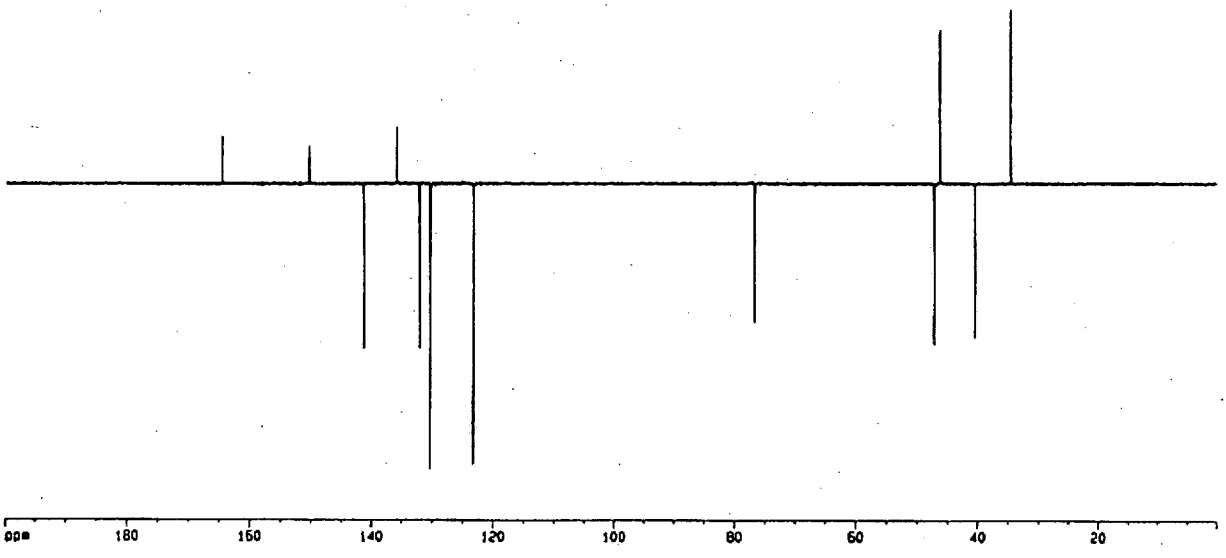


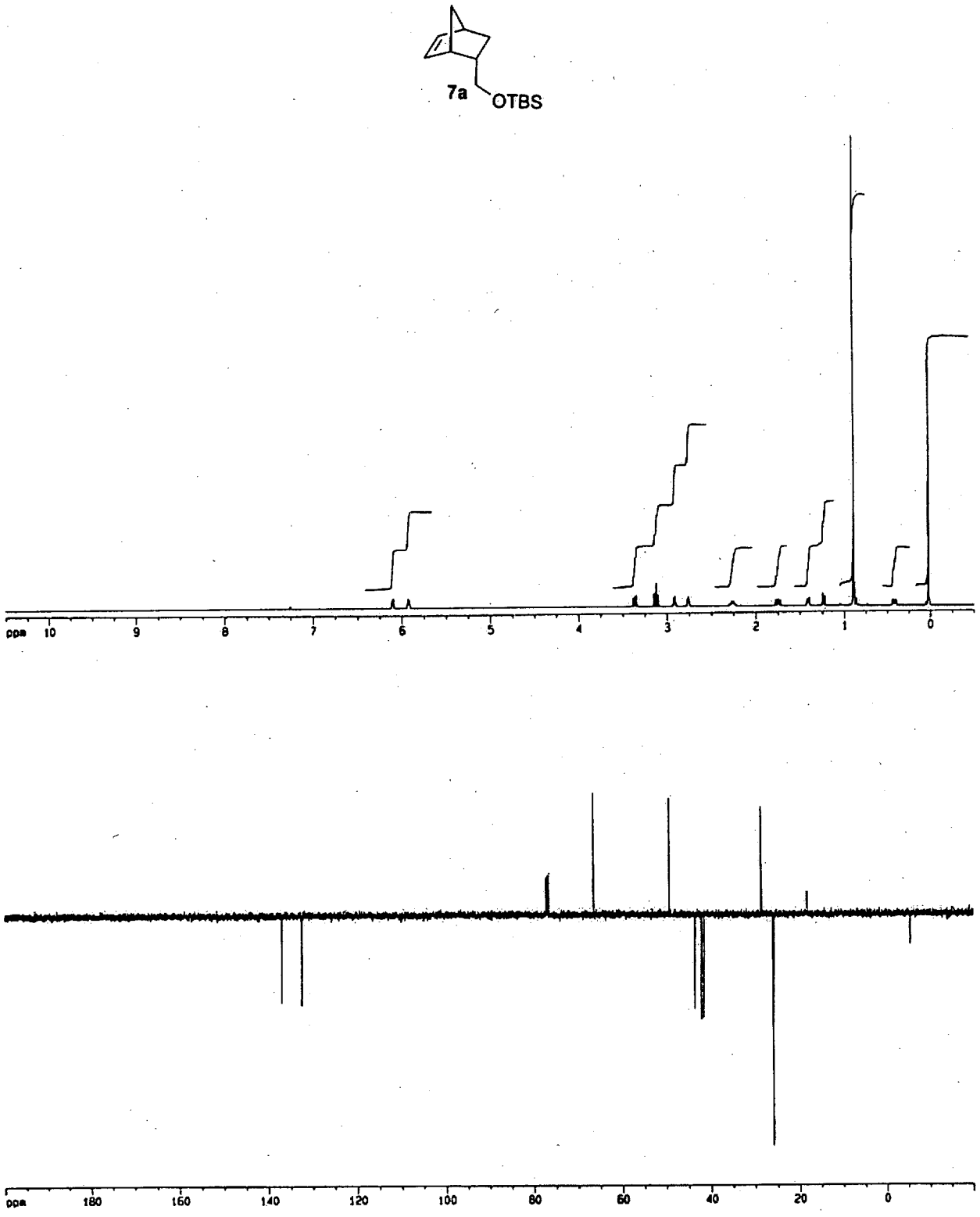


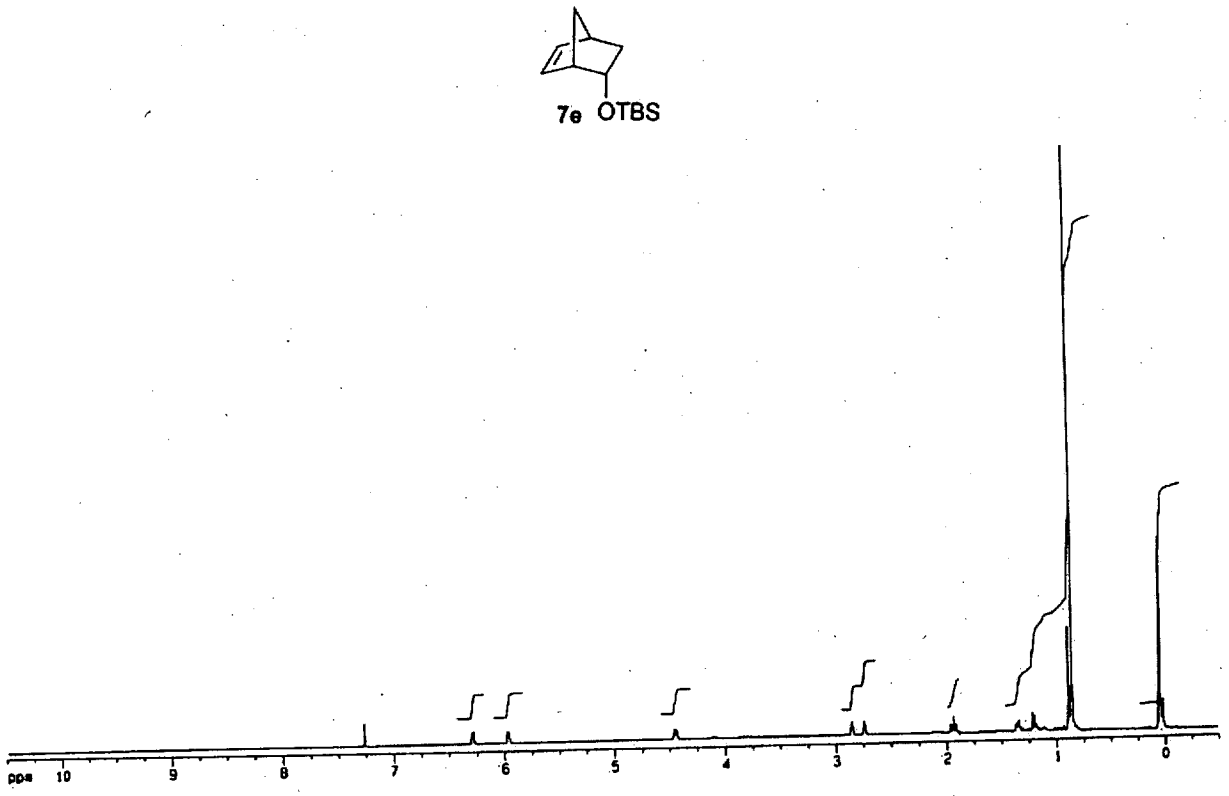

OCO-C6H4-p-NO2

6g


ppm
10
9
8
7
6
5
4
3
2
1
0


ppm
180
160
140
120
100
80
60
40
20


7a
OTBS
ppm 10 9 8 7 6 5 4 3 2 1 0
ppm 180 160 140 120 100 80 60 40 20 0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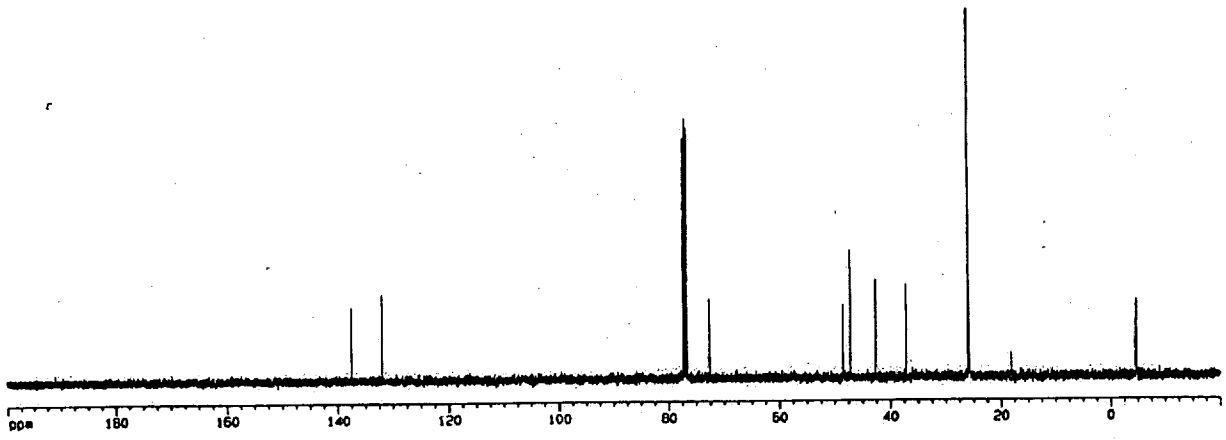
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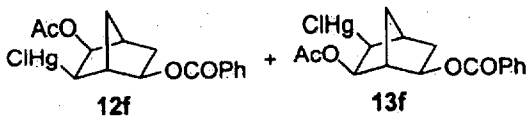
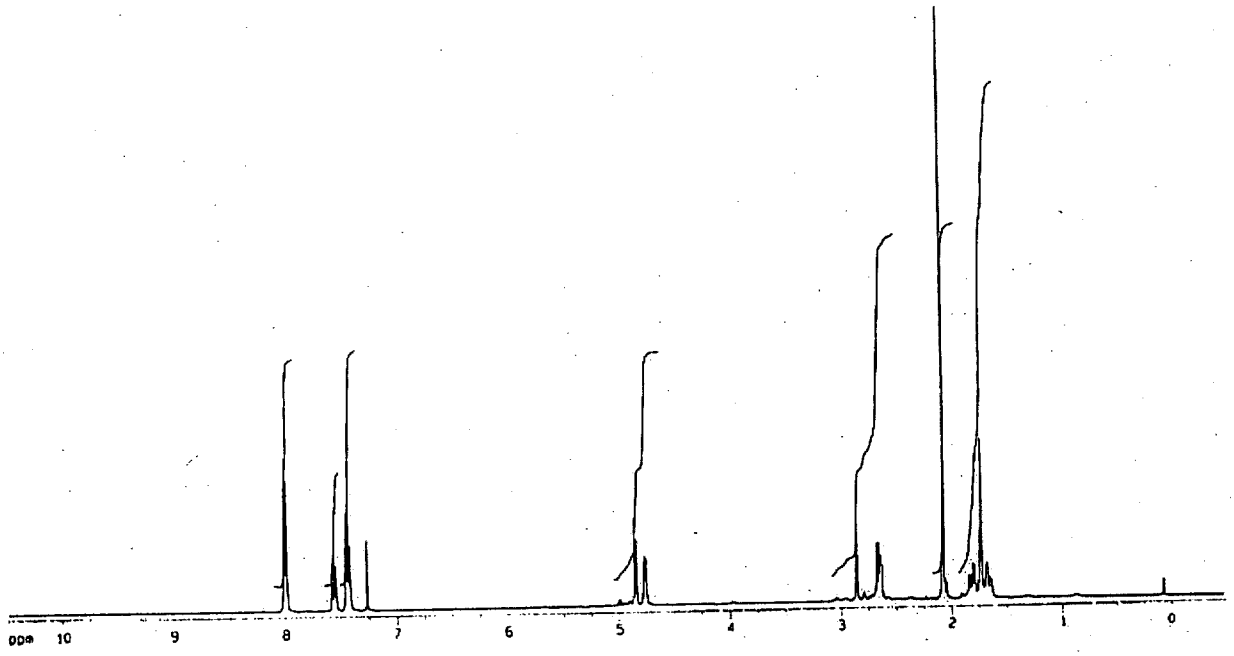

AcO
ClHg
OCOPh
12f
+
ClHg
AcO
OCOPh
13f

(12 : 1)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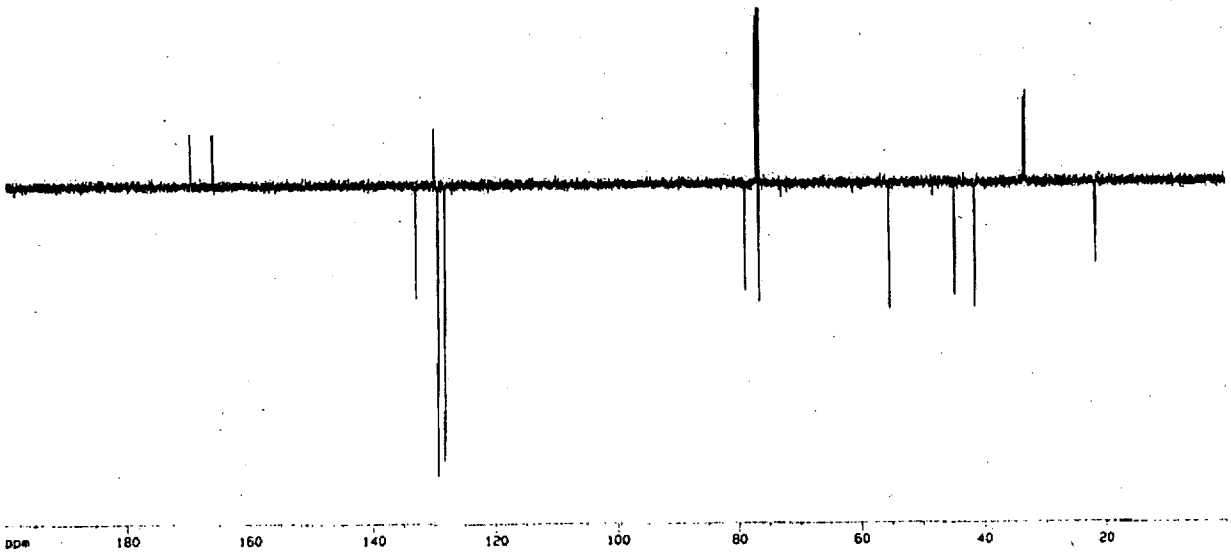
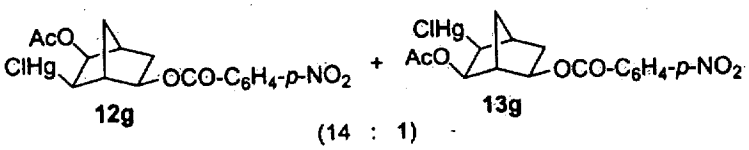
8
7
6
5
4
3
2
1
0


ppm
180
160
140
120
100
80
60
40
20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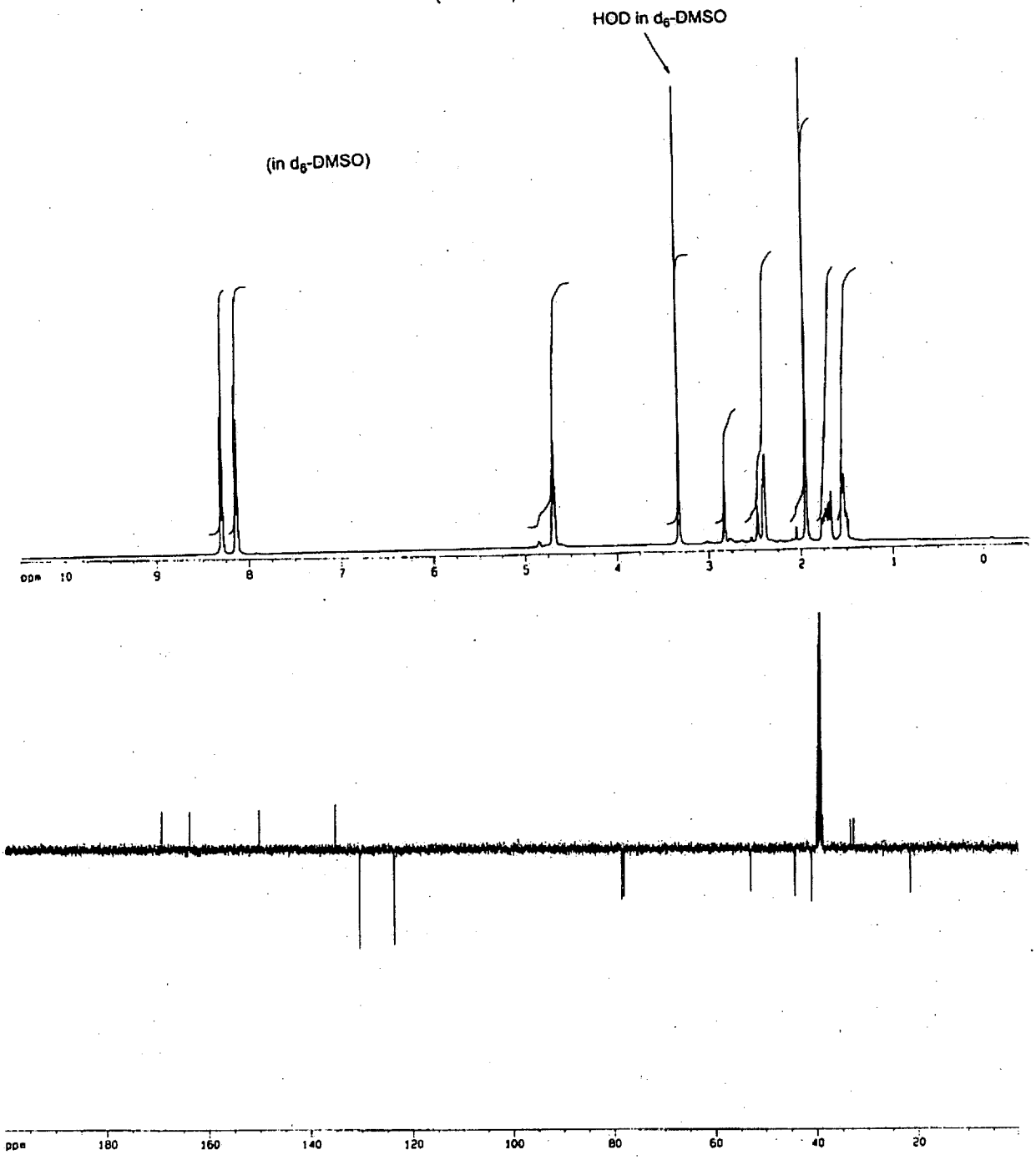
ClHg
OCO-C6H4-p-NO2
12g
+
ClHg
AcO
OCO-C6H4-p-NO2
13g

(14 : 1)


HOD in d6-DMSO
(in d6-DMSO)
ppm 10
9
8
7
6
5
4
3
2
1
0
ppm
180
160
140
120
100
80
60
40
20