SUPPLEMENTARY MATERIAL

Tables with the geometric parameters, figures with liner fit curves, and other results of all the optimized structures considered in this work are available from the authors upon request.

Table S-1. Geometry Parameters Obtained from the HF/6-31G* Geometry Optimizations of 1 in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	-4.739634	-1.029004	-0.168968
6	-3.742274	-1.351969	0.113216
6	-1.747291	-2.763070	-0.691605
6	-1.382752	-0.453256	0.618509
6	-0.874125	-1.483592	-0.457143
6	-2.873433	-0.113651	0.320830
6	-3.186942	-2.277576	-0.962993
1	-0.987326	-0.945744	-1.396068
1	-3.209700	-1.754669	-1.914581
1	-3.853101	-1.879036	1.052966
1	-3.247270	0.464705	1.147861
1	-3.839408	-3.139739	-1.068395
6	-1.339327	-0.926968	2.093097
1	-2.200035	-1.534433	2.334647
1	-1.371241	-0.071690	2.751965
0	-0.467642	-1.513509	2.319731
6	-1.278858	-3.482544	-1.972057
1	-2.009284	-4.231830	-2.260332
1	-0.336190	-4.001198	-1.837206
1	-1.171780	-2.794513	-2.806059
6	-1.747939	-3.806755	0.440655
1	-2.399514	-4.629709	0.160547
1	-2.102518	-3.419657	1.383923
1	-0.762725	-4.216351	0.613599
8	-2.924596	0.676299	-0.869004
6	0.645994	-1.730967	-0.381505
1	0.942248	-2.326722	-1.231991
6	-0.526792	0.828667	0.378203
6	1.014985	0.681666	0.497470
6	1.426439	-0.413836	-0.496723
8	0.976303	-2.409473	0.808933
6	1.561166	0.426660	1.908054
1	1.469048	-0.605733	2.196110
1	1.047409	1.024239	2.649758
1	2.611423	0.680704	1.924956

(Table S1). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
6	-0.925596	2.104828	1.096765
8	-1.741810	2.184654	1.966448
8	1.602877	1.848709	-0.064686
6	1.282946	3.175979	0.343351
6	-0.244607	3.332694	0.531341
1	-0.468034	4.183957	1.160218
1	-0.714410	3.504474	-0.434377
6	2.026982	3.574333	1.618909
1	1.644186	3.058832	2.487397
1	1.907758	4.635669	1.800065
1	3.082492	3.352494	1.523650
6	1.706563	4.009209	-0.851428
1	1.259405	3.677166	-1.774662
6	2.519169	5.045675	-0.871680
1	2.730371	5.555308	-1.794564
1	3.006415	5.432099	0.003937
6	1.998455	-3.260921	1.004797
8	2.296497	-3.512179	2.121521
6	2.672613	-3.904483	-0.182071
1	3.228135	-4.753042	0.187840
1	3.364537	-3.210281	-0.639253
1	1.962389	-4.239074	-0.927826
6	-3.686034	1.758188	-1.045429
8	-3.503650	2.427335	-2.007843
6	-4.735961	2.093776	-0.011980
1	-5.348456	1.237328	0.239672
1	-5.357439	2.876009	-0.420705
1	-4.266925	2.453568	0.896433
1	-0.671611	1.085519	-0.664645
1	1.229495	-0.020952	-1.482883
8	2.792517	-0.731285	-0.357314
6	3.783711	-0.360645	-1.183049
8	4.877259	-0.742820	-0.940803
6	3.462023	0.484307	-2.390955
1	2.809096	-0.050506	-3.073309
1	4.393466	0.694519	-2.893898
1	2.978487	1.406388	-2.103003

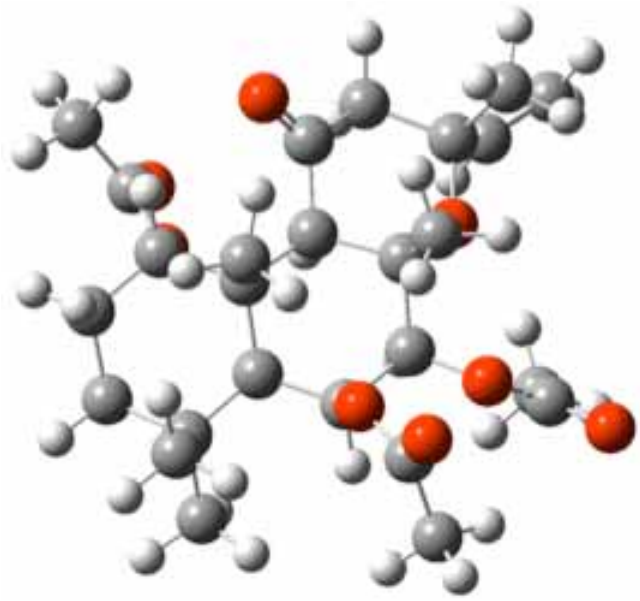

Fig. (S-1). HF/6-31G* geometry optimized of **1** in the gaseous phase.

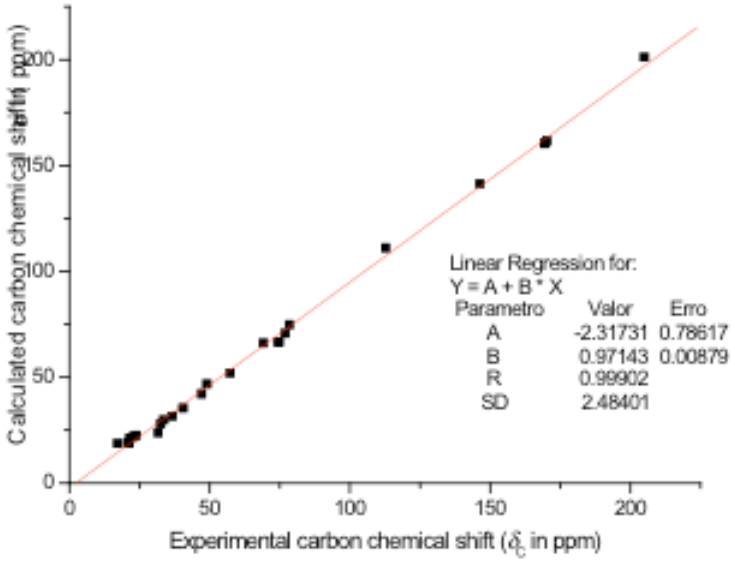

Fig. (S-2). Correlations between ^{13}C NMR data of **1** and HF/6-31G* calculated carbon chemical shifts of labdane diterpenoid isolated from *Plectranthus ornatus* (structure in the gaseous phase).

Table S-2. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 1(C7) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	1.454768	4.438868	0.227078
6	1.678285	3.438112	-0.129924
6	2.928712	1.279024	0.490964
6	0.554627	1.201164	-0.740591
6	1.565740	0.539616	0.264751
6	0.360931	2.695400	-0.344950

(Table S2). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
6	2.586348	2.734613	0.872410
1	1.072082	0.647090	1.225666
1	2.100942	2.740488	1.843873
1	2.182775	3.566159	-1.079821
1	-0.205752	3.167895	-1.128564
1	3.507146	3.300738	0.982716
6	0.989579	1.205526	-2.228492
1	1.614569	2.058975	-2.451193
1	0.123404	1.286544	-2.868481
1	1.549613	0.328845	-2.502778
6	3.655997	0.665197	1.703591
1	4.475469	1.309727	2.005768
1	4.086661	-0.305160	1.482011
1	2.994523	0.555501	2.558314
6	3.921829	1.267147	-0.686424
1	4.819152	1.806146	-0.395068
1	3.537918	1.739693	-1.578063
1	4.217212	0.263691	-0.958226
8	-0.384790	2.745015	0.872681
6	1.670817	-0.992077	0.121925
1	2.230766	-1.365979	0.963273
6	-0.796046	0.453286	-0.508682
6	-0.778886	-1.081188	-0.733496
6	0.294802	-1.682350	0.192341
8	2.332629	-1.349253	-1.077297
6	-0.534785	-1.548232	-2.177230
1	0.502959	-1.507557	-2.457768
1	-1.090063	-0.957176	-2.892764
1	-0.864580	-2.576917	-2.257326
6	-2.045888	1.009644	-1.160322
8	-2.077463	1.878564	-1.981692
8	-1.988444	-1.638667	-0.257400
6	-3.279870	-1.155382	-0.603728
6	-3.307471	0.391064	-0.599629
1	-4.163429	0.758005	-1.149953
1	-3.389182	0.749611	0.423355
1	0.397558	-2.733594	-0.026925
8	-0.154773	-1.539324	1.532565
6	0.030397	-2.535016	2.391020
8	0.668870	-3.508103	2.145219
6	-0.662562	-2.266247	3.696767
1	-0.402711	-1.280730	4.063155

(Table S2). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	-0.385832	-3.022026	4.416377
1	-1.734698	-2.286630	3.537409
6	-3.741262	-1.692699	-1.960070
1	-3.190066	-1.249858	-2.777394
1	-4.786453	-1.456682	-2.118646
1	-3.616404	-2.767571	-1.999904
6	-4.145682	-1.654281	0.536873
1	-3.735683	-1.414108	1.504007
6	-5.288504	-2.305115	0.466109
1	-5.810379	-2.590617	1.361851
1	-5.753639	-2.585295	-0.460642
6	3.051175	-2.468399	-1.262973
8	3.356278	-2.755638	-2.369953
6	3.471747	-3.276249	-0.059020
1	4.030451	-4.126306	-0.419808
1	2.628030	-3.618281	0.526092
1	4.109888	-2.684580	0.588743
6	-1.342271	3.629929	1.156158
8	-1.942878	3.509175	2.171847
6	-1.638680	4.734130	0.167603
1	-0.745470	5.275266	-0.118246
1	-2.336097	5.411699	0.636196
1	-2.087716	4.325982	-0.730353
1	-1.007626	0.544288	0.548396

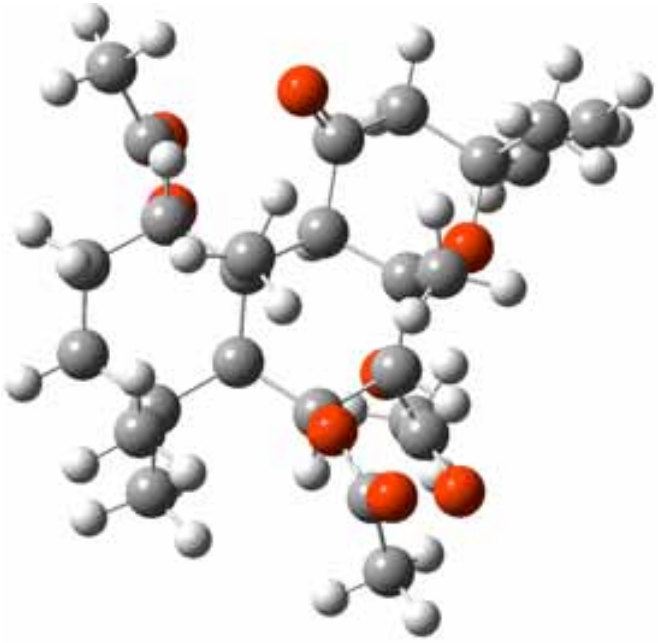

Fig. (S-3). HF/6-31G* geometry optimized of **1** in the gaseous phase.

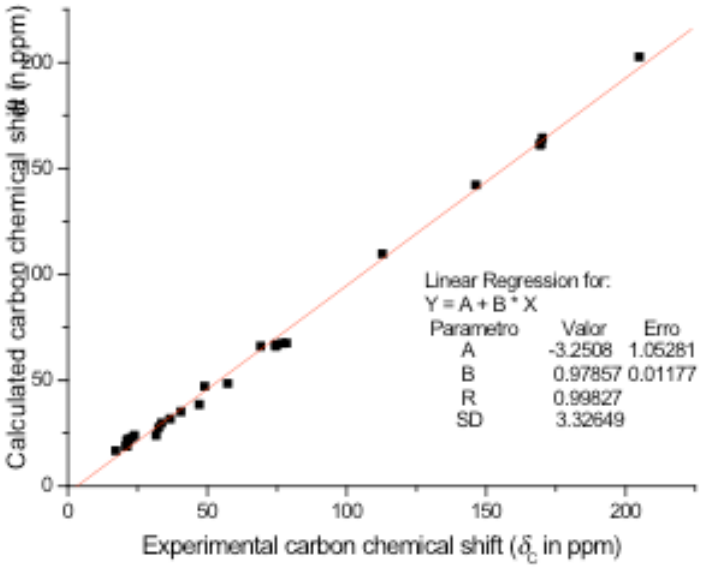

Fig. (S-4). Correlations between ^{13}C NMR data of **1(C7)** and HF/6-31G* calculated carbon chemical shifts of labdane diterpenoid isolated from *Plectranthus ornatus* (structure in the gaseous phase).

Table S-3. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 1(C8) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	4.681960	-0.951289	-0.912899
6	3.614447	-1.081314	-1.063421
6	1.654968	-2.661658	-0.499175
6	1.341208	0.005777	-0.604241
6	0.906344	-1.375005	0.003184
6	2.886808	0.118783	-0.461357
6	3.172647	-2.390788	-0.417632
1	3.470826	-2.371868	0.625495
1	3.462581	-1.100383	-2.135913
1	3.206529	1.028355	-0.939178
1	3.704679	-3.219809	-0.875918
6	1.010916	0.205799	-2.098076
1	1.391729	1.165367	-2.434600
1	-0.047073	0.165388	-2.277054
1	1.470475	-0.540607	-2.723813
6	1.365330	-3.821055	0.477942
1	2.045761	-4.643587	0.282165
1	0.360378	-4.215828	0.371446
1	1.506235	-3.522308	1.512779
6	1.286225	-3.170639	-1.905772
1	1.791290	-4.116759	-2.077436
1	1.583655	-2.504077	-2.701265
1	0.224171	-3.344381	-2.010437
8	3.203035	0.174054	0.927602
6	-0.621093	-1.514692	0.107219

(Table S3). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	-0.861277	-2.462085	0.568994
6	0.677177	1.151540	0.261124
6	-0.821089	1.013679	0.624609
6	-1.137578	-0.428173	1.046574
8	-1.204041	-1.442897	-1.169259
6	0.886162	2.528752	-0.363033
8	1.975587	3.020391	-0.414937
6	-1.648627	2.584893	-1.067360
6	-0.302116	3.331809	-0.874437
1	0.016589	3.785707	-1.804906
1	-0.408423	4.153903	-0.173690
6	-2.384125	-1.943144	-1.563943
8	-2.846473	-1.542347	-2.576846
6	-3.037726	-3.040787	-0.758769
1	-3.720217	-3.556191	-1.418074
1	-3.605747	-2.617003	0.058457
1	-2.321862	-3.749972	-0.361673
6	4.142587	0.945780	1.482869
8	4.248112	0.940006	2.663743
6	5.018314	1.791584	0.590749
1	5.472519	1.209069	-0.201553
1	5.791736	2.223256	1.207776
1	4.432105	2.583008	0.140992
6	-1.924521	2.363077	-2.559898
1	-1.073272	1.920911	-3.059969
1	-2.148844	3.308869	-3.042838
1	-2.773064	1.702136	-2.673557
6	-2.805807	3.403044	-0.516938
1	-2.739292	4.463554	-0.707705
6	-3.879529	2.913173	0.067467
1	-4.683046	3.557483	0.377142
1	-3.994562	1.861007	0.251926
6	-1.132914	1.917741	1.833427
1	-2.174869	1.844083	2.107753
1	-0.928712	2.961263	1.640943
1	-0.520913	1.623500	2.679756
1	1.229544	-1.305489	1.038334
1	1.228384	1.177510	1.190523
8	-1.620823	1.292358	-0.491644
1	-0.636173	-0.592204	1.988411
8	-2.533052	-0.573123	1.210482
6	-3.144630	-1.038974	2.305038
8	-4.308901	-1.247972	2.252973
6	-2.338528	-1.282286	3.561273
1	-1.593210	-2.055378	3.409101
1	-3.026532	-1.605838	4.326844
1	-1.830736	-0.384579	3.892188

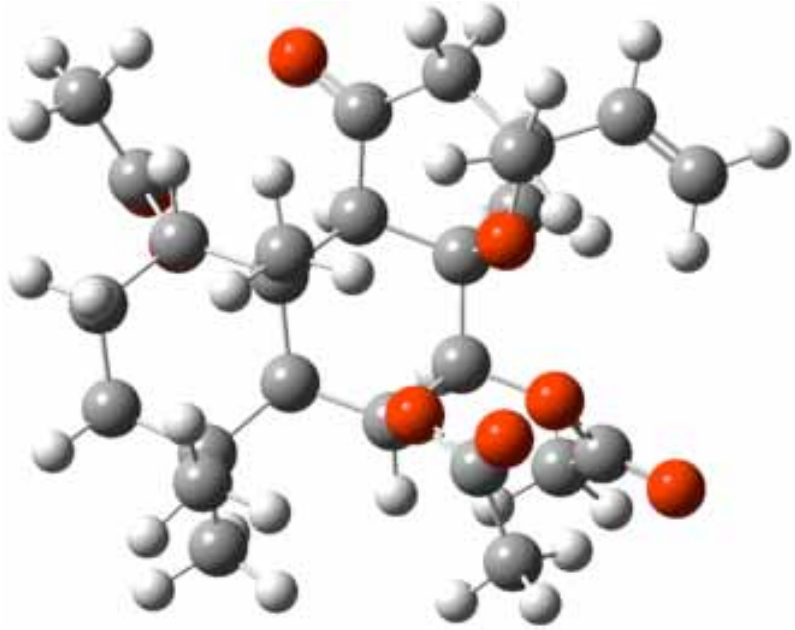

Fig. (S-5). HF/6-31G* geometry optimized of **1(C8)** in the gaseous phase.

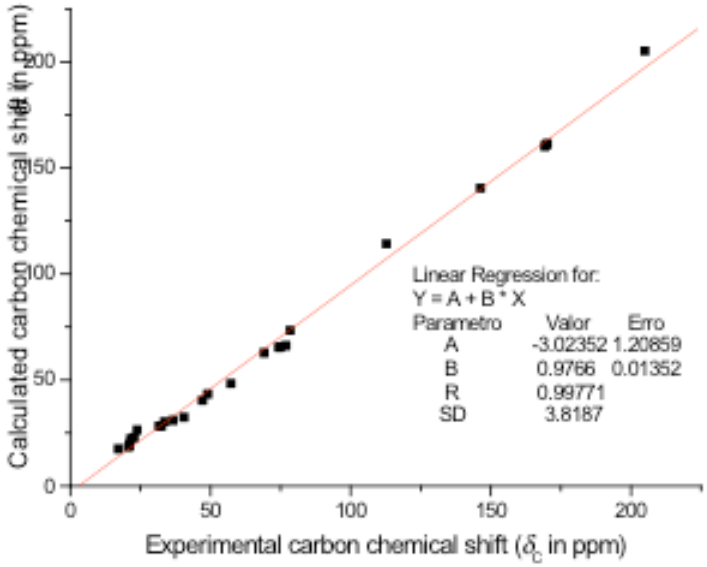

Fig. (S-6). Correlations between ^{13}C NMR data of **1(C8)** and HF/6-31G* calculated carbon chemical shifts of labdane diterpenoid isolated from *Plectranthus ornatus* (structure in the gaseous phase).

Table S-4. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 1(C13) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	4.431845	-1.917123	-0.065663
6	3.384733	-2.009415	-0.337078
6	1.173900	-3.103329	0.392716
6	1.231065	-0.626627	-0.625293
6	0.561263	-1.662014	0.353174
6	2.766322	-0.613379	-0.361277
6	2.686691	-2.937830	0.649687

(Table S4). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	2.833885	-2.550362	1.653517
1	3.370585	-2.430196	-1.335003
1	3.224236	-0.020382	-1.133621
1	3.161289	-3.914681	0.622647
6	1.059549	-0.908692	-2.139983
1	1.180373	0.007198	-2.699780
1	0.105915	-1.343148	-2.379956
1	1.817523	-1.590564	-2.499712
6	0.607452	-3.876038	1.600312
1	1.186442	-4.779671	1.762323
1	-0.420692	-4.186380	1.451600
1	0.656314	-3.289950	2.513848
6	0.945083	-3.976297	-0.854959
1	1.425821	-4.938876	-0.704554
1	1.351783	-3.549329	-1.759286
1	-0.104903	-4.161206	-1.033122
8	2.997750	0.002686	0.907198
6	-0.980640	-1.603354	0.337157
1	-1.355980	-2.227199	1.134471
6	0.645614	0.757201	-0.205934
6	-0.899263	0.914857	-0.265363
6	-1.476953	-0.183024	0.638724
8	-1.483527	-2.062809	-0.897419
6	1.272287	2.011500	-0.789965
8	2.085063	2.038444	-1.665891
6	-0.696414	3.376713	0.077457
6	0.830586	3.266668	-0.069259
1	1.253710	4.130817	-0.558772
1	1.265686	3.210228	0.925204
6	-2.651858	-2.692787	-1.107560
8	-3.044243	-2.771646	-2.220242
6	-3.364612	-3.334517	0.057921
1	-4.189911	-3.902875	-0.342838
1	-3.747294	-2.586990	0.737917
1	-2.705464	-3.999277	0.604323
6	3.965551	0.882452	1.173424
8	3.947686	1.444000	2.218153
6	5.032691	1.137251	0.134541
1	5.458424	0.217671	-0.246414
1	5.806447	1.728460	0.600344
1	4.618927	1.690383	-0.700530
1	0.807683	-1.273989	1.339167
1	0.864008	0.856385	0.850916
1	-1.158156	0.046003	1.644984
8	-2.884102	-0.202455	0.565143

(Table S4). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
6	-3.715429	0.433346	1.409344
8	-4.845492	0.565614	1.088623
6	-3.188328	0.875815	2.753139
1	-2.753067	0.040303	3.291638
1	-4.022873	1.264235	3.316752
1	-2.434863	1.642329	2.642231
6	-1.527104	0.918189	-1.662565
1	-2.547190	1.266777	-1.584309
1	-1.552124	-0.065970	-2.095014
8	-1.237112	2.109434	0.434253
6	-1.402069	3.932789	-1.146910
1	-2.471322	3.806069	-1.104282
6	-0.875902	4.578017	-2.168772
1	-1.505273	4.968669	-2.948091
1	0.179155	4.740074	-2.291348
6	-1.041290	4.282376	1.262176
1	-0.993533	1.574730	-2.335176
1	-0.633120	5.274860	1.109282
1	-2.116457	4.367095	1.370036
1	-0.633579	3.870510	2.178613

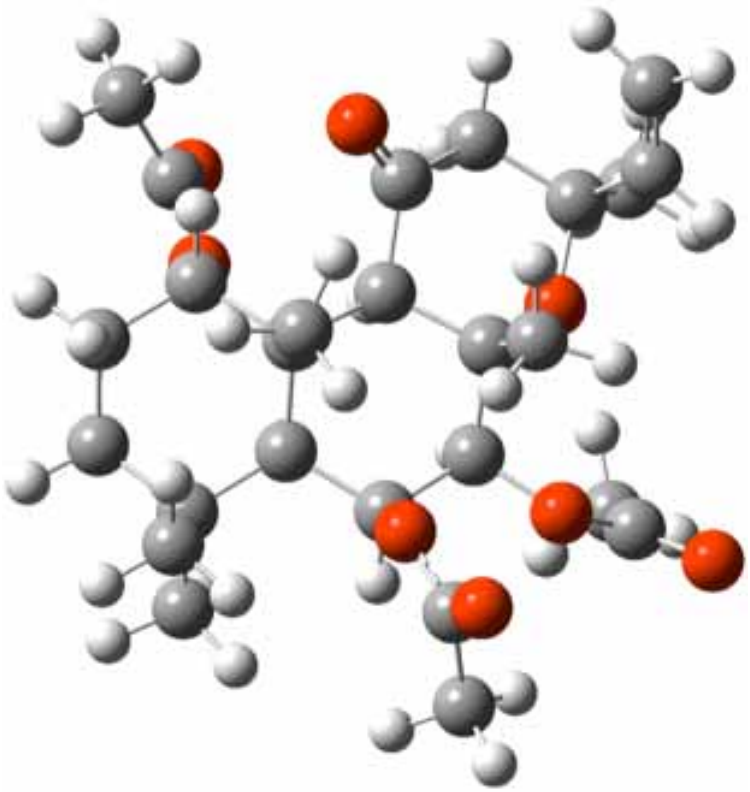

Fig. (S-7). HF/6-31G* geometry optimized of **1(C13)** in the gaseous phase.

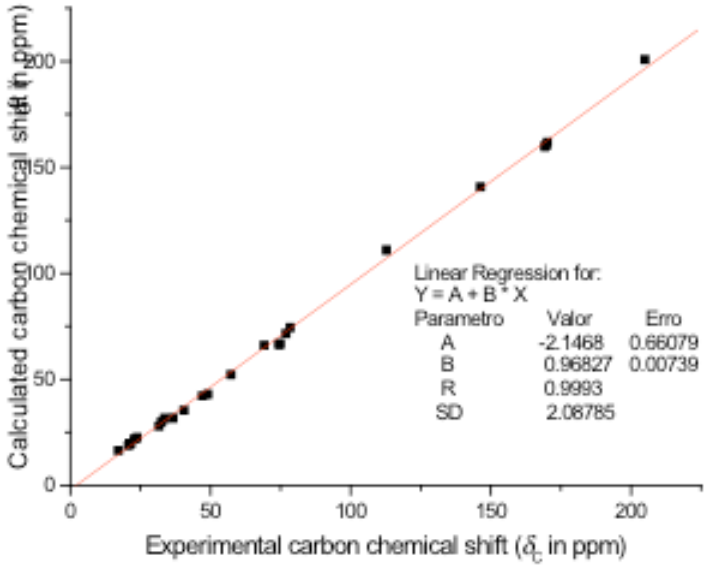

Fig. (S-8). Correlations between ^{13}C NMR data of **1(C13)** and HF/6-31G* calculated carbon chemical shifts of labdane diterpenoid isolated from *Plectranthus ornatus* (structure in the gaseous phase).

Table S-5. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 1(C7,C13) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	0.308332	4.632838	-0.111914
6	0.732377	3.689151	-0.441358
6	2.547061	1.957942	0.119671
6	0.141779	1.202147	-0.772065
6	1.394321	0.896544	0.127350
6	-0.372538	2.634196	-0.436197
6	1.900461	3.315913	0.464386
1	1.003498	0.972905	1.137308
1	1.549043	3.289635	1.491652
1	1.072817	3.853664	-1.456360
1	-1.126916	2.886596	-1.160805
1	2.656711	4.094558	0.415280
6	0.389060	1.182387	-2.302957
1	0.706844	2.151752	-2.661476
1	-0.527096	0.949913	-2.825785
1	1.147982	0.477284	-2.594162
6	3.547690	1.645486	1.249644
1	4.209389	2.492794	1.399571
1	4.178043	0.792918	1.021397
1	3.044700	1.452922	2.193104

(Table S5). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
6	3.359101	2.082830	-1.183350
1	4.126563	2.840023	-1.047973
1	2.763387	2.377701	-2.034229
1	3.854032	1.158139	-1.444046
8	-0.959254	2.606916	0.866292
6	1.860662	-0.572009	0.070489
1	2.584155	-0.719371	0.855621
6	-0.942634	0.172138	-0.324469
6	-0.563418	-1.327369	-0.457891
6	0.717048	-1.561878	0.362042
8	2.456783	-0.870903	-1.178055
6	-0.365115	-1.850961	-1.886875
1	0.554879	-1.512594	-2.328973
1	-1.179740	-1.562739	-2.535441
1	-0.337694	-2.933712	-1.847524
6	-2.359968	0.357493	-0.831145
8	-2.707356	1.140896	-1.665417
8	-1.541109	-2.114039	0.200077
6	-2.927616	-2.000378	-0.084659
6	-3.345911	-0.520896	-0.093584
1	-4.334923	-0.383964	-0.504809
1	-3.364398	-0.167207	0.933519
1	1.054657	-2.573575	0.202573
8	0.394232	-1.401610	1.736257
6	0.865737	-2.269269	2.623836
8	1.659036	-3.116216	2.362712
6	0.273951	-2.030956	3.984131
1	0.410261	-0.995795	4.272940
1	0.741256	-2.686686	4.703310
1	-0.792104	-2.223119	3.945774
6	3.404820	-1.799545	-1.380658
8	3.667077	-2.093005	-2.496904
6	4.119519	-2.389036	-0.188107
1	4.823595	-3.116868	-0.561510
1	3.442712	-2.864461	0.509900
1	4.662582	-1.616644	0.346160
6	-2.066307	3.257693	1.227827

(Table S5). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
8	-2.495382	3.083413	2.319904
6	-2.740538	4.171774	0.230701
1	-2.049073	4.885107	-0.199861
1	-3.524704	4.699653	0.751801
1	-3.175307	3.593943	-0.576402
1	-1.049297	0.302195	0.744302
6	-3.608690	-2.728041	1.076514
1	-3.313910	-2.278946	2.017921
1	-3.315224	-3.771252	1.088412
1	-4.687143	-2.673864	0.978671
6	-3.271575	-2.744822	-1.363715
1	-2.819137	-3.722057	-1.410394
6	-4.068993	-2.364283	-2.342187
1	-4.263104	-3.018752	-3.173115
1	-4.549595	-1.404050	-2.377619

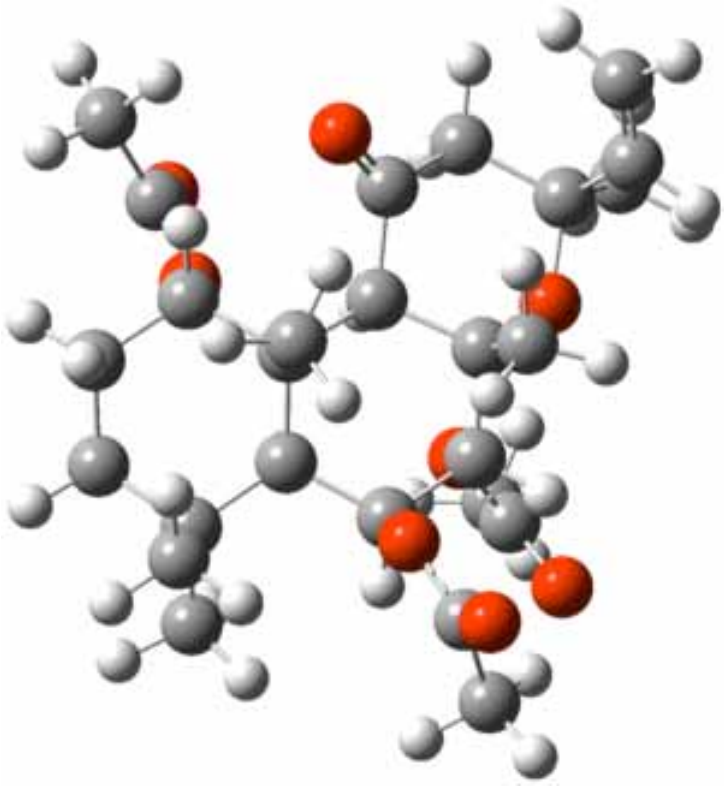

Fig. (S-9). HF/6-31G* geometry optimized of **1(C7,C13)** in the gaseous phase.

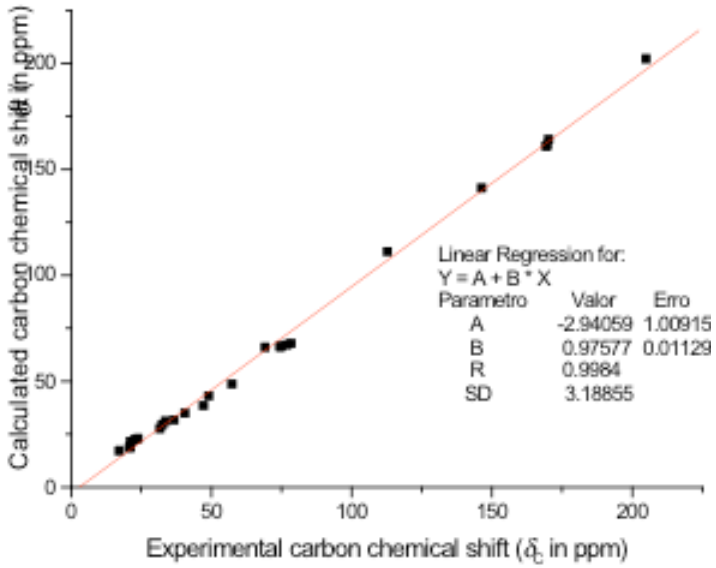

Fig. (S-10). Correlations between ^{13}C NMR data of **1(C7, C13)** and HF/6-31G* calculated carbon chemical shifts of labdane diterpenoid isolated from *Plectranthus ornatus* (structure in the gaseous phase).

Table S-6. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 1(C8,C13) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	x	z
1	4.332796	-1.382466	-1.321790
6	3.251455	-1.357282	-1.373279
6	1.126499	-2.716855	-0.851819
6	1.216243	-0.049485	-0.524718
6	0.615292	-1.434295	-0.103035
6	2.765715	-0.164903	-0.553780
6	2.668526	-2.670886	-0.864020
1	3.031097	-2.840656	0.145741
1	3.003462	-1.201906	-2.416909
1	3.187636	0.744569	-0.946329
1	3.043681	-3.494876	-1.464814
6	0.793355	0.456178	-1.919191
1	1.252720	1.418325	-2.121508
1	-0.271753	0.568243	-1.998554
1	1.114642	-0.205168	-2.707217
6	0.720490	-3.966005	-0.042040
1	1.244577	-4.835857	-0.426313
1	-0.340207	-4.179527	-0.108537
1	0.979078	-3.866802	1.008068
6	0.598512	-2.933844	-2.282910

(Table S6). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	x	z
1	1.000585	-3.867422	-2.665420
1	0.882556	-2.156591	-2.976828
1	-0.479616	-3.017936	-2.305027
8	3.236441	-0.306340	0.791928
6	-0.901169	-1.386773	0.125262
1	-1.239257	-2.339509	0.492605
6	0.802186	0.996406	0.582972
6	-0.688633	1.054786	0.986585
6	-1.225602	-0.363796	1.206081
8	-1.615800	-1.103635	-1.072525
6	1.250892	2.408823	0.235093
8	2.393588	2.739060	0.338886
6	-1.221731	2.982536	-0.467502
6	0.226852	3.452740	-0.194949
1	0.648459	3.939971	-1.061754
1	0.237922	4.201825	0.589969
6	-2.784768	-1.687771	-1.293363
8	-3.268111	-2.515378	-0.588224
6	-3.418734	-1.171563	-2.555766
1	-4.284156	-1.770246	-2.798118
1	-2.706258	-1.189608	-3.371140
1	-3.720129	-0.141641	-2.400009
6	4.464983	0.111119	1.083569
8	5.254147	0.471357	0.273704
6	4.717549	0.066862	2.566283
1	4.116840	0.830414	3.048667
1	5.762882	0.254936	2.761006
1	4.425467	-0.894087	2.972156
6	-0.833750	1.799763	2.327516
1	-1.880008	1.901685	2.582458
1	-0.392481	2.787765	2.309394
1	-0.340743	1.245871	3.118359
1	1.004466	-1.580648	0.902274
1	1.363698	0.733757	1.467724
8	-1.454498	1.647849	-0.032201
1	-0.769038	-0.739264	2.108858
8	-2.624745	-0.293822	1.409754

(Table S6). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	x	z
6	-3.181898	-1.144587	2.273963
8	-2.557450	-1.892722	2.952885
6	-4.678825	-1.028914	2.264289
1	-4.980651	0.010825	2.279645
1	-5.086972	-1.555462	3.114238
1	-5.047235	-1.476720	1.348634
6	-2.234206	3.915561	0.215668
1	-3.242215	3.571472	0.015804
1	-2.132752	4.922315	-0.174765
1	-2.093125	3.947921	1.288009
6	-1.584000	2.954933	-1.945411
1	-2.326285	2.208929	-2.171508
6	-1.167266	3.756822	-2.904269
1	-1.554460	3.662538	-3.902827
1	-0.441598	4.536651	-2.755273

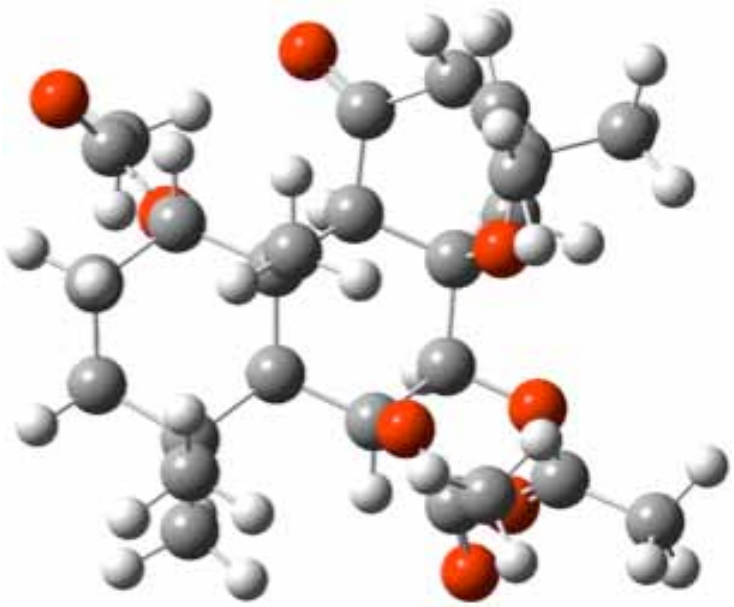

Fig. (S-11). HF/6-31G* geometry optimized of **1(C8,C13)** in the gaseous phase.

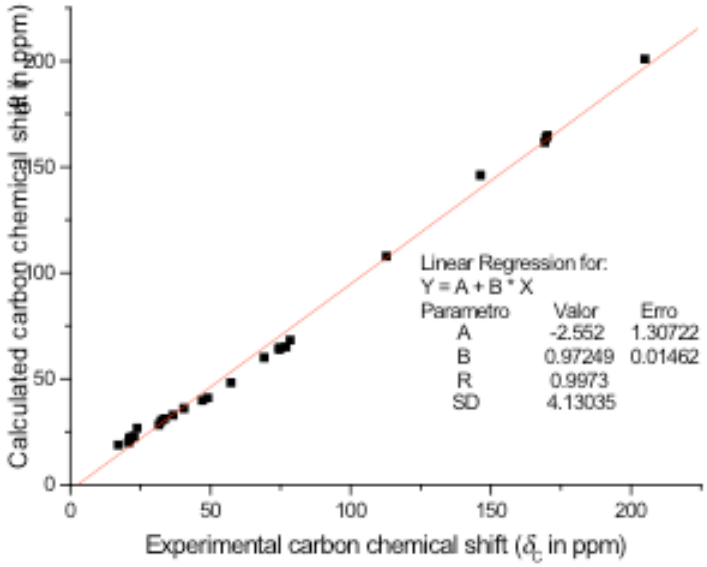

Fig. (S-12). Correlations between ^{13}C NMR data of **1(C8,C13)** and HF/6-31G* calculated carbon chemical shifts of labdane diterpenoid isolated from *Plectranthus ornatus* (structure in the gaseous phase).

Table S-7. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 1(C7,C8,C13) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	4.180801	-0.170493	-1.921606
6	3.120302	-0.388567	-1.900212
6	1.402719	-2.256725	-1.466283
6	0.937875	0.287963	-0.737335
6	0.688783	-1.240083	-0.504174
6	2.465755	0.536316	-0.878496
6	2.889712	-1.856444	-1.559720
1	3.370046	-2.069107	-0.608972
1	2.744662	-0.156252	-2.890045
1	2.639257	1.563582	-1.150700
1	3.381197	-2.485302	-2.297174
6	0.287928	0.878642	-2.005302
1	0.522809	1.935087	-2.087385
1	-0.780518	0.771505	-1.995887
1	0.655097	0.414126	-2.906136
6	1.358464	-3.663139	-0.832608
1	2.027857	-4.327986	-1.370122
1	0.370655	-4.108595	-0.873309
1	1.678565	-3.645568	0.205119
6	0.812371	-2.396585	-2.882664
1	1.376002	-3.150900	-3.424159

(Table S7). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	0.855160	-1.487697	-3.464573
1	-0.218832	-2.721769	-2.858031
8	3.084580	0.325027	0.396337
6	-0.777137	-1.571519	-0.203102
1	-0.866493	-2.617217	0.030577
6	0.418251	1.038546	0.548954
6	-0.993594	0.688600	1.061430
6	-1.286905	-0.825227	1.033028
8	-1.616782	-1.306185	-1.321043
6	0.506796	2.550549	0.404346
8	1.549988	3.123567	0.502802
6	-2.090351	2.623544	-0.044499
6	-0.756867	3.374927	0.184005
1	-0.535975	4.034019	-0.642779
1	-0.832221	4.019374	1.053426
6	-2.723656	-2.028193	-1.466088
8	-3.048581	-2.896662	-0.723596
6	-3.499471	-1.603870	-2.682560
1	-4.329164	-2.277995	-2.834072
1	-2.855939	-1.596010	-3.553886
1	-3.870573	-0.595928	-2.536555
6	4.209660	0.976849	0.672570
8	4.819544	1.616952	-0.119313
6	4.603332	0.797350	2.113846
1	3.898542	1.334511	2.739397
1	5.596354	1.191872	2.269826
1	4.565603	-0.249480	2.389880
6	-1.158859	1.199805	2.501996
1	-2.151470	0.972345	2.869558
1	-1.006873	2.268510	2.572400
1	-0.432435	0.735634	3.154315
1	1.173514	-1.431626	0.448277
1	1.110002	0.787494	1.338537
8	-1.981263	1.225330	0.206271
6	-3.203147	3.202136	0.844307
1	-4.128924	2.666942	0.668311
1	-3.362453	4.247666	0.604072

(Table S7). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	-2.962459	3.124017	1.896143
6	-2.597488	2.703709	-1.476909
1	-3.195047	1.850380	-1.748080
6	-2.461116	3.690073	-2.339718
1	-2.929654	3.639737	-3.306064
1	-1.897213	4.583604	-2.138821
1	-2.349716	-0.960876	1.134092
8	-0.630403	-1.470037	2.124009
6	-1.347584	-1.963649	3.136714
8	-2.516571	-1.813273	3.258911
6	-0.468969	-2.722542	4.092995
1	-0.015530	-3.562797	3.579803
1	-1.060419	-3.074422	4.924752
1	0.330886	-2.082939	4.447727

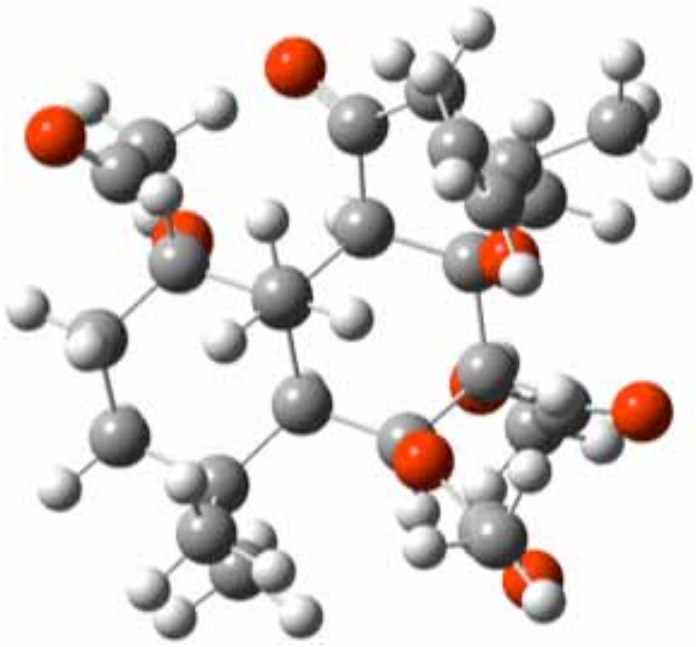

Fig. (S-13). HF/6-31G* geometry optimized of **1(C7,C8,C13)** in the gaseous phase.

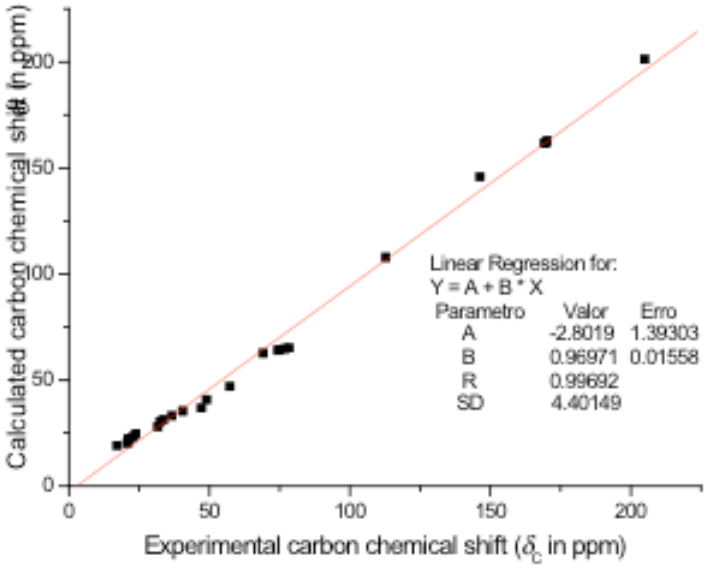

Fig. (S-14). Correlations between ^{13}C NMR data of **1(C7, C8, C13)** and HF/6-31G* calculated carbon chemical shifts of labdane diterpenoid isolated from *Plectranthus ornatus* (structure in the gaseous phase).

Table S-8. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 2 in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	4.359139	-2.537636	-0.691261
6	3.858950	-1.694782	-0.217455
6	3.468102	0.833180	-0.408734
6	1.509075	-0.811168	0.362563
6	1.931824	0.521022	-0.354372
6	2.361819	-2.003941	-0.175684
6	4.162139	-0.415891	-0.990360
1	1.683170	0.354205	-1.395964
1	3.848491	-0.549144	-2.021978
1	4.264540	-1.642059	0.784783
1	2.179658	-2.847753	0.474234
1	5.236004	-0.250532	-1.011750
6	1.760837	-0.811417	1.896793
1	2.748087	-1.188617	2.119805
1	1.070782	-1.466824	2.403049
1	1.697740	0.173318	2.321727
6	3.714655	1.989826	-1.396978
1	4.777183	2.078953	-1.602628
1	3.386307	2.943333	-0.999076
1	3.210817	1.824823	-2.345587

(Table S8). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
6	4.142243	1.231766	0.918599
1	5.193115	1.435618	0.729291
1	4.097103	0.460221	1.673249
1	3.696523	2.121546	1.336789
8	1.949153	-2.367145	-1.491626
1	2.348360	-3.192022	-1.731706
6	1.044253	1.723257	0.024697
1	1.253779	2.518790	-0.683619
6	-0.021978	-1.014055	0.021200
6	-0.952073	0.136629	0.524869
6	-0.451710	1.424004	-0.147500
1	-0.654014	1.324137	-1.197979
8	-0.234491	-0.996994	-1.375538
1	0.406854	-1.572064	-1.780687
8	1.320087	2.198827	1.315421
1	0.694492	2.885688	1.513872
8	-1.129811	2.550019	0.387537
6	-2.199419	3.152833	-0.153590
8	-2.789322	3.940844	0.503753
6	-2.563234	2.840359	-1.583769
1	-1.725092	3.028403	-2.246284
1	-3.385125	3.484212	-1.857911
1	-2.857404	1.805415	-1.687391
6	-1.092321	0.284838	2.046125
1	-0.253732	0.792156	2.486743
1	-1.203742	-0.672493	2.539398
1	-1.977589	0.872967	2.240221
6	-0.664737	-2.318912	0.510209
8	-0.131566	-3.137820	1.194430
8	-2.237210	-0.048322	-0.040983
6	-2.980014	-1.259875	0.028720
6	-2.070719	-2.518799	-0.016029
1	-2.523300	-3.330473	0.537723
1	-1.956426	-2.846798	-1.042023
6	-3.850015	-1.278202	1.287403
1	-3.251174	-1.380653	2.181619
1	-4.535712	-2.117006	1.260937

(Table S8). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	-4.421207	-0.361063	1.360150
6	-3.804358	-1.225311	-1.243886
1	-3.197311	-1.082982	-2.122697
6	-5.109967	-1.349015	-1.368735
1	-5.572312	-1.313569	-2.339098
1	-5.772826	-1.485446	-0.534425

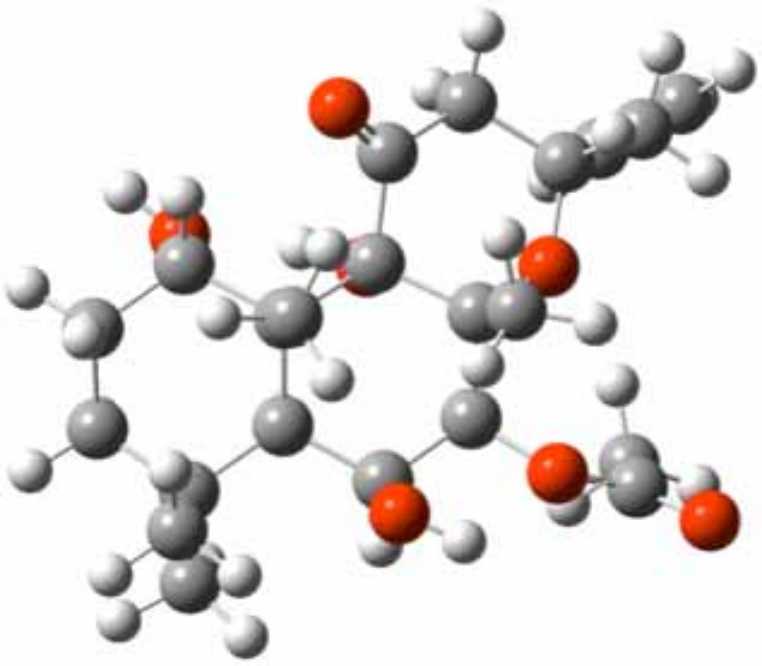

Fig. (S-15). HF/6-31G* geometry optimized of **2** in the gaseous phase.

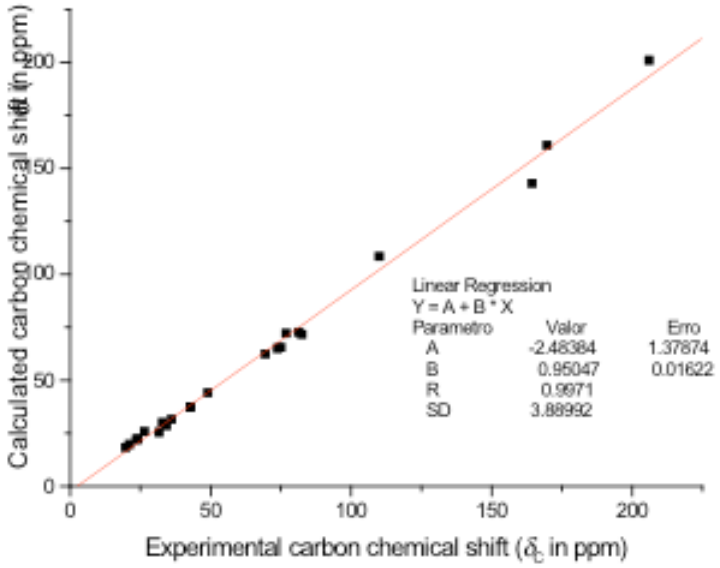

Fig. (S-16). Correlations between ^{13}C NMR data of **2** and HF/6-31G* calculated carbon chemical shifts of **2** (structure in the gaseous phase).

Table S-9. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 2(C7) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	3.778806	-2.714168	-1.614961
6	3.430369	-2.012970	-0.858697
6	3.400977	0.465500	-0.211038
6	1.265277	-1.092005	0.195798
6	1.842041	0.343113	-0.077284
6	1.909809	-2.142202	-0.767458
6	3.857556	-0.598263	-1.230418
1	1.487921	0.586651	-1.071617
1	3.447879	-0.355830	-2.206841
1	3.898496	-2.324851	0.066270
1	1.645169	-3.120250	-0.391641
1	4.939142	-0.557469	-1.328488
6	1.585375	-1.639005	1.616236
1	2.525736	-2.171033	1.613693
1	0.840855	-2.350839	1.934539
1	1.673276	-0.859127	2.349774
6	3.753551	1.841501	-0.809738
1	4.801835	1.863241	-1.092898
1	3.599706	2.649217	-0.102972
1	3.168976	2.054584	-1.700362
6	4.220868	0.320019	1.086161
1	5.278049	0.393200	0.843313
1	4.069971	-0.624790	1.587704
1	3.984987	1.100244	1.793801
8	1.383077	-2.025889	-2.087005
1	1.634986	-2.785270	-2.594072
6	1.190048	1.440711	0.788119
1	1.488635	2.393031	0.372777
6	-0.291914	-0.974102	-0.062272
6	-1.016707	0.057683	0.856922
6	-0.351288	1.447054	0.736534
8	-0.556438	-0.495037	-1.358380
1	-0.030000	-0.992844	-1.974221
8	1.623315	1.386842	2.129117
1	1.399290	2.205664	2.552313
6	-1.063622	-0.312934	2.351350
1	-0.144532	-0.086461	2.862480
1	-1.290873	-1.358752	2.514988
1	-1.852799	0.276354	2.801202
6	-1.100750	-2.273109	0.048275
8	-0.672407	-3.334220	0.387828

(Table S9). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
8	-2.333501	0.243258	0.400118
6	-3.240551	-0.809799	0.107818
6	-2.539142	-2.103643	-0.393370
1	-3.092217	-2.978207	-0.077440
1	-2.515445	-2.106388	-1.476016
1	-0.707532	2.048120	1.559341
8	-0.757189	2.085674	-0.461474
6	-0.944441	3.394176	-0.438366
8	-0.689404	4.089303	0.495475
6	-1.515359	3.882751	-1.740706
1	-0.889930	3.557013	-2.563151
1	-1.586910	4.960186	-1.726662
1	-2.497302	3.446129	-1.882434
6	-4.089088	-1.119320	1.343772
1	-3.495608	-1.577758	2.123499
1	-4.886673	-1.810406	1.097076
1	-4.524810	-0.207603	1.733435
6	-4.062551	-0.240914	-1.032638
1	-3.443833	0.157227	-1.819022
6	-5.374539	-0.200603	-1.145186
1	-5.835922	0.222101	-2.020051
1	-6.044466	-0.572196	-0.391660

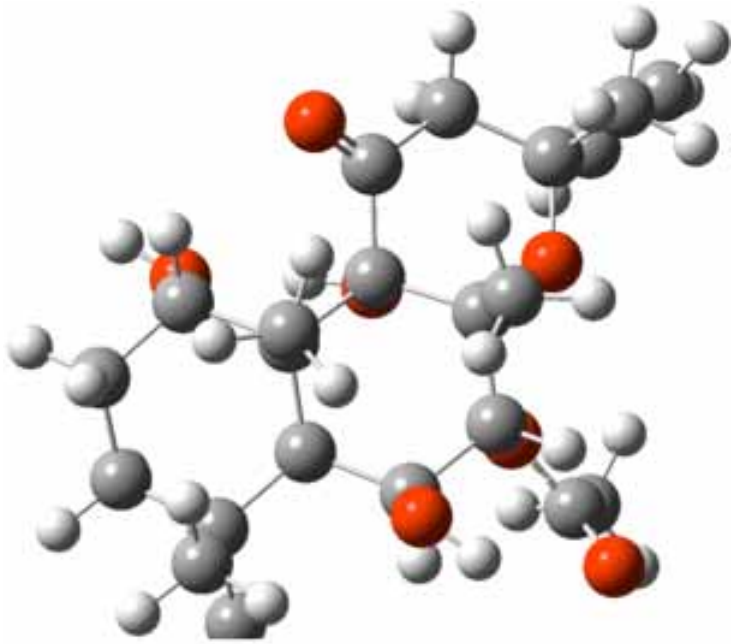

Fig. (S-17). HF/6-31G* geometry optimized of **2(C7)** in the gaseous phase.

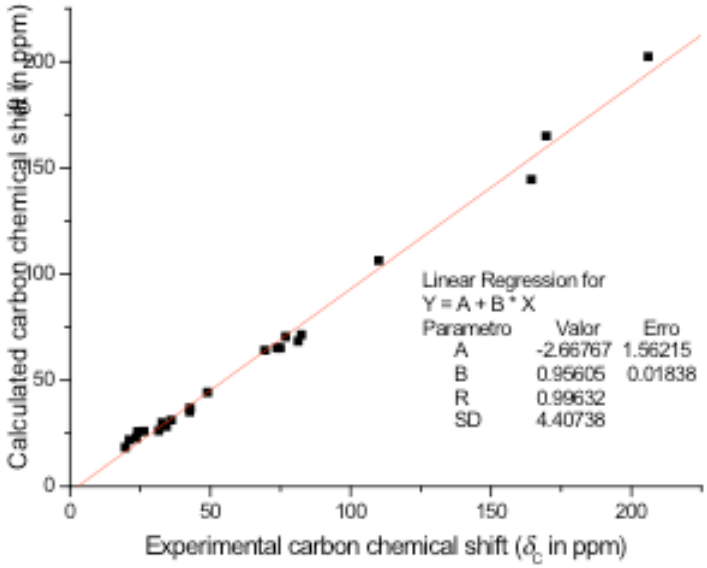

Fig. (S-18). Correlations between ^{13}C NMR data of **2(C7)** and HF/6-31G* calculated carbon chemical shifts of **2** (structure in the gaseous phase).

Table S-10. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 2(C8) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	4.327149	-2.486303	-0.257509
6	3.642331	-1.771218	0.192538
6	3.250828	0.746887	0.543251
6	1.217023	-0.937081	0.060656
6	1.797021	0.516371	-0.008029
6	2.274976	-1.962601	-0.464369
6	4.165456	-0.356279	-0.027835
1	1.904810	0.700809	-1.072761
1	4.284173	-0.201515	-1.095623
1	3.605850	-2.016696	1.246428
1	1.902210	-2.954991	-0.247887
1	5.154354	-0.258308	0.412060
6	0.895137	-1.422365	1.492801
1	1.787768	-1.501555	2.089731
1	0.461086	-2.416996	1.466322
1	0.226655	-0.758139	2.001390
6	3.782036	2.088681	-0.002901
1	4.845254	2.173291	0.200711
1	3.302702	2.942771	0.462218
1	3.648608	2.166759	-1.078307
6	3.397415	0.809956	2.076293
1	4.430377	1.045452	2.318614

(Table S10). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	3.158378	-0.119468	2.572665
1	2.767917	1.575225	2.506028
8	2.465320	-1.866050	-1.872188
1	2.757672	-2.705199	-2.200236
6	0.773832	1.571357	0.448535
1	1.194777	2.552671	0.242836
6	-0.102432	-0.958520	-0.841804
6	-1.169584	0.112358	-0.485249
6	-0.489080	1.486061	-0.404847
8	0.191835	-0.696466	-2.179936
1	0.927891	-1.239454	-2.444974
8	0.484763	1.493592	1.814438
1	-0.372178	1.873636	1.966783
6	-0.787335	-2.331711	-0.738133
8	-0.375847	-3.254188	-1.373735
8	-1.728318	-0.179046	0.771057
6	-2.562510	-1.318063	0.933203
6	-2.009233	-2.538939	0.153982
6	-2.560100	-1.589952	2.443610
6	-3.995534	-0.942390	0.578845
6	-4.965762	-1.735016	0.169938
1	-5.961575	-1.354747	0.029576
1	-4.829733	-2.782269	-0.035530
6	-2.242124	0.194778	-1.587648
1	-3.026042	0.871043	-1.275206
1	-2.697166	-0.762611	-1.801484
1	-1.808055	0.551302	-2.508993
1	-4.213150	0.091991	0.786440
1	-1.737913	-3.331739	0.841830
1	-2.917406	-0.715677	2.974662
1	-1.565740	-1.822589	2.798924
1	-3.218122	-2.420944	2.669893
1	-0.211501	1.742204	-1.413311
8	-1.429706	2.417789	0.109622
6	-1.675457	3.633602	-0.391223
8	-2.401005	4.355625	0.202694
6	-1.033670	4.029024	-1.701620
1	0.048167	4.010363	-1.638118
1	-1.357942	5.032255	-1.931415
1	-1.335590	3.363591	-2.502219
1	-2.759434	-2.963856	-0.499119

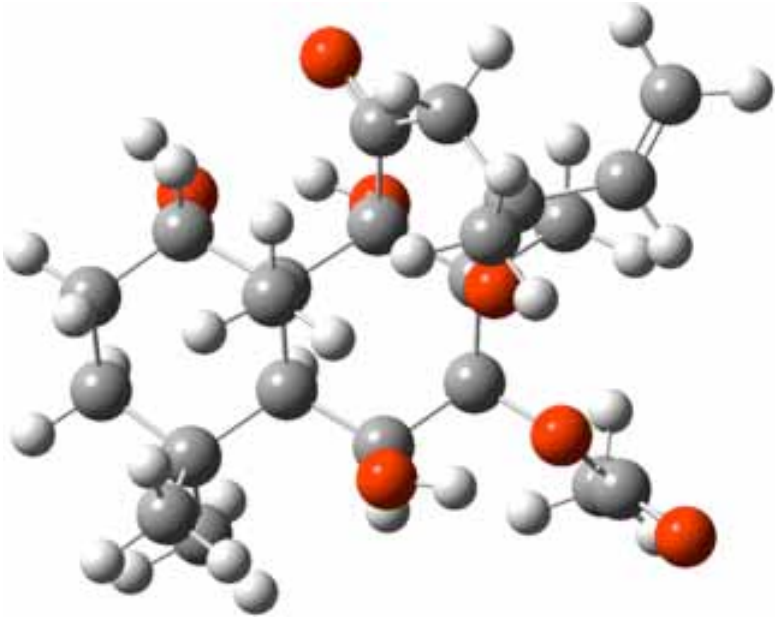

Fig. (S-19). HF/6-31G* geometry optimized of **2(C8)** in the gaseous phase.

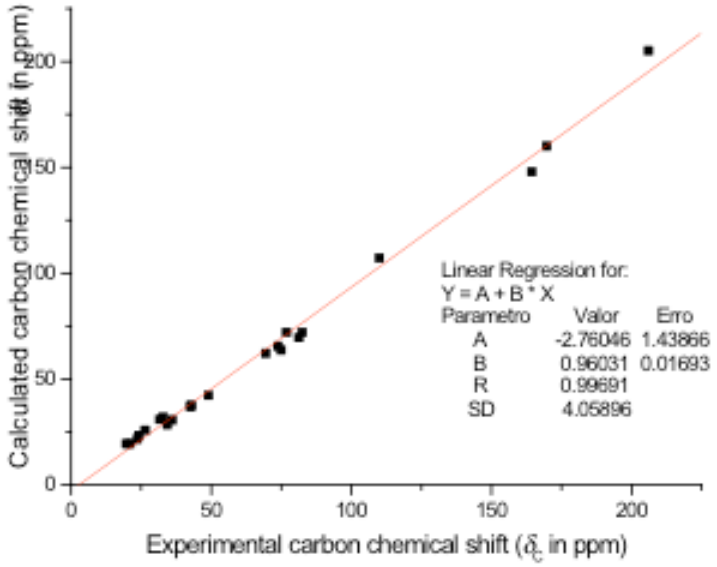

Fig. (S-20). Correlations between ^{13}C NMR data of **2(C8)** and HF/6-31G* calculated carbon chemical shifts of **2** (structure in the gaseous phase).

Table S-11. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 2(C13) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	4.317838	-2.563126	-0.641924
6	3.791267	-1.759113	-0.130685
6	3.488299	0.787596	-0.075786
6	1.416015	-0.855369	0.294891
6	1.948768	0.527677	-0.226993

(Table S11). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
6	2.290754	-2.013524	-0.282794
6	4.211899	-0.415308	-0.716024
1	1.819062	0.474495	-1.301437
1	4.013411	-0.422403	-1.784166
1	4.086033	-1.833088	0.908261
1	2.016760	-2.916235	0.243900
1	5.285214	-0.289466	-0.600942
6	1.503785	-1.030920	1.837270
1	2.438135	-1.496216	2.115651
1	0.726724	-1.685368	2.198260
1	1.451717	-0.093055	2.359267
6	3.873522	2.036310	-0.892609
1	4.954340	2.107281	-0.970243
1	3.526671	2.951284	-0.425849
1	3.475171	1.996781	-1.902933
6	4.018561	1.010953	1.353969
1	5.087506	1.202321	1.303919
1	3.876814	0.159454	2.003376
1	3.545817	1.860581	1.822881
8	2.015419	-2.213234	-1.667793
1	2.411452	-3.024519	-1.954747
6	1.052858	1.718847	0.168985
1	1.357794	2.568790	-0.433568
6	-0.075057	-0.960942	-0.221931
6	-1.020951	0.166836	0.310798
6	-0.422889	1.489193	-0.189840
1	-0.509129	1.488967	-1.260360
8	-0.129888	-0.778279	-1.622236
1	0.535232	-1.330825	-2.020113
8	1.199939	2.062559	1.521144
1	0.571083	2.746150	1.720392
8	-1.129402	2.588009	0.365853
6	-2.132807	3.246449	-0.232406
8	-2.807227	3.962907	0.425696
6	-2.312944	3.090919	-1.722626
1	-1.403055	3.359350	-2.249021
1	-3.108589	3.754487	-2.025870

(Table S11). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	-2.566283	2.071658	-1.978052
6	-1.292297	0.184295	1.820356
1	-0.464907	0.582505	2.377257
1	-1.527160	-0.798612	2.203688
1	-2.145440	0.823908	1.994341
6	-0.800813	-2.291471	0.036709
8	-0.361263	-3.206896	0.662522
8	-2.257192	0.069897	-0.381170
6	-3.034778	-1.119717	-0.386139
6	-2.151589	-2.357089	-0.644549
1	-2.645394	-3.268882	-0.345077
1	-1.958331	-2.418588	-1.707256
6	-4.003485	-0.928040	-1.555827
1	-3.445000	-0.757461	-2.468856
1	-4.644976	-0.072426	-1.377832
1	-4.629140	-1.805420	-1.677452
6	-3.863206	-1.202051	0.886316
1	-4.311698	-0.257142	1.146691
6	-4.130830	-2.257092	1.629951
1	-4.782911	-2.171401	2.480809
1	-3.722353	-3.234115	1.448636

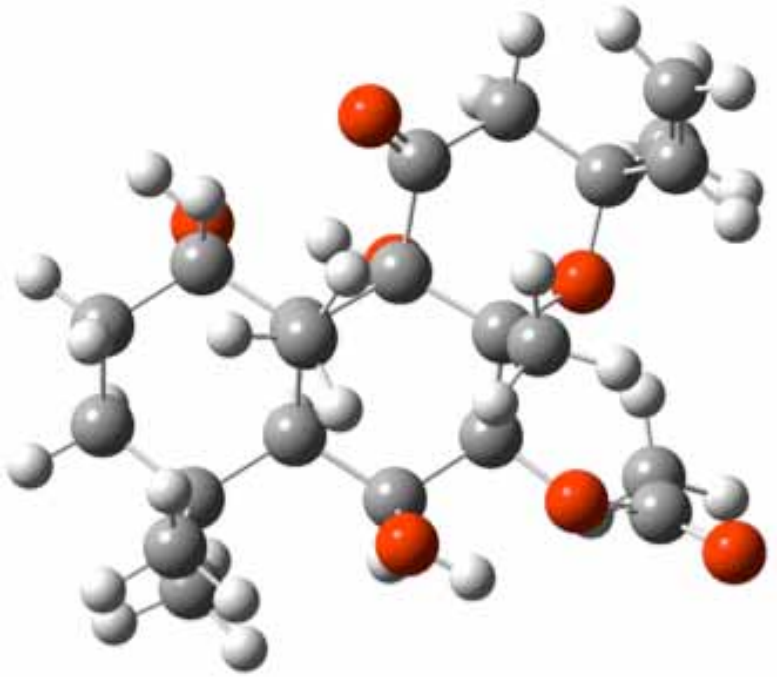

Fig. (S-21). HF/6-31G* geometry optimized of **2(C13)** in the gaseous phase.

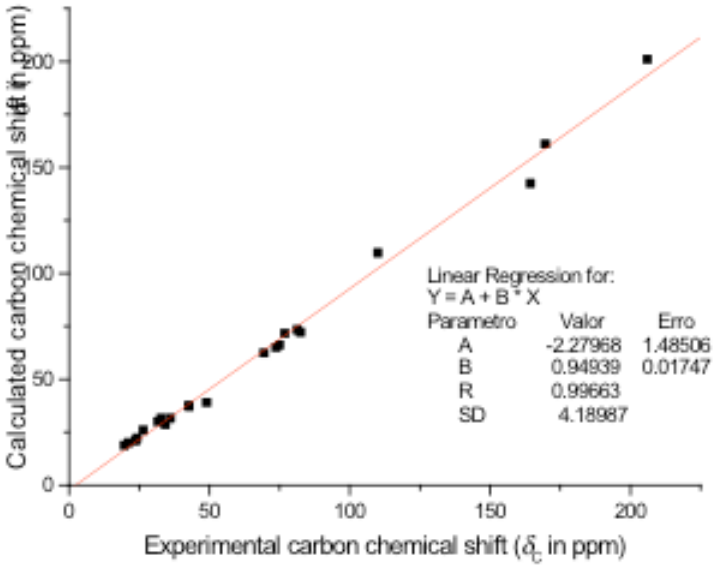

Fig. (S-22). Correlations between ^{13}C NMR data of **2(C13)** and HF/6-31G* calculated carbon chemical shifts of **2** (structure in the gaseous phase).

Table S-12. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 2(C7,C13) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	3.544050	-3.040076	-1.467874
6	3.201582	-2.336121	-0.711455
6	3.418489	0.087566	0.089580
6	1.064136	-1.177760	0.147944
6	1.852580	0.175704	0.028728
6	1.677332	-2.258244	-0.802559
6	3.854287	-0.977668	-0.937510
1	1.663123	0.503876	-0.985746
1	3.604784	-0.632983	-1.936997
1	3.508487	-2.755745	0.238128
1	1.242852	-3.207579	-0.523984
1	4.935567	-1.082757	-0.905972
6	1.138130	-1.831610	1.557212
1	1.978911	-2.507583	1.618408
1	0.261504	-2.427683	1.754692
1	1.263767	-1.108875	2.342398
6	4.021824	1.429338	-0.370153
1	5.090814	1.319067	-0.527248
1	3.889029	2.213320	0.366991
1	3.586108	1.766884	-1.306452
6	4.043716	-0.236139	1.460928
1	5.123651	-0.293510	1.349123

(Table S12). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	3.712527	-1.177872	1.873756
1	3.822210	0.529729	2.188454
8	1.335286	-2.005596	-2.163171
1	1.538035	-2.769607	-2.685028
6	1.246728	1.319581	0.867921
1	1.711083	2.237394	0.535183
6	-0.421308	-0.832647	-0.275334
6	-1.109921	0.242368	0.625729
6	-0.266478	1.535319	0.649944
8	-0.451746	-0.250276	-1.555404
1	0.074069	-0.785392	-2.139352
8	1.513657	1.161533	2.243530
1	1.341045	1.984679	2.682145
6	-1.354881	-0.175682	2.086913
1	-0.464052	-0.110051	2.685362
1	-1.758644	-1.174204	2.175683
1	-2.082987	0.511772	2.498862
6	-1.402403	-2.013762	-0.356759
8	-1.158958	-3.142495	-0.054566
8	-2.341625	0.606087	0.043044
6	-3.341996	-0.347875	-0.275932
6	-2.741131	-1.606414	-0.934898
1	-3.415158	-2.447345	-0.875311
1	-2.570951	-1.391521	-1.981128
6	-4.235769	0.380574	-1.282784
1	-3.638133	0.705035	-2.126016
1	-4.684361	1.254258	-0.823857
1	-5.029550	-0.271992	-1.630493
6	-4.181725	-0.640063	0.958866
1	-4.440980	0.256789	1.498209
6	-4.652456	-1.793912	1.389135
1	-5.279980	-1.834761	2.261753
1	-4.440037	-2.736830	0.920077
1	-0.631880	2.143727	1.463217
8	-0.450958	2.274128	-0.545244
6	-0.456968	3.593357	-0.468830
8	-0.224310	4.207304	0.526016
6	-0.788455	4.210958	-1.799271
1	-0.093492	3.856722	-2.551303
1	-0.742194	5.287231	-1.723861
1	-1.781865	3.899190	-2.099955

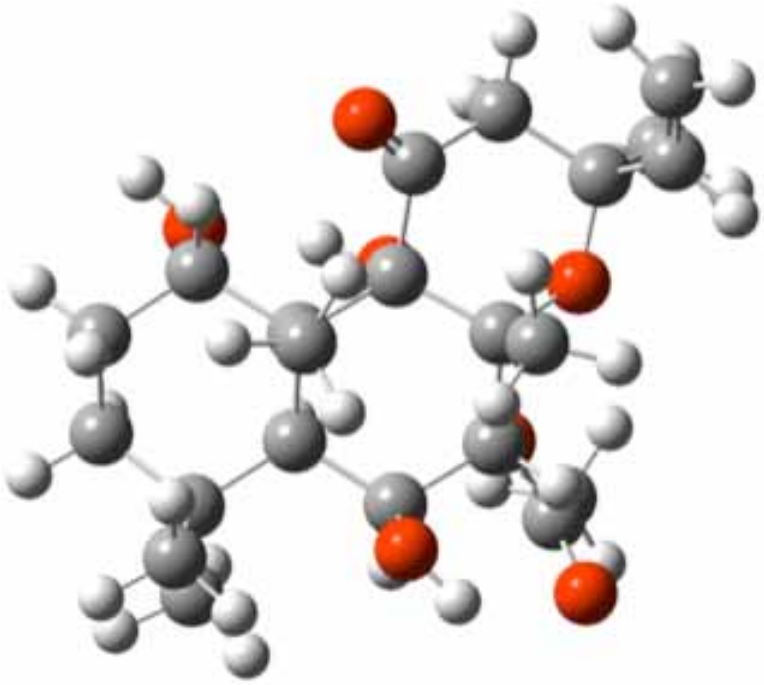

Fig. (S-23). HF/6-31G* geometry optimized of **2(C7,C13)** in the gaseous phase.

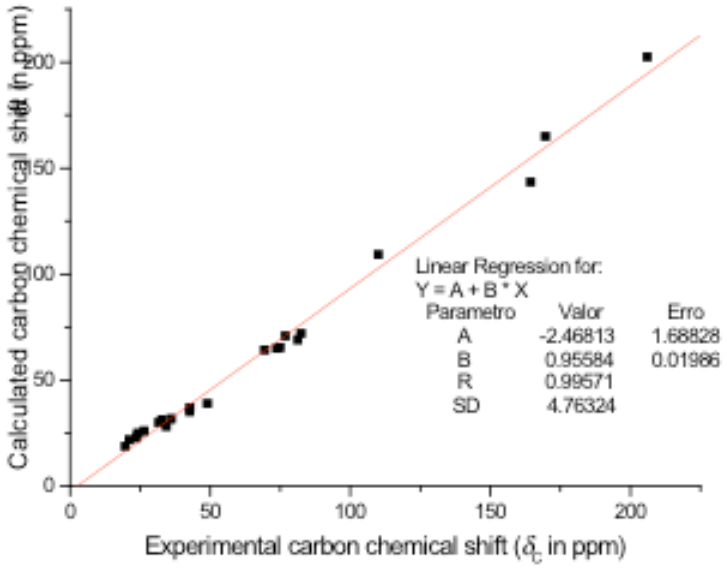

Fig. (S-24). Correlations between ^{13}C NMR data of **2(C7, C13)** and HF/6-31G* calculated carbon chemical shifts of **2** (structure in the gaseous phase).

Table S-13. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 2(C8, C13) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	4.403323	-2.288186	-0.159719
6	3.647482	-1.643972	0.283903
6	3.107687	0.815788	0.810717
6	1.208213	-0.894690	-0.005217

(Table S13). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
6	1.722830	0.580270	0.105955
6	2.355687	-1.828388	-0.513579
6	4.121675	-0.195746	0.237795
1	1.918308	0.864051	-0.923985
1	4.331287	0.059352	-0.796227
1	3.528195	-1.985853	1.304191
1	2.010959	-2.849685	-0.418906
1	5.059978	-0.099991	0.777657
6	0.785292	-1.513708	1.344816
1	1.626303	-1.624440	2.007870
1	0.385944	-2.512077	1.196340
1	0.059773	-0.908714	1.848603
6	3.623981	2.220366	0.434358
1	4.659083	2.326710	0.744672
1	3.065316	3.010644	0.923085
1	3.586010	2.389157	-0.638246
6	3.108067	0.747840	2.350520
1	4.100457	1.005132	2.711211
1	2.872220	-0.231700	2.740779
1	2.402705	1.443785	2.780576
8	2.668401	-1.598546	-1.883260
1	3.056197	-2.383442	-2.245108
6	0.613475	1.549639	0.553379
1	1.007887	2.560191	0.480168
6	-0.026706	-0.890501	-1.020995
6	-1.166803	0.114776	-0.692535
6	-0.551584	1.498055	-0.429764
8	0.374408	-0.514517	-2.303480
1	1.154753	-1.006640	-2.539567
8	0.195890	1.335863	1.870642
1	-0.701669	1.633702	1.961015
6	-0.660395	-2.291797	-1.086896
8	-0.150228	-3.145849	-1.746097
8	-1.855051	-0.284831	0.466644
6	-2.626663	-1.484205	0.500422
6	-1.956971	-2.607532	-0.344363
6	-2.107386	0.267010	-1.904131

(Table S13). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	-2.974341	0.842194	-1.609322
1	-2.439374	-0.685169	-2.296651
1	-1.603162	0.770577	-2.714019
1	-1.741143	-3.470017	0.275554
1	-0.180092	1.844814	-1.379117
8	-1.576748	2.354063	0.050670
6	-1.796715	3.608362	-0.359007
8	-2.602779	4.259598	0.212179
6	-1.024289	4.136821	-1.546648
1	0.044012	4.130833	-1.364104
1	-1.348642	5.151618	-1.718172
1	-1.217580	3.545297	-2.434212
1	-2.641025	-2.966729	-1.105679
6	-4.062997	-1.229796	0.030413
1	-4.483373	-0.386995	0.564271
1	-4.672336	-2.105714	0.221054
1	-4.119532	-1.026849	-1.026636
6	-2.618906	-1.882198	1.969021
1	-1.638145	-2.024037	2.381056
6	-3.655205	-2.070227	2.761102
1	-3.506491	-2.357916	3.786638
1	-4.675562	-1.947158	2.450960

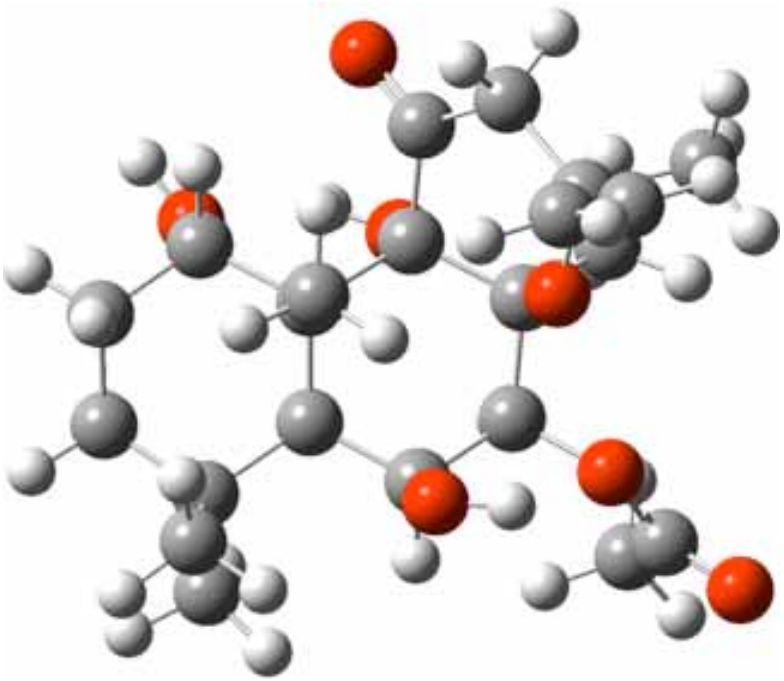

Fig. (S-25). HF/6-31G* geometry optimized of **2(C8,C13)** in the gaseous phase.

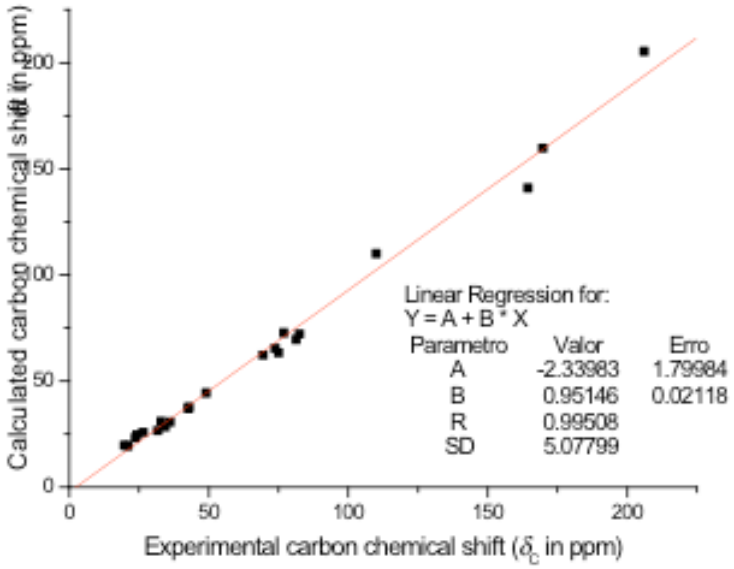

Fig. (S-26). Correlations between ^{13}C NMR data of **2(C8,C13)** and HF/6-31G* calculated carbon chemical shifts of **2** (structure in the gaseous phase).

Table S-14. Geometry Parameters (Standard Orientation) Obtained from the HF/6-31G* Geometry Optimizations of 2(C7,C8,C13) in the Gaseous Phase

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	1.946073	-4.207804	-0.989813
6	1.755764	-3.370295	-0.327512
6	2.810162	-1.301314	0.740267
6	0.257827	-1.282671	-0.110136
6	1.561335	-0.488585	0.248918
6	0.568421	-2.606340	-0.903531
6	2.995501	-2.495303	-0.215570
1	1.893845	-0.083775	-0.700373
1	3.252531	-2.127995	-1.205786
1	1.498618	-3.789612	0.638022
1	-0.307776	-3.235029	-0.822022
1	3.838567	-3.093401	0.120159
6	-0.543521	-1.777691	1.115107
1	0.002663	-2.546676	1.640916
1	-1.477343	-2.230779	0.800351
1	-0.760699	-0.998313	1.816657
6	4.070105	-0.421914	0.604151
1	4.958373	-1.024773	0.768215
1	4.096700	0.382942	1.330229
1	4.149778	0.014003	-0.387755
6	2.768375	-1.794560	2.199298
1	3.670076	-2.365488	2.405731

(Table S14). Contd…..

Atomic Number	Coordinates (Angstroms)		
	x	y	z
1	1.923980	-2.432440	2.416593
1	2.729019	-0.968691	2.894683
8	0.828062	-2.433531	-2.289447
1	0.001848	-2.549579	-2.746480
6	1.262405	0.772196	1.075819
1	2.184669	1.329101	1.166142
6	-0.611871	-0.286348	-0.996873
6	-0.938514	1.080535	-0.335400
6	0.287468	1.720966	0.359748
8	0.057757	0.064811	-2.171706
1	0.539380	-0.688625	-2.496122
8	0.801509	0.469050	2.367464
1	0.792241	1.266323	2.880603
6	-1.942052	-0.963524	-1.373706
8	-1.971936	-1.813875	-2.215257
8	-1.851067	0.893916	0.726505
6	-3.160157	0.370623	0.528652
6	-4.166181	1.530418	0.448089
1	-3.993263	2.160080	-0.413848
1	-4.089713	2.142616	1.339123
1	-5.175846	1.138560	0.391432
6	-3.462264	-0.372446	1.823055
1	-2.905917	0.011432	2.660557
6	-4.348722	-1.327200	2.019657
1	-4.510752	-1.729438	3.003329
1	-4.952378	-1.748630	1.234914
1	-0.106647	2.421821	1.078650
8	1.038940	2.451281	-0.607605
6	1.677852	3.545177	-0.214296
8	1.686524	3.940033	0.908125
6	2.381784	4.208399	-1.365833
1	3.069256	3.508738	-1.826242
1	2.915228	5.078113	-1.012530
1	1.656559	4.497251	-2.117831
6	-1.488601	2.074689	-1.371743
1	-2.363954	1.691093	-1.877743
1	-0.752004	2.294577	-2.122594
1	-1.768198	2.991356	-0.863704
6	-3.247775	-0.522537	-0.730573
1	-3.788353	-0.009999	-1.520052
1	-3.808911	-1.424104	-0.533587

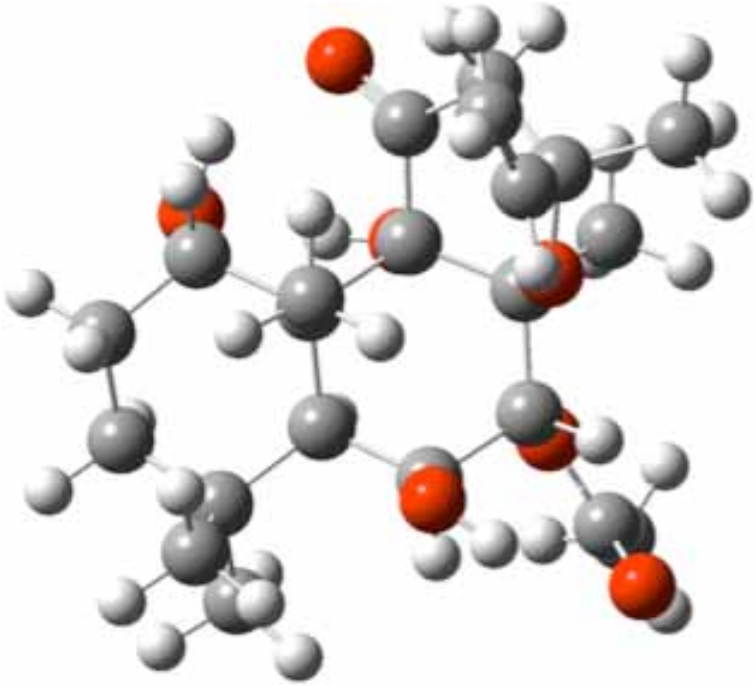

Fig. (S-27). HF/6-31G* geometry optimized of **2(C7,C8,C13)** in the gaseous phase.

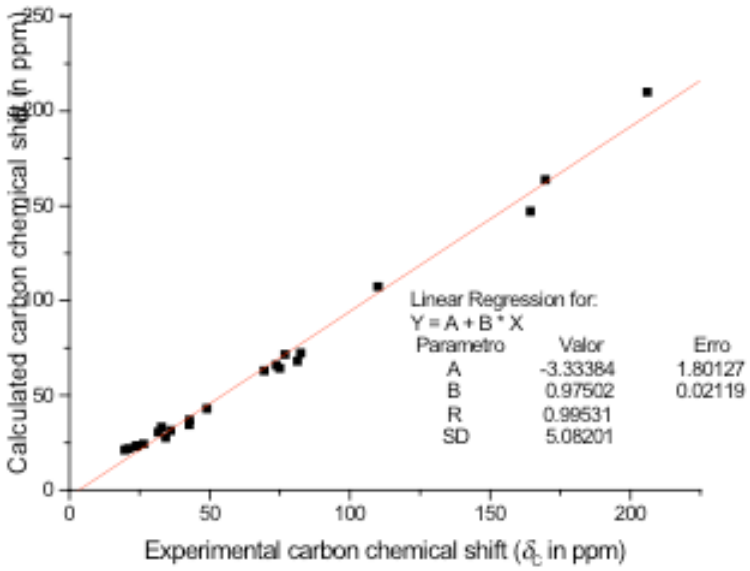

Fig. (S-28). Correlations between ^{13}C NMR data of **2(C7,C8,C13)** and HF/6-31G* calculated carbon chemical shifts of **2** (structure in the gaseous phase).