Supporting Information

4-Arylflavan-3-ols as Proanthocyanidin Models: Absolute Configuration via Density Functional Calculation of Electronic Circular Dichroism

Yuanqing Ding,[†] Xing-Cong Li,[*,†,‡] and Daneel Ferreira[*,†,‡]

National Center for Natural Products Research, Research Institute of Pharmaceutical Sciences, and Department of Pharmacognosy, School of Pharmacy, The University of Mississippi, University, Mississippi 38677

Supporting Information Table of Contents

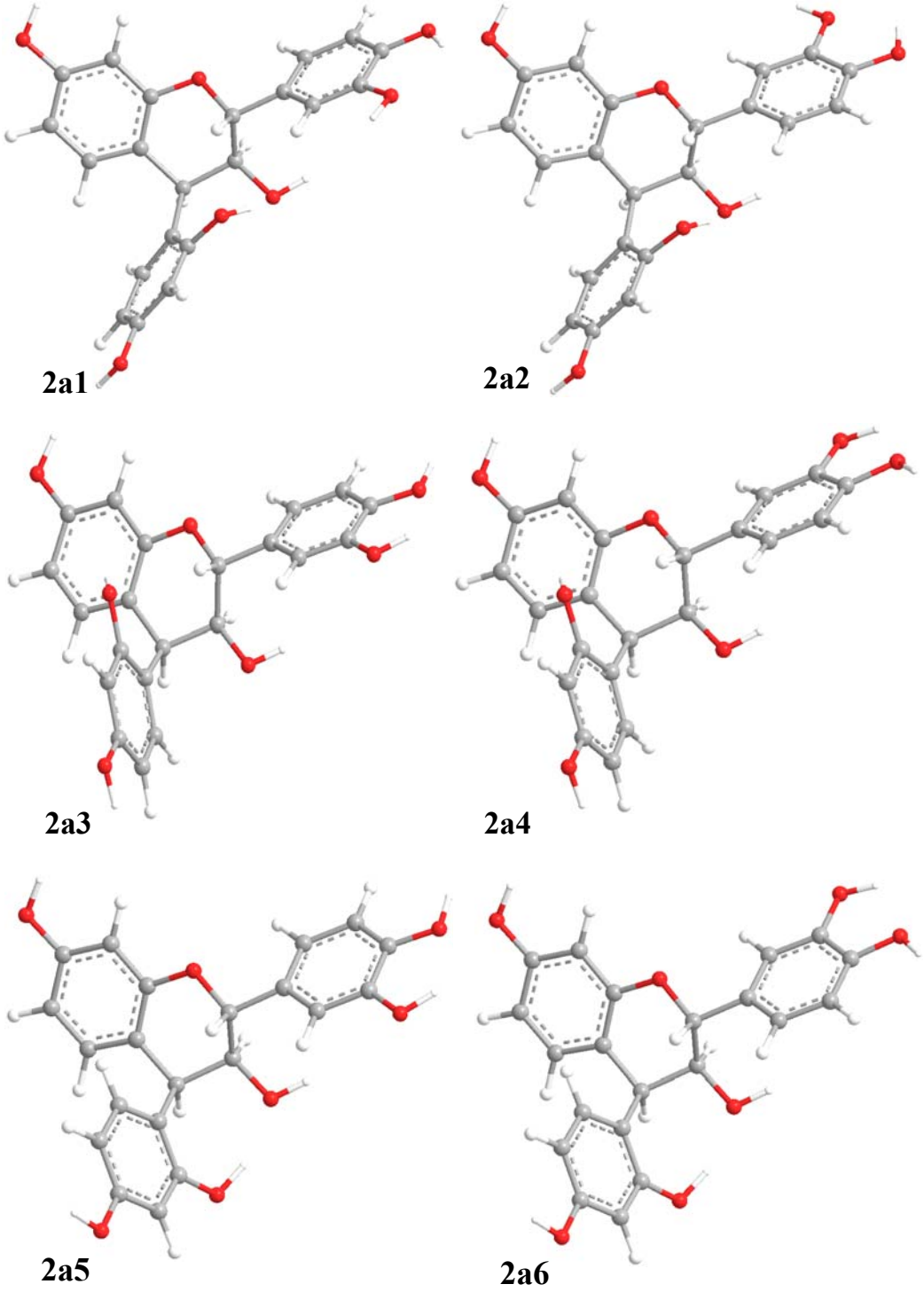

Figure S1. Optimized geometries of (2R,3S,4S)-2,3-trans-3,4-cis-4-arylflavan-3-ol (**2a**) at B3LYP/6-31G* level in the gas phase.

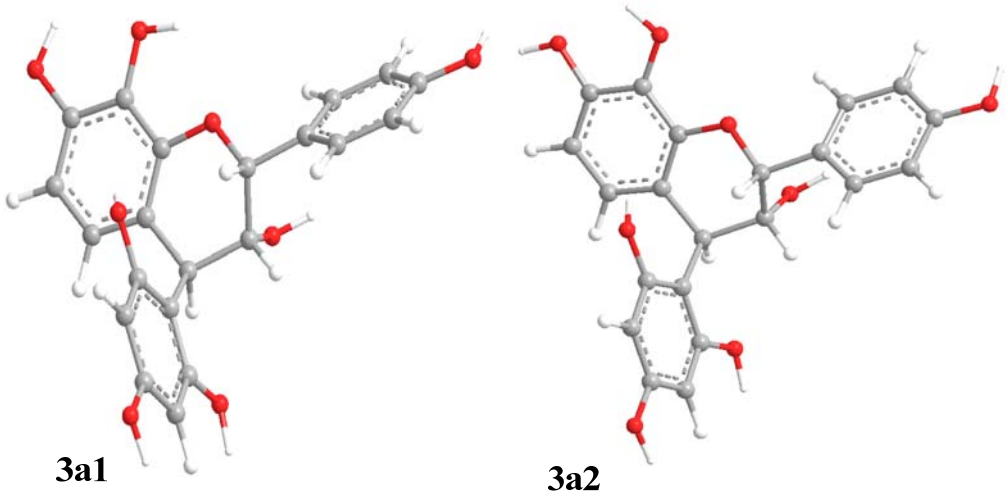

Figure S2. Optimized geometries of (2R,3R,4R)-2,3-cis-3,4-trans-4-arylflavan-3-ol (**3a**) at B3LYP/6-31G* level in the gas phase.

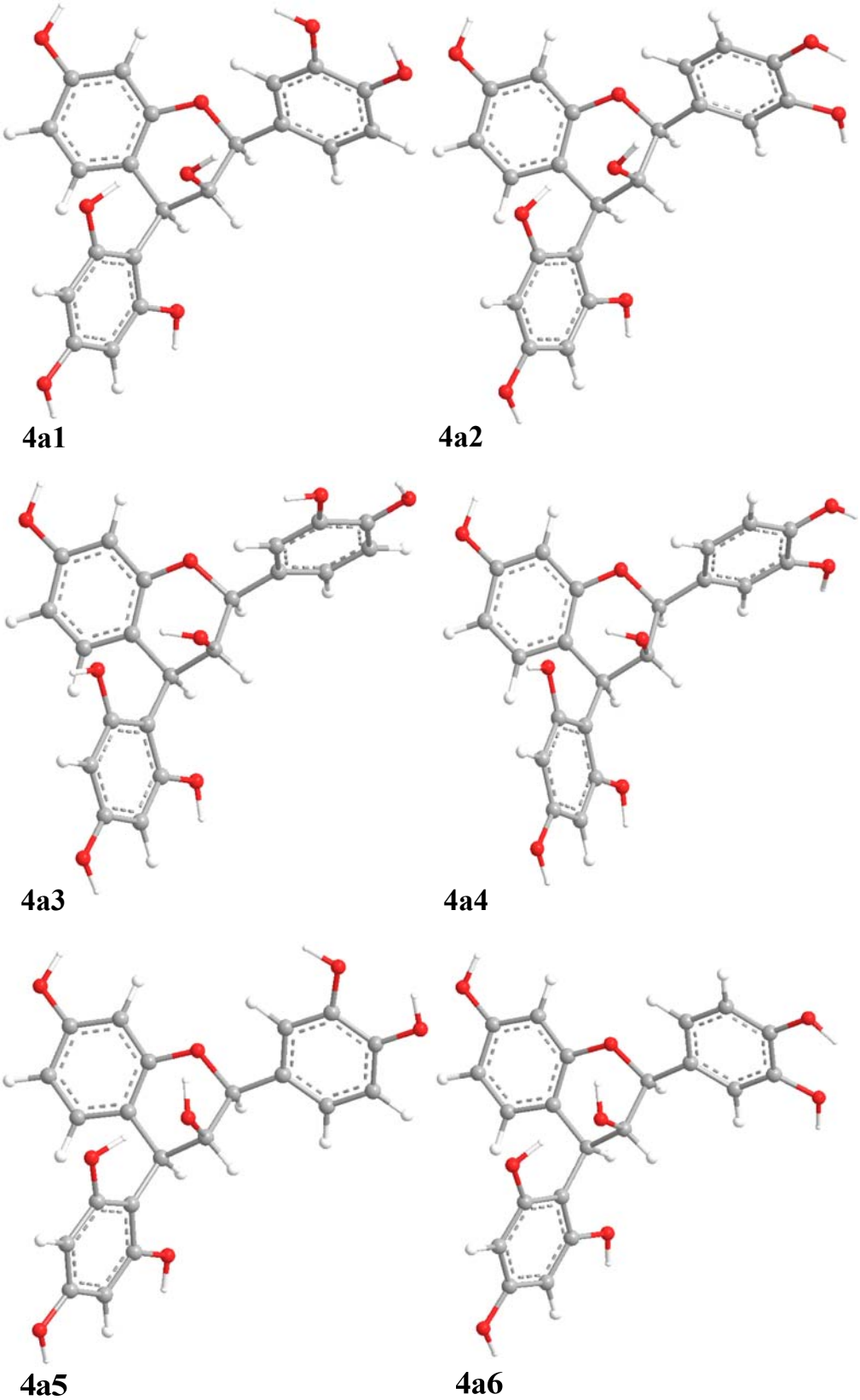

Figure S3. Optimized geometries of (2S,3S,4R)-2,3-cis-3,4-cis-4-arylflavan-3-ol (**4a**) at B3LYP/6-31G* level in the gas phase.

Table S1. Important Thermodynamic Parameters of Compound **1a** (au)

Species	E	E′=E+ZPE	H	G	E″	E_s
1a1	-1412.816686	-1412.455740	-1412.429638	-1412.510199	-1413.2570038	-1412.8563442
1a2	-1412.816420	-1412.455544	-1412.429420	-1412.510126	-1413.2569767	-1412.8566353
1a3	-1412.8075349	-1412.447698	-1412.420971	-1412.503556	-1413.2491781	-1412.853544
1a4	-1412.807477	-1412.447776	-1412.420966	-1412.504349	-1413.249353	-1412.853609
1a5	-1412.7994602	-1412.439431	-1412.412875	-1412.494917		-1412.8428011
1a6	-1412.7998667	-1412.439659	-1412.413232	-1412.494377		-1412.8426887

E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy at B3LYP/6-31G level; E'': single point energy at B3LYP/AUG-cc-pVDZ//B3LYP/6-31G* level in the gas phase; Es: single point energy in methanol solution at B3LYP-SCRF/6-31G*//B3LYP/6-31G* level with COSMO model.*

Table S2. Important Thermodynamic Parameters of Compound **1b** (au)

Species	In Gas Phase				In Methanol
	E	*E´=E+ZPE*	*H*	*G*	E_s
1b1	-1801.308869	-1800.738366	-1800.699787	-1800.811788	-1801.338614
1b2	-1801.309634	-1800.739151	-1800.700573	-1800.812682	-1801.338739
1b3	-1801.308569	-1800.738297	-1800.699583	-1800.811884	-1801.335801
1b4	-1801.308806	-1800.738591	-1800.699817	-1800.811878	-1801.335412

E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy at B3LYP/6-31G level; Es: single point energy in methanol solution at B3LYP-SCRF/6-31G*//B3LYP/6-31G* level with COSMO model.*

Table S3. Important Thermodynamic Parameters of Compound **2a** (au)

Species	E	E′=E+ZPE	H	G	Es
2a1	-1337.593180	-1337.235234	-1337.210805	-1337.288203	-1337.629679
2a2	-1337.592794	-1337.234802	-1337.210358	-1337.287728	-1337.628942
2a3	-1337.5954927	-1337.238807	-1337.213877	-1337.292294	-1337.631035
2a4	-1337.5949927	-1337.238462	-1337.213484	-1337.292091	-1337.63061
2a5	-1337.6033945	-1337.246247	-1337.221508	-1337.299460	-1337.638955
2a6	-1337.6031397	-1337.246038	-1337.221291	-1337.299079	-1337.638666

E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy at B3LYP/6-31G level; Es: single point energy in methanol solution at B3LYP-SCRF/6-31G*//B3LYP/6-31G* level with COSMO model.*

Table S4. Conformational Analysis of Compound **2a**.

Species	ΔE^a	$P_E\%^b$	$\Delta E'^c$	$P_{E'}\%^d$	ΔG^e	$P_G\%^f$	ΔE_s^g	$P_{Es}\%^h$
2a1	6.41	0.0	6.91	0.0	7.06	0.0	5.82	0.0
2a2	6.65	0.0	7.18	0.0	7.36	0.0	6.28	0.0
2a3	4.96	0.0	4.67	0.0	4.50	0.0	4.97	0.0
2a4	5.27	0.0	4.89	0.0	4.62	0.0	5.24	0.0
2a5	0.00	56.7	0.00	55.5	0.00	59.9	0.00	57.6
2a6	0.16	43.3	0.13	44.5	0.24	40.0	0.18	42.4

[a,c,e] Relative energy, relative energy with ZPE, and relative Gibbs free energy at B3LYP/6-31G level in the gas phase, respectively (kcal/mol). [b,d,f] Conformational distribution calculated by using the respective parameters above at B3LYP/6-31G* level in the gas phase. [g,h] Relative energy (kcal/mol) and conformational distribution in methanol solution at B3LYP-SCRF/6-31G*//B3LYP/6-31G* level with COSMO model, respectively.*

Table S5. Important Thermodynamic Parameters of Compounds **3a** (au)

Species	E	E′=E+ZPE	H	G	Es
3a1	-1412.813887	-1412.452850	-1412.426754	-1412.507309	-1412.852188
3a2	-1412.8064063	-1412.446001	-1412.420578	-1412.501058	-1412.848942

E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy at B3LYP/6-31G level; Es: single point energy in methanol solution at B3LYP-SCRF/6-31G*//B3LYP/6-31G* level with COSMO model.*

Table S6: Important Thermodynamic Parameters of Compound **4a** (au).

Species	In Gas Phase				In Methanol
	E	*E′=E+ZPE*	*H*	*G*	E_s
4a1	-1412.817301	-1412.4563	-1412.430214	-1412.5109	-1412.8595
4a2	-1412.817956	-1412.4569	-1412.430853	-1412.5114	-1412.8596
4a3	-1412.809054	-1412.4485	-1412.422065	-1412.5038	-1412.855
4a4	-1412.81094	-1412.4501	-1412.423825	-1412.5053	-1412.8555
4a5	-1412.815785	-1412.4547	-1412.428595	-1412.5097	-1412.8584
4a6	-1412.816243	-1412.4551	-1412.428988	-1412.5102	-1412.8585

E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy in the gas phase at B3LYP/6-31G level; E_s: single point energy in methanol solution at B3LYP-SCRF/6-31G*//B3LYP/6-31G* level with COSMO model.*

Table S7. Conformational Analysis of Compound **4a**.

Species	In Gas Phase						In Methanol	
	ΔE^a	$P_E\%^b$	$\Delta E'^c$	$P_{E'}\%^d$	ΔG^e	$P_G\%^f$	ΔEs^g	$P_{Es}\%^h$
4a1	0.41	28.3	0.40	29.2	0.34	28.0	0.05	36.0
4a2	0.00	56.7	0.00	57.6	0.00	50.0	0.00	39.5
4a3	5.59	0.0	5.32	0.0	4.80	0.0	2.91	0.3
4a4	4.40	0.0	4.29	0.0	3.85	0.1	2.56	0.5
4a5	1.36	5.7	1.40	5.4	1.09	7.9	0.76	11.0
4a6	1.08	9.2	1.18	7.8	0.75	14.0	0.67	12.7

[a,c,e] Relative energy, relative energy with ZPE, and relative Gibbs free energy at B3LYP/6-31G level in the gas phase, respectively (kcal/mol). [b,d,f] Conformational distribution calculated by using the respective parameters above at B3LYP/6-31G* level in the gas phase. [g,h] Relative energy (kcal/mol) and conformational distribution in methanol solution at B3LYP-SCRF/6-31G*//B3LYP/6-31G* level with COSMO model, respectively.*

Table S8. The geometric parameters for the possible stationary points of compounds **1a** and **1b** in gas phase (Å).

1a1				**1a2**			
C	1.743264	4.156181	-0.242098	C	1.442204	4.201617	-0.118753
C	2.777555	3.324637	-0.688893	C	2.565938	3.463378	-0.510051
C	2.541660	1.960854	-0.837514	C	2.444157	2.092899	-0.720497
C	1.299538	1.387602	-0.551444	C	1.228338	1.423420	-0.557186
C	0.274786	2.250412	-0.135631	C	0.112862	2.195130	-0.199171
C	0.485872	3.620073	0.027116	C	0.209707	3.568411	0.027954
C	1.049368	-0.105917	-0.724637	C	1.104751	-0.076123	-0.801226
C	-0.350022	-0.501718	-0.228448	C	-0.300619	-0.587582	-0.449418
C	-1.385071	0.600526	-0.527405	C	-1.381258	0.454306	-0.795882
O	-0.995262	1.800063	0.145505	O	-1.139821	1.645165	-0.043352
C	-2.774350	0.218334	-0.066669	C	-2.773927	-0.045646	-0.484716
C	-3.597685	-0.541813	-0.912634	C	-3.323291	0.122568	0.794534
C	-4.854334	-0.963952	-0.487060	C	-4.579110	-0.393792	1.094272
C	-5.300224	-0.620929	0.800715	C	-5.295931	-1.101256	0.111046

C	-4.491484	0.135728	1.641127	C	-4.756429	-1.276444	-1.156870
C	-3.227337	0.550809	1.213346	C	-3.496255	-0.746542	-1.456629
C	2.123699	-1.034557	-0.167363	C	2.189293	-0.948952	-0.177570
O	-0.679719	-1.708400	-0.927304	O	-0.485037	-1.779322	-1.224580
C	2.800826	-0.808279	1.046525	C	2.734845	-0.724152	1.101204
C	3.863178	-1.612622	1.462720	C	3.808519	-1.471064	1.588998
C	4.241967	-2.703727	0.678082	C	4.333046	-2.503666	0.809055
C	3.539848	-3.015836	-0.484174	C	3.763630	-2.817584	-0.423281
C	2.471992	-2.202770	-0.876189	C	2.681610	-2.063139	-0.887253
O	-6.557902	-1.082338	1.121719	O	-6.526226	-1.570477	0.514885
O	-5.644634	-1.698076	-1.319976	O	-5.110361	-0.215838	2.335790
O	1.904044	5.504947	-0.065638	O	1.490171	5.550151	0.115966
O	2.373151	0.236463	1.820051	O	2.164857	0.258985	1.862702
O	1.785629	-2.585699	-1.993771	O	2.127996	-2.448464	-2.076071
O	5.291942	-3.458210	1.124958	O	5.388631	-3.201793	1.328393
H	3.758539	3.739715	-0.912070	H	3.528237	3.955361	-0.638575
H	3.351651	1.314365	-1.164765	H	3.323062	1.518312	-1.001021
H	-0.328649	4.258958	0.349340	H	-0.672230	4.134862	0.304912
H	1.025066	-0.291803	-1.808383	H	1.192282	-0.220334	-1.888095
H	-0.333596	-0.673213	0.855753	H	-0.365630	-0.810185	0.623547
H	-1.386995	0.778347	-1.613515	H	-1.300165	0.680856	-1.869859
H	-3.283246	-0.796407	-1.920700	H	-2.787956	0.677160	1.557004
H	-4.847951	0.403292	2.634386	H	-5.320482	-1.814589	-1.916459
H	-2.601958	1.149934	1.864933	H	-3.087935	-0.868517	-2.455839
H	4.387498	-1.415475	2.393845	H	4.231347	-1.274616	2.570462
H	3.769770	-3.899486	-1.072847	H	4.107131	-3.661020	-1.015518
H	5.442890	-4.179530	0.494615	H	5.648239	-3.886480	0.692620
H	2.961639	0.316885	2.586751	H	2.665210	0.343568	2.689228
H	0.842121	-2.364426	-1.852745	H	1.162752	-2.294512	-2.017478
H	-1.496948	-2.077208	-0.555053	H	-1.312822	-2.205505	-0.949420
H	-6.808089	-0.763185	2.001635	H	-6.971350	-2.004232	-0.228353
H	-6.479721	-1.871634	-0.852318	H	-5.990084	-0.630638	2.340684

H	2.811714	5.742664	-0.310044	H	2.396241	5.858520	-0.039065
1a3				**1a4**			
C	-0.010886	-0.009185	-0.026852	C	-0.039780	0.014803	0.010222
C	-0.021952	0.001519	1.372987	C	-0.032567	0.020823	1.410325
C	1.188168	-0.003518	2.062582	C	1.186391	0.014597	2.084033
C	2.419349	-0.020840	1.402675	C	2.408669	0.001911	1.407345
C	2.400599	-0.006546	-0.001594	C	2.371665	0.019859	0.003576
C	1.199970	-0.007430	-0.715257	C	1.161697	0.019980	-0.694171
C	3.744871	-0.002387	2.153945	C	3.742861	0.018756	2.143206
C	4.929292	-0.323590	1.218675	C	4.918625	-0.291090	1.193315
C	4.754161	0.426069	-0.120602	C	4.723938	0.453400	-0.145669
O	3.541826	-0.007868	-0.758278	O	3.502660	0.022263	-0.767423
C	5.892711	0.195722	-1.089242	C	5.849534	0.215674	-1.126760
C	7.027526	1.014530	-1.027792	C	5.803374	-0.867864	-2.013741
C	8.103880	0.799017	-1.880542	C	6.858510	-1.109635	-2.886883
C	8.047739	-0.247464	-2.815747	C	7.979604	-0.263374	-2.873812
C	6.924283	-1.062378	-2.885219	C	8.032751	0.812412	-1.995279
C	5.847192	-0.844250	-2.021385	C	6.967538	1.052611	-1.124020
C	3.800153	-0.849869	3.417021	C	3.811859	-0.843335	3.395807
O	6.168247	0.018959	1.823882	O	6.161170	0.074165	1.781377
C	4.361887	-0.329485	4.594847	C	4.360908	-0.331901	4.583077
C	4.443641	-1.054554	5.783326	C	4.448903	-1.072948	5.761295
C	3.979112	-2.369351	5.801255	C	4.003879	-2.394619	5.758436
C	3.455666	-2.947167	4.643818	C	3.493700	-2.963303	4.590515
C	3.389393	-2.192573	3.466027	C	3.419710	-2.192566	3.423809
O	9.161757	-0.372375	-3.621553	O	8.968716	-0.587025	-3.780849
O	9.203770	1.606456	-1.812887	O	6.801467	-2.164111	-3.753669
O	-1.159991	-0.011754	-0.773510	O	-1.198848	0.013849	-0.720467
O	4.858168	0.953777	4.526269	O	4.839737	0.959225	4.534616
O	2.927413	-2.744405	2.306704	O	2.968332	-2.732051	2.255092
O	4.074294	-3.048241	6.982652	O	4.105120	-3.089385	6.929810
H	-0.965085	0.008270	1.916099	H	-0.968600	0.023934	1.965661

H	1.178131	-0.011094	3.149494	H	1.190714	0.003039	3.171041
H	1.217113	0.002794	-1.799275	H	1.165087	0.031195	-1.778243
H	3.904124	1.036029	2.476994	H	3.902431	1.053992	2.475684
H	4.952527	-1.397160	0.997201	H	4.951392	-1.365116	0.975381
H	4.671015	1.502211	0.098933	H	4.648938	1.530394	0.072425
H	7.093861	1.823158	-0.307527	H	4.938543	-1.520629	-2.045778
H	6.885952	-1.867483	-3.617465	H	8.903254	1.466317	-1.992626
H	4.965182	-1.470730	-2.086834	H	7.018182	1.887965	-0.433159
H	4.876024	-0.627774	6.683631	H	4.871947	-0.653131	6.669272
H	3.116789	-3.982253	4.647360	H	3.169666	-4.003056	4.577521
H	3.738795	-3.949380	6.858208	H	3.784008	-3.993621	6.790569
H	5.219514	1.196172	5.393018	H	5.184715	1.197523	5.409104
H	2.666212	-3.663562	2.471258	H	2.724833	-3.659058	2.401748
H	5.989829	0.617318	2.567721	H	5.979596	0.635282	2.552812
H	9.031426	-1.108379	-4.237630	H	9.702222	0.039575	-3.694026
H	9.832702	1.292719	-2.484764	H	7.624440	-2.155874	-4.271417
H	-1.919207	0.010527	-0.170943	H	-1.949523	0.030686	-0.107153
1a5				**1a6**			
C	-0.155861	0.312032	0.227544	C	4.374546	-0.626805	-1.150238
C	-0.018936	0.684322	1.571100	C	4.145808	0.743078	-1.335032
C	1.242742	0.646680	2.156616	C	3.073877	1.342454	-0.681003
C	2.379380	0.235635	1.454464	C	2.205726	0.621457	0.143822
C	2.214617	-0.122730	0.105963	C	2.465132	-0.748363	0.320148
C	0.958737	-0.083958	-0.507267	C	3.541993	-1.370887	-0.318129
C	3.752886	0.218296	2.097832	C	1.052027	1.288540	0.868527
C	4.815188	0.355979	0.976015	C	0.743409	0.457995	2.141950
C	4.585598	-0.615977	-0.197776	C	0.595917	-1.051981	1.862511
O	3.247317	-0.496285	-0.715960	O	1.721728	-1.567692	1.129851
C	4.961687	-2.073486	0.040850	C	-0.722225	-1.480366	1.231056
C	6.255209	-2.384515	0.489066	C	-0.757147	-2.182668	0.022612
C	6.656126	-3.705295	0.648948	C	-1.971068	-2.576399	-0.531478
C	5.761545	-4.744169	0.341604	C	-3.169965	-2.304072	0.143453

C	4.486133	-4.447023	-0.120796	C	-3.143163	-1.637435	1.363765
C	4.087176	-3.114707	-0.275017	C	-1.923259	-1.226633	1.904728
C	4.045422	-0.900039	3.100234	C	-0.181742	1.659165	0.041846
O	4.837481	1.693040	0.479922	O	1.763753	0.660487	3.117845
C	3.396756	-2.147300	3.178664	C	-0.578997	1.083323	-1.181172
C	3.737100	-3.105159	4.140059	C	-1.726410	1.502534	-1.864236
C	4.749350	-2.837965	5.056652	C	-2.513128	2.521651	-1.336984
C	5.416858	-1.613237	5.023256	C	-2.156173	3.128606	-0.132222
C	5.055343	-0.673540	4.053959	C	-1.005477	2.690802	0.529357
O	6.258207	-6.017888	0.529325	O	-4.314335	-2.746467	-0.488579
O	7.916223	-3.988264	1.092834	O	-1.988453	-3.222034	-1.737802
O	-1.362966	0.325999	-0.420266	O	5.410440	-1.287621	-1.755254
O	2.399706	-2.414440	2.286769	O	0.194193	0.093249	-1.710205
O	5.693616	0.538834	3.990124	O	-0.629391	3.262640	1.718657
O	5.043476	-3.811333	5.970611	O	-3.624305	2.890117	-2.044239
H	-0.886310	1.004063	2.145268	H	4.801008	1.329483	-1.976095
H	1.353979	0.935517	3.199462	H	2.892463	2.405837	-0.821378
H	0.858658	-0.358479	-1.551523	H	3.724034	-2.428449	-0.162776
H	3.860647	1.150167	2.664140	H	1.423906	2.237563	1.270669
H	5.810194	0.192598	1.391102	H	-0.172594	0.824097	2.607719
H	5.210113	-0.236714	-1.015648	H	0.677882	-1.537795	2.842097
H	6.979287	-1.608241	0.717952	H	0.158576	-2.416034	-0.505161
H	3.801498	-5.255734	-0.373013	H	-4.073805	-1.436601	1.891779
H	3.095931	-2.887260	-0.646440	H	-1.918580	-0.711272	2.861388
H	3.220209	-4.059736	4.182679	H	-2.009048	1.046653	-2.808731
H	6.211226	-1.391559	5.734566	H	-2.763396	3.927633	0.291259
H	5.769656	-3.504189	6.534729	H	-4.064739	3.618620	-1.580362
H	2.140080	-3.343454	2.384730	H	-0.286968	-0.322994	-2.442783
H	6.357953	0.583982	4.694424	H	-1.250081	3.974203	1.937203
H	3.942431	1.898686	0.162462	H	2.613136	0.449366	2.695387
H	5.600761	-6.667110	0.238424	H	-5.088727	-2.513001	0.044330
H	8.001816	-4.956606	1.118368	H	-2.915541	-3.441717	-1.933070

H	-2.043415	0.625802	0.201944	H	5.902531	-0.655937	-2.301924

1b1				**1b2**			
C	1.802676	4.473839	-0.336796	C	1.493102	4.486934	-0.336420
C	2.866265	3.612598	-0.634352	C	2.637899	3.709195	-0.550756
C	2.616156	2.244154	-0.751936	C	2.498510	2.330708	-0.720255
C	1.345269	1.695117	-0.580132	C	1.259027	1.691498	-0.687117
C	0.295484	2.585575	-0.295740	C	0.125429	2.500539	-0.493947
C	0.515948	3.955588	-0.171759	C	0.235614	3.878017	-0.315700
C	1.083130	0.196078	-0.720373	C	1.121767	0.180572	-0.872512
C	-0.301933	-0.147699	-0.141298	C	-0.290478	-0.268349	-0.455968
C	-1.347929	0.877422	-0.618798	C	-1.345419	0.693404	-1.033289
O	-0.998450	2.168473	-0.100820	O	-1.149136	1.989760	-0.446059
C	-2.756021	0.559079	-0.170712	C	-2.768111	0.265691	-0.763853
C	-3.628484	-0.107140	-1.047864	C	-3.321059	0.418140	0.519805
C	-4.919346	-0.450350	-0.655146	C	-4.615109	-0.009367	0.795750
C	-5.361948	-0.121265	0.650781	C	-5.388292	-0.613518	-0.230413
C	-4.494371	0.543885	1.514468	C	-4.836405	-0.762455	-1.499722
C	-3.197605	0.879976	1.108088	C	-3.532505	-0.321372	-1.764531
C	2.185594	-0.689295	-0.159498	C	2.214484	-0.635864	-0.198247
O	-0.694687	-1.441013	-0.647284	O	-0.530152	-1.575997	-1.015452
C	2.528140	-0.680935	1.210798	C	2.403092	-0.622487	1.201518
C	3.525241	-1.508863	1.725659	C	3.394096	-1.384972	1.819021
C	4.210103	-2.371312	0.864797	C	4.227647	-2.187217	1.034200
C	3.909305	-2.410941	-0.497621	C	4.080850	-2.230159	-0.352982
C	2.898719	-1.568661	-0.990066	C	3.074720	-1.452360	-0.949764
O	-6.639942	-0.490910	0.950258	O	-6.643917	-1.002216	0.131532
O	-5.833066	-1.090335	-1.442052	O	-5.233664	0.102321	2.004901
O	1.915600	5.830099	-0.192459	O	1.496419	5.842314	-0.147301
O	1.822456	0.193242	1.981405	O	1.556039	0.189514	1.895095
O	2.551501	-1.551935	-2.316328	O	2.878029	-1.439145	-2.306199
O	5.169144	-3.143030	1.458361	O	5.168075	-2.897547	1.725788
H	3.874382	3.985621	-0.771078	H	3.625655	4.153859	-0.578586
H	3.445715	1.575733	-0.966482	H	3.390811	1.727339	-0.864301
H	-0.313259	4.618371	0.049435	H	-0.656243	4.476245	-0.165491
H	1.018874	-0.033547	-1.789473	H	1.194570	-0.034234	-1.944041
H	-0.288380	-0.177104	0.947107	H	-0.394730	-0.317598	0.626903
H	-1.314535	0.916674	-1.718545	H	-1.189373	0.768591	-2.119740
H	-3.282386	-0.352050	-2.045985	H	-2.725888	0.893318	1.289842
H	-4.819969	0.808121	2.514076	H	-5.416271	-1.213959	-2.296591
H	-2.540236	1.408661	1.789852	H	-3.122451	-0.441244	-2.763639
H	3.789662	-1.514270	2.774621	H	3.542958	-1.384490	2.890450
H	4.440646	-3.076911	-1.161277	H	4.727134	-2.848586	-0.957900
C	5.899094	-4.052173	0.653262	C	2.741988	6.516184	-0.181049

H	6.594580	-4.556844	1.326678	H	3.239964	6.400568	-1.153303
H	5.241658	-4.798462	0.187250	H	2.516811	7.571831	-0.015861
H	6.467743	-3.533686	-0.130537	H	3.417018	6.162715	0.610242
C	3.242931	-2.391747	-3.222607	C	-7.459089	-1.608658	-0.854966
H	4.315935	-2.160082	-3.254356	H	-8.403625	-1.841877	-0.359736
H	3.111010	-3.453737	-2.975485	H	-7.649390	-0.929863	-1.697569
H	2.804643	-2.195181	-4.203127	H	-7.011452	-2.536506	-1.236936
C	2.044959	0.205640	3.383225	C	-4.495789	0.669555	3.074355
H	1.824911	-0.771611	3.830040	H	-3.593396	0.084340	3.296291
H	3.076216	0.495001	3.622779	H	-4.207471	1.707762	2.861300
H	1.358349	0.953067	3.784224	H	-5.162537	0.650105	3.938602
C	-5.454984	-1.413542	-2.767380	C	3.719421	-2.221081	-3.134205
H	-5.201260	-0.516002	-3.347858	H	4.771408	-1.918215	-3.046623
H	-4.601333	-2.105458	-2.789906	H	3.632838	-3.291907	-2.906604
H	-6.323627	-1.899722	-3.215777	H	3.378969	-2.043268	-4.156230
C	-7.132297	-0.181076	2.242165	C	6.046167	-3.740821	1.000689
H	-6.542669	-0.670802	3.028986	H	5.500115	-4.525350	0.459839
H	-7.141699	0.902340	2.423329	H	6.658465	-3.171737	0.288110
H	-8.155781	-0.559977	2.269845	H	6.697987	-4.204202	1.743853
C	3.194372	6.414111	-0.366348	C	1.638177	0.216992	3.311586
H	3.057786	7.486803	-0.214439	H	1.449732	-0.774296	3.742127
H	3.917893	6.034673	0.368009	H	2.615848	0.583316	3.649939
H	3.586671	6.239297	-1.377398	H	0.861287	0.910228	3.638758
C	-0.873034	-2.449804	0.244564	C	-0.795610	-2.597728	-0.161810
O	-0.701688	-2.354613	1.438147	C	-1.076220	-3.861730	-0.940778
C	-1.327308	-3.699835	-0.473093	H	-0.259527	-4.067281	-1.639597
H	-1.359200	-4.532402	0.230546	H	-1.200430	-4.695908	-0.249393
H	-2.325701	-3.536828	-0.893593	H	-1.990074	-3.731210	-1.530320
H	-0.652343	-3.930035	-1.303024	O	-0.812461	-2.503285	1.044492
1b3				**1b4**			
C	1.703974	4.530527	-0.295885	C	1.083020	4.581776	-0.206191
C	2.796719	3.730917	-0.664305	C	2.309526	3.940945	-0.439383
C	2.618034	2.365478	-0.835971	C	2.332854	2.573739	-0.675562
C	1.373535	1.745300	-0.655264	C	1.165264	1.797706	-0.692461
C	0.297776	2.567853	-0.306224	C	-0.045164	2.463947	-0.475106
C	0.449203	3.948632	-0.120458	C	-0.099011	3.842633	-0.228721
C	1.179049	0.243032	-0.856646	C	1.196007	0.293817	-0.963326
C	-0.170441	-0.190763	-0.256265	C	-0.155033	-0.328145	-0.568684
C	-1.276287	0.803202	-0.662388	C	-1.311328	0.536032	-1.106482
O	-0.973891	2.087287	-0.101371	O	-1.260676	1.820580	-0.466758
C	-2.653396	0.397360	-0.189558	C	-2.677243	-0.060343	-0.857537
C	-3.491529	-0.346431	-1.030494	C	-3.243031	-0.009909	0.424833
C	-4.741949	-0.783634	-0.607131	C	-4.481876	-0.597928	0.681587
C	-5.187906	-0.469926	0.696023	C	-5.179149	-1.240393	-0.368315

C	-4.362747	0.289432	1.530219	C	-4.608989	-1.287910	-1.635889
C	-3.105742	0.713259	1.091183	C	-3.363418	-0.705267	-1.885137
C	2.336168	-0.614850	-0.366692	C	2.378756	-0.436234	-0.344039
O	-0.517384	-1.478671	-0.804452	O	-0.252203	-1.629723	-1.180913
C	3.070134	-1.418251	-1.264818	C	3.327437	-1.091125	-1.158051
C	4.118778	-2.233880	-0.836179	C	4.407071	-1.790042	-0.615515
C	4.452605	-2.260567	0.520879	C	4.556925	-1.845758	0.773030
C	3.757140	-1.478936	1.444920	C	3.647591	-1.206339	1.617266
C	2.710411	-0.664428	0.987072	C	2.573056	-0.507714	1.046025
O	-6.419347	-0.950391	1.044115	O	-6.376479	-1.879707	-0.155003
O	-5.489155	-1.569602	-1.453705	O	-5.092493	-0.612127	1.903949
O	1.964122	5.864221	-0.139734	O	1.146782	5.927990	0.025888
O	2.690676	-1.341492	-2.577719	O	3.123907	-0.990862	-2.507788
O	1.990382	0.139271	1.821918	O	1.649204	0.155354	1.800631
O	5.487856	-3.090500	0.847591	O	5.638789	-2.555517	1.211406
H	3.766268	4.198096	-0.802480	H	3.220698	4.529923	-0.424065
H	3.471222	1.748470	-1.104348	H	3.286563	2.079075	-0.837968
H	-0.428551	4.522157	0.150588	H	-1.071940	4.290920	-0.069419
H	1.095894	0.057296	-1.932950	H	1.282463	0.149414	-2.045698
H	-0.124530	-0.262885	0.829219	H	-0.249243	-0.433364	0.510930
H	-1.276682	0.887516	-1.759811	H	-1.168046	0.673909	-2.188475
H	-3.178489	-0.610291	-2.036655	H	-2.701814	0.500683	1.211906
H	-4.686718	0.547432	2.532159	H	-5.161886	-1.792846	-2.422336
H	-2.478894	1.303854	1.750707	H	-2.933976	-0.749174	-2.882265
H	4.688493	-2.854126	-1.515152	H	5.139457	-2.297171	-1.229356
H	4.014222	-1.500459	2.493593	H	3.763849	-1.248194	2.690061
C	5.877688	-3.179938	2.207673	C	5.852970	-2.667007	2.608485
H	6.219838	-2.211037	2.595369	H	6.754834	-3.271043	2.725252
H	5.060307	-3.552551	2.839209	H	6.013452	-1.685031	3.073296
H	6.706040	-3.890564	2.235170	H	5.013835	-3.169589	3.107507
C	2.231001	0.081868	3.218128	C	1.721252	0.073710	3.214235
H	1.521236	0.777920	3.668565	H	1.630722	-0.963133	3.561662
H	2.053565	-0.925802	3.614187	H	2.653249	0.509984	3.596845
H	3.252383	0.400305	3.464679	H	0.876091	0.655258	3.586811
C	3.385021	-2.121494	-3.536207	C	4.049174	-1.610150	-3.385246
H	4.448469	-1.853098	-3.582472	H	4.081785	-2.697322	-3.236594
H	3.293901	-3.195148	-3.326147	H	3.692364	-1.393942	-4.394103
H	2.914715	-1.900055	-4.496254	H	5.059674	-1.199708	-3.261158
C	-6.685584	-0.972897	-1.957616	C	-4.389785	-0.060380	3.006846
H	-7.393675	-0.750991	-1.153181	H	-3.430254	-0.569192	3.164019
H	-6.459428	-0.052146	-2.512493	H	-4.211352	1.015207	2.876304
H	-7.124536	-1.705472	-2.639294	H	-5.031055	-0.216880	3.876323
C	-6.882844	-0.704307	2.362110	C	-7.488121	-1.036507	0.153723
H	-7.856720	-1.192454	2.432037	H	-7.667914	-0.315636	-0.655528

H	-6.206274	-1.133877	3.112283	H	-8.352289	-1.699014	0.244228
H	-7.000754	0.370124	2.556616	H	-7.336796	-0.500067	1.095165
C	0.892258	6.713164	0.231801	C	-0.064784	6.620626	0.271208
H	1.314963	7.717314	0.304685	H	-0.577155	6.236428	1.163630
H	0.093197	6.710261	-0.521834	H	0.212979	7.663676	0.435981
H	0.467082	6.427287	1.203459	H	-0.747936	6.559035	-0.586690
C	-0.665924	-2.522164	0.053582	C	-0.425277	-2.705022	-0.368642
O	-0.485811	-2.461517	1.248562	O	-0.465860	-2.655730	0.839904
C	-1.105072	-3.754005	-0.702087	C	-0.577777	-3.959261	-1.196133
H	-1.069314	-4.619778	-0.039811	H	-0.565779	-4.831700	-0.541896
H	-2.130244	-3.611437	-1.061932	H	-1.530053	-3.920829	-1.736714
H	-0.466999	-3.916018	-1.575758	H	0.222187	-4.028715	-1.939075

Table S9. The geometric parameters for the possible stationary points of compound **2a** in gas phase (Å).

2a1				**2a2**			
C	1.626193	4.064124	-0.495630	C	-4.368872	-0.861948	-0.954240
C	2.736776	3.372843	0.004503	C	-4.368872	-0.861948	0.446385
C	2.580387	2.069947	0.456902	C	-3.158258	-0.861948	1.125304
C	1.342088	1.407863	0.446115	C	-1.917786	-0.857532	0.466691
C	0.254578	2.123543	-0.071965	C	-1.954757	-0.829849	-0.935370
C	0.384745	3.435749	-0.539985	C	-3.161065	-0.835468	-1.644815
C	1.176793	0.012266	1.076764	C	-0.593979	-0.995006	1.246968
C	-0.310861	-0.427532	0.983421	C	0.571211	-1.103665	0.231950
C	-1.046219	0.166531	-0.242230	C	0.325657	-0.263548	-1.043201
O	-1.011622	1.592518	-0.142659	O	-0.818697	-0.805705	-1.707715
C	-2.489980	-0.274929	-0.302125	C	1.501265	-0.296357	-1.990688
C	-3.471261	0.394520	0.447560	C	2.421430	0.765591	-1.986246
C	-4.785405	-0.050523	0.431995	C	3.538924	0.729708	-2.812431
C	-5.152694	-1.185128	-0.316667	C	3.762436	-0.367443	-3.662747
C	-4.182277	-1.852974	-1.056197	C	2.849649	-1.419787	-3.669813
C	-2.859941	-1.397329	-1.051725	C	1.730408	-1.387620	-2.836069
C	2.271129	-0.969831	0.631033	C	-0.477132	0.001585	2.413785
O	-0.388106	-1.856617	0.976861	O	1.800334	-0.739493	0.871265
C	2.244806	-1.781422	-0.525312	C	0.095851	1.293179	2.372724

C	3.374727	-2.483580	-0.943659	C	-0.032674	2.178168	3.443369
C	4.554343	-2.429224	-0.201535	C	-0.696395	1.789727	4.606204
C	4.589946	-1.698177	0.988570	C	-1.198423	0.490348	4.713040
C	3.453932	-0.992624	1.382546	C	-1.072842	-0.373563	3.626846
O	-6.443127	-1.618037	-0.324532	O	4.853978	-0.400178	-4.475713
O	-5.818975	0.544077	1.119705	O	4.492018	1.720352	-2.881169
O	1.821186	5.343861	-0.936096	O	-5.580332	-0.870106	-1.588115
O	1.106421	-1.939955	-1.274647	O	0.831694	1.733861	1.299835
O	5.626155	-3.140411	-0.668132	O	-0.786764	2.706809	5.617588
H	3.703545	3.864801	0.022610	H	-5.314772	-0.865892	0.977536
H	3.451014	1.542772	0.833417	H	-3.173901	-0.861658	2.210140
H	-0.494036	3.932451	-0.943554	H	-3.123196	-0.805130	-2.730824
H	1.358516	0.142831	2.151441	H	-0.631034	-1.976627	1.737045
H	-0.832626	-0.042616	1.871048	H	0.635184	-2.149388	-0.099622
H	-0.518329	-0.141207	-1.153422	H	0.108594	0.770490	-0.749836
H	-3.200514	1.280404	1.016568	H	2.248634	1.632261	-1.349609
H	-4.477627	-2.717257	-1.642416	H	3.029374	-2.255753	-4.338525
H	-2.118746	-1.908450	-1.660694	H	1.014720	-2.202778	-2.861497
H	3.316493	-3.098718	-1.834637	H	0.421576	3.160381	3.375409
H	5.489721	-1.677702	1.600045	H	-1.678283	0.154602	5.630025
H	0.979463	5.693656	-1.267170	H	-5.433000	-0.862757	-2.546640
H	6.362239	-3.037493	-0.045352	H	-1.248482	2.299110	6.366490
H	0.388899	-2.080102	-0.617965	H	1.407018	0.973907	1.056258
H	-1.332787	-2.092096	0.945516	H	2.510943	-0.880340	0.221311
H	-5.498084	1.341502	1.567154	H	4.234350	2.465201	-2.317147
H	-6.960007	-1.009918	0.231717	H	5.347377	0.426858	-4.337889
H	3.496572	-0.421020	2.307405	H	-1.467597	-1.382566	3.723695
2a3				**2a4**			
C	-4.424746	-0.514114	-0.601422	C	2.511888	3.876510	-0.322564
C	-4.413393	-0.500531	0.801818	C	3.442584	3.070906	0.351105
C	-3.195139	-0.492370	1.464376	C	3.043652	1.825613	0.813325
C	-1.964936	-0.491392	0.782515	C	1.738848	1.334411	0.629258

C	-2.006711	-0.495904	-0.623506	C	0.828978	2.159983	-0.055832
C	-3.227464	-0.505421	-1.312356	C	1.212254	3.421842	-0.531136
C	-0.642160	-0.563882	1.539922	C	1.306061	-0.003980	1.220552
C	0.456182	-1.013550	0.547003	C	-0.239834	-0.023743	1.274867
C	0.368738	-0.203556	-0.766848	C	-0.837534	0.432556	-0.075838
O	-0.887984	-0.490660	-1.408509	O	-0.467279	1.805986	-0.305720
C	1.478750	-0.547246	-1.733296	C	-2.346703	0.344923	-0.102204
C	1.349277	-1.619591	-2.627799	C	-2.952773	-0.861750	-0.487350
C	2.398396	-1.961836	-3.473686	C	-4.338250	-0.996730	-0.466390
C	3.602881	-1.236375	-3.419818	C	-5.133757	0.088097	-0.058702
C	3.742062	-0.177811	-2.531062	C	-4.539760	1.286249	0.320978
C	2.679538	0.170113	-1.689698	C	-3.148072	1.415165	0.306471
C	-0.275734	0.672316	2.365618	C	1.929029	-1.250729	0.586813
O	1.717291	-0.887191	1.169525	O	-0.667419	-1.317005	1.645037
C	-0.532505	2.009038	1.987775	C	2.218947	-1.408670	-0.786785
C	-0.121115	3.079037	2.785511	C	2.747462	-2.602378	-1.282981
C	0.555302	2.843625	3.979832	C	2.999931	-3.668303	-0.423214
C	0.810543	1.530917	4.390400	C	2.738385	-3.538366	0.944997
C	0.390998	0.478901	3.582649	C	2.214525	-2.340553	1.419917
O	4.575497	-1.661308	-4.297334	O	-6.490926	-0.146504	-0.080464
O	2.258275	-2.996850	-4.348831	O	-4.914194	-2.171332	-0.845944
O	-5.642733	-0.524517	-1.217577	O	2.940408	5.096434	-0.760557
O	-1.167683	2.355396	0.823188	O	1.986029	-0.436118	-1.724398
O	0.932482	3.934202	4.716049	O	3.517223	-4.810776	-0.971061
H	-5.354884	-0.501084	1.340205	H	4.452345	3.437423	0.500380
H	-3.179824	-0.485993	2.551688	H	3.759377	1.198405	1.339455
H	-3.209325	-0.502071	-2.399146	H	0.476916	4.021392	-1.061581
H	-0.734368	-1.383268	2.263915	H	1.634468	-0.011284	2.267542
H	0.254336	-2.064669	0.278629	H	-0.557473	0.723759	2.022146
H	0.405249	0.865964	-0.525332	H	-0.414741	-0.184476	-0.878288
H	0.423108	-2.179591	-2.691015	H	-2.356465	-1.704680	-0.824294
H	4.673102	0.384989	-2.499622	H	-5.163820	2.123265	0.629404

H	2.786591	1.009342	-1.008636	H	-2.687795	2.354388	0.590798
H	-0.342054	4.092673	2.470367	H	2.965871	-2.687234	-2.341569
H	1.330278	1.334769	5.326075	H	2.939679	-4.361446	1.627635
H	-5.511587	-0.531623	-2.178636	H	2.208968	5.545455	-1.212430
H	1.382369	3.625130	5.517471	H	3.639841	-5.463984	-0.265025
H	-1.706886	1.600648	0.526434	H	1.958183	0.427820	-1.276351
H	2.386264	-1.170512	0.524288	H	-1.638437	-1.305633	1.675584
H	3.087720	-3.069281	-4.851667	H	-5.878211	-2.058812	-0.781999
H	5.354378	-1.089593	-4.224920	H	-6.965878	0.658500	0.174611
H	0.605717	-0.539154	3.896586	H	1.996493	-2.249165	2.480598
2a5				**2a6**			
C	1.601336	4.203373	-0.251124	C	2.479252	3.921071	-0.334324
C	2.615377	3.648857	0.542091	C	3.373578	3.163834	0.434745
C	2.492238	2.333451	0.968433	C	2.976045	1.915030	0.892962
C	1.388657	1.535403	0.633459	C	1.709791	1.380662	0.614445
C	0.389893	2.115443	-0.160943	C	0.835455	2.159409	-0.156220
C	0.490549	3.440152	-0.603222	C	1.212854	3.421927	-0.630285
C	1.267401	0.100661	1.117225	C	1.289047	0.016799	1.133461
C	-0.236479	-0.241050	1.114883	C	-0.251988	0.021981	1.191649
C	-0.844164	0.053157	-0.272084	C	-0.832760	0.424362	-0.179816
O	-0.755309	1.458766	-0.539207	O	-0.441746	1.771755	-0.479013
C	-2.296784	-0.359613	-0.363669	C	-2.343804	0.349867	-0.212317
C	-3.317702	0.515193	0.035755	C	-2.962917	-0.865742	-0.546887
C	-4.646399	0.107162	0.005791	C	-4.350239	-0.985101	-0.522273
C	-4.966814	-1.198078	-0.413513	C	-5.134160	0.124598	-0.161689
C	-3.961464	-2.072945	-0.804434	C	-4.527097	1.331690	0.166235
C	-2.625882	-1.653885	-0.783100	C	-3.134273	1.445224	0.148280
C	2.151307	-0.886988	0.345903	C	1.898197	-1.154394	0.353468
O	-0.400316	-1.608067	1.474983	O	-0.700773	-1.266750	1.594487
C	2.536150	-2.113324	0.940473	C	2.023579	-2.427038	0.962090
C	3.446419	-2.963831	0.313313	C	2.694380	-3.468807	0.322191
C	3.971771	-2.627347	-0.934522	C	3.229842	-3.277038	-0.951696

C	3.581644	-1.440547	-1.561032	C	3.089076	-2.042237	-1.591042
C	2.689015	-0.588709	-0.910719	C	2.436848	-1.002603	-0.928566
O	-6.310438	-1.496245	-0.400785	O	-6.492918	-0.096674	-0.174762
O	-5.631484	0.967946	0.383474	O	-4.937314	-2.168275	-0.852846
O	1.754927	5.501300	-0.652801	O	2.903266	5.146247	-0.769371
O	2.071172	-2.500022	2.165656	O	1.534128	-2.681087	2.212155
O	4.855232	-3.505927	-1.501866	O	3.871278	-4.339049	-1.529992
H	3.472643	4.256744	0.810421	H	4.355151	3.566989	0.659304
H	3.276751	1.897967	1.582746	H	3.666766	1.322273	1.487932
H	-0.309771	3.847363	-1.215983	H	0.501301	3.989812	-1.224536
H	1.591900	0.063104	2.166444	H	1.637511	-0.078815	2.171306
H	-0.743850	0.405736	1.846865	H	-0.572227	0.779356	1.923530
H	-0.256461	-0.495802	-1.020515	H	-0.411552	-0.250386	-0.937450
H	-3.087594	1.527378	0.348544	H	-2.376909	-1.728023	-0.852430
H	-4.215454	-3.077255	-1.137943	H	-5.142224	2.187894	0.437464
H	-1.845765	-2.334651	-1.112145	H	-2.663318	2.390567	0.391825
H	3.728220	-3.893780	0.794361	H	2.779974	-4.431266	0.814066
H	3.986117	-1.171192	-2.534741	H	3.502443	-1.884966	-2.585351
H	0.986089	5.758748	-1.184944	H	2.194398	5.558202	-1.287310
H	5.130087	-3.154736	-2.362924	H	4.178745	-4.072246	-2.410088
H	1.128909	-2.241607	2.219225	H	0.673884	-2.221186	2.290782
H	-1.343540	-1.836026	1.420371	H	-1.672451	-1.279303	1.595047
H	-6.480831	0.503901	0.286197	H	-5.900384	-2.045205	-0.792702
H	-6.450517	-2.398636	-0.724706	H	-6.960761	0.721413	0.050302
H	2.429119	0.352757	-1.384540	H	2.374785	-0.034145	-1.415165

Table S10. The geometric parameters for the possible stationary points of compound **3a** in gas phase (Å).

3a1				**3a2**			
C	-0.007608	0.060836	-0.036568	C	0.000000	0.000000	0.000000
C	-0.008969	0.027288	1.361324	C	0.000000	0.000000	1.395248
C	1.198345	-0.004628	2.053395	C	1.215748	0.000000	2.072688

C	2.436064	0.003256	1.387428	C	2.438428	0.016199	1.384430
C	2.415522	0.038579	-0.014198	C	2.417967	0.034041	-0.023137
C	1.209105	0.069815	-0.721042	C	1.197632	0.019094	-0.719813
C	3.760769	-0.109854	2.131186	C	3.762725	-0.087676	2.132944
C	4.880880	-0.522163	1.147103	C	4.880349	-0.511031	1.154894
C	4.796656	0.296232	-0.162939	C	4.791209	0.306251	-0.151487
O	3.533608	0.053031	-0.811810	O	3.535702	0.067154	-0.801656
C	5.892198	-0.053907	-1.142171	C	5.889257	-0.050591	-1.129428
C	5.771246	-1.138963	-2.019633	C	5.694174	-1.000125	-2.138725
C	6.818453	-1.489850	-2.872851	C	6.739906	-1.361637	-2.990385
C	8.010521	-0.759447	-2.853645	C	8.000128	-0.777776	-2.838596
C	8.144819	0.327853	-1.981899	C	8.208155	0.175154	-1.833863
C	7.091974	0.672009	-1.141485	C	7.158929	0.530405	-0.994070
C	4.161972	1.097599	2.979910	C	4.161164	1.125691	2.973998
C	3.875928	2.447565	2.678390	C	3.859324	2.473035	2.675371
C	4.321956	3.499554	3.483675	C	4.301196	3.528806	3.479067
C	5.070562	3.223248	4.622338	C	5.062769	3.259594	4.610299
C	5.373194	1.901890	4.965940	C	5.382015	1.941188	4.950364
C	4.919140	0.868345	4.144416	C	4.930642	0.903998	4.132099
O	9.072402	-1.051287	-3.661955	O	9.063633	-1.088366	-3.640169
O	-1.182917	0.097616	-0.725826	O	-1.136820	-0.005791	-0.779539
O	3.171705	2.819553	1.569481	O	3.141544	2.842254	1.575703
O	5.215662	-0.439218	4.436486	O	5.238729	-0.401083	4.423233
O	5.484291	4.284406	5.378192	O	5.472604	4.324434	5.363908
H	-0.960306	0.024345	1.882736	H	-0.940741	-0.010061	1.941129
H	1.192376	-0.037122	3.139509	H	1.227356	-0.016240	3.158886
H	3.676491	-0.958391	2.816592	H	3.671817	-0.930148	2.825308
H	4.854793	1.362316	0.095148	H	4.856513	1.372722	0.106716
H	4.840753	-1.697040	-2.052649	H	4.708271	-1.430828	-2.278205
H	9.071451	0.892847	-1.985250	H	9.189043	0.629062	-1.734563
H	7.202430	1.524489	-0.475133	H	7.327634	1.278990	-0.222977
H	4.071874	4.520136	3.220004	H	4.041139	4.547197	3.216532

H	5.959782	1.678522	5.856246	H	5.978141	1.723012	5.835654
H	-0.964393	0.129511	-1.673277	H	-1.919815	-0.006271	-0.209425
H	5.710284	-0.471074	5.269467	H	5.752022	-0.427141	5.245002
H	5.975947	3.953176	6.145270	H	5.982043	3.997090	6.120945
H	2.647917	2.057135	1.259211	H	2.652344	2.067962	1.240524
H	8.847572	-1.813058	-4.218632	H	8.781197	-1.742777	-4.297934
O	4.721834	-1.909612	0.894084	O	4.707022	-1.896140	0.901471
H	5.417265	-2.174730	0.269506	H	5.306344	-2.137004	0.174750
H	5.855122	-0.314877	1.610745	H	5.856882	-0.313017	1.618628
O	1.175475	0.112186	-2.093051	O	1.203431	0.023650	-2.082993
H	2.096636	0.180765	-2.399089	H	0.273398	0.019323	-2.367699
H	6.705002	-2.329724	-3.556240	H	6.569765	-2.093106	-3.778742

Table S11. The geometric parameters for the possible stationary points of compound **4a** in gas phase (Å).

4a1				**4a2**			
C	-1.214549	4.152187	-0.082174	C	1.624315	4.129116	0.219770
C	-2.411156	3.431123	-0.158483	C	2.731442	3.286759	0.370710
C	-2.361970	2.056866	-0.359664	C	2.527837	1.918666	0.505254
C	-1.154292	1.359443	-0.493703	C	1.249554	1.345203	0.500527
C	0.027983	2.109976	-0.423615	C	0.159158	2.215502	0.360509
C	0.005880	3.492534	-0.214987	C	0.337268	3.594631	0.215689
C	-1.092701	-0.143165	-0.769076	C	1.014214	-0.152744	0.697200
C	0.296433	-0.676432	-0.382017	C	-0.380476	-0.523754	0.165900
C	1.392919	0.215088	-1.004956	C	-1.432699	0.453640	0.734829
O	1.284172	1.560129	-0.532961	O	-1.150401	1.794684	0.336175
C	2.783958	-0.283954	-0.676098	C	-2.831168	0.111105	0.265101
C	-2.256303	-0.960326	-0.216119	C	2.136770	-1.061383	0.206236
C	3.460191	0.180847	0.463961	C	-3.573079	-0.858987	0.958109
C	4.709820	-0.333467	0.792565	C	-4.824014	-1.247363	0.498259
C	5.304891	-1.332585	0.003147	C	-5.367531	-0.676529	-0.668334

C	4.632159	-1.796672	-1.124529	C	-4.636665	0.287363	-1.353894
C	3.382359	-1.274145	-1.461164	C	-3.374704	0.677524	-0.893021
C	-2.687957	-0.925394	1.132928	C	2.685771	-1.018196	-1.099580
C	-3.836450	-1.604853	1.552188	C	3.795848	-1.792924	-1.452672
C	-4.561121	-2.364613	0.640557	C	4.362335	-2.654394	-0.519957
C	-4.145829	-2.460508	-0.691053	C	3.825981	-2.757984	0.767169
C	-3.007286	-1.759609	-1.095909	C	2.728963	-1.962930	1.107677
O	-2.582170	-1.827904	-2.402800	O	2.188388	-2.037875	2.371691
O	6.529044	-1.833722	0.326674	O	-6.596677	-1.055914	-1.114137
O	-2.043910	-0.209771	2.086624	O	2.200594	-0.206188	-2.068691
O	-5.668944	-3.019034	1.104366	O	5.438417	-3.398323	-0.919523
O	0.406104	-0.679297	1.039875	O	-0.362969	-0.463998	-1.257467
O	5.455991	0.068229	1.877312	O	-5.626698	-2.182470	1.110711
O	-1.298815	5.503396	0.119266	O	1.860449	5.470551	0.085881
H	-3.355288	3.954311	-0.051195	H	3.728622	3.713664	0.370232
H	-3.290464	1.495693	-0.404279	H	3.387721	1.263140	0.605510
H	0.950991	4.028214	-0.169291	H	-0.541679	4.225548	0.108434
H	-1.140576	-0.277087	-1.855585	H	0.950090	-0.334173	1.776037
H	0.413703	-1.696958	-0.771620	H	-0.634350	-1.540770	0.496848
H	1.250063	0.203434	-2.095995	H	-1.387024	0.386614	1.832920
H	3.019557	0.977880	1.057380	H	-3.172700	-1.308409	1.866244
H	5.106298	-2.559722	-1.733603	H	-5.070035	0.730483	-2.244988
H	2.875068	-1.639128	-2.350642	H	-2.826098	1.455793	-1.412288
H	-4.138714	-1.552899	2.591249	H	4.191423	-1.731585	-2.459384
H	-4.697301	-3.072594	-1.403722	H	4.252467	-3.448017	1.494327
H	6.834803	-1.368267	1.124262	H	-6.939546	-1.725886	-0.497939
H	5.009343	0.799802	2.329514	H	-5.190990	-2.519460	1.907829
H	1.319109	-0.903561	1.286185	H	-1.277506	-0.485666	-1.588192
H	-3.230097	-2.337211	-2.912716	H	2.747551	-2.616708	2.911624
H	-6.070360	-3.514475	0.374177	H	5.724894	-3.957915	-0.181613
H	-1.106517	-0.102759	1.826056	H	1.260571	-0.007167	-1.879520
H	-0.402256	5.870957	0.154993	H	1.012526	5.927889	-0.024318

4a3				**4a4**			
C	0.043881	-0.069637	-0.047355	C	1.253846	4.183328	-0.037272
C	0.025351	-0.155439	1.350041	C	2.423109	3.494561	0.307330
C	1.229652	-0.138180	2.043468	C	2.351219	2.131443	0.568574
C	2.469054	-0.040542	1.397247	C	1.149095	1.414711	0.503258
C	2.458290	0.017386	-0.004726	C	-0.011280	2.135734	0.181103
C	1.257975	0.012192	-0.724874	C	0.037750	3.507008	-0.096262
C	3.790753	-0.034141	2.166582	C	1.075598	-0.083379	0.802998
C	4.964689	0.393093	1.242855	C	-0.286633	-0.667243	0.340652
C	4.809435	-0.343279	-0.107241	C	-1.401908	0.300971	0.794764
O	3.601634	0.096958	-0.756076	O	-1.250545	1.557335	0.101558
C	5.957949	-0.142370	-1.064650	C	-2.806974	-0.195756	0.567086
C	3.765683	0.744780	3.475314	C	2.264069	-0.896558	0.305412
C	6.879359	-1.180688	-1.262246	C	-3.324454	-0.330588	-0.730693
C	7.965368	-1.008628	-2.112336	C	-4.612769	-0.807192	-0.918770
C	8.148182	0.203212	-2.796222	C	-5.418821	-1.163851	0.177215
C	7.229700	1.233393	-2.608280	C	-4.909383	-1.030695	1.464334
C	6.145755	1.064383	-1.746667	C	-3.613020	-0.544067	1.653705
C	3.296468	2.066587	3.591293	C	2.760236	-0.838645	-1.009954
C	3.283435	2.759334	4.801583	C	3.852425	-1.591601	-1.439764
C	3.769379	2.134155	5.949252	C	4.478816	-2.455768	-0.542462
C	4.259255	0.830024	5.883516	C	4.015415	-2.561195	0.768696
C	4.254309	0.159370	4.654754	C	2.919675	-1.788345	1.170851
O	4.737067	-1.120692	4.562715	O	2.441326	-1.878516	2.451825
O	9.208587	0.369570	-3.639439	O	-6.685150	-1.631549	-0.021103
O	2.825026	2.670100	2.451151	O	2.130683	0.014648	-1.884183
O	3.741948	2.852693	7.110267	O	5.540942	-3.176202	-1.008751
O	5.078264	1.790282	1.056928	O	-0.363312	-0.923079	-1.051314
O	8.920294	-1.973481	-2.366645	O	-5.208427	-0.972897	-2.152756
O	-1.160529	-0.081257	-0.699304	O	1.360760	5.523976	-0.296331
H	-0.926397	-0.227522	1.865898	H	3.362802	4.034380	0.358942
H	1.213615	-0.185569	3.129355	H	3.262327	1.593958	0.818523

H	1.304195	0.060974	-1.810110	H	-0.889255	4.019758	-0.341222
H	4.010013	-1.071333	2.443686	H	1.076261	-0.198038	1.892579
H	5.905054	0.067217	1.702686	H	-0.443228	-1.629269	0.842242
H	4.709515	-1.419002	0.108234	H	-1.267275	0.485945	1.871364
H	6.745741	-2.134601	-0.752536	H	-2.703056	-0.075068	-1.582719
H	7.381260	2.165358	-3.144152	H	-5.539431	-1.302311	2.305495
H	5.441751	1.873007	-1.596483	H	-3.230926	-0.433008	2.665427
H	2.914215	3.778860	4.865748	H	4.217605	-1.526905	-2.460709
H	4.647045	0.338834	6.774886	H	4.494922	-3.240092	1.472395
H	9.717661	-0.458930	-3.630158	H	-6.835971	-1.652652	-0.981805
H	8.707643	-2.776992	-1.869403	H	-4.570179	-0.750371	-2.846899
H	4.187998	2.178561	1.101704	H	0.233648	-0.306169	-1.508252
H	5.008896	-1.418129	5.444187	H	2.994301	-2.497079	2.952810
H	4.115351	2.314614	7.825151	H	5.879365	-3.740326	-0.296472
H	2.532672	3.569986	2.664586	H	2.569363	-0.034187	-2.747847
H	-0.998129	-0.016700	-1.653167	H	0.480710	5.870024	-0.511136
4a5				**4a6**			
C	-1.175452	4.123329	-0.244499	C	-1.590400	4.120135	-0.287114
C	-2.369497	3.411056	-0.403901	C	-2.686629	3.279565	-0.512090
C	-2.327251	2.026538	-0.515824	C	-2.486057	1.907085	-0.596430
C	-1.125711	1.306606	-0.476263	C	-1.218224	1.324515	-0.466448
C	0.053111	2.050539	-0.322793	C	-0.139823	2.194942	-0.252024
C	0.040552	3.441942	-0.203382	C	-0.312533	3.577488	-0.157063
C	-1.061624	-0.213698	-0.646172	C	-0.977850	-0.180939	-0.602855
C	0.292594	-0.715537	-0.103264	C	0.385284	-0.524868	0.032114
C	1.412404	0.124524	-0.754866	C	1.448229	0.427693	-0.555808
O	1.304522	1.460674	-0.233250	O	1.159756	1.749336	-0.076911
C	2.811107	-0.388021	-0.485303	C	2.870500	0.079537	-0.167632
C	-2.294593	-0.976086	-0.172011	C	-2.145374	-1.068856	-0.184863
C	3.672065	0.252599	0.414996	C	3.461280	-1.061215	-0.735493
C	4.939195	-0.265891	0.657582	C	4.750229	-1.434209	-0.382380
C	5.374474	-1.433865	0.010827	C	5.486784	-0.673082	0.544231

C	4.520983	-2.067339	-0.888954	C	4.906605	0.461594	1.098826
C	3.251040	-1.545393	-1.135447	C	3.606298	0.835938	0.745778
C	-2.805411	-0.928507	1.148623	C	-2.742885	-1.049283	1.099959
C	-4.019769	-1.533551	1.488090	C	-3.899562	-1.783301	1.382302
C	-4.736298	-2.231907	0.522351	C	-4.467280	-2.582859	0.396490
C	-4.247569	-2.339600	-0.783333	C	-3.886065	-2.663741	-0.872827
C	-3.043102	-1.711094	-1.109020	C	-2.742705	-1.907531	-1.142698
O	-2.550519	-1.787026	-2.391332	O	-2.161936	-1.958051	-2.389734
O	6.617532	-1.938069	0.250291	O	6.753724	-1.038583	0.886320
O	-2.163681	-0.274359	2.145213	O	-2.247843	-0.300846	2.112711
O	-5.911075	-2.815790	0.907853	O	-5.589653	-3.290744	0.726747
O	0.398293	-0.594679	1.325240	O	0.376757	-0.385400	1.461758
O	5.856909	0.296408	1.517792	O	5.413156	-2.531319	-0.885942
O	-1.258112	5.484250	-0.138493	O	-1.827674	5.464604	-0.208601
H	-3.309353	3.952090	-0.430850	H	-3.676145	3.713484	-0.608495
H	-3.255862	1.474565	-0.624160	H	-3.339889	1.255134	-0.754250
H	0.985284	3.967437	-0.087735	H	0.559433	4.204690	0.010995
H	-1.007579	-0.413540	-1.722571	H	-0.836415	-0.388585	-1.669917
H	0.421301	-1.774923	-0.341485	H	0.642844	-1.565741	-0.186139
H	1.234891	0.154351	-1.838742	H	1.349815	0.418418	-1.650975
H	3.359259	1.170681	0.904557	H	2.912831	-1.661202	-1.461084
H	4.868385	-2.964604	-1.391132	H	5.485171	1.046759	1.806662
H	2.600351	-2.048859	-1.846369	H	3.174059	1.734389	1.170361
H	-4.378770	-1.476263	2.508636	H	-4.328713	-1.743101	2.376233
H	-4.795176	-2.902909	-1.537927	H	-4.315083	-3.305408	-1.641553
H	7.046809	-1.358351	0.902733	H	6.966226	-1.852274	0.397718
H	5.474214	1.082693	1.934749	H	4.830615	-3.020735	-1.485707
H	0.898898	0.221673	1.501757	H	0.840844	0.443795	1.673916
H	-3.192800	-2.259362	-2.942268	H	-2.721895	-2.496794	-2.968874
H	-6.296708	-3.279169	0.148658	H	-5.869711	-3.812882	-0.040535
H	-1.201151	-0.259292	1.938797	H	-1.283516	-0.171048	1.962981
H	-0.365581	5.847202	-0.029352	H	-0.990298	5.923100	-0.038524

Table S12. Frequencies of Compounds **1a** and **1b**

Species	Frequencies (cm^{-1})
1a1	27 28 44 50 55 63 88 133 139 158 181 207 214 222 230 242 253 266 289 310 311 325 332 344 347 351 360 374 375 396 403 439 446 457 467 480 510 532 540 557 573 589 598 608 615 634 638 642 648 651 662 705 717 735 758 780 782 796 799 802 815 856 863 882 885 925 938 967 987 1032 1039 1063 1082 1086 1098 1133 1143 1179 1183 1186 1192 1196 1203 1223 1226 1229 1242 1256 1274 1294 1300 1304 1325 1326 1337 1350 1356 1368 1373 1379 1398 1400 1411 1425 1444 1501 1517 1520 1552 1556 1567 1645 1662 1663 1679 1682 1684 3011 3014 3057 3170 3172 3195 3198 3199 3207 3231 3234 3584 3716 3738 3751 3753 3754 3772
1a2	23 32 43 50 54 62 88 128 141 158 172 208 220 231 232 242 250 268 284 309 313 321 331 344 349 354 360 369 377 396 404 438 447 463 470 477 516 531 537 559 563 586 599 608 615 634 638 642 650 654 659 704 717 735 757 780 783 790 795 802 807 852 862 885 892 910 937 982 994 1031 1039 1062 1077 1085 1098 1138 1143 1177 1184 1187 1192 1195 1206 1223 1227 1228 1243 1254 1268 1288 1296 1301 1328 1329 1339 1349 1360 1369 1372 1381 1398 1400 1414 1429 1445 1503 1518 1519 1553 1555 1565 1645 1658 1662 1679 1681 1684 3010 3014 3058 3169 3173 3195 3197 3200 3202 3231 3235 3586 3717 3737 3750 3753 3754 3771
1a3	23 28 31 42 50 57 75 129 136 155 179 192 206 213 214 234 245 259 270 286 304 311 324 334 338 348 349 358 368 374 399 406 426 445 455 463 478 511 534 535 558 577 590 601 612 614 632 632 642 648 663 702 715 733 745 758 776 785 798 800 805 858 864 877 886 916 933 965 986 1031 1036 1060 1069 1090 1117 1133 1143 1174 1182 1186 1196 1198 1216 1222 1229 1230 1242 1248 1262 1281 1298 1299 1310 1323 1336 1355 1365 1371 1381 1388 1405 1407 1412 1415 1440 1501 1508 1519 1552 1567 1579 1643 1665 1669 1681 1683 1683 3000 3023 3075 3160 3166 3168 3194 3202 3219 3231 3232 3720 3722 3754 3754 3755 3756 3773

1a4	15 26 31 37 48 57 73 126 136 155 169 191 199 211 223 233 243 253 261 284 306 310 326 334 345 347 352 358 368 373 399 406 425 444 462 467 477 517 531 534 560 567 586 601 612 614 632 632 639 649 658 703 715 733 747 757 776 784 788 796 806 855 862 886 889 905 932 978 993 1032 1036 1060 1064 1091 1114 1138 1144 1174 1184 1186 1194 1197 1218 1220 1226 1230 1243 1248 1262 1276 1290 1298 1311 1327 1338 1358 1364 1369 1379 1385 1405 1406 1413 1415 1440 1503 1508 1518 1553 1565 1578 1643 1664 1669 1681 1682 1683 3000 3022 3075 3160 3168 3169 3194 3201 3212 3232 3234 3719 3722 3754 3755 3755 3756 3774
1a5	12 22 37 46 58 62 120 126 146 160 172 196 206 218 228 236 246 248 268 291 306 313 331 333 340 342 352 353 361 375 398 407 428 456 464 476 486 506 533 541 566 587 594 602 607 614 630 634 641 644 698 700 725 735 743 760 783 785 792 801 823 848 855 878 894 910 925 926 961 983 1040 1040 1061 1067 1118 1133 1147 1173 1180 1182 1193 1196 1212 1220 1227 1232 1248 1252 1257 1283 1286 1298 1304 1322 1335 1342 1362 1363 1377 1383 1393 1400 1419 1425 1445 1500 1508 1511 1553 1566 1575 1643 1662 1667 1681 1682 1684 3054 3061 3143 3160 3163 3168 3188 3196 3204 3228 3245 3718 3721 3754 3754 3756 3760 3773
1a6	20 25 38 47 59 63 117 126 146 164 177 191 198 218 232 237 250 258 272 306 314 319 332 334 337 352 354 358 364 377 399 409 437 462 466 471 486 512 535 552 569 583 588 602 605 616 630 633 639 641 697 699 726 734 744 759 778 786 790 799 818 848 855 881 895 910 920 925 965 993 1038 1040 1060 1067 1114 1138 1147 1172 1181 1182 1190 1197 1213 1221 1227 1229 1249 1251 1258 1283 1287 1291 1301 1331 1335 1342 1362 1364 1378 1383 1391 1398 1419 1424 1443 1500 1509 1517 1553 1563 1573 1642 1662 1666 1680 1682 1683 3056 3061 3138 3156 3168 3169 3188 3196 3199 3230 3252 3716 3717 3746 3754 3754 3760 3773
1b1	14 20 23 26 32 33 46 49 53 60 78 81 85 93 93 95 119 128 142 151 154 177

	179 187 189 197 212 221 226 227 240 251 252 254 261 277 290 293 317 319 331 345 368 373 384 391 421 432 461 472 475 490 511 525 536 551 559 581 598 600 608 620 622 641 643 651 654 676 694 713 720 740 750 782 785 787 805 816 825 849 858 862 864 929 932 939 951 963 969 983 1004 1068 1069 1075 1076 1078 1087 1090 1096 1103 1114 1154 1170 1175 1183 1185 1185 1185 1186 1186 1198 1203 1203 1210 1220 1221 1222 1228 1229 1231 1245 1255 1270 1277 1282 1294 1311 1317 1328 1329 1340 1360 1360 1382 1387 1395 1407 1415 1422 1465 1470 1482 1494 1499 1500 1501 1506 1511 1512 1515 1519 1519 1520 1520 1521 1522 1527 1534 1535 1535 1536 1537 1546 1552 1573 1628 1641 1645 1660 1664 1678 1836 3006 3018 3021 3022 3022 3023 3034 3070 3072 3074 3078 3079 3080 3081 3098 3135 3152 3153 3154 3155 3155 3162 3170 3182 3192 3216 3218 3228 3229 3231 3251 3265
1b2	15 19 22 24 31 33 41 50 55 60 80 82 85 93 96 98 113 127 140 149 163 178 181 186 192 197 206 214 225 226 243 248 253 258 266 274 288 291 317 327 332 345 371 375 384 392 424 434 461 472 475 494 512 525 537 551 561 574 595 597 609 620 622 642 643 653 656 674 694 713 721 740 748 775 782 788 800 815 815 846 859 863 878 907 931 939 955 958 982 993 1006 1063 1069 1071 1076 1078 1086 1088 1097 1103 1112 1153 1169 1177 1184 1184 1185 1186 1186 1187 1198 1202 1202 1210 1219 1222 1222 1227 1228 1231 1245 1253 1270 1276 1280 1294 1309 1315 1318 1327 1339 1358 1360 1381 1386 1397 1413 1421 1423 1467 1470 1481 1494 1500 1500 1501 1506 1510 1512 1515 1519 1520 1521 1521 1521 1521 1527 1534 1535 1535 1536 1537 1546 1552 1571 1627 1641 1645 1660 1664 1678 1833 3016 3020 3022 3023 3024 3024 3033 3072 3073 3077 3079 3081 3082 3083 3096 3136 3152 3154 3155 3155 3155 3160 3168 3182 3191 3192 3226 3229 3229 3240 3253 3267
1b3	16 20 22 24 32 37 44 46 58 59 74 81 83 91 98 102 120 132 135 146 150 167 170 177 182 197 207 210 215 225 231 242 254 255 272 277 278 295

	306 323 330 343 350 373 380 405 420 455 463 469 476 483 507 522 529 552 567 583 593 598 607 616 620 638 643 655 665 672 686 717 738 743 749 769 789 796 810 816 828 845 853 868 903 937 941 947 953 959 971 984 1005 1057 1067 1071 1076 1078 1085 1088 1096 1103 1110 1139 1163 1173 1183 1184 1184 1185 1185 1186 1193 1195 1201 1208 1219 1220 1222 1223 1228 1238 1246 1254 1265 1270 1280 1292 1309 1315 1317 1321 1346 1350 1367 1374 1381
1b4	13 19 20 24 31 36 38 45 53 56 78 82 84 88 95 103 113 116 128 146 161 168 176 180 182 195 206 209 218 220 232 244 254 261 274 275 291 295 299 306 330 344 349 373 391 410 427 455 465 470 480 484 510 527 544 557 558 578 585 597 599 605 620 636 643 653 663 670 686 717 737 742 746 771 789 798 811 813 839 846 852 869 877 936 938 948 955 967 982 991 1006 1048 1066 1072 1075 1077 1078 1088 1097 1104 1110 1139 1154 1172 1183 1184 1184 1185 1185 1187 1192 1197 1201 1208 1219 1220 1222 1227 1227 1238 1245 1251 1265 1271 1279 1293 1301 1313 1319 1322 1343 1348 1366 1374 1387

Table S13. Frequencies of Compound **2a**

Species	Frequencies (cm^{-1})
2a1	23 29 40 44 52 78 117 134 161 168 210 214 231 246 253 256 273 285 309 313 339 347 361 362 365 377 414 442 444 457 465 475 479 502 514 523 547 561 573 585 606 633 638 645 655 681 698 709 722 749 757 772 775 790 797 821 831 838 846 862 866 868 934 939 957 982 989 997 1001 1076 1086 1108 1133 1139 1146 1179 1185 1192 1196 1198 1208 1222 1229 1242 1257 1268 1286 1295 1299 1318 1325 1337 1346 1353 1362 1374 1390 1397 1410 1425 1435 1440 1491 1497 1522 1549 1554 1577 1641 1648 1662 1674 1676 1682 3015 3036 3064 3166 3183 3191 3192 3192 3209 3220 3224 3230 3502 3688 3714 3750 3752 3770
2a2	22 29 39 45 52 83 119 144 164 169 205 212

	225 246 248 256 272 279 310 312 335 347 353 364 366 377 413 439 443 453 467 468 476 495 502 525 552 564 580 588 603 634 638 644 659 680 698 709 719 752 759 770 785 792 802 820 831 841 850 864 867 870 939 947 954 963 991 994 1001 1083 1089 1108 1133 1136 1144 1184 1185 1193 1196 1200 1209 1222 1234 1240 1254 1266 1284 1300 1303 1313 1331 1340 1345 1346 1362 1373 1394 1398 1416 1428 1429 1441 1488 1501 1522 1550 1554 1579 1640 1648 1663 1674 1676 1682 3021 3039 3067 3167 3168 3184 3191 3210 3211 3224 3225 3230 3478 3703 3713 3751 3752 3768
2a3	27 29 41 52 54 65 87 134 149 162 186 201 221 232 234 251 257 286 312 325 345 347 356 361 372 375 380 419 435 443 458 464 477 478 494 505 525 551 559 579 591 609 636 640 645 649 668 698 703 728 752 758 771 784 799 805 823 831 855 859 871 893 912 924 953 972 983 998 1001 1065 1086 1125 1139 1141 1149 1177 1184 1191 1196 1204 1214 1226 1228 1239 1251 1264 1266 1288 1305 1312 1319 1330 1346 1352 1365 1373 1378 1384 1397 1409 1422 1444 1496 1515 1519 1551 1553 1565 1642 1645 1660 1674 1679 1687 2978 3043 3066 3171 3175 3189 3195 3195 3206 3226 3230 3234 3659 3716 3718 3750 3753 3771
2a4	23 29 42 50 55 65 88 139 150 162 193 195 220 226 232 251 257 284 311 323 343 346 354 359 368 374 377 418 437 441 455 463 466 477 492 495 524 557 564 586 591 609 637 639 643 650 668 698 702 728 753 759 770 786 799 809 823 830 858 865 871 879 920 923 952 961 983 987 1001 1069 1085 1124 1133 1141 1150 1177 1184 1192 1198 1204 1214 1226 1227 1237 1248 1262 1267 1302 1303 1311 1319 1328 1346 1349 1363 1371 1378 1383 1397 1410 1419 1440 1495 1514 1517 1550 1553 1567 1642 1645 1661 1673 1679 1687 2976 3042 3066 3171 3172 3189 3194 3196 3210 3227 3231 3232 3661 3716 3720 3750 3752 3771
2a5	25 28 44 49 52 78 99 133 154 166 186 210 230 239 247 248 257 294 312

	326 335 343 347 362 367 374 384 423 437 446 461 464 478 480 509 516 545 557 581 595 611 622 630 638 646 650 669 703 708 732 748 765 776 786 801 805 823 829 860 864 871 893 911 937 950 976 991 997 998 1072 1086 1112 1123 1139 1147 1184 1185 1194 1197 1205 1212 1226 1228 1239 1245 1257 1286 1299 1303 1316 1326 1330 1350 1353 1364 1373 1378 1384 1402 1417 1424 1441 1497 1514 1518 1552 1555 1565 1640 1649 1658 1677 1678 1683 3012 3033 3044 3171 3175 3188 3192 3203 3209 3224 3231 3235 3591 3715 3716 3751 3751 3771
2a6	27 30 47 50 51 77 100 138 155 166 189 210 223 229 245 250 255 295 311 325 335 340 346 364 367 371 383 422 441 444 460 464 467 478 507 516 547 567 587 594 612 618 630 638 645 651 670 703 708 731 749 764 777 790 800 812 823 830 864 868 871 879 923 936 952 965 986 994 997 1076 1087 1112 1123 1134 1148 1184 1185 1195 1197 1204 1212 1226 1227 1237 1245 1259 1295 1300 1303 1315 1325 1330 1349 1351 1362 1372 1379 1382 1403 1416 1419 1438 1496 1513 1516 1552 1555 1567 1641 1649 1661 1677 1678 1683 3010 3033 3044 3171 3172 3188 3191 3206 3207 3225 3231 3233 3589 3715 3719 3752 3752 3771

Table S14. Frequencies of Compound **3a**

Species	Frequencies (cm^{-1})
3a1	28 34 42 48 50 57 86 127 135 158 165 194 213 222 237 238 245 283 300 313 326 335 341 342 357 361 370 376 379 398 408 429 442 449 483 512 518 529 533 544 561 572 587 603 606 617 628 638 650 655 666 720 734 738 741 757 793 811 823 832 838 845 849 867 914 926 944 964 987 1008 1032 1033 1054 1072 1103 1108 1138 1176 1176 1191 1202 1209 1211 1225 1232 1242 1249 1258 1262 1272 1303 1311 1312 1322 1330 1343 1357 1380 1385 1396 1407 1411 1412 1420 1437 1488 1510 1520 1560 1563 1566 1648 1653 1659 1676 1682 1690 3036 3049 3090 3157 3170

	3185 3195 3215 3220 3223 3240 3623 3711 3713 3717 3751 3755 3759
3a2	28 33 42 47 50 57 85 127 134 158 164 193 213 221 236 238 244 282 299 312 325 334 341 342 357 360 369 375 378 397 408 428 441 448 483 512 517 528 533 543 561 571 587 603 606 617 627 638 650 655 665 720 733 737 740 756 792 810 823 831 837 845 848 867 913 925 943 963 986 1008 1032 1032 1053 1072 1102 1107 1138 1175 1176 1190 1202 1209 1210 1225 1231 1241 1248 1257 1261 1271 1303 1311 1311 1321 1329 1342 1356 1380 1384 1395 1406 1411 1412 1419 1437 1487 1510 1520 1559 1562 1566 1648 1653 1658 1676 1681 1689 3035 3048 3090 3157 3170 3185 3195 3215 3219 3223 3240 3622 3711 3713 3717 3750 3754 3758

Table S15. Frequencies of Compound **4a**

Species	Frequencies (cm^{-1})
4a1	29 32 37 47 49 61 93 127 148 167 182 211 223 224 239 253 255 261 267 287 311 317 325 335 337 343 355 358 388 395 401 443 464 469 469 503 520 532 538 558 572 591 602 607 621 627 633 638 656 682 701 705 726 744 754 775 787 801 817 824 832 836 844 862 881 922 938 960 978 981 1014 1033 1065 1083 1128 1137 1139 1176 1181 1188 1194 1203 1210 1211 1214 1226 1243 1252 1275 1286 1297 1315 1328 1331 1338 1348 1360 1366 1370 1390 1400 1416 1422 1431 1446 1490 1495 1520 1553 1567 1576 1650 1652 1664 1674 1678 1691 3014 3040 3068 3155 3188 3189 3196 3205 3220 3225 3239 3587 3713 3715 3753 3755 3760 3769
4a2	25 33 38 47 49 62 95 129 149 176 186 202 216 223 233 238 251 262 264 286 313 315 330 338 342 348 361 361 390 400 403 439 457 463 469 496 517 531 539 575 584 591 603 608 621 630 634 639 662 683 701 703 726 743 751 778 795 802 816 825 833 839 842 856 877 922 948 959 963 987 1008 1033 1065 1087 1130 1132 1142 1178 1182 1189 1194 1202 1210

	1212 1215 1233 1244 1251 1276 1294 1300 1310 1327 1331 1337 1340 1358 1368 1370 1392 1403 1417 1422 1431 1448 1488 1498 1520 1553 1567 1578 1649 1652 1661 1676 1678 1691 3005 3033 3066 3155 3161 3189 3203 3213 3224 3229 3239 3577 3698 3716 3752 3755 3759 3772
4a3	16 30 41 46 52 58 89 134 149 170 177 197 221 224 235 240 255 263 275 278 312 314 329 334 338 348 350 364 379 393 402 436 440 462 466 469 503 518 533 537 562 590 599 602 616 630 633 638 657 681 703 706 743 746 757 769 787 789 804 820 828 830 841 852 885 916 928 952 965 984 1014 1038 1058 1068 1132 1137 1140 1175 1181 1192 1197 1206 1208 1214 1220 1232 1249 1257 1261 1282 1291 1304 1318 1329 1333 1354 1363 1369 1378 1397 1404 1407 1417 1437 1465 1494 1499 1509 1553 1577 1579 1649 1667 1667 1676 1678 1684 3011 3064 3075 3161 3186 3189 3190 3200 3215 3218 3220 3702 3715 3752 3754 3756 3760 3772
4a4	16 33 39 44 50 58 89 137 149 173 181 192 206 221 224 239 253 260 264 275 309 311 325 333 336 344 349 362 377 393 397 433 435 457 462 471 497 517 534 538 573 590 599 602 615 627 632 637 661 681 703 707 742 744 752 772 788 801 803 817 830 832 840 852 877 917 939 952 959 987 1003 1038 1058 1074 1132 1136 1140 1177 1184 1192 1194 1205 1208 1213 1219 1235 1250 1257 1260 1284 1299 1304 1317 1329 1333 1345 1361 1369 1378 1397 1405 1412 1417 1426 1463 1490 1502 1509 1553 1577 1580 1649 1667 1668 1676 1678 1684 2997 3061 3073 3156 3160 3189 3190 3200 3211 3220 3248 3705 3718 3752 3753 3756 3760 3774
4a5	15 31 37 41 59 62 90 122 143 165 183 213 218 222 226 235 256 262 267 287 311 319 333 339 345 353 355 379 389 400 402 434 463 465 470 504 522 533 544 559 594 601 604 616 619 632 636 657 685 700 702 714 726 747 753 768 790 801 815 828 832 835 844 861 880 924 935 962 976 982 1017 1033 1065 1074 1108 1129 1138 1175 1182 1192 1193 1197 1207 1211 1220 1228 1244 1253 1280 1286 1293 1305 1317 1328 1346 1350 1360 1370 1378 1395 1398 1412 1427 1434 1463 1491 1494 1523 1551

	1570 1580 1647 1654 1667 1678 1679 1691 3032 3064 3109 3156 3184 3190 3196 3208 3219 3225 3240 3464 3690 3717 3753 3755 3761 3773
4a6	23 29 36 39 58 61 89 123 143 170 189 203 214 218 230 233 246 263 270 282 310 314 329 338 342 346 362 383 386 395 402 434 457 462 471 497 517 533 544 579 592 601 603 616 619 633 636 662 684 695 701 705 726 746 750 771 795 803 814 829 832 836 842 858 878 924 946 959 967 986 1010 1033 1066 1079 1111 1129 1138 1179 1183 1190 1194 1198 1208 1210 1219 1236 1248 1254 1279 1285 1299 1305 1316 1326 1341 1348 1353 1369 1381 1395 1400 1414 1432 1434 1462 1487 1495 1522 1550 1570 1580 1647 1653 1665 1679 1679 1691 3021 3063 3097 3155 3158 3191 3204 3214 3224 3235 3240 3466 3695 3717 3753 3755 3759 3772