Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.
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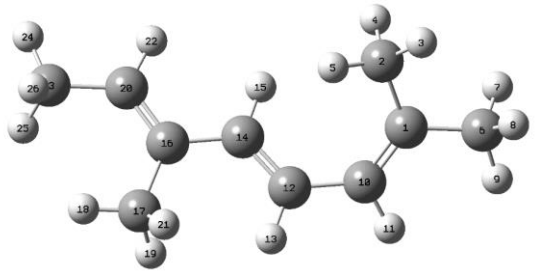
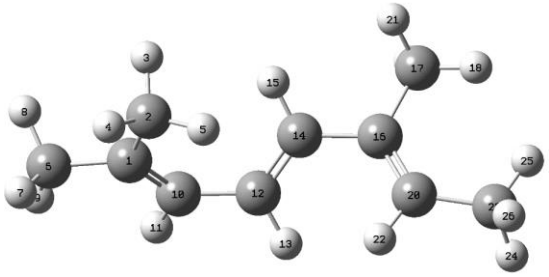
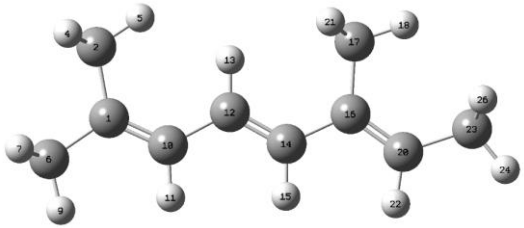
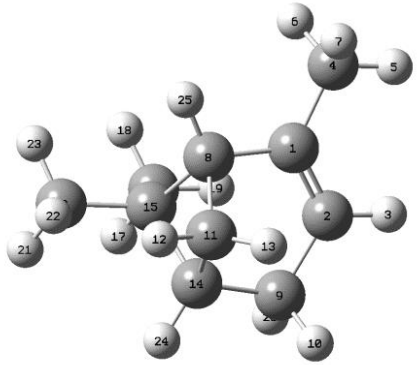
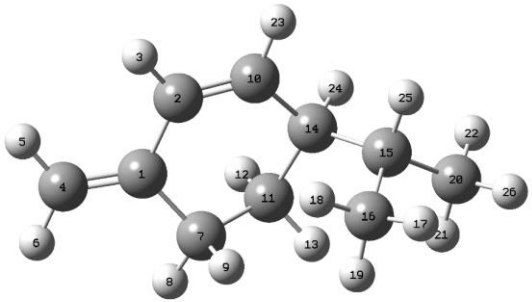
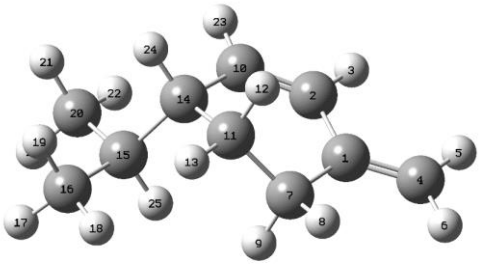
Table S17: **Cartesian coordinates (Å) of optimized gas-phase structures at the target levels of theory, calculated with M06-2X/6-31+G(d,p), M06-2X/6-311+G(2d,p), B3LYP-D3/6-31+G(d, p), B3LYP-D3/6-311+G(2d,p), and DFTBA.**

M06-2X/6-31+G(d,p):

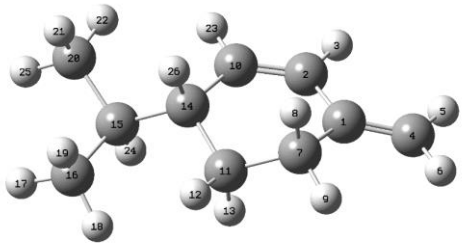
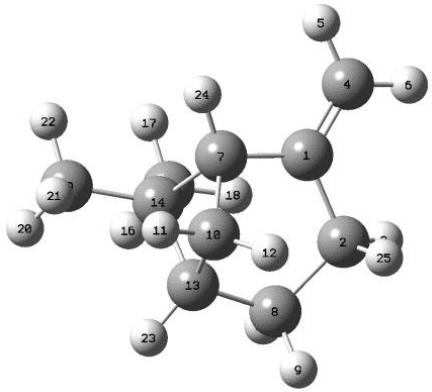
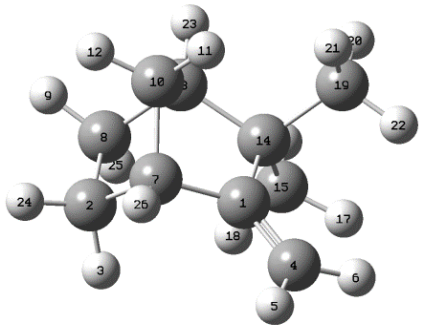
alloocimene- conformer 1				alloocimene- conformer 2				alloocimene- conformer 3			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.058480	0.019380	-0.102900	C	-0.011910	0.035740	0.013960	C	-0.036630	0.006610	0.043400
C	0.160470	-0.240900	1.363710	C	-0.302790	0.177000	1.484360	C	0.272840	0.081800	1.513730
H	1.202900	-0.032720	1.628920	H	0.586810	-0.051720	2.084770	H	1.240380	-0.390910	1.721010
H	-0.461030	0.422060	1.979090	H	-0.580080	1.212120	1.712420	H	0.359720	1.128600	1.828610
H	-0.073920	-1.271860	1.636980	H	-1.107700	-0.485240	1.810120	H	-0.478700	-0.398120	2.140750
C	0.680660	1.211560	-0.649880	C	0.703310	1.208840	-0.601690	C	0.986890	0.664270	-0.842340
H	0.402620	2.120990	-0.103210	H	0.106640	2.123050	-0.497450	H	1.091270	1.726940	-0.591020
H	1.763030	1.086490	-0.524240	H	1.654570	1.392390	-0.087310	H	1.973990	0.207700	-0.698930
H	0.469530	1.370580	-1.710040	H	0.912250	1.048990	-1.662100	H	0.720690	0.584610	-1.898900
C	-0.825400	-0.740210	-0.906570	C	-0.363250	-1.024600	-0.737110	C	-1.124740	-0.588460	-0.481150
H	-0.838280	-0.483220	-1.966160	H	-0.153110	-0.965970	-1.805340	H	-1.233000	-0.574140	-1.566340
C	-1.630310	-1.910770	-0.541920	C	-1.036080	-2.252980	-0.302860	C	-2.195920	-1.262160	0.239040
H	-1.661580	-2.707630	-1.284550	H	-1.738030	-2.689410	-1.014230	H	-2.137610	-1.305430	1.323740
C	-2.353680	-2.047980	0.584860	C	-0.821770	-2.910340	0.850270	C	-3.248310	-1.829270	-0.382920

H	-2.378520	-1.222410	1.295310	H	-0.027840	-2.561750	1.512180	H	-3.296290	-1.779610	-1.471630
C	-3.157390	-3.220320	0.944900	C	-1.535210	-4.131670	1.275110	C	-4.359670	-2.521310	0.272000
C	-3.167270	-4.392890	-0.000030	C	-0.671170	-5.148760	1.979210	C	-4.346960	-2.620980	1.775100
H	-3.766590	-5.219480	0.384040	H	-1.240460	-5.984800	2.386160	H	-5.219360	-3.155170	2.154060
H	-3.572620	-4.102120	-0.975780	H	0.085770	-5.548320	1.295100	H	-3.450060	-3.146700	2.121140
C	-3.850490	-3.211110	2.098760	C	-2.851000	-4.273430	1.039380	C	-5.348120	-3.041680	-0.479530
H	-2.149330	-4.761020	-0.168570	H	-0.132650	-4.673830	2.807140	H	-4.335380	-1.624000	2.229540
H	-3.776560	-2.319620	2.720360	H	-3.360800	-3.430330	0.573700	H	-5.273070	-2.921160	-1.559390
C	-4.719500	-4.325470	2.618090	C	-3.720110	-5.456750	1.346130	C	-6.554680	-3.779060	0.037420
H	-5.255600	-4.012560	3.516080	H	-4.165160	-5.850340	0.425050	H	-7.198680	-4.094720	-0.785430
H	-5.465110	-4.639400	1.880310	H	-3.177990	-6.272560	1.826600	H	-6.272220	-4.677060	0.598210
H	-4.127600	-5.210190	2.880690	H	-4.550910	-5.168730	1.999720	H	-7.156800	-3.153890	0.706210

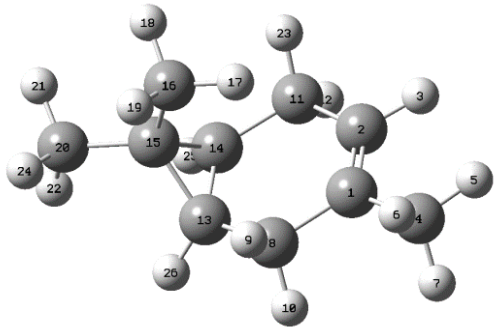
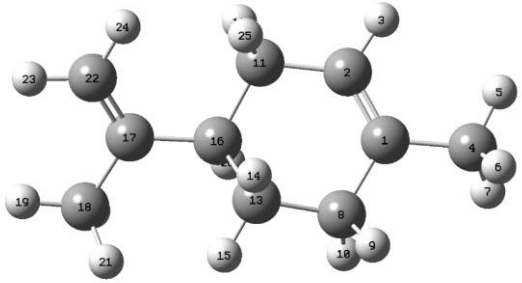
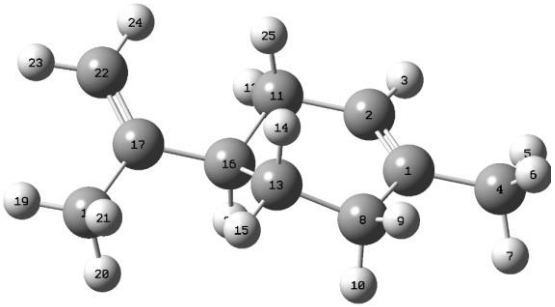
a-pinene	b-phellandrene- conformer 1	b-phellandrene- conformer 2
		

	X	Y	Z		X	Y	Z		X	Y	Z
C	0.001370	0.000830	-0.000370	C	0.240330	-0.200010	0.073750	C	0.002300	-0.002780	-0.003620
C	0.001580	0.001580	1.337900	C	0.057520	-0.150520	1.529780	C	0.005160	-0.000440	1.465850
H	0.932660	0.002770	1.901670	H	0.946990	-0.248930	2.149120	H	0.976190	-0.001790	1.957360
C	1.234330	-0.017390	-0.853020	C	1.404960	-0.568330	-0.475740	C	1.143600	-0.077900	-0.700980
H	2.143080	-0.008570	-0.245540	H	2.257840	-0.837980	0.141080	H	2.107060	-0.120170	-0.200710
H	1.248490	-0.913540	-1.485770	H	1.536070	-0.607280	-1.553150	H	1.144060	-0.096880	-1.786910
H	1.256640	0.847520	-1.526630	C	-0.954640	0.233290	-0.738810	C	-1.355610	0.086720	-0.663260
C	-1.354880	0.019350	-0.681770	H	-0.855250	-0.119820	-1.770320	H	-1.307740	-0.333710	-1.672770
C	-1.311640	-0.036620	2.087700	H	-0.960080	1.328600	-0.775620	H	-1.629180	1.145140	-0.773570
H	-1.381940	0.814380	2.778750	C	-1.143560	0.007160	2.104130	C	-1.117280	-0.012430	2.200810
C	-2.211920	1.095590	0.041780	C	-2.268200	-0.276100	-0.130130	C	-2.415800	-0.628180	0.178980
H	-3.104190	1.385910	-0.512950	H	-2.280680	-1.368490	-0.223980	H	-2.140060	-1.685900	0.267840
H	-1.679590	1.990120	0.376490	H	-3.115830	0.095510	-0.716750	H	-3.388960	-0.595070	-0.318450
C	-2.488410	0.000380	1.102190	C	-2.450430	0.081130	1.358170	C	-2.500510	-0.033260	1.593500
C	-2.300190	-1.053520	-0.035040	C	-3.181150	1.418680	1.642840	C	-3.158310	1.370140	1.654560

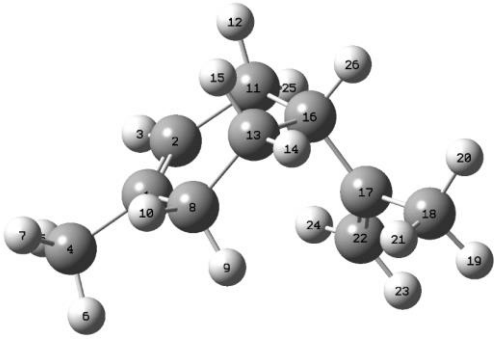
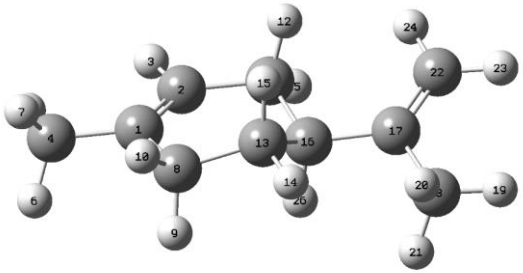
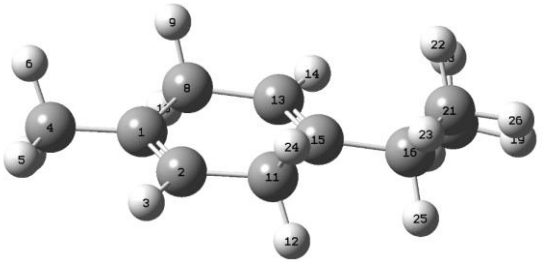
C	-1.741780	-2.426040	0.322000	C	-2.523810	2.628450	0.976930	C	-4.544390	1.381670	1.005780
H	-2.470160	-2.977590	0.928790	H	-2.977140	3.556370	1.339690	H	-5.035140	2.346190	1.169850
H	-1.561670	-3.010120	-0.588320	H	-1.449640	2.669990	1.184250	H	-4.502360	1.214600	-0.073770
H	-0.804120	-2.372740	0.877800	H	-2.665030	2.599450	-0.109770	H	-5.181880	0.603640	1.444710
C	-3.580160	-1.253620	-0.849320	C	-4.663240	1.342190	1.270490	C	-3.260020	1.859470	3.102420
H	-4.312170	-1.823580	-0.265230	H	-4.796870	1.205460	0.191630	H	-3.851000	1.157170	3.703930
H	-4.052620	-0.315510	-1.148440	H	-5.160550	0.510340	1.779990	H	-2.277270	1.964520	3.569380
H	-3.363880	-1.823860	-1.759860	H	-1.207110	0.062370	3.190490	H	-1.036180	-0.009300	3.285470
H	-3.453540	0.007260	1.621810	H	-3.095920	-0.693760	1.799540	H	-3.132160	-0.695560	2.206030
H	-1.280010	0.042140	-1.774860	H	-3.123730	1.566630	2.731420	H	-2.509850	2.070040	1.109250
H	-1.362590	-0.941780	2.709970	H	-5.179610	2.266630	1.547950	H	-3.755490	2.834150	3.146910

b-phellandrene- conformer 3				b-pinene				camphene			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.032590	0.072280	-0.040520	C	0.000850	-0.000290	-0.002150	C	0.000170	0.001320	-0.000780
C	0.025140	0.080050	1.426880	C	0.009270	-0.009570	1.519230	C	0.001590	-0.003380	2.466160
H	0.985060	0.172300	1.931100	H	1.038760	-0.027770	1.890470	H	1.093170	-0.006730	2.395660
C	1.146770	0.314470	-0.742920	C	0.966500	0.563120	-0.730400	C	0.845560	0.576990	-0.853330
H	2.091520	0.518290	-0.246510	H	0.910390	0.589380	-1.814980	H	1.143600	1.615430	-0.739200
H	1.143190	0.314250	-1.828920	H	1.836570	1.018460	-0.264330	H	1.269430	0.030930	-1.692870
C	-1.295530	-0.250330	-0.677990	C	-1.193240	-0.683590	-0.609340	C	-0.645200	0.637620	1.209130
H	-1.432710	-1.341300	-0.666070	C	-0.830970	-1.159320	2.135020	C	-0.608180	-1.436710	2.488000
H	-1.300370	0.064640	-1.726030	H	-1.333860	-0.796330	3.037870	H	-1.270450	-1.562850	3.350220
C	-1.100550	-0.027430	2.148310	C	-2.424840	-0.480520	0.315490	C	-2.024570	-0.051030	1.197490
C	-2.448970	0.394570	0.095250	H	-3.365050	-0.705430	-0.188350	H	-2.621200	0.196930	0.316030
H	-3.396010	0.168220	-0.403400	H	-2.518440	0.485080	0.821670	H	-2.612720	0.158460	2.097440
H	-2.326440	1.487120	0.086100	C	-1.877730	-1.672570	1.140020	C	-1.439310	-1.478680	1.191330
C	-2.488570	-0.087600	1.551580	C	-1.198390	-2.187940	-0.165100	C	-0.508170	-1.446890	-0.057770
C	-3.499740	0.698810	2.418210	C	0.140710	-2.908190	-0.064300	C	0.641040	-2.460580	-0.009880

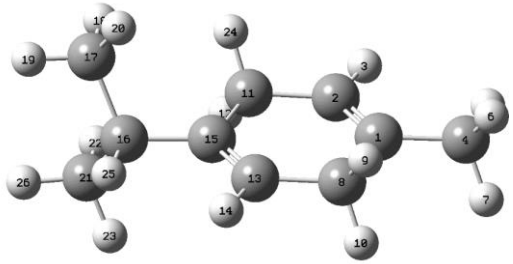
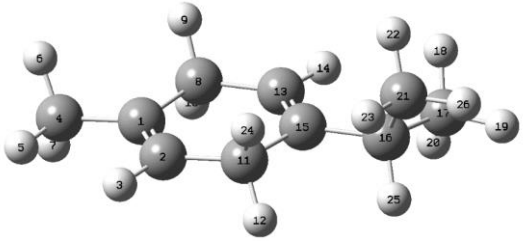
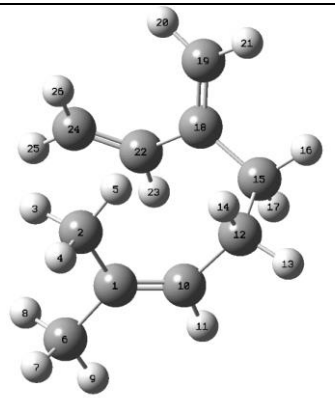
C	-4.857850	0.842590	1.725200	H	0.012900	-3.885040	0.417150	H	0.255780	-3.475110	0.148180
H	-5.577380	1.325530	2.393580	H	0.551020	-3.077060	-1.066540	H	1.186720	-2.452080	-0.959060
H	-4.798500	1.440700	0.812590	H	0.886930	-2.343750	0.499230	H	1.359640	-2.232080	0.781120
H	-5.260140	-0.143560	1.459710	C	-2.150180	-3.029020	-1.016110	C	-1.319870	-1.698950	-1.337860
C	-3.704190	0.038570	3.784930	H	-2.290900	-4.015430	-0.559450	H	-1.680680	-2.733920	-1.358140
H	-4.136740	-0.961590	3.660350	H	-3.136190	-2.571790	-1.130750	H	-2.182440	-1.032510	-1.418040
H	-2.775750	-0.066700	4.351410	H	-1.732090	-3.179640	-2.017840	H	-0.694000	-1.538110	-2.221380
H	-1.017210	-0.043930	3.232400	H	-2.595910	-2.345970	1.622170	H	-2.163340	-2.298800	1.155050
H	-3.083090	1.705550	2.572610	H	-1.287600	-0.475270	-1.680780	H	-0.273930	0.559130	3.363750
H	-4.396180	0.626320	4.395870	H	-0.415170	0.945930	1.850040	H	0.145920	-2.224540	2.545330
H	-2.821790	-1.141360	1.553730	H	-0.186850	-1.988570	2.447040	H	-0.629120	1.729720	1.203730

car-3-ene				limonene- conformer 1				limonene- conformer 2			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.179960	-0.069950	-0.009290	C	-0.015190	-0.012390	-0.010250	C	0.011810	0.013460	0.011640
C	-0.157440	-0.166700	1.322730	C	0.000600	-0.226190	1.310090	C	0.009590	0.083580	1.346930
H	0.706580	-0.632340	1.796320	H	0.956990	-0.393930	1.804080	H	0.941830	-0.086520	1.884530
C	0.942470	-0.585630	-0.868620	C	1.239950	0.035710	-0.837100	C	1.258760	-0.259770	-0.783060
H	1.740520	-1.027490	-0.267020	H	2.134240	-0.083150	-0.220220	H	2.135480	-0.354500	-0.137530
H	0.576770	-1.347180	-1.568190	H	1.236410	-0.754210	-1.597560	H	1.155720	-1.183740	-1.364370
H	1.372930	0.221390	-1.473570	H	1.314870	0.990780	-1.371370	H	1.445270	0.548360	-1.500790
C	-1.325650	0.552590	-0.768740	C	-1.308330	0.204620	-0.760860	C	-1.251410	0.216900	-0.790330
H	-1.718870	-0.194100	-1.477030	H	-1.292890	-0.390380	-1.683550	H	-1.307510	-0.550020	-1.574130
H	-0.911810	1.354520	-1.394640	H	-1.357100	1.255480	-1.084600	H	-1.182320	1.179220	-1.320100
C	-1.237390	0.310780	2.255320	C	-1.231110	-0.251700	2.179020	C	-1.210430	0.385600	2.178520
H	-0.786110	1.005410	2.974610	H	-1.025340	0.237230	3.138780	H	-0.939070	1.053190	3.005330
C	-2.450890	1.122980	0.073140	C	-2.543760	-0.145540	0.069220	C	-2.517580	0.184260	0.066610
C	-2.409240	1.001320	1.581810	H	-2.646140	-1.236110	0.147230	H	-2.749140	-0.850170	0.355100
C	-3.437580	0.234130	0.787990	H	-3.444670	0.225910	-0.429460	H	-3.363690	0.551950	-0.521890
C	-3.319620	-1.269920	0.662080	C	-2.419660	0.423400	1.493950	C	-2.331870	1.011920	1.349180

H	-2.281060	-1.606710	0.617660	C	-3.729130	0.338120	2.251700	C	-3.632420	1.216180	2.100770
H	-3.797850	-1.761340	1.517420	C	-4.780090	1.332540	1.825510	C	-4.732230	1.903000	1.327110
H	-3.828530	-1.616200	-0.245270	H	-5.711820	1.191090	2.377720	H	-5.530470	2.238890	1.992720
C	-4.869070	0.723650	0.866960	H	-4.427490	2.355950	2.000100	H	-4.343410	2.773030	0.785210
H	-5.383720	0.287310	1.731030	H	-5.001700	1.250880	0.756030	H	-5.175960	1.232720	0.583240
H	-4.909360	1.813140	0.965520	C	-3.965540	-0.532530	3.237230	C	-3.820230	0.849170	3.371980
H	-1.593230	-0.540880	2.854740	H	-4.929070	-0.555100	3.738360	H	-4.766530	1.040450	3.870080
H	-5.427550	0.445770	-0.034680	H	-3.221210	-1.241920	3.582390	H	-3.053160	0.355880	3.958650
H	-2.801610	1.852800	2.132960	H	-1.479750	-1.296230	2.414300	H	-1.571870	-0.544130	2.641720
H	-2.867620	2.050080	-0.313670	H	-2.176620	1.494260	1.391960	H	-1.992940	2.014110	1.034690

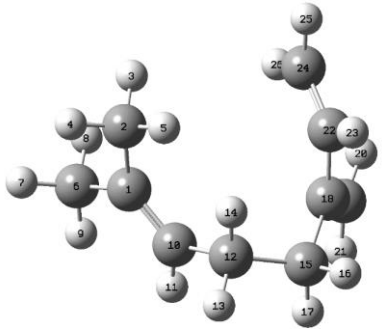
limonene- conformer 3				limonene- conformer 4				gamma-terpinene- conformer 1			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.311580	-0.130340	0.337570	C	0.000830	-0.001380	-0.001260	C	0.002930	0.000270	-0.001860
C	-0.258490	0.450560	1.541460	C	0.001870	-0.005810	1.335860	C	0.000930	-0.004390	1.332620
H	0.668630	0.394930	2.111920	H	0.956190	-0.012560	1.861460	H	0.951650	-0.000490	1.864520
C	0.845650	-0.893550	-0.244250	C	1.266490	-0.037800	-0.812370	C	1.268520	0.011130	-0.812810
H	1.696190	-0.921630	0.441620	H	2.151980	-0.101170	-0.175030	H	2.155040	-0.000410	-0.173830
H	0.550950	-1.925990	-0.469210	H	1.267360	-0.900380	-1.489810	H	1.311920	-0.859830	-1.477750
H	1.176070	-0.444030	-1.188190	H	1.354150	0.858170	-1.438280	H	1.314510	0.901420	-1.451280
C	-1.561610	-0.070900	-0.508460	C	-1.287540	0.030630	-0.788270	C	-1.281900	-0.009250	-0.787760
H	-2.056970	-1.053410	-0.473900	H	-1.431770	-0.948560	-1.269790	H	-1.322890	-0.923070	-1.401320
H	-1.282970	0.093510	-1.557350	H	-1.190090	0.753500	-1.609010	H	-1.264170	0.816200	-1.515640
C	-1.407230	1.191840	2.179480	C	-1.243060	-0.001600	2.185200	C	-1.241020	-0.032150	2.177580
H	-1.196280	2.270140	2.156010	H	-1.392360	1.004580	2.603340	H	-1.199790	0.771860	2.928450
C	-2.522520	1.021830	-0.042740	C	-2.506030	0.372940	0.070030	C	-2.520520	0.095880	0.057610
H	-3.471280	0.957480	-0.585300	H	-3.418920	0.166540	-0.496940	H	-3.456750	0.190820	-0.487080
H	-2.090800	2.004240	-0.271690	H	-2.508320	1.445440	0.307950	C	-2.527520	0.091730	1.394080

C	-2.746980	0.936410	1.479940	C	-2.483060	-0.413450	1.391220	C	-3.789990	0.223600	2.226600
C	-3.425590	-0.370660	1.853540	C	-3.787050	-0.300520	2.156060	C	-5.045800	0.532510	1.413930
C	-4.822540	-0.544070	1.308950	C	-5.017920	-0.773870	1.420700	H	-5.298090	-0.301500	0.749290
H	-5.314730	-1.411510	1.754450	H	-5.860300	-0.899790	2.104500	H	-5.895600	0.689530	2.084610
H	-5.434730	0.343270	1.507520	H	-5.319030	-0.060960	0.645740	H	-4.922370	1.431960	0.803840
H	-4.809140	-0.687240	0.222380	H	-4.830110	-1.731700	0.921660	C	-4.022030	-1.030470	3.084650
C	-2.854660	-1.324240	2.594380	C	-3.875470	0.157530	3.408360	H	-4.141000	-1.909490	2.441200
H	-3.392710	-2.237250	2.834050	H	-4.833970	0.195450	3.918250	H	-3.194410	-1.221010	3.772720
H	-1.840070	-1.238800	2.969620	H	-3.013270	0.503310	3.967770	H	-1.252260	-0.963860	2.762040
H	-1.480040	0.926740	3.241010	H	-1.108450	-0.671830	3.042860	H	-3.622280	1.066130	2.915670
H	-3.442080	1.739670	1.763970	H	-2.369030	-1.478570	1.125380	H	-4.931660	-0.920550	3.683520

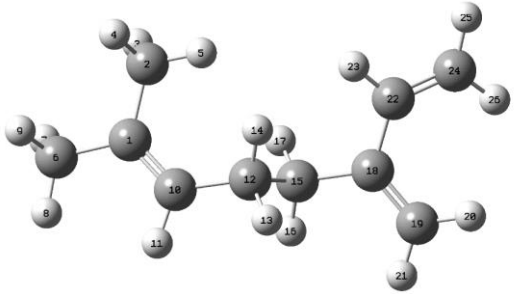
gamma-terpinene- conformer 2				gamma-terpinolene- conformer 3				myrcene- conformer 1			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.011570	-0.250690	-0.062410	C	-0.002230	0.000730	0.000390	C	-0.131010	-0.232240	-0.383720
C	0.096310	-0.068470	1.257140	C	-0.000380	0.001770	1.337300	C	0.892470	-1.064740	0.339110
H	1.025170	-0.322490	1.766690	H	0.953720	0.010420	1.863660	H	1.799040	-1.140990	-0.273930
C	1.149210	-0.795030	-0.880430	C	1.262460	0.042560	-0.811760	H	1.181860	-0.587850	1.283500
H	2.022170	-1.012200	-0.259870	H	2.148470	0.117040	-0.176240	H	0.550310	-2.079620	0.549290
H	0.852750	-1.717820	-1.393360	H	1.356670	-0.854590	-1.435030	C	0.381090	1.099680	-0.864160
H	1.446950	-0.080380	-1.657050	H	1.254830	0.902680	-1.492280	H	0.796930	1.683470	-0.034380
C	-1.245320	0.080570	-0.824710	C	-1.295380	-0.046550	-0.777260	H	1.192970	0.952600	-1.588070
H	-1.596970	-0.821680	-1.348870	H	-1.172900	-0.713280	-1.641200	H	-0.404920	1.689710	-1.342070
H	-1.002620	0.794780	-1.626800	H	-1.513430	0.950440	-1.186930	C	-1.386780	-0.622230	-0.635430
C	-1.012580	0.468950	2.117630	C	-1.238270	0.026760	2.203350	H	-2.023130	0.063430	-1.198280
H	-0.653460	1.354500	2.662370	H	-1.111290	0.813820	2.951520	C	-2.029120	-1.930060	-0.264470
C	-2.347740	0.634190	0.032080	C	-2.462410	-0.523730	0.094000	H	-3.041880	-1.733270	0.107730
H	-3.272860	0.899000	-0.479450	H	-2.298030	-1.585970	0.326930	H	-1.488010	-2.423680	0.548650
C	-2.266340	0.819710	1.352760	H	-3.401860	-0.464590	-0.457010	C	-2.139610	-2.910060	-1.451580

C	-3.431400	1.392490	2.135370	C	-2.503570	0.236110	1.397660	H	-2.771380	-3.754700	-1.157820
C	-3.941830	0.419050	3.205850	C	-3.527000	1.007870	1.801260	H	-2.645810	-2.403630	-2.285060
H	-3.200800	0.279670	4.000350	C	-4.766500	1.272640	0.979540	C	-0.802470	-3.435210	-1.925960
H	-4.851810	0.809690	3.672550	H	-5.629350	0.736610	1.394280	C	-0.407970	-4.681890	-1.632810
H	-4.169650	-0.560580	2.774870	H	-5.012160	2.340410	1.019910	H	0.527720	-5.085650	-2.007590
C	-3.086960	2.747400	2.768140	H	-4.667730	0.997310	-0.070170	H	-1.025590	-5.337130	-1.024930
H	-2.329150	2.638610	3.551400	C	-3.575770	1.703470	3.141890	C	0.031750	-2.531670	-2.750820
H	-2.706200	3.448240	2.019180	H	-3.445150	2.786550	3.023450	H	-0.511830	-1.812400	-3.363580
H	-1.253380	-0.267030	2.899040	H	-4.562180	1.554750	3.596750	C	1.367550	-2.527530	-2.784050
H	-4.245000	1.556860	1.416810	H	-1.302540	-0.919510	2.765060	H	1.911490	-1.854930	-3.439290
H	-3.975510	3.187870	3.231860	H	-2.830530	1.344310	3.851500	H	1.953400	-3.182620	-2.144320

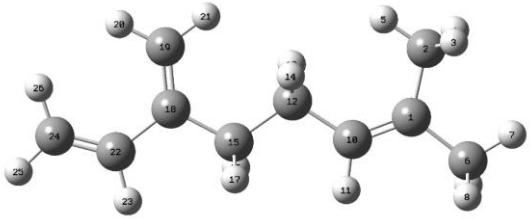
myrcene- conformer 2



myrcene- conformer 3

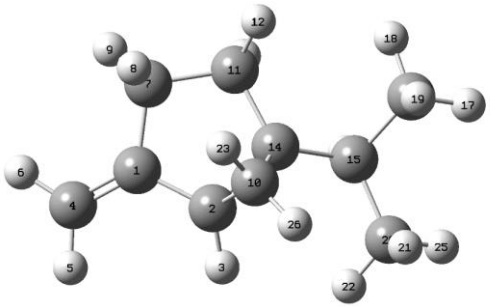
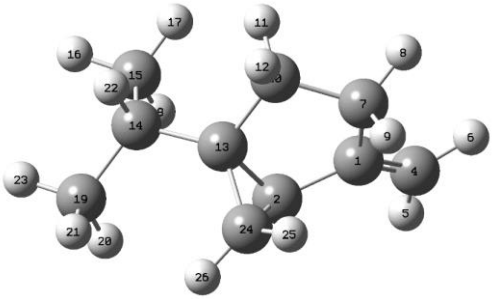
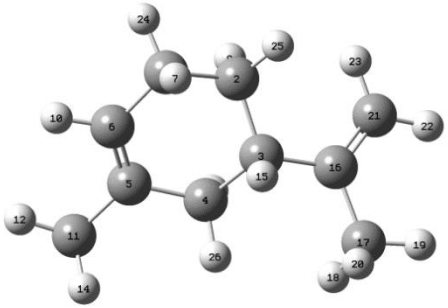


myrcene- conformer 4

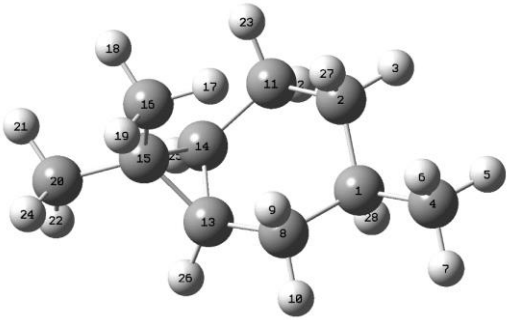
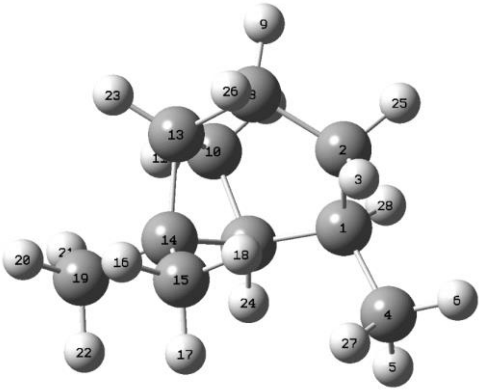
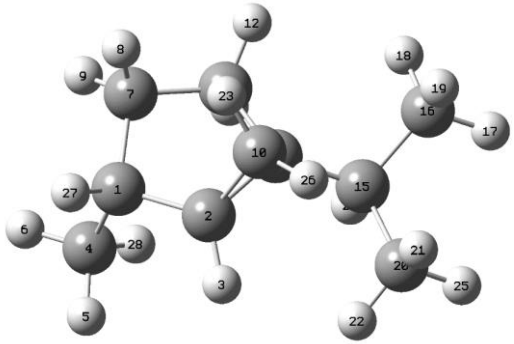


	X	Y	Z		X	Y	Z		X	Y	Z
C	0.065560	-0.023160	-0.215130	C	0.029630	-0.003370	-0.174220	C	0.003730	0.006460	-0.015340
C	0.264890	0.290510	1.244640	C	-0.293010	0.038750	1.296750	C	0.144570	0.250400	1.463100
H	1.335230	0.364310	1.471380	H	0.631660	0.013180	1.885490	H	1.203720	0.324830	1.738250
H	-0.179130	1.264360	1.484820	H	-0.804200	0.974680	1.552100	H	-0.320550	1.204870	1.738250
H	-0.165060	-0.457070	1.911640	H	-0.919990	-0.793480	1.622170	H	-0.310440	-0.537700	2.065960
C	0.712400	0.967670	-1.149280	C	0.919380	1.113920	-0.652850	C	0.611560	1.059260	-0.921720
H	0.339700	1.981780	-0.961180	H	1.876120	1.106170	-0.117140	H	1.074890	1.861760	-0.341160
H	1.797340	0.993250	-0.990260	H	1.123520	1.036740	-1.723460	H	1.384000	0.630350	-1.567360
H	0.524590	0.720330	-2.196860	H	0.455280	2.088570	-0.459380	H	-0.146100	1.513750	-1.567360
C	-0.619640	-1.069440	-0.693470	C	-0.417960	-0.947550	-1.012110	C	-0.615270	-1.065680	-0.520290
H	-0.679390	-1.170910	-1.779460	H	-0.098390	-0.891690	-2.053070	H	-0.668440	-1.157770	-1.607440
C	-1.298880	-2.166090	0.075740	C	-1.286410	-2.124140	-0.652550	C	-1.258280	-2.179400	0.273950
H	-2.376260	-2.153550	-0.133710	H	-1.891840	-2.415280	-1.517920	H	-2.040170	-1.774790	0.930780
H	-1.186060	-2.016340	1.153450	H	-1.994070	-1.856410	0.139610	H	-0.516930	-2.654240	0.930780
C	-0.746970	-3.554120	-0.306730	C	-0.451840	-3.345460	-0.212560	C	-1.869440	-3.237970	-0.636910
H	-1.283980	-4.320210	0.268940	H	0.229350	-3.621710	-1.024810	H	-2.603690	-2.760290	-1.302410
H	-0.941230	-3.752430	-1.366770	H	0.170460	-3.054000	0.643580	H	-1.088640	-3.635000	-1.302410

C	0.733530	-3.673090	-0.036840	C	-1.317050	-4.528710	0.153550	C	-2.543830	-4.406050	0.044840
C	1.622030	-3.947050	-0.998410	C	-1.480640	-5.568770	-0.673450	C	-2.617750	-4.534070	1.375180
H	2.678100	-4.062960	-0.773830	H	-2.167210	-6.377160	-0.441040	H	-3.108360	-5.383830	1.839090
H	1.310150	-4.073950	-2.031270	H	-0.940030	-5.626710	-1.613960	H	-2.191770	-3.796260	2.045450
C	1.150310	-3.455610	1.365970	C	-2.010150	-4.446800	1.458260	C	-3.117230	-5.399200	-0.897670
H	0.517170	-3.904970	2.133340	H	-2.290250	-3.447610	1.794350	H	-2.979100	-5.159940	-1.952440
C	2.203990	-2.723520	1.734690	C	-2.268460	-5.486450	2.255790	C	-3.767240	-6.525050	-0.592520
H	2.472320	-2.600580	2.779250	H	-2.782830	-5.356320	3.202200	H	-4.143640	-7.176990	-1.373240
H	2.815520	-2.213990	0.993890	H	-1.959160	-6.493570	1.989450	H	-3.946130	-6.834900	0.432990

sabinene- conformer 1				sabinene- conformer 2				sylvestrene			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.000550	0.003400	-0.002300	C	-0.318030	-0.116850	0.063200	C	0.143030	-0.162130	-0.075950
C	0.003490	0.003090	1.483130	C	-0.118590	0.305180	1.473110	C	0.054120	-0.142840	1.450190
H	0.954730	0.007750	2.005260	H	0.410020	-0.355210	2.154980	C	1.438690	0.043510	2.068220
C	1.047130	-0.238680	-0.791580	C	0.287760	-1.136560	-0.546950	C	2.014160	1.401550	1.627750
H	2.008690	-0.530420	-0.379820	H	1.058390	-1.715580	-0.046940	C	1.823250	1.686960	0.156100
H	0.971490	-0.151030	-1.871220	H	0.029030	-1.419960	-1.562690	C	0.991960	0.964750	-0.602620
C	-1.385510	0.422700	-0.454220	C	-1.408630	0.759410	-0.523410	H	0.555590	-1.123780	-0.414110
H	-2.015570	-0.465360	-0.584280	H	-1.974160	0.245210	-1.304300	H	-0.593730	0.686600	1.765370
H	-1.366600	0.945150	-1.413680	H	-0.958900	1.647260	-0.983750	H	1.544740	2.204080	2.218420
C	-1.181850	-0.655340	2.168410	C	-2.274830	1.157910	0.689870	H	0.910800	1.198430	-1.663630
C	-1.916990	1.296390	0.699390	H	-3.095780	0.442540	0.809920	C	2.628440	2.833430	-0.391720
H	-3.005460	1.233080	0.802970	H	-2.717950	2.154420	0.584080	H	2.404320	3.015860	-1.445650
H	-1.659400	2.349030	0.523550	C	-1.353910	1.073430	1.909090	H	2.421860	3.753600	0.168180
C	-1.179790	0.827200	1.955350	C	-2.017070	0.856080	3.265460	H	3.702830	2.636880	-0.295270
C	-1.120490	1.808490	3.116670	C	-2.547090	-0.577510	3.385140	H	2.097160	-0.735850	1.649080
C	-2.536120	2.153370	3.591590	H	-3.115740	-0.705510	4.311590	C	1.488910	-0.096680	3.576390
H	-2.506000	2.854190	4.431970	H	-3.200190	-0.848560	2.550990	C	2.867510	-0.055870	4.187570

H	-3.132120	2.609390	2.795740	H	-1.712910	-1.288050	3.398280	H	3.311020	0.941910	4.096680
H	-3.052880	1.245330	3.924420	C	-1.108190	1.172950	4.453580	H	2.838050	-0.314650	5.248430
C	-0.277010	1.329520	4.298870	H	-0.196020	0.563690	4.426260	H	3.541540	-0.754310	3.677970
H	-0.750100	0.481070	4.805300	H	-0.815670	2.226230	4.473230	C	0.400570	-0.233350	4.338930
H	0.730510	1.030920	3.994680	H	-2.874460	1.544430	3.310370	H	0.485150	-0.326070	5.418020
H	-1.843640	-1.281480	1.576610	H	-1.623060	0.948780	5.392590	H	-0.601670	-0.255430	3.924250
H	-0.657140	2.726220	2.723700	C	-0.053540	1.797040	1.740460	H	-0.861520	-0.098050	-0.510310
H	-0.177070	2.132280	5.035540	H	0.074030	2.472920	0.899600	H	-0.402710	-1.070290	1.811500
H	-0.997940	-1.023470	3.172090	H	0.490290	2.087840	2.631880	H	3.087210	1.449830	1.854920

hydrogenated car-3-ene				hydrogenated pinene				hydrogenated sabinene			
											
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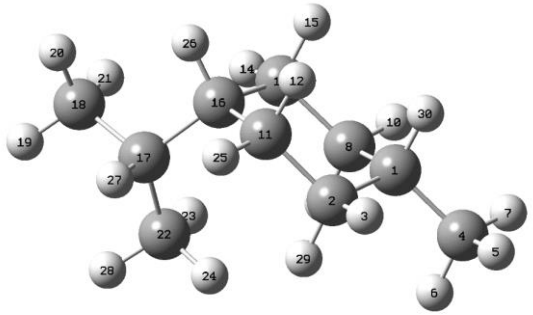
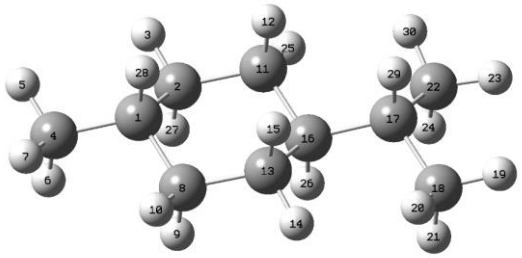
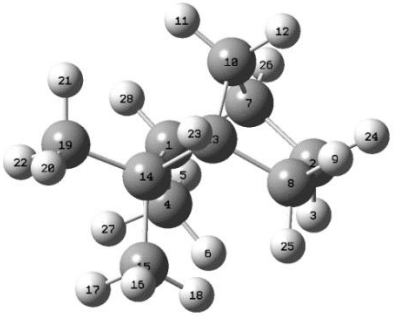
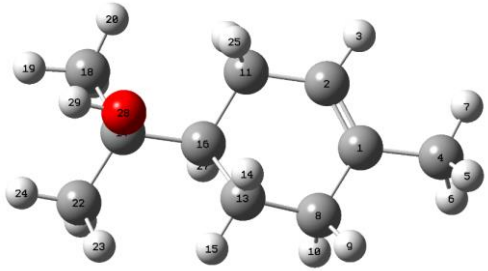
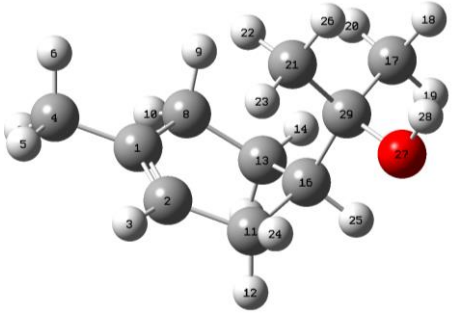
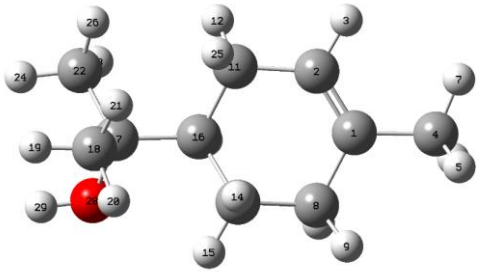
C	0.010330	-0.019870	-0.103060	C	-0.278570	0.321980	0.039050	C	-0.168020	-0.501650	0.030030
C	0.175850	-0.038490	1.416930	C	0.018230	-0.029520	1.527290	C	-0.222000	-0.364240	1.544120
H	1.220350	0.167230	1.680910	H	1.054080	-0.378620	1.596380	H	0.706370	-0.479330	2.097430
C	1.003890	-0.959940	-0.779650	C	1.003370	0.426470	-0.789400	C	1.029300	0.273500	-0.523450
H	2.037030	-0.682460	-0.546850	H	0.781470	0.751580	-1.811410	H	1.971690	-0.111880	-0.120790
H	0.848700	-1.990410	-0.437550	H	1.690130	1.156220	-0.346930	H	1.073900	0.206110	-1.615130
H	0.885520	-0.947680	-1.868180	C	-1.316980	-0.631230	-0.565430	C	-1.507130	0.107520	-0.438490
C	-1.434770	-0.388500	-0.461200	C	-0.918190	-1.098290	2.164360	H	-2.288380	-0.658630	-0.452210
H	-1.608130	-1.434530	-0.168090	H	-1.519640	-0.645190	2.960990	H	-1.439990	0.510760	-1.453830
H	-1.562270	-0.353270	-1.548760	C	-2.564580	-0.600940	0.352960	C	-1.503680	-0.722660	2.253400
C	-0.725010	0.987170	2.128550	H	-3.485550	-0.912640	-0.140920	C	-1.844950	1.191700	0.603370
H	-0.203780	1.951530	2.111260	H	-2.748030	0.336440	0.890710	H	-2.925490	1.353020	0.688100
C	-2.453200	0.538180	0.188900	C	-1.875070	-1.731400	1.150970	H	-1.392200	2.153320	0.326000
C	-2.093300	1.216850	1.498740	C	-1.135010	-2.129980	-0.159090	C	-1.212960	0.715120	1.909020

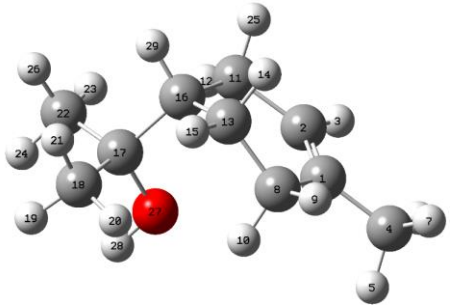
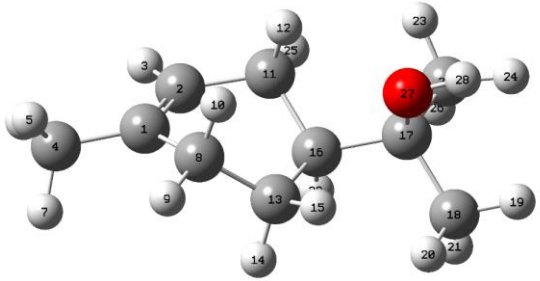
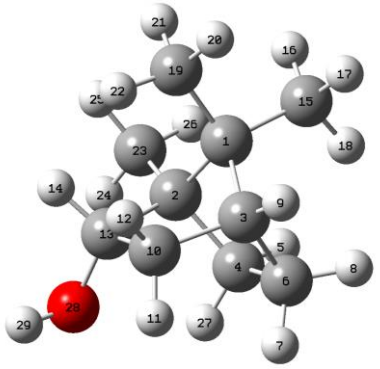
C	-3.193300	0.188830	1.460560	C	0.252590	-2.755860	-0.044120	C	-0.995760	1.764430	2.989400
C	-3.010430	-1.158490	2.124550	H	0.165170	-3.767810	0.369920	C	-2.342760	2.285130	3.501770
H	-1.987110	-1.530720	2.064990	H	0.719450	-2.844690	-1.031980	H	-2.202060	3.056530	4.265830
H	-3.277190	-1.092310	3.185650	H	0.931140	-2.194450	0.599250	H	-2.942770	2.716240	2.694890
H	-3.665940	-1.905930	1.661620	C	-1.989560	-3.043320	-1.042430	H	-2.916850	1.464210	3.947800
C	-4.610880	0.712960	1.579100	H	-2.049320	-4.046950	-0.605740	C	-0.136150	1.288360	4.161110
H	-4.895650	0.834780	2.630870	H	-3.010000	-2.675540	-1.173850	H	-0.628870	0.482140	4.715920
H	-4.715370	1.685240	1.087400	H	-1.538730	-3.137310	-2.037180	H	0.843230	0.930300	3.831190
H	-0.832390	0.718030	3.187240	H	-2.504640	-2.496030	1.621920	H	-2.281570	-1.249280	1.707020
H	-5.323340	0.021550	1.113920	H	-1.456990	-0.426580	-1.634990	H	-0.465660	2.601460	2.508760
H	-2.447220	2.240660	1.604190	H	-0.013960	0.887580	2.123380	H	0.029610	2.111000	4.863480
H	-3.021940	1.146200	-0.511330	H	-0.314050	-1.880000	2.639810	H	-1.416270	-1.018790	3.293740
H	-0.027250	-1.058430	1.769800	H	1.527400	-0.532150	-0.847100	H	-0.091110	-1.552280	-0.277980
H	0.194100	1.006710	-0.456410	H	-0.750440	1.314470	0.014900	H	0.959150	1.333150	-0.250230

hydrogenated limonane- conformer 1				hydrogenated limonane- conformer 2				hydrogenated camphane			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.482580	0.187510	0.091780	C	0.402720	0.246570	-0.078230	**C**	0.390832	0.897105	-0.657134
C	-0.023440	-0.058600	1.515400	C	0.021400	-0.004630	1.381050	**C**	-1.82225	0.624298	0.559266
H	0.793900	-0.440250	2.140410	H	0.867070	-0.448940	1.920520	**H**	-1.505543	1.442202	1.213585
C	1.063110	-1.081040	-0.527150	C	0.840660	-1.039520	-0.773990	**C**	0.806778	2.223787	-0.030115
H	1.884330	-1.479370	0.077780	H	1.692870	-1.498770	-0.262320	**H**	0.426625	3.05786	-0.629481
H	0.292700	-1.858190	-0.599870	H	0.021530	-1.768690	-0.780860	**H**	0.431912	2.350885	0.988938
H	1.444130	-0.892970	-1.536370	H	1.129670	-0.851520	-1.813270	**C**	-1.127089	0.669642	-0.819686
C	-0.651990	0.755800	-0.764790	C	-0.775010	0.903530	-0.799060	**C**	-1.422364	-0.774954	1.114819
H	-1.415770	-0.022770	-0.881600	H	-1.608660	0.185040	-0.830470	**H**	-2.291235	-1.440612	1.146114
H	-0.278760	0.975600	-1.773220	H	-0.507050	1.118030	-1.841080	**C**	-1.139747	-0.814595	-1.223828
C	-0.586340	1.221560	2.136700	C	-0.439080	1.270910	2.090820	**H**	-0.58476	-1.010595	-2.14636
H	0.248580	1.928160	2.247810	H	0.403730	1.977440	2.152120	**H**	-2.147672	-1.232381	-1.321174
C	-1.259760	2.031410	-0.166000	C	-1.241080	2.185600	-0.104920	**C**	-0.426585	-1.285608	0.058225
H	-2.106520	2.365610	-0.778740	H	-2.096730	2.596030	-0.650050	**C**	0.872669	-0.421764	0.0633
H	-0.503590	2.825380	-0.237100	H	-0.440050	2.939770	-0.158140	**C**	1.4292	-0.192403	1.472343
C	-1.686600	1.917150	1.311960	C	-1.605040	1.963740	1.370440	**H**	1.581324	-1.153118	1.978434

C	-3.114640	1.355940	1.540480	C	-2.020320	3.275570	2.068580	**H**	2.399001	0.314926	1.424684
C	-4.159560	2.443810	1.266000	C	-3.186570	3.964580	1.352010	**H**	0.772754	0.416285	2.098887
H	-5.171970	2.072810	1.455730	H	-3.517330	4.843560	1.914060	**C**	1.967466	-1.106874	-0.762842
H	-3.996650	3.322490	1.898050	H	-2.921410	4.299360	0.346390	**H**	2.338842	-2.004356	-0.254495
H	-4.119870	2.770360	0.220030	H	-4.041800	3.281970	1.267950	**H**	1.603466	-1.403749	-1.751632
C	-3.490790	0.098580	0.749190	C	-2.391590	3.052400	3.538520	**H**	2.815635	-0.427391	-0.910188
H	-3.527140	0.308720	-0.325980	H	-2.763780	3.979390	3.985820	**H**	-0.217669	-2.358357	0.132686
H	-2.798240	-0.730970	0.910180	H	-3.185800	2.299730	3.623070	**H**	-2.907337	0.709547	0.445671
H	-0.959060	1.023940	3.149260	H	-0.719660	1.025440	3.119760	**H**	-1.011363	-0.739515	2.125948
H	-1.736680	2.944440	1.699700	H	-2.474970	1.283570	1.404770	**H**	-1.590565	1.367412	-1.523942
H	-3.178540	1.104910	2.609600	H	-0.791750	-0.746520	1.405710	**H**	1.897615	2.314711	0.007745
H	-4.488430	-0.239950	1.048140	H	1.245670	0.955960	-0.090810	**H**	0.815516	0.884454	-1.671505
H	-0.786110	-0.848400	1.489590	H	-1.151680	3.952220	2.034950				
H	1.279840	0.946520	0.147780	H	-1.542730	2.716770	4.138870				

a-terpineol- conformer 1				a-terpineol- conformer 2				a-terpineol- conformer 3		
										
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.145340	0.578300	-0.347800	C	-0.039020	-0.048000	0.017800	C	0.001940	0.001590	-0.000620
C	0.268100	0.633010	0.922390	C	-0.060320	0.040170	1.352680	C	0.001130	0.004240	1.337070
H	0.754250	1.541280	1.278070	H	0.889690	0.064940	1.887140	H	0.955170	0.009420	1.863560
C	0.004470	1.732080	-1.300490	C	1.240270	-0.150720	-0.766080	C	1.271130	0.035800	-0.806490
H	0.640500	1.456480	-2.150150	H	2.115720	-0.147250	-0.111750	H	1.360660	-0.861470	-1.430340
H	-0.969760	2.020910	-1.713730	H	1.258180	-1.074640	-1.358000	H	1.273390	0.896480	-1.486340
H	0.441980	2.606040	-0.811130	H	1.333770	0.681460	-1.474010	H	2.155070	0.101230	-0.167000
C	-0.795710	-0.665050	-0.903500	C	-1.312470	-0.061510	-0.792360	C	-1.286890	-0.035550	-0.787970
H	-0.397790	-0.859400	-1.908370	H	-1.456860	-1.060680	-1.230760	H	-1.170630	-0.724610	-1.634810
H	-1.871480	-0.475500	-1.040750	H	-1.195430	0.613030	-1.651110	H	-1.467050	0.955660	-1.230310
C	0.094890	-0.476610	1.927400	C	-1.309590	0.104790	2.195400	C	-1.241080	0.025360	2.192480
H	-0.252870	-0.036050	2.869180	H	-1.415390	1.122850	2.595420	H	-1.104270	0.764780	2.990420
C	-0.581470	-1.888130	-0.012610	C	-2.531050	0.362200	0.027200	C	-2.477350	-0.452240	0.073670
H	0.461100	-2.220040	-0.080220	H	-3.453920	0.171000	-0.529130	H	-2.382440	-1.521410	0.308840
H	-1.203340	-2.712870	-0.372810	H	-2.479500	1.448380	0.174760	H	-3.417470	-0.310850	-0.467760
C	-0.886050	-1.557280	1.453350	C	-2.584930	-0.269570	1.425390	C	-2.496090	0.351380	1.376540
C	-0.870810	-2.804430	2.364510	C	-4.060200	-2.144250	0.558890	C	-3.811110	0.190680	2.163780

C	-1.016050	-2.420620	3.840020	H	-4.386000	-3.172470	0.752160	C	-4.185460	-1.272120	2.412710
H	-1.095650	-3.322600	4.458240	H	-4.909270	-1.477030	0.737040	H	-5.102360	-1.327070	3.011730
H	-0.149460	-1.850410	4.181370	H	-3.771720	-2.078560	-0.494980	H	-4.364220	-1.790550	1.467710
H	-1.918940	-1.822630	4.003940	C	-1.709110	-2.715540	1.215480	H	-3.402040	-1.802320	2.962710
C	-1.986880	-3.783850	1.989260	H	-1.328550	-2.620540	0.196220	C	-3.758640	0.955370	3.487670
H	-1.863880	-4.155310	0.970300	H	-0.889860	-2.516210	1.909640	H	-3.447250	1.990650	3.317140
H	-1.971790	-4.646420	2.665420	H	-1.207730	-0.545320	3.072390	H	-4.752020	0.967610	3.950720
H	1.065800	-0.945370	2.143970	H	-3.438390	0.177850	1.950370	H	-1.352920	-0.946790	2.697160
H	-2.969210	-3.308160	2.076470	H	-2.031200	-3.756070	1.350950	H	-3.068440	0.488980	4.196850
H	-1.904450	-1.140550	1.506840	O	-3.312760	-1.974670	2.844950	H	-2.452460	1.417760	1.106440
O	0.401390	-3.423900	2.155270	H	-3.423100	-2.919010	3.007480	O	-4.799270	0.791560	1.319350
H	0.480740	-4.181820	2.746290	C	-2.896140	-1.786460	1.484150	H	-5.665660	0.682610	1.728970

a-terpineol- conformer 4				a-terpineol- conformer 5				borneol			
											
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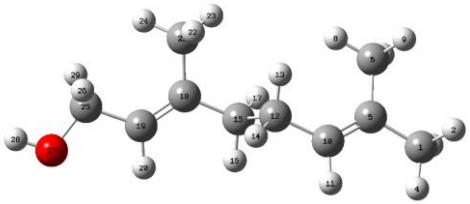
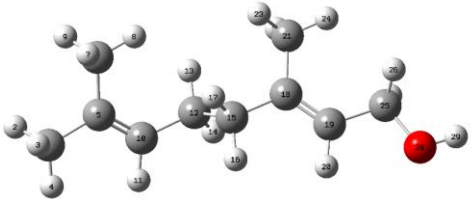
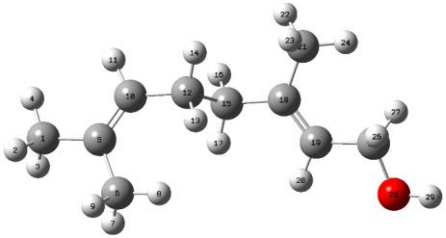
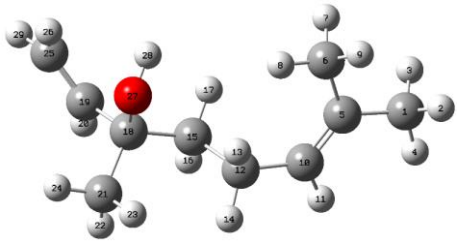
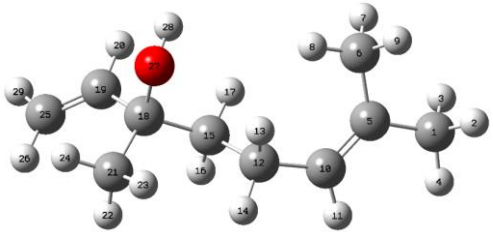
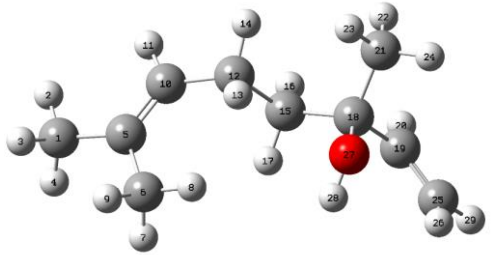
C	0.111130	-0.175550	1.230120	C	0.117260	-0.240800	1.311940	C	-0.005290	-0.015970	1.563340
H	1.050090	-0.408300	1.732250	H	1.083050	-0.368800	1.797050	C	1.550030	0.014390	-0.088050
C	1.272660	-0.520630	-0.947780	C	1.212560	0.280120	-0.887880	C	0.880700	-1.246720	1.866240
H	1.492410	0.315630	-1.623040	H	1.201460	1.290190	-1.314810	H	0.275430	-2.158710	1.856480
H	2.158060	-0.705540	-0.333870	H	2.156210	0.142490	-0.353180	C	1.933000	-1.240940	0.721260
H	1.096260	-1.401070	-1.577400	H	1.185410	-0.421250	-1.730510	H	2.957790	-1.174710	1.098440
C	-1.208630	0.094630	-0.846470	C	-1.357530	0.233280	-0.547470	H	1.870900	-2.145970	0.109810
H	-1.302070	-0.585480	-1.703650	H	-1.334370	0.312630	-1.639890	H	1.956840	0.037270	-1.104490
H	-1.142610	1.111470	-1.257940	H	-1.793230	1.169970	-0.171250	C	1.930300	1.234420	0.774110
C	-1.045160	0.187680	2.127330	C	-1.146450	-0.402140	2.114800	H	2.926830	1.126280	1.214500
H	-0.692920	0.927040	2.855300	H	-1.607000	0.581480	2.291660	H	1.917890	2.166040	0.200240
C	-2.432330	-0.048790	0.057580	C	-2.270700	-0.933810	-0.129580	C	0.847270	1.228920	1.890850
H	-2.550750	-1.111350	0.307500	H	-2.001630	-1.812060	-0.726270	H	0.214760	2.125710	1.835370
H	-3.344270	0.247600	-0.469970	H	-3.299320	-0.667770	-0.386840	C	-0.657370	-1.211250	-0.640460
C	-2.286270	0.716690	1.380950	C	-2.176800	-1.289740	1.378910	H	-1.743950	-1.177720	-0.502870

C	-2.289600	2.261140	1.249510	C	-3.562420	-1.256030	2.058920	H	-0.463560	-1.215410	-1.719300
C	-3.338690	2.745600	0.244450	C	-4.487490	-2.318620	1.457710	H	-0.301250	-2.160060	-0.235410
H	-3.398140	3.840060	0.262920	H	-5.486790	-2.244710	1.902530	C	-0.657700	1.251940	-0.621080
H	-3.079230	2.437010	-0.770910	H	-4.587820	-2.195720	0.376910	H	-0.527970	1.231930	-1.709110
H	-4.331730	2.353040	0.488640	H	-4.104110	-3.323700	1.661710	H	-1.735130	1.253970	-0.421190
C	-2.572050	2.909300	2.609700	C	-3.462450	-1.474380	3.571100	H	-0.253040	2.200410	-0.261740
H	-1.853200	2.584260	3.365370	H	-2.954310	-0.636010	4.052230	C	-1.350790	-0.029140	2.263100
H	-2.503600	4.000470	2.526250	H	-4.464590	-1.562110	4.007340	H	-1.210410	-0.017010	3.348750
H	-1.329940	-0.696870	2.714110	H	-0.919730	-0.828580	3.095630	H	-1.951540	0.846560	1.990780
H	-3.580660	2.664760	2.957570	H	-2.917130	-2.396410	3.799670	H	-1.920330	-0.928690	2.004900
O	-0.987740	2.646040	0.803490	O	-4.088700	0.049260	1.800140	H	1.331740	-1.163540	2.856730
H	-0.950890	3.608680	0.753930	H	-4.947100	0.131090	2.231800	O	1.366660	1.122900	3.208880
H	-3.172730	0.484700	1.987270	H	-1.819590	-2.324170	1.467840	H	1.756330	1.966080	3.461440

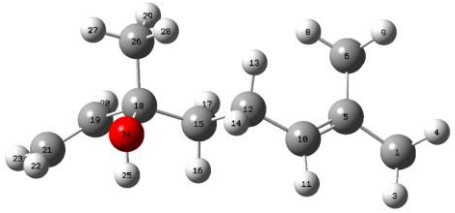
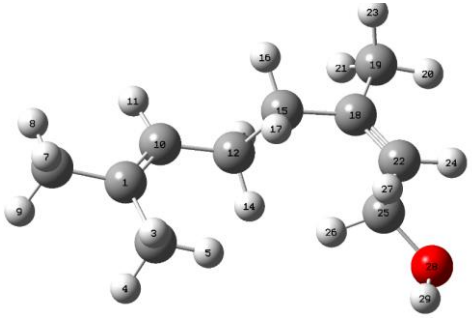
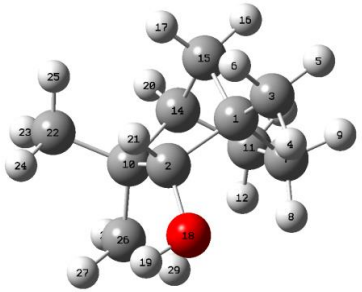
geraniol- conformer 1				geraniol- conformer 2				geraniol- conformer 3			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.033010	-0.018350	-0.000390	C	-0.150170	0.009210	-0.136530	C	-0.174750	0.276840	0.087780
H	-0.023930	-0.015820	1.096310	H	-0.130530	-0.000100	0.959970	H	0.558900	0.652050	0.811630
H	1.013880	-0.043310	-0.326110	H	0.892680	-0.036020	-0.472740	H	0.349850	-0.444750	-0.549780
H	-0.520270	-0.936170	-0.338290	H	-0.661750	-0.893520	-0.479020	H	-0.958200	-0.252460	0.635510
C	-0.727750	1.208600	-0.530590	C	-0.821810	1.257390	-0.646490	C	-0.735870	1.407030	-0.735080
C	-0.110170	2.512500	-0.096450	C	-0.167280	2.541950	-0.208770	C	0.293140	2.185170	-1.513140
H	0.938110	2.557350	-0.415560	H	0.876490	2.565950	-0.544480	H	0.857750	1.511070	-2.167990
H	-0.622190	3.386510	-0.503370	H	-0.665220	3.431890	-0.598350	H	-0.141820	2.969610	-2.134640
H	-0.110520	2.592350	0.997250	H	-0.148310	2.609910	0.885520	H	1.019600	2.647100	-0.833690
C	-1.800360	1.115060	-1.327290	C	-1.906520	1.197480	-1.429800	C	-2.048640	1.670580	-0.754720
H	-2.143910	0.115580	-1.595730	H	-2.277460	0.209330	-1.703700	H	-2.701810	1.021920	-0.169770
C	-2.556980	2.258590	-1.949040	C	-2.643780	2.365610	-2.028890	C	-2.735790	2.750970	-1.546600
H	-2.551700	3.131080	-1.286640	H	-2.612820	3.228180	-1.354420	H	-2.085120	3.622750	-1.676990
H	-3.607920	1.976340	-2.082290	H	-3.702000	2.107950	-2.154980	H	-3.611450	3.099280	-0.986190
C	-1.976870	2.648990	-3.323050	C	-2.068610	2.763220	-3.402760	C	-3.181500	2.255140	-2.936700
H	-1.955390	1.764520	-3.969700	H	-2.069910	1.887590	-4.061570	H	-3.853980	1.395730	-2.801530
H	-0.932420	2.959930	-3.174910	H	-1.017100	3.052030	-3.259720	H	-2.302650	1.888780	-3.479270
C	-2.745180	3.757110	-3.996390	C	-2.819310	3.896480	-4.054950	C	-3.877520	3.318250	-3.748320
C	-3.365940	3.567000	-5.164210	C	-3.447130	3.731920	-5.223360	C	-3.354720	3.766970	-4.893560

H	-3.317280	2.599520	-5.661370	H	-3.417470	2.766840	-5.726940	H	-2.416350	3.356790	-5.263650
C	-2.794810	5.074590	-3.261840	C	-2.841470	5.198630	-3.293120	C	-5.161870	3.863030	-3.174060
H	-3.542000	5.050740	-2.459120	H	-3.580380	5.167580	-2.483240	H	-5.754220	3.061640	-2.718530
H	-1.828160	5.294410	-2.794230	H	-1.866930	5.393960	-2.830860	H	-4.959470	4.599620	-2.387030
H	-3.047420	5.908380	-3.922040	H	-3.090980	6.050310	-3.930950	H	-5.779680	4.353000	-3.931110
C	-4.168230	4.603740	-5.901890	C	-4.242360	4.780640	-5.949450	C	-3.947150	4.836900	-5.768530
H	-5.000580	4.962830	-5.277500	H	-3.672930	5.719440	-6.018610	H	-3.945670	5.806000	-5.245710
O	-4.659310	3.996520	-7.086600	H	-5.175890	4.997930	-5.407020	H	-4.991830	4.596140	-6.017820
H	-5.176110	4.639160	-7.582270	O	-4.529100	4.275840	-7.245050	O	-3.157290	4.906140	-6.945700
H	-3.538050	5.473330	-6.146460	H	-5.054530	4.921520	-7.727670	H	-3.493400	5.605960	-7.514170

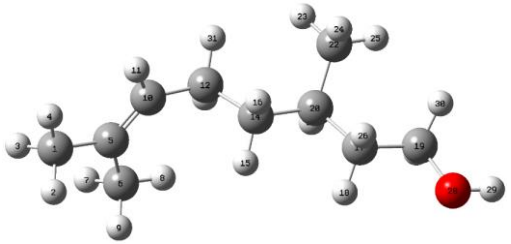
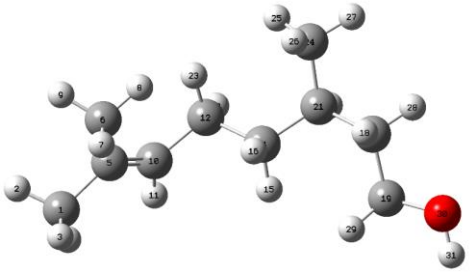
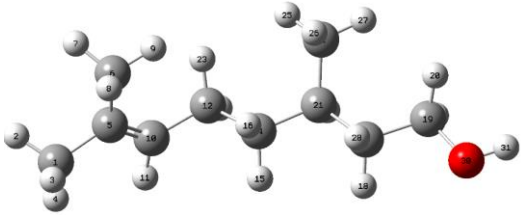
linalool- conformer 1	linalool- conformer 2	linalool- conformer 3
		

	X	Y	Z		X	Y	Z		X	Y	Z
C	-0.053980	0.118270	-0.185260	C	-0.040000	0.091390	-0.171180	C	-0.199400	0.148300	0.015550
H	0.716160	0.506000	0.492360	H	0.141010	0.216870	0.903170	H	0.848980	-0.018740	-0.243300
H	0.470150	-0.323200	-1.041610	H	0.942070	-0.010200	-0.648600	H	-0.794680	-0.666320	-0.414200
H	-0.598440	-0.675700	0.331680	H	-0.593130	-0.839110	-0.320110	H	-0.302110	0.075510	1.105090
C	-0.973680	1.223180	-0.634030	C	-0.784440	1.276680	-0.727500	C	-0.689280	1.483760	-0.479060
C	-0.291780	2.355790	-1.356930	C	-0.074900	2.596590	-0.570170	C	-2.129730	1.785500	-0.155840
H	0.191270	1.984800	-2.269350	H	0.897490	2.565290	-1.077130	H	-2.277520	1.801290	0.931080
H	-0.979600	3.156130	-1.637410	H	-0.643110	3.436340	-0.975500	H	-2.463810	2.743820	-0.558730
H	0.500300	2.788160	-0.734310	H	0.128290	2.800440	0.487980	H	-2.785320	1.001000	-0.551740
C	-2.292570	1.174920	-0.406440	C	-1.978990	1.141340	-1.317490	C	0.114510	2.324820	-1.142530
H	-2.685530	0.296260	0.105470	H	-2.391510	0.135410	-1.398590	H	1.147910	2.016500	-1.302180
C	-3.302800	2.207990	-0.836680	C	-2.795750	2.250650	-1.929970	C	-0.264210	3.691450	-1.654140
H	-2.890890	3.219800	-0.758080	H	-2.713750	3.173270	-1.345860	H	-1.295420	3.703050	-2.023040
H	-4.162550	2.168770	-0.159520	H	-3.852600	1.964430	-1.913910	H	0.374420	3.941520	-2.507950
C	-3.776400	1.980790	-2.279730	C	-2.367460	2.543680	-3.375540	C	-0.117480	4.770250	-0.571180
H	-4.371320	1.059910	-2.336100	H	-2.616780	1.694270	-4.023830	H	0.943850	4.915670	-0.331370
H	-2.899690	1.816070	-2.923210	H	-1.271960	2.641140	-3.404630	H	-0.592650	4.415510	0.355200
C	-4.582250	3.151460	-2.874280	C	-2.974430	3.829340	-3.969380	C	-0.753280	6.125330	-0.936040

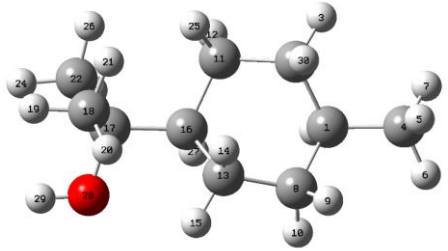
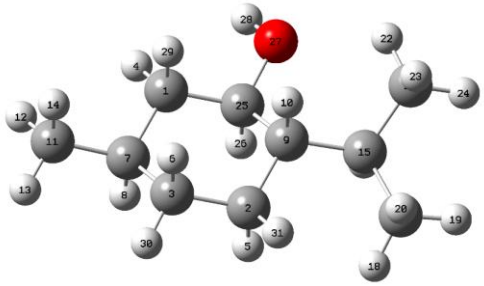
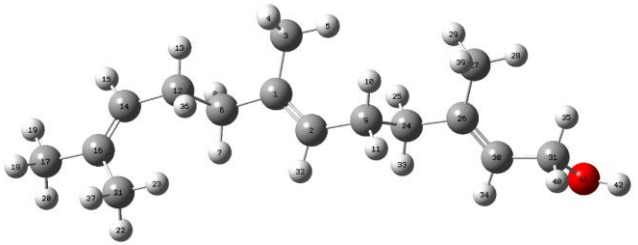
C	-5.061670	2.762650	-4.257020	C	-2.445100	3.993290	-5.378480	C	-0.459540	7.116730	0.170130
H	-5.586680	1.808760	-4.315430	H	-1.361050	4.123450	-5.434980	H	0.590300	7.199440	0.452880
C	-5.782150	3.524860	-2.004420	C	-4.494240	3.831330	-3.900630	C	-0.225550	6.669960	-2.262900
H	-6.443360	2.663180	-1.870820	H	-4.909160	2.940250	-4.381100	H	0.862770	6.779140	-2.228210
H	-5.443410	3.869300	-1.024350	H	-4.812320	3.847930	-2.856120	H	-0.489830	5.993080	-3.078920
H	-6.342860	4.330940	-2.483220	H	-4.891020	4.723840	-4.390590	H	-0.673570	7.646530	-2.460400
C	-4.892000	3.493190	-5.357060	C	-3.147800	3.967960	-6.507990	C	-1.371500	7.866770	0.785150
H	-4.397370	4.459680	-5.321290	H	-4.225350	3.833090	-6.513830	H	-2.419780	7.824520	0.503380
O	-3.769430	4.318950	-2.919090	O	-2.563010	4.956420	-3.184420	O	-2.154550	5.962020	-1.124310
H	-3.006190	4.135360	-3.482310	H	-1.612310	5.084280	-3.292100	H	-2.536010	5.641220	-0.296670
H	-5.262850	3.155200	-6.318920	H	-2.661030	4.080520	-7.471260	H	-1.091640	8.560040	1.571300

linalool- conformer 4				nerol				fenchol		
										
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.476360	-0.114150	-0.171800	C	-0.131060	-0.376980	-0.211480	C	0.000400	-0.003870	0.001790
H	0.569130	-0.342410	-0.411430	C	0.856080	-1.339400	-0.818580	C	-0.000120	0.002710	1.539720
H	-1.107980	-0.887910	-0.614880	H	0.933370	-1.167520	-1.899120	C	1.391260	-0.002410	-0.602670
H	-0.572320	-0.174000	0.919040	H	1.857020	-1.178940	-0.400820	H	1.935450	-0.905570	-0.308250
C	-0.850510	1.259710	-0.664720	H	0.585220	-2.384990	-0.661250	H	1.340870	0.028080	-1.696330
C	-0.022640	2.376020	-0.083050	C	0.226340	1.076120	-0.383660	H	1.965720	0.867190	-0.263230
H	1.041390	2.193090	-0.274100	H	0.311450	1.331600	-1.446790	C	-0.904630	-1.169050	-0.469210
H	-0.274100	3.355650	-0.492520	H	-0.521000	1.732150	0.069100	H	-0.678310	-2.085390	0.083220
H	-0.145160	2.417120	1.005900	H	1.198980	1.293540	0.073810	H	-0.730100	-1.369080	-1.531720
C	-1.841720	1.434000	-1.548440	C	-1.248880	-0.750670	0.424750	C	-1.473400	0.398440	1.929260
H	-2.350460	0.540190	-1.913050	H	-1.902580	0.038010	0.799060	C	-2.347550	-0.646920	-0.218590
C	-2.314950	2.732870	-2.143360	C	-1.737960	-2.159510	0.628700	H	-2.974860	-1.350960	0.332260
H	-2.087410	3.569680	-1.476510	H	-2.301560	-2.217330	1.566960	H	-2.854670	-0.436550	-1.165930
H	-3.404980	2.711250	-2.256620	H	-0.904240	-2.862690	0.731450	C	-2.101360	0.673520	0.531280
C	-1.684050	2.978750	-3.520040	C	-2.643470	-2.630320	-0.530250	C	-0.898900	1.216310	-0.264580
H	-1.759580	2.063070	-4.124990	H	-3.458830	-1.906480	-0.657300	H	-1.116930	1.350890	-1.329990
H	-0.610100	3.171670	-3.397190	H	-2.062490	-2.602070	-1.459350	H	-0.477820	2.148840	0.127370

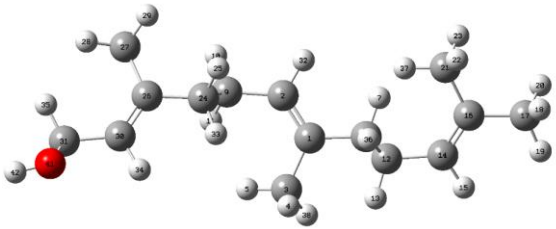
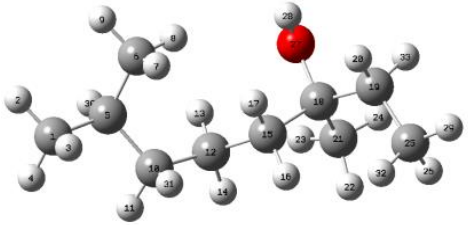
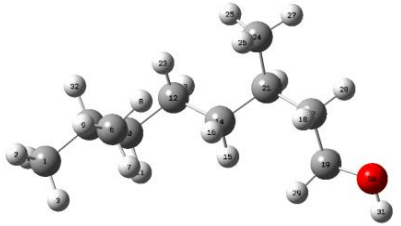
C	-2.324120	4.128110	-4.322400	C	-3.221750	-4.004230	-0.278020	O	0.454570	-1.248460	2.023050
C	-1.558440	4.301370	-5.617060	C	-4.486320	-4.042970	0.538040	H	0.582200	-1.197100	2.976060
H	-0.478950	4.407310	-5.505870	H	-4.790810	-5.068310	0.760300	H	-2.982050	1.322290	0.587610
C	-2.105230	4.335340	-6.830440	H	-4.355590	-3.510970	1.488050	H	0.689440	0.791680	1.883590
H	-3.180060	4.258140	-6.967910	C	-2.636930	-5.120960	-0.721740	C	-1.480160	1.678190	2.772940
H	-1.494440	4.460790	-7.718230	H	-5.305620	-3.546110	0.005200	H	-2.502980	1.947660	3.059480
O	-3.696370	3.845770	-4.566240	H	-3.074350	-6.094070	-0.503340	H	-0.900870	1.537110	3.693670
H	-3.754000	3.024030	-5.070770	C	-1.382820	-5.179140	-1.547640	H	-1.046200	2.527350	2.235640
C	-2.313560	5.443920	-3.544340	H	-0.669550	-4.407230	-1.224710	C	-2.186220	-0.703610	2.715440
H	-2.735860	6.237560	-4.165250	H	-1.616870	-4.994270	-2.608320	H	-1.800130	-0.758800	3.740340
H	-2.918250	5.351190	-2.638960	O	-0.825110	-6.474790	-1.385190	H	-3.258150	-0.484660	2.781510
H	-1.291450	5.718240	-3.265360	H	-0.055730	-6.561940	-1.956790	H	-2.055560	-1.689030	2.264070

citronellol- conformer 1				citronellol- conformer 2				citronellol- conformer 3			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.125120	0.077810	-0.005160	C	-0.353780	-0.038140	-0.031580	C	-0.140880	0.012010	-0.185740
H	-0.769390	-0.376050	0.757460	H	-0.161820	0.073280	1.042450	H	-0.173830	-0.008750	0.910390
H	0.776440	0.430400	0.510370	H	0.584350	-0.375380	-0.488330	H	0.911990	-0.093900	-0.473450
H	0.167520	-0.699290	-0.715410	H	-1.103780	-0.821200	-0.166740	H	-0.689180	-0.854950	-0.562100
C	-0.828740	1.221270	-0.688520	C	-0.800070	1.270050	-0.631500	C	-0.711830	1.303240	-0.711390
C	-1.249870	2.335660	0.233850	C	0.191410	2.394220	-0.479700	C	-0.006490	2.542110	-0.223750
H	-0.374870	2.784580	0.719280	H	1.156220	2.104620	-0.912610	H	-0.071750	2.618110	0.868370
H	-1.802860	3.126520	-0.275510	H	-0.128780	3.318460	-0.963160	H	1.059740	2.489280	-0.473960
H	-1.886960	1.940250	1.033810	H	0.372530	2.605440	0.581080	H	-0.406500	3.460770	-0.656350
C	-1.050210	1.214970	-2.009300	C	-1.985670	1.384460	-1.244170	C	-1.757190	1.313260	-1.548550
H	-0.721420	0.338950	-2.569660	H	-2.604200	0.487850	-1.310650	H	-2.165600	0.349190	-1.854830
C	-1.755300	2.277530	-2.810760	C	-2.551430	2.610910	-1.907630	C	-2.404580	2.524610	-2.166320
H	-1.612990	3.267010	-2.359520	H	-3.632580	2.657490	-1.718020	H	-3.480350	2.338900	-2.283220
C	-3.259820	1.997290	-2.941080	C	-2.316100	2.597360	-3.425210	C	-1.804580	2.852650	-3.541050
H	-3.674000	1.880560	-1.930840	H	-2.630140	1.618540	-3.810010	H	-1.815620	1.941050	-4.153380
H	-3.406770	1.030960	-3.445530	H	-1.234420	2.670350	-3.616510	H	-0.745340	3.119150	-3.410130
C	-5.553280	2.764280	-3.589170	C	-2.700900	3.682080	-5.686500	C	-1.935440	4.077490	-5.720900
H	-5.842380	2.670720	-2.535290	H	-1.640630	3.931960	-5.828720	H	-2.038200	3.112070	-6.231080

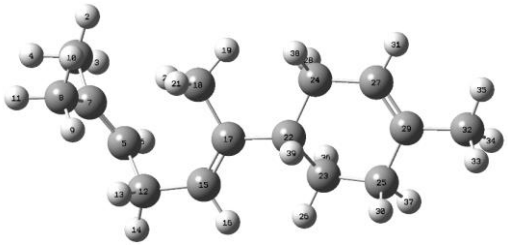
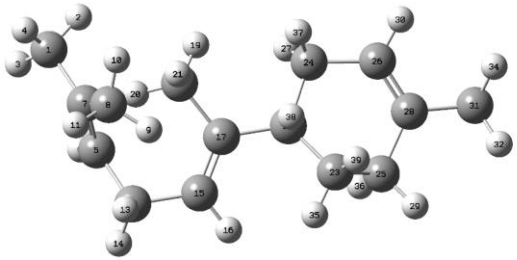
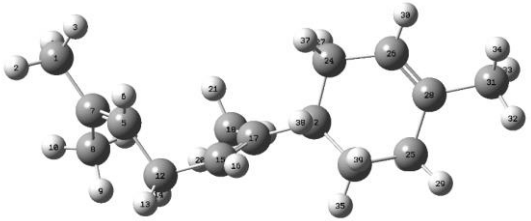
C	-6.454210	3.814980	-4.215110	C	-2.988700	2.358580	-6.374600	C	-2.597060	5.127790	-6.596500
C	-4.055830	3.078550	-3.683370	H	-4.011980	2.029650	-6.132830	H	-2.364720	6.137530	-6.232210
H	-3.878060	4.036570	-3.168660	C	-3.042570	3.710000	-4.192420	C	-2.517600	3.974070	-4.306640
C	-3.598870	3.225090	-5.137500	H	-4.125500	3.536300	-4.088890	H	-3.579850	3.696060	-4.396590
H	-2.532650	3.456550	-5.205780	H	-2.123770	3.518110	-1.472020	H	-2.312070	3.386530	-1.498780
H	-3.778810	2.292690	-5.687710	C	-2.726290	5.093870	-3.620170	C	-2.434000	5.308800	-3.560380
H	-4.134980	4.027260	-5.652930	H	-3.102790	5.212440	-2.600590	H	-2.841440	5.232350	-2.548720
H	-5.759890	1.794160	-4.061330	H	-1.641840	5.260710	-3.602470	H	-1.388800	5.634290	-3.481390
H	-6.177450	4.811730	-3.836450	H	-3.175340	5.879960	-4.235120	H	-2.993680	6.097140	-4.072420
O	-7.791730	3.496500	-3.860820	H	-3.279760	4.454600	-6.207280	H	-0.859600	4.292450	-5.664160
H	-8.391670	4.117470	-4.285940	H	-2.292650	1.582330	-6.029440	H	-3.690710	4.999130	-6.567680
H	-6.340450	3.823740	-5.307460	O	-2.844900	2.566100	-7.771850	O	-2.104410	4.953750	-7.916630
H	-1.298450	2.324360	-3.805210	H	-2.959220	1.729280	-8.233410	H	-2.467700	5.638890	-8.486580

hydrogenated terpinol				menthol				farnesol- conformer 1			
											
	X	Y	Z		X	Y	Z		X	Y	Z
C	0.339320	0.285950	0.011640	C	-0.023020	0.236550	-0.001050	C	0.022740	0.097620	-0.007770
C	-0.261580	-0.168450	1.343630	C	0.025960	-0.221280	2.874760	C	-0.019030	-0.282340	1.276250
H	0.442140	-0.811420	1.884640	C	1.318800	-0.153800	2.059670	C	1.291940	0.510220	-0.714230
C	0.930810	-0.877060	-0.779750	H	-0.178110	0.893950	-0.869130	H	1.377570	1.602050	-0.771530
H	0.166480	-1.642280	-0.961640	H	-0.209690	0.779810	3.267590	H	2.188760	0.130030	-0.220440
H	1.305720	-0.542790	-1.753110	H	1.598360	-1.168760	1.738440	C	-1.234730	0.157640	-0.839820
H	1.758930	-1.348580	-0.240650	C	1.171450	0.726610	0.818200	H	-2.082790	-0.233660	-0.266160
C	-0.737750	1.031400	-0.805940	H	0.956030	1.752570	1.155900	H	-1.123080	-0.487240	-1.723400
H	-1.249620	0.313310	-1.460340	C	-1.165280	-0.733870	2.048220	C	1.149560	-0.394490	2.216870
H	-0.251180	1.761170	-1.464170	H	-0.911230	-1.743080	1.682220	H	1.962520	0.269080	1.904740
C	-0.653990	1.036830	2.219620	C	2.449150	0.750710	-0.016720	H	0.846980	-0.065620	3.218990
H	0.200440	1.332650	2.839330	H	2.340280	1.397950	-0.893050	C	-1.576990	1.583440	-1.316630
C	-1.775000	1.738940	0.085240	H	3.298620	1.114630	0.570090	H	-0.740660	1.981640	-1.903010
H	-2.575700	1.034180	0.347050	H	2.693170	-0.257460	-0.371640	C	-2.822060	1.609810	-2.162400
H	-2.240540	2.570950	-0.451050	C	-2.493110	-0.832230	2.847190	H	-2.675250	1.426010	-3.227450
C	-1.113990	2.241870	1.371840	H	-3.012410	0.131610	2.734120	C	-4.078170	1.786760	-1.732840
C	-1.978250	3.250460	2.150900	C	-2.293760	-1.080090	4.346430	C	-5.243760	1.762530	-2.686790

C	-3.390620	2.734320	2.433930	H	-1.751940	-0.270650	4.843160	H	-5.796260	2.709020	-2.648520
H	-3.949530	3.473070	3.020750	H	-3.267330	-1.178810	4.837020	H	-4.919060	1.595650	-3.716690
H	-3.928720	2.562680	1.498450	H	-1.743750	-2.013630	4.518390	H	-5.952090	0.970770	-2.415020
H	-3.375720	1.802780	3.007820	C	-3.401850	-1.933960	2.288000	C	-4.454140	2.014560	-0.291860
C	-1.289310	3.666230	3.452020	H	-3.566000	-1.816060	1.217010	H	-5.151710	1.236900	0.041610
H	-0.272210	4.013850	3.245960	H	-2.943490	-2.915640	2.462880	H	-3.596010	2.006940	0.382260
H	-1.843350	4.485270	3.925200	H	-4.371400	-1.926880	2.797430	C	1.665460	-1.844200	2.314430
H	-1.449540	0.734300	2.912730	C	-1.309110	0.173200	0.820620	H	1.998360	-2.156050	1.313820
H	-1.243140	2.839180	4.166610	H	-1.544540	1.187880	1.191510	C	2.803330	-2.004380	3.292930
H	-0.224160	2.817470	1.075880	O	-2.389150	-0.292740	0.021620	C	4.045170	-1.213330	2.962860
O	-2.060430	4.387820	1.284520	H	-2.451310	0.259840	-0.765490	H	4.939830	-1.609530	3.446400
H	-2.629780	5.049840	1.694380	H	0.184490	-0.769580	-0.394100	H	4.216960	-1.214710	1.880490
H	-1.144030	-0.787940	1.129820	H	2.140020	0.216160	2.685560	C	2.664820	-2.783980	4.372190
H	1.153560	0.989460	0.240230	H	0.179620	-0.867700	3.743390	C	3.667550	-3.023880	5.457250
								H	-0.985670	-0.580440	1.685040
								H	0.836050	-2.503510	2.593600
								H	1.724180	-3.314830	4.517970
								H	4.658230	-2.643450	5.179650
								H	-1.677040	2.232450	-0.439620
								H	-4.973590	2.973600	-0.178090
								H	1.291130	0.135180	-1.743830
								H	3.937900	-0.165870	3.268250
								H	3.349520	-2.493210	6.368020
								O	3.714370	-4.424830	5.701670
								H	4.237400	-4.590250	6.492790

farnesol- conformer 2				hydrogenated linalool				hydrogenated citronellol			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.903340	-0.943630	-0.457280	**C**	-4.27442	-0.186468	0.527007	**C**	-4.369722	-1.003064	-0.035261
C	0.418150	-1.335770	0.728700	**H**	-5.013866	0.575972	0.261693	**H**	-5.14079	-0.822336	0.720375
C	2.301170	-0.410980	-0.646180	**H**	-4.13449	-0.153033	1.614341	**H**	-4.026168	-2.038433	0.07887
H	2.287660	0.675940	-0.792160	**H**	-4.691369	-1.16656	0.273028	**H**	-4.833676	-0.9106	-1.022696
H	2.948480	-0.619090	0.208560	**C**	-2.945108	0.055008	-0.188532	**C**	-3.197532	-0.033719	0.122781
C	0.044870	-0.985050	-1.697500	**C**	-2.393535	1.437941	0.161788	**C**	-2.585438	-0.162019	1.51852
H	-0.919020	-1.453220	-1.466950	**H**	-2.15943	1.499446	1.232344	**H**	-2.133287	-1.153108	1.650063
H	0.526710	-1.611010	-2.462390	**H**	-1.482924	1.664014	-0.402798	**H**	-1.810189	0.589855	1.696301
C	1.154860	-1.293280	2.042700	**H**	-3.128496	2.217293	-0.064614	**H**	-3.351359	-0.037642	2.290837
H	0.689220	-1.997240	2.741130	**C**	-1.954606	-1.074176	0.127404	**C**	-2.169945	-0.257673	-0.99515
H	2.194920	-1.620080	1.920270	**H**	-2.421009	-2.020534	-0.172206	**H**	-1.829497	-1.303686	-0.953817
C	-0.215240	0.410450	-2.300630	**C**	-0.580999	-0.930921	-0.552098	**C**	-0.951116	0.681855	-0.954213
H	0.738240	0.865190	-2.591610	**H**	-0.673497	-0.309283	-1.452429	**H**	-0.684062	0.98959	-1.973679
C	-1.118060	0.348400	-3.505030	**H**	-0.236848	-1.913937	-0.891855	**C**	0.289369	0.054486	-0.311173
H	-0.624060	0.269090	-4.473830	**C**	0.489056	-0.3294	0.364753	**H**	0.503653	-0.879893	-0.846653
C	-2.457270	0.338330	-3.488480	**H**	0.771126	-1.076275	1.117982	**H**	0.074122	-0.231394	0.728974
C	-3.259680	0.247210	-4.759920	**H**	0.06772	0.52024	0.921473	**C**	2.72944	0.256082	0.354735
H	-3.921990	1.115140	-4.863810	**C**	1.746593	0.167665	-0.36415	**H**	2.512884	0.111324	1.42206
H	-2.615550	0.198720	-5.641230	**C**	2.779478	0.726943	0.627686	**C**	3.118882	-1.081391	-0.251731

H	-3.901400	-0.642070	-4.751730	**H**	2.293697	1.522238	1.212568	**H**	3.216679	-0.978073	-1.344206
C	-3.281270	0.408030	-2.229230	**C**	2.356277	-0.914309	-1.249286	**C**	1.539781	0.944387	-0.324778
H	-3.944830	1.280850	-2.251650	**H**	2.520589	-1.83893	-0.688289	**H**	1.810387	1.130891	-1.376345
H	-3.925390	-0.476220	-2.151360	**H**	1.687774	-1.129407	-2.086238	**H**	-1.229198	1.601869	-0.424278
C	1.155810	0.119800	2.660290	**H**	3.312215	-0.571306	-1.656751	**C**	1.28317	2.296064	0.347359
H	0.113640	0.427640	2.826230	**C**	3.40768	-0.287516	1.582131	**H**	0.558583	2.899448	-0.205606
C	1.916510	0.195850	3.961730	**H**	3.934405	-1.075223	1.035499	**H**	0.896214	2.149783	1.36393
C	1.363820	-0.653470	5.079580	**O**	1.383121	1.216969	-1.269369	**H**	2.209469	2.874257	0.422645
H	1.693070	-0.320420	6.065470	**H**	1.098285	1.982868	-0.755113	**H**	3.60933	0.908379	0.298068
H	0.268500	-0.633340	5.063470	**H**	4.135218	0.203699	2.233866	**H**	2.349438	-1.838794	-0.050584
C	3.015640	0.953910	4.056810	**H**	-3.129255	0.03285	-1.272846	**O**	4.355889	-1.467022	0.328957
C	3.912650	1.113820	5.244480	**H**	-1.822195	-1.134101	1.218943	**H**	4.601958	-2.339848	0.00693
H	-0.614980	-1.682750	0.761750	**H**	2.660333	-0.762335	2.224244	**H**	-3.583073	0.991142	0.015065
H	1.583510	0.821190	1.935340	**H**	3.564548	1.207955	0.031892	**H**	-2.689867	-0.146588	-1.954442
H	3.331750	1.530140	3.187180								
H	3.455700	0.698490	6.150970								
H	-0.639650	1.054330	-1.521460								
H	-2.674270	0.461970	-1.323600								
H	2.761110	-0.846580	-1.540890								
H	1.665800	-1.701050	4.964510								
H	4.852680	0.569430	5.065150								
O	4.177910	2.502780	5.402900								
H	4.865030	2.618560	6.067240								

a-bisabolene- conformer 1				a-bisabolene- conformer 2				a-bisabolene- conformer 3			
											
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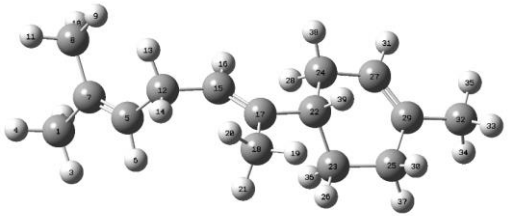
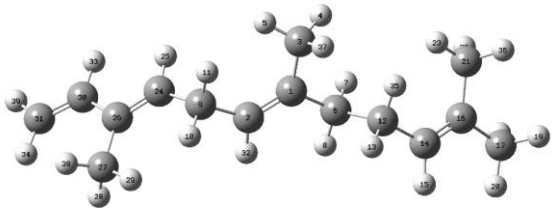
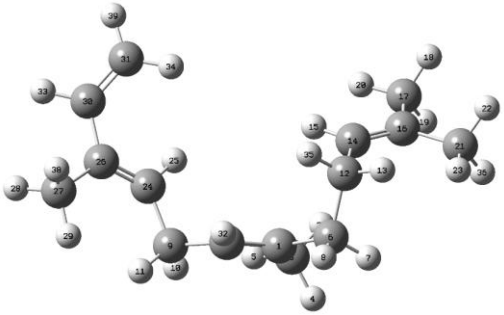
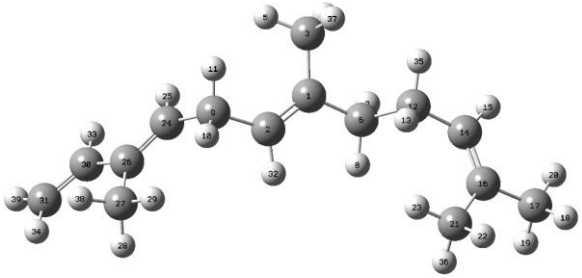
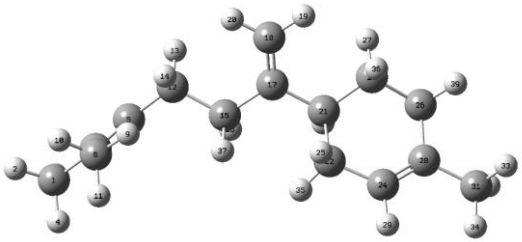
C	0.23392	0.0631	0.19026	C	1.33312	-1.70083	0.19882	C	-0.20983	0.09404	-0.35048
H	0.09579	0.08711	1.2784	H	1.27252	-0.94519	0.99173	H	-0.58879	0.50716	0.59206
H	1.29981	-0.05834	-0.01704	H	1.8093	-2.5932	0.61207	H	0.88122	0.06579	-0.29987
H	-0.08311	1.04118	-0.19107	H	1.98514	-1.29033	-0.58159	H	-0.50009	0.79503	-1.14276
C	0.0031	-2.02056	-1.12887	C	-0.53568	-3.24667	-0.30496	C	-0.0002	-2.34463	-0.7323
H	1.08825	-1.97818	-1.23428	H	0.08593	-4.02029	0.14896	H	1.07551	-2.18575	-0.64336
C	-0.58412	-1.04414	-0.4251	C	-0.03723	-2.00474	-0.35126	C	-0.79275	-1.27231	-0.60853
C	-2.06254	-0.9354	-0.15736	C	-0.74986	-0.80564	-0.92012	C	-2.2955	-1.28709	-0.7141
H	-2.65473	-1.69016	-0.67607	H	-1.72048	-1.04316	-1.35771	H	-2.71438	-2.28818	-0.82422
H	-2.26062	-1.02475	0.91849	H	-0.90204	-0.04972	-0.13925	H	-2.74139	-0.83367	0.17889
H	-2.43044	0.05003	-0.46595	H	-0.13775	-0.33631	-1.69924	H	-2.62139	-0.6839	-1.5712
C	-0.63565	-3.228	-1.76945	C	-1.89075	-3.72887	-0.76066	C	-0.39545	-3.76976	-1.02939
H	-1.7209	-3.21745	-1.62672	H	-2.48858	-2.90206	-1.15672	H	-0.10708	-4.40633	-0.18478
H	-0.46756	-3.19137	-2.852	H	-1.75928	-4.43465	-1.5893	H	-1.48222	-3.86012	-1.12553
C	-0.04628	-4.51479	-1.22543	C	-2.63063	-4.43292	0.36052	C	0.28379	-4.28364	-2.2825
H	0.63253	-5.05125	-1.88418	H	-2.70634	-5.51316	0.2707	H	1.0949	-4.99845	-2.14714
C	-0.26765	-4.98703	0.00847	C	-3.1412	-3.83225	1.44332	C	-0.01094	-3.89499	-3.5299
C	-1.17057	-4.27098	0.98548	C	-3.07741	-2.33392	1.61327	C	-1.09037	-2.8815	-3.82518

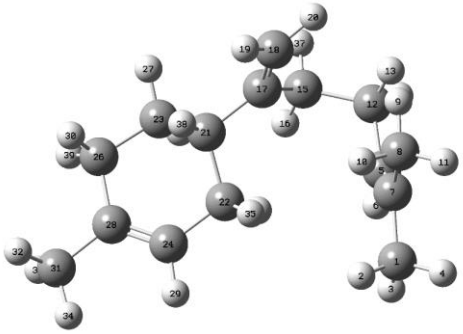
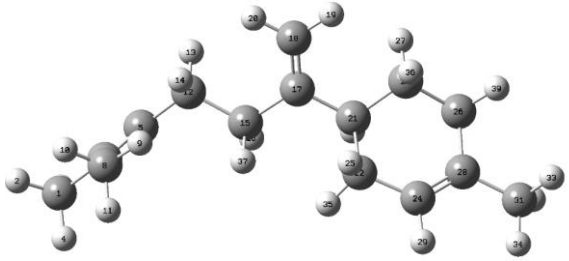
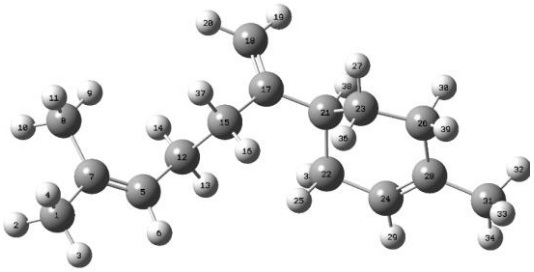
H	-0.61481	-3.51027	1.54826	H	-4.01781	-1.9489	2.02411	H	-1.53929	-3.05162	-4.8095
H	-1.9924	-3.75658	0.48083	H	-2.27433	-2.05215	2.30531	H	-1.88738	-2.9027	-3.07742
H	-1.60037	-4.97253	1.70793	H	-2.88452	-1.82245	0.6687	H	-0.67618	-1.86556	-3.82277
C	0.40773	-6.22809	0.55352	C	-3.87404	-4.59023	2.54488	C	0.75473	-4.438	-4.71636
C	1.1999	-7.05213	-0.45986	C	-3.67914	-6.11243	2.52432	C	-0.14527	-5.30096	-5.6456
C	1.33387	-5.85444	1.72545	C	-3.49874	-4.09673	3.95495	C	1.46061	-3.30732	-5.50213
C	1.67717	-8.36243	0.16755	C	-2.22936	-6.52609	2.80992	C	-0.0498	-4.92241	-7.13681
H	0.59027	-7.2602	-1.34592	C	-2.14411	-4.59871	4.38403	C	2.0961	-3.85092	-6.75415
C	2.14675	-7.02649	2.21046	H	-3.52461	-3.00436	4.01035	H	0.7217	-2.53777	-5.77233
H	1.99956	-5.0385	1.40452	C	-1.56	-5.68706	3.87131	C	1.3756	-4.64412	-7.55469
C	2.29739	-8.16854	1.53128	H	-2.2047	-7.57882	3.1229	H	-0.49164	-5.7138	-7.75197
H	0.83744	-9.06821	0.25609	H	-1.62416	-4.03796	5.15998	H	3.12777	-3.59971	-6.99219
H	2.62938	-6.9242	3.18213	C	-0.19464	-6.14834	4.30012	C	1.88469	-5.24683	-8.83137
C	3.0802	-9.33406	2.07003	H	-0.23575	-7.16358	4.71228	H	1.83293	-6.34147	-8.79292
H	2.45315	-10.233	2.11319	H	0.48786	-6.17996	3.44193	H	1.27133	-4.92927	-9.68307
H	3.92847	-9.56975	1.41656	H	0.23503	-5.48609	5.05597	H	2.92025	-4.95586	-9.02603
H	3.46259	-9.13438	3.07415	H	-4.01989	-6.54368	1.57725	H	-1.19152	-5.23743	-5.32588
H	2.07153	-6.47166	-0.79184	H	-1.61506	-6.47328	1.90138	H	-0.65157	-4.01868	-7.31681
H	2.40675	-8.85063	-0.49182	H	-4.26357	-4.44624	4.66309	H	2.19485	-2.82129	-4.85257
H	0.74488	-5.45315	2.55898	H	-4.94523	-4.37895	2.40312	H	1.55195	-5.08141	-4.32743
H	-0.3828	-6.87944	0.96266	H	-4.32486	-6.53361	3.3045	H	0.14408	-6.35029	-5.5306

a-bisabolene- conformer 4				a-farnesene- conformer 1				a-farnesene- conformer 2			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-1.1405	-0.01284	-1.80437	C	0.28159	-0.03476	0.1961	C	0.36036	0.89478	0.42428
H	-0.21468	0.48457	-2.11778	C	0.40859	-0.8912	1.21797	C	0.52977	0.32223	1.6229
H	-1.77254	-0.14945	-2.68506	C	1.27418	1.05354	-0.13238	C	1.44275	1.60212	-0.34922
H	-1.65093	0.67121	-1.11569	H	0.74616	1.96857	-0.42504	H	1.20992	2.67101	-0.43062
C	-1.317	-2.47657	-1.61141	H	1.92777	1.29896	0.70622	H	2.43117	1.50158	0.10236
H	-1.9159	-2.43017	-2.52224	C	-0.90134	-0.12702	-0.73738	C	-0.99068	0.82077	-0.26136
C	-0.83717	-1.32441	-1.12584	H	-1.45385	0.82392	-0.72996	H	-1.08174	1.64001	-0.98613
C	0.02826	-1.19634	0.10063	H	-1.59504	-0.89848	-0.38452	H	-1.79065	0.94858	0.47668
H	0.26103	-2.15335	0.56879	C	1.51689	-0.95034	2.24123	C	1.81079	0.20404	2.41333
H	0.97483	-0.70627	-0.15663	H	1.91762	-1.96778	2.27801	H	2.5306	0.96468	2.0937
H	-0.46248	-0.56134	0.84789	H	2.34811	-0.30174	1.9465	H	1.60367	0.39293	3.47015
C	-1.09836	-3.87291	-1.08335	C	-0.50366	-0.43523	-2.19486	C	-1.21221	-0.51948	-0.99759
H	-0.62677	-3.84312	-0.09588	H	0.09872	-1.35147	-2.20494	H	-2.19943	-0.5057	-1.47063
H	-2.07126	-4.35752	-0.95365	C	-1.71049	-0.6149	-3.07673	C	-0.13563	-0.83144	-2.00168
C	-0.23077	-4.66249	-2.03309	H	-2.1242	-1.62317	-3.11583	H	0.77542	-1.268	-1.58862
H	0.788	-4.2887	-2.11386	C	-2.34627	0.34173	-3.76539	C	-0.16385	-0.59652	-3.32007
C	-0.60789	-5.70181	-2.78925	C	-3.57036	0.0351	-4.58795	C	1.01067	-0.94072	-4.19915

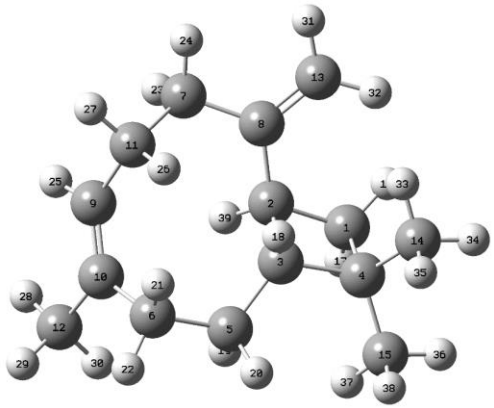
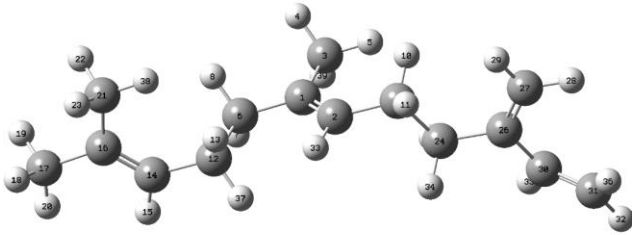
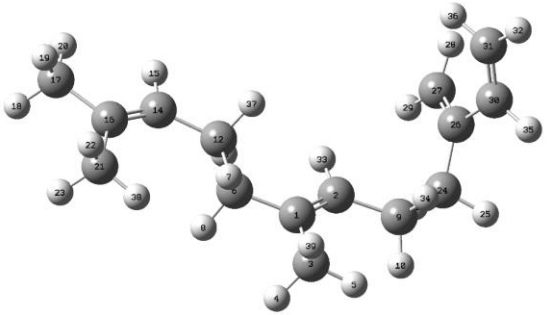
C	-2.00801	-6.2787	-2.74316	H	-4.43041	0.61836	-4.23739	H	0.71491	-1.64331	-4.9876
H	-2.00711	-7.31778	-3.08758	H	-3.40989	0.30693	-5.63821	H	1.39503	-0.04455	-4.70172
H	-2.42557	-6.26671	-1.73423	H	-3.8327	-1.02461	-4.54336	H	1.8257	-1.39019	-3.62646
H	-2.6956	-5.72361	-3.39212	C	-1.92592	1.78843	-3.78594	C	-1.32334	0.03211	-4.04789
C	0.32122	-6.39277	-3.769	H	-2.74215	2.42227	-3.41899	H	-1.69912	-0.64243	-4.8266
C	-0.19602	-6.27946	-5.21293	H	-1.04488	1.987	-3.17292	H	-2.15357	0.29182	-3.38956
C	1.77599	-5.92655	-3.73922	C	1.0098	-0.52267	3.59231	C	2.40826	-1.16464	2.21227
C	0.58203	-7.21032	-6.14369	H	0.73869	0.53237	3.6561	H	2.73059	-1.36779	1.19036
H	-1.26509	-6.50984	-5.26881	C	0.81239	-1.27741	4.68884	C	2.55165	-2.15053	3.11244
C	2.59361	-6.57288	-4.82885	C	1.10055	-2.75258	4.77652	C	2.21466	-2.04589	4.57885
H	1.81866	-4.83444	-3.85981	H	0.19028	-3.30245	5.03958	H	3.09779	-2.27788	5.18536
C	2.07386	-7.16117	-5.91187	H	1.48165	-3.16107	3.84084	H	1.861	-1.0553	4.86602
H	0.23843	-8.24766	-6.01038	C	0.27492	-0.62767	5.89532	C	3.09514	-3.46466	2.69968
H	3.67663	-6.54851	-4.71311	C	0.02492	-1.23194	7.06252	C	2.79543	-4.09953	1.56326
C	2.92524	-7.81903	-6.96263	H	-0.38401	-1.62553	1.36759	H	-0.3319	-0.17452	2.07341
H	2.63416	-8.86817	-7.09603	H	0.07272	0.43879	5.80157	H	3.76878	-3.94651	3.41029
H	2.79485	-7.32757	-7.93416	H	0.20579	-2.29154	7.21614	H	2.08463	-3.68193	0.85471
H	3.98562	-7.78836	-6.69983	H	0.13963	0.36359	-2.57891	H	-1.23377	-1.31725	-0.24547
H	-0.0743	-5.23678	-5.53691	H	-1.71197	2.11166	-4.81171	H	-0.99627	0.94783	-4.55518
H	0.37181	-6.96066	-7.19215	H	1.9083	0.76594	-0.97933	H	1.48993	1.21025	-1.37151
H	2.22146	-6.14488	-2.76091	H	1.8378	-2.95292	5.5618	H	1.44326	-2.77638	4.84663
H	0.31472	-7.46542	-3.51048	H	-0.37278	-0.67551	7.90419	H	3.24352	-5.0567	1.31718

a-farnesene- conformer 3				a-farnesene- conformer 4				b-bisabolene- conformer 1			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.30096	-0.26009	-0.46724	C	0.05785	1.26798	-0.02908	C	0.31317	-0.12173	0.03348
C	0.73088	0.06415	0.75944	C	0.56697	0.33567	0.7872	H	0.33221	-0.11593	1.13004
C	1.2004	-0.70577	-1.59395	C	0.59832	2.67074	-0.16049	H	1.33313	-0.27594	-0.32684
H	1.36901	0.10795	-2.30918	H	-0.22778	3.38705	-0.23438	H	-0.01878	0.87409	-0.28353
H	2.17502	-1.05225	-1.24648	H	1.22182	2.96561	0.68505	C	-0.19144	-2.16563	-1.2794
C	-1.16721	-0.17195	-0.80922	C	-1.12112	0.94447	-0.91543	H	0.86077	-2.14972	-1.56753
H	-1.74248	0.09862	0.0835	H	-1.95229	1.62748	-0.6884	C	-0.62452	-1.18551	-0.47603
H	-1.53047	-1.15724	-1.13497	H	-1.47832	-0.07011	-0.70532	C	-2.04781	-1.03807	-0.00452
C	2.14923	0.03959	1.2757	C	1.73425	0.47718	1.73391	H	-2.72355	-1.77706	-0.43763
H	2.85731	-0.07809	0.44915	H	2.43775	-0.34308	1.56258	H	-2.10019	-1.12215	1.08773
H	2.37861	1.00211	1.74265	H	2.28411	1.40176	1.53097	H	-2.42727	-0.04229	-0.26247
C	-1.46901	0.85217	-1.92189	C	-0.79613	1.05358	-2.41886	C	-1.00527	-3.2832	-1.8737
H	-0.94405	0.56124	-2.83874	H	0.06837	0.41627	-2.63775	H	-0.40873	-4.20361	-1.87029
C	-2.94357	0.95421	-2.2126	C	-1.97454	0.68312	-3.28107	H	-1.89256	-3.4859	-1.26578
H	-3.3266	0.29751	-2.99423	H	-2.63408	1.50122	-3.57198	C	-1.42729	-2.96753	-3.31281
C	-3.82243	1.73882	-1.57573	C	-2.30392	-0.55167	-3.68161	H	-0.53914	-2.67428	-3.89179
C	-5.28425	1.73984	-1.93874	C	-3.52458	-0.8058	-4.52664	C	-2.14031	-4.07374	-4.06071
H	-5.60762	2.74304	-2.24188	H	-3.24734	-1.28325	-5.47431	C	-2.54701	-5.19866	-3.46443

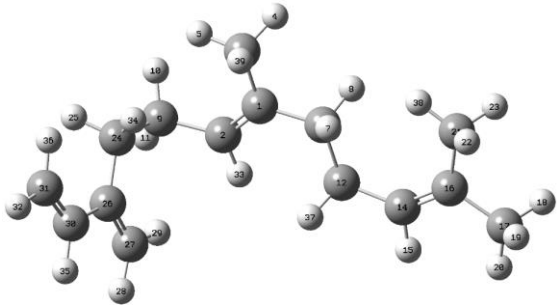
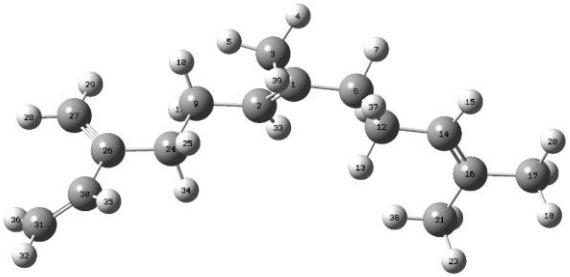
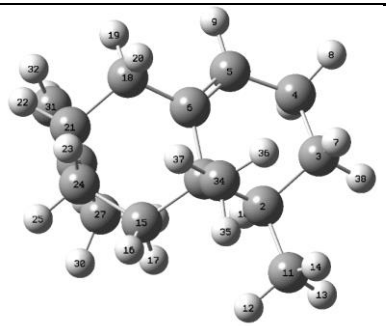
H	-5.49779	1.04757	-2.75681	H	-4.21436	-1.48904	-4.01684	H	-3.06054	-5.98322	-4.0095
H	-5.89867	1.45541	-1.07612	H	-4.06013	0.11981	-4.75138	H	-2.38013	-5.37716	-2.40743
C	-3.45369	2.67346	-0.45315	C	-1.51382	-1.78605	-3.33266	C	-2.36539	-3.79675	-5.53532
H	-4.0326	2.42825	0.44536	H	-1.15763	-2.28515	-4.24195	C	-3.31137	-2.59718	-5.73521
H	-2.39466	2.6311	-0.19192	H	-0.65206	-1.57642	-2.69628	C	-2.88925	-4.98358	-6.34372
C	2.33572	-1.09096	2.2518	C	1.25703	0.48841	3.16146	C	-3.70655	-2.40827	-7.17662
H	2.27806	-2.08439	1.80419	H	0.68187	1.37422	3.43549	H	-4.20774	-2.74156	-5.11302
C	2.51415	-1.02468	3.584	C	1.41169	-0.46133	4.10222	C	-2.89251	-4.65985	-7.83711
C	2.58548	0.25382	4.37568	C	2.14427	-1.76014	3.89524	H	-2.28076	-5.87419	-6.1536
H	3.54766	0.33153	4.8937	H	1.47656	-2.60685	4.08855	C	-3.50791	-3.31422	-8.1399
H	2.4632	1.13873	3.75145	H	2.53384	-1.86293	2.88265	H	-4.17346	-1.45837	-7.43553
C	2.64841	-2.28449	4.33339	C	0.82602	-0.22766	5.43231	H	-1.86545	-4.67995	-8.23173
C	2.8347	-2.39221	5.65401	C	0.89358	-1.06468	6.47403	C	-3.8725	-3.06155	-9.5766
H	-0.01593	0.35258	1.50054	H	0.07846	-0.63944	0.81312	H	-2.99474	-3.17807	-10.224
H	2.58914	-3.19331	3.73547	H	0.29883	0.71825	5.55192	H	-4.6203	-3.78496	-9.92236
H	2.90164	-1.52332	6.30195	H	1.40447	-2.02117	6.4159	H	-4.27304	-2.05498	-9.72059
H	-1.05759	1.82375	-1.62488	H	-0.49122	2.07967	-2.65343	H	-2.83572	-1.67748	-5.37496
H	-3.70275	3.70858	-0.71634	H	-2.1535	-2.50561	-2.80766	H	-3.91441	-5.21383	-6.02264
H	0.73066	-1.52597	-2.14859	H	1.19704	2.77866	-1.07265	H	-2.06605	-2.07338	-3.29488
H	1.80276	0.26933	5.14197	H	2.98366	-1.84327	4.5943	H	-1.3904	-3.51179	-5.96452
H	2.92465	-3.36433	6.12625	H	0.43267	-0.81163	7.42253	H	-3.43814	-5.43653	-8.38878

b-bisabolene- conformer 2				b-bisabolene- conformer 3				b-bisabolene- conformer 4			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.10634	-0.06691	-0.44192	C	0.42977	-0.45883	-0.17723	C	-0.27825	0.27847	-0.18441
H	0.10731	-0.05484	0.6345	H	-0.00278	0.01672	0.71136	H	-0.22387	0.29898	0.91076
H	0.83735	0.05343	-0.98003	H	1.3471	-0.97249	0.12041	H	0.72413	0.45453	-0.58215
H	-0.73691	0.80598	-0.64881	H	0.69457	0.34742	-0.87164	H	-0.92132	1.11414	-0.48554
C	-0.26793	-2.18324	-1.71634	C	-0.27464	-2.70444	-0.96261	C	-0.15432	-1.83403	-1.48327
H	0.69575	-1.89963	-2.14508	H	0.7086	-3.04511	-0.63458	H	0.82938	-1.49278	-1.80908
C	-0.8101	-1.34324	-0.82551	C	-0.55895	-1.40488	-0.80803	C	-0.84644	-1.03194	-0.66379
C	-2.11277	-1.57171	-0.10618	C	-1.85375	-0.76088	-1.23063	C	-2.22958	-1.33718	-0.15064
H	-2.62564	-2.47868	-0.42635	H	-2.52795	-1.447	-1.7454	H	-2.62704	-2.28161	-0.52598
H	-1.93361	-1.65741	0.97279	H	-2.37938	-0.35021	-0.36006	H	-2.23321	-1.37403	0.94532
H	-2.78364	-0.71695	-0.254	H	-1.65197	0.08129	-1.90304	H	-2.92308	-0.53924	-0.44157
C	-0.78492	-3.52055	-2.16757	C	-1.14938	-3.76131	-1.58094	C	-0.6112	-3.14937	-2.053
H	-1.84819	-3.63516	-1.93898	H	-1.03883	-4.69514	-1.01634	H	0.24574	-3.82705	-2.14191
H	-0.68976	-3.59263	-3.25792	H	-2.20547	-3.4816	-1.51488	H	-1.32346	-3.64845	-1.38861
C	0.00438	-4.68557	-1.53423	C	-0.77399	-4.01596	-3.04484	C	-1.27355	-2.97985	-3.43761
H	1.06994	-4.54227	-1.74874	H	0.30778	-4.20411	-3.11109	H	-0.58689	-2.4368	-4.09855

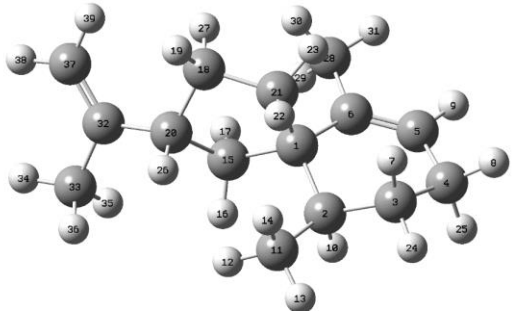
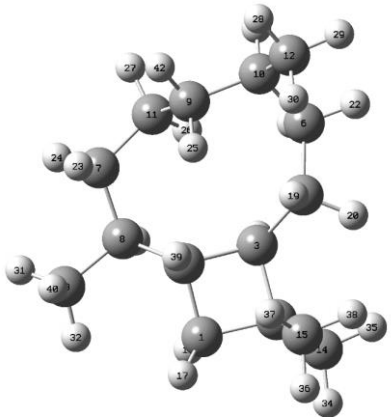
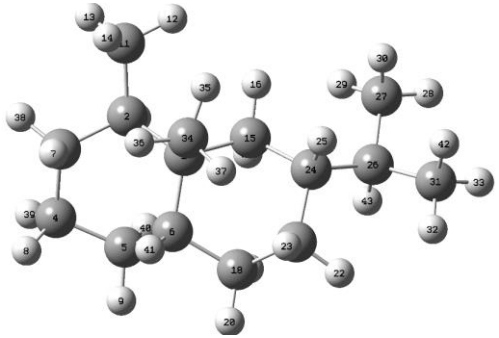
C	-0.21473	-4.82658	-0.03544	C	-1.49877	-5.1514	-3.73543	C	-1.68025	-4.30381	-4.05199
C	-1.43723	-5.03716	0.46029	C	-2.53343	-5.78829	-3.17845	C	-2.79419	-4.92195	-3.64834
H	-1.60266	-5.14671	1.52854	H	-3.04786	-6.59821	-3.68418	H	-3.08777	-5.88803	-4.0499
H	-2.31262	-5.11	-0.18149	H	-2.90415	-5.52334	-2.19391	H	-3.44973	-4.47692	-2.90272
C	0.98824	-4.76857	0.88011	C	-0.96388	-5.49827	-5.11218	C	-0.8016	-4.90378	-5.12719
C	1.70088	-3.40969	0.84482	C	-1.16517	-4.32899	-6.09507	C	0.66729	-5.04072	-4.70241
C	2.00332	-5.88146	0.57831	C	-1.54233	-6.77173	-5.7288	C	-0.86661	-4.10348	-6.43835
C	3.00108	-3.43476	1.60555	C	-0.81846	-4.70135	-7.51305	C	1.54949	-5.46479	-5.84876
H	1.88536	-3.10398	-0.19508	H	-2.21082	-3.99018	-6.03781	H	1.03277	-4.08367	-4.30113
C	3.08794	-5.92126	1.65471	C	-0.79972	-7.13431	-7.01415	C	-0.15116	-4.85661	-7.56008
H	1.4935	-6.84918	0.51371	H	-1.4866	-7.6013	-5.01585	H	-1.91043	-3.91368	-6.71056
C	3.63026	-4.55099	1.99019	C	-0.6295	-5.95404	-7.94103	C	1.19303	-5.40127	-7.13634
H	3.44195	-2.47059	1.85781	H	-0.70624	-3.88064	-8.22099	H	2.53661	-5.84963	-5.59433
H	2.69095	-6.38048	2.57255	H	0.19204	-7.54715	-6.77552	H	-0.77647	-5.69093	-7.9118
C	4.90749	-4.52709	2.78363	C	-0.23379	-6.27529	-9.35562	C	2.09114	-5.86932	-8.24798
H	4.7894	-5.0814	3.72276	H	0.70081	-6.84917	-9.37433	H	1.59383	-6.64222	-8.84664
H	5.72046	-5.01103	2.22949	H	-0.99625	-6.89429	-9.84304	H	2.32936	-5.04419	-8.92956
H	5.21369	-3.50605	3.02467	H	-0.0916	-5.36978	-9.95075	H	3.02772	-6.28187	-7.86478
H	1.03645	-2.64009	1.25824	H	-0.55079	-3.47258	-5.79349	H	0.74834	-5.7653	-3.88251
H	2.47071	-5.69409	-0.39755	H	-2.60427	-6.61013	-5.95948	H	-0.38549	-3.12711	-6.29243
H	-0.28421	-5.62219	-2.02666	H	-0.93847	-3.08663	-3.608	H	-2.15566	-2.3407	-3.31501
H	0.62879	-4.92547	1.90738	H	0.12384	-5.64783	-5.00956	H	-1.18233	-5.91279	-5.34243
H	3.916	-6.56689	1.3336	H	-1.33445	-7.93313	-7.54447	H	-0.01467	-4.20009	-8.42936

b-caryophyllene				b-farnesene- conformer 1				b-farnesene- conformer 2			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.17405	-0.46202	0.05482	C	-0.04064	0.02024	0.11505	C	0.00401	0.01633	-0.07043
C	-0.02227	-0.40942	1.59525	C	0.03925	-0.04507	1.45066	C	-0.05924	-0.23654	1.24331
C	1.53191	-0.2239	1.4039	C	1.16463	0.10948	-0.78736	C	1.29321	0.297	-0.80158
C	1.30674	-0.05062	-0.13825	H	1.11434	1.01213	-1.40763	H	1.20966	1.22339	-1.38198
C	2.43363	-1.3819	1.82038	H	2.10962	0.12273	-0.24173	H	2.15346	0.38967	-0.13649
C	2.73795	-1.44659	3.32798	C	-1.35334	0.00975	-0.63546	C	-1.20958	0.03716	-0.97722
C	-0.88656	0.52739	3.84479	H	-1.33722	-0.82222	-1.35499	H	-1.01836	-0.66056	-1.80444
C	-0.73529	0.69255	2.34639	H	-1.40706	0.91811	-1.25408	H	-1.26604	1.03609	-1.43142
C	0.61875	-1.33262	4.68506	C	1.30764	-0.05664	2.26666	C	1.12017	-0.29777	2.18527
C	1.6107	-2.04424	4.13902	H	2.07353	0.58215	1.81335	H	1.82542	0.50914	1.95997
C	0.39706	0.15252	4.62111	H	1.09958	0.36463	3.25689	H	0.78224	-0.12226	3.21279
C	1.64916	-3.54617	4.25856	C	-2.63296	-0.0834	0.20209	C	-2.5372	-0.30637	-0.3142
C	-1.2538	1.77549	1.75623	H	-2.67951	0.76573	0.8927	H	-2.71721	0.408	0.50167
C	1.48125	1.40287	-0.57277	C	-3.86138	-0.1371	-0.66825	C	-3.80084	-0.36354	-1.13818
C	2.09475	-0.9585	-1.07686	H	-4.16561	-1.13098	-0.99848	H	-4.65324	-0.65558	-0.52176

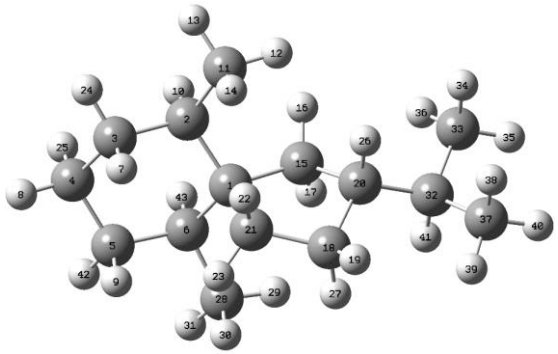
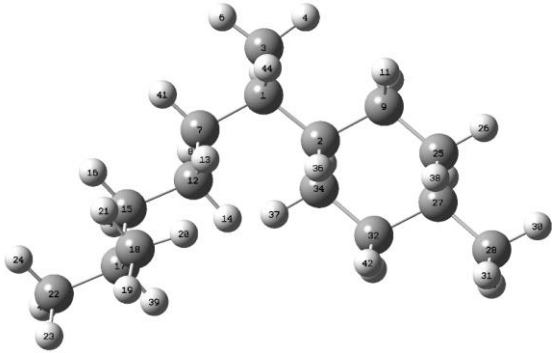
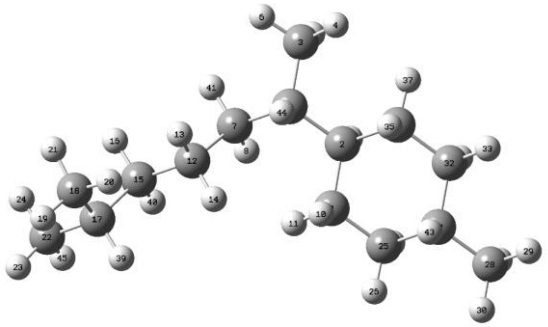
H	-0.92107	0.1991	-0.39372	C	-4.58011	0.90616	-1.10221	C	-4.09224	-0.14095	-2.42779
H	-0.37067	-1.48038	-0.29629	C	-5.78217	0.71684	-1.99039	C	-5.516	-0.3115	-2.90573
H	1.90685	0.70035	1.86469	H	-6.68124	1.13068	-1.51812	H	-5.89689	0.62542	-3.32988
H	1.99569	-2.33638	1.49513	H	-5.65031	1.24701	-2.94112	H	-5.56845	-1.06339	-3.70268
H	3.38438	-1.28122	1.28138	H	-5.96295	-0.33885	-2.20677	H	-6.18533	-0.62	-2.09941
H	2.99495	-0.44277	3.68353	C	-4.27176	2.34193	-0.76507	C	-3.16224	0.27393	-3.54093
H	3.6313	-2.06551	3.47772	H	-4.10962	2.91712	-1.68444	H	-3.15847	-0.4934	-4.32476
H	-1.6384	-0.25355	4.03151	H	-5.12047	2.80576	-0.24829	H	-3.53589	1.19344	-4.00741
H	-1.29866	1.4568	4.25034	C	1.86221	-1.47418	2.43105	C	1.88224	-1.6276	2.1223
H	-0.15726	-1.88052	5.22419	H	2.06169	-1.89474	1.43434	H	2.8259	-1.53602	2.67987
H	1.25723	0.67346	4.18923	C	3.11899	-1.60481	3.26133	C	1.15887	-2.84647	2.65201
H	0.28673	0.52711	5.64642	C	3.74708	-0.57147	3.83585	C	-0.02363	-2.81245	3.2777
H	0.77555	-3.93418	4.78806	H	4.67717	-0.71854	4.37612	H	-0.45554	-3.71588	3.69684
H	2.55045	-3.8683	4.79361	H	3.3655	0.44215	3.77463	H	-0.58354	-1.8923	3.40454
H	1.68552	-4.01492	3.26716	C	3.63657	-2.98662	3.38517	C	1.89124	-4.11997	2.46459
H	-1.73636	2.55044	2.34517	C	4.18081	-3.5031	4.48951	C	1.3252	-5.29185	2.16712
H	-1.23224	1.92822	0.6828	H	4.54922	-4.52341	4.51244	H	1.91925	-6.19224	2.05038
H	0.94568	2.08822	0.08994	H	-0.88301	-0.13295	2.02197	H	-1.03202	-0.44462	1.68093
H	1.10993	1.54946	-1.59419	H	1.08624	-2.1204	2.86481	H	2.16778	-1.82431	1.07942
H	2.54202	1.68032	-0.55269	H	3.52315	-3.62084	2.50499	H	2.97753	-4.06266	2.54792
H	1.71106	-0.84555	-2.09773	H	4.26108	-2.92058	5.40343	H	0.25181	-5.37717	2.02088
H	2.00313	-2.01433	-0.80453	H	-2.5949	-0.98693	0.82152	H	-2.43385	-1.28308	0.17909
H	3.15989	-0.70033	-1.09149	H	-3.38585	2.45436	-0.13788	H	-2.13582	0.44673	-3.23211
H	-0.25742	-1.36457	2.07649	H	1.1847	-0.74492	-1.4744	H	1.50738	-0.50688	-1.51647

b-farnesene- conformer 3				b-farnesene- conformer 4				valencene			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.02565	-0.03098	-0.06173	C	0.2853	1.25432	-0.22715	C	0.06316	0.20606	-0.13043
C	-0.03967	-0.19282	1.26628	C	-0.24868	1.23268	1.00173	C	-0.03996	-0.03571	1.39972
C	1.32213	0.14144	-0.81369	C	1.77061	1.27804	-0.48586	C	1.31584	-0.3784	2.01681
H	1.26328	1.006	-1.48508	H	2.01328	2.00176	-1.27262	C	1.85091	-1.68119	1.4318
H	2.18294	0.27961	-0.15698	H	2.34779	1.53533	0.405	C	1.72695	-1.68621	-0.06738
C	-1.1912	-0.01568	-0.96379	C	-0.5946	1.22778	-1.45262	C	0.97096	-0.8377	-0.77284
H	-1.02319	-0.75238	-1.76182	H	-0.3809	2.10481	-2.08058	H	2.02677	0.4356	1.82103
H	-1.22258	0.96462	-1.459	H	-1.6471	1.30063	-1.15509	H	2.89958	-1.83087	1.71458
C	1.14423	-0.24491	2.20341	C	0.51464	1.21578	2.30183	H	2.30827	-2.43279	-0.60917
H	1.87484	0.52359	1.92904	H	1.36901	1.90201	2.25843	H	-0.67316	-0.92798	1.52434
H	0.82244	-0.0004	3.22179	H	-0.13388	1.57849	3.10677	C	-0.7072	1.12	2.14689
C	-2.52457	-0.29688	-0.28284	C	-0.41104	-0.04236	-2.30774	H	-1.63414	1.44605	1.66304
H	-2.69066	0.46197	0.49508	H	-0.57777	-0.91956	-1.67195	H	-0.95166	0.81783	3.1699
C	-3.78971	-0.37478	-1.10301	C	-1.32787	-0.05487	-3.50243	H	-0.03925	1.98576	2.21125
H	-4.64344	-0.64369	-0.47801	H	-0.93589	0.40251	-4.41149	C	-1.37015	0.11299	-0.75638
C	-4.08044	-0.19001	-2.39863	C	-2.58046	-0.52762	-3.53673	H	-1.66557	1.10829	-1.11115
C	-5.50534	-0.36675	-2.87135	C	-3.41317	-0.45823	-4.78998	H	-2.09519	-0.15234	0.02005

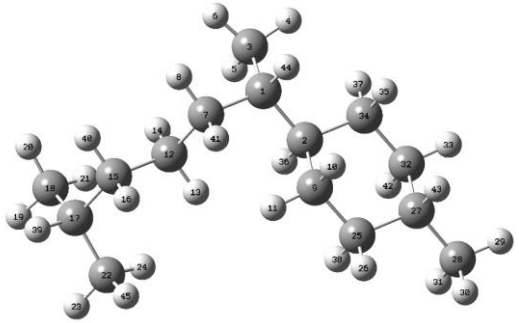
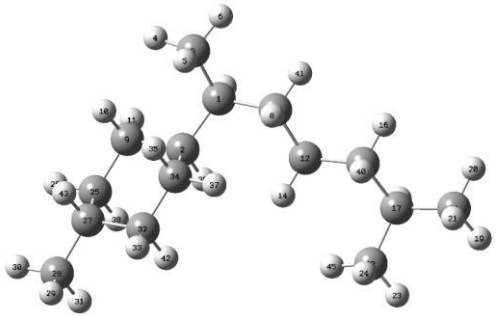
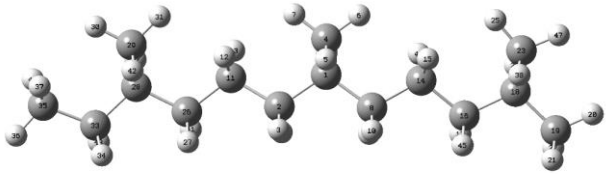
H	-5.88272	0.56095	-3.3186	H	-3.72094	-1.46192	-5.10707	C	1.00303	-0.85555	-2.28866
H	-5.56113	-1.1381	-3.64907	H	-4.33176	0.11449	-4.61456	H	1.37137	-1.83443	-2.60915
H	-6.17497	-0.6524	-2.05687	H	-2.86758	0.00992	-5.61284	H	1.73815	-0.12149	-2.64354
C	-3.14944	0.19012	-3.52323	C	-3.27608	-1.15412	-2.35629	C	-0.3678	-0.54878	-2.92873
H	-3.16667	-0.58814	-4.29596	H	-4.1855	-0.59128	-2.11378	H	-0.4856	-1.09939	-3.86744
H	-3.5075	1.11022	-4.00116	H	-3.5923	-2.17655	-2.59517	H	-0.43099	0.51429	-3.19151
C	1.86444	-1.6004	2.20508	C	1.0168	-0.18785	2.65174	C	-1.51126	-0.84776	-1.95722
H	2.81373	-1.50963	2.75106	H	1.6544	-0.55053	1.83222	H	-2.46228	-0.58267	-2.44472
C	1.10157	-2.76463	2.79245	C	1.78832	-0.31325	3.94595	C	-1.65362	-2.32074	-1.59257
C	-0.08618	-2.64834	3.4031	C	2.03216	0.71054	4.77359	C	-2.54482	-2.63888	-0.41815
H	-0.58122	-3.52003	3.82157	H	2.63705	0.57169	5.66425	H	-2.77578	-3.70565	-0.38029
H	-0.5967	-1.69798	3.50887	H	1.65233	1.70858	4.58329	H	-2.06216	-2.36334	0.52629
C	1.72764	-4.09625	2.70384	C	2.28561	-1.67642	4.24124	H	-3.48757	-2.08137	-0.47276
C	2.91575	-4.36812	2.15339	C	2.30386	-2.23485	5.45391	C	-1.10455	-3.30863	-2.30534
H	3.30255	-5.38137	2.1377	H	2.68982	-3.23704	5.60877	H	-0.45637	-3.12743	-3.15595
H	-1.01805	-0.32599	1.71988	H	-1.33548	1.19436	1.07853	H	-1.28966	-4.34762	-2.04826
H	2.13224	-1.8531	1.17026	H	0.16504	-0.88154	2.68226	C	0.65295	1.59854	-0.43675
H	1.15113	-4.91173	3.13907	H	2.62624	-2.2595	3.38456	H	-0.00548	2.39457	-0.07545
H	3.53813	-3.59918	1.70585	H	1.92126	-1.7054	6.32241	H	1.63886	1.72501	0.02204
H	-2.43928	-1.24892	0.26006	H	0.62674	-0.10332	-2.65446	H	0.76885	1.73699	-1.51656
H	-2.11738	0.34595	-3.22404	H	-2.65321	-1.18751	-1.46064	H	1.21801	-0.45646	3.10628
H	1.51632	-0.73603	-1.44261	H	2.12204	0.29936	-0.8344	H	1.29911	-2.53537	1.85183

premnaspirodiene				b-caryophyllane				valencane			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.00202	0.04224	-0.02876	C	0.39889	1.07148	0.04643	C	0.23852	0.00688	-0.01107
C	-0.0013	0.12022	1.52362	C	0.07272	0.46905	1.43686	C	0.21194	0.06232	1.54758
C	1.42258	-0.01914	2.06275	C	1.60158	0.12641	1.56323	C	1.57475	0.49829	2.09849
C	1.9595	-1.41462	1.7597	C	1.72087	0.28335	0.0148	C	2.67619	-0.53581	1.79975
C	1.64116	-1.82545	0.34849	C	2.21145	-1.16247	2.13126	C	2.30984	-1.39593	0.58523
C	0.77361	-1.20447	-0.46211	C	2.59219	-1.19563	3.62407	C	1.59999	-0.59308	-0.50838
H	2.06463	0.74055	1.59539	C	-1.08725	0.90404	3.74595	H	1.83594	1.46819	1.65494
H	3.04367	-1.45837	1.91706	C	-0.65375	1.44435	2.37592	H	3.62709	-0.02259	1.61693
H	2.18084	-2.68867	-0.04019	C	0.15224	-1.24474	4.30002	H	3.20582	-1.87179	0.16845
H	-0.56149	-0.76553	1.86373	C	1.54169	-1.82196	4.55948	H	0.02116	-0.96244	1.90182
C	-0.70208	1.34619	2.11057	C	0.03608	0.25945	4.55966	C	-0.89556	0.95131	2.11953
H	-1.7455	1.41917	1.79009	C	1.52195	-3.3467	4.42587	H	-1.87602	0.73318	1.68516
H	-0.69991	1.28028	3.20316	C	-1.89058	2.00405	1.66155	H	-0.97202	0.80205	3.20111
H	-0.19878	2.28107	1.84112	C	2.95677	1.01956	-0.48206	H	-0.68019	2.01182	1.94965

C	-1.46822	0.05916	-0.55466	C	1.54664	-1.03284	-0.74438	C	-0.90342	-0.89801	-0.50573
H	-2.17673	-0.21395	0.23478	H	0.58446	2.15007	0.13304	H	-1.84865	-0.57292	-0.05701
H	-1.60853	-0.65796	-1.37031	H	-0.31184	0.89968	-0.76951	H	-0.72372	-1.919	-0.13275
C	-0.3549	1.81111	-1.74202	H	2.10217	0.99102	2.02782	C	1.42047	-1.48589	-1.74971
H	-0.23706	2.87669	-1.96324	H	1.57128	-2.01895	1.88049	H	1.15758	-2.50068	-1.4162
C	-1.71116	1.47289	-1.12496	H	3.13568	-1.31759	1.55794	H	2.38144	-1.58062	-2.26843
C	0.65349	1.29752	-0.70731	H	2.83265	-0.1772	3.95214	C	0.34265	-0.99908	-2.71674
H	0.8434	2.07274	0.04285	H	3.52061	-1.76835	3.74034	H	0.31065	-1.67606	-3.57714
H	1.62125	1.05134	-1.15443	H	-1.90222	0.17749	3.60624	H	0.62819	-0.01985	-3.11803
H	1.43942	0.17114	3.14218	H	-1.52378	1.74336	4.30118	C	-1.05208	-0.93328	-2.03832
H	1.52291	-2.14009	2.4617	H	-0.11913	-1.46053	3.25843	H	-1.55041	-0.00112	-2.34594
H	-1.88019	2.16125	-0.28173	H	0.97847	0.76396	4.31282	C	-1.96246	-2.09034	-2.50391
H	-0.24322	1.26172	-2.68569	H	-0.12121	0.4242	5.632	C	-3.23607	-2.21591	-1.66209
C	0.6163	-1.67393	-1.88891	H	0.80177	-3.79236	5.11959	H	-3.8975	-2.98173	-2.07968
H	-0.34731	-2.16434	-2.06112	H	2.50625	-3.77757	4.63556	H	-3.02627	-2.48649	-0.62437
H	0.67678	-0.83519	-2.59281	H	1.23238	-3.64953	3.41274	H	-3.78692	-1.26641	-1.66026
H	1.40292	-2.38703	-2.14626	H	-2.43247	2.70106	2.30889	C	-2.35739	-1.92261	-3.97467
C	-2.9223	1.56483	-2.02069	H	-1.63246	2.53275	0.74032	H	-1.49334	-1.80096	-4.6334
C	-4.22295	1.14664	-1.38297	H	3.07023	1.98297	0.02618	H	-2.92756	-2.78729	-4.32844
H	-5.07309	1.34622	-2.03925	H	2.89568	1.20779	-1.56049	C	0.06283	1.42348	-0.58437
H	-4.2169	0.0766	-1.14618	H	3.86342	0.42968	-0.29789	H	-0.9518	1.80146	-0.41894
H	-4.37982	1.6814	-0.43834	H	1.4304	-0.82489	-1.81414	H	0.76462	2.12583	-0.12077
C	-2.86897	1.99328	-3.2849	H	0.65775	-1.58082	-0.41433	H	0.25328	1.44455	-1.65991
H	-3.76785	2.05154	-3.89226	H	2.41404	-1.69074	-0.62405	H	1.49837	0.67457	3.17752
H	-1.93958	2.30158	-3.75264	H	-0.52133	-0.44984	1.32168	H	2.83473	-1.18341	2.66935
				H	-2.57722	1.18939	1.40015	H	1.64759	-2.21762	0.89239
				H	0.04383	2.27897	2.55893	H	2.25269	0.25121	-0.78239
				H	-0.59046	-1.77141	4.91393	H	-2.99165	-1.03512	-4.09011
				H	1.83225	-1.57809	5.59227	H	-1.38623	-3.02382	-2.39737

premnaspirodienehyd				bisabolane- conformer 1				bisabolane- conformer 2			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.02722	0.11279	0.04243	C	0.07366	0.01517	-0.03545	C	-0.52543	0.08979	0.33061
C	0.08524	0.02707	1.59502	C	0.02483	0.021	1.50642	C	-0.12142	-0.05391	1.8135
C	1.52147	-0.12915	2.10284	C	1.49713	-0.05923	-0.59733	C	0.64618	0.55122	-0.54336
C	2.16927	-1.39135	1.54291	H	2.10408	0.79827	-0.29512	H	1.01235	1.54265	-0.26651
C	2.12659	-1.37395	0.01815	H	2.00694	-0.97057	-0.26496	H	1.48293	-0.1549	-0.46787
C	0.71319	-1.1571	-0.54328	H	1.47294	-0.07843	-1.69179	H	0.34206	0.59561	-1.59381
H	2.10914	0.75333	1.80712	C	-0.78038	-1.10421	-0.65268	C	-1.12862	-1.2169	-0.23594
H	3.20293	-1.48755	1.89353	H	-0.28725	-2.07276	-0.48493	H	-0.8198	-2.07021	0.3846
H	2.7842	-0.57276	-0.34991	C	0.84338	1.15977	2.12956	C	-1.30292	-0.49249	2.69117
H	-0.45375	-0.8972	1.86284	H	1.91069	1.00543	1.91784	H	-2.10718	0.25386	2.59415
C	-0.61232	1.18102	2.32053	H	0.56367	2.11669	1.66986	H	-1.71278	-1.44335	2.33306
H	-1.64455	1.32276	1.98777	C	-2.22354	-1.18077	-0.15374	C	-2.65338	-1.20257	-0.36522
H	-0.6371	0.98015	3.39636	H	-2.6934	-0.19408	-0.26468	H	-2.93552	-0.37025	-1.02293
H	-0.08223	2.12929	2.18205	H	-2.24119	-1.41331	0.92028	H	-3.11338	-0.99175	0.61031
C	-1.4545	0.19582	-0.42704	C	-3.03946	-2.24167	-0.89289	C	-3.20949	-2.51451	-0.91576
H	-2.14654	-0.04546	0.38661	H	-3.14629	-1.95472	-1.95013	H	-2.8205	-2.67488	-1.9333

H	-1.64805	-0.53883	-1.21886	C	-4.43165	-2.50109	-0.30547	C	-4.73992	-2.60292	-0.95434
C	-0.29602	1.97338	-1.54897	C	-5.30741	-1.24688	-0.33483	C	-5.35733	-1.49824	-1.81421
H	-0.16585	3.04759	-1.71241	H	-6.31396	-1.46371	0.03698	H	-6.44326	-1.61884	-1.88328
C	-1.68029	1.6072	-0.99769	H	-4.89285	-0.44224	0.27885	H	-5.15884	-0.50198	-1.40918
C	0.67914	1.41636	-0.5057	H	-5.40307	-0.87385	-1.36251	H	-4.95078	-1.53628	-2.83289
H	0.80002	2.14999	0.29872	C	-5.11919	-3.64827	-1.04709	C	-5.17742	-3.97786	-1.46117
H	1.67893	1.24714	-0.91814	H	-6.0957	-3.87695	-0.60818	H	-6.26727	-4.07965	-1.44615
H	1.52103	-0.15061	3.1996	H	-5.27897	-3.38191	-2.09898	H	-4.84138	-4.12756	-2.49447
H	1.62356	-2.26977	1.91495	C	0.64769	1.21706	3.6463	C	-0.91946	-0.62712	4.16614
H	-1.90941	2.29703	-0.16778	H	1.24203	2.032	4.07785	H	-1.79343	-0.92956	4.75624
H	-0.15286	1.47254	-2.51699	C	1.01868	-0.10874	4.31918	C	-0.33113	0.66891	4.72721
C	0.78835	-1.17945	-2.07397	C	0.78223	-0.05204	5.82615	C	0.06401	0.51782	6.19389
H	-0.18642	-1.06477	-2.55594	H	1.0619	-0.99402	6.30906	H	0.46832	1.45273	6.59551
H	1.44166	-0.3814	-2.44501	H	1.36213	0.75263	6.28988	H	-0.79407	0.22692	6.80868
H	1.21238	-2.13042	-2.412	H	-0.27753	0.13284	6.0392	H	0.83353	-0.25562	6.30465
C	-2.82117	1.69624	-2.01548	C	0.24311	-1.26076	3.67283	C	0.85709	1.10054	3.86581
C	-4.15434	1.27378	-1.39349	H	0.54607	-2.21299	4.12529	H	1.26558	2.04846	4.2375
H	-4.4039	1.92832	-0.54885	C	0.43128	-1.30919	2.15441	C	0.48897	1.23348	2.38613
H	-4.96828	1.34412	-2.12218	H	1.48599	-1.52184	1.92791	H	-0.23797	2.05177	2.26232
H	-4.1235	0.24449	-1.02373	H	-1.02374	0.20718	1.78841	H	0.64915	-0.84375	1.86672
C	-2.93624	3.10048	-2.61192	H	-0.15372	-2.13933	1.7417	H	1.38243	1.51705	1.82164
H	-3.11136	3.83912	-1.81974	H	-0.40648	1.44177	3.8702	H	-0.17202	-1.42795	4.27649
H	-2.02856	3.39118	-3.14858	H	-4.29969	-2.80208	0.74468	H	-5.10837	-2.48255	0.07534
H	-3.77401	3.15936	-3.31408	H	-2.47482	-3.185	-0.88668	H	-2.82583	-3.3457	-0.30686
H	-2.58311	0.99416	-2.83102	H	-0.79244	-0.96308	-1.74256	H	-0.70898	-1.41073	-1.23208
H	2.52986	-2.3105	-0.38615	H	-0.82725	-1.13143	3.89764	H	1.65613	0.3506	3.97286
H	0.09479	-2.01189	-0.22184	H	2.0912	-0.2859	4.14009	H	-1.10472	1.4499	4.65176
				H	-0.3614	0.97399	-0.35974	H	-1.30365	0.86936	0.28437
				H	-4.51332	-4.55988	-1.0205	H	-4.75242	-4.78155	-0.851

bisabolane- conformer 3				bisabolane- conformer 4				farnesane- conformer 1			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.26784	-0.03706	0.02853	C	0.00251	-0.00121	-0.00072	C	-0.25661	0.02622	-0.06832
C	-0.14719	-0.147	1.56338	C	0.00422	-0.00045	1.5415	C	-0.144	0.00238	1.46109
C	1.09201	0.23232	-0.62902	C	1.40817	-0.00268	-0.60977	H	0.92	-0.03535	1.7399
H	1.47171	1.2287	-0.39035	H	1.98363	0.88053	-0.31993	C	0.38271	1.28394	-0.66134
H	1.84208	-0.4965	-0.30017	H	1.97208	-0.89092	-0.30338	H	1.45405	1.3135	-0.42364
H	1.01431	0.16339	-1.7192	H	1.34834	-0.01442	-1.70296	H	0.27814	1.3152	-1.74934
C	-0.94894	-1.25909	-0.61541	C	-0.81543	-1.15924	-0.596	H	-0.0753	2.19409	-0.26437
H	-0.98068	-1.10066	-1.70212	H	-0.26953	-2.1033	-0.45318	C	0.35515	-1.25103	-0.65718
C	-1.47733	-0.52689	2.22792	C	0.76931	1.18683	2.14138	H	-0.10991	-2.11862	-0.16745
H	-2.23582	0.22257	1.95208	H	1.83697	1.10076	1.89543	H	1.42347	-1.28821	-0.39526
H	-1.83543	-1.48939	1.84677	H	0.41463	2.1247	1.69438	C	-0.81332	1.17572	2.17826
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H	-0.23072	-2.77085	0.75052	H	-2.76494	-0.35159	-0.13143	H	-1.82629	1.30564	1.77433
H	0.76061	-2.58093	-0.69024	H	-2.19227	-1.54882	1.02362	C	0.20085	-1.40579	-2.17063
C	-1.02633	-3.76357	-0.99349	C	-3.02605	-2.39955	-0.77093	H	0.79636	-0.64469	-2.69246

H	-2.06967	-3.74818	-0.64667	H	-2.98362	-2.21288	-1.85309	C	0.63292	-2.78948	-2.65679
C	-0.44585	-5.16318	-0.73476	C	-4.49619	-2.51508	-0.35018	H	-0.04701	-3.54892	-2.24117
C	0.96821	-5.31695	-1.29941	C	-5.19907	-3.59481	-1.17464	C	0.6816	-2.95266	-4.18013
H	1.30998	-6.35363	-1.2155	H	-6.26322	-3.65588	-0.92512	C	1.18568	-4.34906	-4.54804
H	1.00864	-5.03154	-2.35611	H	-5.11232	-3.3972	-2.248	H	1.27366	-4.46767	-5.63264
H	1.68273	-4.69123	-0.7534	H	-4.75244	-4.57688	-0.97679	H	2.16628	-4.54794	-4.10355
C	-0.47777	-5.53712	0.74939	C	-4.64668	-2.80728	1.14436	H	0.48967	-5.11369	-4.18223
H	-0.19416	-6.58474	0.89253	H	-5.69844	-2.95913	1.40756	C	-0.68032	-2.69027	-4.8267
H	0.22356	-4.92639	1.32848	H	-4.09934	-3.72031	1.41104	H	-1.43733	-3.36416	-4.40569
C	-1.36645	-0.60487	3.75189	C	0.6181	1.229	3.6637	H	-1.01843	-1.66244	-4.66799
H	-2.33951	-0.86241	4.1881	H	1.17228	2.07953	4.07974	C	-0.87224	0.96754	3.69185
C	-0.84352	0.69514	4.36592	C	1.09397	-0.07136	4.31953	H	0.12947	0.68456	4.04592
C	-0.71357	0.58595	5.88299	C	0.90355	-0.03219	5.83358	C	-1.35164	2.17993	4.49956
H	-0.35751	1.52436	6.32075	H	1.26302	-0.95304	6.30426	C	-2.76188	2.60868	4.08816
H	-1.67249	0.33592	6.34858	H	1.44165	0.81013	6.28055	H	-3.09797	3.48272	4.65262
H	0.00316	-0.20066	6.14804	H	-0.15885	0.07924	6.08169	H	-2.81134	2.86889	3.02735
C	0.49025	1.06451	3.71442	C	0.37294	-1.26999	3.69478	H	-3.47455	1.79368	4.26964
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C	0.38652	1.15073	2.18986	C	0.51388	-1.30359	2.17079	H	-0.25569	1.51595	6.22572
H	-0.29104	1.97528	1.91796	H	1.572	-1.44905	1.9093	C	-1.59848	3.05115	6.91307
H	0.58237	-0.94293	1.78973	H	-1.04403	0.12013	1.85821	H	-1.40868	2.80043	7.96062
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H	-1.09392	-5.8728	-1.26773	H	-4.98208	-1.5508	-0.56146	H	-1.32812	0.03312	-0.32461
H	-1.06077	-3.59103	-2.07847	H	-2.53578	-3.372	-0.60753	H	-0.58973	-0.933	1.82868
H	-1.99651	-1.31172	-0.29289	H	-0.8717	-1.01089	-1.68332	H	-1.52803	0.11181	3.91369
H	1.23499	0.29994	3.98434	H	-0.69557	-1.21018	3.95486	H	-0.66463	3.01602	4.29205
H	-1.56572	1.49359	4.13235	H	2.16921	-0.17926	4.10523	H	-1.94535	1.03191	6.22312
H	-0.91656	0.82869	-0.17929	H	-0.49051	0.93534	-0.30693	H	-2.64754	3.34939	6.83293

H	-1.47765	-5.39642	1.17435	H	-4.26353	-1.99177	1.76417	H	1.6283	-3.01268	-2.24681
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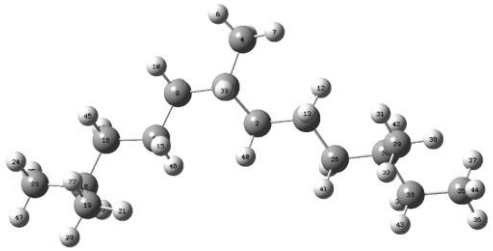
								H	-0.64024	-2.86537	-5.90664

farnesane- conformer 2



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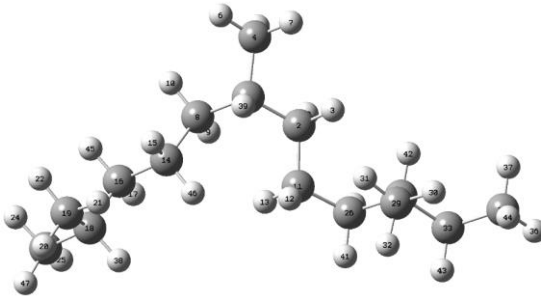
C	1.37358	1.28485	-0.23409
H	2.24418	1.12526	0.41476
H	1.73524	1.37417	-1.26361
H	0.91911	2.23993	0.0429
C	1.00177	-1.15205	-0.6995
H	1.93154	-1.38536	-0.15849
H	1.29717	-0.94259	-1.73735
C	-0.6201	1.15223	2.03638
H	0.16783	1.90637	2.16491

farnesane- conformer 3



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C	1.38679	-0.64986	-0.29969
H	1.5201	-1.66551	0.0923
H	1.45635	-0.70095	-1.39088
H	2.21734	-0.03736	0.06637
C	-1.12314	-0.9694	-0.35858
H	-1.42073	-1.66677	0.43898
H	-0.77084	-1.59838	-1.18743
C	-1.26635	0.64593	2.26164
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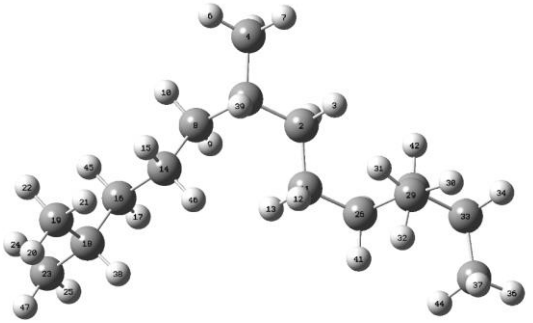
farnesane- conformer 4



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C	1.37388	-1.19958	-0.456
H	1.40863	-2.22609	-0.07127
H	1.38697	-1.25188	-1.54929
H	2.28503	-0.68797	-0.12881
C	-1.15929	-1.21853	-0.41153
H	-1.53412	-1.84912	0.4084
H	-0.91317	-1.9089	-1.22959
C	-0.99672	0.38232	2.21884
H	-1.0852	1.39596	1.80359

H	-1.37842	1.60162	1.381	H	-2.09593	-0.02691	2.01105	H	-1.92428	-0.13809	1.94917
C	0.0888	-2.37871	-0.69053	C	-2.34666	-0.1905	-0.84746	C	-2.27243	-0.28704	-0.89702
H	-0.89074	-2.09454	-1.09837	H	-2.04315	0.42153	-1.70667	H	-1.9133	0.23734	-1.792
C	0.67063	-3.54267	-1.49293	C	-3.51037	-1.10082	-1.23717	C	-3.57196	-1.02779	-1.2065
H	1.7057	-3.71615	-1.16566	H	-3.72082	-1.78197	-0.40019	H	-3.88119	-1.58272	-0.30906
C	-0.1087	-4.85728	-1.37399	C	-4.80528	-0.36749	-1.60586	C	-4.73368	-0.13317	-1.6541
C	-1.55814	-4.70828	-1.84114	C	-4.61401	0.5709	-2.79894	C	-4.41933	0.60803	-2.95522
H	-2.07779	-5.67139	-1.81361	H	-5.56224	1.03835	-3.08354	H	-5.28056	1.19754	-3.28581
H	-2.12188	-4.00905	-1.21713	H	-3.90053	1.37108	-2.58276	H	-3.572	1.29061	-2.84689
H	-1.58908	-4.34011	-2.87444	H	-4.24256	0.01196	-3.66729	H	-4.17821	-0.10794	-3.75126
C	0.59232	-5.9642	-2.16293	C	-5.92148	-1.37244	-1.89384	C	-6.01003	-0.96093	-1.8123
H	0.60886	-5.71911	-3.23196	H	-5.66637	-1.98738	-2.7655	H	-5.87795	-1.72032	-2.59273
H	1.6281	-6.09561	-1.83341	H	-6.0819	-2.04474	-1.04466	H	-6.26834	-1.47814	-0.88249
C	-1.22784	0.83224	3.40272	C	-1.22781	0.79856	3.78578	C	-0.92111	0.4468	3.74935
H	-0.50633	0.23123	3.97431	H	-1.12561	-0.1981	4.23795	H	-0.97548	-0.57621	4.14891
C	-1.61783	2.05475	4.24286	C	-0.12118	1.70242	4.34913	C	0.33116	1.12674	4.32027
C	-2.65769	2.92095	3.52893	C	-0.14092	3.0871	3.69958	C	0.49493	2.55143	3.78425
H	-2.9213	3.8035	4.11817	H	0.6298	3.74	4.11805	H	1.31407	3.07063	4.29378
H	-2.29096	3.27452	2.56139	H	0.03307	3.02949	2.62072	H	0.71688	2.55281	2.71245
H	-3.57569	2.34542	3.35289	H	-1.11502	3.568	3.85686	H	-0.41977	3.13749	3.93207
C	-2.10813	1.60349	5.62514	C	-0.26095	1.78795	5.87503	C	0.34031	1.08959	5.85823
H	-1.35212	0.93757	6.06072	H	-0.34141	0.76783	6.27253	H	1.32488	1.42765	6.20637
C	-2.38898	2.74424	6.60259	C	0.88897	2.50718	6.57919	C	-0.73855	1.933	6.53999
H	-2.6212	2.35803	7.59908	H	0.78506	2.44202	7.66595	H	-0.66807	1.84009	7.62751
H	-1.5172	3.40186	6.6939	H	1.85196	2.06019	6.30832	H	-0.63294	2.99434	6.29464
H	-0.1187	-5.1456	-0.31217	H	-5.10372	0.23827	-0.73715	H	-4.90445	0.61468	-0.86533
H	-0.5111	0.36624	-0.69045	H	-0.07989	0.9133	-0.31104	H	0.10419	0.52515	-0.38971
H	-0.80927	-0.88276	1.38858	H	0.24908	-0.8776	2.13579	H	0.29076	-1.33266	2.02119
H	-2.11569	0.1962	3.26591	H	-2.19705	1.19215	4.12502	H	-1.81241	0.97183	4.11733

H	-0.71028	2.66166	4.39184	H	0.85291	1.2364	4.13692	H	1.20552	0.54464	3.99769
H	-3.01549	0.99613	5.49632	H	-1.21106	2.28659	6.11456	H	0.24113	0.04542	6.18236
H	-3.23722	3.35592	6.28309	H	0.92748	3.56846	6.31786	H	-1.74585	1.61987	6.2493
H	0.72804	-3.25971	-2.55525	H	-3.2103	-1.73815	-2.08348	H	-3.38679	-1.78401	-1.98516
H	-0.08735	-2.71237	0.3407	H	-2.68274	0.51378	-0.07472	H	-2.46821	0.49021	-0.14572
H	0.07507	-6.92227	-2.04862	H	-6.86716	-0.86468	-2.10874	H	-6.85917	-0.33223	-2.09852

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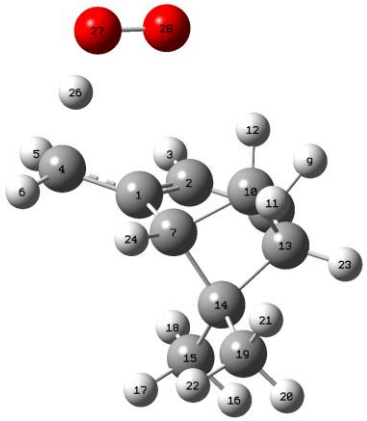	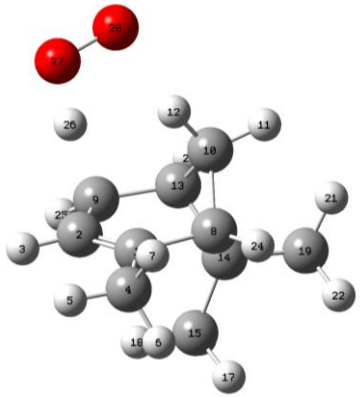	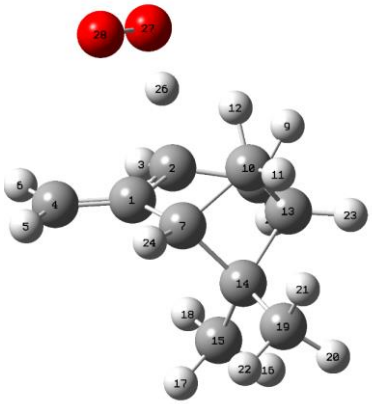

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C	0.07242	0.02129	1.09878	C	0.00000	0.00000	1.36105	C	0.00000	0.00000	1.44002
H	1.01282	0.07420	1.64158	H	0.93162	0.00000	1.92212	H	0.97331	0.00000	1.93492
C	1.24171	-0.38445	-1.02473	C	1.23705	0.00067	-0.83950	C	1.07822	0.38573	-0.73414
H	2.17136	-0.59608	-0.49682	H	2.14131	0.04375	-0.22788	H	1.03583	0.42057	-1.81758
H	1.15927	-0.81496	-2.02109	H	1.27673	-0.90272	-1.46097	H	2.00449	0.68738	-0.25436
C	-1.30525	-0.23151	-0.90781	H	1.23786	0.85601	-1.52602	C	-1.30394	-0.42157	-0.62930
C	-1.22378	0.21409	1.83461	C	-1.35066	-0.04816	-0.67307	C	-1.14911	-0.70282	2.15197
H	-1.21541	1.18565	2.34806	C	-1.27293	-0.04651	2.05071	H	-1.55059	-0.07196	2.95638
C	-2.06894	1.01456	-0.37712	C	-2.25548	0.99714	0.03565	C	-2.47326	0.16312	0.20883
H	-2.94406	1.26218	-0.97720	H	-3.16565	1.23216	-0.51412	H	-3.42334	0.12619	-0.32337
H	-1.46948	1.91256	-0.20878	H	-1.77114	1.92442	0.34946	H	-2.33880	1.16584	0.62306
C	-2.40750	0.14661	0.86027	C	-2.47101	-0.08645	1.12831	C	-2.26534	-1.04365	1.15825
C	-2.29925	-1.10629	-0.06571	C	-2.24640	-1.15958	-0.00689	C	-1.70521	-1.83076	-0.06799

C	-1.81279	-2.42466	0.52620	C	-1.62712	-2.50296	0.35365	C	-0.60997	-2.86652	0.15818
H	-2.57063	-2.83092	1.20625	H	-2.34166	-3.09955	0.93219	H	-1.01532	-3.72915	0.69984
H	-1.65432	-3.15986	-0.27117	H	-1.39275	-3.06350	-0.55896	H	-0.22746	-3.22603	-0.80390
H	-0.87599	-2.32927	1.07882	H	-0.71085	-2.41101	0.93816	H	0.24047	-2.47935	0.72377
C	-3.59922	-1.37091	-0.82695	C	-3.52241	-1.41960	-0.80713	C	-2.81976	-2.47251	-0.89467
H	-4.35464	-1.78183	-0.14768	H	-4.22256	-2.01455	-0.21014	H	-3.22747	-3.34160	-0.36602
H	-4.01836	-0.47350	-1.28697	H	-4.03847	-0.50820	-1.11464	H	-3.64765	-1.79018	-1.10077
H	-3.42864	-2.10620	-1.62116	H	-3.28658	-1.99302	-1.71099	H	-2.42509	-2.82047	-1.85570
H	-3.36169	0.31066	1.37288	H	-3.42298	-0.10601	1.66570	H	-3.13850	-1.46783	1.66618
H	-1.25283	-0.40901	-1.98703	H	-1.27752	-0.04420	-1.76614	H	-1.30396	-0.28083	-1.71477
H	-1.32120	-0.54645	2.62345	H	-1.31962	-0.61135	2.98503	H	-0.77853	-1.61616	2.63780
H	1.46741	1.00351	-1.30916	H	-1.46363	1.23968	2.63853	H	-0.24606	1.41825	1.60652
O	1.59231	2.16375	-1.30267	O	-1.80007	2.26204	3.07734	O	-0.39345	2.55612	1.63435
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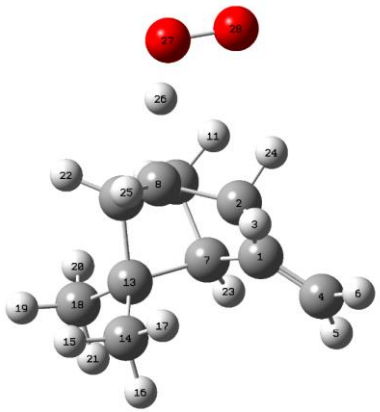	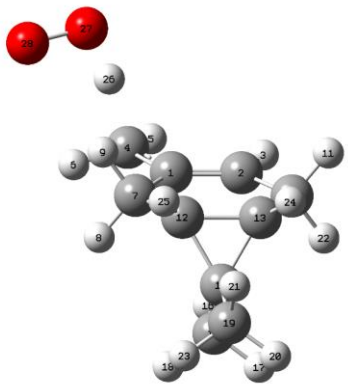	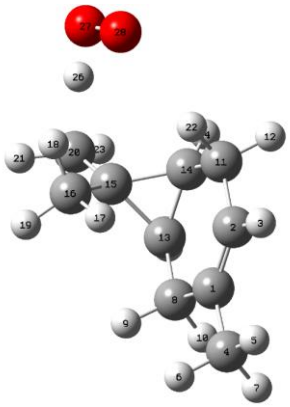

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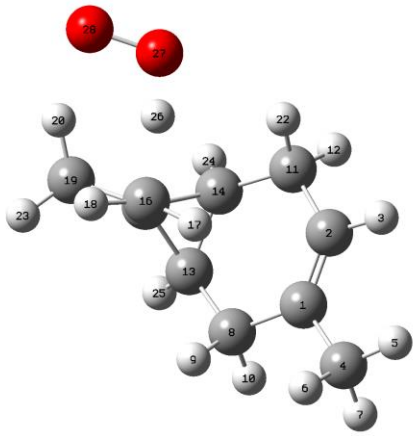
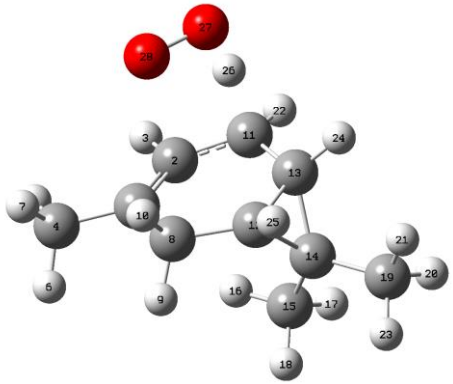
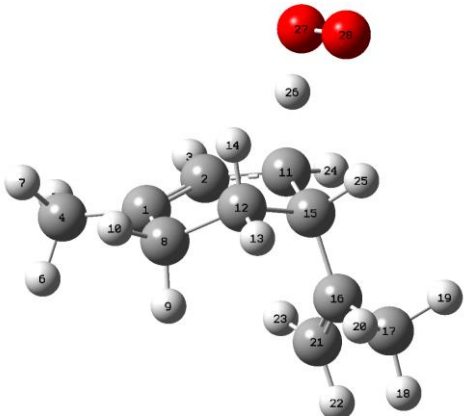
C	0.16108	-0.29990	1.65181	C	0.03739	-0.06536	1.35921	C	-0.28199	0.33816	1.24685
H	1.20852	-0.41918	1.94557	H	0.97832	-0.06780	1.90774	H	0.54670	0.50356	1.93429
C	0.94200	0.63551	-0.54211	C	1.34942	-0.20126	-0.68404	C	1.39979	-0.27506	-0.48324
H	0.82304	0.80925	-1.60768	H	2.24656	-0.37338	-0.09114	H	2.12968	-0.08006	0.30595
H	1.81805	1.06251	-0.06138	H	1.36441	-0.62075	-1.69258	H	1.53394	-1.30725	-0.82874
C	-1.17093	-0.69996	-0.48082	C	-1.15761	-0.14110	-0.85782	H	1.62903	0.37786	-1.33371
C	-0.67580	-1.47296	2.11768	H	-1.15997	-1.05490	-1.46952	C	-1.08012	-0.31485	-1.03003
C	-2.35646	-0.60286	0.51703	H	-1.05682	0.68797	-1.56831	H	-0.99776	-1.35905	-1.36935
H	-3.32130	-0.77909	0.04279	C	-1.20985	0.02605	2.18081	H	-0.85744	0.29534	-1.91530
H	-2.41955	0.30009	1.13146	H	-1.13247	0.92510	2.80645	C	-1.65684	0.56892	1.81037
C	-1.77919	-1.87581	1.18867	C	-2.47474	0.00305	-0.11932	H	-1.69985	1.58534	2.21977
C	-1.15499	-2.24338	-0.21710	C	-2.50361	0.08470	1.39182	C	-2.49949	-0.01251	-0.59027
C	0.18402	-2.96757	-0.25564	C	-3.06248	-1.12691	0.68836	C	-2.78547	0.41089	0.81034
H	0.07325	-3.99498	0.10974	C	-2.32915	-2.44928	0.77217	C	-3.23298	-0.98216	0.36534

H	0.55142	-3.01526	-1.28700	H	-1.24248	-2.33268	0.78902	C	-2.51112	-2.20735	0.88709
H	0.95415	-2.47318	0.34154	H	-2.62303	-2.99014	1.67906	H	-1.44603	-2.02481	1.04320
C	-2.15648	-2.99097	-1.09552	H	-2.58484	-3.07992	-0.08694	H	-2.94238	-2.51373	1.84554
H	-2.27367	-4.02085	-0.74054	C	-4.57025	-1.27311	0.66963	H	-2.61486	-3.03873	0.18134
H	-3.14509	-2.52641	-1.10867	H	-4.92517	-1.77180	1.57880	C	-4.66624	-1.15851	0.12729
H	-1.79059	-3.03184	-2.12766	H	-5.06149	-0.29711	0.60660	H	-5.02689	-2.15868	-0.11454
H	-2.46637	-2.60619	1.62885	H	-1.22784	-0.81526	2.89097	H	-1.82685	-0.09878	2.66575
H	-1.31520	-0.37174	-1.51543	H	-4.89311	-1.86943	-0.19131	H	-5.20925	-0.34125	-0.34841
H	-0.19220	0.61634	2.15560	H	-3.24822	0.75505	1.81353	H	-3.60716	1.11018	0.94339
H	-0.17620	-2.26403	2.67966	H	-3.20222	0.62340	-0.63656	H	-3.13350	0.40618	-1.36613
H	-1.48705	-0.84101	3.28508	H	1.52661	1.13442	-1.16243	H	-5.20081	-1.02964	1.57297
O	-2.07259	-0.29409	4.00871	O	1.57390	2.14624	-1.70963	O	-5.45707	-0.90227	2.62294
O	-1.85032	0.96104	3.81184	O	1.14477	1.95725	-2.89612	O	-4.35573	-0.67445	3.25169

car-3-ene- TS- 3				car-3-ene- TS- 4				d-limonene- TS- 1			
											
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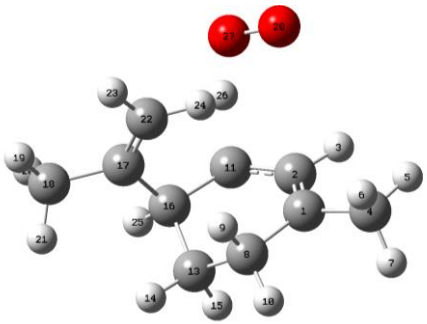
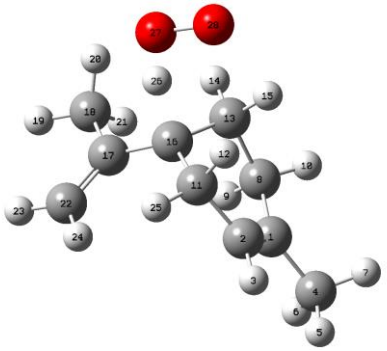
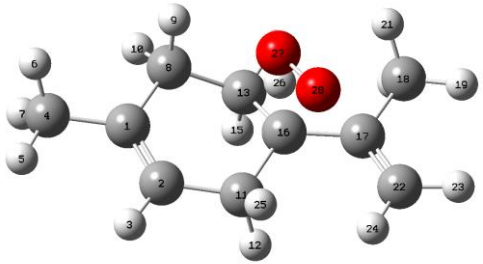
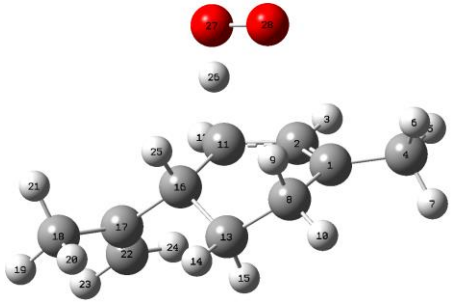
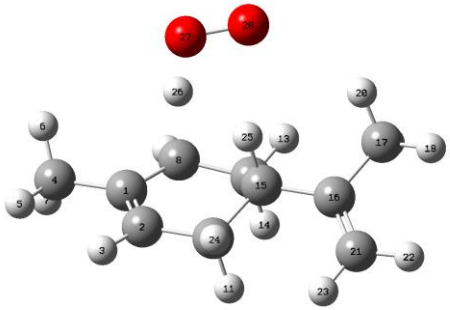
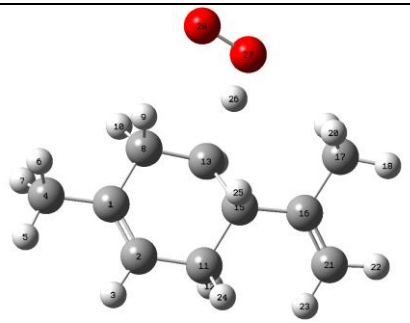
C	-0.00130	0.02430	-0.00760	C	-0.01241	-0.09366	0.33890	C	0.12853	0.00938	0.01308
C	0.00590	-0.12503	1.31993	C	-0.08478	-0.41223	1.66289	C	0.14231	-0.14717	1.36432
H	0.96441	-0.21645	1.82909	H	0.83761	-0.64254	2.19280	H	1.10087	-0.18794	1.87906
C	1.26570	0.06540	-0.81766	C	1.29008	-0.05210	-0.39816	C	1.38585	0.08666	-0.79722
H	2.15072	-0.02694	-0.18389	H	2.12810	-0.33355	0.24334	H	2.27804	-0.03109	-0.17805
H	1.28250	-0.74686	-1.55428	H	1.27107	-0.72431	-1.26490	H	1.39260	-0.69159	-1.57018
H	1.33963	1.00469	-1.37827	H	1.47531	0.95845	-0.78334	H	1.44894	1.04918	-1.31920
C	-1.27218	0.16895	-0.80816	C	-1.23371	0.26210	-0.46402	C	-1.17443	0.05670	-0.73909
H	-1.27105	-0.57862	-1.61580	H	-1.22331	-0.32618	-1.39543	H	-1.34006	-0.93152	-1.19539
H	-1.24080	1.14389	-1.31291	H	-1.12105	1.31008	-0.77418	H	-1.08924	0.76477	-1.57260
C	-1.21136	-0.16981	2.20219	C	-1.29670	-0.34554	2.42378	C	-1.05755	-0.24800	2.15857
H	-1.15574	0.66805	2.90835	C	-2.57256	0.10579	0.23724	C	-2.35824	0.43215	0.15172
C	-2.56164	0.08201	-0.01840	C	-2.59947	-0.22929	1.71348	H	-3.29708	0.31619	-0.39824
C	-2.53517	-0.08438	1.46692	C	-3.09203	-1.23581	0.68129	H	-2.28254	1.48937	0.43198

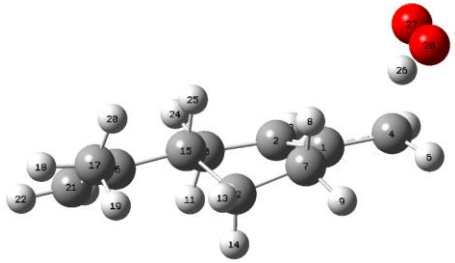
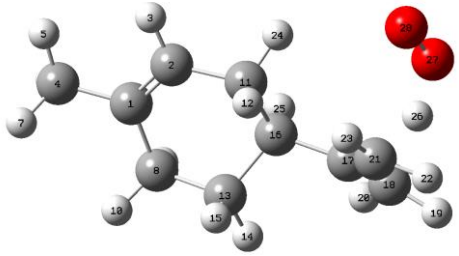
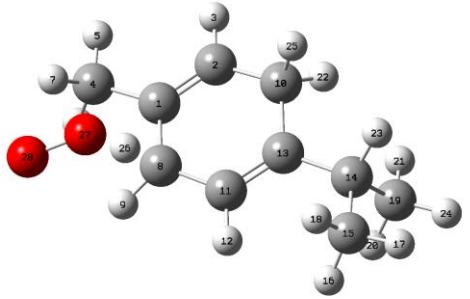
C	-3.03998	-1.23991	0.60460	C	-2.32625	-2.50673	0.38509	C	-2.38418	-0.40464	1.44799
C	-2.21462	-2.44435	0.46492	H	-1.24444	-2.37329	0.42508	C	-2.76143	-1.85473	1.17112
H	-1.13892	-2.33916	0.33527	H	-2.59719	-3.28625	1.10591	C	-4.23199	-2.09418	0.94319
H	-2.67035	-3.29926	-0.03730	H	-2.58756	-2.87330	-0.61454	H	-4.43162	-3.13800	0.69143
C	-4.53651	-1.48714	0.61146	C	-4.59556	-1.42323	0.63311	H	-4.80372	-1.83849	1.84248
H	-4.81534	-2.15258	1.43478	H	-4.91850	-2.17125	1.36583	H	-4.61788	-1.46651	0.13250
H	-5.08635	-0.54894	0.73007	H	-5.11977	-0.48741	0.85057	C	-1.87054	-2.84896	1.12037
H	-1.18144	-1.07575	2.82425	H	-1.30462	-0.85071	3.39095	H	-2.18359	-3.86558	0.90022
H	-4.85785	-1.95193	-0.32673	H	-4.91064	-1.76379	-0.35987	H	-0.81192	-2.68205	1.29432
H	-3.32816	0.40961	2.02270	H	-3.39174	0.22985	2.30173	H	-0.96346	-0.77242	3.11222
H	-3.38022	0.67051	-0.42635	H	-3.33118	0.80569	-0.10481	H	-3.17234	0.01392	2.09060
H	-2.28383	-3.03821	1.84110	H	-1.14545	0.99751	2.82204	H	-1.21057	1.05910	2.67924
O	-2.47208	-3.47249	2.83865	O	-1.04687	2.18065	2.86260	O	-1.47896	2.12939	3.06759
O	-3.51917	-4.21169	2.73787	O	-0.42888	2.51643	1.80513	O	-2.74359	2.27793	3.01728

d-limonene- TS- 2				d-limonene- TS- 3				d-limonene- TS- 4			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.07015	0.09863	0.19354	C	-0.00704	0.09015	-0.04979	C	-0.01459	0.02036	-0.03074
C	-0.21350	0.34776	1.50736	C	0.06185	-0.03146	1.28014	C	-0.03546	0.14826	1.29940
H	0.59439	0.66949	2.16184	H	1.03584	-0.02846	1.76721	H	0.90645	0.26504	1.83322
C	1.46279	0.16600	-0.34990	C	1.21794	0.19748	-0.91542	C	1.26363	0.00272	-0.82168
H	2.19424	0.37485	0.43364	H	2.13503	0.11900	-0.32691	H	2.13981	0.07618	-0.17308
H	1.73057	-0.78597	-0.82522	H	1.22550	-0.59592	-1.67228	H	1.34305	-0.92418	-1.40235
H	1.54281	0.93795	-1.12490	H	1.23216	1.15226	-1.45355	H	1.29039	0.83206	-1.53811
C	-1.03771	-0.21892	-0.77379	C	-1.33242	0.12062	-0.77704	C	-1.28868	-0.13847	-0.82329
H	-1.05721	-1.30259	-0.96124	H	-1.47234	-0.83545	-1.30356	H	-1.40374	-1.19457	-1.11006
H	-0.81652	0.25199	-1.73964	H	-1.30659	0.89663	-1.55262	H	-1.20641	0.42088	-1.76351
C	-1.51281	0.16536	2.08288	C	-1.15052	-0.17206	2.17901	C	-1.27615	0.10479	2.15145
H	-1.77180	0.84119	2.90141	H	-1.33904	0.78969	2.68064	H	-1.39803	1.06167	2.68581
C	-2.39956	0.24855	-0.25906	C	-2.51513	0.37591	0.17479	C	-2.52363	0.33219	-0.05113
H	-3.19521	-0.09259	-0.93026	H	-3.46584	0.23760	-0.34663	H	-3.42920	0.04884	-0.59291
H	-2.42242	1.34471	-0.25073	H	-2.47689	1.41497	0.52328	H	-2.51250	1.43349	-0.00148
C	-2.66366	-0.26023	1.17852	C	-2.36974	-0.54538	1.36798	C	-2.53814	-0.19653	1.36830

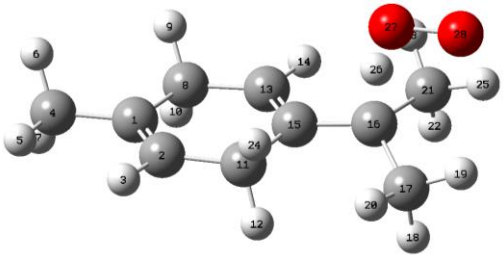
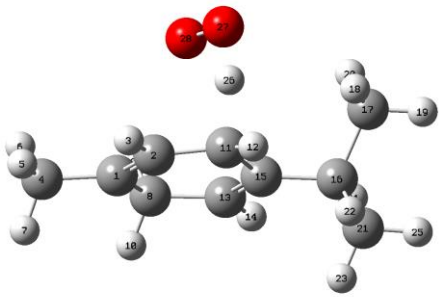
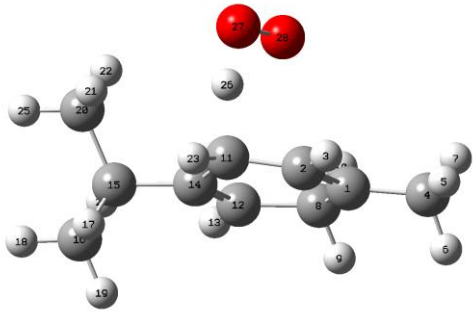
C	-2.95295	-1.75708	1.13334	C	-2.77171	-1.94587	1.21201	C	-3.79601	-0.30943	2.08935
C	-4.40545	-2.10993	0.94711	C	-3.95202	-2.22558	0.30842	C	-5.07498	-0.41271	1.29100
H	-4.54303	-3.18386	0.80420	H	-4.26747	-3.26681	0.39544	H	-5.92285	-0.61177	1.94899
H	-4.99031	-1.79853	1.82040	H	-4.80457	-1.58581	0.56144	H	-5.27851	0.51240	0.74160
H	-4.82829	-1.58975	0.07924	H	-3.70164	-2.03446	-0.74060	H	-5.01746	-1.22468	0.55732
C	-1.99904	-2.68949	1.18961	C	-2.15557	-2.96573	1.84922	C	-3.83953	-0.40361	3.44217
H	-2.24534	-3.74437	1.10950	H	-2.50411	-3.98571	1.72223	H	-4.78493	-0.54461	3.95578
H	-0.95049	-2.43835	1.32840	H	-1.28933	-2.82121	2.48357	H	-2.95072	-0.34740	4.05864
H	-3.57400	0.22968	1.54474	H	-0.95374	-0.89373	2.97583	H	-1.13757	-0.65261	2.93532
H	-1.17235	-0.88384	2.99781	H	-3.43045	-0.05117	2.19858	H	-2.35037	-1.61334	1.18403
O	-0.67130	-1.60964	3.76643	O	-4.17553	0.54877	2.82812	O	-2.12264	-2.74138	1.25238
O	0.51048	-1.81839	3.34758	O	-3.74532	1.74959	2.88864	O	-2.26387	-3.05854	2.47810

d-limonene- TS- 5				d-limonene- TS- 6				d-limonene- TS- 7			
											
	X	Y	Z		X	Y	Z		X	Y	Z
C	0.00000	0.00000	0.00000	C	0.08876	0.09511	0.00113	C	-0.03208	0.07809	0.00889
C	0.00000	0.00000	1.36802	C	0.04892	-0.05330	1.35086	C	-0.00117	-0.10548	1.33161
H	0.95390	0.00000	1.89275	H	0.98577	-0.14237	1.89768	H	0.96128	-0.25749	1.81762
C	1.25572	-0.03794	-0.80946	C	1.38493	0.09000	-0.76705	C	1.19855	0.06336	-0.85344
H	2.14656	-0.05414	-0.17756	H	2.23963	-0.06060	-0.10384	H	2.09574	-0.14372	-0.26538
H	1.26560	-0.93600	-1.44023	H	1.38868	-0.71036	-1.51512	H	1.11344	-0.69958	-1.63588
H	1.31546	0.82501	-1.48368	H	1.52492	1.03560	-1.30123	H	1.33091	1.02657	-1.35938
C	-1.31524	0.01109	-0.72888	C	-1.14305	0.24439	-0.74482	C	-1.33946	0.31001	-0.73060
H	-1.60994	-1.02772	-0.94522	H	-1.06309	0.75660	-1.70756	H	-1.50826	-0.55018	-1.39957
H	-1.19786	0.50942	-1.69841	C	-1.22435	-0.05693	2.14722	H	-1.23898	1.17601	-1.39524
C	-1.19130	-0.15932	2.14114	H	-1.36464	0.94273	2.58840	C	-1.21894	-0.10991	2.21627
H	-1.12705	0.07170	3.20440	C	-2.43306	0.43371	0.01359	H	-1.30722	0.85887	2.72685
C	-2.39574	0.70493	0.10235	H	-3.27866	0.17147	-0.63019	C	-2.50326	0.49346	0.20247
H	-3.35334	0.69733	-0.42862	H	-2.55449	1.49513	0.28598	H	-2.86617	1.51360	0.35568
H	-2.11253	1.75289	0.25810	C	-2.44102	-0.41812	1.29483	C	-2.51328	-0.39191	1.42494
C	-2.55559	0.03617	1.48295	C	-3.76939	-0.33848	2.01824	C	-3.78534	-0.26649	2.24248

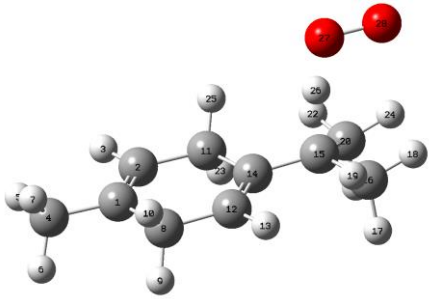
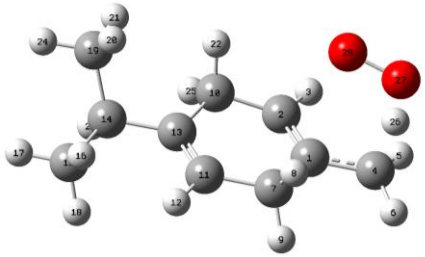
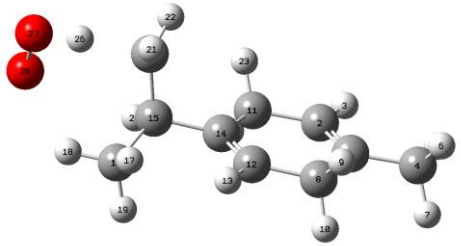
C	-3.54521	0.81676	2.33047	C	-4.96418	-0.80235	1.22154	C	-5.06844	-0.52426	1.49321
C	-4.98876	0.42897	2.14906	H	-5.83703	-0.93422	1.86460	H	-5.91434	-0.60286	2.17914
H	-5.65689	1.09022	2.70503	H	-5.22745	-0.07963	0.44150	H	-5.28672	0.28445	0.78575
H	-5.27275	0.46370	1.09065	H	-4.75024	-1.75051	0.71604	H	-5.00791	-1.44917	0.90854
H	-5.15418	-0.59983	2.48927	C	-3.89966	0.08591	3.27848	C	-3.79576	0.02939	3.54475
C	-3.17378	1.81202	3.13927	H	-4.87369	0.10428	3.75883	H	-4.73350	0.08532	4.08962
H	-3.90757	2.38334	3.69991	H	-3.05749	0.42132	3.87428	H	-2.89197	0.22044	4.11241
H	-2.13136	2.09398	3.25949	H	-1.13406	-0.74994	2.99164	H	-1.11036	-0.86696	3.00179
H	-3.00196	-0.95535	1.29911	H	-2.32361	-1.46643	0.97585	H	-2.44703	-1.43613	1.07415
H	-1.11438	-1.56226	2.20787	H	-1.35523	-1.06991	-1.26752	H	-3.63446	-0.01430	-0.76645
O	-1.06762	-2.72868	1.98827	O	-1.69334	-2.11117	-1.65045	O	-4.32024	-0.39130	-1.50674
O	-0.37421	-2.85300	0.93036	O	-2.95694	-2.20021	-1.50030	O	-3.64644	-0.63987	-2.57719

d-limonene- TS- 8				d-limonene- TS- 9				gamma-terpinene- TS- 1			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.06809	0.15917	0.00878	C	-0.14078	-0.25105	0.16436	C	-0.06795	-0.09568	-0.04253
C	0.03810	0.08507	1.36950	C	-0.31836	-0.41171	1.48034	C	-0.02827	0.12173	1.28703
H	0.98226	0.11388	1.91120	H	0.52643	-0.72893	2.09012	H	0.93056	0.12662	1.80147
C	1.31385	0.19567	-0.70551	C	1.17498	-0.52008	-0.51234	C	1.16675	-0.32291	-0.87088
H	2.22674	0.34514	-0.13051	H	1.92304	-0.88898	0.19350	H	2.06900	-0.28986	-0.25596
H	1.31302	0.62741	-1.70852	H	1.05550	-1.26561	-1.30772	H	1.12266	-1.29602	-1.37168
C	-1.21414	0.12587	-0.79439	H	1.56365	0.38961	-0.98490	H	1.25020	0.43880	-1.65351
H	-1.30395	-0.86368	-1.26367	C	-1.26355	0.20454	-0.73907	C	-1.35495	-0.06169	-0.74032
H	-1.14139	0.84338	-1.61961	H	-1.56710	-0.63908	-1.37708	H	-1.39969	-0.61045	-1.68767
C	-1.21838	-0.00436	2.18263	H	-0.88477	0.97412	-1.42414	C	-1.25159	0.37250	2.11480
H	-1.40949	0.97949	2.63879	C	-1.62639	-0.18355	2.19473	C	-2.57100	-0.03763	0.05855
C	-2.45279	0.40835	0.05601	H	-1.57400	0.77758	2.72525	H	-3.51539	-0.16481	-0.46372
H	-3.34827	0.19168	-0.53346	C	-2.47078	0.73747	0.03280	C	-2.55713	0.16977	1.39379
H	-2.49324	1.47226	0.32699	H	-3.33438	0.83683	-0.63392	C	-3.79996	0.19690	2.25606
C	-2.42888	-0.42441	1.34851	H	-2.25252	1.73909	0.42698	C	-5.08139	0.53037	1.49231
C	-3.74630	-0.37708	2.09721	C	-2.80146	-0.18508	1.21749	H	-5.34774	-0.27255	0.79645
C	-4.94922	-0.86503	1.32723	C	-4.14490	0.16931	1.82604	H	-5.91490	0.64403	2.19150

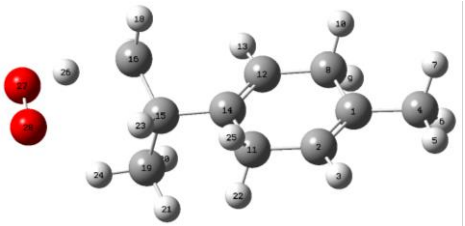
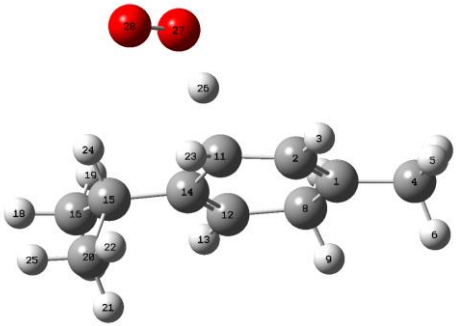
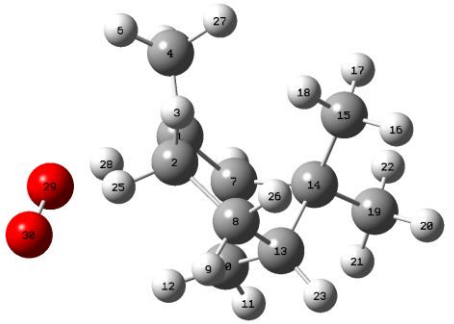
H	-5.79932	-1.03221	1.99211	C	-5.30359	-0.33776	1.16715	H	-4.98006	1.45849	0.92271
H	-5.25710	-0.14035	0.56612	H	-6.27830	0.06041	1.44345	C	-3.96325	-1.13889	3.00221
H	-4.72650	-1.80364	0.80695	H	-5.21021	-0.68776	0.13953	H	-4.15230	-1.94505	2.28574
C	-3.86669	0.03892	3.36130	C	-4.27677	0.89349	2.98086	H	-3.07161	-1.40083	3.57874
H	-4.83350	0.03248	3.85625	H	-5.26269	1.12388	3.37188	H	-1.22466	-0.25141	3.02080
H	-3.02575	0.39361	3.94712	H	-3.42474	1.24532	3.54865	H	-3.64164	0.98103	3.01197
H	-1.06879	-0.69838	3.01895	H	-1.78290	-0.95251	2.95966	H	-4.80907	-1.08893	3.69491
H	-2.27764	-1.47486	1.04721	H	-2.89288	-1.20831	0.82085	H	-1.22727	1.40725	2.50045
H	1.44395	-1.13406	-1.20226	H	-5.31530	-1.63775	1.85360	H	-1.30581	1.14188	-1.38537
O	1.41997	-2.14407	-1.76317	O	-5.14467	-2.57183	2.48151	O	-1.15939	2.10714	-2.10221
O	0.81005	-1.94576	-2.86555	O	-4.19848	-2.28648	3.28602	O	-0.74287	1.69341	-3.22546

gamma-terpinene- TS- 2				gamma-terpinene- TS- 3				gamma-terpinene- TS- 4			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.00262	-0.10141	-0.03431	C	0.04700	0.06371	0.23192	C	0.04235	-0.06271	0.23229
C	-0.25433	-0.95841	0.95519	C	-0.04427	0.31452	1.55752	C	-0.04986	-0.30666	1.55910
H	0.44889	-1.76625	1.15155	H	0.85426	0.57354	2.11358	H	0.84549	-0.57886	2.11399
C	1.22693	-0.19881	-0.90015	C	1.34325	0.13121	-0.51726	C	1.33534	-0.15544	-0.51982
H	1.86192	-1.03693	-0.60379	H	2.17264	0.40897	0.13694	H	2.16152	-0.44477	0.13343
H	0.94943	-0.33129	-1.95247	H	1.57267	-0.84052	-0.97097	H	1.26236	-0.88582	-1.33426
H	1.81981	0.72155	-0.83978	H	1.28484	0.85944	-1.33479	H	1.58023	0.81039	-0.97803
C	-0.93267	1.03624	-0.34663	C	-1.17216	-0.30076	-0.56591	C	-1.17238	0.31958	-0.56396
H	-1.20242	1.00325	-1.41366	H	-1.03762	-1.31727	-0.97067	H	-1.24665	-0.33133	-1.44977
H	-0.39802	1.99169	-0.22588	H	-1.23320	0.34809	-1.45425	H	-1.02153	1.33219	-0.97273
C	-1.45688	-0.89284	1.85280	C	-1.28575	0.16777	2.29488	C	-1.28681	-0.13573	2.29891
H	-1.12403	-0.73879	2.88936	H	-1.35084	0.68052	3.25569	C	-2.45475	0.27749	0.20936
C	-2.18386	1.05111	0.47769	C	-2.45548	-0.23400	0.20410	H	-3.37417	0.44657	-0.34810
H	-2.90347	1.82707	0.23263	H	-3.37628	-0.38975	-0.35496	C	-2.52339	0.03570	1.53549
C	-2.45321	0.18479	1.48159	C	-2.52320	0.01420	1.52909	C	-3.84838	-0.00487	2.26944
C	-3.71924	0.21410	2.21720	C	-3.84907	0.08000	2.25964	C	-4.13793	-1.40507	2.82498
C	-3.74179	-0.30001	3.64179	C	-3.92852	-0.96612	3.37842	H	-3.40516	-1.68698	3.58883

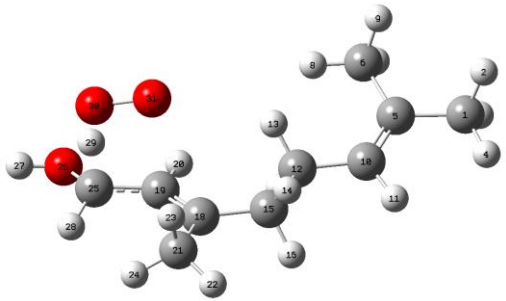
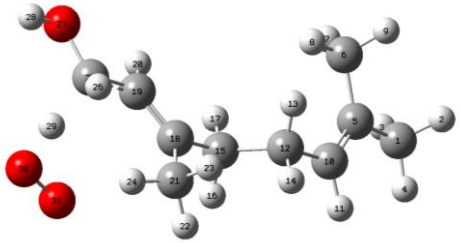
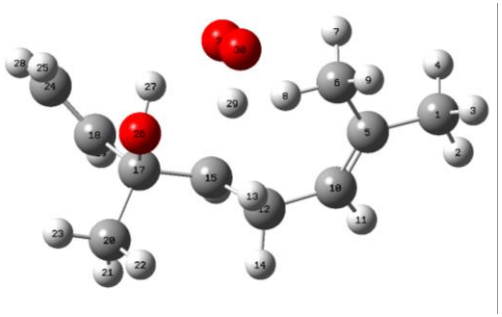
H	-3.30332	0.44833	4.31822	H	-3.18671	-0.76527	4.16016	H	-5.12758	-1.43322	3.29165
H	-4.77220	-0.47571	3.96376	H	-4.91629	-0.94504	3.84909	H	-4.10776	-2.15816	2.03243
H	-3.18499	-1.23100	3.76642	H	-3.74778	-1.97404	2.99436	C	-3.90745	1.04677	3.38431
C	-4.70444	1.33074	1.95485	C	-4.11626	1.48705	2.80905	H	-3.16721	0.83650	4.16505
H	-4.34002	2.27684	2.37904	H	-3.38074	1.75948	3.57369	H	-3.71073	2.05001	2.99587
H	-4.88578	1.48507	0.88833	H	-4.07139	2.23643	2.01369	H	-1.35820	-0.64343	3.26195
H	-1.96453	-1.86875	1.85707	H	-4.63077	-0.14943	1.52455	H	-4.62790	0.23486	1.53533
H	-5.66306	1.09873	2.42703	H	-5.10645	1.53373	3.27308	H	-4.89428	1.04413	3.85742
H	-4.40943	-0.85528	1.60040	H	-1.12365	-1.14188	2.73073	H	-1.10142	1.17274	2.72899
O	-5.15036	-1.67615	1.24378	O	-0.96319	-2.33586	2.78017	O	-0.92075	2.36409	2.77328
O	-6.17793	-1.62022	1.99675	O	-0.80218	-2.70448	1.57941	O	-0.75642	2.72525	1.57072

gamma-terpinene- TS- 5				gamma-terpinene- TS- 6				gamma-terpinene- TS- 7			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.02293	-0.01117	-0.01580	C	0.07314	0.34736	-0.15478	C	0.00282	0.02736	0.05051
C	-0.01740	-0.28495	1.28929	C	0.07835	0.11001	1.19411	C	-0.00215	0.03822	1.38533
H	0.91448	-0.47962	1.81807	H	1.03569	0.05706	1.70928	H	0.94696	0.01958	1.91890
C	1.30484	0.04038	-0.79812	C	1.28488	0.43174	-0.89375	C	1.27088	-0.01155	-0.75562
H	2.16935	-0.17284	-0.16487	H	2.21369	0.58739	-0.34678	H	2.15466	-0.02368	-0.11336
H	1.28960	-0.68808	-1.61761	H	1.25566	0.84935	-1.89927	H	1.29734	-0.90091	-1.39626
H	1.44499	1.02849	-1.25186	C	-1.23172	0.38500	-0.91370	H	1.33729	0.86015	-1.41736
C	-1.23444	0.26490	-0.79632	H	-1.25669	-0.47094	-1.60484	C	-1.27642	0.05833	-0.74538
H	-1.33006	-0.47303	-1.60854	H	-1.24976	1.27889	-1.55115	H	-1.29175	-0.79679	-1.43825
H	-1.13583	1.23281	-1.31239	C	-1.14861	-0.15536	2.00060	H	-1.27564	0.94624	-1.39612
C	-1.27314	-0.35958	2.10989	C	-2.45459	0.36296	-0.03907	C	-1.24556	0.08634	2.22683
C	-2.48494	0.27199	0.02872	H	-3.39654	0.55678	-0.54545	C	-2.52280	0.04536	0.09382
H	-3.40136	0.51289	-0.50274	C	-2.44435	0.12586	1.27555	H	-3.46646	0.03319	-0.44736
C	-2.53476	-0.00308	1.35302	C	-3.68720	0.11677	2.14530	C	-2.52512	0.05459	1.42988
C	-3.78170	0.07522	2.11729	C	-4.96621	0.50983	1.40999	C	-3.80916	0.01012	2.25686
C	-5.08439	0.31813	1.38831	H	-5.21597	-0.22716	0.63840	C	-5.03506	0.60411	1.56406
H	-5.38413	-0.57461	0.82161	H	-5.80307	0.55106	2.11309	H	-5.34301	-0.00469	0.70773

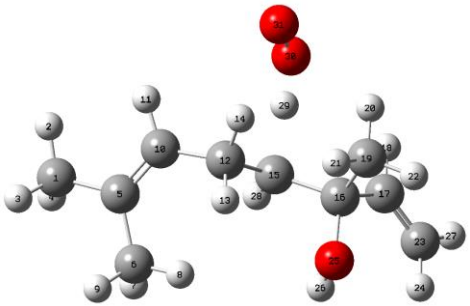
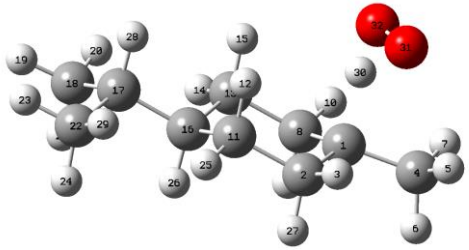
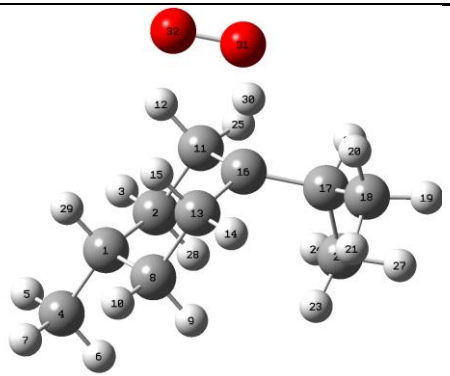
H	-5.87696	0.54014	2.10829	H	-4.87510	1.49013	0.93344	H	-5.87538	0.64917	2.26216
H	-5.02176	1.15689	0.69054	C	-3.87140	-1.25037	2.82364	H	-4.82765	1.61660	1.20865
C	-3.92668	-0.77763	3.36025	H	-3.97033	-2.03639	2.06678	C	-4.03941	-1.43179	2.62928
H	-4.14635	-1.81795	3.07816	H	-3.03038	-1.50725	3.47323	H	-4.55849	-2.05355	1.89895
H	-3.02850	-0.78095	3.98106	H	-1.12167	-1.21079	2.31556	H	-3.28028	-1.94667	3.21691
H	-1.37181	-1.37335	2.52393	H	-3.51615	0.85835	2.94163	H	-1.23707	-0.74454	2.94779
H	-4.75895	-0.41629	3.97114	H	-4.77646	-1.25160	3.43870	H	-3.62169	0.58271	3.17643
H	-1.17798	0.29946	2.98576	H	-1.11537	0.42060	2.93776	H	-1.24008	0.99594	2.84685
H	-3.62969	1.33353	2.74487	H	1.38279	-1.00236	-1.18520	H	-5.15253	-1.27190	3.74842
O	-3.71459	2.31937	3.35405	O	1.29126	-2.14343	-1.24540	O	-5.83432	-1.01728	4.53055
O	-4.75033	2.22748	4.09217	O	0.40315	-2.46817	-0.38851	O	-5.55797	0.19136	4.89117

gamma-terpinene- TS- 8				gamma-terpinene- TS- 9				pinane- TS			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.00871	0.05619	0.07208	C	0.00000	0.00000	0.00000	C	0.00000	0.00000	0.00000
C	-0.10249	0.38312	1.36164	C	0.00000	0.00000	1.35054	C	0.00000	0.00000	1.52441
H	0.79998	0.58891	1.93536	H	0.94676	0.00000	1.88654	H	1.03868	0.00000	1.87861
C	1.33528	-0.04206	-0.62793	C	1.25958	-0.00644	-0.81323	C	1.30183	0.29348	-0.70116
H	2.16314	0.18973	0.04636	H	2.14797	0.00477	-0.17787	H	1.14942	0.46108	-1.77202
H	1.48920	-1.05054	-1.02969	H	1.30290	-0.89366	-1.45595	H	1.78707	1.17941	-0.27812
H	1.37837	0.64962	-1.47759	H	1.29771	0.86742	-1.47493	C	-0.95232	-0.97974	-0.62652
C	-1.20109	-0.23682	-0.77776	C	-1.29400	0.00917	-0.76306	C	-0.79444	-1.17645	2.16938
H	-1.08740	-1.23078	-1.23642	H	-1.26818	-0.78080	-1.53050	H	-1.47747	-0.78132	2.92822
H	-1.22351	0.46332	-1.62708	H	-1.35697	0.94607	-1.34386	C	-2.28358	-0.96360	0.17207
C	-1.40751	0.50124	2.09619	C	-1.22753	0.04561	2.12788	H	-3.11478	-1.39471	-0.38592
C	-2.50352	-0.17293	-0.03140	C	-2.52375	-0.14425	0.08172	H	-2.59430	-0.00186	0.59260
H	-3.39959	-0.41732	-0.60021	H	-3.46609	-0.25021	-0.44915	C	-1.60505	-1.96230	1.13752
C	-2.61156	0.14838	1.26062	C	-2.50151	-0.15504	1.42999	C	-0.70962	-2.42819	-0.04654
C	-3.94227	0.14554	2.00765	C	-3.73078	-0.34249	2.29930	C	0.71435	-2.88141	0.25108
C	-5.10027	0.48537	1.11671	C	-5.04929	-0.07966	1.57433	H	0.69683	-3.83921	0.78459
H	-5.63438	-0.32451	0.61880	H	-5.23354	-0.83432	0.80123	H	1.27120	-3.03239	-0.68117

H	-5.07048	1.43068	0.57678	H	-5.88065	-0.12971	2.28320	H	1.27435	-2.17223	0.86548
C	-4.16723	-1.19507	2.72243	H	-5.05996	0.90737	1.10285	C	-1.39327	-3.48929	-0.90851
H	-4.28715	-1.99572	1.98526	C	-3.73280	-1.75286	2.90961	H	-1.40791	-4.44964	-0.38024
H	-3.31852	-1.44924	3.36275	H	-3.82633	-2.50272	2.11652	H	-2.42498	-3.23198	-1.15978
H	-1.38795	-0.13200	2.99572	H	-2.81318	-1.95959	3.46436	H	-0.84436	-3.63016	-1.84638
H	-3.87211	0.92921	2.77877	H	-1.17260	-0.33496	3.15391	H	-2.22535	-2.72823	1.61719
H	-5.06188	-1.15482	3.35120	H	-3.64624	0.37920	3.12426	H	-0.98655	-0.88510	-1.71847
H	-1.52819	1.52687	2.47707	H	-4.57537	-1.87229	3.59759	H	-0.42750	0.94900	1.88003
H	-6.18546	0.84390	2.21593	H	-1.34091	1.32901	2.57584	H	-0.10552	-1.85328	2.68714
O	-6.80477	1.09908	3.04930	O	-1.53385	2.37535	3.16122	H	2.00436	-0.54609	-0.59362
O	-6.02277	1.33063	4.04883	O	-1.81918	2.09510	4.36334	H	-0.70850	1.26887	-0.26973
								O	-1.24391	2.24157	-0.39783
								O	-1.81462	2.51508	0.72055

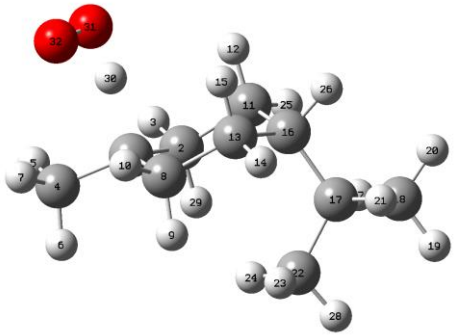
geraniol- TS -1				geraniol- TS -2				linalool- TS- 1			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.08911	0.09226	0.05391	C	0.01470	-0.03642	-0.10293	C	-0.05212	-0.03603	-0.10255
H	-0.10625	0.13555	1.14945	H	0.05030	-0.06864	0.99254	H	-0.05131	-0.11031	0.98735
H	0.96502	0.05443	-0.24549	H	1.05321	-0.03677	-0.45445	H	0.98677	-0.05126	-0.45206
H	-0.57060	-0.83664	-0.26092	H	-0.46955	-0.94903	-0.45825	H	-0.54008	-0.92881	-0.51042
C	-0.76847	1.30069	-0.53575	C	-0.70762	1.19830	-0.57511	C	-0.75462	1.20813	-0.57683
C	-0.15420	2.61834	-0.14083	C	-0.09163	2.49556	-0.12004	C	-0.77624	1.38742	-2.07231
H	0.90313	2.64079	-0.43037	H	0.94875	2.55634	-0.46057	H	-1.24436	0.51657	-2.54472
H	-0.64764	3.47749	-0.59788	H	-0.61823	3.37579	-0.49228	H	-1.32222	2.27827	-2.39157
H	-0.18564	2.74432	0.94786	H	-0.06840	2.54593	0.97500	H	0.24594	1.45651	-2.46236
C	-1.82928	1.17802	-1.34421	C	-1.80249	1.11416	-1.34170	C	-1.31867	2.06130	0.28725
H	-2.17109	0.16932	-1.57910	H	-2.14130	0.11907	-1.63133	H	-1.26670	1.82813	1.34992
C	-2.58147	2.29870	-2.00893	C	-2.59922	2.26460	-1.89662	C	-2.07848	3.31243	-0.08940
H	-2.54785	3.21744	-1.41631	H	-2.56680	3.13039	-1.22638	H	-1.65376	3.79202	-0.97657
H	-3.63978	2.02497	-2.09158	H	-3.65171	1.96778	-1.97027	H	-1.98841	4.04218	0.73053
C	-2.02426	2.60376	-3.41845	C	-2.09139	2.69420	-3.28942	C	-3.54249	3.04895	-0.33048
H	-2.08906	1.69067	-4.02692	H	-2.15001	1.82968	-3.96619	H	-4.09872	2.60935	0.50423

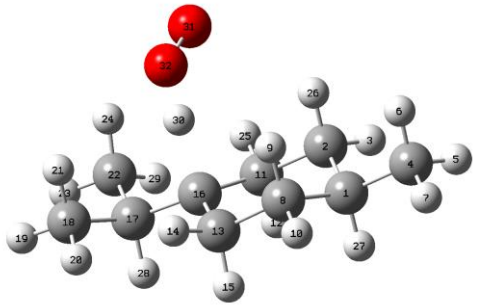
H	-0.96287	2.85957	-3.33027	H	-1.03376	2.96859	-3.21267	C	-4.32407	4.00360	-1.21906
C	-2.77489	3.71676	-4.09081	C	-2.88058	3.82900	-3.87799	C	-5.75365	3.52594	-1.37144
C	-2.17474	4.91359	-4.32390	C	-2.28096	5.00915	-4.17788	H	-6.23282	3.18115	-0.45598
H	-1.13751	5.05628	-4.02468	H	-1.20563	5.11209	-4.04099	C	-4.31127	5.41203	-0.60341
C	-4.22748	3.46822	-4.39038	C	-4.34842	3.58501	-4.10015	H	-4.77508	5.40514	0.38672
H	-4.41325	2.40356	-4.56081	H	-4.51506	2.54938	-4.41323	H	-3.28270	5.77193	-0.51770
H	-4.84803	3.78003	-3.54055	H	-4.91693	3.74257	-3.17497	H	-4.87177	6.08532	-1.25656
H	-4.57172	4.01755	-5.27086	H	-4.76858	4.23309	-4.87222	C	-6.42510	3.51580	-2.51984
C	-2.83908	6.09027	-4.81400	C	-2.93080	6.13369	-4.79994	H	-5.97500	3.86669	-3.44422
O	-1.98091	7.12360	-5.14475	H	-3.98119	6.32694	-4.56027	O	-3.67646	4.13832	-2.47808
H	-2.48278	7.88696	-5.44938	O	-2.13583	7.26258	-4.87717	H	-3.79485	3.31434	-2.97136
H	-3.69289	5.96556	-5.48815	H	-2.61914	7.98014	-5.30008	H	-7.44942	3.16269	-2.56464
H	-3.53128	6.42852	-3.62325	H	-3.08175	5.57561	-6.10425	H	-3.60361	1.75245	-1.14582
O	-4.09112	6.58547	-2.59356	O	-3.20903	5.00476	-7.12456	O	-3.81792	0.85737	-1.73022
O	-3.79888	5.58449	-1.86269	O	-2.88764	3.79000	-6.91338	O	-4.87907	0.32884	-1.22845

linalool- TS- 2				limonane- TS- 1				limonane- TS- 2			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.02145	-0.01838	-0.01729	C	-0.12173	-0.13205	0.05378	C	-0.03742	0.05573	-0.06857
H	-0.05178	-0.06502	1.07360	C	-0.01508	0.01404	1.54833	C	-0.04232	-0.10106	1.45374
H	1.02801	0.00012	-0.33386	H	1.03901	0.06519	1.84547	H	0.98591	-0.13050	1.83357
H	-0.45745	-0.94216	-0.41539	C	0.77007	-1.15834	-0.58615	C	0.72346	-1.08556	-0.73974
C	-0.75540	1.18660	-0.54284	H	1.81129	-1.02753	-0.27418	H	1.75728	-1.13617	-0.38383
C	-0.77207	1.31310	-2.04417	H	0.45863	-2.16970	-0.28024	H	0.24492	-2.04715	-0.51938
H	-1.26858	0.44306	-2.49099	H	0.72007	-1.11403	-1.67821	H	0.74473	-0.96272	-1.82712
H	-1.28368	2.21281	-2.39265	C	-1.51053	0.02766	-0.50461	C	-1.47583	0.14571	-0.58315
H	0.25084	1.32762	-2.43788	H	-2.07779	-0.88806	-0.25327	H	-1.98603	-0.80667	-0.38135
C	-1.34281	2.06271	0.28167	H	-1.47949	0.07282	-1.59977	H	-1.47964	0.28464	-1.67091
H	-1.29015	1.88039	1.35419	C	-0.78558	1.21925	2.09707	C	-0.80760	1.04476	2.14799
C	-2.11644	3.28392	-0.14751	H	-0.27292	2.14513	1.79659	H	-0.23443	1.97042	1.98412
H	-1.60763	3.81528	-0.96853	C	-2.25224	1.24148	0.06505	C	-2.24321	1.30768	0.08017
H	-2.15934	4.00063	0.68301	H	-3.27883	1.22955	-0.31107	H	-3.27213	1.35029	-0.28792
C	-3.51298	2.96280	-0.60741	H	-1.78571	2.16455	-0.31106	H	-1.75378	2.24316	-0.23278
C	-4.35897	4.04169	-1.26519	C	-2.23740	1.27682	1.60021	C	-2.20143	1.23047	1.59014

C	-5.79988	3.58299	-1.33826	C	-2.99025	2.50373	2.15631	C	-3.36343	0.64528	2.37845
H	-6.23412	3.26692	-0.38932	C	-4.44255	2.55580	1.66897	C	-4.73219	1.11428	1.87678
C	-4.27295	5.37565	-0.52500	H	-4.97703	3.38192	2.14745	H	-5.51216	0.82256	2.58589
H	-4.61398	5.26831	0.50889	H	-4.51912	2.70031	0.58886	H	-4.77203	2.20216	1.75883
H	-3.24236	5.73847	-0.52174	H	-4.96698	1.62690	1.92640	H	-4.97950	0.65841	0.91247
H	-4.90143	6.10832	-1.03557	C	-2.97085	2.54231	3.68838	C	-3.31765	-0.89341	2.42813
C	-6.53713	3.56223	-2.44615	H	-3.58822	3.36656	4.05798	H	-3.39712	-1.31718	1.42132
H	-6.14144	3.90321	-3.39859	H	-3.37824	1.61053	4.10069	H	-2.39227	-1.25605	2.88346
O	-3.81762	4.28862	-2.56469	H	-0.75370	1.18137	3.18922	H	-0.84964	0.87923	3.23103
H	-3.91501	3.48566	-3.09435	H	-2.76032	0.37498	1.96639	H	-3.24431	1.00012	3.41329
H	-7.56791	3.22555	-2.42556	H	-0.42078	-0.91055	2.00028	H	-4.15682	-1.27278	3.02042
H	-3.67116	1.95309	-1.00131	H	-2.47175	3.40130	1.78496	H	-0.50192	-1.06723	1.70321
H	-4.17686	2.72298	0.80279	H	-1.96544	2.68105	4.09214	H	0.46606	1.00479	-0.31030
O	-4.54645	2.68356	1.80749	H	0.60191	1.13527	-0.37300	H	-2.39782	2.66852	1.90057
O	-3.81957	3.48769	2.50819	O	2.35076	1.73115	0.11176	O	-2.40051	3.76918	2.04831
				O	1.28443	1.96755	-0.57261	O	-1.37770	4.22552	1.41717

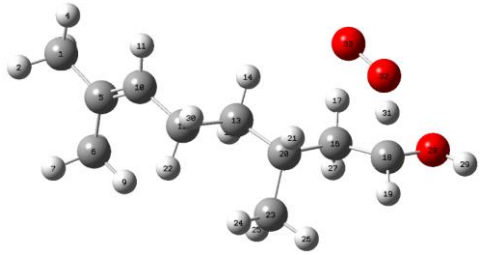
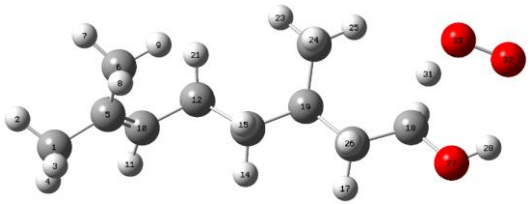
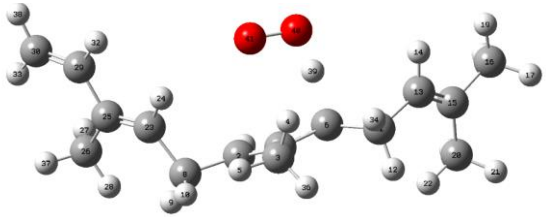
limonane- TS- 3	limonane- TS- 4



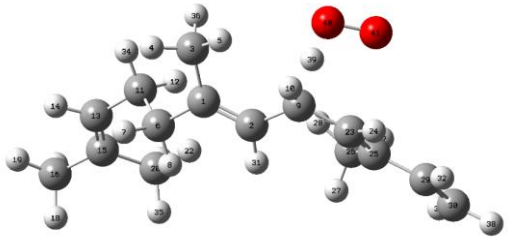
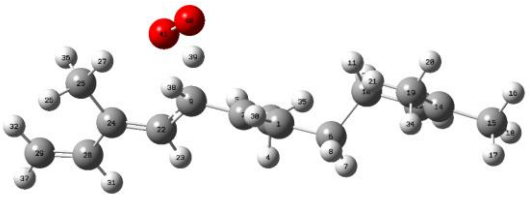
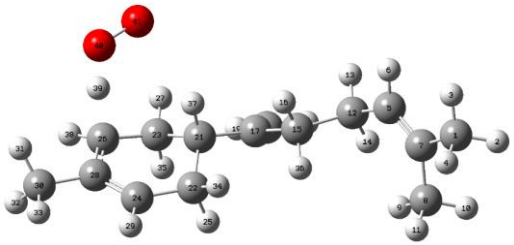


	X	Y	Z		X	Y	Z
C	-0.10304	-0.15398	0.11003	C	-0.01491	-0.00134	0.02350
C	-0.02161	0.01518	1.60544	C	-0.05430	-0.03527	1.55144
H	1.02909	0.04369	1.92004	H	0.96292	-0.07320	1.95800
C	0.74838	-1.22738	-0.50850	C	0.74220	-1.20063	-0.54067
H	1.76226	-1.22765	-0.09703	H	1.77028	-1.23248	-0.16636
H	0.30898	-2.21754	-0.30836	H	0.24938	-2.13489	-0.24743
H	0.80833	-1.10926	-1.59530	H	0.77952	-1.16904	-1.63424
C	-1.45408	0.06276	-0.52245	C	-1.44736	0.05539	-0.50785
H	-2.03145	-0.86666	-0.39339	H	-1.96850	-0.86545	-0.20753
H	-1.32803	0.18432	-1.60595	H	-1.44802	0.07513	-1.60388
C	-0.75103	1.27242	2.08851	C	-0.79274	1.16571	2.14926
H	-0.18410	2.14622	1.73907	H	-0.18269	2.07859	2.00808
C	-2.22326	1.26858	0.04100	C	-2.21347	1.26990	0.02362
H	-3.25759	1.24212	-0.32190	H	-3.25345	1.22664	-0.31426
H	-1.77609	2.17576	-0.38542	H	-1.78746	2.18820	-0.42312
C	-2.19500	1.40793	1.57543	C	-2.14554	1.42972	1.52717

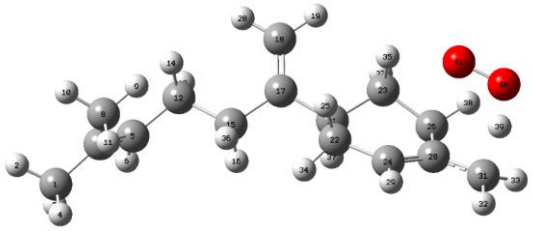
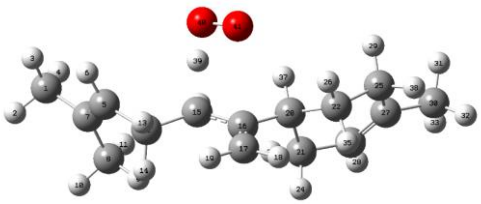
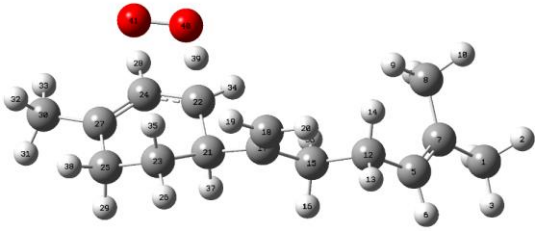
C	-3.23224	0.54504	2.34026	C	-2.96860	2.56175	2.12669
C	-4.60322	1.23134	2.32087	C	-4.42381	2.56497	1.63938
H	-5.34522	0.64455	2.87150	H	-4.97850	3.37302	2.12434
H	-4.55749	2.22809	2.76992	H	-4.50396	2.71396	0.56031
H	-4.96779	1.34230	1.29267	H	-4.91890	1.62051	1.89453
C	-3.40211	-0.90091	1.85947	C	-2.93304	2.58385	3.65977
H	-3.84329	-0.92778	0.85652	H	-3.57688	3.38381	4.03583
H	-2.46392	-1.46066	1.83283	H	-3.29596	1.63561	4.07247
H	-0.74086	1.31311	3.18361	H	-0.89114	1.02758	3.23041
H	-2.48330	2.44567	1.79220	H	-0.55470	-0.96031	1.87132
H	-2.89696	0.50960	3.38716	H	0.50226	0.92052	-0.28837
H	-4.08567	-1.43401	2.52797	H	-2.49672	3.49616	1.76786
H	-0.44823	-0.88290	2.08419	H	-1.92727	2.75939	4.04817
H	0.60328	1.07866	-0.41971	H	-2.89155	0.18938	2.02686
O	1.06529	1.89888	-0.98258	O	-2.69606	-0.99391	3.52303
O	0.76698	1.70033	-2.22052	O	-3.36496	-0.69524	2.46097

citronellol- TS- 1				citronellol- TS- 2				a-farnesene- TS- 1			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	-0.24344	-0.11699	-0.11240	C	0.09362	0.00529	-0.01766	C	-0.14064	-0.50816	0.32957
H	-0.18505	-0.11714	0.98271	H	0.08713	-0.01472	1.07868	C	-0.08626	-0.39898	1.69253
H	0.77782	-0.26110	-0.48469	H	1.14357	0.06489	-0.32779	C	1.07531	-0.41209	-0.55761
H	-0.84737	-0.97231	-0.42442	H	-0.31982	-0.93853	-0.38096	H	0.94292	0.39277	-1.28845
C	-0.81700	1.18257	-0.61472	C	-0.68335	1.18899	-0.53228	H	1.98498	-0.19852	0.00291
C	-0.03432	2.40584	-0.21288	C	-0.16807	2.52531	-0.06459	C	-1.42688	-0.62793	-0.30634
H	0.00137	2.49811	0.87925	H	-0.20825	2.59126	1.02917	H	-2.26215	-0.86385	0.35838
H	1.00321	2.31668	-0.55602	H	0.88423	2.64204	-0.34923	C	1.12291	-0.13198	2.54304
H	-0.44395	3.33111	-0.62169	H	-0.72260	3.36891	-0.47926	H	1.07960	-0.75424	3.44076
C	-1.92881	1.21101	-1.36056	C	-1.73760	1.03137	-1.34290	H	2.04228	-0.40368	2.01466
H	-2.39230	0.25633	-1.61149	H	-2.00111	0.01457	-1.63598	C	-1.58831	-1.15380	-1.72132
C	-2.59022	2.42960	-1.94741	C	-2.57934	2.12560	-1.94523	H	-1.36535	-2.23029	-1.73412
C	-2.11517	2.69736	-3.38206	C	-2.06018	2.54644	-3.32756	C	-2.96847	-0.88709	-2.26769
H	-2.21485	1.77416	-3.96680	H	-1.93942	1.64513	-3.94319	H	-3.10691	0.08530	-2.74063
H	-1.04220	2.94127	-3.36119	H	-1.05388	2.97556	-3.21332	C	-4.02868	-1.70047	-2.18703
C	-2.32481	3.97191	-5.53004	C	-2.41964	3.73883	-5.49730	C	-5.36409	-1.30142	-2.75850
H	-2.08889	2.98745	-5.95434	H	-2.35941	2.76491	-6.00684	H	-5.69307	-2.02579	-3.51298
C	-3.28071	4.66070	-6.45682	C	-3.25805	4.65169	-6.34144	H	-6.13165	-1.28676	-1.97591
H	-3.85488	5.50926	-6.06711	C	-2.95402	3.54493	-4.07332	H	-5.32637	-0.31333	-3.22267

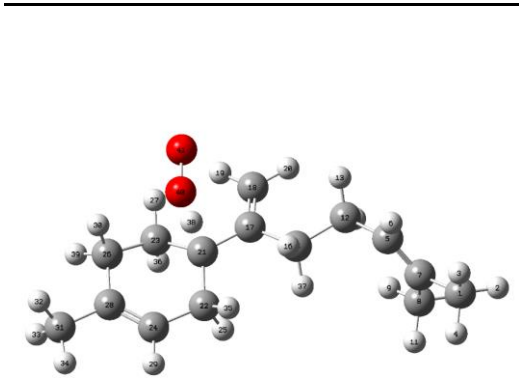
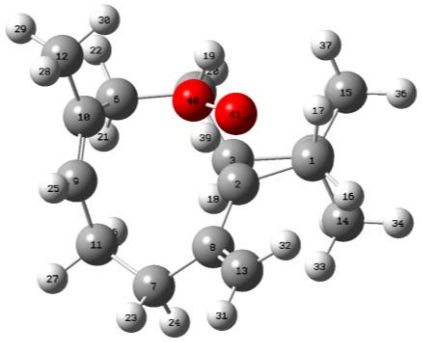
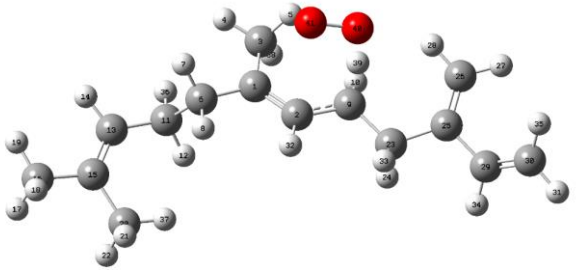
C	-2.87507	3.81435	-4.10494	H	-3.96143	3.10600	-4.14527	C	-4.00873	-3.05730	-1.53274
H	-3.92802	3.50248	-4.17544	H	-2.61436	2.99022	-1.27603	H	-4.26510	-3.83704	-2.25963
H	-2.40409	3.30640	-1.31966	C	-3.06040	4.87992	-3.33072	H	-3.04441	-3.30699	-1.08733
C	-2.80782	5.13967	-3.33984	H	-3.41846	4.74310	-2.30729	C	1.16309	1.33400	2.89833
H	-3.34121	5.08436	-2.38738	H	-2.07956	5.36974	-3.28405	H	1.22299	1.99691	2.03505
H	-1.76342	5.40211	-3.12911	H	-3.75611	5.56842	-3.82061	C	1.08822	1.89800	4.11766
H	-3.24740	5.96365	-3.91134	H	-1.39296	4.12967	-5.46356	C	0.97376	1.13968	5.41293
H	-1.37966	4.53898	-5.50673	O	-2.80519	4.76264	-7.62260	H	0.07076	1.44393	5.95296
O	-2.77019	4.83780	-7.71548	H	-3.31304	5.44805	-8.08583	H	0.93249	0.06053	5.26724
H	-3.35006	5.39629	-8.24611	H	-3.61345	1.77179	-2.04671	C	1.12441	3.36721	4.20231
H	-3.67792	2.28045	-1.95760	H	-4.35050	4.56727	-6.24126	C	1.08692	4.08440	5.33104
H	-4.33094	3.60580	-6.54600	H	-3.13874	6.05185	-5.89649	H	-1.03279	-0.43125	2.23178
O	-5.00087	2.71128	-6.59125	O	-3.54539	7.42831	-7.17729	H	1.18458	3.88920	3.24835
O	-4.33644	1.71233	-6.13065	O	-3.18518	7.17943	-5.96972	H	1.02493	3.62203	6.31156
								H	-0.84735	-0.68699	-2.37981
								H	-4.76648	-3.10251	-0.74179
								H	1.22488	-1.34237	-1.11628
								H	1.82849	1.36097	6.06133
								H	1.11680	5.16805	5.30192
								H	-1.65587	0.78060	-0.47298
								O	-1.65958	1.93575	-0.57967
								O	-0.63317	2.35073	0.05276

a-farnesene- TS- 2				a-farnesene- TS- 3				b-bisabolene- TS- 1			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.34255	0.13795	-0.35305	C	-0.73142	0.28525	0.47814	C	-0.03447	-0.01484	-0.09596
C	0.43598	0.78275	0.82770	C	-0.97940	-0.05114	1.75977	H	-0.05233	-0.00972	1.00050
C	1.52544	-0.48777	-1.04294	C	0.56774	0.87325	-0.00833	H	1.00752	0.01975	-0.42294
H	1.42923	-0.40234	-2.13040	H	0.45125	1.94564	-0.21098	H	-0.53160	0.90498	-0.42638
H	2.47364	-0.03444	-0.74589	H	1.38938	0.74854	0.69986	C	-0.11767	-2.11197	-1.42119
C	-0.99341	-0.04675	-1.02179	C	-1.77060	0.03051	-0.58555	H	0.92193	-1.90670	-1.67914
H	-0.96352	0.37648	-2.03582	H	-1.80423	0.87951	-1.28161	C	-0.74540	-1.22991	-0.63284
H	-1.76768	0.49947	-0.47143	H	-2.76591	-0.04909	-0.13411	C	-2.18700	-1.34668	-0.21089
C	1.68249	1.02145	1.57413	C	-0.07548	0.11889	2.91191	H	-2.69155	-2.21525	-0.63726
H	2.54217	1.27700	0.95132	C	-1.49665	-1.25972	-1.38930	H	-2.26311	-1.40681	0.88144
C	-1.40879	-1.53034	-1.12201	H	-1.50089	-2.10736	-0.69632	H	-2.74113	-0.45115	-0.51650
H	-1.38265	-1.96939	-0.11829	C	-2.49767	-1.45250	-2.49733	C	-0.70788	-3.35215	-2.03856
C	-2.76721	-1.69325	-1.75140	H	-2.24297	-0.99742	-3.45490	H	0.06315	-4.12910	-2.09893
H	-2.78307	-1.82431	-2.83352	C	-3.67648	-2.08117	-2.40326	H	-1.50772	-3.75545	-1.40919
C	-3.94367	-1.64842	-1.11305	C	-4.60784	-2.18400	-3.58271	C	-1.24906	-3.07413	-3.44553
C	-5.24636	-1.80119	-1.85356	H	-4.80961	-3.23388	-3.82643	H	-0.46170	-2.59122	-4.04262
H	-5.81171	-2.65853	-1.46927	H	-5.57475	-1.71934	-3.35592	C	-1.76527	-4.27150	-4.21448
H	-5.87845	-0.91611	-1.71469	H	-4.19213	-1.69921	-4.46919	C	-1.95052	-5.46617	-3.64558

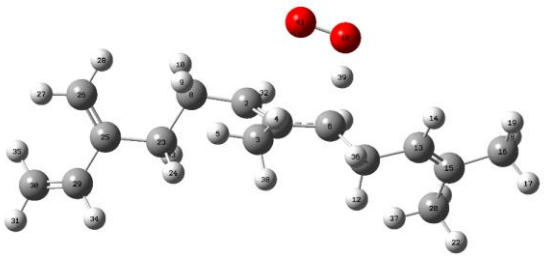
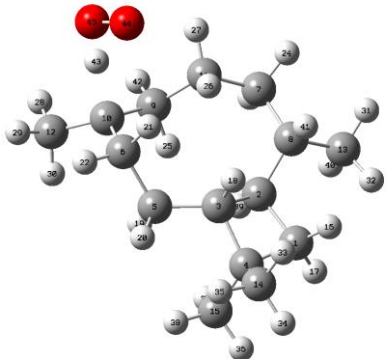
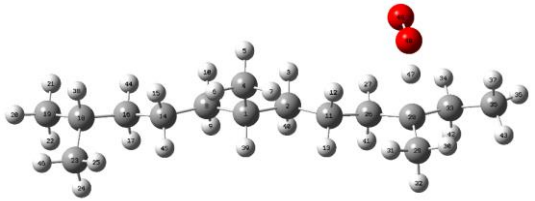
H	-5.08755	-1.94645	-2.92470	C	-4.18803	-2.72931	-1.14315	H	-2.31600	-6.32085	-4.20381
C	-4.08699	-1.44064	0.37235	H	-4.38000	-3.79571	-1.31053	H	-1.73192	-5.63702	-2.59695
H	-4.61945	-2.28375	0.82815	H	-3.49908	-2.63392	-0.30208	C	-2.03999	-4.00527	-5.68291
H	-3.12959	-1.32423	0.88374	C	0.58866	1.37318	3.15550	C	-3.08319	-2.88797	-5.86719
C	1.69778	1.65681	2.86978	H	0.48903	2.13524	2.38380	C	-2.45978	-5.23825	-6.48572
H	2.55375	2.29805	3.07608	C	1.37807	1.68226	4.23371	C	-3.48879	-2.69930	-7.30037
C	0.82129	1.46830	3.90656	C	1.68388	0.70891	5.33463	H	-3.97391	-3.12057	-5.26084
C	-0.30350	0.47030	3.88324	H	1.37615	1.10976	6.30653	C	-2.66325	-4.89194	-7.93923
H	-1.27884	0.96606	3.80504	H	1.19373	-0.25384	5.18913	H	-1.70416	-6.02534	-6.38670
H	-0.20732	-0.23580	3.05789	C	1.96764	3.01172	4.30053	C	-3.29090	-3.62989	-8.26904
C	1.01984	2.25472	5.11901	C	2.76093	3.46079	5.28666	H	-3.98546	-1.76628	-7.56108
C	0.22240	2.23850	6.19847	H	-1.93312	-0.53450	1.97289	C	-3.68933	-3.39078	-9.70228
H	-0.48102	1.16399	1.27382	H	1.73260	3.67734	3.47129	H	-2.81814	-3.46550	-10.36249
H	1.88578	2.91520	5.11816	H	3.03314	2.84219	6.13612	H	-4.41511	-4.14029	-10.03478
H	-0.66048	1.60977	6.25715	H	-0.48853	-1.21777	-1.81646	H	-4.13106	-2.40046	-9.83326
H	-0.66792	-2.07570	-1.71711	H	-5.14380	-2.27874	-0.85006	H	-2.69680	-1.93863	-5.48002
H	-4.68705	-0.54441	0.57026	H	0.86287	0.40648	-0.95397	H	-3.40241	-5.64292	-6.08177
H	1.58844	-1.55708	-0.80629	H	2.76336	0.52626	5.37775	H	-2.04826	-2.32434	-3.35987
H	-0.29827	-0.10507	4.81398	H	3.16296	4.46740	5.26311	H	-1.09679	-3.64121	-6.11979
H	0.43630	2.86539	7.05685	H	-0.38492	-0.42851	3.80372	H	-2.88484	-5.72642	-8.61024
H	2.06189	-0.24682	1.97012	H	1.03149	-0.64983	2.61441	H	-1.30851	-4.69311	-8.36483
O	2.32201	-1.32023	2.45630	O	2.10682	-1.17571	2.42910	O	-0.17433	-4.60779	-8.57051
O	2.41234	-1.14192	3.70570	O	2.97615	-0.26510	2.55567	O	0.44863	-5.12209	-7.58269

b-bisabolene- TS- 2				b-bisabolene- TS- 3				b-bisabolene- TS- 4			
											
	X	Y	Z		X	Y	Z		X	Y	Z
C	0.12598	-0.00037	0.04228	C	-0.09304	0.08292	-0.17444	C	-0.03278	-0.04840	-0.02618
H	0.35480	-0.10871	1.10921	H	-0.49352	0.35712	0.80863	H	-0.35773	0.12186	1.00718
H	1.06780	0.09770	-0.50281	H	0.96413	-0.16703	-0.05865	H	1.04531	-0.22580	-0.02257
H	-0.43649	0.93435	-0.06815	H	-0.17005	0.97373	-0.80897	H	-0.22878	0.87906	-0.57725
C	-0.24323	-1.95438	-1.44345	C	-0.27995	-2.21463	-1.09624	C	-0.14682	-2.28275	-1.10307
H	0.71426	-1.69914	-1.89897	H	0.79436	-2.30223	-0.93817	H	0.94188	-2.29084	-1.04306
C	-0.68313	-1.17232	-0.44936	C	-0.87357	-1.06093	-0.76599	C	-0.78515	-1.20184	-0.63679
C	-1.99613	-1.36743	0.26323	C	-2.34357	-0.79100	-0.95595	C	-2.28070	-1.02379	-0.67487
H	-2.57851	-2.20228	-0.12985	H	-2.88695	-1.64290	-1.36956	H	-2.80143	-1.86407	-1.13722
H	-1.83019	-1.53765	1.33364	H	-2.80814	-0.51682	-0.00158	H	-2.67724	-0.88977	0.33854
H	-2.60719	-0.46091	0.17952	H	-2.48634	0.06091	-1.63172	H	-2.53717	-0.11714	-1.23579
C	-0.95508	-3.13892	-2.04198	C	-0.96336	-3.40691	-1.72151	C	-0.77932	-3.48705	-1.75079
H	-0.21547	-3.88453	-2.35623	H	-0.36653	-4.30542	-1.52768	H	-0.16510	-4.37021	-1.54146
H	-1.59143	-3.62707	-1.29679	H	-1.94059	-3.58741	-1.25050	H	-1.76775	-3.68850	-1.32389
C	-1.80256	-2.73183	-3.25247	C	-1.15745	-3.23464	-3.21538	C	-0.90851	-3.31128	-3.26669
H	-1.17187	-2.17528	-3.96112	C	-1.64313	-4.28280	-4.06982	H	0.08439	-3.10267	-3.69169
C	-2.48795	-3.85468	-4.00061	C	-1.72659	-5.57632	-3.64853	C	-1.51565	-4.46652	-4.02891
C	-2.49739	-5.11601	-3.56008	H	-2.04618	-6.37073	-4.31304	C	-1.85182	-5.62627	-3.45897
H	-2.99738	-5.90984	-4.10419	H	-1.46946	-5.86049	-2.63422	H	-2.28694	-6.44046	-4.02905

H	-2.00609	-5.40111	-2.63596	C	-2.01951	-3.86995	-5.48062	H	-1.71380	-5.80098	-2.39725
C	-3.17478	-3.43179	-5.28666	C	-3.42937	-3.25620	-5.50570	C	-1.73578	-4.18467	-5.50599
C	-4.34976	-2.48033	-4.99014	C	-1.94244	-4.98329	-6.52499	C	-3.00445	-3.37023	-5.72466
C	-3.67627	-4.58152	-6.16124	C	-3.88541	-2.95734	-6.91048	C	-1.78575	-5.42454	-6.40585
C	-5.19971	-2.20201	-6.18945	H	-4.13004	-3.95095	-5.01853	C	-3.48603	-3.23889	-7.06487
H	-4.98213	-2.92866	-4.20649	C	-2.12933	-4.39982	-7.92531	C	-1.94596	-5.02908	-7.87539
C	-4.16364	-4.05673	-7.51036	H	-0.98444	-5.50798	-6.44927	H	-0.88101	-6.02464	-6.26619
H	-2.87925	-5.31605	-6.31517	C	-3.30169	-3.44935	-8.00916	C	-3.03241	-4.01033	-8.09776
C	-5.13412	-2.90442	-7.36759	H	-4.74064	-2.29154	-7.02082	H	-4.28432	-2.52493	-7.25930
H	-5.94020	-1.40854	-6.10275	H	-1.21705	-3.87062	-8.23847	H	-1.00162	-4.61676	-8.26493
H	-3.30927	-3.72393	-8.11619	C	-3.76217	-3.09297	-9.39558	C	-3.56814	-3.87942	-9.48852
C	-6.03201	-2.63281	-8.43691	H	-2.93727	-2.66589	-9.97859	H	-2.75363	-3.71914	-10.20549
H	-6.58804	-1.69666	-8.42140	H	-4.10285	-3.98534	-9.93389	H	-4.07547	-4.80520	-9.78685
H	-5.79054	-3.01943	-9.42641	H	-4.57995	-2.36836	-9.37581	H	-4.27812	-3.05415	-9.57597
H	-3.98864	-1.53059	-4.57783	H	-3.45055	-2.33687	-4.90651	H	-3.17103	-2.52451	-5.05574
H	-4.50677	-5.09141	-5.65632	H	-2.74038	-5.71472	-6.33728	H	-2.63921	-6.04969	-6.12071
H	-2.55719	-2.00938	-2.91085	H	-1.39037	-2.21385	-3.53239	H	-1.49638	-2.40281	-3.46415
H	-2.43621	-2.86369	-5.87609	H	-1.31179	-3.08436	-5.78890	H	-0.88795	-3.56282	-5.84540
H	-4.64957	-4.86060	-8.07524	H	-2.27048	-5.20800	-8.65461	H	-2.15609	-5.91710	-8.48431
H	-7.05256	-3.59163	-8.03354	H	0.20265	-3.26351	-3.71352	H	-4.02643	-4.25124	-5.23294
O	-7.71384	-4.38722	-7.52953	O	1.24887	-3.45804	-4.14641	O	-4.84039	-5.06160	-5.03558
O	-7.14516	-4.65298	-6.41952	O	1.15878	-4.52849	-4.83078	O	-5.24823	-5.43855	-6.18213

b-bisabolene- TS- 5				b-carophyllene- TS				b-farnesene- TS- 1			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.00000	0.00000	0.00000	C	0.00007	-0.00026	0.00000	C	-0.12026	-0.21893	0.15738
H	0.00000	0.00000	1.09660	C	0.00003	-0.00009	1.53003	C	0.27848	-1.01020	1.20239
H	1.03704	0.00000	-0.34407	C	1.53606	-0.00005	1.57950	C	0.85292	0.66728	-0.57113
H	-0.46966	0.93875	-0.31735	C	1.50015	0.40197	0.06299	H	0.33385	1.34428	-1.25386
C	-0.17871	-2.08912	-1.32815	C	2.20357	-1.34235	1.89575	H	1.42802	1.27752	0.13364
H	0.86521	-1.92525	-1.59731	C	2.28038	-1.67695	3.39723	C	-1.54587	-0.21162	-0.30700
C	-0.76297	-1.18544	-0.53107	C	-0.53840	1.30352	3.70666	H	-1.91554	0.82317	-0.32692
C	-2.20339	-1.24771	-0.09407	C	-0.92012	0.78116	2.33135	H	-2.17969	-0.76548	0.39415
H	-2.74231	-2.10253	-0.50618	C	0.12690	-1.02839	4.52950	C	1.59805	-1.05325	1.74219
H	-2.27075	-1.29335	0.99944	C	0.93466	-1.97285	4.02866	H	2.40713	-0.72414	1.08515
H	-2.72896	-0.33657	-0.40407	C	0.41573	0.44468	4.56517	C	-1.70939	-0.82195	-1.71734
C	-0.82703	-3.30410	-1.93891	C	0.54324	-3.42758	4.02779	H	-1.36048	-1.85951	-1.69270
H	-0.07799	-4.09835	-2.03620	C	-2.17174	1.01642	1.85969	C	-3.13068	-0.73250	-2.20435
H	-1.61468	-3.69426	-1.28543	C	1.65747	1.91408	-0.07840	H	-3.40228	0.19728	-2.70504
C	-1.41163	-2.98656	-3.31907	C	2.42788	-0.33043	-0.89704	C	-4.08981	-1.65293	-2.04210
H	-0.61718	-2.55353	-3.94376	H	-0.67267	0.70860	-0.49278	C	-5.48685	-1.42764	-2.55858

C	-2.03859	-4.14643	-4.07068	H	-0.15400	-0.99404	-0.43698	H	-5.76733	-2.21282	-3.27070
C	-2.10373	-5.38496	-3.52489	H	1.97775	0.78301	2.21077	H	-6.21443	-1.46723	-1.73937
H	-2.53781	-6.22592	-4.05002	H	1.67892	-2.15046	1.36616	H	-5.58242	-0.46058	-3.05778
H	-1.72050	-5.58519	-2.53132	H	3.22560	-1.32157	1.49817	C	-3.88799	-2.97099	-1.34109
C	-2.49877	-3.87175	-5.43029	H	2.79220	-0.85858	3.91524	H	-4.58167	-3.05627	-0.49635
C	-2.86139	-2.44060	-5.78131	H	2.91832	-2.56085	3.51601	H	-4.11160	-3.80378	-2.01827
C	-3.30186	-4.91256	-6.18254	H	-1.46688	1.47313	4.26191	C	1.96638	-2.14935	2.71199
C	-3.28965	-2.25226	-7.21151	H	-0.07570	2.29187	3.57955	H	2.08468	-3.09658	2.16081
H	-3.67274	-2.10812	-5.10962	H	-0.84079	-1.33850	4.92742	C	3.22709	-1.93254	3.52150
C	-3.28360	-4.68629	-7.69723	H	1.44825	0.63035	4.26581	C	3.97131	-0.82149	3.47120
H	-2.92993	-5.91801	-5.97190	H	0.33024	0.80754	5.59719	H	4.89168	-0.74861	4.04171
C	-3.46998	-3.24283	-8.08978	H	-0.48179	-3.57154	4.37636	H	3.69868	0.03690	2.86620
H	-3.44135	-1.22328	-7.53414	H	1.21958	-4.00325	4.67114	C	3.60071	-3.07217	4.38886
H	-2.33620	-5.05069	-8.11948	H	0.61760	-3.85044	3.01911	C	4.10208	-2.95890	5.62092
C	-3.84902	-2.99255	-9.52265	H	-2.91111	1.52953	2.46689	H	4.36556	-3.83464	6.20459
H	-3.11062	-3.43933	-10.19904	H	-2.47683	0.68730	0.87257	H	-0.49154	-1.58323	1.72084
H	-4.81504	-3.45609	-9.75480	H	0.97416	2.44378	0.59582	H	1.13147	-2.32138	3.40573
H	-3.91521	-1.92429	-9.74252	H	1.43529	2.23266	-1.10268	H	3.41412	-4.06684	3.98210
H	-2.02315	-1.76607	-5.56816	H	2.68144	2.22123	0.16251	H	4.24983	-1.98612	6.08177
H	-4.34110	-4.86820	-5.81943	H	2.19375	-0.04187	-1.92775	H	-1.05327	-0.29224	-2.41804
H	-2.15675	-2.18793	-3.20117	H	2.32088	-1.41634	-0.82223	H	-2.87476	-3.10373	-0.95836
H	-1.21841	-4.06751	-6.06317	H	3.47682	-0.07498	-0.70753	H	1.56847	0.08019	-1.16014
H	-4.07028	-5.29265	-8.16331	H	-0.51179	-1.27961	1.80979	H	1.48035	0.14198	2.53540
O	-0.24268	-4.45439	-6.53560	O	-1.12325	-2.28123	1.76120	O	1.26399	1.16124	3.05779
O	-0.10141	-5.65247	-6.12082	O	-2.11323	-2.07543	0.99048	O	0.15568	1.57329	2.58453

b-farnesene- TS- 2				b-caryophyllane- TS				farnesane- TS- 1			
											
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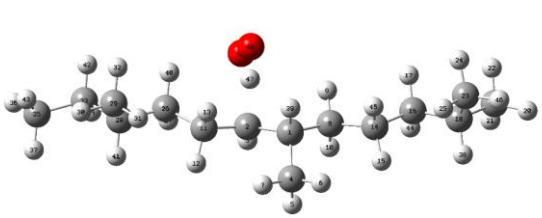
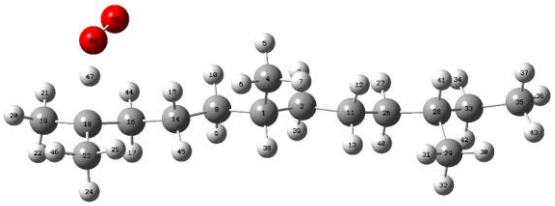
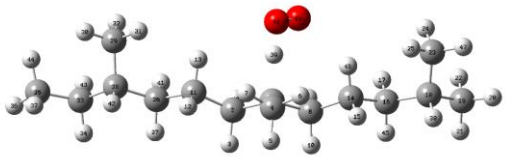
C	-0.12648	-0.52095	0.07326	C	0.00190	0.02995	-0.01303	C	-0.10592	-0.11337	0.05288
C	0.00789	-0.23189	1.40485	C	-0.01159	-0.00410	1.53674	C	-0.09205	-0.09316	1.58653
C	1.06078	-0.67863	-0.84364	C	1.55861	-0.00467	1.47555	H	0.95079	-0.05811	1.93487
H	1.01654	0.05579	-1.65540	C	1.46006	-0.46407	-0.01381	C	0.50243	1.16254	-0.53397
H	2.00817	-0.54318	-0.32105	C	2.51316	-0.84135	2.33522	H	1.55134	1.26023	-0.22660
C	-1.44150	-0.58811	-0.50415	C	3.05872	-0.22515	3.64966	H	0.46987	1.15735	-1.62674
H	-2.26803	-0.65006	0.20887	C	-0.96120	1.13747	3.69712	H	-0.03005	2.05660	-0.19822
C	1.29915	-0.04438	2.14345	C	-0.82686	1.13543	2.16796	C	0.61324	-1.36974	-0.45455
H	2.02564	0.48567	1.51729	C	0.77174	-0.37752	4.77550	H	0.16390	-2.24883	0.02899
H	1.12043	0.58591	3.02091	C	2.25360	-0.61851	4.86494	H	1.66130	-1.33876	-0.12061
C	-1.71132	-1.26507	-1.83601	C	0.36556	1.06748	4.45401	C	-0.86954	1.05894	2.22351
H	-1.59246	-2.35191	-1.72044	C	2.67958	-1.88199	5.56538	H	-0.36919	2.01264	2.01248
C	-3.08085	-0.93077	-2.37148	C	-2.23492	1.14556	1.55907	H	-1.86692	1.11513	1.76732
H	-3.14621	-0.01105	-2.95310	C	2.42236	0.21384	-0.97844	C	0.57318	-1.57404	-1.96953
C	-4.20856	-1.62224	-2.16574	C	1.51479	-1.98288	-0.18746	H	1.15839	-0.79310	-2.47281
C	-5.52171	-1.16423	-2.74456	H	-0.06413	1.06493	-0.37208	C	1.11845	-2.94206	-2.38112

H	-5.94498	-1.93543	-3.39901	H	-0.73635	-0.57746	-0.54751	H	0.45419	-3.72957	-1.99352
H	-6.25446	-0.98520	-1.94905	H	1.89862	1.04262	1.48425	C	1.29025	-3.14094	-3.89145
H	-5.40977	-0.24463	-3.32335	H	2.07383	-1.82756	2.53985	C	1.89595	-4.51548	-4.17979
C	-4.29077	-2.88957	-1.35538	H	3.38560	-1.03495	1.69713	H	2.07396	-4.65495	-5.25072
H	-5.01985	-2.76927	-0.54559	H	3.10622	0.86626	3.54234	H	2.84832	-4.64929	-3.65671
H	-4.64507	-3.71995	-1.97750	H	4.09116	-0.55984	3.79865	H	1.21610	-5.30933	-3.84740
C	1.89664	-1.38222	2.59900	H	-1.60636	0.30042	4.00477	C	-0.03062	-2.97234	-4.64524
H	2.05304	-2.02364	1.71957	H	-1.50185	2.05047	3.97273	H	-0.78222	-3.67143	-4.25723
C	3.20040	-1.29245	3.35991	H	0.38621	-1.04600	3.98558	H	-0.43165	-1.95935	-4.55027
C	3.82646	-0.14248	3.63728	H	1.14210	1.56159	3.85853	C	-0.99101	0.88558	3.73922
H	4.78789	-0.14359	4.14103	H	0.30838	1.63281	5.39009	H	-0.00073	0.65533	4.15613
H	3.41382	0.82215	3.36177	H	2.14594	-2.02131	6.51014	C	-1.56572	2.05827	4.49782
C	3.76330	-2.59814	3.77244	H	3.75569	-1.89302	5.76311	C	-2.78829	2.72818	3.92982
C	4.37542	-2.83217	4.93556	H	2.45576	-2.75682	4.93313	H	-3.01162	3.67106	4.43492
H	4.77514	-3.81194	5.17499	H	-2.84238	1.94342	1.99768	H	-2.68366	2.93130	2.86124
H	-0.90809	-0.14016	1.98731	H	-2.21742	1.29398	0.47642	H	-3.66594	2.07229	4.05487
H	1.16369	-1.91577	3.21949	H	2.35698	1.30374	-0.89677	C	-1.46060	1.93887	6.00110
H	3.62733	-3.42179	3.07051	H	2.20006	-0.06433	-2.01513	H	-0.43176	1.64977	6.25084
H	4.48213	-2.05111	5.68335	H	3.45835	-0.08057	-0.76982	C	-1.85258	3.18687	6.79204
H	-0.95707	-0.95772	-2.56913	H	1.22284	-2.24312	-1.21095	H	-1.64756	3.04304	7.85563
H	-3.33818	-3.17799	-0.90816	H	0.82928	-2.49796	0.49402	H	-1.28051	4.05877	6.45726
H	1.06461	-1.67405	-1.30094	H	2.52221	-2.37776	-0.01792	H	1.99143	-2.37399	-4.25250
H	-1.53838	0.80549	-0.84266	H	-0.38765	-0.97564	1.89062	H	-1.15679	-0.17461	-0.27249
O	-1.43569	1.93453	-1.08490	H	-2.74093	0.19310	1.75938	H	-0.50724	-1.04318	1.95213
O	-0.37886	2.32663	-0.48908	H	-0.32238	2.07355	1.88327	H	-1.61811	0.00019	3.95179
				H	0.27642	-0.70334	5.69843	H	-2.09396	1.09112	6.31704
				H	2.70908	0.47436	5.83091	H	-2.91641	3.41726	6.68888
				O	3.27407	2.29634	5.63569	H	2.09181	-3.09531	-1.89399
				O	3.04200	1.31603	6.44067	H	-0.46263	-1.46214	-2.31718

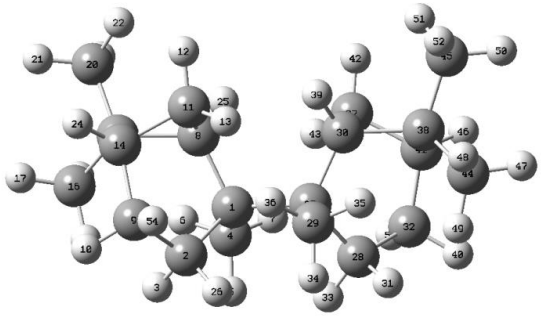
	H	0.09947	-3.18006	-5.71212
	H	-0.44494	3.05998	4.25780
	O	0.48381	3.63131	4.16721
	O	1.42467	2.86337	4.60010

farnesane- TS- 2				farnesane- TS- 3				farnesane- TS- 4			
											
	X	**Y**	**Z**		**X**	**Y**	**Z**		**X**	**Y**	**Z**
C	0.00891	0.01529	-0.02152	C	-0.14685	-0.06137	-0.02404	C	0.00000	0.00000	0.00000
C	-0.04001	-0.02099	1.48509	C	-0.08267	-0.01124	1.50780	C	0.00000	0.00000	1.51110
H	0.93464	0.00967	1.98982	H	0.96812	0.09651	1.81618	H	1.05131	0.00000	1.85326
C	0.15218	1.47164	-0.50553	C	0.35697	1.23917	-0.65427	C	0.33636	1.29365	-0.69352
H	1.11009	1.88928	-0.17432	H	1.40971	1.40553	-0.39322	H	1.40325	1.53044	-0.54612
H	0.11362	1.52568	-1.59674	H	0.28228	1.21590	-1.74487	H	0.15923	1.23596	-1.77021
H	-0.65089	2.10110	-0.11276	H	-0.21791	2.10243	-0.30842	H	-0.24035	2.13339	-0.29723
C	1.13696	-0.87719	-0.55772	C	0.63633	-1.27708	-0.53499	C	0.48810	-1.28301	-0.62857
H	1.00446	-1.89233	-0.16034	H	0.26208	-2.17512	-0.02290	H	-0.04295	-2.12360	-0.16121
H	2.09504	-0.51329	-0.15846	H	1.69189	-1.17158	-0.24377	H	1.55214	-1.41466	-0.35742
C	-1.16271	0.65398	2.22097	C	-0.91443	1.09590	2.15677	C	-0.74120	1.15825	2.18358
H	-0.97715	1.74330	2.21960	H	-0.49335	2.07955	1.91054	H	-0.24104	2.10886	1.95671
H	-2.09967	0.50669	1.66868	H	-1.92731	1.07377	1.73321	H	-1.75337	1.22347	1.76442
C	1.21964	-0.95573	-2.08236	C	0.56129	-1.50470	-2.04449	C	0.34097	-1.38699	-2.14803
H	1.51608	0.01676	-2.49736	H	1.08000	-0.69384	-2.57055	H	1.04289	-0.70406	-2.64588
C	2.21751	-2.01675	-2.54772	C	1.19382	-2.83950	-2.44385	C	0.58924	-2.81299	-2.63813
H	1.85364	-3.01188	-2.25106	H	0.58081	-3.66753	-2.04152	H	-0.20850	-3.46412	-2.25064
C	2.49607	-2.02045	-4.05514	C	1.36270	-3.06597	-3.92581	C	0.65809	-2.96406	-4.16180
C	3.55064	-3.07459	-4.39564	C	2.13929	-4.29815	-4.30700	C	0.94855	-4.41849	-4.53586

H	3.79976	-3.05752	-5.46127	H	2.40184	-4.30052	-5.36910	H	1.05355	-4.53639	-5.61892
H	4.47298	-2.91385	-3.82831	H	3.05689	-4.39064	-3.71784	H	1.86956	-4.77567	-4.06356
H	3.17907	-4.07779	-4.15467	H	1.53330	-5.19819	-4.11664	H	0.12812	-5.06696	-4.20600
C	1.22391	-2.25642	-4.87201	C	0.21486	-2.69880	-4.82862	C	-0.62677	-2.48484	-4.84043
H	0.75022	-3.20047	-4.57486	H	-0.64514	-3.35773	-4.62609	H	-1.49303	-3.02875	-4.44373
H	0.49253	-1.45467	-4.73595	H	-0.12291	-1.67036	-4.67424	H	-0.80125	-1.41663	-4.68288
C	-1.30571	0.18976	3.67559	C	-0.97607	0.95181	3.67811	C	-0.80606	0.98169	3.70062
H	-0.30626	0.14119	4.12876	H	0.04556	0.80918	4.05789	H	0.21051	0.79099	4.07347
C	-2.20149	1.08356	4.54131	C	-1.61057	2.13512	4.41956	C	-1.39331	2.17238	4.46813
C	-3.62083	1.17363	3.97620	C	-3.05452	2.37252	3.97193	C	-2.85084	2.43027	4.07997
H	-4.25677	1.81998	4.58672	H	-3.50281	3.22475	4.48975	H	-3.25539	3.30552	4.59541
H	-3.62798	1.58075	2.96097	H	-3.11585	2.57637	2.89947	H	-2.95991	2.60758	3.00657
H	-4.08126	0.17798	3.94466	H	-3.66824	1.48733	4.18333	H	-3.47254	1.56508	4.34356
C	-2.19716	0.57251	5.98816	C	-1.51673	1.91130	5.93486	C	-1.24259	1.94113	5.97774
H	-1.15514	0.46701	6.31515	H	-0.47279	1.68579	6.18733	H	-0.18744	1.72780	6.19180
C	-2.94284	1.46723	6.97766	C	-1.99036	3.09184	6.78221	C	-1.70211	3.11003	6.84793
H	-2.80207	1.11580	8.00344	H	-1.78651	2.91891	7.84262	H	-1.45677	2.93435	7.89909
H	-2.57602	2.49836	6.92446	H	-1.47519	4.01329	6.48880	H	-1.21236	4.04120	6.54137
H	2.89854	-1.03251	-4.32424	H	-1.20216	-0.19644	-0.31060	H	1.49119	-2.34322	-4.52396
H	-0.95068	-0.36669	-0.40467	H	-0.41993	-0.97990	1.90344	H	-1.48538	-0.16577	-0.28161
H	-1.69875	-0.83622	3.69402	H	-1.52844	0.03466	3.93334	H	-0.42479	-0.95152	1.86070
H	-1.76672	2.09614	4.54244	H	-1.02401	3.03594	4.17788	H	-1.39333	0.08133	3.93586
H	-2.62836	-0.43818	6.00607	H	-2.09680	1.01433	6.19487	H	-0.80385	3.06613	4.20674
H	-4.01867	1.48398	6.78271	H	-3.06555	3.26260	6.67952	H	-1.80170	1.03518	6.25209
H	3.16704	-1.86647	-2.01505	H	2.17494	-2.93123	-1.95892	H	-2.78288	3.26403	6.78524
H	0.22154	-1.17728	-2.48343	H	-0.48885	-1.47328	-2.36523	H	1.52990	-3.18162	-2.20397
H	1.45270	-2.31934	-5.94059	H	0.48128	-2.82240	-5.88211	H	-0.66934	-1.06912	-2.43498
H	-0.22774	-1.49968	1.81481	H	2.38732	-1.97778	-4.20042	H	-0.58602	-2.65917	-5.92042
O	-0.26266	-2.54355	2.13105	O	3.18233	-1.22812	-4.27020	O	-2.53830	-0.40972	-0.45892

O	0.66512	-2.69269	3.01211	O	3.77356	-1.20605	-3.12535	O	-2.61566	-1.69285	-0.55756

Pinene-dimer 1



Atom		X	Y	Z
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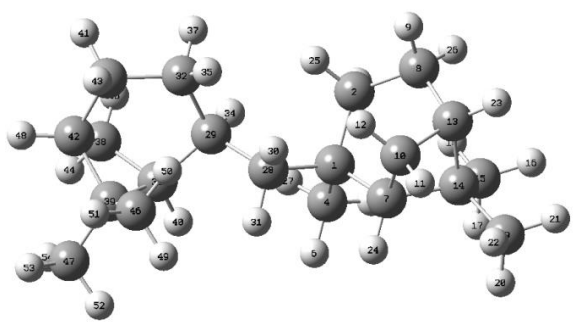
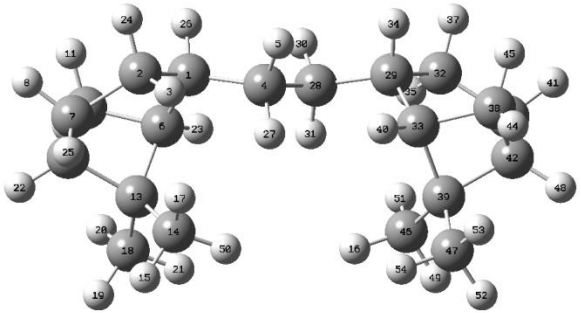
H	3	-2.256948	-2.294677	-0.218858
C	4	-0.804574	-1.197586	-1.763369
H	5	-0.795465	-2.289098	-1.842985
H	6	-1.725557	-0.852290	-2.236454
H	7	0.026519	-0.826111	-2.362947
C	8	-1.410200	0.669761	-0.200655
C	9	-2.694792	-1.081169	1.506385
H	10	-3.637985	-1.638488	1.455583
C	11	-1.597334	1.133161	1.272375
H	12	-1.684491	2.216733	1.360498
H	13	-0.882257	0.792181	2.018705
C	14	-2.952419	0.407324	1.230131
C	15	-2.990793	0.690905	-0.293647
C	16	-3.847258	-0.231285	-1.165857
H	17	-4.898565	-0.076165	-0.892830

Pinene-dimer 2



Atom		X	Y	Z
C	1	1.177761	-0.090070	-0.428849
C	2	1.582141	1.410126	-0.651592
H	3	1.642715	1.602573	-1.728848
C	4	1.022586	-0.847112	-1.759032
H	5	1.929762	-0.836304	-2.362252
H	6	0.760496	-1.893996	-1.563818
C	7	2.241336	-0.773109	0.451849
C	8	2.909055	1.889863	0.021642
H	9	2.693677	2.735881	0.684382
C	10	2.525997	0.102771	1.704095
H	11	2.932064	-0.463869	2.542804
H	12	1.716572	0.739336	2.073274
C	13	3.598182	0.802172	0.847513
C	14	3.729843	-0.506202	0.025954
C	15	4.167536	-0.365088	-1.430293
H	16	5.215645	-0.041361	-1.452970
H	17	4.108049	-1.323448	-1.958228

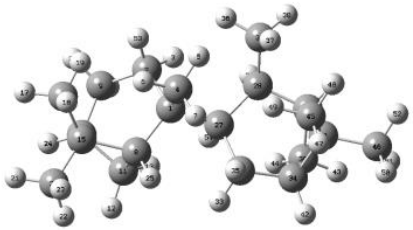
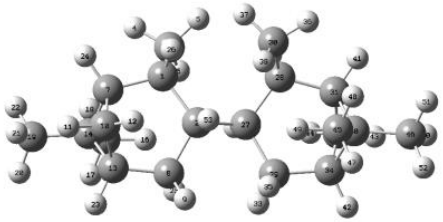
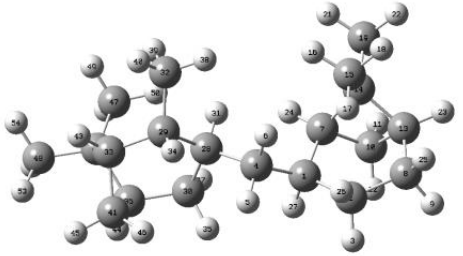
Pinene-dimer 3



Atom		X	Y	Z
C	1	-1.958113	1.333538	0.168250
C	2	-2.899058	1.364499	1.411386
H	3	-2.329588	1.011035	2.278086
C	4	-0.493792	1.130168	0.583881
H	5	-0.226443	1.936935	1.283382
C	6	-2.468013	0.344968	-0.888082
C	7	-4.208231	0.527392	1.295524
H	8	-5.081253	1.187798	1.351020
C	9	-3.949961	0.693694	-1.176834
H	10	-4.302289	0.346845	-2.149045
H	11	-4.235822	1.744170	-1.048228
C	12	-4.294864	-0.261645	-0.012511
C	13	-2.967465	-1.017955	-0.308522
C	14	-2.246549	-1.691858	0.856989
H	15	-2.809283	-2.579065	1.172177
H	16	1.245637	-2.024494	-0.552246
H	17	-2.131920	-1.047379	1.730215

H	**18**	-3.751447	0.023722	-2.227295	**H**	**18**	3.587705	0.369498	-1.992266	**C**	**18**	-3.132284	-2.054573	-1.422990
H	**19**	-3.637757	-1.293868	-1.055803	**C**	**19**	4.664779	-1.519104	0.693906	**H**	**19**	-3.704333	-2.916837	-1.061113
C	**20**	-3.463517	2.118289	-0.608616	**H**	**20**	4.581150	-2.493202	0.198143	**H**	**20**	-3.647484	-1.657055	-2.301026
H	**21**	-4.534655	2.217960	-0.398162	**H**	**21**	5.706664	-1.188758	0.610427	**H**	**21**	-2.150116	-2.416905	-1.749337
H	**22**	-2.940453	2.889797	-0.040816	**H**	**22**	4.446121	-1.667546	1.754039	**H**	**22**	-5.224433	-0.841129	-0.068432
H	**23**	-3.311851	2.332847	-1.672803	**H**	**23**	4.503144	1.182942	1.336994	**H**	**23**	-1.787583	0.291156	-1.745717
H	**24**	-3.778150	0.792954	1.841176	**H**	**24**	1.972707	-1.825251	0.619729	**H**	**24**	-3.151656	2.404231	1.640195
H	**25**	-0.911905	1.371402	-0.878071	**H**	**25**	0.768150	2.048768	-0.292297	**H**	**25**	-4.284929	-0.159152	2.146778
H	**26**	-1.088122	-2.476123	1.033431	**H**	**26**	3.600155	2.266211	-0.741011	**H**	**26**	-2.003916	2.320109	-0.317957
C	**27**	0.759057	-0.738170	0.282937	**H**	**27**	0.222098	-0.413707	-2.368158	**H**	**27**	-0.395981	0.195304	1.147619
C	**28**	1.684694	-1.723497	-0.514384	**C**	**28**	-0.185467	-0.186297	0.302159	**C**	**28**	0.494372	1.130972	-0.583364
C	**29**	0.804714	-1.197625	1.763488	**C**	**29**	-1.359082	0.538895	-0.403036	**C**	**29**	1.958755	1.333875	-0.167654
C	**30**	1.410254	0.669703	0.200766	**H**	**30**	-0.075664	0.199194	1.320528	**H**	**30**	0.226936	1.938662	-1.281760
H	**31**	2.256640	-2.294944	0.218738	**H**	**31**	-0.424482	-1.254143	0.410362	**H**	**31**	0.396546	0.196892	-1.148357
C	**32**	2.694598	-1.081265	-1.506401	**C**	**32**	-1.960173	1.735221	0.410080	**C**	**32**	2.899675	1.365089	-1.410834
H	**33**	1.087689	-2.476002	-1.033525	**C**	**33**	-2.460784	-0.430553	-0.849225	**C**	**33**	2.468530	0.344868	0.888320
H	**34**	0.795192	-2.289126	1.843137	**H**	**34**	-0.963859	0.970366	-1.332116	**H**	**34**	2.004776	2.320269	0.318891
H	**35**	1.725970	-0.852724	2.236317	**H**	**35**	-1.439479	1.813587	1.370424	**H**	**35**	2.329854	1.012871	-2.277816
H	**36**	-0.026053	-0.825725	2.363262	**C**	**36**	-3.495551	1.681617	0.673136	**C**	**36**	4.208176	0.526793	-1.295800
C	**37**	1.597274	1.133130	-1.272269	**H**	**37**	-1.728682	2.664694	-0.119783	**H**	**37**	3.153170	2.404799	-1.638744
C	**38**	2.990858	0.690872	0.293600	**C**	**38**	-3.619758	0.390496	-1.464952	**C**	**38**	3.950751	0.692749	1.176671
H	**39**	0.912020	1.371339	0.878235	**C**	**39**	-3.431265	-0.830653	0.306016	**C**	**39**	2.967023	-1.018166	0.308287
H	**40**	3.637760	-1.638640	-1.455635	**H**	**40**	-2.033916	-1.251290	-1.440733	**H**	**40**	1.788345	0.291222	1.746158
C	**41**	2.952323	0.407220	-1.230167	**H**	**41**	-3.962705	2.607195	0.317857	**H**	**41**	5.081732	1.186463	-1.351632
H	**42**	1.684508	2.216699	-1.360364	**C**	**42**	-4.168176	0.499838	-0.022693	**C**	**42**	4.294774	-0.262547	0.012042
H	**43**	0.882100	0.792247	-2.018545	**H**	**43**	-3.692009	1.629485	1.750179	**H**	**43**	4.283866	-0.159672	-2.147204
C	**44**	3.847499	-0.231209	1.165755	**H**	**44**	-4.260218	-0.187679	-2.132251	**H**	**44**	4.303182	0.345492	2.148699
C	**45**	3.463568	2.118285	0.608456	**H**	**45**	-3.343999	1.329222	-1.959300	**H**	**45**	4.237162	1.743094	1.048214
H	**46**	3.777999	0.792821	-1.841303	**C**	**46**	-2.905276	-1.023556	1.725787	**C**	**46**	2.245104	-1.691168	-0.857113

H	**47**	4.898782	-0.075776	0.892816	**C**	**47**	-4.269464	-2.054630	-0.068674	**C**	**47**	3.131568	-2.055180	1.422417
H	**48**	3.751554	0.023652	2.227218	**H**	**48**	-5.255159	0.514681	0.123101	**H**	**48**	5.224029	-0.842568	0.067566
H	**49**	3.638308	-1.293833	1.055554	**H**	**49**	-2.336028	-1.956491	1.807256	**H**	**49**	2.806190	-2.579484	-1.172072
H	**50**	4.534678	2.217986	0.397871	**H**	**50**	-2.258043	-0.210380	2.061523	**H**	**50**	-1.247871	-2.027138	0.552255
H	**51**	2.940413	2.889754	0.040686	**H**	**51**	-3.748398	-1.089200	2.424647	**H**	**51**	2.131534	-1.046668	-1.730474
H	**52**	3.312021	2.332878	1.672652	**H**	**52**	-3.651493	-2.959761	-0.047790	**H**	**52**	3.703089	-2.917641	1.060177
H	**53**	2.335695	-1.176552	-2.539104	**H**	**53**	-5.087145	-2.189447	0.648928	**H**	**53**	3.647177	-1.658150	2.300436
H	**54**	-2.335914	-1.176492	2.539093	**H**	**54**	-4.710914	-1.975544	-1.065543	**H**	**54**	2.149289	-2.417089	1.748901

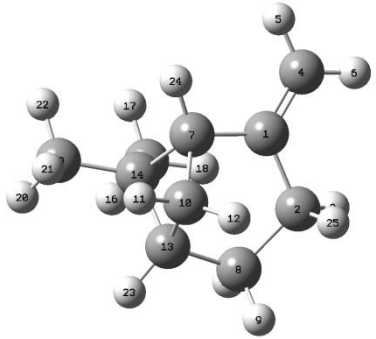
Pinene-dimer 4					Pinene-dimer 5					Pinene-dimer 6				
														
Atom		X	Y	Z	**Atom**		X	Y	Z	**Atom**		X	Y	Z
C	**1**	-0.860550	0.429284	0.183769	**C**	**1**	-1.563833	1.176657	0.325200	**C**	**1**	1.530180	-1.087668	-0.055841
C	**2**	-1.523156	1.505923	-0.746854	**C**	**2**	-0.629357	-0.086728	0.444717	**C**	**2**	2.665355	-1.830199	0.716523
H	**3**	-0.785518	1.856147	-1.474525	**C**	**3**	-1.455731	2.033874	-0.950856	**H**	**3**	2.580776	-2.904151	0.524319
C	**4**	-0.661371	0.962741	1.614558	**H**	**4**	-2.395056	2.572782	-1.115826	**C**	**4**	0.366885	-0.747987	0.888339
H	**5**	-0.071712	1.879469	1.642502	**H**	**5**	-0.666848	2.785214	-0.861757	**H**	**5**	0.057097	-1.676022	1.394596
H	**6**	-1.619771	1.178277	2.088037	**H**	**6**	-1.252217	1.458783	-1.855604	**H**	**6**	0.720225	-0.072996	1.678783
H	**7**	-0.161080	0.217153	2.241099	**C**	**7**	-3.023793	0.793252	0.626895	**C**	**7**	2.090563	0.097895	-0.854480
C	**8**	-1.814867	-0.789593	0.276925	**C**	**8**	-1.405476	-1.432765	0.299823	**C**	**8**	4.118149	-1.360008	0.410761
C	**9**	-2.802688	1.063588	-1.525749	**H**	**9**	-0.937326	-2.176228	0.954751	**H**	**9**	4.685252	-2.173309	-0.056734
H	**10**	-2.587356	1.024347	-2.600039	**C**	**10**	-3.046038	-0.243886	1.778358	**C**	**10**	3.246581	-0.441656	-1.734498
C	**11**	-2.180222	-1.315181	-1.139517	**H**	**11**	-4.007723	-0.300969	2.288594	**H**	**11**	3.460714	0.176467	-2.607321
H	**12**	-2.506460	-2.355792	-1.135385	**H**	**12**	-2.254019	-0.174998	2.530609	**H**	**12**	3.169286	-1.488697	-2.049508
H	**13**	-1.451904	-1.186693	-1.944533	**C**	**13**	-2.885087	-1.308069	0.665454	**C**	**13**	4.165417	-0.152088	-0.526266
C	**14**	-3.342498	-0.305117	-1.102029	**C**	**14**	-3.599493	-0.321421	-0.302153	**C**	**14**	3.155679	0.948276	-0.089028
C	**15**	-3.341122	-0.433457	0.441532	**C**	**15**	-3.240308	-0.378362	-1.784146	**C**	**15**	3.006328	1.243201	1.401236
C	**16**	-3.864728	0.762778	1.236131	**H**	**16**	-2.165815	-0.375333	-1.971370	**H**	**16**	2.147159	1.901226	1.579403
H	**17**	-4.935943	0.875307	1.026904	**H**	**17**	-3.648760	-1.296617	-2.224159	**H**	**17**	2.876148	0.348459	2.012346
H	**18**	-3.759591	0.601073	2.314774	**H**	**18**	-3.676895	0.470919	-2.321966	**H**	**18**	3.900679	1.764603	1.763816
H	**19**	-3.382706	1.708483	0.987014	**C**	**19**	-5.124593	-0.403224	-0.188510	**C**	**19**	3.410134	2.276058	-0.807597

C	**20**	-4.116568	-1.664444	0.925518	**H**	**20**	-5.489135	-1.336580	-0.633125	**H**	**20**	3.527161	2.159381	-1.887945
H	**21**	-5.194062	-1.509385	0.796812	**H**	**21**	-5.479117	-0.365774	0.844100	**H**	**21**	2.575214	2.965410	-0.635317
H	**22**	-3.846360	-2.579853	0.394808	**H**	**22**	-5.589661	0.428988	-0.729713	**H**	**22**	4.320585	2.748782	-0.421398
H	**23**	-3.927564	-1.831485	1.992170	**H**	**23**	-3.350507	-2.291044	0.807225	**H**	**23**	5.197744	0.164846	-0.718485
H	**24**	-4.271823	-0.549747	-1.631603	**H**	**24**	-3.634691	1.698778	0.736847	**H**	**24**	1.294111	0.655564	-1.361151
H	**25**	-1.430963	-1.518085	1.001023	**H**	**25**	-1.314907	-1.829865	-0.718650	**H**	**25**	4.634117	-1.121854	1.348237
H	**26**	-3.583248	1.822409	-1.396515	**H**	**26**	-1.277639	1.835521	1.155675	**H**	**26**	2.477266	-1.716124	1.789815
C	**27**	0.492997	-0.032249	-0.447756	**C**	**27**	0.629344	-0.086745	-0.444673	**H**	**27**	1.133700	-1.779392	-0.812876
C	**28**	1.575436	1.067794	-0.798434	**C**	**28**	1.563825	1.176645	-0.325221	**C**	**28**	-0.870873	-0.129561	0.227564
C	**29**	1.078460	-1.308470	0.218958	**C**	**29**	1.405463	-1.432778	-0.299739	**C**	**29**	-1.876155	0.353434	1.317049
C	**30**	1.634055	2.410115	-0.053887	**C**	**30**	1.455753	2.033928	0.950791	**C**	**30**	-1.490173	-1.074154	-0.843981
C	**31**	2.967530	0.414881	-0.874504	**C**	**31**	3.023780	0.793225	-0.626928	**H**	**31**	-0.530478	0.775767	-0.287742
H	**32**	1.350109	1.351994	-1.837290	**H**	**32**	1.277617	1.835474	-1.155720	**C**	**32**	-1.654319	1.826827	1.663635
H	**33**	0.505999	-2.169566	-0.148741	**H**	**33**	0.937299	-2.176265	-0.954628	**C**	**33**	-3.328750	0.034470	0.941858
C	**34**	2.557839	-1.513236	-0.118595	**C**	**34**	2.885068	-1.308098	-0.665403	**H**	**34**	-1.674848	-0.225069	2.232208
H	**35**	0.953962	-1.304850	1.307888	**H**	**35**	1.314913	-1.829837	0.718751	**H**	**35**	-1.103229	-2.093049	-0.704922
H	**36**	0.683554	2.947898	-0.107188	**H**	**36**	2.395077	2.572856	1.115701	**C**	**36**	-3.017905	-1.152558	-0.777773
H	**37**	1.918427	2.330270	0.995162	**H**	**37**	0.666861	2.785254	0.861679	**H**	**37**	-1.166244	-0.757010	-1.843807
H	**38**	2.387337	3.036322	-0.545835	**H**	**38**	1.252281	1.458883	1.855579	**H**	**38**	-0.607119	2.009930	1.931022
C	**39**	2.842498	-0.978707	-1.544193	**C**	**39**	3.046001	-0.243959	-1.778351	**H**	**39**	-1.902257	2.477359	0.819311
C	**40**	3.403840	-0.329816	0.429654	**C**	**40**	3.599501	-0.321415	0.302147	**H**	**40**	-2.274264	2.126391	2.514940
H	**41**	3.693669	1.123058	-1.294814	**H**	**41**	3.634677	1.698745	-0.736929	**C**	**41**	-3.411593	-1.489422	0.679439
H	**42**	2.894179	-2.525318	0.137938	**H**	**42**	3.350481	-2.291080	-0.807147	**C**	**42**	-3.668269	0.245709	-0.569938
H	**43**	3.784995	-1.342305	-1.953852	**H**	**43**	4.007677	-0.301063	-2.288602	**H**	**43**	-4.025541	0.474731	1.667012
H	**44**	2.062367	-1.104662	-2.301259	**H**	**44**	2.253969	-0.175096	-2.530591	**H**	**44**	-3.420744	-1.776348	-1.584930
C	**45**	3.054232	0.208969	1.813144	**C**	**45**	3.240359	-0.378301	1.784153	**H**	**45**	-4.414830	-1.904515	0.780413
C	**46**	4.904477	-0.634910	0.414665	**C**	**46**	5.124598	-0.403221	0.188466	**H**	**46**	-2.708391	-2.115149	1.241532
H	**47**	3.281987	-0.554691	2.567815	**H**	**47**	3.648825	-1.296539	2.224188	**C**	**47**	-3.122188	1.434361	-1.357902
H	**48**	3.653364	1.095838	2.049254	**H**	**48**	3.676961	0.471002	2.321929	**C**	**48**	-5.183490	0.204964	-0.795552

H	**49**	2.002693	0.475553	1.921184	**H**	**49**	2.165872	-0.375265	1.971407	**H**	**49**	-3.568083	2.370355	-1.001254
H	**50**	5.151323	-1.357326	1.201490	**H**	**50**	5.479092	-0.365815	-0.844157	**H**	**50**	-2.038106	1.539604	-1.306276
H	**51**	5.250014	-1.047530	-0.535971	**H**	**51**	5.589679	0.429017	0.729618	**H**	**51**	-3.392739	1.325444	-2.415305
H	**52**	5.477691	0.279130	0.608304	**H**	**52**	5.489154	-1.336557	0.633111	**H**	**52**	-5.405007	0.097442	-1.863676
H	**53**	-1.765021	2.386352	-0.141741	**H**	**53**	-0.268389	-0.079444	1.482193	**H**	**53**	-5.673992	-0.617253	-0.269317
H	**54**	0.207840	-0.377154	-1.444903	**H**	**54**	0.268369	-0.079501	-1.482147	**H**	**54**	-5.640702	1.139809	-0.451084

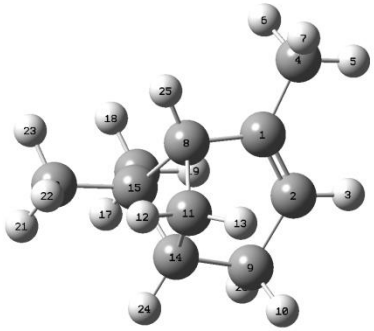
M06-2X/6-311+G(2d,p)

α-Pinene



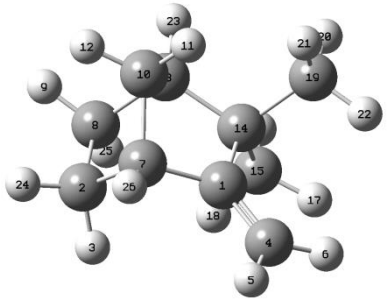
Atom	X	Y	Z
C1	1.378171	-0.519624	-0.276523
C2	1.728406	0.806716	0.374286
H5	2.393085	0.644701	1.224307
C6	2.199755	-1.562043	-0.277833
H5	1.937303	-2.482450	-0.785908
H6	3.160648	-1.524615	0.223055
C7	0.019084	-0.546645	-0.910942
C8	0.487990	1.641203	0.781432
H11	0.693141	2.699639	0.606297
C12	-0.314377	0.865314	-1.464696
H11	-1.145106	0.849717	-2.164774
H12	0.505841	1.436282	-1.900980
C13	-0.745101	1.222111	-0.020876
C14	-1.060716	-0.287854	0.196689

β-Pinene



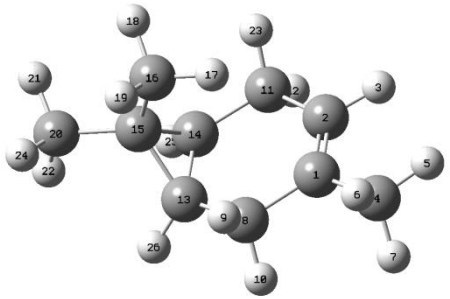
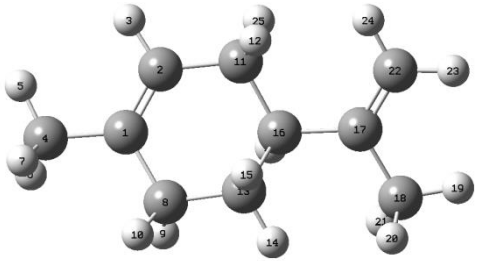
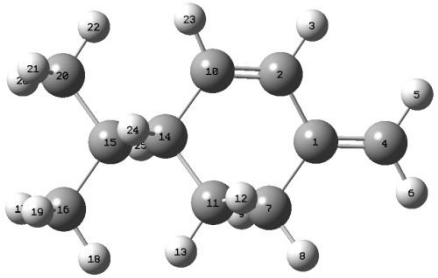
Atom	X	Y	Z
C1	1.439159	-0.278370	-0.091276
C2	1.504128	0.921874	0.497080
H3	2.416079	1.262661	0.983863
C4	2.563550	-1.269076	-0.133394
H5	3.458754	-0.882042	0.360313
H6	2.269634	-2.202426	0.362716
H7	2.819466	-1.526237	-1.168140
C8	0.123772	-0.641193	-0.756245
C9	0.281108	1.811720	0.521806
H10	0.510564	2.788999	0.075750
C11	-0.322909	0.596185	-1.584322
H12	-1.107497	0.374848	-2.307917
H13	0.475230	1.164666	-2.069507
C14	-0.872748	1.151867	-0.246683

Camphene



Atom	X	Y	Z
C1	-0.407037	1.035757	-0.028826
C2	1.872449	0.447953	-0.749132
H3	1.602701	0.878882	-1.713817
C4	-1.162882	2.070278	-0.364209
H5	-0.775349	3.082070	-0.342597
H6	-2.194957	1.942963	-0.672902
C7	1.038616	1.068973	0.400455
C8	1.539252	-1.068753	-0.650382
H9	2.418889	-1.636582	-0.342785
C10	1.060461	-0.070989	1.435522
H11	0.437247	0.129909	2.306176
H12	2.069912	-0.322602	1.766761
C13	0.480448	-1.117396	0.464184
C14	-0.837324	-0.435736	-0.004605

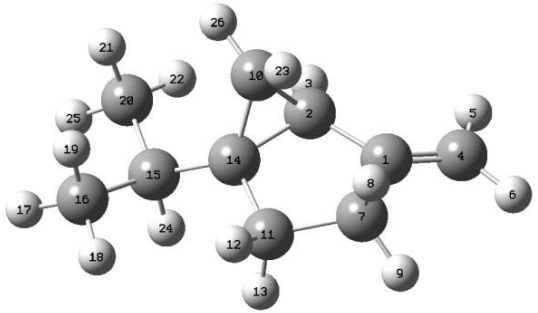
C15	-0.832506	-0.895047	1.572038	**C15**	-1.074400	-0.328708	0.207939	**C15**	-1.335905	-0.908220	-1.372415
H16	-1.556916	-0.496167	2.287991	**C16**	-0.950797	-0.664330	1.689554	**H16**	-1.447643	-1.996142	-1.387451
H17	-0.966515	-1.979203	1.528581	**H17**	-1.783785	-0.214703	2.243539	**H17**	-2.312209	-0.467397	-1.584453
H18	0.168575	-0.708541	1.958868	**H18**	-1.004060	-1.749438	1.837779	**H18**	-0.664007	-0.614672	-2.178696
C21	-2.462173	-0.655791	-0.282283	**H19**	-0.016876	-0.310727	2.129704	**C19**	-1.954243	-0.668351	1.020771
H20	-3.209326	-0.276062	0.419772	**C20**	-2.391270	-0.912882	-0.307798	**H20**	-2.244444	-1.722542	1.026993
H21	-2.694206	-0.250356	-1.266918	**H21**	-3.234493	-0.490437	0.251096	**H21**	-1.651698	-0.389558	2.030164
H22	-2.572192	-1.742141	-0.332325	**H22**	-2.564655	-0.716762	-1.368092	**H22**	-2.832906	-0.074244	0.762226
H23	-1.572202	1.922269	0.115354	**H23**	-2.405916	-1.998991	-0.162271	**H23**	0.314313	-2.114744	0.873670
H24	-0.120339	-1.418180	-1.553063	**H24**	-1.762302	1.791828	-0.272401	**H24**	2.935943	0.629996	-0.586659
H25	2.304992	1.380144	-0.356656	**H25**	0.149218	-1.625365	-1.237613	**H25**	1.195842	-1.494281	-1.591719
H26	0.282015	1.534923	1.848647	**H26**	-0.016917	2.011608	1.561214	**H26**	1.385351	2.047849	0.726918

Car-3-ene	Limonene	Phellandrene
		

Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C1	1.795973	-0.130957	-0.056970	**C1**	-2.154834	0.043202	-0.031806	**C1**	2.118377	0.011967	-0.233870
C2	1.505372	1.146926	0.160740	**C2**	-1.513966	1.206265	-0.104278	**C2**	1.457452	1.263882	0.147675
H3	2.283581	1.797850	0.550591	**H3**	-2.092051	2.117743	-0.229338	**H3**	2.045463	2.173292	0.073410
C4	3.157559	-0.700225	0.221816	**C4**	-3.647082	-0.066967	-0.148148	**C4**	3.406221	-0.013081	-0.576502
H5	3.837943	0.056559	0.611542	**H5**	-4.109127	0.903869	-0.326658	**H5**	3.996578	0.895384	-0.601306
H6	3.092849	-1.514241	0.949957	**H6**	-3.920457	-0.735913	-0.969577	**H6**	3.902292	-0.938993	-0.841693
H7	3.594171	-1.122847	-0.687668	**H7**	-4.076240	-0.492983	0.763176	**C7**	1.254214	-1.225180	-0.213428
C8	0.795161	-1.121237	-0.590966	**C8**	-1.413360	-1.254293	0.165151	**H8**	1.878902	-2.112522	-0.097584
H9	0.706131	-1.944373	0.131135	**H9**	-1.465373	-1.833165	-0.765869	**H9**	0.746817	-1.318770	-1.179941
H10	1.226442	-1.574415	-1.489951	**H10**	-1.937631	-1.854601	0.915896	**C10**	0.197103	1.319203	0.583700
C11	0.171726	1.794858	-0.078680	**C11**	-0.018891	1.356346	-0.025015	**C11**	0.212048	-1.138270	0.901941
H12	0.321537	2.646617	-0.749036	**H12**	0.252900	1.742366	0.964736	**H12**	0.731795	-1.060256	1.861055
C13	-0.571810	-0.568544	-0.930536	**C13**	0.044097	-1.057134	0.575208	**H13**	-0.387595	-2.047909	0.939294
C14	-0.885669	0.888352	-0.672998	**H14**	0.578052	-2.004071	0.483835	**C14**	-0.678204	0.100777	0.738409
C15	-1.560178	-0.186294	0.140290	**H15**	0.099126	-0.754612	1.626671	**C15**	-1.702230	-0.000531	-0.418835
C16	-1.191581	-0.365399	1.594198	**C16**	0.706237	0.036754	-0.274618	**C16**	-2.581575	-1.244219	-0.294749
H17	-0.138706	-0.160812	1.786822	**C17**	2.205199	0.097126	-0.077206	**H17**	-3.374349	-1.225991	-1.044964

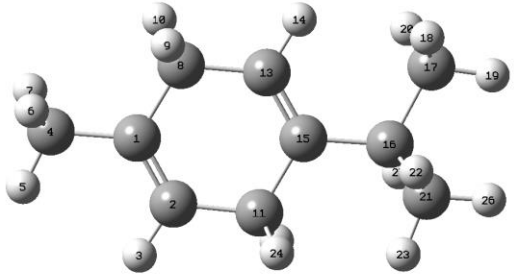
H18	-1.785910	0.304760	2.221460	**C18**	2.954571	-1.173759	-0.384657	**H18**	-2.019825	-2.168008	-0.434299
H19	-1.402914	-1.389126	1.915703	**H19**	4.025211	-0.988388	-0.461164	**H19**	-3.056023	-1.281898	0.690786
C20	-3.019815	-0.448966	-0.152501	**H20**	2.798328	-1.924581	0.393236	**C20**	-2.581398	1.249667	-0.475106
H21	-3.660025	0.223710	0.424914	**H21**	2.608280	-1.609776	-1.325795	**H21**	-3.109154	1.388239	0.473595
H22	-3.242000	-0.300035	-1.210829	**C22**	2.854428	1.189414	0.313652	**H22**	-1.999647	2.149609	-0.675493
H23	-0.186973	2.226989	0.864311	**H23**	3.933282	1.183894	0.415765	**H23**	-0.226239	2.283055	0.845403
H24	-3.291051	-1.476008	0.107649	**H24**	2.349322	2.118813	0.539386	**H24**	-1.266392	0.221553	1.657527
H25	-1.522618	1.366665	-1.407790	**H25**	0.315091	2.107603	-0.746399	**H25**	-1.142975	-0.058708	-1.358982
H26	-1.012891	-0.992381	-1.825158	**H26**	0.542883	-0.237928	-1.327598	**H26**	-3.331698	1.156635	-1.262220

Sabinene



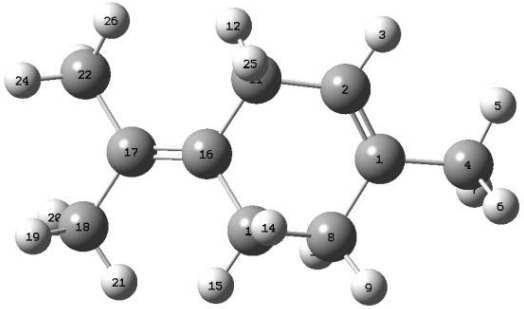
Atom		X	Y	Z
C	**1**	-2.020063	-0.251883	-0.114754
C	**2**	-0.723980	-0.912506	0.163122
H	**3**	-0.559828	-1.919387	-0.195436
C	**4**	-3.119339	-0.844567	-0.563234
H	**5**	-3.163350	-1.918194	-0.700818
H	**6**	-4.006135	-0.272245	-0.807073
C	**7**	-1.832174	1.233252	0.105226
H	**8**	-2.071872	1.483861	1.142155
H	**9**	-2.487472	1.829252	-0.528842
C	**10**	0.004858	-0.479481	1.422624
C	**11**	-0.337655	1.473682	-0.174836
H	**12**	0.069077	2.296640	0.416351
H	**13**	-0.188806	1.718670	-1.231384
C	**14**	0.360615	0.146259	0.111123
C	**15**	1.714951	-0.065000	-0.541312
C	**16**	2.692006	1.027333	-0.100974
H	**17**	3.672331	0.878004	-0.557813

γ-Terpinene



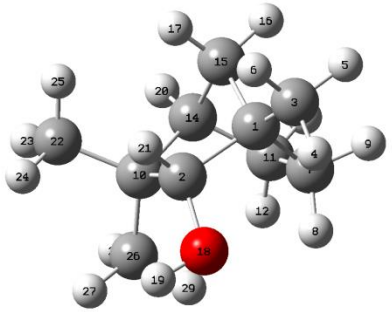
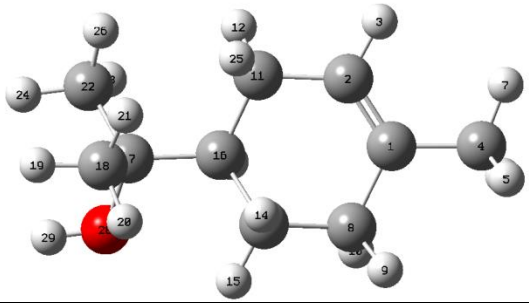
Atom		X	Y	Z
C	**1**	-2.218985	-0.026794	0.017362
C	**2**	-1.593179	-1.167594	-0.244737
H	**3**	-2.180531	-2.062642	-0.430820
C	**4**	-3.714105	0.085082	0.069463
H	**5**	-4.194384	-0.875102	-0.118269
H	**6**	-4.040615	0.449075	1.047986
H	**7**	-4.074977	0.803603	-0.672154
C	**8**	-1.456961	1.240082	0.286156
H	**9**	-1.691941	1.592792	1.299672
H	**10**	-1.831849	2.030767	-0.376882
C	**11**	-0.102476	-1.322861	-0.288680
H	**12**	0.194769	-1.808993	-1.227231
C	**13**	0.028428	1.110413	0.120213
H	**14**	0.594501	2.030335	0.216431
C	**15**	0.659760	-0.029500	-0.143132
C	**16**	2.159752	-0.130625	-0.333322
C	**17**	2.877949	1.214227	-0.354743

Terpinolene



Atom		X	Y	Z
C	**1**	2.086499	0.061028	-0.143382
C	**2**	1.486015	1.208015	0.159502
H	**3**	2.057487	2.130963	0.108030
C	**4**	3.518717	-0.009684	-0.585900
H	**5**	3.965318	0.981435	-0.664644
H	**6**	4.112867	-0.604734	0.113452
H	**7**	3.593940	-0.499758	-1.561202
C	**8**	1.351248	-1.251418	-0.055292
H	**9**	2.020068	-2.009119	0.366214
H	**10**	1.096839	-1.595156	-1.065089
C	**11**	0.033447	1.348166	0.541987
H	**12**	-0.397512	2.144533	-0.065071
C	**13**	0.085123	-1.134500	0.796019
H	**14**	0.393527	-0.977464	1.836829
H	**15**	-0.480355	-2.062952	0.772984
C	**16**	-0.735806	0.057046	0.375556
C	**17**	-1.985937	-0.006857	-0.093407

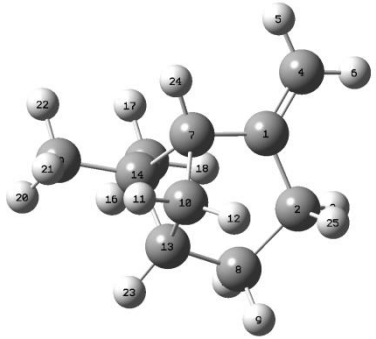
H	**18**	2.339652	2.021573	-0.379111	**H**	**18**	2.802917	1.712210	0.615290	**C**	**18**	-2.740549	-1.291270	-0.327253
H	**19**	2.816725	1.003188	0.985212	**H**	**19**	3.937598	1.067284	-0.569422	**H**	**19**	-3.516165	-1.427373	0.432884
C	**20**	2.325130	-1.440442	-0.283220	**H**	**20**	2.465941	1.880546	-1.113935	**H**	**20**	-3.254471	-1.240499	-1.291269
H	**21**	2.620177	-1.549816	0.762903	**C**	**21**	2.795122	-1.039257	0.728180	**H**	**21**	-2.111797	-2.177569	-0.335213
H	**22**	1.639102	-2.251006	-0.533812	**H**	**22**	2.616640	-0.630816	1.726194	**C**	**22**	-2.813879	1.205968	-0.438960
H	**23**	-0.536941	0.098812	2.160283	**H**	**23**	2.394849	-2.052549	0.697888	**H**	**23**	-2.922307	1.305003	-1.523700
H	**24**	1.557081	0.034966	-1.622602	**H**	**24**	0.204760	-2.021982	0.498686	**H**	**24**	-3.822656	1.084921	-0.034315
H	**25**	3.224283	-1.567373	-0.888470	**H**	**25**	2.316452	-0.608935	-1.309250	**H**	**25**	-0.031175	1.691549	1.584229
H	**26**	0.689888	-1.206834	1.835875	**H**	**26**	3.874040	-1.104636	0.575254	**H**	**26**	-2.412874	2.137262	-0.047328

Fenchol					Terpineol				
									
Atom		X	Y	Z	**Atom**		X	Y	Z
C	**1**	1.244449	-0.102365	0.226571	**C**	**1**	2.441387	0.088227	-0.028911
C	**2**	0.021289	-1.026034	0.149257	**C**	**2**	1.754408	1.213431	0.149862
C	**3**	2.527939	-0.828808	0.568203	**H**	**3**	2.297740	2.148495	0.256830
H	**4**	2.766685	-1.562338	-0.204837	**C**	**4**	3.939461	0.064954	-0.118673
H	**5**	3.362654	-0.128458	0.645811	**H**	**5**	4.365954	-0.543067	0.684188
H	**6**	2.436563	-1.357354	1.520737	**H**	**6**	4.260199	-0.387317	-1.061868
C	**7**	1.301936	0.724888	-1.078730	**H**	**7**	4.362876	1.067333	-0.055921
H	**8**	1.153796	0.087322	-1.950662	**C**	**8**	1.748171	-1.245123	-0.153417
H	**9**	2.281064	1.197992	-1.175399	**H**	**9**	2.308395	-1.992780	0.417313
C	**10**	-1.209310	-0.048637	0.182518	**H**	**10**	1.790491	-1.574337	-1.199199
C	**11**	0.176982	1.780996	-0.901591	**C**	**11**	0.251446	1.301133	0.191072
H	**12**	-0.497730	1.841575	-1.753731	**H**	**12**	-0.065155	2.144976	-0.427880
H	**13**	0.601514	2.775911	-0.754298	**C**	**13**	0.301039	-1.189894	0.324274
C	**14**	-0.510256	1.323628	0.393199	**H**	**14**	0.296669	-1.090578	1.415223
C	**15**	0.720935	0.936784	1.230970	**H**	**15**	-0.226328	-2.110784	0.071269
H	**16**	1.416831	1.766668	1.372173	**C**	**16**	-0.414562	0.011718	-0.292123
H	**17**	0.487570	0.502816	2.205493	**C**	**17**	-1.937280	-0.020010	-0.075244

O	**18**	0.120087	-1.861796	-0.988629	**C**	**18**	-2.329181	-0.215588	1.387925
H	**19**	-0.592152	-2.506264	-0.968977	**H**	**19**	-3.417838	-0.183780	1.488253
H	**20**	-1.177788	2.070539	0.826921	**H**	**20**	-1.981923	-1.181887	1.752906
H	**21**	0.006137	-1.653113	1.051331	**H**	**21**	-1.917603	0.569881	2.024006
C	**22**	-2.115366	-0.367477	1.373769	**C**	**22**	-2.599315	1.236950	-0.634367
H	**23**	-2.982395	0.297939	1.387214	**H**	**23**	-2.283008	1.405223	-1.665540
H	**24**	-2.483941	-1.395572	1.312301	**H**	**24**	-3.686032	1.119610	-0.623283
H	**25**	-1.593079	-0.258830	2.326098	**H**	**25**	-0.071069	1.539785	1.212840
C	**26**	-2.046432	-0.119727	-1.093191	**H**	**26**	-2.353873	2.118462	-0.039918

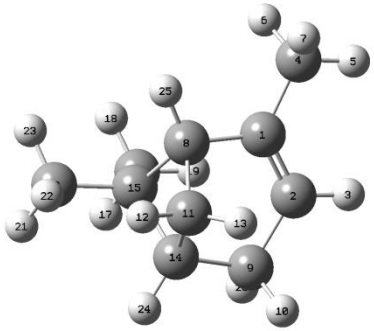
B3LYP-D3/6-31+G(d,p)

α-Pinene



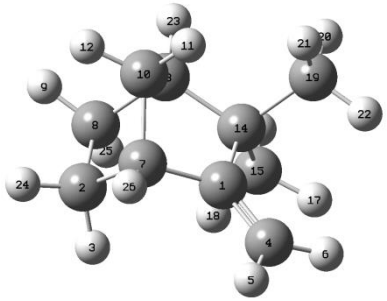
Atom	X	Y	Z
C1	1.391623	-0.526343	-0.271141
C2	1.746519	0.805799	0.383750
H5	2.408715	0.645371	1.240862
C6	2.219099	-1.578030	-0.278512
H5	1.955920	-2.501445	-0.787804
H6	3.185107	-1.548304	0.219901
C7	0.026441	-0.547030	-0.910210
C8	0.500035	1.649848	0.787745
H11	0.708898	2.711525	0.611537
C12	-0.306629	0.871954	-1.469589
H11	-1.137692	0.856664	-2.176389
H12	0.512953	1.445842	-1.913554
C13	-0.740990	1.232296	-0.019596
C14	-1.073192	-0.286085	0.195339
C15	-0.871119	-0.906718	1.579047

β-Pinene



Atom	X	Y	Z
C1	1.446455	-0.285491	-0.087318
C2	1.516275	0.914489	0.510617
H3	2.427670	1.250401	1.001838
C4	2.568583	-1.281495	-0.140075
H5	3.468666	-0.908330	0.358519
H6	2.273641	-2.223556	0.342184
H7	2.826588	-1.529591	-1.178520
C8	0.126413	-0.637356	-0.759802
C9	0.296760	1.814838	0.536729
H10	0.534145	2.793309	0.094358
C11	-0.312865	0.612801	-1.585645
H12	-1.094859	0.400506	-2.316427
H13	0.487670	1.181057	-2.068660
C14	-0.866192	1.165323	-0.240091
C15	-1.085450	-0.327035	0.205505

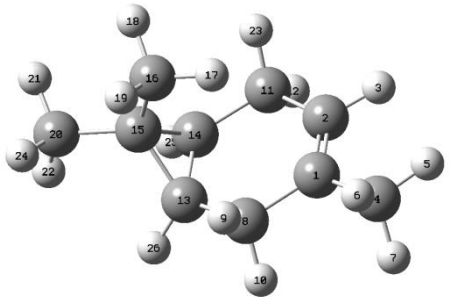
Camphene



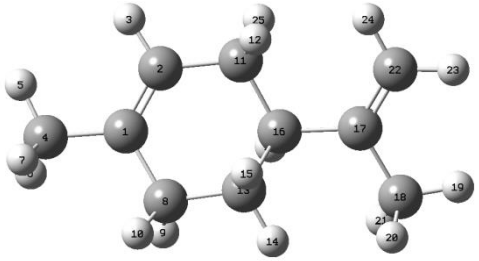
Atom	X	Y	Z
C1	-0.406373	1.042696	-0.027855
C2	1.896590	0.450673	-0.743276
H3	1.643672	0.893742	-1.711056
C4	-1.158102	2.093892	-0.362145
H5	-0.762104	3.105706	-0.335575
H6	-2.193672	1.981311	-0.673436
C7	1.044755	1.066384	0.409090
C8	1.552253	-1.072954	-0.662791
H9	2.427984	-1.655722	-0.357169
C10	1.062472	-0.087023	1.440991
H11	0.437332	0.105078	2.317046
H12	2.072373	-0.342119	1.781735
C13	0.480906	-1.128086	0.453254
C14	-0.847558	-0.434983	-0.008732
C15	-1.362763	-0.905453	-1.381393

H16	-1.598566	-0.497613	2.291135	**C16**	-0.975420	-0.683820	1.689728	**H16**	-1.507401	-1.992701	-1.389646
H17	-1.022607	-1.991562	1.530959	**H17**	-1.804279	-0.230581	2.247813	**H17**	-2.327076	-0.436325	-1.603144
H18	0.129353	-0.741569	1.983301	**H18**	-1.042692	-1.770354	1.825921	**H18**	-0.680311	-0.640677	-2.192595
C21	-2.481729	-0.647204	-0.300782	**H19**	-0.039697	-0.350624	2.141630	**C19**	-1.966344	-0.671136	1.029933
H20	-3.236714	-0.268006	0.398821	**C20**	-2.409148	-0.902018	-0.324536	**H20**	-2.249160	-1.730687	1.048749
H21	-2.710713	-0.235233	-1.287234	**H21**	-3.254123	-0.484298	0.236575	**H21**	-1.663642	-0.381130	2.039506
H22	-2.598167	-1.736031	-0.360242	**H22**	-2.582422	-0.693660	-1.383104	**H22**	-2.854789	-0.085213	0.772579
H23	-1.566370	1.941463	0.116565	**H23**	-2.429475	-1.990758	-0.194113	**H23**	0.312299	-2.133106	0.852166
H24	-0.114960	-1.419353	-1.557463	**H24**	-1.749253	1.814911	-0.264964	**H24**	2.962257	0.629929	-0.563455
H25	2.332172	1.379415	-0.345513	**H25**	0.148223	-1.617047	-1.249724	**H25**	1.212095	-1.487307	-1.614491
H26	0.292323	1.547920	1.858822	**H26**	-0.002272	2.017195	1.576010	**H26**	1.395120	2.045161	0.746323

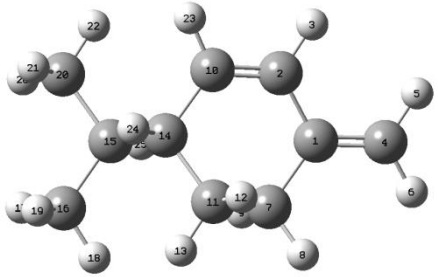
Car-3-ene



Limonene

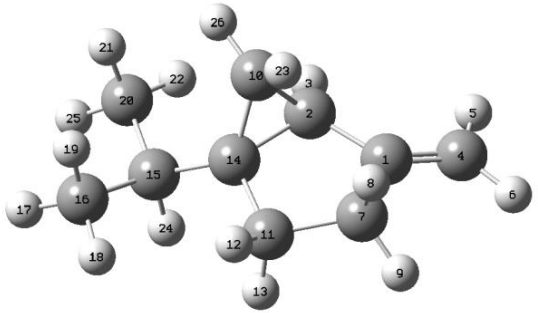
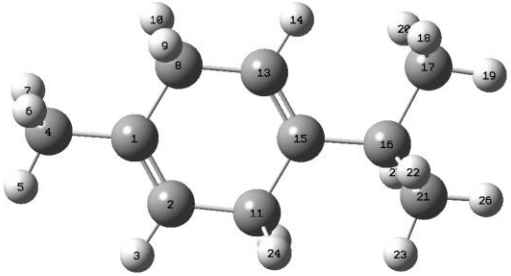
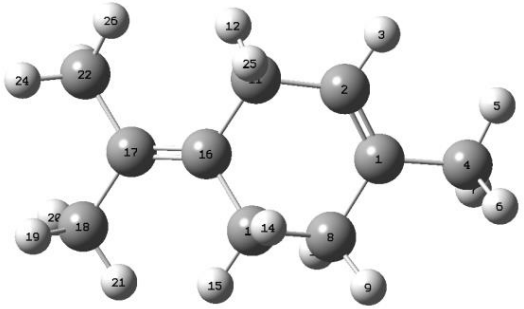


Phellandrene



Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C1	1.806197	-0.133576	-0.057032	**C1**	-2.166824	0.031948	-0.044361	**C1**	2.152170	0.020689	-0.223857
C2	1.509979	1.151531	0.181141	**C2**	-1.522409	1.188944	-0.259957	**C2**	1.476234	1.249144	0.201578
H3	2.281414	1.797127	0.600914	**H3**	-2.101859	2.078603	-0.505726	**H3**	2.057729	2.169188	0.174466
C4	3.166517	-0.713315	0.238762	**C4**	-3.663734	-0.098732	-0.159723	**C4**	3.454685	0.012840	-0.562375
H5	3.848927	0.035020	0.652960	**H5**	-4.134896	0.841238	-0.462972	**H5**	4.049019	0.922798	-0.549573
H6	3.091308	-1.541292	0.956938	**H6**	-3.933493	-0.868271	-0.896000	**H6**	3.958749	-0.901103	-0.863920
H7	3.624462	-1.127641	-0.669634	**H7**	-4.106130	-0.411240	0.795770	**C7**	1.288185	-1.224528	-0.268593
C8	0.808738	-1.110801	-0.638919	**C8**	-1.417441	-1.232562	0.320683	**H8**	1.911151	-2.121317	-0.181460
H9	0.729185	-1.975949	0.039140	**H9**	-1.460258	-1.928228	-0.532640	**H9**	0.798883	-1.277893	-1.251305
H10	1.239424	-1.514898	-1.566465	**H10**	-1.942235	-1.742996	1.140666	**C10**	0.198981	1.281554	0.628325
C11	0.179491	1.811144	-0.076173	**C11**	-0.024128	1.359682	-0.182333	**C11**	0.215693	-1.199089	0.833012
H12	0.340455	2.655332	-0.761350	**H12**	0.226675	1.874235	0.756392	**H12**	0.716366	-1.186197	1.809322
C13	-0.574825	-0.556649	-0.947121	**C13**	0.043349	-0.975825	0.715987	**H13**	-0.381434	-2.114616	0.800082
C14	-0.891893	0.903975	-0.665513	**H14**	0.591634	-1.923507	0.755270	**C14**	-0.681306	0.055198	0.734258
C15	-1.564826	-0.190510	0.143270	**H15**	0.087230	-0.541141	1.723211	**C15**	-1.738911	-0.004894	-0.413589
C16	-1.203783	-0.393105	1.605205	**C16**	0.714834	0.014432	-0.263676	**C16**	-2.704002	-1.189716	-0.243891
H17	-0.150137	-0.195254	1.812469	**C17**	2.219184	0.079279	-0.052392	**H17**	-3.460791	-1.184486	-1.036058

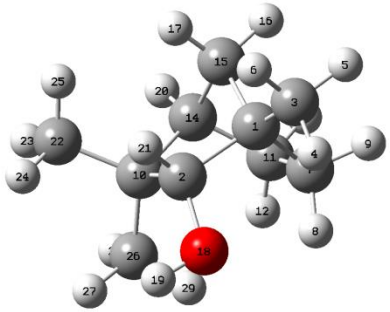
H18	-1.801083	0.272580	2.240730	**C18**	2.996594	-1.048372	-0.692030	**H18**	-2.195114	-2.156793	-0.285597
H19	-1.420677	-1.423805	1.912687	**H19**	4.060568	-1.005461	-0.442764	**H19**	-3.229148	-1.126542	0.718019
C20	-3.034474	-0.452908	-0.147303	**H20**	2.612834	-2.027023	-0.377897	**C20**	-2.541398	1.303809	-0.511464
H21	-3.675014	0.219043	0.438283	**H21**	2.898193	-1.009734	-1.785030	**H21**	-3.047180	1.521754	0.438499
H22	-3.270425	-0.300185	-1.206227	**C22**	2.838632	1.037464	0.650676	**H22**	-1.906181	2.158431	-0.760699
H23	-0.181755	2.265951	0.859835	**H23**	3.916205	1.021939	0.790959	**H23**	-0.230500	2.235707	0.923811
H24	-3.306705	-1.484580	0.110296	**H24**	2.306372	1.864576	1.108303	**H24**	-1.256293	0.137469	1.670201
H25	-1.535674	1.399006	-1.390518	**H25**	0.321916	2.021579	-0.986517	**H25**	-1.195274	-0.133370	-1.359907
H26	-1.020436	-0.975162	-1.847961	**H26**	0.548901	-0.382117	-1.278276	**H26**	-3.311968	1.226931	-1.286298

Sabinene	γ-Terpinene	Terpinolene
		

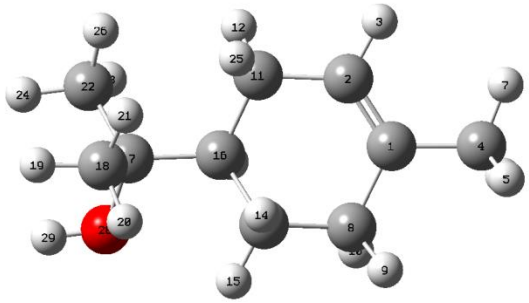
Atom		X	Y	Z	Atom		X	Y	Z	Atom		X	Y	Z
C	**1**	-2.029328	-0.261228	-0.093833	**C**	**1**	-2.231414	-0.013957	0.019993	**C**	**1**	2.108200	0.061145	-0.144188
C	**2**	-0.723283	-0.889132	0.232958	**C**	**2**	-1.615874	-1.161115	-0.292476	**C**	**2**	1.497624	1.213172	0.168120
H	**3**	-0.557080	-1.923304	-0.051706	**H**	**3**	-2.212370	-2.055904	-0.468485	**H**	**3**	2.062782	2.144126	0.124019
C	**4**	-3.134790	-0.902983	-0.489697	**C**	**4**	-3.727829	0.104619	0.143185	**C**	**4**	3.545317	-0.006728	-0.591210
H	**5**	-3.174110	-1.987792	-0.538512	**H**	**5**	-4.230401	-0.847409	-0.052979	**H**	**5**	4.002125	0.985647	-0.655728
H	**6**	-4.032298	-0.361989	-0.776474	**H**	**6**	-4.013293	0.441549	1.149034	**H**	**6**	4.144104	-0.616824	0.098507
C	**7**	-1.853580	1.244735	0.009608	**H**	**7**	-4.121593	0.850541	-0.560527	**H**	**7**	3.623485	-0.482458	-1.578348
H	**8**	-2.111035	1.578113	1.023196	**C**	**8**	-1.445658	1.250718	0.271484	**C**	**8**	1.365964	-1.254508	-0.063558
H	**9**	-2.508169	1.788834	-0.677257	**H**	**9**	-1.687455	1.633330	1.277489	**H**	**9**	2.028127	-2.023083	0.359948
C	**10**	0.018153	-0.365582	1.463056	**H**	**10**	-1.801224	2.039813	-0.412359	**H**	**10**	1.116683	-1.597412	-1.079373
C	**11**	-0.349540	1.481788	-0.272315	**C**	**11**	-0.124995	-1.317604	-0.423700	**C**	**11**	0.042118	1.342660	0.563850
H	**12**	0.044465	2.348209	0.270296	**H**	**12**	0.119388	-1.694931	-1.430958	**H**	**12**	-0.394007	2.165914	-0.009322
H	**13**	-0.194084	1.665246	-1.343416	**C**	**13**	0.046090	1.096359	0.133272	**C**	**13**	0.084637	-1.147123	0.784123
C	**14**	0.365583	0.174636	0.102933	**H**	**14**	0.626897	2.000558	0.298022	**H**	**14**	0.385329	-1.014515	1.834590
C	**15**	1.733235	-0.061680	-0.536485	**C**	**15**	0.667076	-0.051167	-0.171277	**H**	**15**	-0.474098	-2.083240	0.736588
C	**16**	2.752018	0.970607	-0.019594	**C**	**16**	2.179374	-0.191029	-0.285284	**C**	**16**	-0.740991	0.054151	0.375954
H	**17**	3.725857	0.837396	-0.503993	**C**	**17**	2.927263	1.132529	-0.499708	**C**	**17**	-2.004477	-0.002001	-0.095063

H	**18**	2.422306	1.997104	-0.208804	**H**	**18**	2.861670	1.777538	0.384175	**C**	**18**	-2.777202	-1.285857	-0.313001
H	**19**	2.893519	0.856888	1.062137	**H**	**19**	3.989703	0.939899	-0.683585	**H**	**19**	-3.643339	-1.336013	0.361383
C	**20**	2.284712	-1.484416	-0.360278	**H**	**20**	2.525464	1.686077	-1.354479	**H**	**20**	-3.179194	-1.313615	-1.334695
H	**21**	2.490869	-1.710379	0.692319	**C**	**21**	2.761853	-0.931682	0.939384	**H**	**21**	-2.188839	-2.192307	-0.167356
H	**22**	1.594360	-2.241879	-0.743874	**H**	**22**	2.612412	-0.335185	1.846734	**C**	**22**	-2.830352	1.214629	-0.457517
H	**23**	-0.514487	0.260830	2.174276	**H**	**23**	2.290141	-1.906546	1.095947	**H**	**23**	-3.079451	1.208360	-1.527685
H	**24**	1.600609	0.104535	-1.616663	**H**	**24**	0.216908	-2.113852	0.255938	**H**	**24**	-3.786677	1.193506	0.082466
H	**25**	3.228896	-1.590647	-0.904937	**H**	**25**	2.370644	-0.822341	-1.167372	**H**	**25**	-0.012908	1.658074	1.620515
H	**26**	0.711301	-1.061638	1.925302	**H**	**26**	3.837789	-1.099162	0.814167	**H**	**26**	-2.349148	2.166601	-0.230572

Fenchol



Terpineol

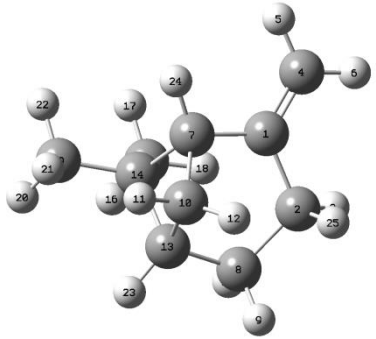


Atom		X	Y	Z	Atom		X	Y	Z
C	**1**	1.252172	-0.111217	0.231525	**C**	**1**	2.463005	0.089109	-0.028551
C	**2**	0.013843	-1.032910	0.137357	**C**	**2**	1.767083	1.222801	0.145466
C	**3**	2.532320	-0.846639	0.598115	**H**	**3**	2.306550	2.164660	0.245040
H	**4**	2.786160	-1.583712	-0.171003	**C**	**4**	3.966663	0.066126	-0.125164
H	**5**	3.371372	-0.147853	0.693476	**H**	**5**	4.402879	-0.541278	0.679302
H	**6**	2.423064	-1.377171	1.551971	**H**	**6**	4.289163	-0.390149	-1.071049
C	**7**	1.339884	0.723806	-1.078018	**H**	**7**	4.397682	1.070453	-0.067996
H	**8**	1.223936	0.088335	-1.959227	**C**	**8**	1.764302	-1.248995	-0.146275
H	**9**	2.321469	1.205833	-1.143474	**H**	**9**	2.322040	-2.002125	0.427795
C	**10**	-1.223556	-0.043629	0.185246	**H**	**10**	1.807694	-1.585442	-1.194192
C	**11**	0.196586	1.775590	-0.927951	**C**	**11**	0.259665	1.307426	0.199515
H	**12**	-0.471642	1.814406	-1.791274	**H**	**12**	-0.066870	2.157341	-0.412297
H	**13**	0.605703	2.783580	-0.796339	**C**	**13**	0.307696	-1.197930	0.330591
C	**14**	-0.505194	1.333295	0.376112	**H**	**14**	0.300086	-1.111154	1.425511
C	**15**	0.723482	0.943996	1.228918	**H**	**15**	-0.215926	-2.121720	0.069452
H	**16**	1.426432	1.772437	1.373226	**C**	**16**	-0.417330	0.011397	-0.282662
H	**17**	0.482838	0.525098	2.211852	**C**	**17**	-1.952420	-0.017568	-0.072105

O	**18**	0.113910	-1.856806	-1.024826	**C**	**18**	-2.364912	-0.158487	1.401274
H	**19**	-0.602056	-2.503466	-1.017744	**H**	**19**	-3.458423	-0.151217	1.488328
H	**20**	-1.167984	2.096008	0.798453	**H**	**20**	-1.999092	-1.099476	1.818632
H	**21**	-0.006656	-1.681343	1.027598	**H**	**21**	-1.982481	0.667801	2.008707
C	**22**	-2.113558	-0.353704	1.403691	**C**	**22**	-2.624764	1.214936	-0.696170
H	**23**	-2.968462	0.331702	1.444218	**H**	**23**	-2.308631	1.337442	-1.736760
H	**24**	-2.507917	-1.376121	1.345815	**H**	**24**	-3.714775	1.094848	-0.681795
H	**25**	-1.569555	-0.264589	2.349221	**H**	**25**	-0.053945	1.543574	1.228186
C	**26**	-2.094231	-0.120896	-1.077573	**H**	**26**	-2.387817	2.129942	-0.144670

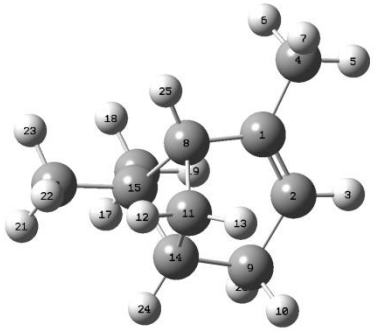
B3LYP-D3/6-311+G(2d,p)

α-Pinene



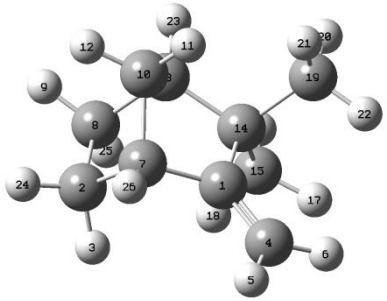
Atom	X	Y	Z
C1	1.387122	-0.526278	-0.274312
C2	1.743774	0.799446	0.383036
H5	2.402373	0.635089	1.238035
C6	2.206242	-1.574231	-0.280872
H5	1.941603	-2.494378	-0.789643
H6	3.169213	-1.547324	0.217841
C7	0.025929	-0.543811	-0.910460
C8	0.501823	1.643366	0.788442
H11	0.712215	2.701925	0.613883
C12	-0.305840	0.874694	-1.464112
H11	-1.135730	0.861632	-2.167061
H12	0.511332	1.447201	-1.905306
C13	-0.737494	1.230875	-0.015404
C14	-1.070342	-0.285328	0.196029
C15	-0.867175	-0.907675	1.573719

β-Pinene



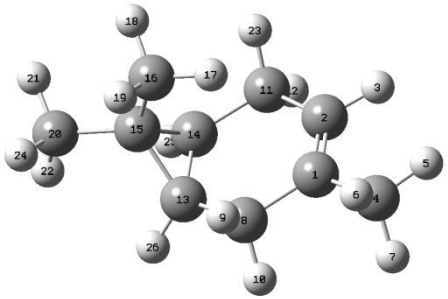
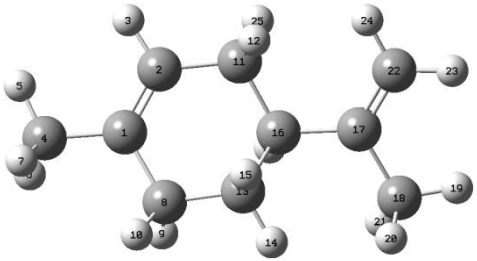
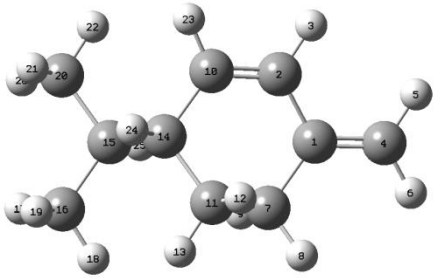
Atom	X	Y	Z
C1	1.442239	-0.282552	-0.089883
C2	1.512763	0.906572	0.510955
H3	2.421930	1.238097	1.003088
C4	2.560582	-1.276861	-0.145869
H5	3.458000	-0.908160	0.354464
H6	2.263880	-2.218423	0.330012
H7	2.818418	-1.519551	-1.182713
C8	0.125731	-0.631665	-0.762120
C9	0.297815	1.806444	0.542552
H10	0.535871	2.783776	0.105382
C11	-0.314988	0.619940	-1.579493
H12	-1.096853	0.410395	-2.306062
H13	0.481652	1.188970	-2.059669
C14	-0.864728	1.164725	-0.232560
C15	-1.082916	-0.327661	0.205323

Camphene



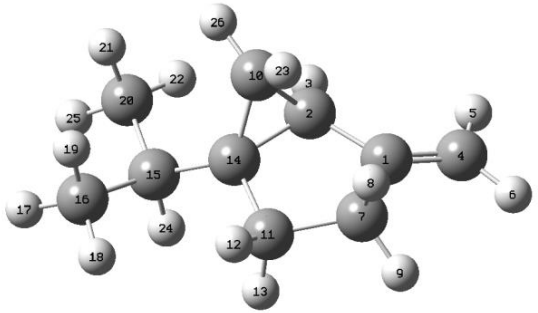
Atom	X	Y	Z
C1	-0.401082	1.042144	-0.027544
C2	1.893684	0.445660	-0.739818
H3	1.644551	0.891524	-1.703474
C4	-1.142056	2.090510	-0.361831
H5	-0.741895	3.097841	-0.334028
H6	-2.174839	1.983653	-0.675331
C7	1.045485	1.059517	0.410872
C8	1.542746	-1.073412	-0.664882
H9	2.414296	-1.659511	-0.365222
C10	1.059302	-0.093995	1.437817
H11	0.436338	0.097202	2.311387
H12	2.065593	-0.352442	1.775957
C13	0.475380	-1.128117	0.449580
C14	-0.848105	-0.430598	-0.009207
C15	-1.365989	-0.898215	-1.377401

H16	-1.593912	-0.504366	2.285567	**C16**	-0.969127	-0.690679	1.683131	**H16**	-1.514492	-1.982106	-1.385149
H17	-1.015990	-1.989998	1.523109	**H17**	-1.794542	-0.242233	2.244663	**H17**	-2.326805	-0.427579	-1.597142
H18	0.129948	-0.741536	1.978103	**H18**	-1.036132	-1.775055	1.814120	**H18**	-0.685929	-0.637495	-2.188008
C21	-2.475322	-0.642334	-0.300366	**H19**	-0.034855	-0.360453	2.133262	**C19**	-1.962927	-0.661428	1.029241
H20	-3.228486	-0.265262	0.397909	**C20**	-2.403464	-0.897791	-0.325839	**H20**	-2.249832	-1.716910	1.048130
H21	-2.702037	-0.228643	-1.283411	**H21**	-3.245910	-0.484912	0.237089	**H21**	-1.657714	-0.374288	2.035780
H22	-2.593029	-1.728029	-0.362170	**H22**	-2.576418	-0.683336	-1.380235	**H22**	-2.847098	-0.073258	0.774531
H23	-1.559366	1.938013	0.122224	**H23**	-2.423884	-1.984419	-0.201983	**H23**	0.304972	-2.130286	0.845352
H24	-0.117341	-1.410526	-1.558549	**H24**	-1.744588	1.812522	-0.253105	**H24**	2.956965	0.618087	-0.559263
H25	2.329987	1.372387	-0.341532	**H25**	0.147435	-1.605315	-1.255844	**H25**	1.199752	-1.479887	-1.615075
H26	0.296922	1.541473	1.856807	**H26**	0.002563	2.005267	1.580357	**H26**	1.397515	2.033047	0.750600

Car-3-ene				Limonene				Phellandrene			
											
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C1	1.800652	-0.131934	-0.057152	**C1**	-2.161164	0.034144	-0.043385	**C1**	2.155056	0.023418	-0.218543
C2	1.506857	1.144989	0.180904	**C2**	-1.520380	1.186549	-0.240259	**C2**	1.473821	1.238177	0.222138
H3	2.276461	1.788408	0.600529	**H3**	-2.097716	2.077864	-0.472604	**H3**	2.050201	2.158718	0.214956
C4	3.156988	-0.711383	0.237940	**C4**	-3.654155	-0.094415	-0.160914	**C4**	3.455405	0.022015	-0.533350
H5	3.837355	0.034141	0.652757	**H5**	-4.123462	0.847410	-0.450274	**H5**	4.047699	0.929122	-0.489411
H6	3.080122	-1.538489	0.952607	**H6**	-3.922292	-0.851970	-0.905967	**H6**	3.962655	-0.883274	-0.846054
H7	3.613313	-1.123557	-0.668828	**H7**	-4.095221	-0.419786	0.787637	**C7**	1.293380	-1.215757	-0.304959
C8	0.806011	-1.105528	-0.639019	**C8**	-1.415038	-1.232252	0.304072	**H8**	1.913323	-2.112797	-0.240424
H9	0.729291	-1.970774	0.034396	**H9**	-1.462496	-1.916483	-0.554336	**H9**	0.812348	-1.238300	-1.289601
H10	1.235951	-1.506732	-1.564875	**H10**	-1.938644	-1.748973	1.116883	**C10**	0.200395	1.258868	0.635418
C11	0.180520	1.804418	-0.074842	**C11**	-0.025776	1.356156	-0.161022	**C11**	0.215956	-1.222194	0.787145
H12	0.341924	2.646792	-0.757697	**H12**	0.224361	1.855970	0.782444	**H12**	0.708503	-1.243182	1.764190
C13	-0.573778	-0.554036	-0.944672	**C13**	0.043925	-0.986008	0.698773	**H13**	-0.381205	-2.132328	0.719831
C14	-0.889310	0.902247	-0.662158	**H14**	0.587293	-1.933282	0.720450	**C14**	-0.675910	0.033308	0.722855
C15	-1.560998	-0.190021	0.143653	**H15**	0.091183	-0.570640	1.710793	**C15**	-1.745815	-0.008917	-0.409183
C16	-1.200131	-0.393688	1.600818	**C16**	0.713603	0.017240	-0.262650	**C16**	-2.744206	-1.155199	-0.204302
H17	-0.148830	-0.198416	1.807614	**C17**	2.214503	0.082730	-0.054821	**H17**	-3.493288	-1.157849	-0.999842

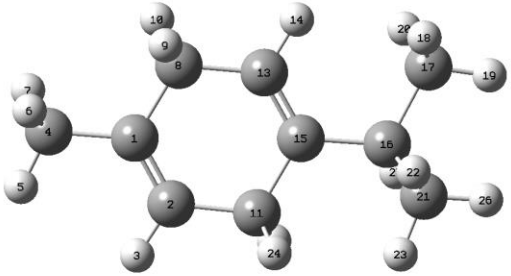
H18	-1.794350	0.270056	2.236468	**C18**	2.987134	-1.067961	-0.648773	**H18**	-2.265381	-2.135120	-0.204804
H19	-1.418140	-1.421303	1.907918	**H19**	4.051569	-1.004193	-0.419648	**H19**	-3.272255	-1.040290	0.747837
C20	-3.026357	-0.450083	-0.147881	**H20**	2.618303	-2.030134	-0.281193	**C20**	-2.505704	1.319123	-0.524731
H21	-3.665768	0.219436	0.436493	**H21**	2.871104	-1.083660	-1.737768	**H21**	-2.982537	1.578096	0.426523
H22	-3.260553	-0.296374	-1.203949	**C22**	2.835503	1.062722	0.599355	**H22**	-1.850571	2.143529	-0.809021
H23	-0.177908	2.259748	0.858576	**H23**	3.911105	1.049849	0.734580	**H23**	-0.234245	2.204234	0.941367
H24	-3.299737	-1.478941	0.107857	**H24**	2.308988	1.908765	1.021033	**H24**	-1.237491	0.099141	1.664788
H25	-1.532087	1.396160	-1.383321	**H25**	0.317105	2.029044	-0.953372	**H25**	-1.219299	-0.173647	-1.356135
H26	-1.019760	-0.970045	-1.842086	**H26**	0.549885	-0.363210	-1.280924	**H26**	-3.292725	1.246900	-1.279127

Sabinene



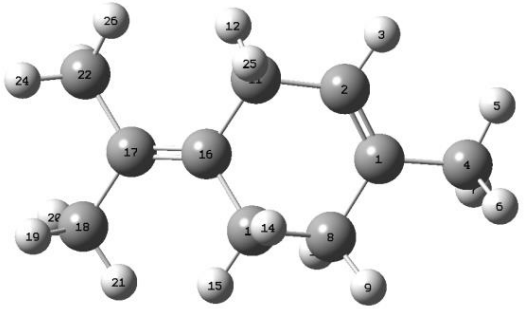
Atom		X	Y	Z
C	**1**	-2.024041	-0.261850	-0.092845
C	**2**	-0.722278	-0.887322	0.231831
H	**3**	-0.554210	-1.917511	-0.052562
C	**4**	-3.122497	-0.900192	-0.487014
H	**5**	-3.161157	-1.982388	-0.536285
H	**6**	-4.017633	-0.360377	-0.773479
C	**7**	-1.850164	1.240684	0.007264
H	**8**	-2.111563	1.575167	1.015949
H	**9**	-2.500721	1.779915	-0.682037
C	**10**	0.017523	-0.364921	1.458776
C	**11**	-0.348998	1.478263	-0.270435
H	**12**	0.041951	2.341748	0.272660
H	**13**	-0.192220	1.664953	-1.337735
C	**14**	0.364242	0.174762	0.102723
C	**15**	1.728251	-0.060758	-0.534262
C	**16**	2.745222	0.968308	-0.017944

γ-Terpinene



Atom		X	Y	Z
C	**1**	-2.224778	-0.015602	0.019521
C	**2**	-1.612357	-1.155734	-0.288819
H	**3**	-2.207360	-2.047997	-0.466901
C	**4**	-3.717798	0.103316	0.136403
H	**5**	-4.218564	-0.846017	-0.061012
H	**6**	-4.005521	0.440268	1.138535
H	**7**	-4.106595	0.847910	-0.567105
C	**8**	-1.441844	1.244645	0.274372
H	**9**	-1.682668	1.622550	1.279410
H	**10**	-1.798137	2.034371	-0.403848
C	**11**	-0.125055	-1.312999	-0.412338
H	**12**	0.123252	-1.697486	-1.412791
C	**13**	0.045589	1.092215	0.133617
H	**14**	0.623889	1.995820	0.293274
C	**15**	0.663737	-0.048196	-0.166948
C	**16**	2.172096	-0.184414	-0.288944

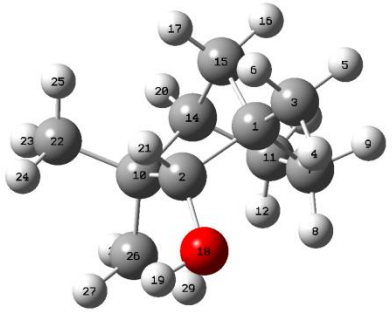
Terpinolene



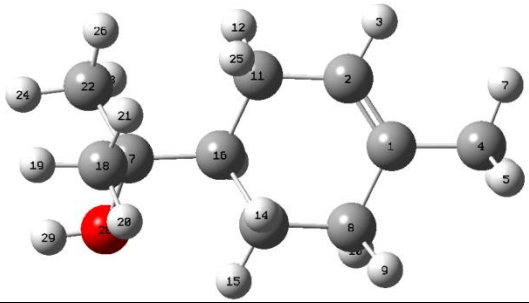
Atom		X	Y	Z
C	**1**	2.100288	0.062654	-0.142343
C	**2**	1.493144	1.207348	0.167446
H	**3**	2.056336	2.136211	0.121348
C	**4**	3.533311	-0.004012	-0.589829
H	**5**	3.987508	0.986209	-0.655592
H	**6**	4.131348	-0.611710	0.098163
H	**7**	3.609800	-0.479916	-1.573911
C	**8**	1.363419	-1.251316	-0.059725
H	**9**	2.025748	-2.013342	0.367748
H	**10**	1.121599	-1.598343	-1.072764
C	**11**	0.040974	1.337533	0.560851
H	**12**	-0.392874	2.156556	-0.014444
C	**13**	0.081360	-1.146907	0.780169
H	**14**	0.375359	-1.017885	1.830028
H	**15**	-0.476606	-2.079671	0.727869
C	**16**	-0.741042	0.052578	0.374756

H	**17**	3.715893	0.835935	-0.502386	**C**	**17**	2.916276	1.139627	-0.485207	**C**	**17**	-1.996411	-0.001825	-0.094392
H	**18**	2.416309	1.992355	-0.204898	**H**	**18**	2.850602	1.771140	0.404783	**C**	**18**	-2.766803	-1.281824	-0.316912
H	**19**	2.888088	0.853493	1.060590	**H**	**19**	3.976160	0.951574	-0.672062	**H**	**19**	-3.619011	-1.343811	0.369576
C	**20**	2.277910	-1.480478	-0.360474	**H**	**20**	2.515077	1.702988	-1.330150	**H**	**20**	-3.185079	-1.295271	-1.329265
H	**21**	2.481139	-1.708520	0.689193	**C**	**21**	2.760436	-0.943483	0.916744	**H**	**21**	-2.174313	-2.185554	-0.195070
H	**22**	1.590533	-2.235131	-0.746691	**H**	**22**	2.614959	-0.365153	1.833036	**C**	**22**	-2.819158	1.213787	-0.451996
H	**23**	-0.514370	0.259193	2.167124	**H**	**23**	2.293020	-1.919398	1.057778	**H**	**23**	-3.049497	1.222581	-1.523483
H	**24**	1.596945	0.106773	-1.611349	**H**	**24**	0.213058	-2.101879	0.273101	**H**	**24**	-3.781888	1.179380	0.069858
H	**25**	3.221009	-1.585321	-0.901712	**H**	**25**	2.357756	-0.799033	-1.180342	**H**	**25**	-0.015922	1.655362	1.613590
H	**26**	0.708984	-1.059266	1.917896	**H**	**26**	3.833251	-1.105910	0.783884	**H**	**26**	-2.347000	2.161108	-0.201800

Fenchol



Terpineol

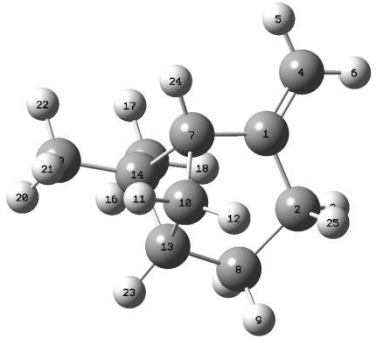


Atom		X	Y	Z	Atom		X	Y	Z
C	**1**	1.249568	-0.109832	0.230738	**C**	**1**	2.456356	0.090132	-0.028197
C	**2**	0.015271	-1.030177	0.135321	**C**	**2**	1.764499	1.216462	0.144273
C	**3**	2.526209	-0.843475	0.597116	**H**	**3**	2.302272	2.156187	0.243610
H	**4**	2.781193	-1.578228	-0.169952	**C**	**4**	3.956175	0.067415	-0.123960
H	**5**	3.363574	-0.147223	0.693667	**H**	**5**	4.390423	-0.537926	0.679278
H	**6**	2.416493	-1.373836	1.547739	**H**	**6**	4.277615	-0.389152	-1.066820
C	**7**	1.337924	0.724582	-1.074896	**H**	**7**	4.385478	1.069303	-0.067827
H	**8**	1.225750	0.093114	-1.955360	**C**	**8**	1.761086	-1.245302	-0.144696
H	**9**	2.315148	1.208398	-1.137882	**H**	**9**	2.317430	-1.993403	0.431658
C	**10**	-1.221000	-0.043889	0.184352	**H**	**10**	1.809913	-1.583842	-1.188528
C	**11**	0.193989	1.771168	-0.926495	**C**	**11**	0.260801	1.302120	0.196005
H	**12**	-0.472483	1.805392	-1.787103	**H**	**12**	-0.062368	2.149013	-0.416435
H	**13**	0.599716	2.777473	-0.798119	**C**	**13**	0.306396	-1.197325	0.326350
C	**14**	-0.504808	1.330008	0.374886	**H**	**14**	0.294548	-1.115076	1.418509
C	**15**	0.720824	0.942329	1.226250	**H**	**15**	-0.213212	-2.118962	0.062137
H	**16**	1.420563	1.769151	1.370199	**C**	**16**	-0.416824	0.010027	-0.283505
H	**17**	0.479865	0.524112	2.205608	**C**	**17**	-1.948271	-0.016928	-0.070797

O	**18**	0.115455	-1.855522	-1.022812	**C**	**18**	-2.356385	-0.150461	1.400306
H	**19**	-0.596029	-2.503222	-1.009710	**H**	**19**	-3.446970	-0.143066	1.488344
H	**20**	-1.165059	2.090597	0.796206	**H**	**20**	-1.990746	-1.087084	1.820125
H	**21**	-0.005428	-1.674881	1.023966	**H**	**21**	-1.974024	0.676635	2.001508
C	**22**	-2.107313	-0.353675	1.400832	**C**	**22**	-2.618270	1.210918	-0.697010
H	**23**	-2.961052	0.328687	1.441319	**H**	**23**	-2.306950	1.326345	-1.736903
H	**24**	-2.499182	-1.373996	1.344109	**H**	**24**	-3.705591	1.092939	-0.677494
H	**25**	-1.564130	-0.262762	2.343338	**H**	**25**	-0.052604	1.541374	1.220767
C	**26**	-2.091093	-0.120991	-1.074093	**H**	**26**	-2.377378	2.126099	-0.153305

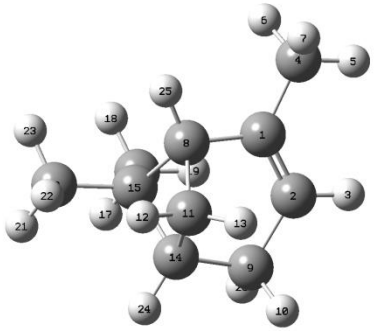
DFTBA

α-Pinene



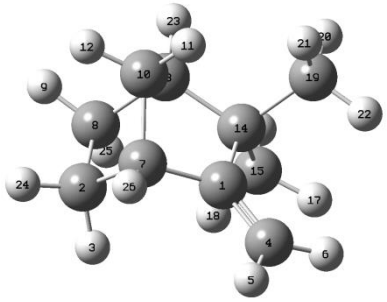
Atom	X	Y	Z
C1	1.369057	-0.515258	-0.265410
C2	1.705275	0.810317	0.388637
H5	2.336470	0.645340	1.284397
C6	2.218084	-1.542625	-0.275782
H5	1.964622	-2.482007	-0.779616
H6	3.195173	-1.481522	0.216646
C7	0.007799	-0.567351	-0.912577
C8	0.470534	1.651411	0.749306
H11	0.684138	2.721852	0.552730
C12	-0.304839	0.835026	-1.476884
H11	-1.139431	0.824597	-2.200836
H12	0.540114	1.403890	-1.906931
C13	-0.754577	1.216303	-0.052384
C14	-1.059855	-0.292577	0.197398

β-Pinene



Atom	X	Y	Z
C1	1.417556	-0.278395	-0.100732
C2	1.465557	0.912262	0.513244
H3	2.377124	1.259047	1.026402
C4	2.567180	-1.234808	-0.153015
H5	3.446132	-0.831825	0.370831
H6	2.295414	-2.197908	0.312052
H7	2.851482	-1.448691	-1.197566
C8	0.111980	-0.640981	-0.781420
C9	0.249013	1.805288	0.528304
H10	0.495664	2.791409	0.074643
C11	-0.321570	0.612705	-1.574802
H12	-1.103058	0.402893	-2.327830
H13	0.486650	1.205956	-2.041996
C14	-0.893219	1.144925	-0.244652

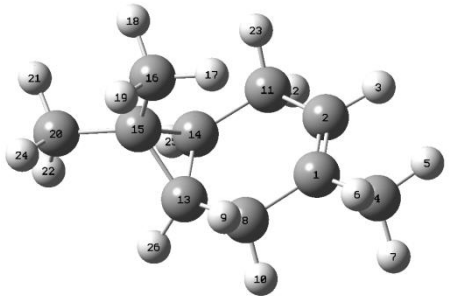
Camphene



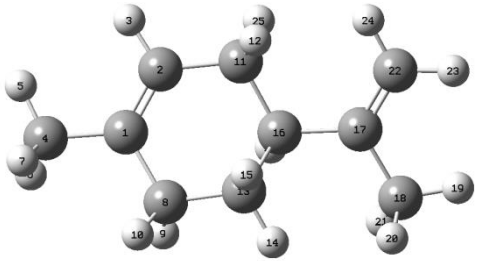
Atom	X	Y	Z
C1	-0.391869	1.036086	-0.010101
C2	1.874370	0.451431	-0.728463
H3	1.614608	0.929251	-1.692030
C4	-1.123628	2.093941	-0.343037
H5	-0.709776	3.108304	-0.303623
H6	-2.165899	1.987557	-0.666045
C7	1.056259	1.036588	0.440670
C8	1.513390	-1.044325	-0.699955
H9	2.401132	-1.656959	-0.446409
C10	1.057210	-0.135875	1.431059
H11	0.418559	0.038450	2.316325
H12	2.072724	-0.411929	1.772150
C13	0.472455	-1.139346	0.426613
C14	-0.843787	-0.429647	-0.009021

C15	-0.800606	-0.870747	1.584151	**C15**	-1.064331	-0.339542	0.206530	**C15**	-1.370150	-0.865745	-1.379325
H16	-1.469761	-0.407451	2.326243	**C16**	-0.880681	-0.676809	1.682021	**H16**	-1.504476	-1.957997	-1.416720
H17	-0.995967	-1.954268	1.584729	**H17**	-1.663470	-0.189687	2.284418	**H17**	-2.346501	-0.396965	-1.575197
H18	0.236917	-0.716827	1.910729	**H18**	-0.963633	-1.763964	1.837642	**H18**	-0.691508	-0.570865	-2.192012
C21	-2.469015	-0.671044	-0.252797	**H19**	0.097400	-0.352723	2.063897	**C19**	-1.948480	-0.660067	1.030070
H20	-3.217086	-0.279981	0.454780	**C20**	-2.385643	-0.934535	-0.277097	**H20**	-2.244171	-1.720806	1.049454
H21	-2.703191	-0.269424	-1.249332	**H21**	-3.226990	-0.530681	0.308070	**H21**	-1.620364	-0.378435	2.041145
H22	-2.582393	-1.765763	-0.292145	**H22**	-2.575523	-0.714361	-1.337448	**H22**	-2.838834	-0.062184	0.783437
H23	-1.600482	1.933456	0.052513	**H23**	-2.385197	-2.029045	-0.153082	**H23**	0.315400	-2.173468	0.803698
H24	-0.132870	-1.454133	-1.569612	**H24**	-1.805409	1.783466	-0.285782	**H24**	2.959149	0.606210	-0.565765
H25	2.338394	1.387186	-0.320401	**H25**	0.134959	-1.624104	-1.301282	**H25**	1.138178	-1.413462	-1.672078
H26	0.254218	1.574333	1.834165	**H26**	-0.056591	2.019539	1.576743	**H26**	1.427153	2.015049	0.812608

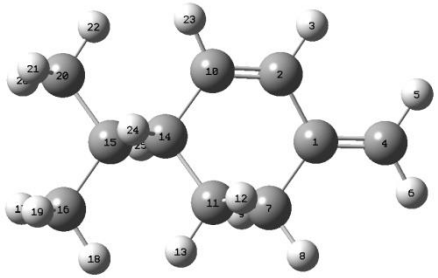
Car-3-ene



Limonene



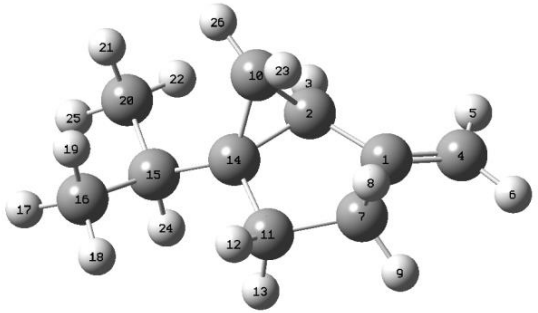
Phellandrene



Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C1	1.755446	-0.135280	-0.067314	**C1**	-2.144986	0.074459	-0.050382	**C1**	2.104511	0.017330	-0.218134
C2	1.464532	1.138505	0.215084	**C2**	-1.460607	1.221248	0.018445	**C2**	1.449607	1.234607	0.269217
H3	2.232191	1.767552	0.698067	**H3**	-2.006517	2.179944	0.029573	**H3**	2.047042	2.161233	0.270521
C4	3.101291	-0.715241	0.263005	**C4**	-3.642932	0.054113	-0.142232	**C4**	3.385284	0.023156	-0.611627
H5	3.751645	0.029257	0.744327	**H5**	-4.057160	1.072531	-0.152146	**H5**	3.980926	0.942532	-0.585210
H6	2.999643	-1.579097	0.942028	**H6**	-3.971110	-0.464023	-1.059451	**H6**	3.875973	-0.888481	-0.969645
H7	3.605197	-1.078658	-0.648891	**H7**	-4.080394	-0.491206	0.711461	**C7**	1.258053	-1.230350	-0.275021
C8	0.795932	-1.083414	-0.740474	**C8**	-1.457299	-1.268773	-0.066069	**H8**	1.897285	-2.131671	-0.191753
H9	0.733698	-2.019728	-0.138715	**H9**	-1.506014	-1.685032	-1.097581	**H9**	0.765805	-1.285681	-1.270968
H10	1.237073	-1.391793	-1.714766	**H10**	-2.018730	-1.980674	0.574932	**C10**	0.185453	1.250821	0.708817
C11	0.162434	1.819537	-0.084973	**C11**	0.035743	1.297267	0.107575	**C11**	0.197460	-1.232925	0.816963
H12	0.354030	2.650259	-0.801601	**H12**	0.330685	1.565970	1.147447	**H12**	0.696318	-1.268758	1.806414
C13	-0.589327	-0.525794	-0.985769	**C13**	-0.008542	-1.187416	0.390316	**H13**	-0.419216	-2.150287	0.740777
C14	-0.905441	0.914552	-0.660626	**H14**	0.511319	-2.139917	0.164301	**C14**	-0.685949	0.018426	0.760906
C15	-1.527114	-0.199103	0.162706	**H15**	0.032054	-1.050471	1.489574	**C15**	-1.689061	-0.010944	-0.420810
C16	-1.080401	-0.423758	1.591266	**C16**	0.707458	-0.019887	-0.294999	**C16**	-2.725715	-1.115032	-0.239405
H17	-0.010491	-0.212427	1.719928	**C17**	2.193976	-0.001476	0.030937	**H17**	-3.439155	-1.112674	-1.077245

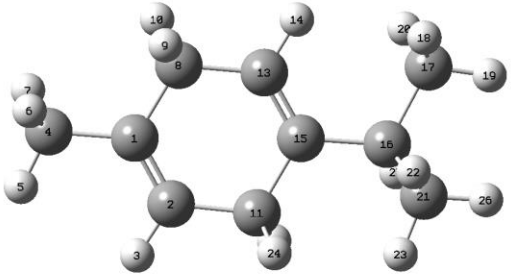
H18	-1.645714	0.226533	2.279045	**C18**	3.132761	-0.063212	-1.137718	**H18**	-2.257358	-2.109425	-0.200188
H19	-1.265144	-1.467761	1.893968	**H19**	4.182715	-0.036522	-0.813112	**H19**	-3.295737	-0.969200	0.691365
C20	-3.001704	-0.472651	-0.061937	**H20**	2.969031	-0.987258	-1.717386	**C20**	-2.390868	1.333807	-0.582076
H21	-3.623818	0.179596	0.572673	**H21**	2.955740	0.784246	-1.821129	**H21**	-2.910888	1.621460	0.344944
H22	-3.283136	-0.297604	-1.111037	**C22**	2.642411	0.069622	1.284018	**H22**	-1.673307	2.128153	-0.833736
H23	-0.211151	2.314870	0.841567	**H23**	3.715770	0.083986	1.503863	**H23**	-0.255395	2.196630	1.065060
H24	-3.250913	-1.516612	0.189608	**H24**	1.954272	0.116318	2.135689	**H24**	-1.287366	0.065535	1.703884
H25	-1.596004	1.420702	-1.361078	**H25**	0.407243	2.122032	-0.536642	**H25**	-1.119040	-0.216129	-1.359073
H26	-1.081000	-0.929211	-1.890939	**H26**	0.593193	-0.145598	-1.398740	**H26**	-3.138539	1.283383	-1.388115

Sabinene



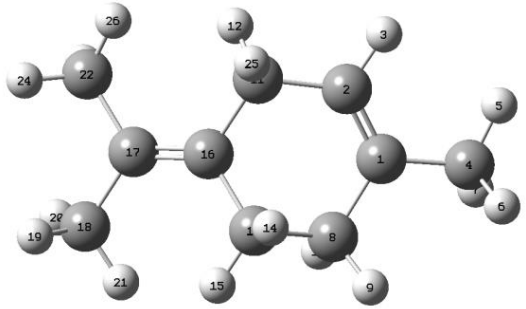
Atom		X	Y	Z
C	**1**	-2.013211	-0.256641	-0.100021
C	**2**	-0.695913	-0.890709	0.187613
H	**3**	-0.516278	-1.933839	-0.120161
C	**4**	-3.149362	-0.902594	-0.359637
H	**5**	-3.195799	-1.996824	-0.343633
H	**6**	-4.071394	-0.360145	-0.594852
C	**7**	-1.837320	1.245324	-0.096224
H	**8**	-2.195314	1.661074	0.869467
H	**9**	-2.436065	1.732364	-0.889387
C	**10**	0.006695	-0.372504	1.426006
C	**11**	-0.336563	1.499986	-0.269467
H	**12**	0.012023	2.340083	0.364684
H	**13**	-0.108025	1.776309	-1.319231
C	**14**	0.367385	0.188714	0.077285
C	**15**	1.751763	-0.034096	-0.534043
C	**16**	2.766910	0.909022	0.107641
H	**17**	3.756472	0.793779	-0.359669

γ-Terpinene



Atom		X	Y	Z
C	**1**	-2.203246	-0.001285	0.019095
C	**2**	-1.610505	-1.156426	-0.295041
H	**3**	-2.225750	-2.055930	-0.467711
C	**4**	-3.694393	0.111901	0.146359
H	**5**	-4.187256	-0.851377	-0.048668
H	**6**	-3.976121	0.448393	1.158744
H	**7**	-4.092104	0.856465	-0.564274
C	**8**	-1.420419	1.259437	0.265327
H	**9**	-1.669667	1.657840	1.277968
H	**10**	-1.763611	2.052043	-0.442540
C	**11**	-0.129837	-1.324641	-0.436927
H	**12**	0.108233	-1.697737	-1.462593
C	**13**	0.062460	1.084374	0.145196
H	**14**	0.668351	1.985079	0.338019
C	**15**	0.657872	-0.068642	-0.170547
C	**16**	2.170072	-0.223317	-0.269768
C	**17**	2.893501	1.082947	-0.574399

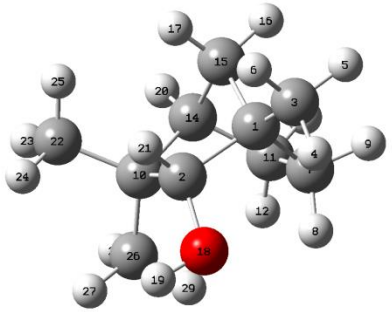
Terpinolene



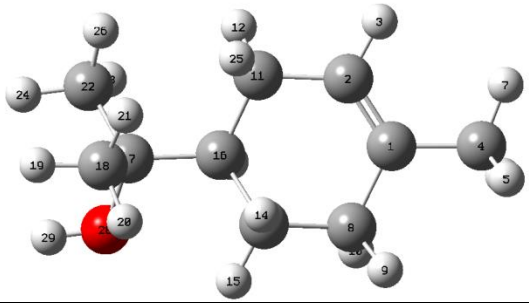
Atom		X	Y	Z
C	**1**	-2.159947	0.071550	0.066886
C	**2**	-1.498960	1.210818	-0.159927
H	**3**	-2.060470	2.141409	-0.348554
C	**4**	-3.658364	0.006585	0.072852
H	**5**	-4.102451	0.993728	-0.120654
H	**6**	-4.023463	-0.696556	-0.695232
H	**7**	-4.029285	-0.356834	1.046442
C	**8**	-1.413223	-1.207921	0.344751
H	**9**	-2.025348	-2.079709	0.035123
H	**10**	-1.255422	-1.312992	1.441114
C	**11**	-0.005078	1.328594	-0.125935
H	**12**	0.289093	1.919128	0.775667
C	**13**	-0.070852	-1.236700	-0.373816
H	**14**	-0.251289	-1.339148	-1.467848
H	**15**	0.497484	-2.136194	-0.065317
C	**16**	0.736063	0.012966	-0.127477
C	**17**	2.074790	-0.009232	0.025969

H	**18**	2.454304	1.957622	-0.006051	**H**	**18**	2.819051	1.789482	0.266096	**C**	**18**	2.868040	-1.288918	-0.006115
H	**19**	2.871050	0.698435	1.182963	**H**	**19**	3.962066	0.891598	-0.755217	**H**	**19**	2.837919	-1.755738	-1.006137
C	**20**	2.226624	-1.478410	-0.432753	**H**	**20**	2.475681	1.566643	-1.469504	**H**	**20**	3.922557	-1.104209	0.244070
H	**21**	2.309326	-1.800898	0.616275	**C**	**21**	2.722527	-0.853431	1.008853	**H**	**21**	2.475491	-2.029389	0.711263
H	**22**	1.536152	-2.161243	-0.949278	**H**	**22**	2.554124	-0.194488	1.873861	**C**	**22**	2.840592	1.271832	0.220316
H	**23**	-0.563945	0.255698	2.123940	**H**	**23**	2.235917	-1.818682	1.214137	**H**	**23**	2.500237	1.808305	1.124069
H	**24**	1.681658	0.226867	-1.620537	**H**	**24**	0.221769	-2.134908	0.246084	**H**	**24**	3.918531	1.083320	0.323058
H	**25**	3.218780	-1.585244	-0.896204	**H**	**25**	2.375595	-0.932104	-1.111710	**H**	**25**	0.334824	1.949381	-0.989383
H	**26**	0.725015	-1.052589	1.903268	**H**	**26**	3.805531	-1.027817	0.918421	**H**	**26**	2.693225	1.958056	-0.632711

Fenchol



Terpineol



Atom		X	Y	Z	Atom		X	Y	Z
C	**1**	1.248613	-0.116157	0.234578	**C**	**1**	2.443322	0.080527	-0.030430
C	**2**	0.003960	-1.029693	0.167896	**C**	**2**	1.761806	1.222159	0.112370
C	**3**	2.525940	-0.834938	0.632691	**H**	**3**	2.310035	2.175197	0.204959
H	**4**	2.777387	-1.611098	-0.104929	**C**	**4**	3.942634	0.061215	-0.095840
H	**5**	3.370711	-0.131262	0.692740	**H**	**5**	4.362633	-0.549331	0.721748
H	**6**	2.412882	-1.320050	1.615070	**H**	**6**	4.286300	-0.387183	-1.043600
C	**7**	1.331590	0.645263	-1.106244	**H**	**7**	4.360268	1.075657	-0.020811
H	**8**	1.191624	-0.039820	-1.962554	**C**	**8**	1.749473	-1.253484	-0.156478
H	**9**	2.321136	1.129820	-1.224369	**H**	**9**	2.305888	-2.017838	0.426110
C	**10**	-1.203068	-0.029706	0.204941	**H**	**10**	1.796115	-1.585131	-1.218021
C	**11**	0.208015	1.688808	-1.002883	**C**	**11**	0.262712	1.302277	0.174000
H	**12**	-0.483195	1.666354	-1.865501	**H**	**12**	-0.081425	2.166856	-0.433211
H	**13**	0.625356	2.714414	-0.953718	**C**	**13**	0.301513	-1.192751	0.305007
C	**14**	-0.475067	1.341672	0.327146	**H**	**14**	0.271320	-1.118958	1.411626
C	**15**	0.744085	0.984454	1.186268	**H**	**15**	-0.228376	-2.123021	0.023993
H	**16**	1.455896	1.824106	1.292408	**C**	**16**	-0.403592	0.014987	-0.314511
H	**17**	0.487796	0.605756	2.194025	**C**	**17**	-1.928234	-0.015306	-0.065384

O	**18**	0.040786	-1.849640	-1.011890	**C**	**18**	-2.304949	-0.032688	1.419936
H	**19**	-0.748084	-2.431285	-0.994108	**H**	**19**	-3.399591	-0.068210	1.535310
H	**20**	-1.128628	2.152130	0.719033	**H**	**20**	-1.883645	-0.913031	1.925062
H	**21**	-0.028526	-1.703391	1.075283	**H**	**21**	-1.942019	0.868790	1.935166
C	**22**	-2.069054	-0.272922	1.446690	**C**	**22**	-2.629886	1.150549	-0.772737
H	**23**	-2.893992	0.454641	1.495054	**H**	**23**	-2.358240	1.182458	-1.837716
H	**24**	-2.509791	-1.282138	1.423320	**H**	**24**	-3.723372	1.041874	-0.702128
H	**25**	-1.482506	-0.182748	2.373405	**H**	**25**	-0.046729	1.526084	1.221240
C	**26**	-2.097476	-0.134733	-1.032129	**H**	**26**	-2.357825	2.114091	-0.317581