Supplementary Information (SI) for RSC Advances.

SUPPLEMENTARY FILE

Docking-Based Computational Analysis of Guava *(Psidium guajava)* Leaves Derived Bioactive Compounds as a Coagulation Factor IXa Inhibitor

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Figure S1. *Structural Representation of Identified CFIXa Active Sites*

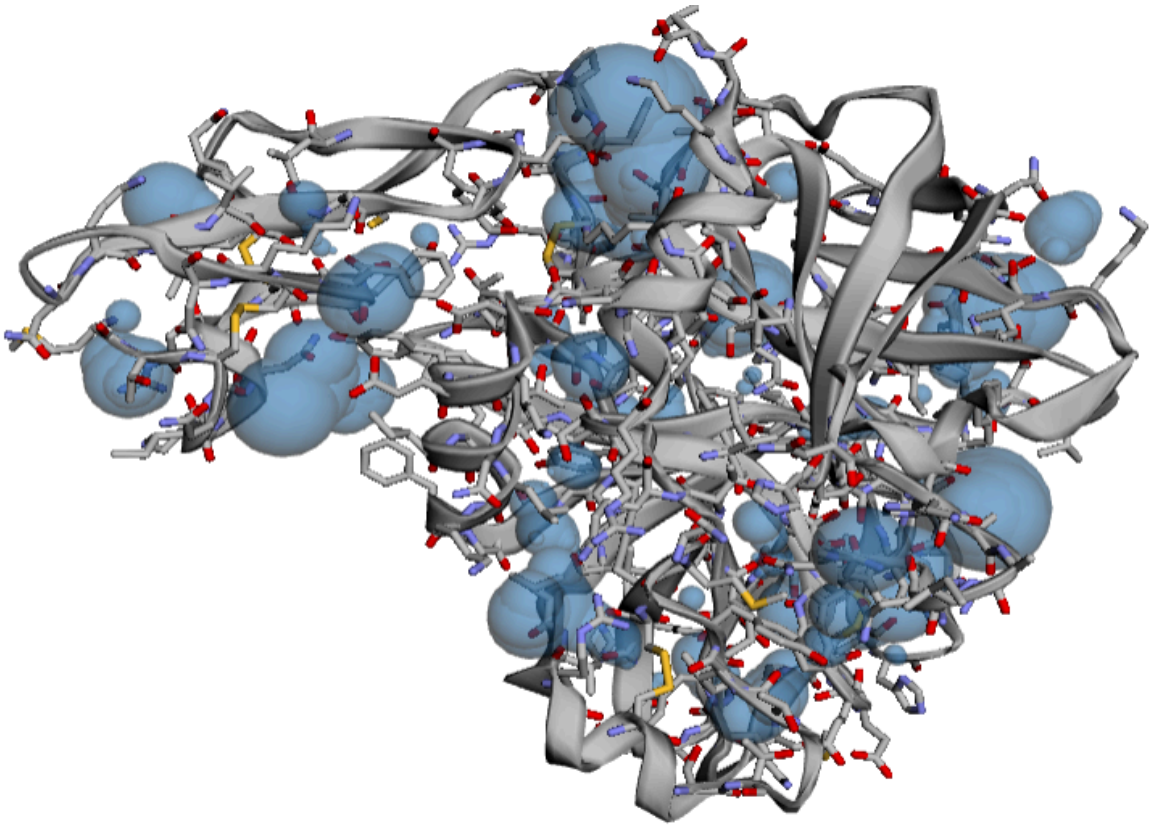


Table S1. *Characteristic of All CFIXa Active Sites*

Active Site ID	Area (Å^2)	Volume (Å^3)	Active Site ID	Area (Å^2)	Volume (Å^3)	Active Site ID	Area (Å^2)	Volume (Å^3)
1	215.899	128.236	15	15.795	2.932	29	1.052	0.037
2	122.970	49.494	16	15.658	2.191	30	0.814	0.026
3	90.078	45.053	17	15.300	2.035	31	0.381	0.024
4	46.643	29.920	18	5.682	1.332	32	0.476	0.013
5	55.432	25.515	19	8.210	0.866	33	0.445	0.011
6	44.564	16.115	20	5.331	0.485	34	0.374	0.009
7	61.362	15.776	21	3.829	0.446	35	0.382	0.007
8	44.347	7.487	22	5.476	0.443	36	0.378	0.006
9	19.565	6.010	23	4.648	0.426	37	0.244	0.005
10	25.308	5.975	24	3.502	0.282	38	0.198	0.004
11	18.459	5.680	25	2.816	0.257	39	0.094	0.001
12	23.415	4.408	26	1.059	0.114	40	0.005	0.000
13	8.783	4.150	27	2.275	0.091	41	0.003	0.000
14	11.694	3.888	28	1.258	0.044	42	0.011	0.000

Table S2. *Coagulation Factor IXa Chosen Active Sites Information*

Active Site ID	Area (Å²)	Volume (Å³)	Amino Acid	Atom	Bond	Bond Length (Å)	Amino Acid	Atom	Bond	Bond Length (Å)
II	122.970	49.494	H:HIS57	NE2	CD2-NE2	1.36914	H:GLY216	N	N-CA	1.45804
			H:TYR99	CE1	CE1-CZ	1.37854		CA		
				OH	CZ-OH	1.37181		O	C-O	1.23484
			H:ASP189	CG	CG-OD1	1.25708	H:GLU217	N	N-CA	1.44962
				OD1				O	C-O	1.24217
				OD2	CG-OD2	1.27266	H:GLU219	O	C-O	1.24331
			H:SER190	C	C-O	1.22405	H:CYS220	CA	CA-CB	1.52297
				O				SG	CB-SG	1.79269
				CB	CB-OG	1.41759	H:ALA221	N	N-CA	1.45148
				OG				CA		
			H:CYS191	N	N-CA	1.4671	H:MET221	N	N-CA	1.45196
				CA			H:LYS224	C	C-O	1.24155
				C	C-O	1.22405		O		
				O				CB	CA-CB	1.61694
			H:GLN192	N	N-CA	1.47061	H:TYR225	N	N-CA	1.4459
				CA				CA		
				CG	CG-CD	1.50074		C	C-O	1.19949
				CD				O		
				NE2	CD-NE2	1.33314	H:GLY226	CA	CA-C	1.51956
			H:SER195	OG	CB-OG	1.41511	H:ILE227	N	N-CA	1.45471
			H:ILE213	CG2	CB-CG1	1.51821		O	C-O	1.24276
			H:SER214	C	C-O	1.24355	H:TYR228	CE2	CE2-CZ	1.39065
				O				CZ		
			H:TRP215	N	N-CA	1.48185				
				CA						
				C	C-O	1.22822				
				O						
				CB	CA-CB	1.55715				
III	90.078	45.053	H:VAL32	CG1	CB-CG1	1.51508	H:THR76	N	N-CA	1.44632
				CG2	CB-CG2	1.50644		CA		
			H:ASN34	OD1	CD-OD1	1.26025		OG1	CB-OG1	1.43909

				ND2	CG-ND2	1.31645		CG2	CB-CG2	1.51245
			H:ASP39	CB	CB-CG	1.52305	H:GLU80	CD	CG-CD	1.51131
				CG				OE1	CD-OE1	1.25032
				OD2	CG-OD2	1.23287		OE2	CD-OE2	1.24772
			H:ALA40	CB	CA-CB	1.54078	H:LYS82	CE	CE-NZ	1.49946
			H:VAL67	CG1	CB-CG1	1.51674		NZ		
				CG2	CB-CG2	1.52517				
			H:GLU70	OE1	CD-OE1	1.2454				
			H:ILE73	CA	CA-C	1.56548				
				O	C-O	1.22965				
				CB	CB-CG2	1.51392				
				CG2						
				CD1	CG1-CD1	1.52142				
			H:GLU74	CD	CG-CD	1.51932				
				OE1	CD-OE1	1.25042				
				OE2	CD-OE2	1.25686				
			H:GLU75	N	N-CA	1.46232				
				C	C-O	1.2445				
				O						
V	55.432	25.515	H:ASP125	OD2	CG-OD2	1.25402	L:CYS88	C	C-O	1.21921
			H:GLU127	CD	CD-CE	1.50033		O		
				OE1	CD-OE1	1.25442		CB	CA-CB	1.51823
				OE2	CD-OE2	1.25241	L:ASN89	N	N-CA	1.46728
			H:TYR128	CD2	CD2-CE2	1.39727		CA		
				CE2				OD1	CG-OD1	1.2463
				CZ	CZ-OH	1.37223	L:ASN92	OD1	CG-OD1	1.22565
				OH			L:PHE98	CB	CA-CB	1.53733
			H:ILE129B	CD1	CG1-CD1	1.57649	L:CYS99	O	C-O	1.2262
							L:LYS100	CG	CG-CD	1.51948

***Table S3**. Extraction Set-Ups Percent Yield*

Set-up	Solvent	Leaf Texture	Dry Sample Weight (g)	Extract Weight (g)	Percent Yield (%)
A	30% Ethanol	Powdered	50 g	15.83	31.66
B	95% Ethanol	Powdered	25 g	3.4	13.6
C	95% Ethanol	Shredded	200 g	78.541	39.27

Computation:

$$Extract\ Weight\ (g)\ =\ Flask\ w/\ Crude\ Extract\ Weight\ (g)\ -\ Empty\ Flask\ Weight\ (g)$$

$$Percent\ Yield\ (\%)\ =\ \frac{Extract\ Weight\ (g)}{Dry\ Sample\ Weight\ (g)} x\ 100$$

30% Ethanol | Powdered

$$Extract Weight(g) = Flask w/ Crude Extract Weight(g) - Empty Flask Weight(g)$$

$$= 403.61\ g\ -\ 387.78\ g\ =\ 15.83\ g$$

$$Percent\ Yield\ (\%)\ =\ \frac{Extract\ Weight\ (g)}{Dry\ Sample\ Weight\ (g)} x\ 100$$

$$=\ \frac{15.83\ g}{50\ g} x\ 100\ =\ 31.66\%$$

95% Ethanol | Powdered

$$Extract Weight(g) = Flask w/ Crude Extract Weight(g) - Empty Flask Weight(g)$$

$$= 391.18\ g\ -\ 387.78\ g\ =\ 3.4\ g$$

$$Percent\ Yield\ (\%)\ =\ \frac{Extract\ Weight\ (g)}{Dry\ Sample\ Weight\ (g)} x\ 100$$

$$=\ \frac{3.4\ g}{25\ g} x\ 100\ =\ 13.6\%$$

95% Ethanol | Shredded

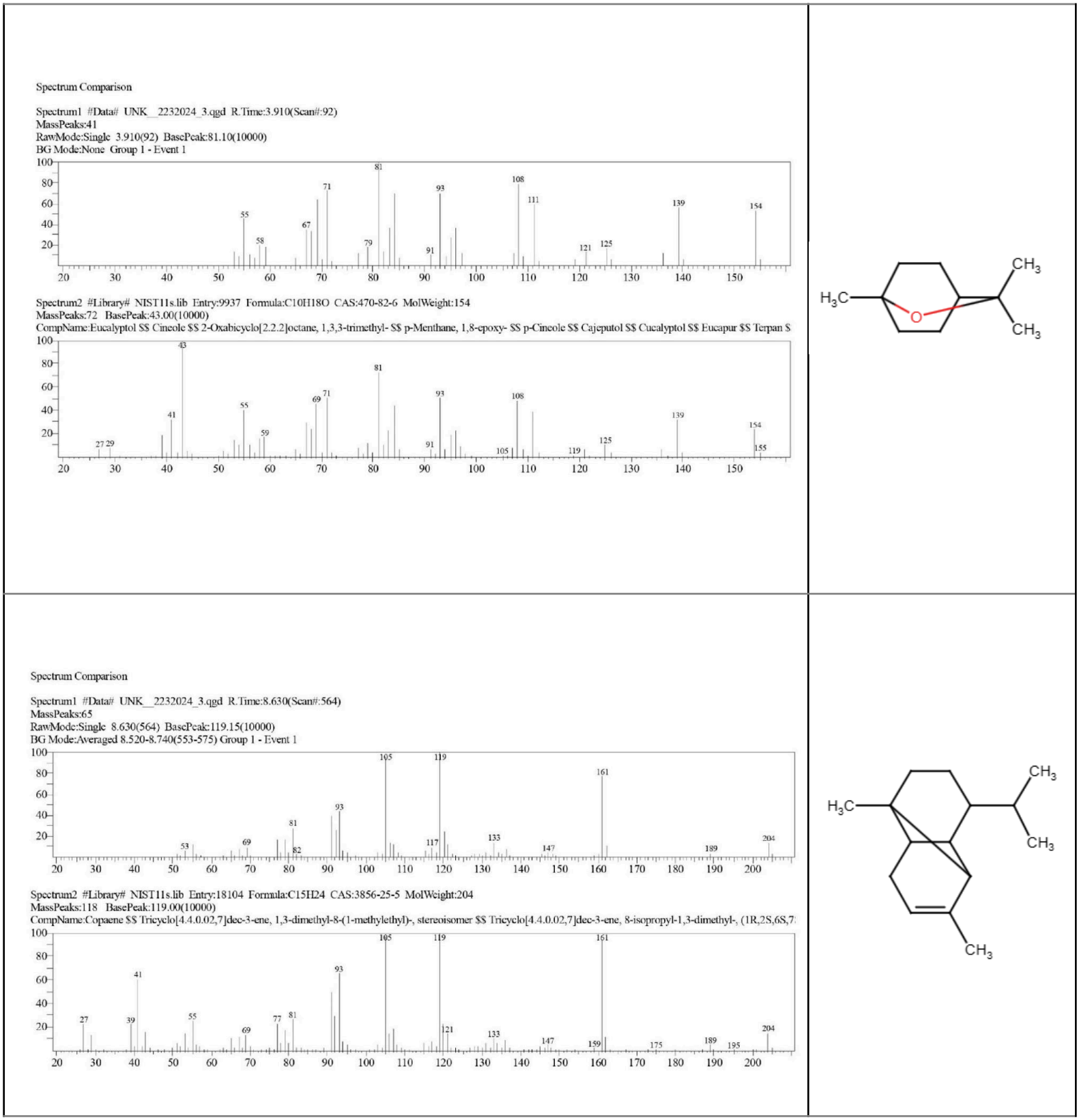
$$Extract Weight(g) = Flask w/ Crude Extract Weight(g) - Empty Flask Weight(g)$$

$$= 186.26\ g\ -\ 107.719\ g\ =\ 78.541\ g$$

$$Percent\ Yield\ (\%)\ =\ \frac{Extract\ Weight\ (g)}{Dry\ Sample\ Weight\ (g)} x\ 100$$

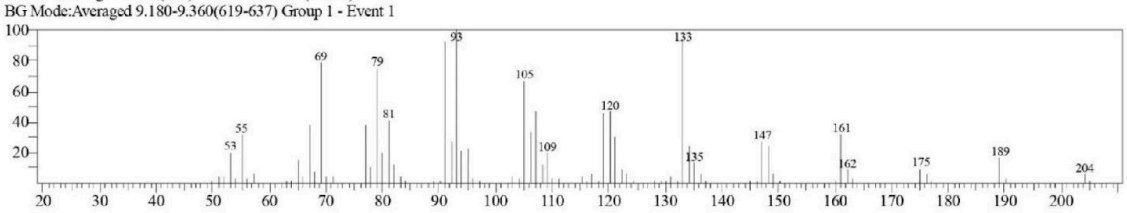
$$=\ \frac{78.541\ g}{200\ g} x\ 100\ =\ 39.271\%$$

Figure S2. *GC-MS Mass Spectra and Chromatogram*

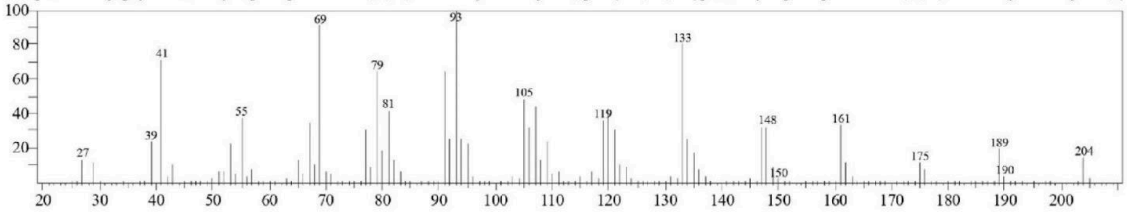


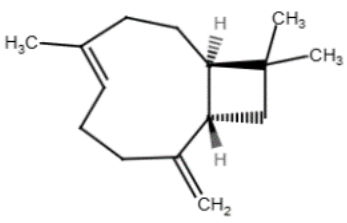
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:9.260(Scan#:627)
MassPeaks:81
RawMode:Single 9.260(627) BasePeak:93.10(10000)
BG Mode:Averaged 9.180-9.360(619-637) Group 1 - Event 1



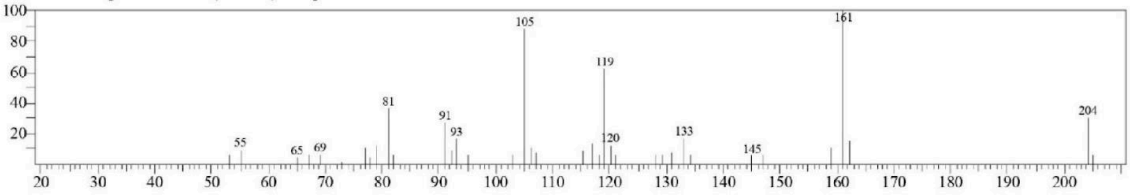
Spectrum2 #Library# NIST11s.lib Entry:18069 Formula:C15H24 CAS:87-44-5 MolWeight:204
MassPeaks:176 BasePeak:93.00(10000)
CompName:Caryophyllene $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)]- $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (



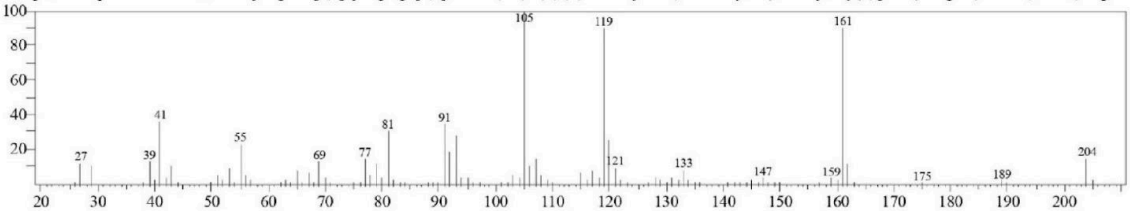


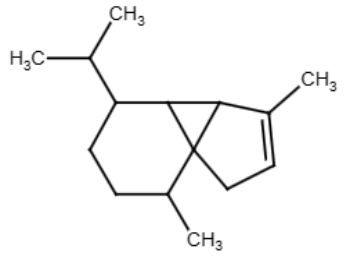
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:9.620(Scan#:663)
MassPeaks:37
RawMode:Single 9.620(663) BasePeak:161.15(10000)
BG Mode:Averaged 9.560-9.660(657-667) Group 1 - Event 1



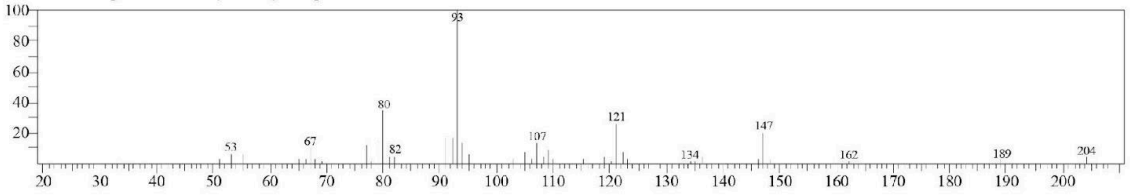
Spectrum2 #Library# NIST11s.lib Entry:18090 Formula:C15H24 CAS:17699-14-8 MolWeight:204
MassPeaks:99 BasePeak:105.00(10000)
CompName:.alpha.-Cubebene $$ 1H-Cyclopenta[1,3]cyclopropa[1,2]benzene, 3a,3b,4,5,6,7-hexahydro-3,7-dimethyl-4-(1-methylethyl)-, [3aS-(3a.alpha.,3b.beta.,4.beta.,7.alpha.



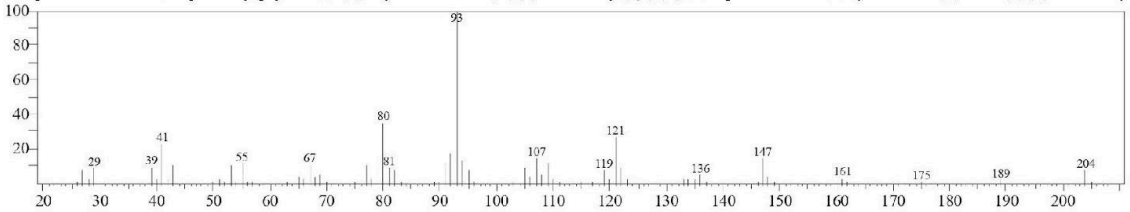


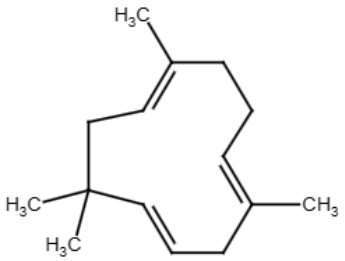
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:9.720(Scan#:673)
MassPeaks:42
RawMode:Single 9.720(673) BasePeak:93.10(10000)
BG Mode:Averaged 9.680-9.800(669-681) Group 1 - Event 1



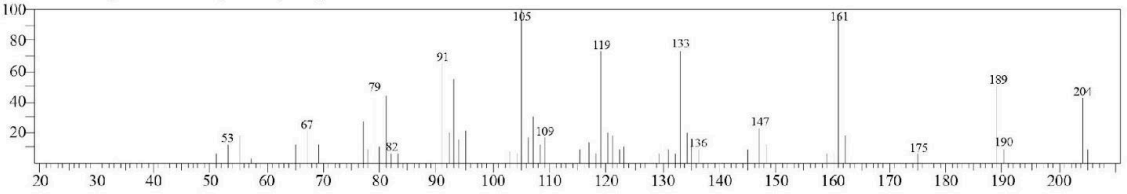
Spectrum2 #Library# NIST11s.lib Entry:18070 Formula:C15H24 CAS:6753-98-6 MolWeight:204
MassPeaks:70 BasePeak:93.00(10000)
CompName:Humulene $$ .alpha.-Caryophyllene $$ 1,4,8-Cycloundecatriene, 2,6,6,9-tetramethyl-, (E,E,E)- $$ .alpha.-Humulene $$ Cycloundeca-1,4,8-triene,2,6,6,9-tetramethy



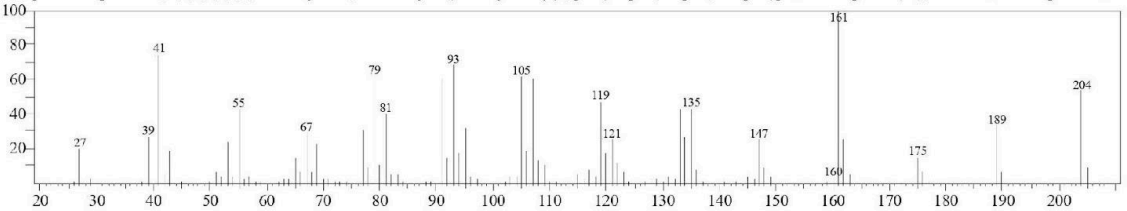


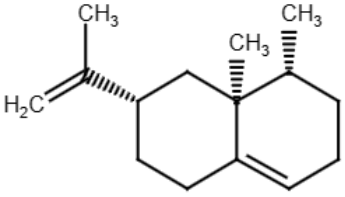
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:9.920(Scan#:693)
MassPeaks:54
RawMode:Single 9.920(693) BasePeak:105.10(10000)
BG Mode:Averaged 9.880-10.000(689-701) Group 1 - Event 1



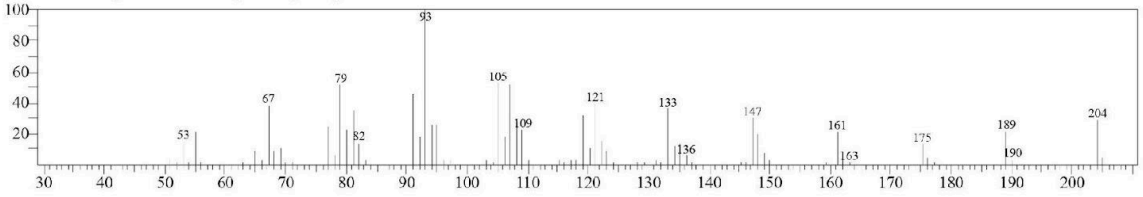
Spectrum2 #Library# NIST11s.lib Entry:18118 Formula:C15H24 CAS:10219-75-7 MolWeight:204
MassPeaks:100 BasePeak:161.00(10000)
CompName:Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,7.alpha.,8a.alpha.)]- $$ Eremophila-1(10),11-diene $$ Eremophilene $$



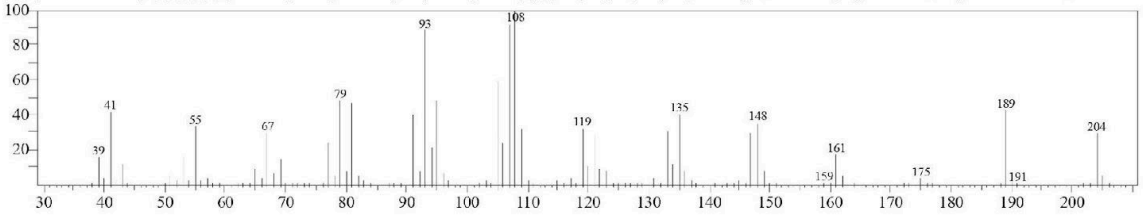


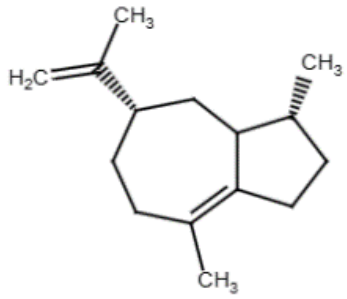
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:10.170(Scan#:718)
MassPeaks:75
RawMode:Single 10.170(718) BasePeak:93.10(10000)
BG Mode:Averaged 10.120-10.210(713-722) Group 1 - Event 1



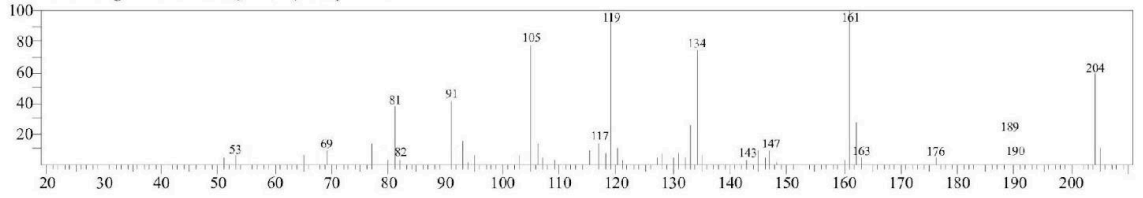
Spectrum2 #Library# NIST11s.lib Entry:18097 Formula:C15H24 CAS:3691-11-0 MolWeight:204
MassPeaks:117 BasePeak:108.00(10000)
CompName:Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,7.alpha.,8a.beta.)]- $$ Guaia-1(10),11-diene $$ .alpha.-Bulnesene $$ .delta.-Gi



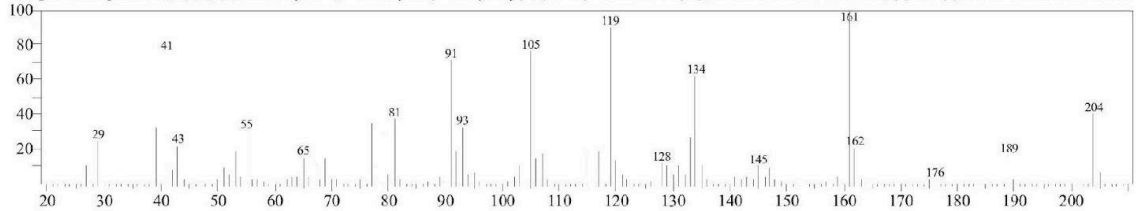


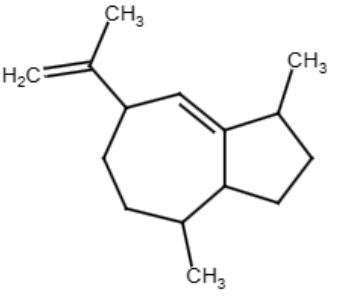
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:10.470(Scan#:748)
MassPeaks:54
RawMode:Single 10.470(748) BasePeak:161.15(10000)
BG Mode:Averaged 10.410-10.500(742-751) Group 1 - Event 1



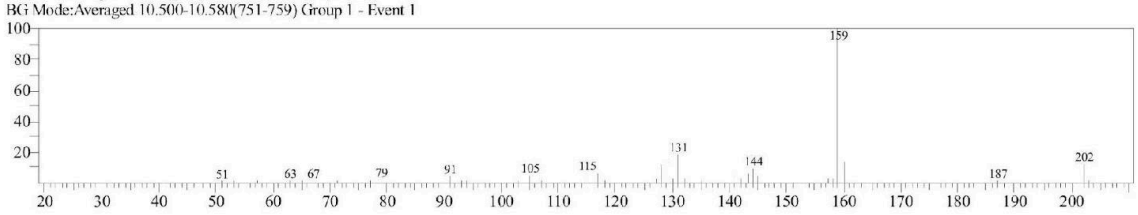
Spectrum2 #Library# NIST11s.lib Entry:18135 Formula:C15H24 CAS:483-76-1 MolWeight:204
MassPeaks:88 BasePeak:161.00(10000)
CompName:Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)- $$ Cadina-1(10),4-diene $$ .delta.-Cadinene, (+)- $$ (+)-.delta.-Cadinene $$ .delta.-



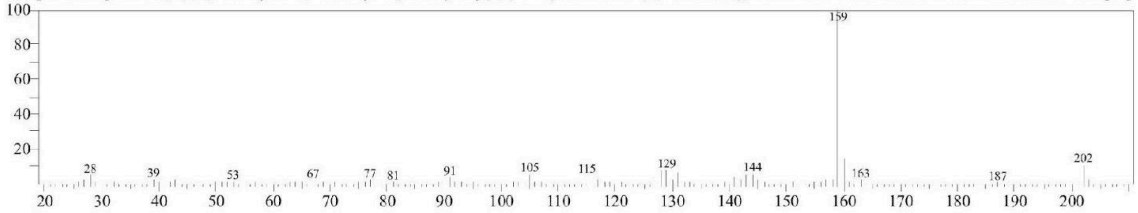


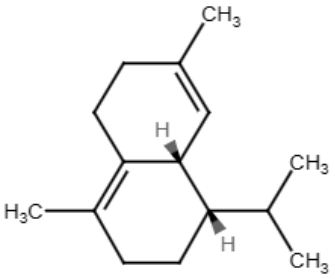
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:10.540(Scan#:755)
MassPeaks:48
RawMode:Single 10.540(755) BasePeak:159.15(10000)
BG Mode:Averaged 10.500-10.580(751-759) Group 1 - Event 1



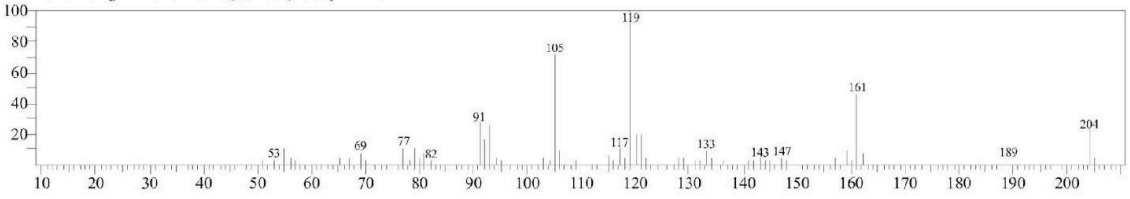
Spectrum2 #Library# NIST11s.lib Entry:17784 Formula:C15H22 CAS:483-77-2 MolWeight:202
MassPeaks:74 BasePeak:159.00(10000)
CompName:Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)- $$ Cadina-1,3,5-triene $$ (-)-Calamenene $$ L-calamenene $$ Calamenene $$ 4-Isoprop



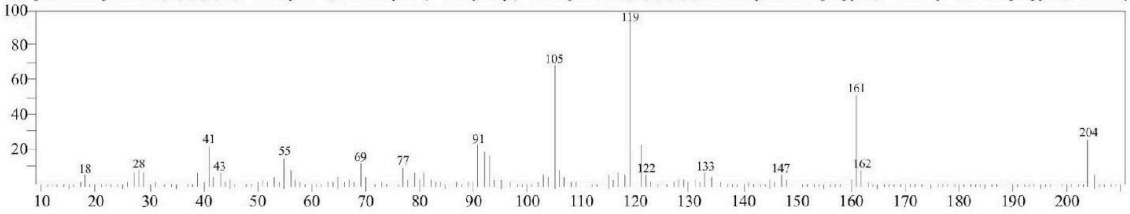


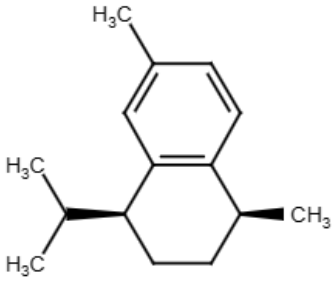
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:10.680(Scan#:769)
MassPeaks:57
RawMode:Single 10.680(769) BasePeak:119.10(10000)
BG Mode:Averaged 10.640-10.710(765-772) Group 1 - Event 1



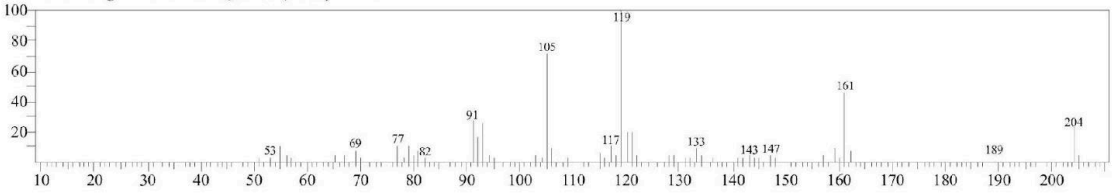
Spectrum2 #Library# NIST11s.lib Entry:18105 Formula:C15H24 CAS:16728-99-7 MolWeight:204
MassPeaks:92 BasePeak:119.00(10000)
CompName:Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)- $$ Naphthalene, 1,2,3,4,6,8a-hexahydro-1-isopropyl-4,7-dimethyl- $$ 4-Isopropyl-1,6-dimeth



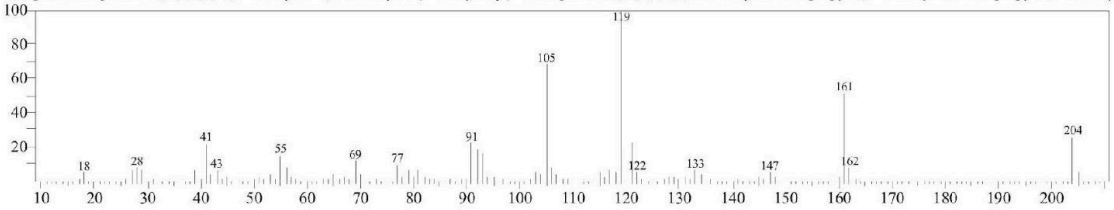


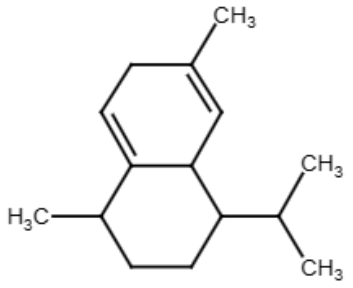
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:10.680(Scan#:769)
MassPeaks:57
RawMode:Single 10.680(769) BasePeak:119.10(10000)
BG Mode:Averaged 10.640-10.710(765-772) Group 1 - Event 1



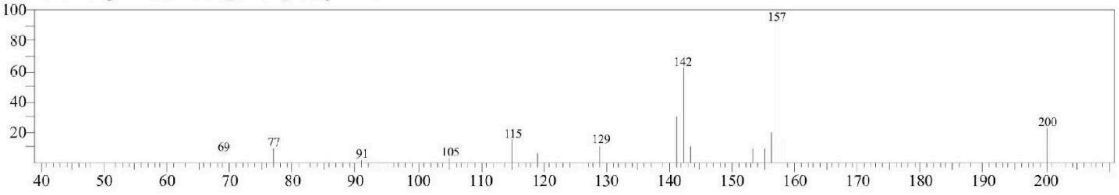
Spectrum2 #Library# NIST11s.lib Entry:18105 Formula:C15H24 CAS:16728-99-7 MolWeight:204
MassPeaks:92 BasePeak:119.00(10000)
CompName:Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)- $$ Naphthalene, 1,2,3,4,6,8a-hexahydro-1-isopropyl-4,7-dimethyl- $$ 4-Isopropyl-1,6-dimeth



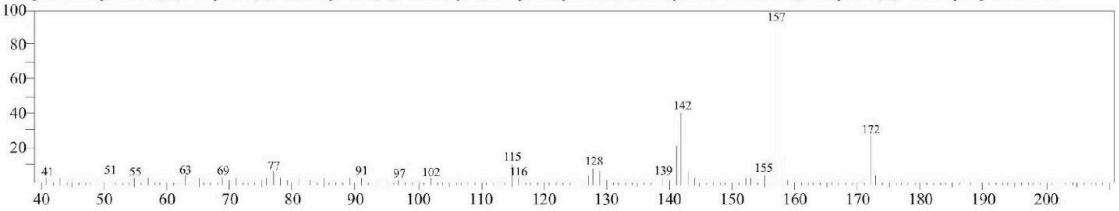


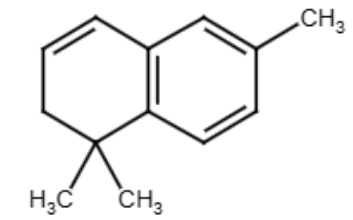
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:10.800(Scan#:781)
MassPeaks:17
RawMode:Single 10.800(781) BasePeak:157.10(10000)
BG Mode:Averaged 10.770-10.830(778-784) Group 1 - Event 1



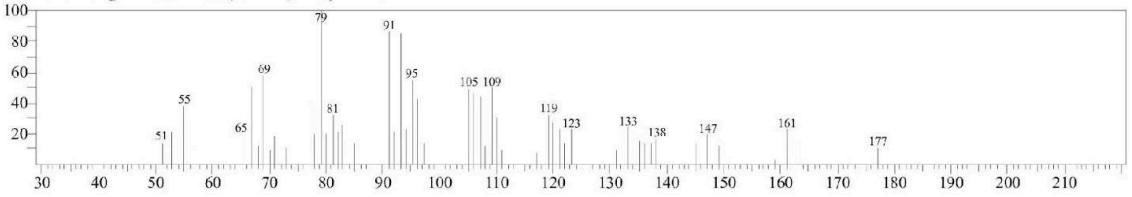
Spectrum2 #Library# NIST11s.lib Entry:13177 Formula:C13H16 CAS:30364-38-6 MolWeight:172
MassPeaks:44 BasePeak:157.00(10000)
CompName:Naphthalene, 1,2-dihydro-1,1,6-trimethyl- $$ 1,1,6-Trimethyl-1,2-dihydronaphthalene $$ Dehydro-ar-ionene $$ 1,2-Dihydro-1,1,6-trimethylnaphthalene $$



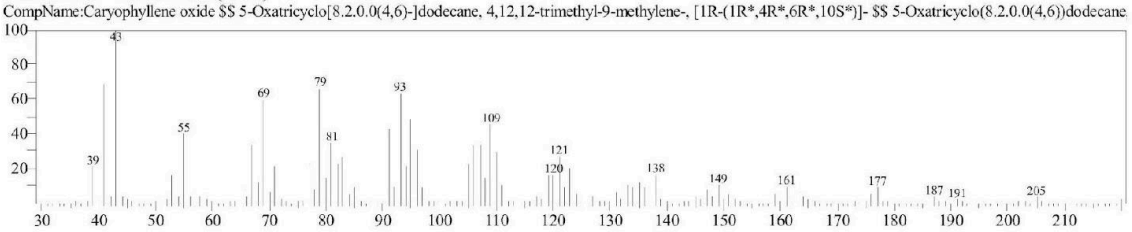


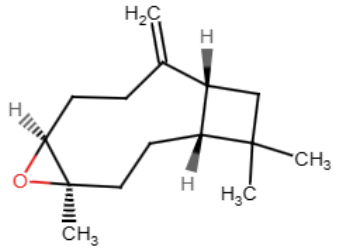
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:11.390(Scan#:840)
MassPeaks:53
RawMode:Single 11.390(840) BasePeak:79.05(10000)
BG Mode:Averaged 11.330-11.430(834-844) Group 1 - Event 1



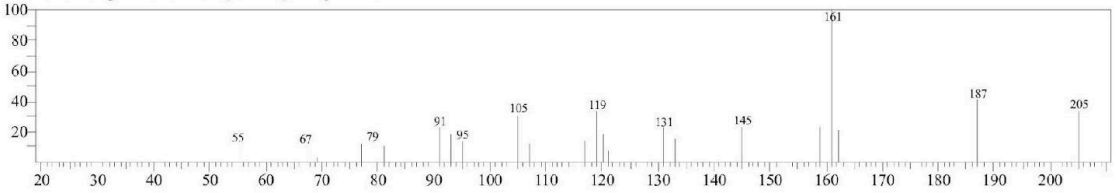
Spectrum2 #Library# NIST11s.lib Entry:20008 Formula:C15H24O CAS:1139-30-6 MolWeight:220
MassPeaks:130 BasePeak:43.00(10000)
CompName:Caryophyllene oxide $$ 5-Oxatricyclo[8.2.0.0(4,6)-]dodecane, 4,12,12-trimethyl-9-methylene-, [1R-(1R*,4R*,6R*,10S*)]- $$ 5-Oxatricyclo(8.2.0.0(4,6))dodecane



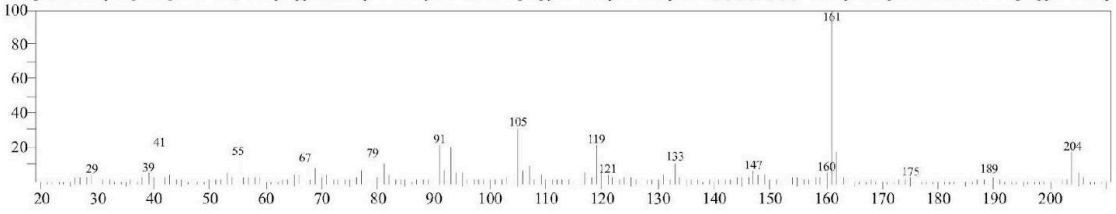


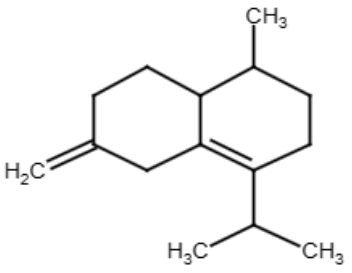
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:11.540(Scan#:855)
MassPeaks:23
RawMode:Single 11.540(855) BasePeak:161.15(10000)
BG Mode:Averaged 11.510-11.580(852-859) Group 1 - Event 1



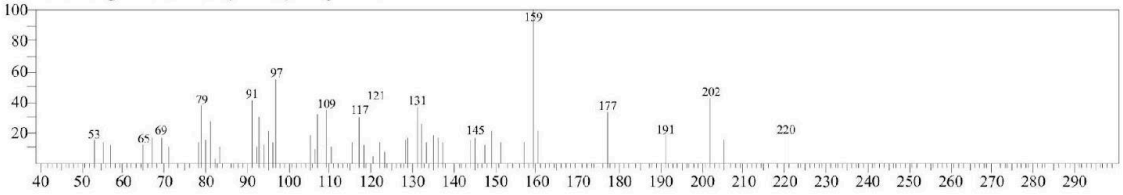
Spectrum2 #Library# NIST11s.lib Entry:18129 Formula:C15H24 CAS:150320-52-8 MolWeight:204
MassPeaks:141 BasePeak:161.00(10000)
CompName:Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene- $$ 8-Isopropyl-5-methyl-2-methylene-1,2,3,4,4a,5,6,7-octahydronaphthalene # $$ 2-Isopropyl-5-methy



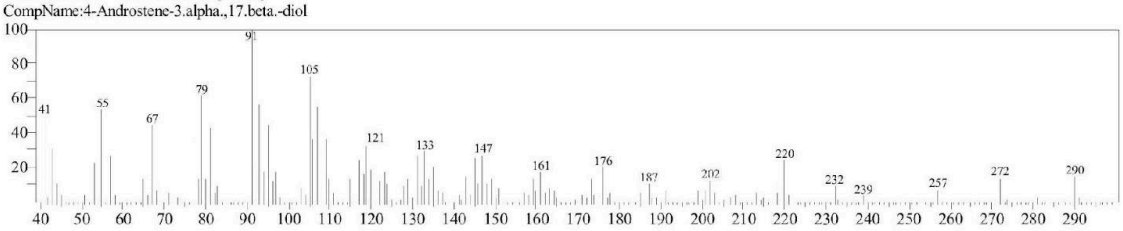


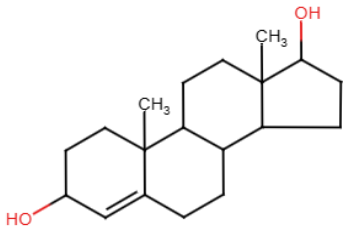
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:11.860(Scan#:887)
MassPeaks:55
RawMode:Single 11.860(887) BasePeak:159.15(10000)
BG Mode:Averaged 11.830-11.890(884-890) Group 1 - Event 1



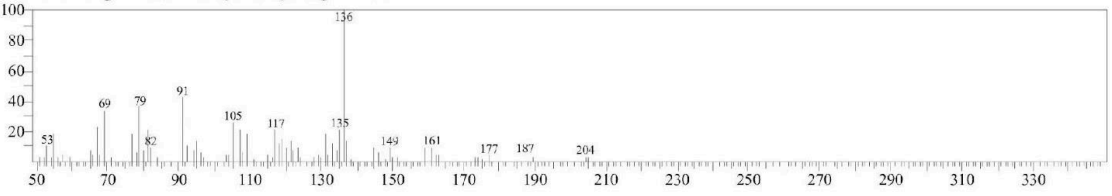
Spectrum2 #Library# SWGDRUG MS LIBRARY VERSION 3.10.lib Entry:2918 Formula:C19H30O2 CAS:1852-61-5 MolWeight:290
MassPeaks:125 BasePeak:91.00(10000)
CompName:4-Androstene-3.alpha.,17.beta.-diol



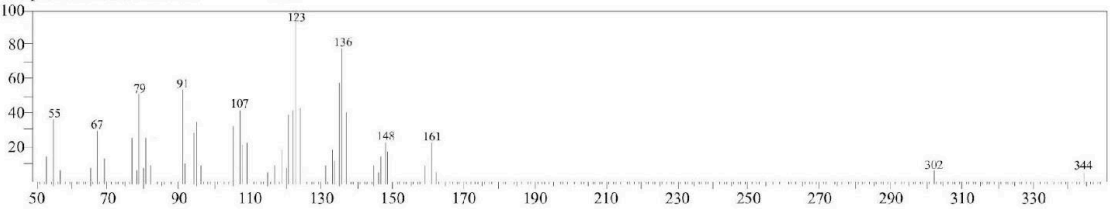


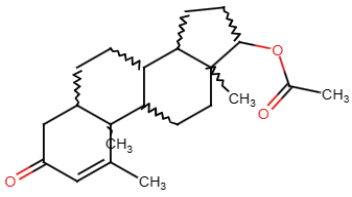
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:12.040(Scan#:905)
MassPeaks:81
RawMode:Single 12.040(905) BasePeak:136.15(10000)
BG Mode:Averaged 11.970-12.090(898-910) Group 1 - Event 1



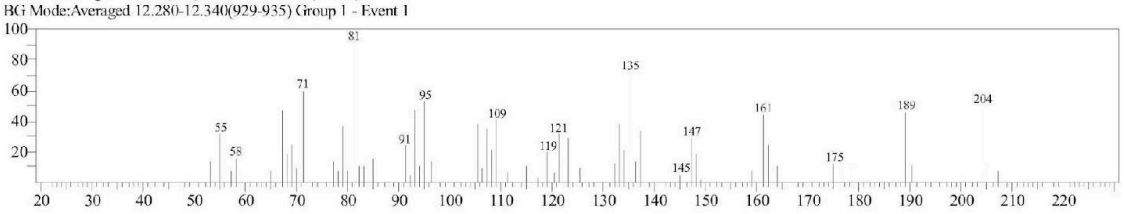
Spectrum2 #Library# MPW2011.lib Entry:5616 Formula:C22H32O3 CAS:0-00-0 MolWeight:344
MassPeaks:50 BasePeak:123.00(10000)
CompName:Metenolone acetate P983



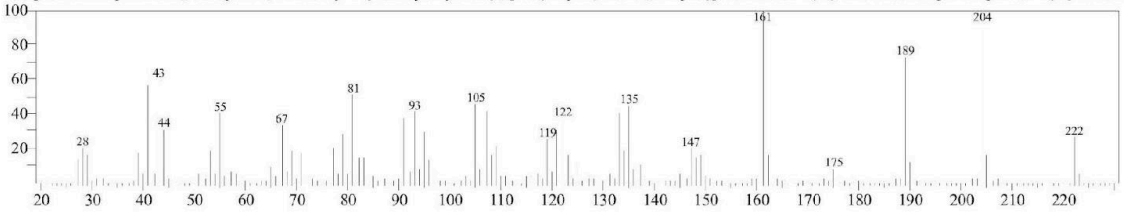


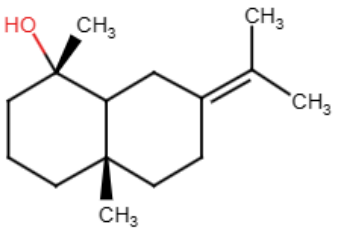
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:12.320(Scan#:933)
MassPeaks:64
RawMode:Single 12.320(933) BasePeak:81.10(10000)
BG Mode:Averaged 12.280-12.340(929-935) Group 1 - Event 1



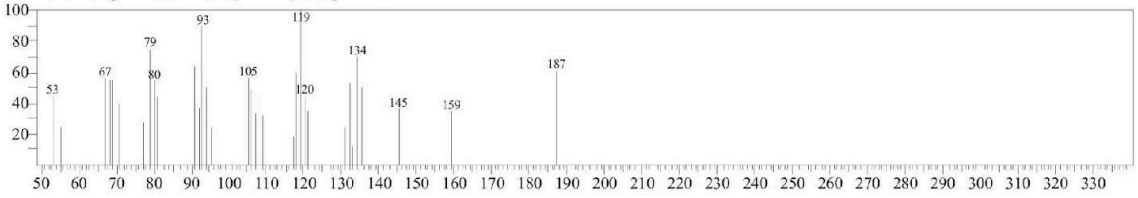
Spectrum2 #Library# NIST11s.lib Entry:20299 Formula:C15H26O CAS:473-04-1 MolWeight:222
MassPeaks:140 BasePeak:161.00(10000)
CompName:1-Naphthalenol, decahydro-1,4a-dimethyl-7-(1-methylethylidene)-, [1R-(1.alpha.,4a.beta.,8a.alpha.)]- $$ Eudesm-7(11)-en-4-ol $$ Juniper camphor $$ 7(11)-Seline



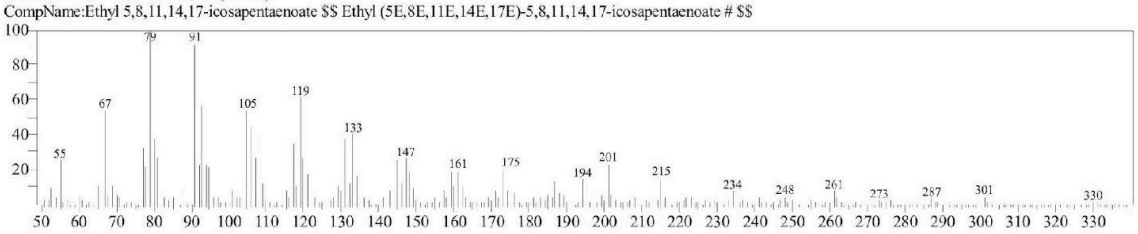


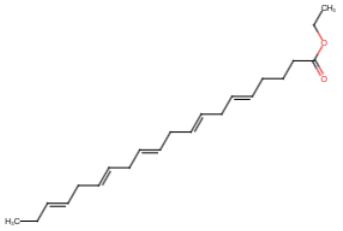
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:12.560(Scan#:957)
MassPeaks:33
RawMode:Single 12.560(957) BasePeak:119.10(10000)
BG Mode:Averaged 12.530-12.590(954-960) Group 1 - Event 1



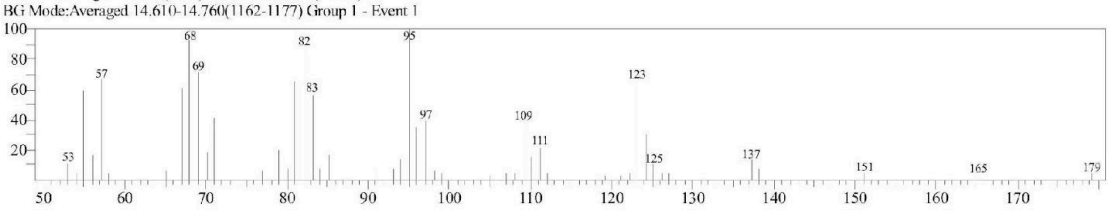
Spectrum2 #Library# NIST11s.lib Entry:27690 Formula:C22H34O2 CAS:84494-70-2 MolWeight:330
MassPeaks:192 BasePeak:79.00(10000)
CompName:Ethyl 5,8,11,14,17-icosapentaenoate $$ Ethyl (5E,8E,11E,14E,17E)-5,8,11,14,17-icosapentaenoate # $$



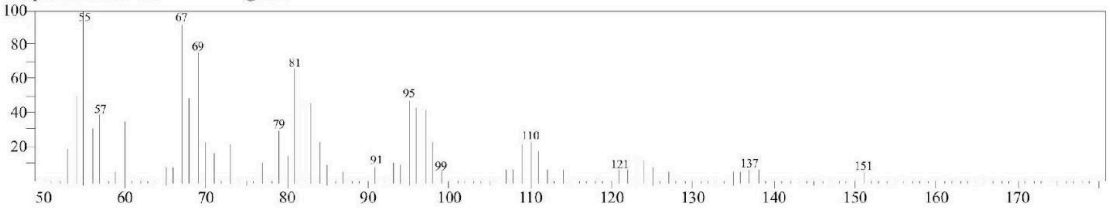


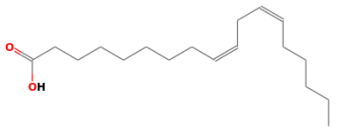
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:14.680(Scan#:1169)
MassPeaks:48
RawMode:Single 14.680(1169) BasePeak:95.10(10000)
BG Mode:Averaged 14.610-14.760(1162-1177) Group 1 - Event 1



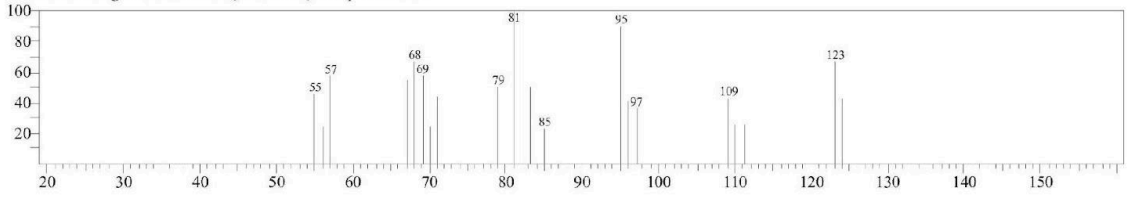
Spectrum2 #Library# MPW2011.lib Entry:3284 Formula:C18H32O2 CAS:60-33-3 MolWeight:280
MassPeaks:50 BasePeak:55.00(10000)
CompName:Linoleic acid @P651



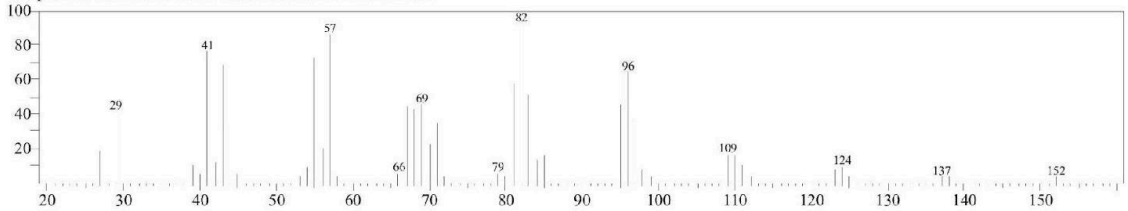


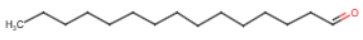
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:15.110(Scan#:1212)
MassPeaks:21
RawMode:Single 15.110(1212) BasePeak:81.10(10000)
BG Mode:Averaged 15.060-15.190(1207-1220) Group 1 - Event 1



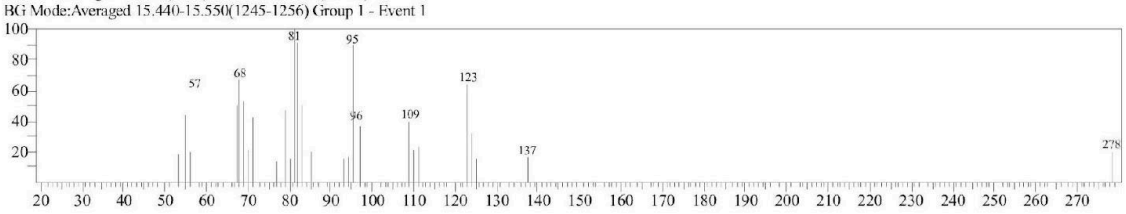
Spectrum2 #Library# NIST11s.lib Entry:20737 Formula:C15H30O CAS:2765-11-9 MolWeight:226
MassPeaks:44 BasePeak:82.00(10000)
CompName:Pentadecanal- $$ 1-Pentadecanal $$ n-Pentadecanal $$



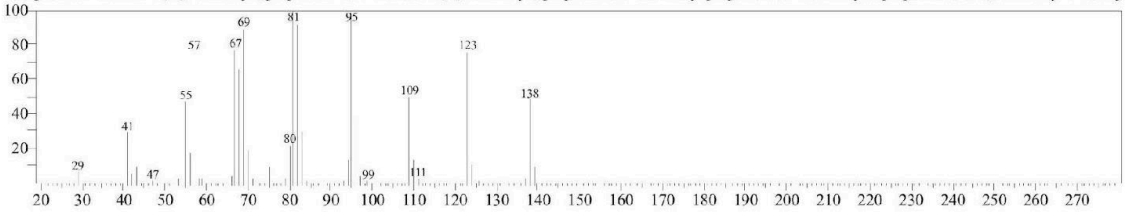


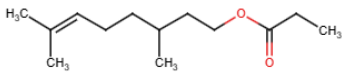
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:15.490(Scan#:1250)
MassPeaks:29
RawMode:Single 15.490(1250) BasePeak:81.10(10000)
BG Mode:Averaged 15.440-15.550(1245-1256) Group 1 - Event 1



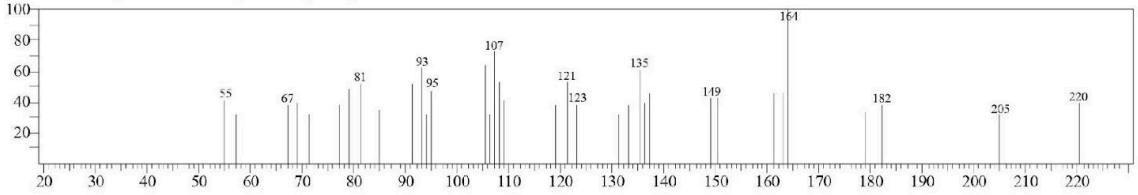
Spectrum2 #Library# NIST11s.lib Entry:19101 Formula:C13H24O2 CAS:141-14-0 MolWeight:212
MassPeaks:40 BasePeak:81.00(10000)
CompName:6-Octen-1-ol, 3,7-dimethyl-, propanoate $$ 6-Octen-1-ol, 3,7-dimethyl-, propionate $$ Citronellyl propionate $$ Citronellyl n-proprionate $$ 3,7-Dimethyl-6-octeny



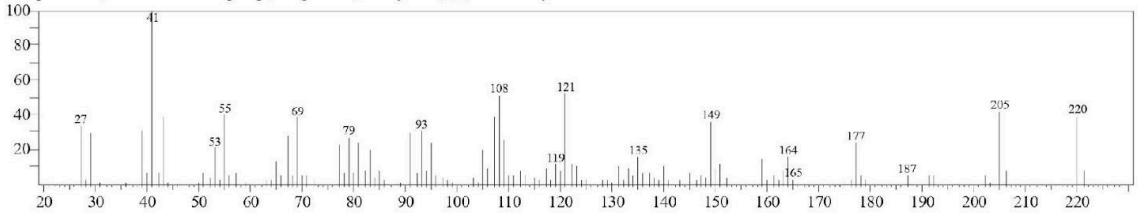


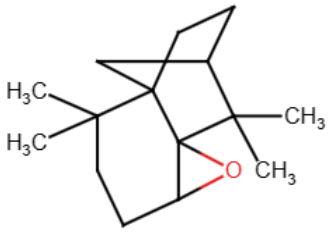
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:16.000(Scan#:1301)
MassPeaks:35
RawMode:Single 16.000(1301) BasePeak:164.10(10000)
BG Mode:Averaged 15.910-16.050(1292-1306) Group 1 - Event 1



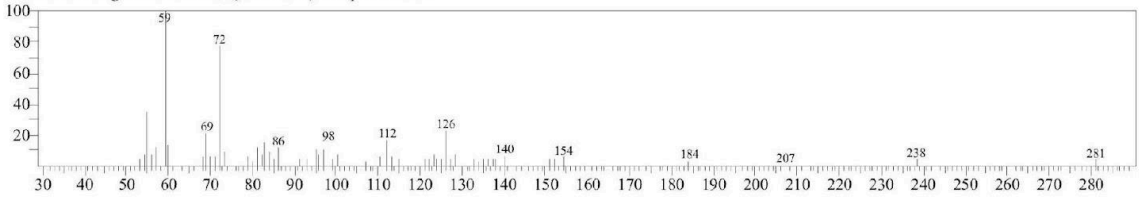
Spectrum2 #Library# NIST11s.lib Entry:20007 Formula:C15H24O CAS:67999-56-8 MolWeight:220
MassPeaks:116 BasePeak:41.00(10000)
CompName:4a,7-Methano-4aH-naphth[1,8a-b]oxirene, octahydro-4,4,8,8-tetramethyl-



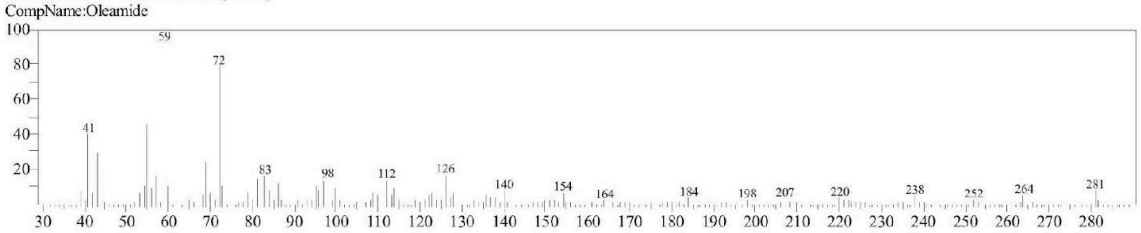


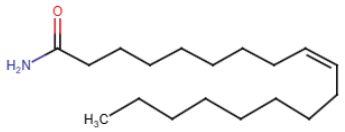
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:22.730(Scan#:1974)
MassPeaks:60
RawMode:Single 22.730(1974) BasePeak:59.05(10000)
BG Mode:Averaged 22.620-22.870(1963-1988) Group 1 - Event 1



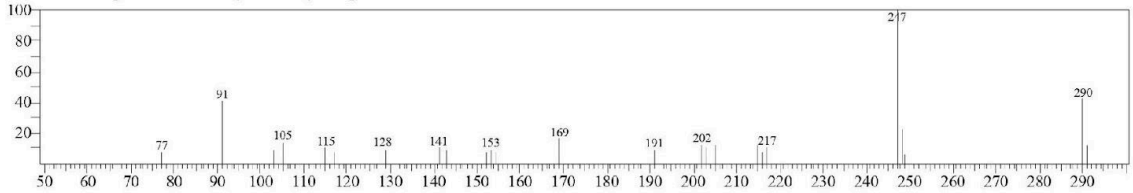
Spectrum2 #Library# SWGDRUG MS LIBRARY VERSION 3.10.lib Entry:424 Formula:C18H35NO CAS:301-02-0 MolWeight:281
MassPeaks:128 BasePeak:59.00(10000)
CompName:Oleamide



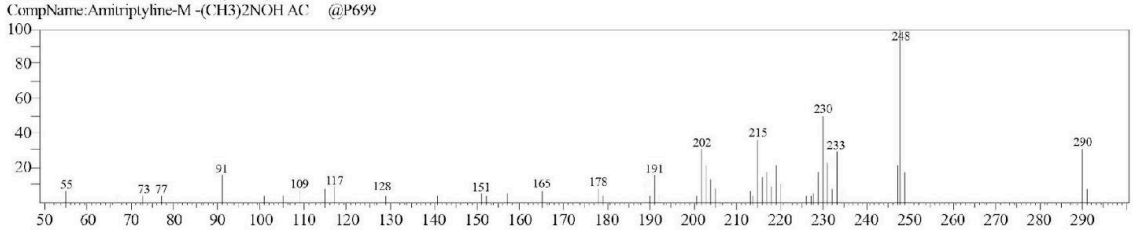


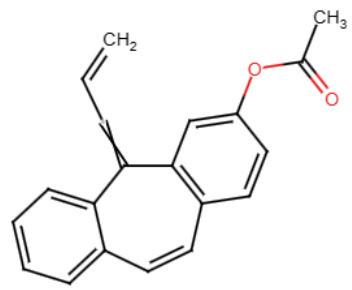
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:26.350(Scan#:2336)
MassPeaks:27
RawMode:Single 26.350(2336) BasePeak:247.15(10000)
BG Mode:Averaged 26.220-26.430(2323-2344) Group 1 - Event 1



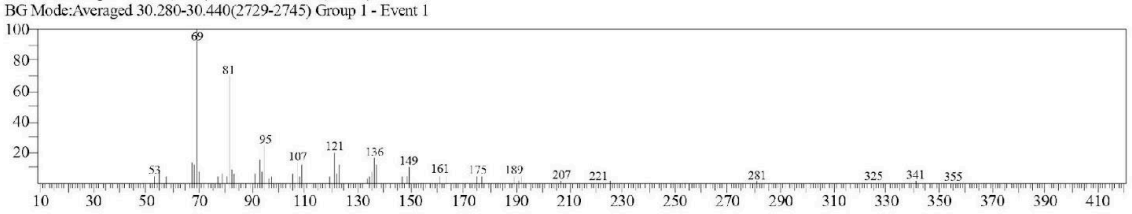
Spectrum2 #Library# MPW2011.lib Entry:3649 Formula:C20H18O2 CAS:0-00-0 MolWeight:290
MassPeaks:50 BasePeak:248.00(10000)
CompName:Amitriptyline-M -(CH3)2NOH AC @P699



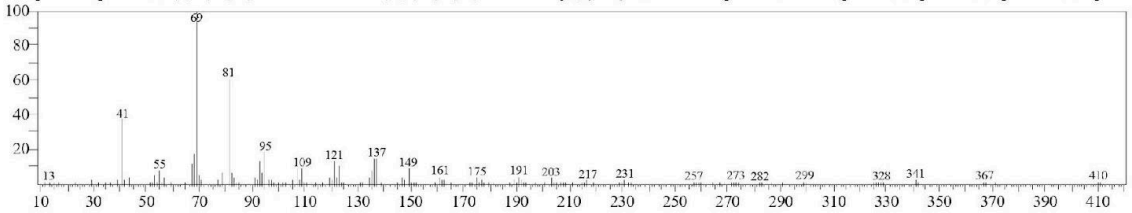


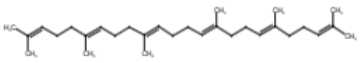
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:30.350(Scan#:2736)
MassPeaks:58
RawMode:Single 30.350(2736) BasePeak:69.10(10000)
BG Mode:Averaged 30.280-30.440(2729-2745) Group 1 - Event 1



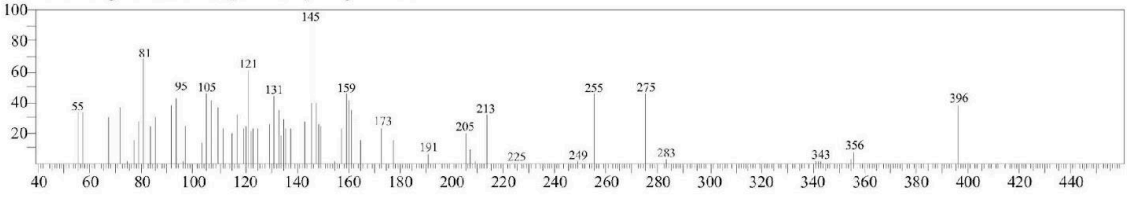
Spectrum2 #Library# NIST11s.lib Entry:29859 Formula:C30H50 CAS:111-02-4 MolWeight:410
MassPeaks:146 BasePeak:69.00(10000)
CompName:Squalene $$ 2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)- $$ all-trans-Squalene $$ trans-Squalene $$ Spinacen $$ Spinacene $$ Squalen



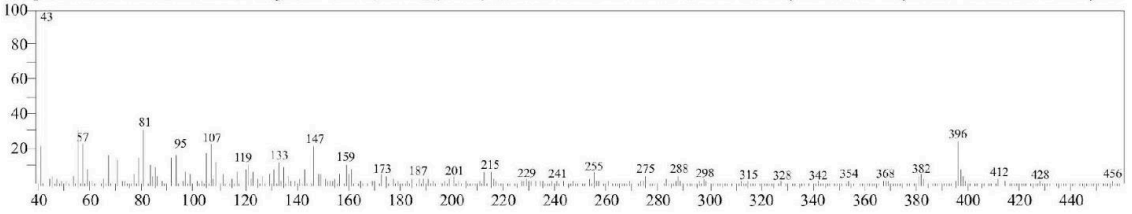


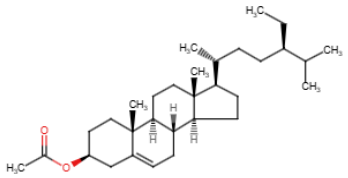
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:32.110(Scan#:2912)
MassPeaks:72
RawMode:Single 32.110(2912) BasePeak:145.15(10000)
BG Mode:Averaged 32.030-32.170(2904-2918) Group 1 - Event 1



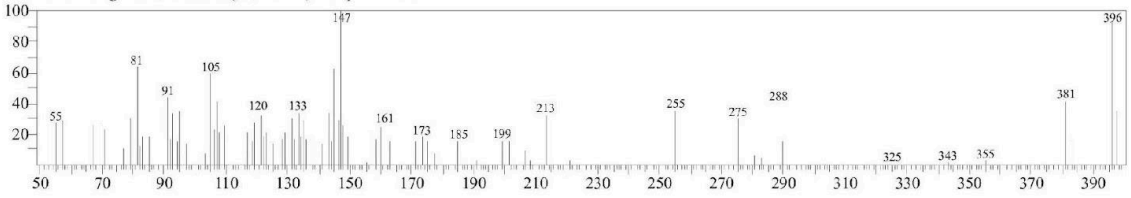
Spectrum2 #Library# NIST11s.lib Entry:30335 Formula:C31H52O2 CAS:915-05-9 MolWeight:456
MassPeaks:157 BasePeak:43.00(10000)
CompName:.beta.-Sitosterol acetate $$ Stigmast-5-en-3-ol, acetate, (3.beta.)- $$ .beta.-Sitosterol 3-acetate $$ .beta.-Sitosteryl acetate $$ Acetyl-.beta.-sitosterol $$ Sitosteryl ace



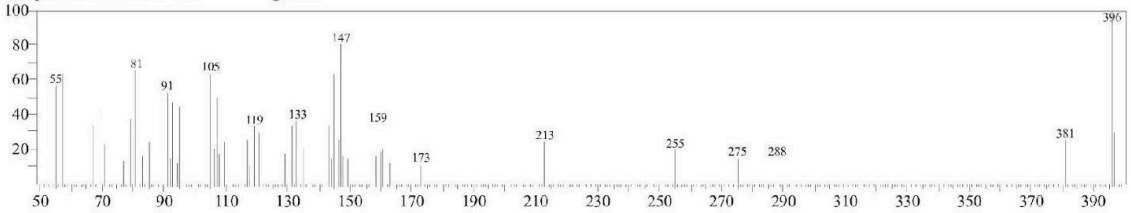


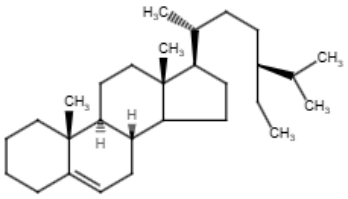
Spectrum Comparison

Spectrum1 #Data# UNK__2232024_3.qgd R.Time:33.810(Scan#:3082)
MassPeaks:92
RawMode:Single 33.810(3082) BasePeak:147.15(10000)
BG Mode:Averaged 33.700-33.900(3071-3091) Group 1 - Event 1



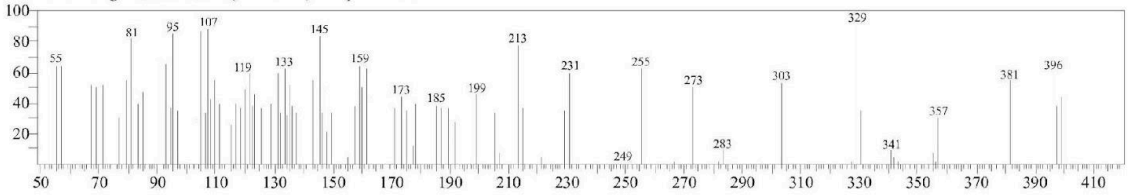
Spectrum2 #Library# MPW2011.lib Entry:7013 Formula:C29H48 CAS:0-00-0 MolWeight:396
MassPeaks:50 BasePeak:396.00(10000)
CompName:Clionasterol -H2O @P1182



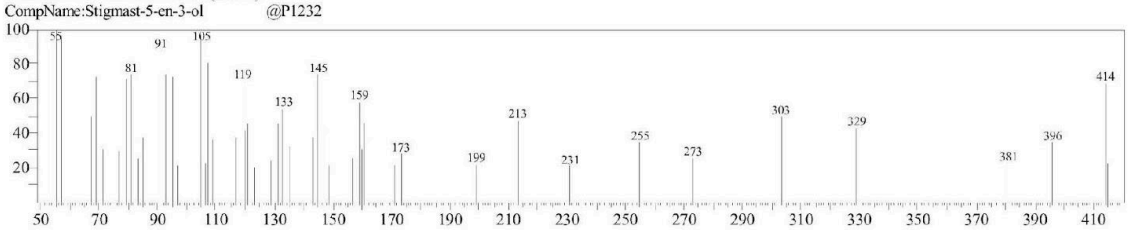


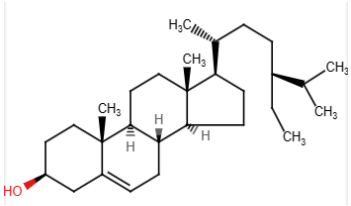
Spectrum Comparison

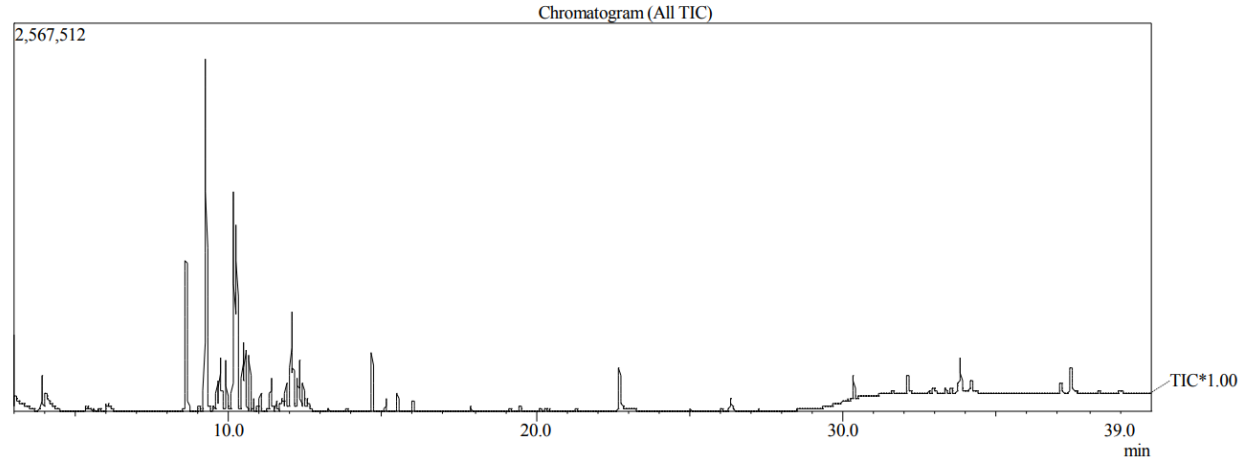
Spectrum1 #Data# UNK__2232024_3.qgd R.Time:37.420(Scan#:3443)
MassPeaks:95
RawMode:Single 37.420(3443) BasePeak:329.30(10000)
BG Mode:Averaged 37.330-37.510(3434-3452) Group 1 - Event 1



Spectrum2 #Library# MPW2011.lib Entry:7358 Formula:C29H50O CAS:83-47-6 MolWeight:414
MassPeaks:50 BasePeak:55.00(10000)
CompName:Stigmast-5-en-3-ol @P1232






Chromatogram (All TIC)
2,567,512
TIC*1.00
10.0
20.0
30.0
39.0
min

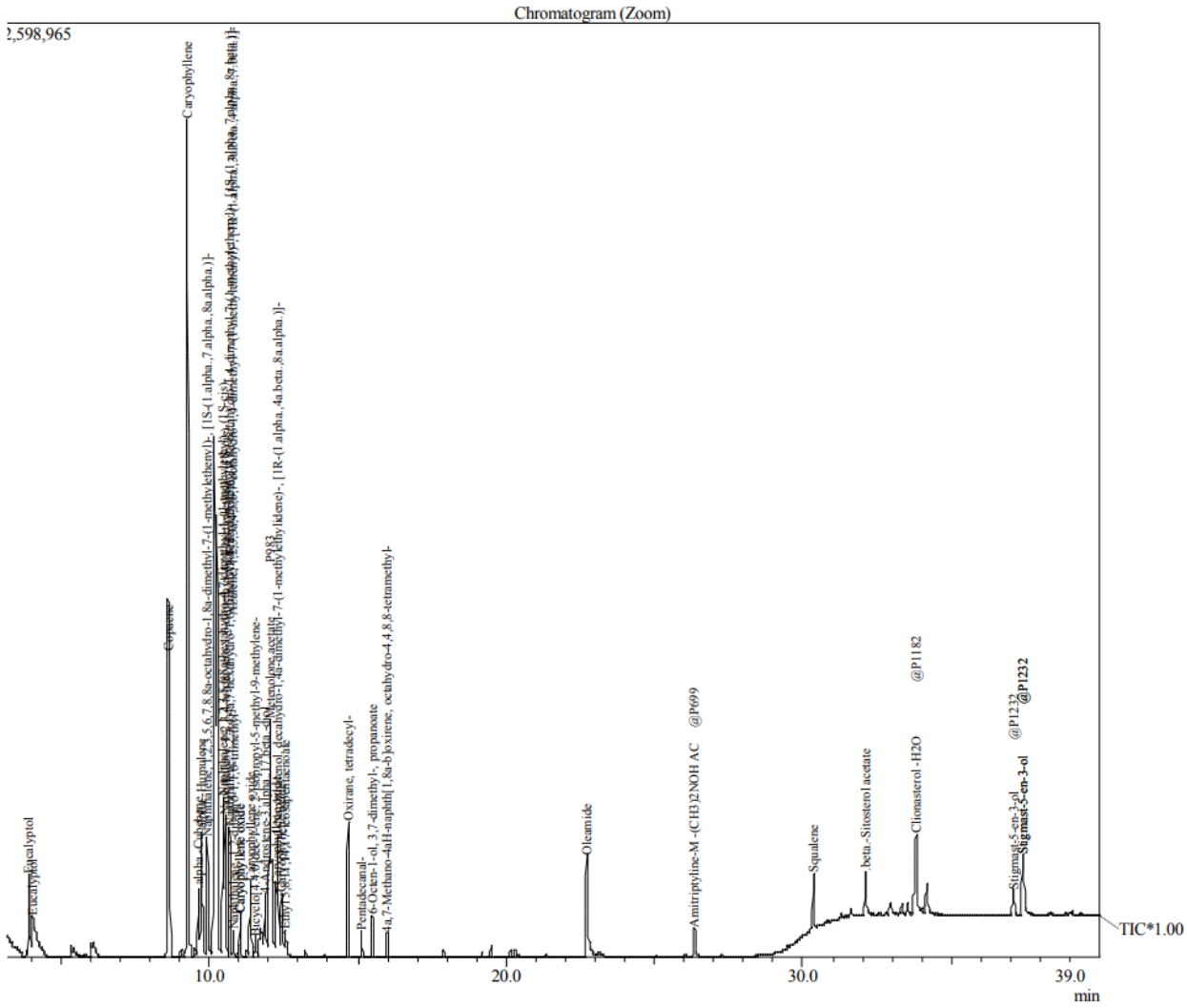
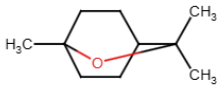
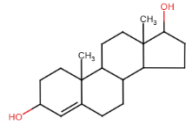
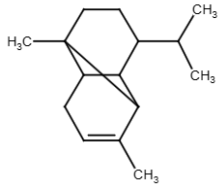
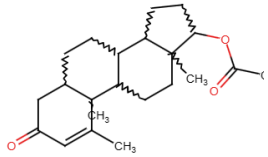
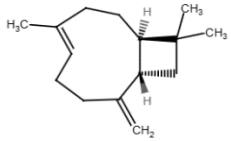
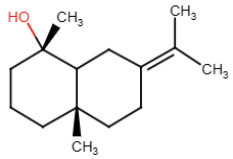
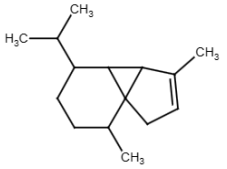
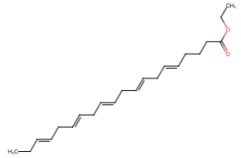
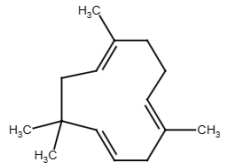
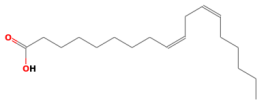
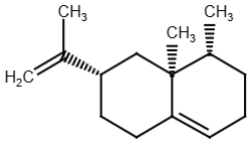
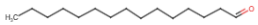
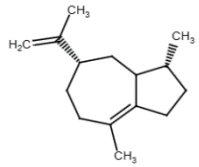
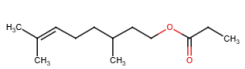
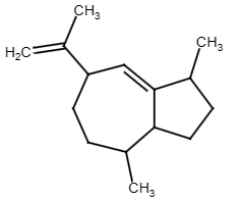
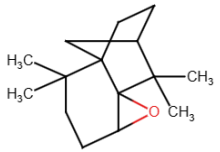
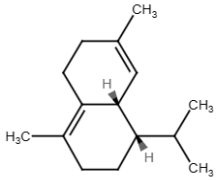
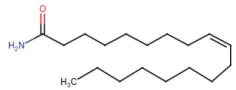
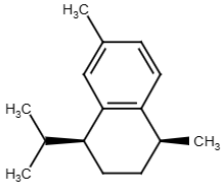
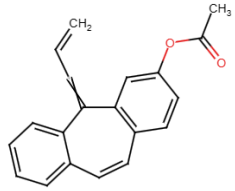
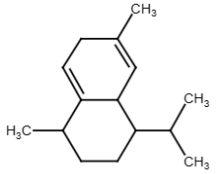
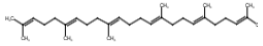
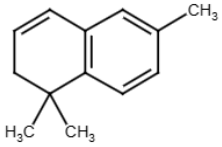
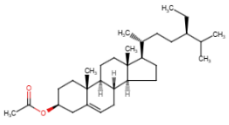
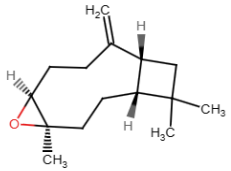
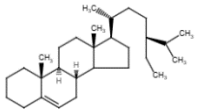
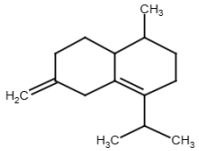
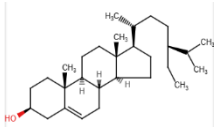

Chromatogram (Zoom)
2,598,965
Caryophyllene
Oxirane, tetradecyl-
Pentadecanal-
Oleamide
Amitriptyline-M -(CH3)2NOH AC
@P699
@P1182
Squalene
beta.-Sitosterol acetate
Clionasterol -H2O
@P1232
Stigmast-5-en-3-ol
TIC*1.00
10.0
20.0
30.0
39.0
min

Table S4. *Identified Bioactive Compounds Structures and Description*

CID	Name	Structure	Type of Phytochemical	SMILES	CID	Name	Structure	Type of Phytochemical	SMILES
1	Eucalyptol		Terpenoid	CC12CCC(CC1)C(C)(C)O2	15	4-Androstene-3.α.,17.β.-diol		Steroid	CC12CCC3C(CCC4=CC(O)CCC34C)C1CCC2O
2	α-Copaene		Terpenoid	CC(C)C1CCC2(C)C3CC=C(C)C2C13	16	Methenolone acetate		Steroid	CC(=O)OC1CCC2C3CCC4CC(=O)C=C(C)C4(C)C3CCC12C
3	Caryophyllene		Terpenoid	[H][C@]12CC(C)(C)[C@]1([H])CC\C(C)=C\CCC2=C	17	Juniper camphor		Terpenoid	CC(C)=C1CC[C@]2(C)CCC[C@](C)(O)C2C1
4	α-Cubebene		Terpenoid	CC(C)C1CCC(C)C23CC=C(C)C2C13	18	Ethyl 5,8,11,14,17-icos apentaenoate		Fatty acid	CCOC(=O)CCC\C=C\C\C=C\C\C=C\C\C=C\C\C=C\C\C=C\CC
5	Humulene		Terpenoid	C\C1=C/CC(C)(C)\C=C\C\C(C)=C\CC1	19	Linoleic Acid		Fatty Acid	CCCCCCCCCCCCCCCC1CO1
6	Valencene		Terpenoid	C[C@@H]1CCC=C2CC[C@@H](C[C@@]12C)C(C)=C	20	1-Pentadecanal		Fatty Aldehyde	CCCCCCCCCCCCCCC=O

7	α-Bulnesene		Terpenoid	C[C@@H]1CCC2=C(C)CC[C@@H](CC12)C(C)=C	21	6-Octen-1-ol, 3,7-dimethyl-, propanoate		Terpenoid/terpene alcohol	CCC(=O)OCCC(C)CCC=C(C)C
8	γ-Gurjunene		Terpenoid	CC1CCC2C(C)CCC(C=C12)C(C)=C	22	4a,7-Methano-4aH-naphth[1,8a-b]oxirene, octahydro-4,4,8,8-tetramethyl-		Terpenoid	CC1(CCC2C3(C14CCC(C4)C3(C)C)O2)C
9	δ-Cadinene, (+)-		Terpenoid	[H][C@]1(CCC(C)=C2CCC(C)=C[C@]12[H])C(C)C	23	Oleamide		Fatty Acid amide	CCCCCCCCC=CCCCCCCC(=O)N
10	(-)-Calamenene		Terpenoid	CC(C)[C@@H]1CC[C@H](C)C2=C1C=C(C)C=C2	24	Amitriptyline-M-(CH3)2NOHAC		Amine	C=1C2CCCCC2\C(=C\C=C)C2CC(CCC2C1)OC(C)=O
11	Cadinadiene-1,4		Terpenoid	CC(C)C1CCC(C)C2=CCC(C)=CC12	25	Squalene		Terpenoid	CC(=CCCC(=CCCC(=CCCC=C(C)CCC=C(C)CCC=C(C)C)C)C)C
12	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-		Benzenoids, Aromatic	CC1=CC2=C(C=C1)C(C)(C)CC=C2	26	β-Sitosterol acetate		Terpenoid	CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)OC(=O)C)C)C)C(C)C

13	Caryophyllene oxide		Terpenoid	[H][C@]12CCC(=C)[C@]3([H])CC(C)(C)[C@]3([H])CC[C@@]1(C)O2	27	Clionasterol -H2O		Phytosterol	[H][C@@]12CC=C3CCCC[C@]3(C)[C@@]1([H])CC[C@]1(C)[C@H](CCC21)[C@H](C)CC[C@@H](CC)C(C)C
14	Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene -		Terpenoid	CC(C)C1=C2CC(=C)CCC2C(C)CC1	28	Stigmast-5-en-3-ol		Sterol lipid	CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C.O

Note: Compound Identification (CID), Simplified Molecular-Input Line-Entry System (SMILES)

Table S5. *SwissADME Analysis Report of Top Bioactive Compounds*

CLASS	Parameters	Compound #							Control		
		1	**2**	**3**	**4**	**5**	**6**	**7**	**Rivaroxaban**	**Apixaban**	**Betrixaban**
Physico-chemical Properties	MW (g/mol)	220.35	290.44	344.49	222.37	212.33	220.35	288.34	435.88	459.50	451.91
	# Heavy Atoms	16	21	25	16	15	16	22	29	34	32
	# Aromatic Heavy Atoms	0	0	0	0	0	0	12	11	17	18
	Fraction Csp3	0.87	0.89	0.82	0.87	0.77	1	0.05	0.32	0.28	0.13
	# Rotatable Bonds	0	0	2	0	8	0	3	6	5	9
	# H-bond acceptors	1	2	3	1	2	1	2	5	5	5
	# H-bond donors	0	2	0	1	0	0	0	1	1	3
	Molar Refractivity	68.27	86.32	99.9	70.46	65.42	66.11	90.59	114.09	132.70	125.23
	TPSA (Å^2)	12.53	40.46	43.37	20.23	26.3	12.53	26.3	116.42	110.76	107.41
Lipophilicity	iLOGP	3.11	2.92	3.19	3.1	3.57	3.06	3.23	2.95	3.62	2.72
	XLOGP3	3.56	3.41	4.45	3.89	4.24	3.85	4.84	2.49	2.24	3.56
	WLOGP	3.94	3.67	4.7	4.06	3.71	3.77	4.5	1.76	1.94	3.75
	MLOGP	3.67	3.7	4.1	3.67	3.32	3.81	4.24	1.41	1.76	2.83
	Silicos-IT Log P	4.07	2.99	4.13	3.75	3.58	4.18	4.87	2.84	1.96	3.24
	Consensus Log P	3.67	3.34	4.11	3.69	3.68	3.73	4.34	2.29	2.30	3.22
Water Solubility	ESOL Class	Soluble	Soluble	Moderately soluble	Soluble	Soluble	Soluble	Moderately soluble	Soluble	Moderately Soluble	Moderately Soluble
	Ali Class	Soluble	Soluble	Moderately soluble	Moderately soluble	Moderately soluble	Soluble	Moderately soluble	Moderately Soluble	Moderately Soluble	Moderately Soluble
	Silicos-IT Class	Soluble	Soluble	Moderately soluble	Soluble	Soluble	Soluble	Moderately soluble	Moderately Soluble	Moderately Soluble	Poorly Soluble
Pharmacokinetics	GI Absorption	High	High	High	High	High	High	High	High	High	High
	BBB Permeant	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	No	No
	Pgp Substrate	No	Yes	No	No	No	No	No	Yes	Yes	No
	CYP1A2 Inhibitor	No	No	No	No	No	No	No	No	No	No
	CYP2C19 Inhibitor	Yes	No	No	No	No	No	Yes	Yes	Yes	Yes
	CYP2C9 Inhibitor	Yes	No	Yes	Yes	No	No	Yes	Yes	Yes	Yes
	CYP2D6 Inhibitor	No	No	No	No	No	No	No	No	Yes	Yes
	CYP3A4 Inhibitor	No	No	No	No	No	No	No	Yes	Yes	Yes
	Log Kp (cm/s)	-5.12	-5.65	-5.24	-4.89	-4.58	-4.91	-4.62	-7.19	-7.51	-6.53
Drug-likeness	Lipinski #	0	0	0	0	0	0	1	0	0	0
	Ghose #	0	0	0	0	0	0	0	0	1	0
	Veber #	0	0	0	0	0	0	0	0	0	0
	Egan #	0	0	0	0	0	0	0	0	0	0

	Muegge #	1	0	0	1	0	1	0	0	0	0
	Bioavailability Score	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55
Medicinal Chemistry	PAINS # Alerts	0	0	0	0	0	0	0	0	0	0
	Brenk # Alerts	2	1	0	1	1	1	2	0	0	2
	Leadlikeness # Violations	2	0	1	2	3	2	1	1	1	3
	Synthetic Accessibility	4.35	4.96	4.87	3.69	2.84	4.87	3.33	3.63	3.48	3.05

Figure S3. *Radar Plot of the Bioactive Compound*

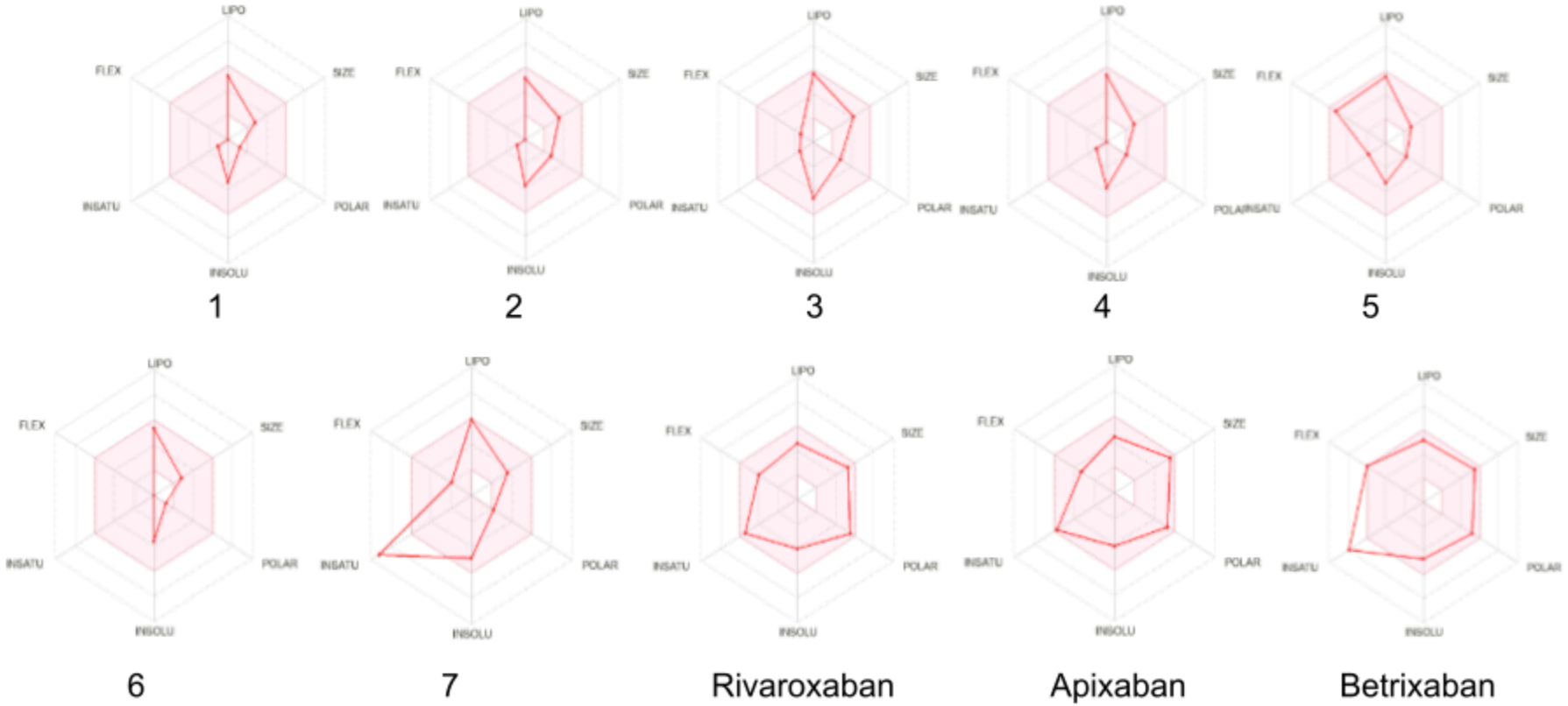
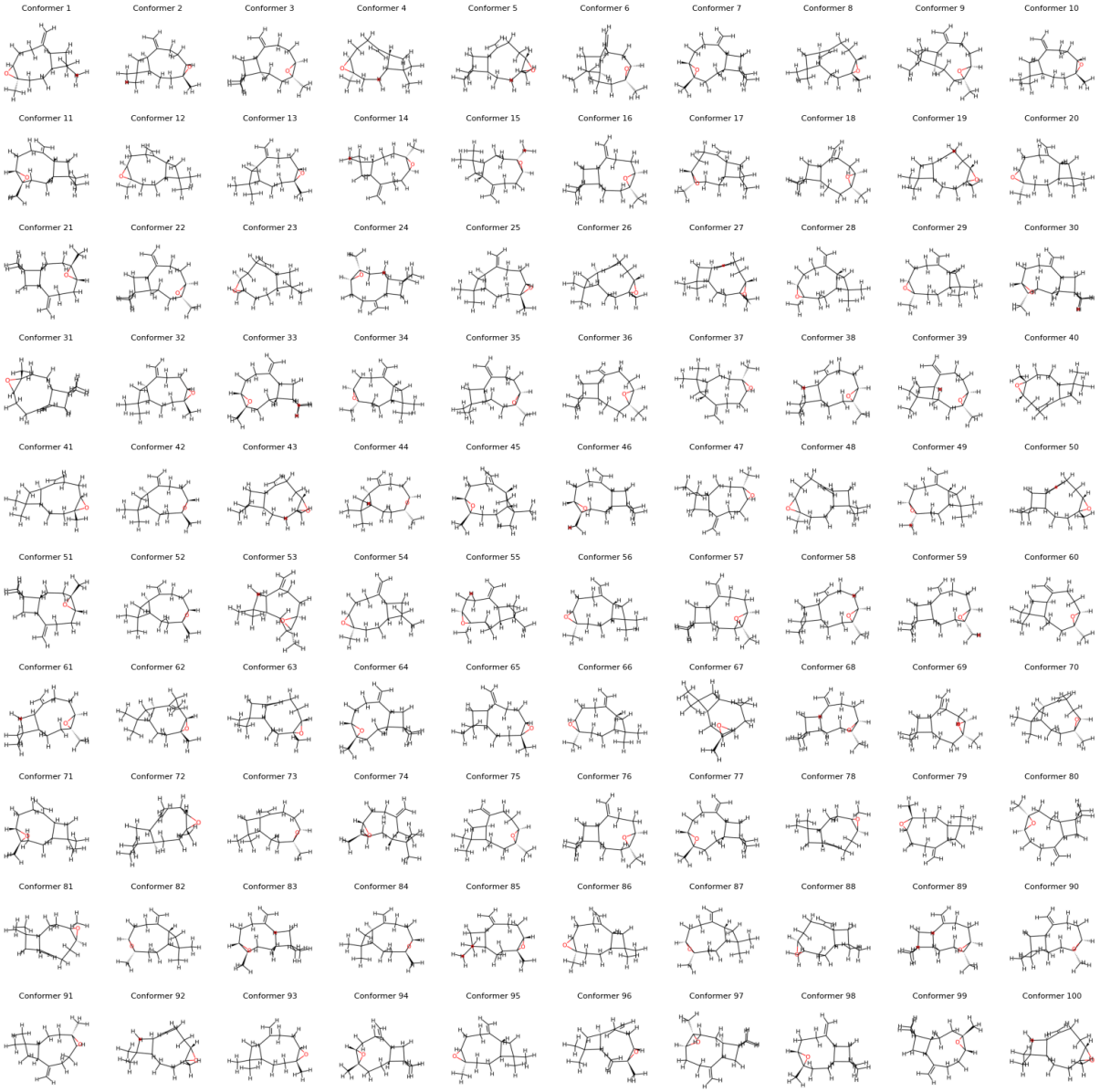


Figure S4. *Conformational Analysis of Compound* ***1***



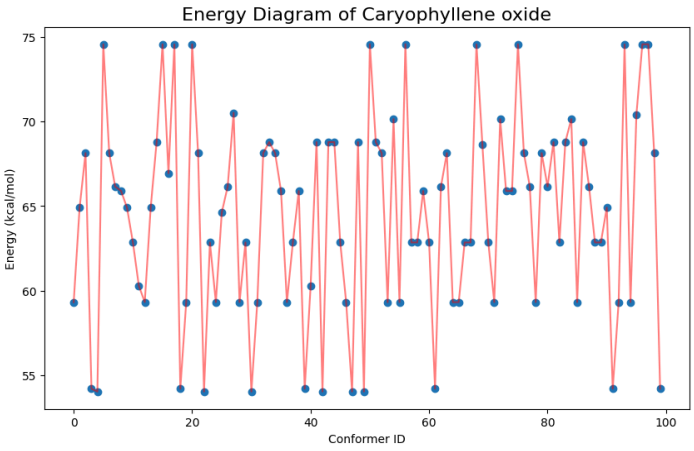


Figure S5. *Conformational Analysis of Compound* ***2***

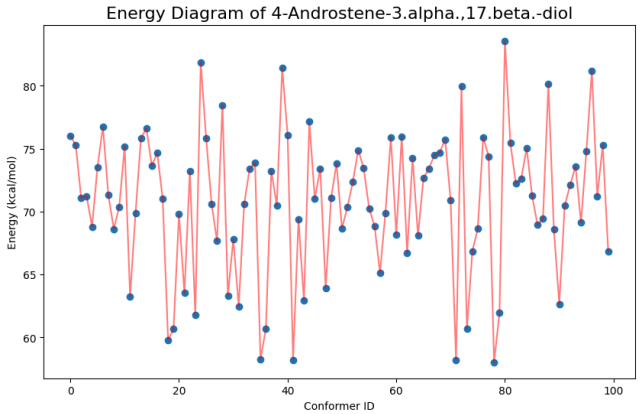
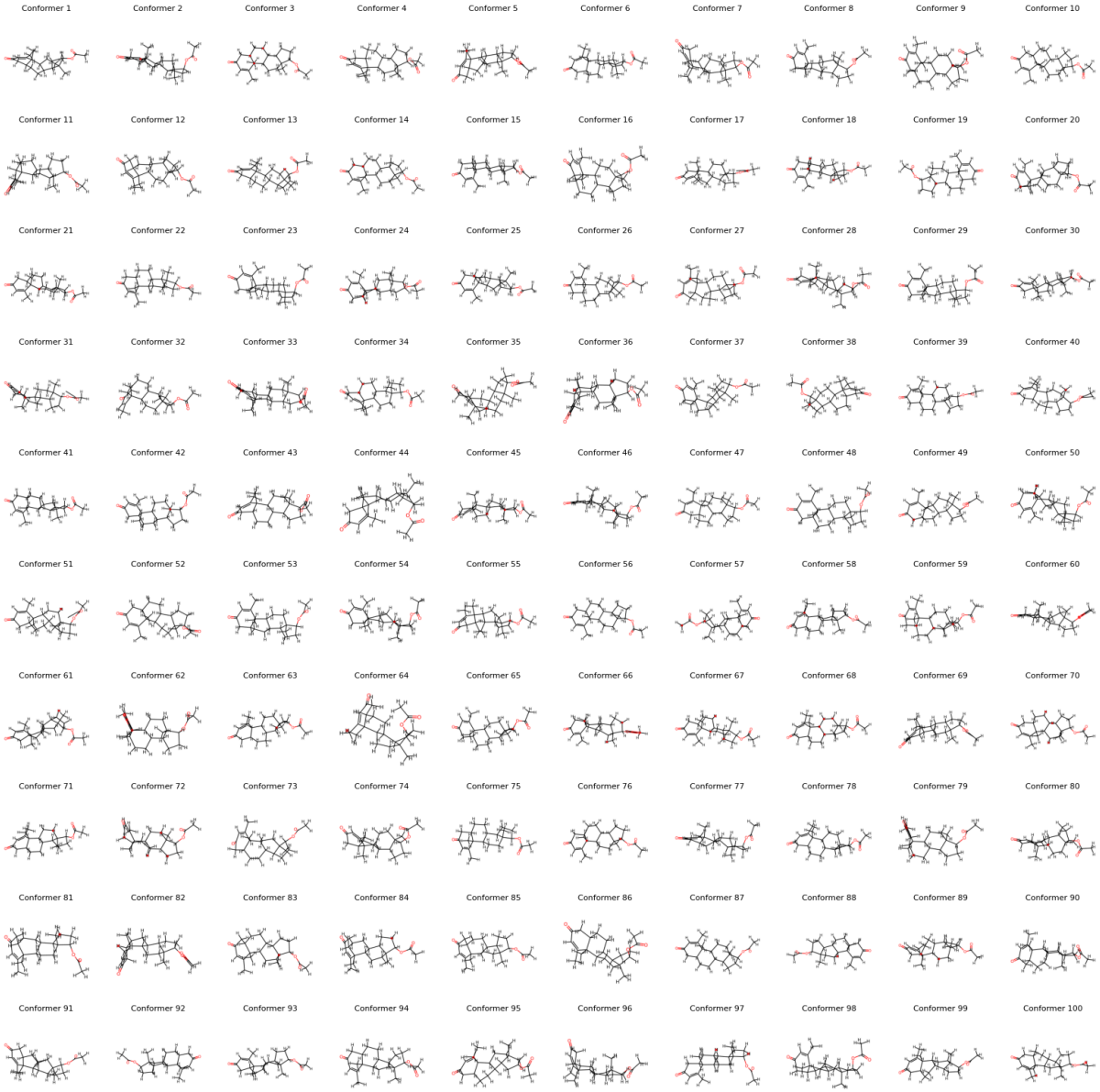


Figure S6. *Conformational Analysis of Compound* ***3***



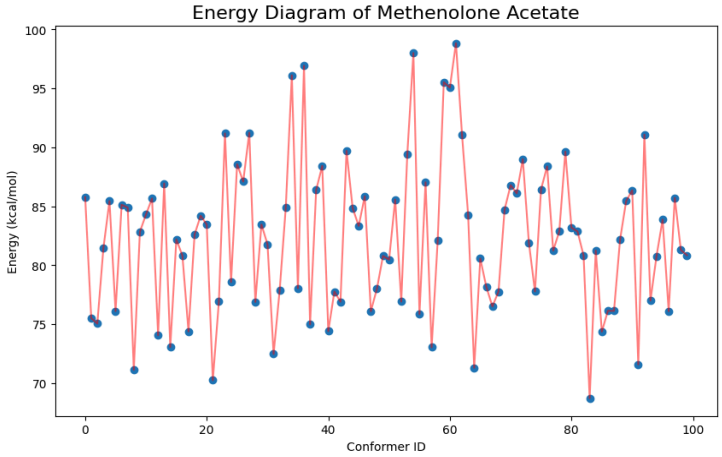
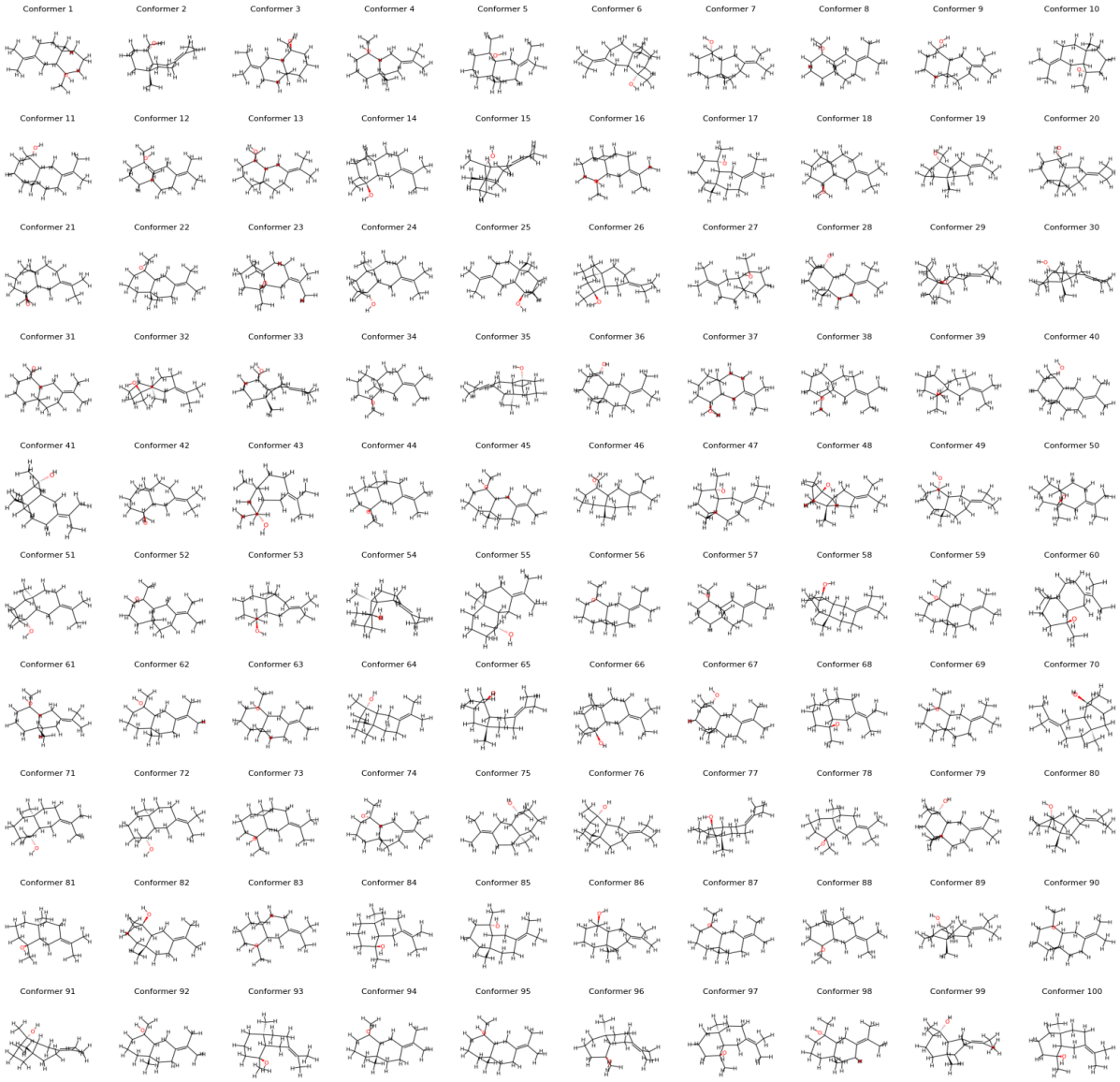


Figure S7. *Conformational Analysis of Compound* ***4***



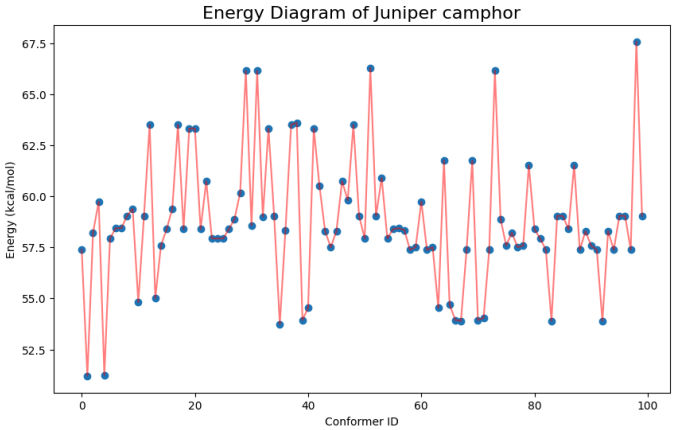
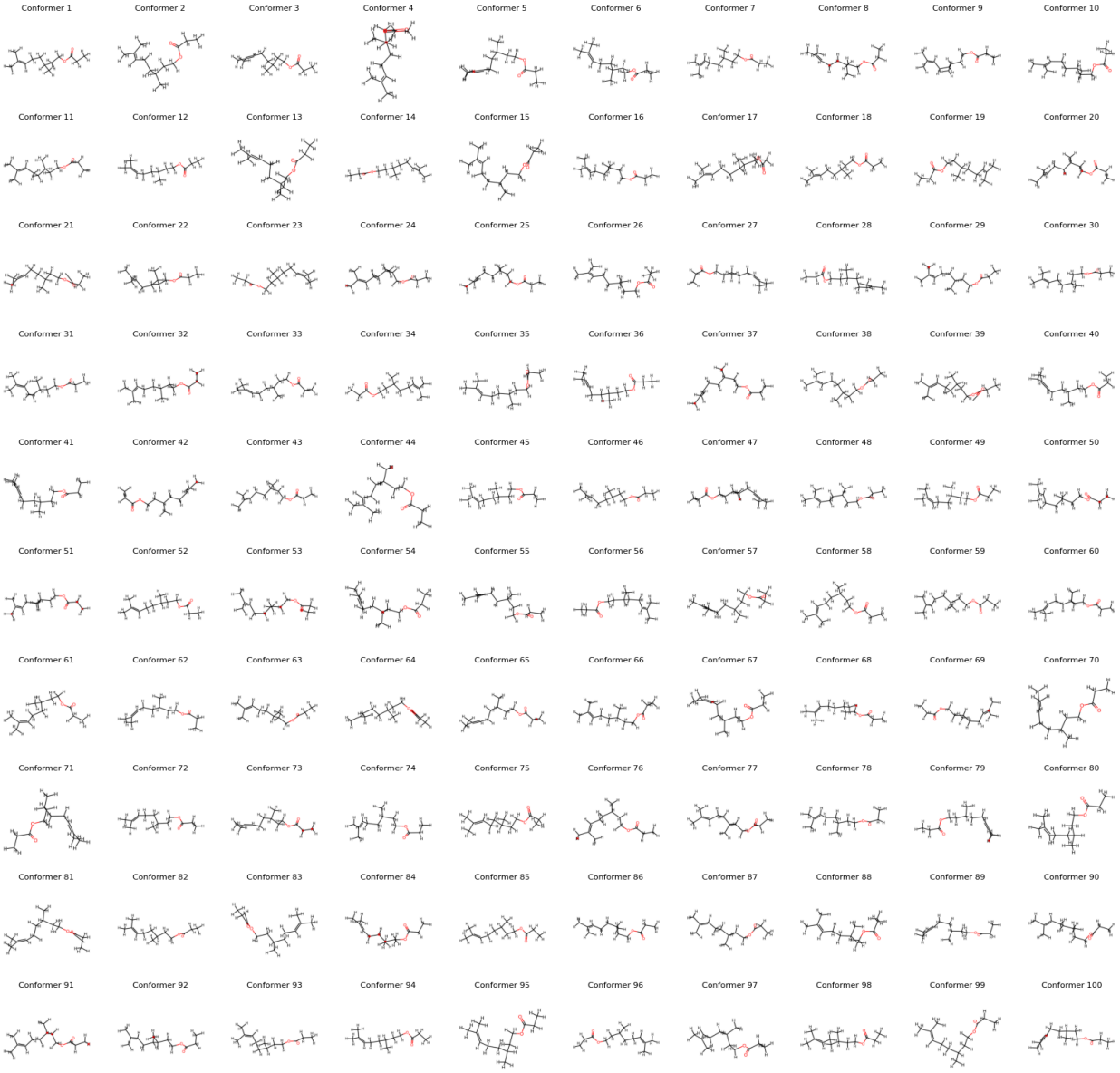


Figure S8. *Conformational Analysis of Compound* ***5***



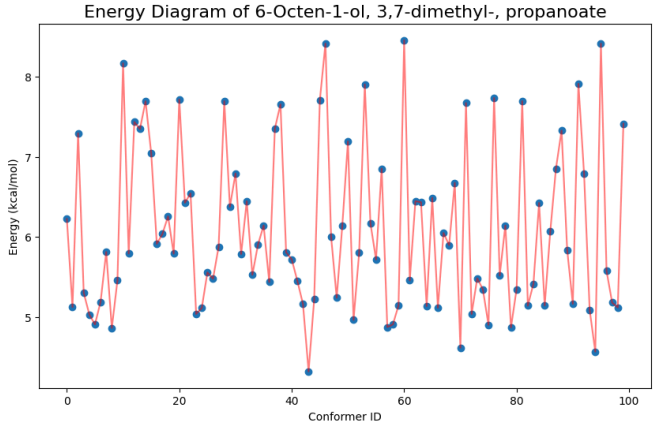
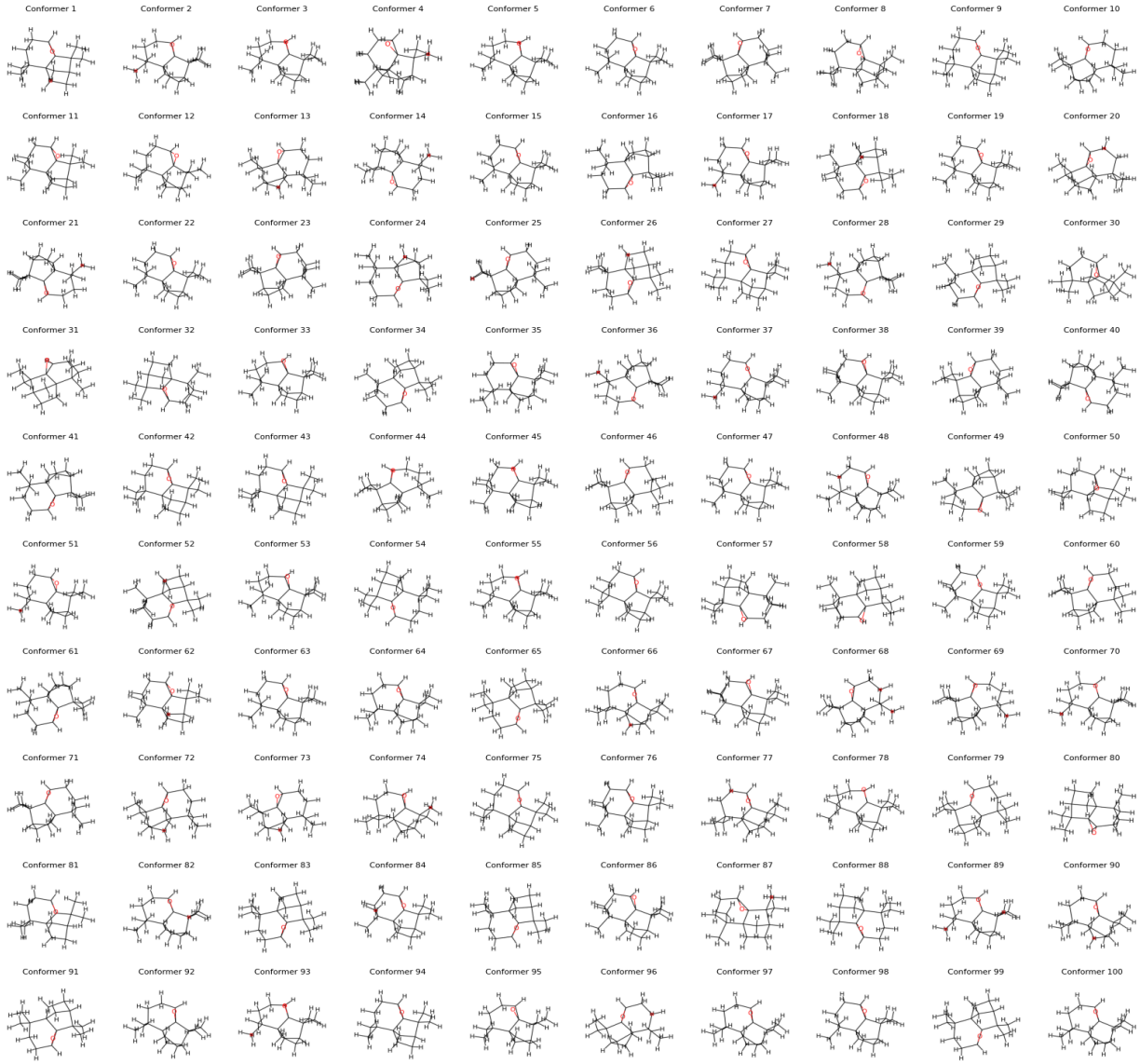


Figure S9. *Conformational Analysis of Compound* ***6***



Energy Diagram of 4a,7-Methano-4aH-naphth[1,8a-b]oxirene, octahydro-4,4,8,8-tetramethyl-

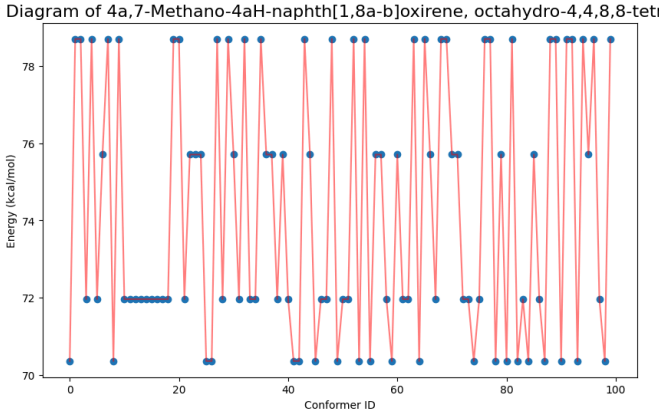
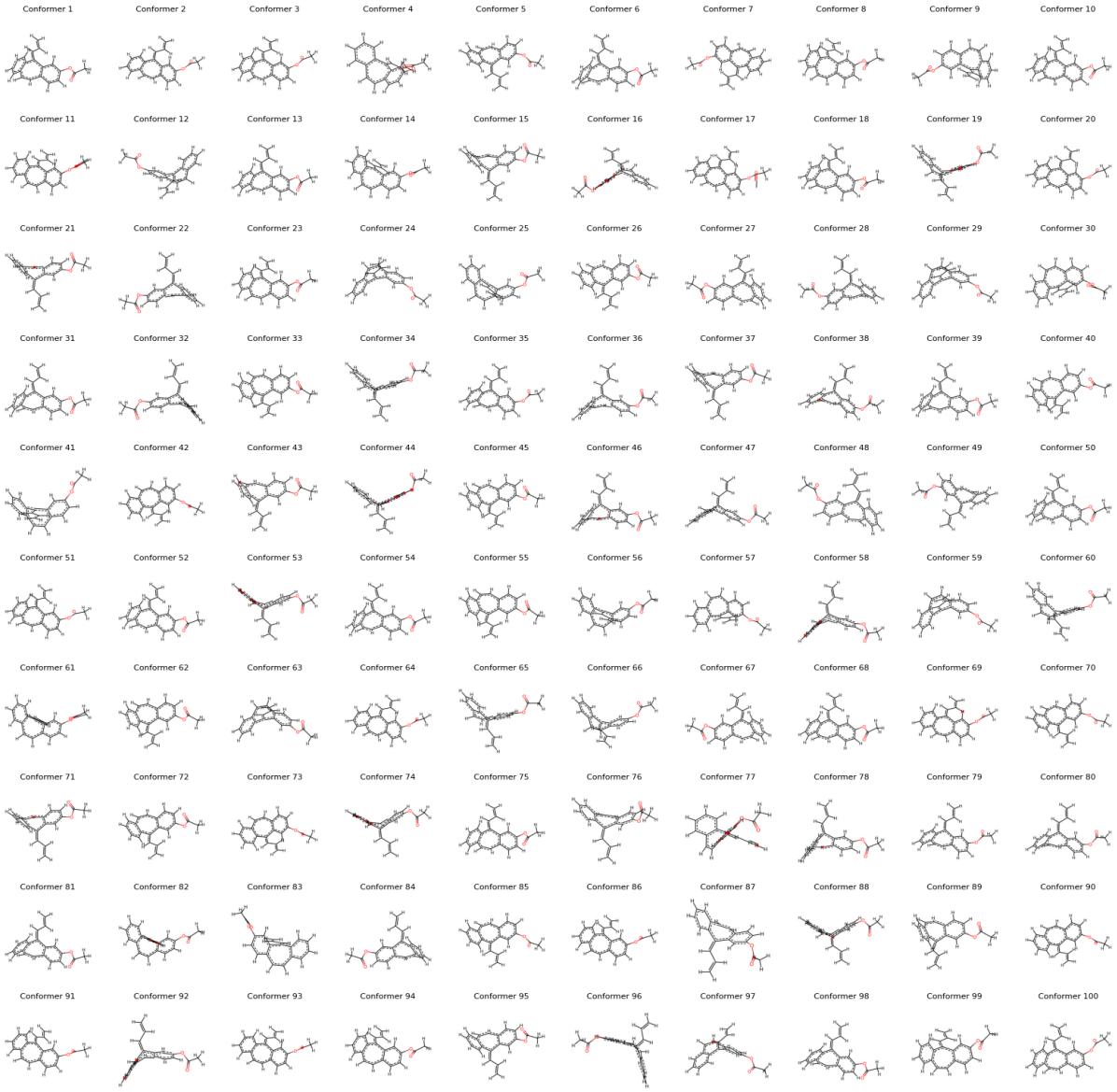


Figure S10. *Conformational Analysis of Compound 7*



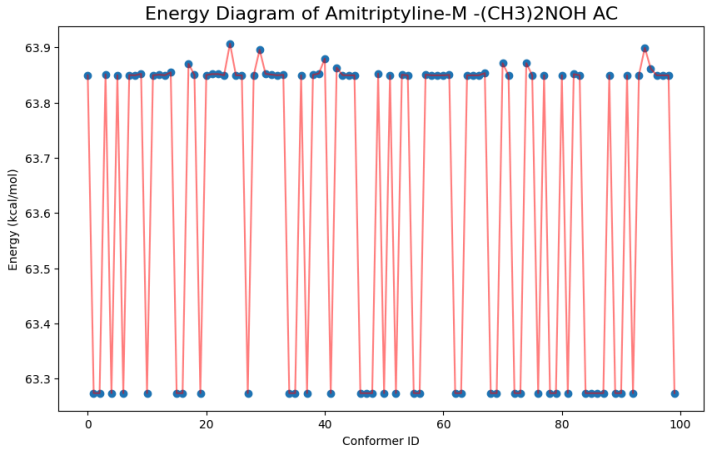


Table S6. *CFIXa Docking Scores*

Active Site	Mode	Compound #													
		1		2		3		4		5		6		7	
		Vina	Vinardo	Vina	Vinardo	Vina	Vinardo	Vina	Vinardo	Vina	Vinardo	Vina	Vinardo	Vina	Vinardo
II	**1**	**-6.5**	**-6.1**	-6.8	-6.0	**-7.6**	**-6.8**	-6.0	-5.3	**-4.7**	**-5.6**	**-5.7**	**-4.8**	**-7.2**	**-6.6**
	2	-6.4	-6.0	-6.6	-5.7	-7.2	-5.9	-5.8	-5.0	-4.7	-5.0	-5.6	-4.6	-6.8	-6.6
	3	-5.9	-5.9	-6.5	-5.6	-6.4	-4.6	-5.7	-4.8	-4.6	-4.8	-5.5	-4.4	-6.7	-6.3
	4	-5.8	-5.7	-6.4	-5.2	-6.3	-3.1	-5.6	-4.7	-4.6	-4.8	-5.3	-3.5	-6.8	-6.2
	5	-5.8	-5.6	-6.4	-5.1	-6.3	-3.1	-5.6	-4.7	-4.4	–4.6	-5.1	-3.3	-6.1	-5.6
	6	-5.6	-5.4	-6.4	-5.0	-6.2	-2.9	-5.6	-4.0	-4.4	-4.4	-4.8	-3.2	-	-
	7	-5.6	-4.4	-6.3	-5.0	-6.2	-	-5.4	-3.6	-4.3	-4.4	-4.6	-3.2	-	-
	8	-5.5	-4.2	-6.2	-4.5	-6.1	-	-5.2	-3.5	-4.3	-4.3	-	-3.1	-	-
	9	-4.5	-	-5.7	-3.8	-	-	-	-3.3	-4.2	-4.2	-	-3.0	-	-
	10	-3.7	-	-4.4	-3.0	-	-	-	-3.1	-4.2	-	-	-2.8	-	-
III	1	-5.5	-4.8	-6.6	-4.8	-7.9	-5.7	-5.2	-4.1	-4.9	-3.5	-5.3	-3.9	-6.9	-4.4
	2	-5.4	-4.6	-6.1	-4.5	-6.6	-4.6	-5.2	-4.0	-4.8	-3.0	-5.2	-3.3	-6.5	-4.3
	3	-5.3	-4.3	-5.6	-4.3	-6.2	-4.5	-5.0	-3.9	-4.7	-3.0	-5.0	-3.3	-6.4	-4.3
	4	-5.2	-4.2	-5.6	-4.3	-6.1	-4.4	-4.9	-3.7	-4.7	-2.9	-4.9	-3.2	-6.3	-4.1
	5	-5.1	-3.9	-5.5	-4.2	-5.5	-4.4	-4.8	-3.6	-4.4	-2.8	-4.8	-3.2	-6.0	-4.1
	6	-5.1	-3.8	-5.5	-4.0	-5.5	-4.4	-4.7	-3.6	-4.2	-2.8	-4.8	-3.1	-5.9	-4.1
	7	–4.8	-3.6	-5.3	-3.9	-5.2	-4.3	-4.7	-3.5	-4.2	-2.8	-4.8	-2.9	-5.7	-4.1
	8	-4.6	-3.6	-5.2	-3.9	-5.1	-4.3	-4.6	-3.4	-4.1	-2.8	-4.8	-2.8	-5.6	-4.0
	9	-4.5	-3.5	-5.2	-3.8	-5.0	-4.2	-4.5	-3.3	-3.9	-2.8	-4.6	-2.8	-5.5	-4.0
	10	-4.4	-3.4	-5.2	-3.6	-4.9	-4.0	-4.5	-3.2	-3.9	-2.5	-4.6	-2.8	-5.3	-3.9
V	1	-5.6	-4.4	**-7.0**	**-6.1**	-7.0	-5.8	**-6.4**	**-5.3**	-4.7	-4.3	-5.0	-3.8	-6.8	-6.1
	2	-5.5	-4.4	-6.7	-5.7	-6.9	-5.6	-6.0	-5.0	-4.6	-4.0	-4.9	-3.5	-6.6	-6.0
	3	-5.3	-4.3	–6.7	-5.6	-6.6	-5.3	-5.3	-4.5	-4.5	-4.0	-4.8	-3.5	-6.5	-6.0
	4	-5.2	-4.3	-6.6	-5.5	-6.6	-5.1	-5.2	-4.4	-4.3	-4.0	-4.7	-3.4	-6.3	-5.9
	5	-5.2	-4.2	-6.6	-5.5	-6.3	-5.0	-5.2	-4.3	-4.3	-3.9	-4.7	-3.4	-6.2	–5.7
	6	-5.1	-4.2	-6.5	-5.5	-6.3	-5.0	-5.0	-4.2	-4.3	-3.9	-4.6	-3.3	-6.0	-5.7
	7	-5.1	-4.1	-6.5	-5.4	-6.2	-4.9	-5.0	-4.1	-4.3	-3.8	-4.5	-3.3	-5.9	-5.6
	8	-5.1	-4.1	-6.4	-5.2	-6.4	-4.9	-4.9	-4.0	-4.3	-3.8	-4.4	-3.3	-5.8	-5.6
	9	-5.1	-4.0	-6.3	-5.1	-6.0	-4.7	-4.9	-4.0	-4.2	-3.7	-4.4	-3.1	-5.7	-5.5
	10	-5.0	-4.0	-6.2	-5.0	-6.0	-4.6	-4.6	-4.0	-4.2	-3.7	-4.4	-3.0	-5.6	-5.3

Table S7. *Conformational Changes on Best Ligand-Complex per Bioactive Compound in CFIXa*

Compound #	Vina Score	Vinardo Score	Active Site	Bond Length (Å)				Bond Angle (Å)			
				Atom	l_i	l_f	Δl	Atom	$\angle_i$	$\angle_f$	Δ∠
							H:TYR99				
				CG - CD1	1.39556	1.39549	-0.00007	α(CD1-CG-CD2)	118.05	118.05	0
				CG - CD2	1.38966	1.38993	0.00027	α(CG-CD2-CE2)	121.11	121.12	0.01
				CD1 - CE1	1.39409	1.39403	-0.00006	α(CD2-CE2-CZ)	119.59	119.57	-0.02
				CD2 - CE2	1.39517	1.39501	-0.00016	α(CE2-CZ-CE1)	120.23	120.23	0
				CE1 - CZ	1.37854	1.37844	-0.00010	α(CZ-CE1-CD1)	119.64	119.67	0.03
				CE2 - CZ	1.38939	1.38949	0.00010	α(CE1-CD1-CG)	121.24	121.21	-0.03
1	-6.5	-6.1	II				H:TRP215				
				CD2 - CE2	1.41412	1.41425	0.00013	α(CE3-CD2-CE2)	118.63	118.63	0
				CD2 - CE3	1.39553	1.39532	-0.00021	α(CD2-CE2-CZ2)	122.34	122.36	0.02
				CE2 - CZ2	1.411	1.41021	-0.00079	α(CE2-CZ2-CH2)	117.54	117.55	0.01
				CE3 - CZ3	1.39216	1.39257	0.00041	α(CZ2-CH2-CZ3)	120.93	120.92	-0.01
				CZ2 - CH2	1.3775	1.37761	0.00011	α(CH2-CZ3-CE3)	121.18	121.20	0.02
				CZ3 - CH2	1.40946	1.40908	-0.00038	α(CZ3-CE3-CD2)	119.30	119.27	-0.03
							L:PHE98				
				CG - CD1	1.39561	1.39508	-0.000530	α(CD1-CG-CD2)	118.35	118.36	0.01
				CG - CD2	1.38125	1.38094	-0.000310	α(CG-CD2-CE2)	120.93	120.94	0.01
				CD1 - CE1	1.40154	1.40109	-0.000450	α(CD2-CE2-CZ)	120.20	120.19	-0.01
				CD2 - CE2	1.39071	1.39084	0.000130	α(CE2-CZ-CE1)	119.86	119.84	-0.02
2	-7.0	-6.1	V	CE1 - CZ	1.37139	1.37223	0.000840	α(CZ-CE1-CD1)	119.83	119.83	0
				CE2 - CZ	1.38619	1.38583	-0.000360	α(CE1-CD1-CG)	120.79	120.80	0.01
							L:LYS100				
				CB - CG	1.51808	1.51855	0.000470	α(CB-CG-CD)	110.42	110.41	-0.01
				CG - CD	1.51948	1.51874	-0.000740				
				CE - NZ	1.49714	1.49794	0.000800	α(CE-NZ-HZ1)	109.30	109.30	0
				HZ1 - NZ	1.01014	1.00985	-0.000290				
							H:TYR99				
				CG - CD1	1.39556	1.39531	-0.000250	α(CD1-CG-CD2)	118.05	118.05	0
3	-7.6	-6.8	II	CG - CD2	1.38966	1.39003	0.000370	α(CG-CD2-CE2)	121.11	121.11	0

				CD1 - CE1	1.39409	1.39417	0.000080	α(CD2-CE2-CZ)	119.59	119.53	-0.06
				CD2 - CE2	1.39517	1.39534	0.000170	α(CE2-CZ-CE1)	120.23	120.27	0.04
				CE1 - CZ	1.37854	1.37766	-0.000880	α(CZ-CE1-CD1)	119.64	119.66	0.02
				CE2 - CZ	1.38939	1.38953	0.000140	α(CE1-CD1-CG)	121.24	121.22	-0.02
				H:TRP215							
				CG - CD1	1.36247	1.3615	-0.000970	α(CE3-CD2-CE2)	118.63	118.67	0.04
				CG - CD2	1.44127	1.44155	0.000280	α(CD2-CE2-CZ2)	122.34	122.33	-0.01
				CD1 - NE1	1.37831	1.37861	0.000300	α(CE2-CZ2-CH2)	117.54	117.55	0.01
				CD2 - CE2	1.41412	1.41369	-0.000430	α(CZ2-CH2-CZ3)	120.93	120.94	0.01
				NE1 - CE2	1.37471	1.37452	-0.000190	α(CH2-CZ3-CE3)	121.18	121.17	-0.01
				CD2 - CE3	1.39553	1.3958	0.000270	α(CZ3-CE3-CD2)	119.30	119.26	-0.04
				CE2 - CZ2	1.411	1.41062	-0.000380	α(CE2-CD2-CG)	107.19	107.18	-0.01
				CE3 - CZ3	1.39216	1.39215	-0.000010	α(CD2-CG-CD1)	106.27	106.26	-0.01
				CZ2 - CH2	1.3775	1.37728	-0.000220	α(CG-CD1-NE1)	110.25	110.29	0.04
				CZ3 - CH2	1.40946	1.4098	0.000340	α(CD1-NE1-CE2)	109.01	108.97	-0.04
				HE1 - NE1	1.00952	1.00894	-0.000580	α(NE1-CE2-CD2)	107.23	107.25	0.02
				H:TYR128							
				CG - CD1	1.39175	1.39183	0.000080	α(CD1-CG-CD2)	118.01	118	-0.01
				CG - CD2	1.3885	1.38838	-0.000120	α(CG-CD2-CE2)	121.21	121.19	-0.02
				CD1 - CE1	1.39351	1.39339	-0.000120	α(CD2-CE2-CZ)	119.57	119.63	0.06
				CD2 - CE2	1.39727	1.39715	-0.000120	α(CE2-CZ-CE1)	120.29	120.25	-0.04
4	-6.4	-5.3	V	CE1 - CZ	1.38569	1.38633	0.000640	α(CZ-CE1-CD1)	119.38	119.36	-0.02
				CE2 - CZ	1.38262	1.3824	-0.000220	α(CE1-CD1-CG)	121.43	121.47	0.04
				H:ILE129B							
				CB - CG1	1.53349	1.53338	-0.000110	α(CD1-CG1-CB)	114.11	114.10	-0.01
				CB - CG2	1.54926	1.54956	0.000300	α(CG1-CB-CG2)	112.14	112.09	-0.05
				CG1 - CD1	1.57649	1.57657	0.000080				
				H:TYR99							
				CG - CD1	1.39556	1.39527	-0.000290	α(CD1-CG-CD2)	118.05	118.08	0.03
				CG - CD2	1.38966	1.38882	-0.000840	α(CG-CD2-CE2)	121.11	121.12	0.01
				CD1 - CE1	1.39409	1.39521	0.001120	α(CD2-CE2-CZ)	119.59	119.54	-0.05
				CD2 - CE2	1.39517	1.39589	0.000720	α(CE2-CZ-CE1)	120.23	120.27	0.04
5	-4.7	-5.6	II	CE1 - CZ	1.37854	1.37795	-0.000590	α(CZ-CE1-CD1)	119.64	119.64	0
				CE2 - CZ	1.38939	1.38904	-0.000350	α(CE1-CD1-CG)	121.24	121.19	-0.05
				H:TRP215							

				CD2 - CE2	1.41412	1.41369	-0.000430	α(CE3-CD2-CE2)	118.63	118.65	0.02
				CD2 - CE3	1.39553	1.39571	0.000180	α(CD2-CE2-CZ2)	122.34	122.29	-0.05
				CE2 - CZ2	1.411	1.41166	0.000660	α(CE2-CZ2-CH2)	117.54	117.57	0.03
				CE3 - CZ3	1.39216	1.393	0.000840	α(CZ2-CH2-CZ3)	120.93	120.95	0.02
				CZ2 - CH2	1.3775	1.37717	-0.000330	α(CH2-CZ3-CE3)	121.18	121.15	-0.03
				CZ3 - CH2	1.40946	1.40887	-0.000590	α(CZ3-CE3-CD2)	119.30	119.30	0
6	-5.7	-4.8	II	H:TYR99							
				CG - CD1	1.39556	1.39634	0.000780	α(CD1-CG-CD2)	118.05	117.99	-0.06
				CG - CD2	1.38966	1.38971	0.000050	α(CG-CD2-CE2)	121.11	121.14	0.03
				CD1 - CE1	1.39409	1.39403	-0.000060	α(CD2-CE2-CZ)	119.59	119.30	-0.29
				CD2 - CE2	1.39517	1.39488	-0.000290	α(CE2-CZ-CE1)	120.23	120.23	0
				CE1 - CZ	1.37854	1.37858	0.000040	α(CZ-CE1-CD1)	119.64	119.63	-0.01
				CE2 - CZ	1.38939	1.38915	-0.000240	α(CE1-CD1-CG)	121.24	121.26	0.02
				H:TRP215							
				CD2 - CE2	1.41412	1.41467	0.000550	α(CE3-CD2-CE2)	118.63	118.61	-0.02
				CD2 - CE3	1.39553	1.39476	-0.000770	α(CD2-CE2-CZ2)	122.34	122.31	-0.03
				CE2 - CZ2	1.411	1.41127	0.000270	α(CE2-CZ2-CH2)	117.54	117.54	0
				CE3 - CZ3	1.39216	1.39205	-0.000110	α(CZ2-CH2-CZ3)	120.93	120.95	0.02
				CZ2 - CH2	1.3775	1.37681	-0.000690	α(CH2-CZ3-CE3)	121.18	121.16	-0.02
				CZ3 - CH2	1.40946	1.40937	-0.000090	α(CZ3-CE3-CD2)	119.30	119.33	0.03
7	-7.2	-6.6	II	H:TYR99							
				CG - CD1	1.39556	1.39527	-0.000290	α(CD1-CG-CD2)	118.05	118.06	0.01
				CG - CD2	1.38966	1.3897	0.000040	α(CG-CD2-CE2)	121.11	121.08	-0.03
				CD1 - CE1	1.39409	1.39499	0.000900	α(CD2-CE2-CZ)	119.59	119.60	0.01
				CD2 - CE2	1.39517	1.39539	0.000220	α(CE2-CZ-CE1)	120.23	120.25	0.02
				CE1 - CZ	1.37854	1.3782	-0.000340	α(CZ-CE1-CD1)	119.64	119.59	-0.05
				CE2 - CZ	1.38939	1.38977	0.000380	α(CE1-CD1-CG)	121.24	121.27	0.03
				CZ - OH	1.37181	1.3714	-0.000410	α(CE1-CZ-OH)	118.89	118.88	-0.01
				HH - OH	0.959771	0.959907	0.000136	α(CZ-OH-HH)	106.98	107.04	0.06

Figure S11. *Compound* ***1*** *Best Binding Mode on CFIXa at Active Site II*

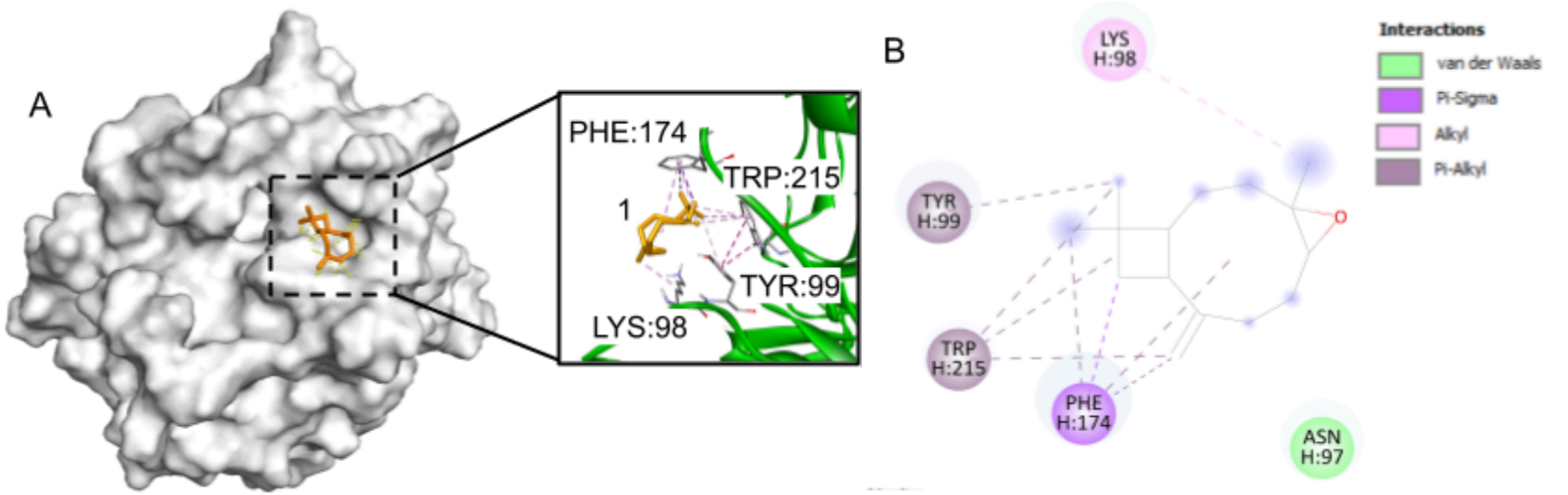


Figure S12. *Compound* ***4*** *Best Binding Mode on CFIXa at Active Site V*

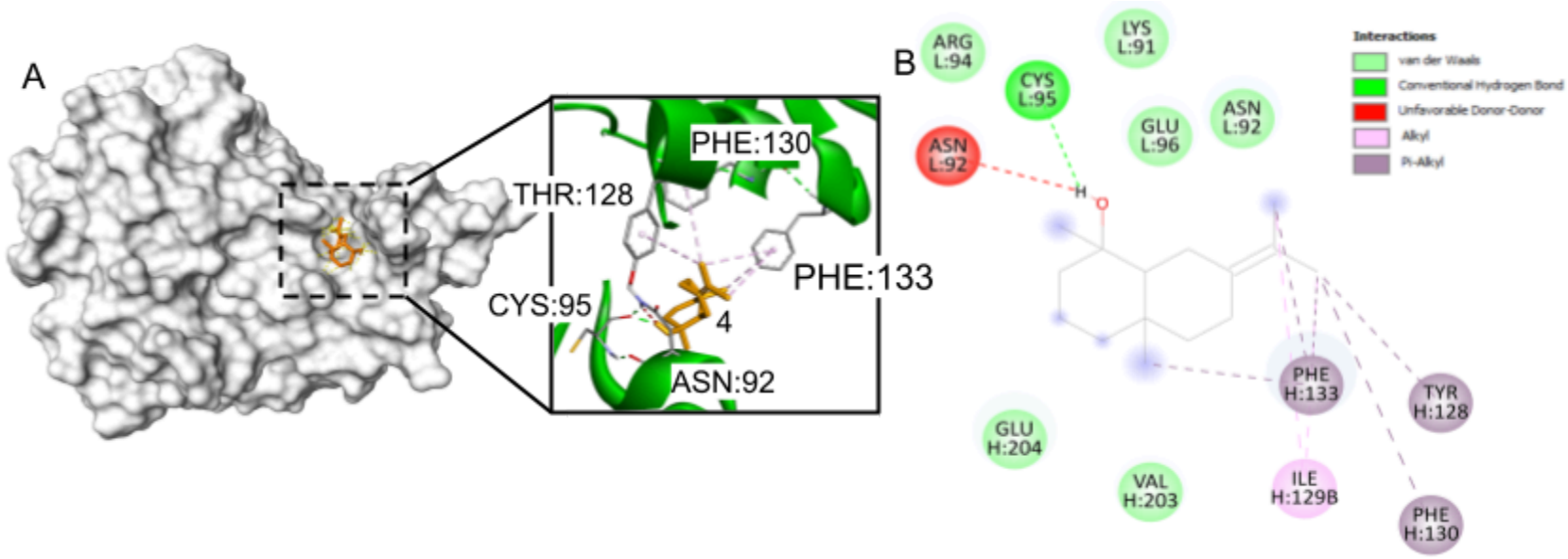


Figure S13. *Compound* ***5*** *Best Binding Mode on CFIXa at Active Site II*

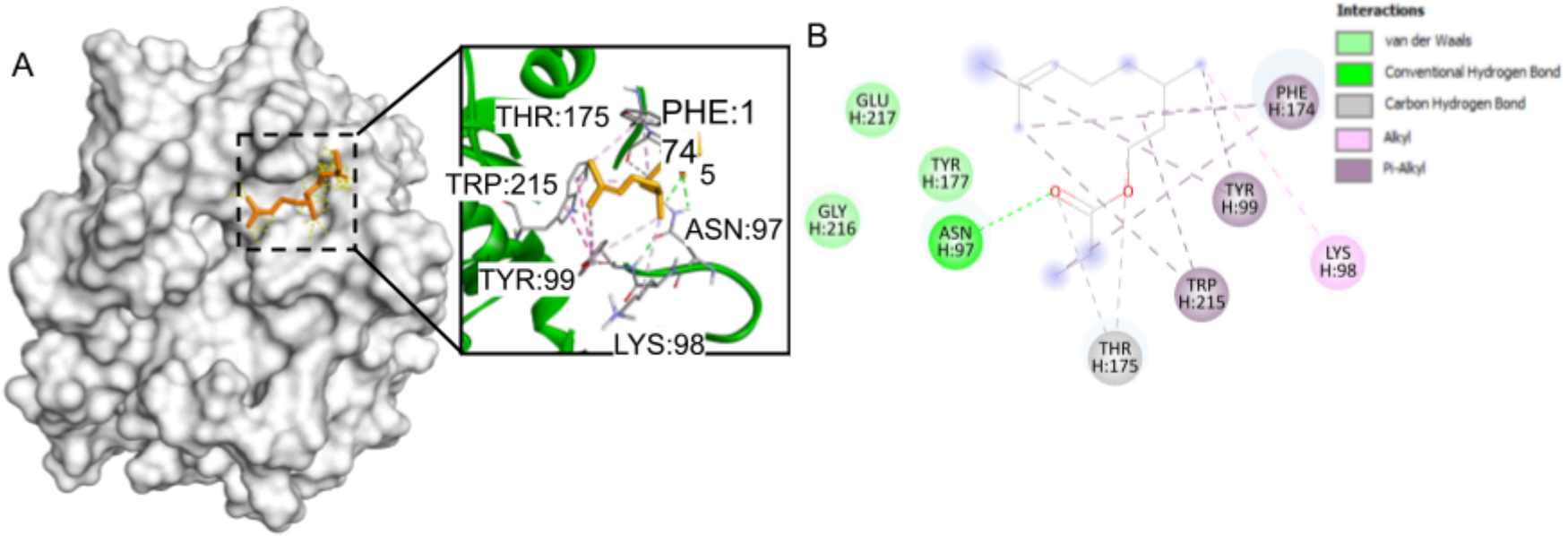


Figure S14. *Compound* ***6*** *Best Binding Mode on CFIXa at Active Site V*