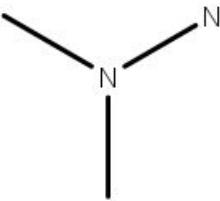
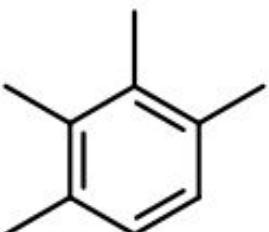
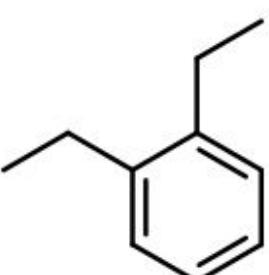
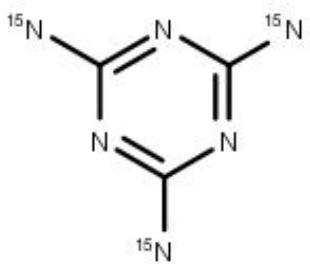
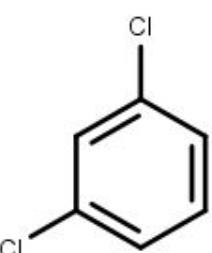


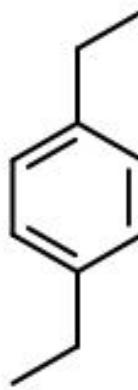
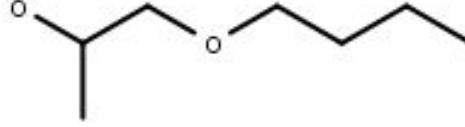
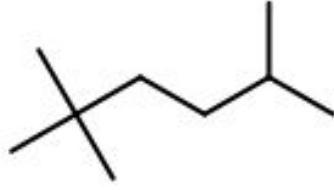
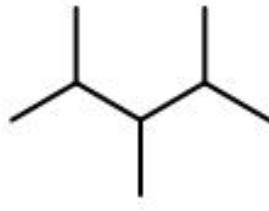
Supplementary Information for

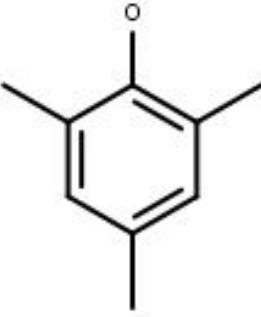
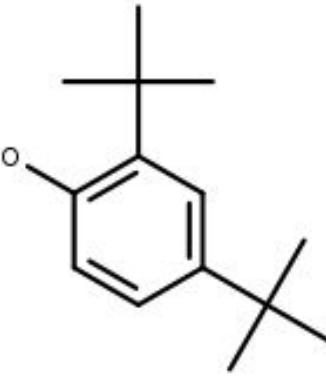
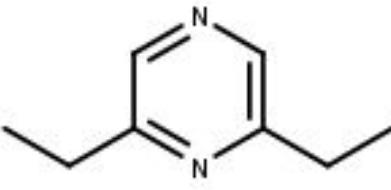
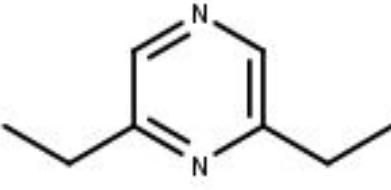
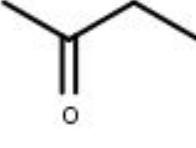
Identification of psychoactive metabolites from *Cannabis sativa*,
its smoke and other phytocannabinoids using machine learning
and multivariate methods

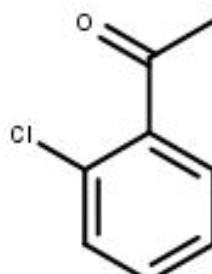
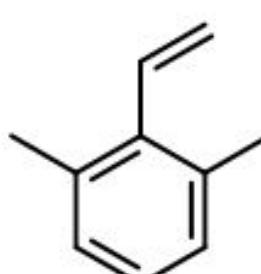
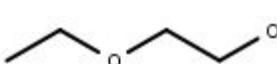
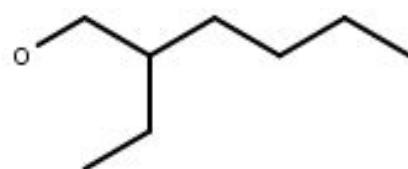
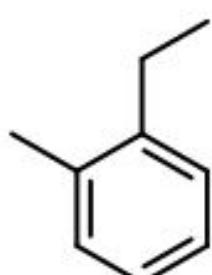
*Ramesh Jagannathan**

International Medical Cannabis Association, Toronto, Ontario, M1S 5E8, CANADA

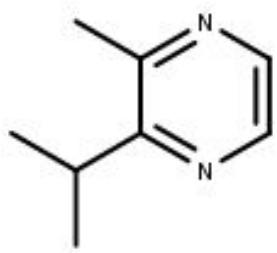
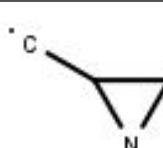
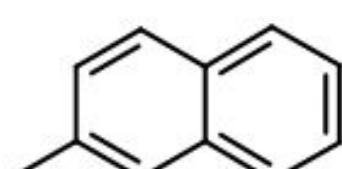
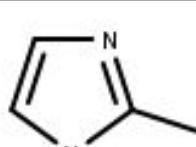
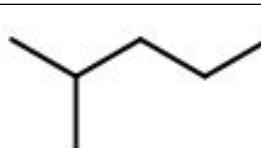
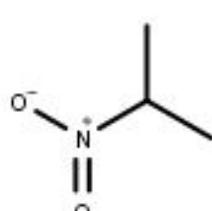
	Metabolite Name	Metabolite Structure
C1	1,1-Dimethylhydrazine	
C2	1,2,3,4-Tetramethylbenzene	
C3	1,2-Diethylbenzene	
C4	1,3,5-Triazine-2,4,6-triamine	
C5	1,3-Dichlorobenzene	

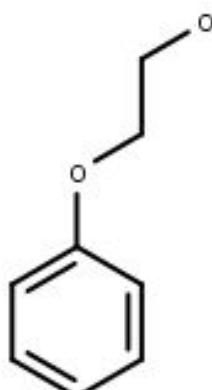
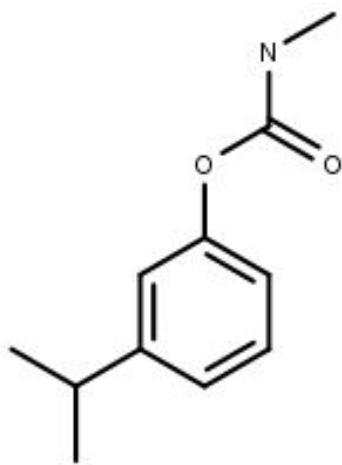
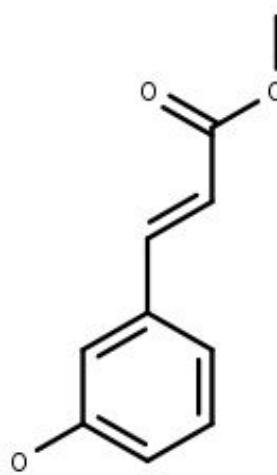
C6	1,4-Diethylbenzene	
C7	1-Butanol	
C8	1-Butoxy-2-Propanol	
C9	Hexan-1-ol	
C10	Undecan-1-ol	
C11	2,2,5-Trimethylhexane	
C12	2,3,4-Trimethylpentane	

C13	2,4,6-Trimethylphenol	
C14	2,4-Ditert-butylphenol	
C15	2,6-Diethylpyrazine	
C16	2,5-Dimethylpyrazine	
C17	Butan-2-one	
C18	2-Butoxyethanol	

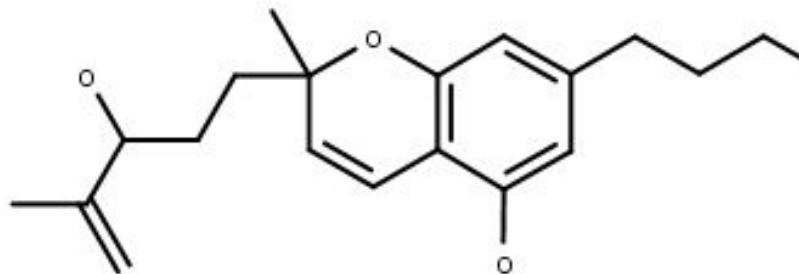
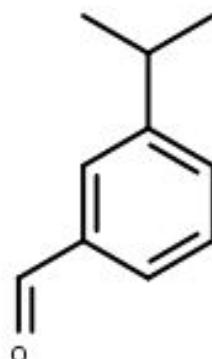
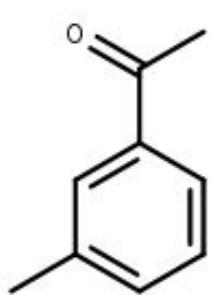
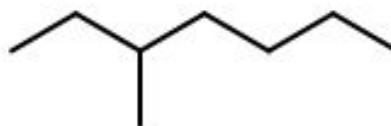
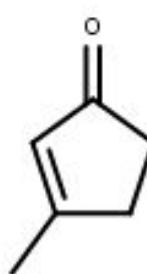
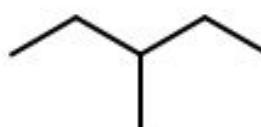
C19	1-(2-Chlorophenyl)Ethenone	
C20	1,3-Dimethyl-2-Vinyl Benzene	
C21	2-Ethoxyethanol	
C22	2-Ethyl-1-hexanol	
C23	2-Ethyl Toluene	

C24	2-Formyl-Delta-9-Tetrahydrocannabinol	
C25	2-Geranyl-5-Hydroxy-3-n-Pentanyl-1,4-Benzoquinone	
C26	2-Heptanone	
C27	2-Hydroxy-Acetophenone	

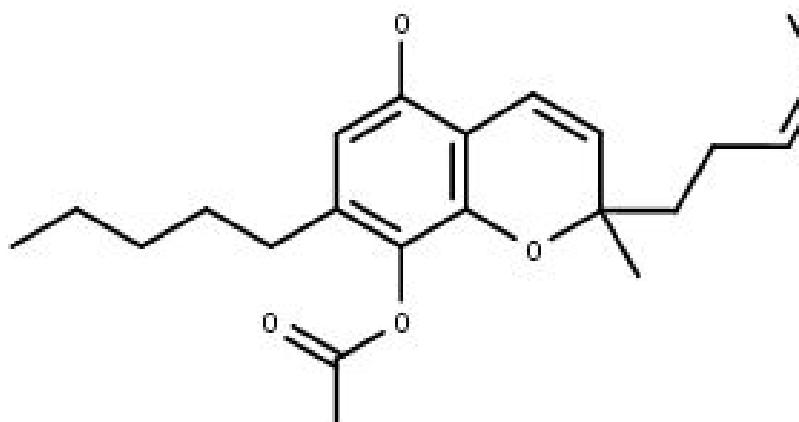
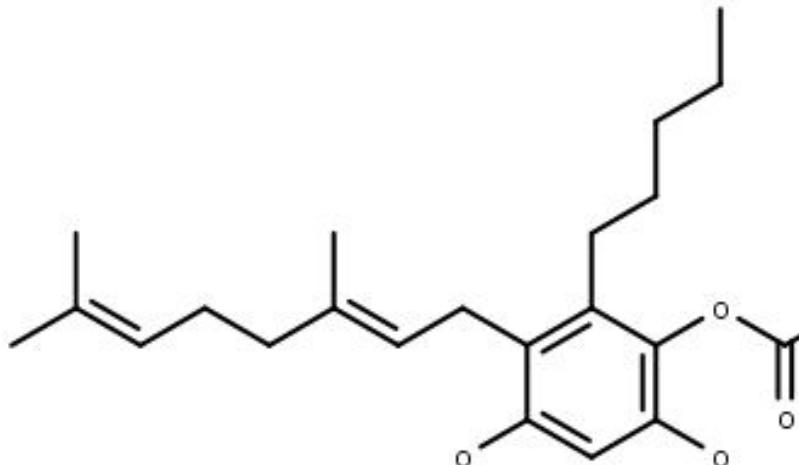
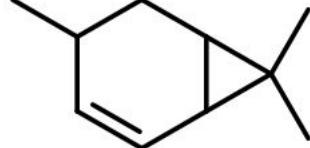
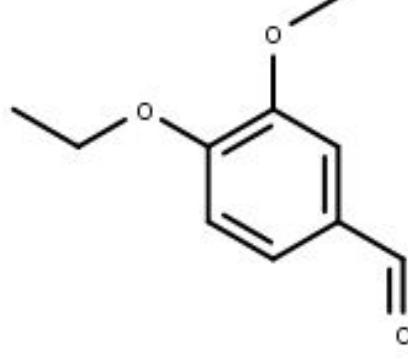
C28	2-Isopropyl-3-methyl-pyrazine	
C29	2-Methylaziridine	
C30	2-Methylnaphthalene	
C31	2-Methyl-1H-imidazole	
C32	2-Methyl-Propanamine	
C33	2-Methylpentane	
C34	2-Nitropropane	

C35	2-Phenoxy Ethanol	
C36	3-(1-Methyl Ethyl)-Phenol Carbamate	
C37	3-(3-Hydroxy Phenyl)-2-Propenoic acid, methyl ester	

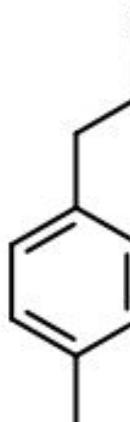
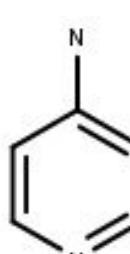
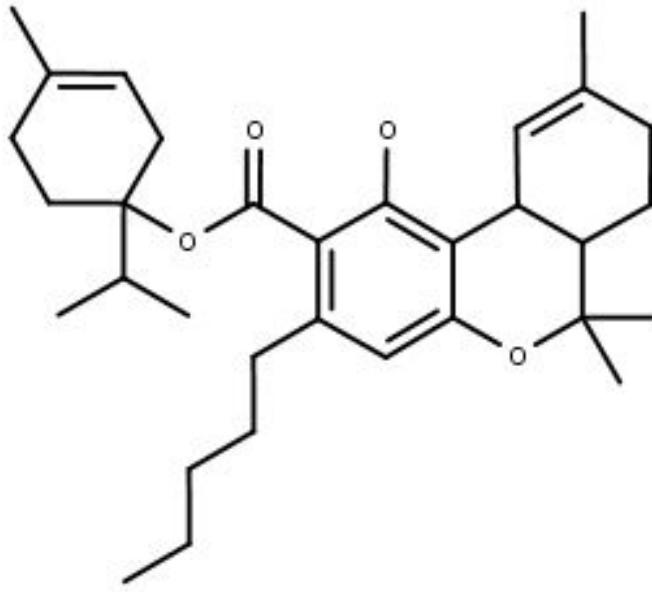
C38	3,4,5,6-Tetrahydro-7-hydroxy-a,a-2-trimethyl-9-n-propyl-2,6-methano-2H-1-Benzoxocin-5-methanol	
C39	3,4,5-Trimethylphenol	
C40	3,4,5-Trimethylhex-1-ene	
C41	3-Ethyl Toulene	
C42	3-Ethyl-O-xylene	

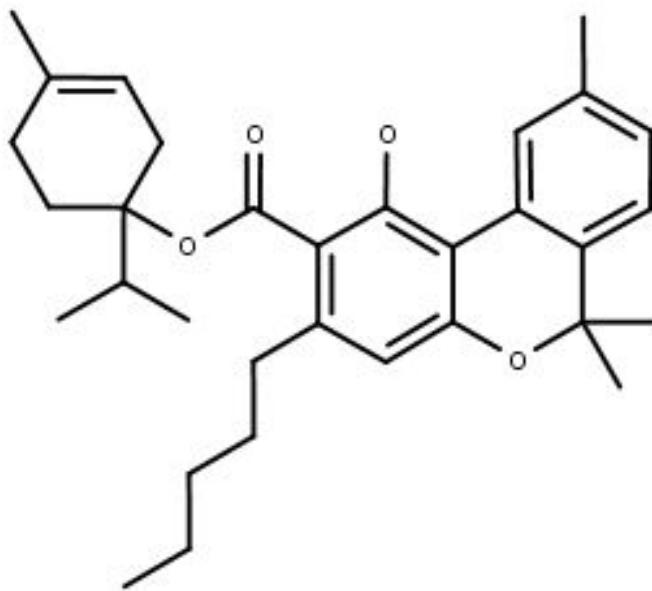
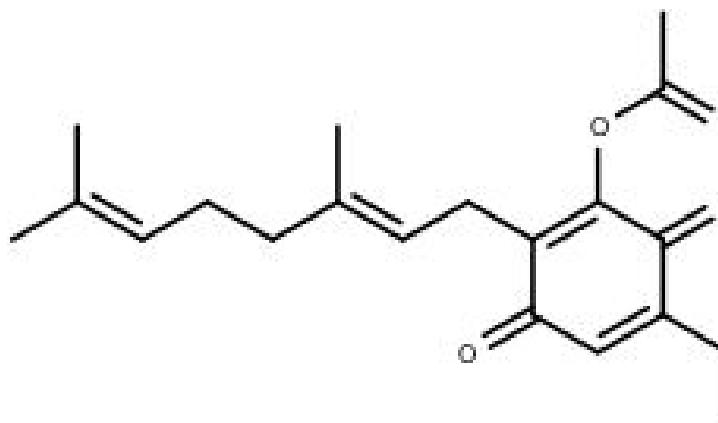
C43	3-Hydroxy-Delta-4,5-Cannabichromene	
C44	3-Isopropyl Benzaldehyde	
C45	3-Methyl Acetophenone	
C46	3-Methyl Heptane	
C47	3-methylcyclopent-2-en-1-one	
C48	3-Methyl Pentane	

C49	3-Methyl-5-(1-Methyl Ethyl)- Phenol Methyl Carbamate	
C50	3-Pentanol	
C51	4,5-Dihydroxy-2,3,6- Trimethoxy-9,10- Dihydrophenanthrene	
C52	4,7-Dimethoxyphenanthrene- 1,2,5-triol	

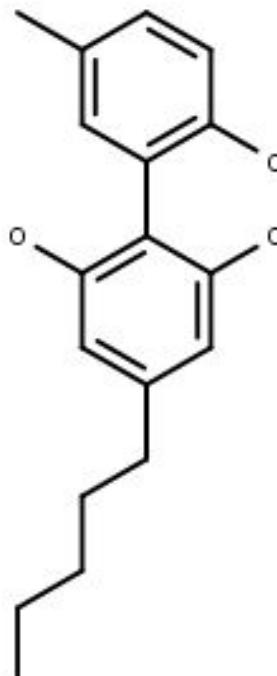
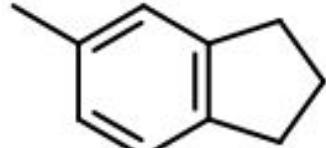
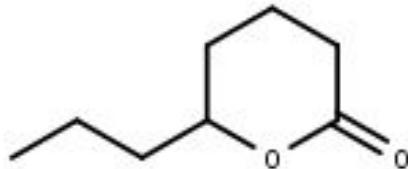
C53	4-Acetoxy Cannabichromene	
C54	4-Acetoxy-2-geranyl-5-hydroxy-3-n-pentylphenol	
C55	4-Carene	
C56	4-Ethoxy-3-anisaldehyde	

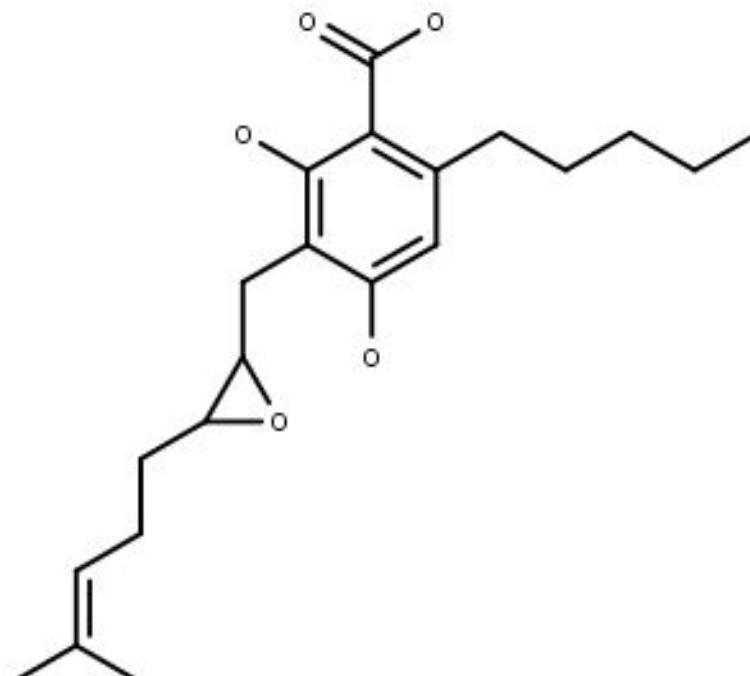
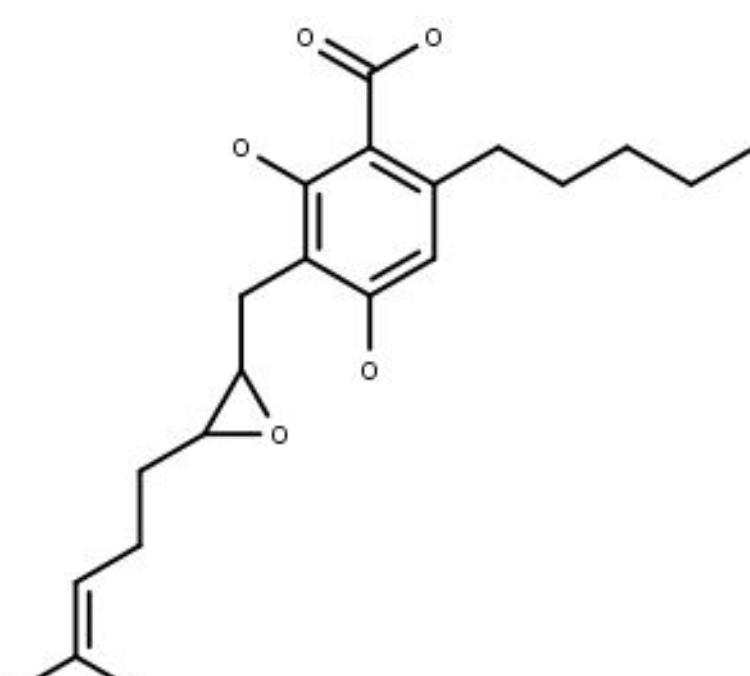
C57	4-Hydroxy-2,3,6,7-tetramethoxy-9,10dihydrophenanthrene	
C58	4-Methoxy-Couramin	
C59	4-Methyl Decane	
C60	4-Methylpyrimidine	
C61	4-Methyl Guaiacol	

C62	4-Methyl Phenyl ethyl amine	
C63	4-Pyridinamine	 CI
C64	4-Terpinal Delta-9-tetrahydrocannabinolate	

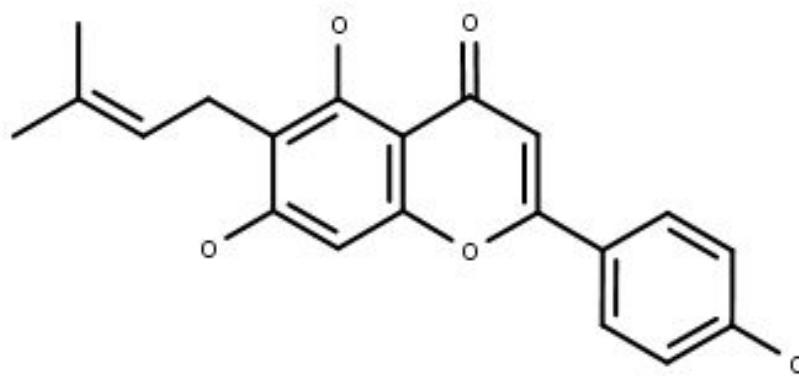
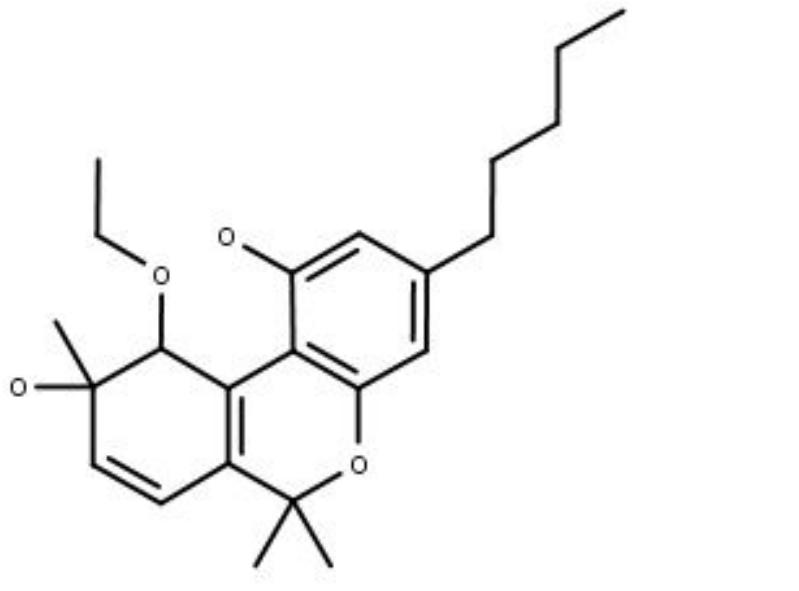
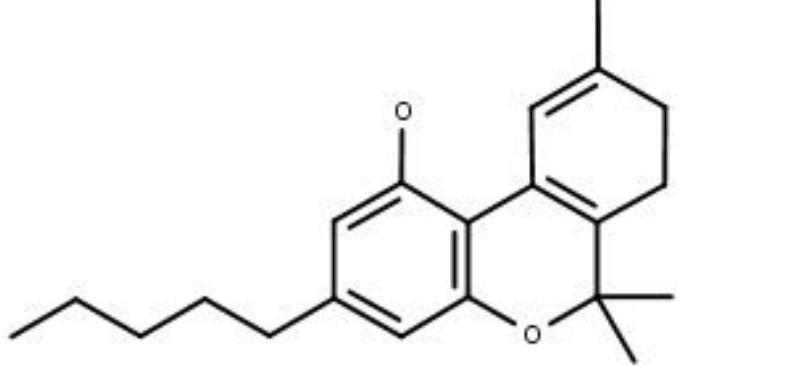
C65	4-Terpenyl Cannabinolate	 The chemical structure shows a 4-terpenyl group (a cyclohexene ring substituted with two isopropyl groups) attached via an ester bond (-COO-) to the 4-position of a cannabinol molecule. The cannabinol core is a bicyclic triterpenoid with a hydroxyl group at the 3-position and a double bond between C2 and C3.
C66	5-Acetoxy-6-Geranyl-3n - Penty1-1,4-Benzoquinone	 The chemical structure shows a geranylgeranyl chain (two farnesyl groups linked by a methylene bridge) attached to the 5-position of a 1,4-benzoquinone molecule. The 1,4-benzoquinone core has a carbonyl group at position 4 and a hydroxyl group at position 5, which is further substituted with an acetyl group (-C(=O)CH ₃) and a pentyl side chain.

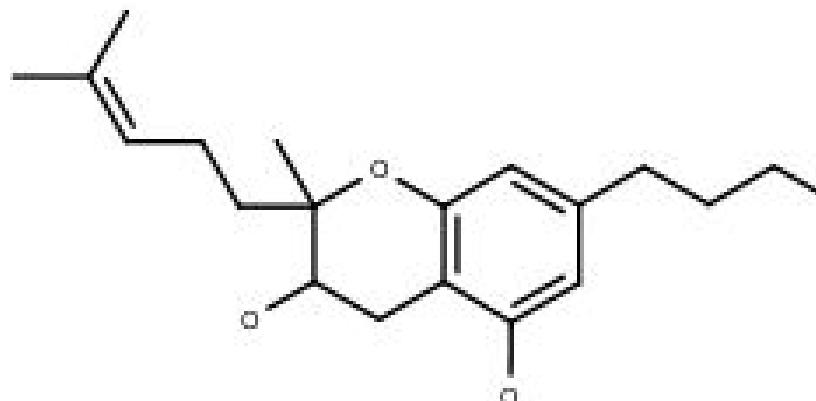
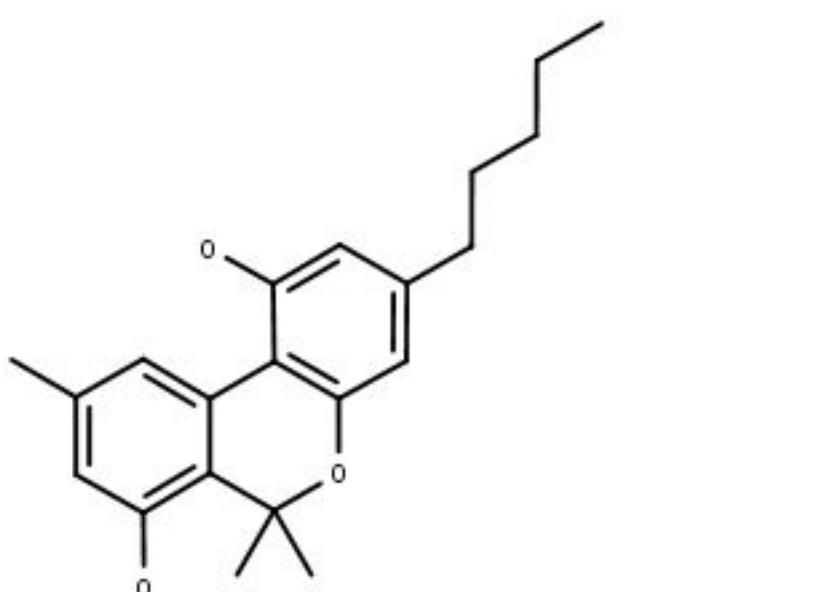
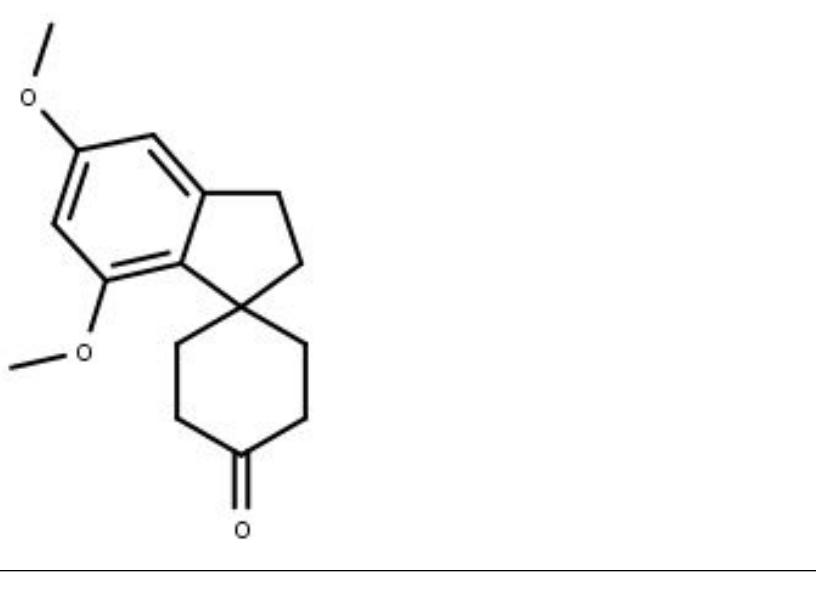
C67	5-Acetyl-4-Hydroxycannabigerol	
C68	5-Ethenyl-2-Methylpyridine	
C69	5-Methoxy Cannabigerolic acid	

C70	5-Methyl-4-Pentyl-Biphenyl-2,2,6-Triol	
C71	5-Methylindane	
C72	5-Octanolide	

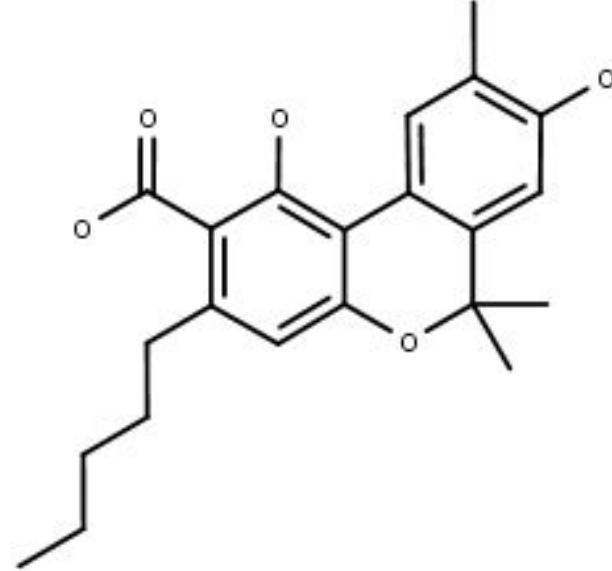
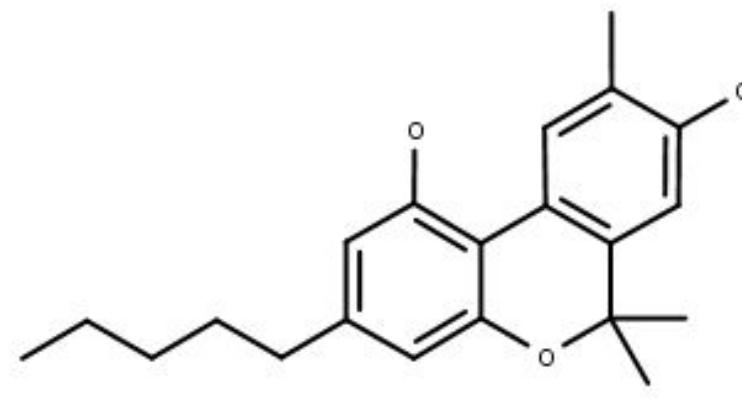
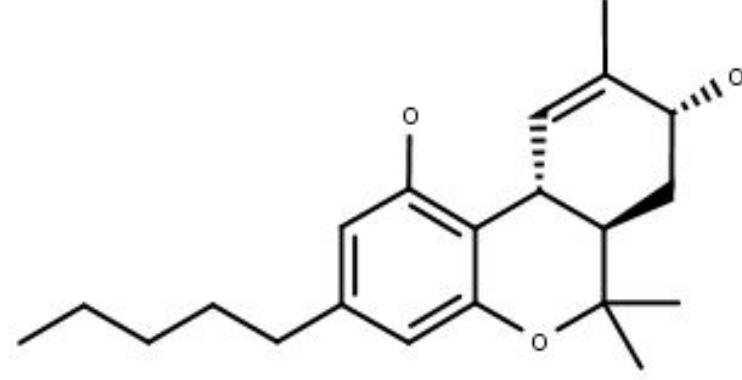
C73	6,7-cis -Epoxycannabigerol	
C74	6,7-cis-Epoxycannabigerolic acid	

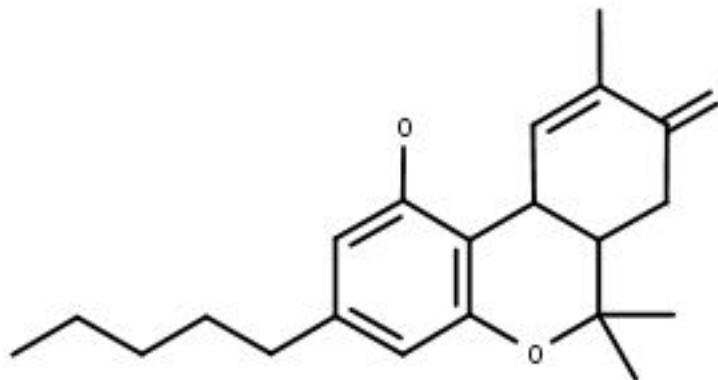
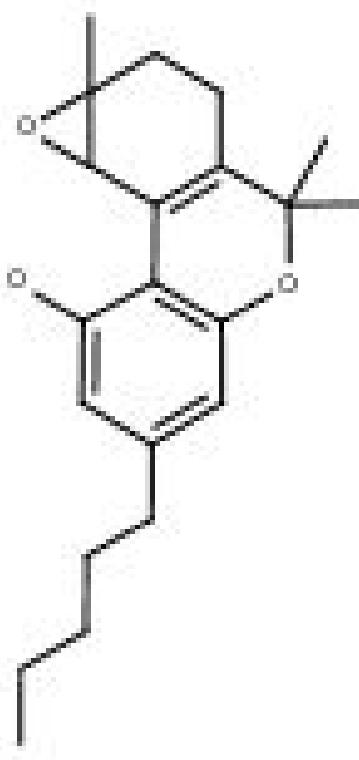
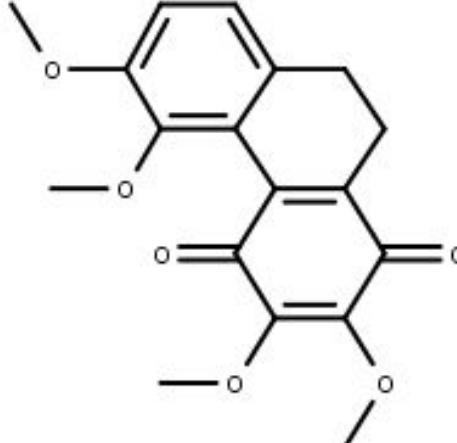
C75	6a-R-Cannabichromanone B	
C76	6a-R-Cannabichromanone C	
C77	6-Metiltetrapterol A	

C78	6-Prenylapigenin	
C79	7,8-Dehydro-10-O-ethylcannabidiol	
C80	7,8-Dihydrocannabinol	

C81	7-Hydroxy Cannabichromane	
C82	7-Hydroxy cannabinol	
C83	7-Methoxy Cannabispiranone	

C84	7-R-Cannabicusmarononic acid	
C85	8,9-Dihydroxy-delta-6a-tetrahydrocannabinol	

C86	8-Hydroxy cannabinolic acid	
C87	8-Hydroxyl cannabinol	
C88	8a-Hydroxy-Delta-9-tetrahydrocannbinol	

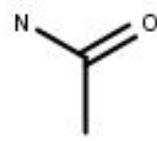
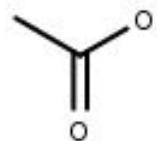
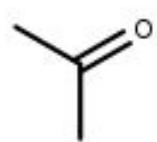
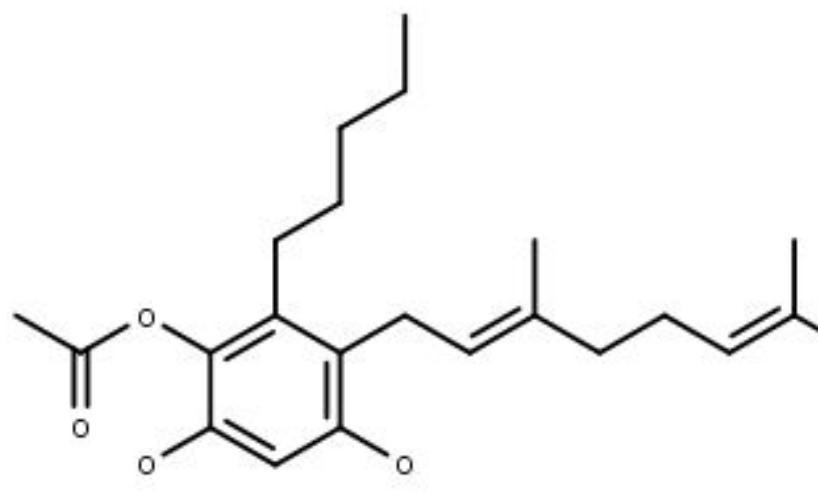
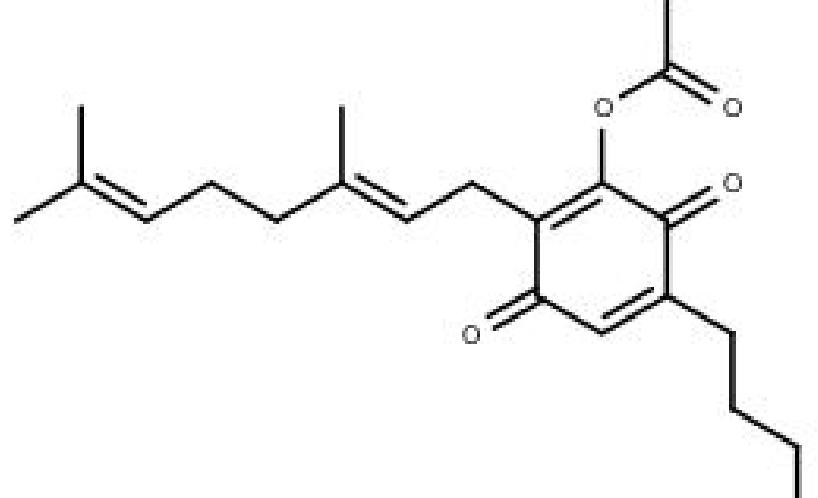
C89	8-oxo-Delta-9-tetrahydrocannbinol	
C90	9,10-Anhydrocannabitriol	
C91	9,10-Dihydro-2,3,5,6-Tetramethoxyphenanthrene-1,4-dione	

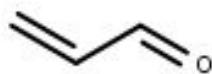
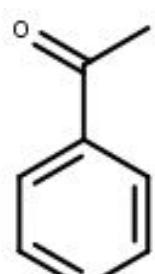
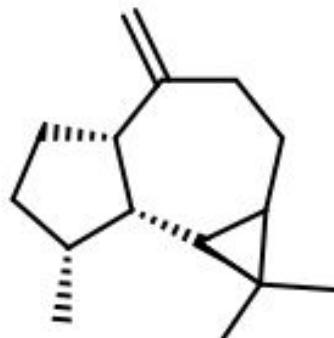
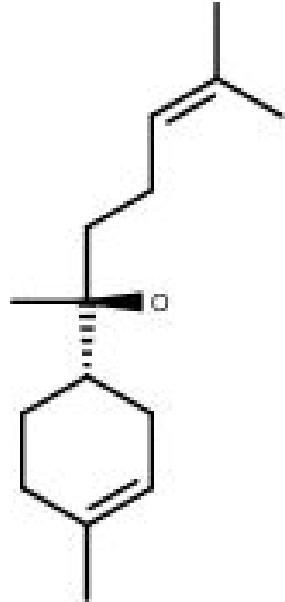
C92	$9\beta,10\beta$ -Epoxyhexahydrocannabinol	
C93	10α -Hydroxy-Delta-9,11-Hexahydrocannabinol	

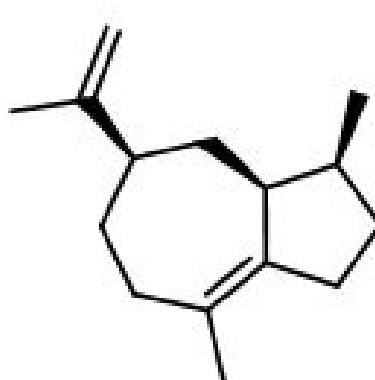
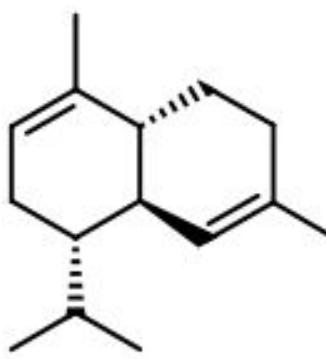
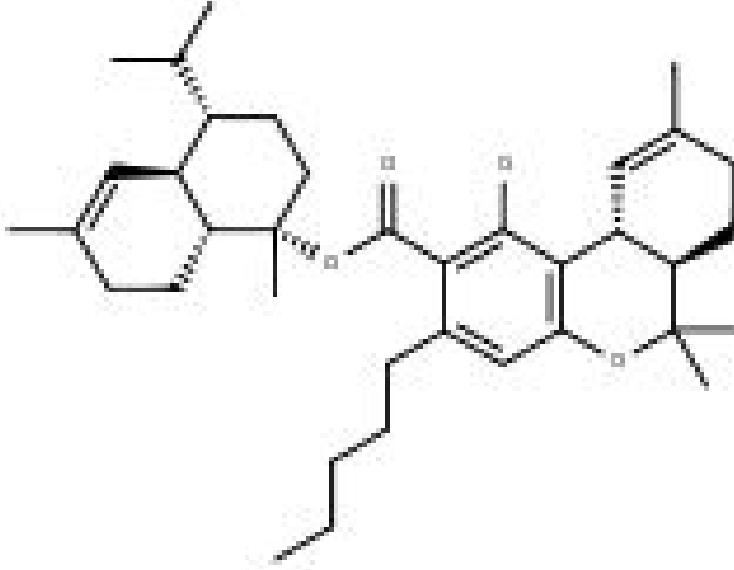
C94	10-Ethoxy-9-hydroxy-delta-6a-Tetrahydrocannabinol	
C95	10-Hydroxy-9-oxo-Delta-8-Tetrahydrocannabinol	
C96	10-O-Ethyl bis-nor Cannabidiol	

C97	10-Oxo-delta-6a-Tetrahydrocannabinol (OTHC)	
C98	11-Acetoxy-Delta-8-Tetrahydrocannbinoic acid	

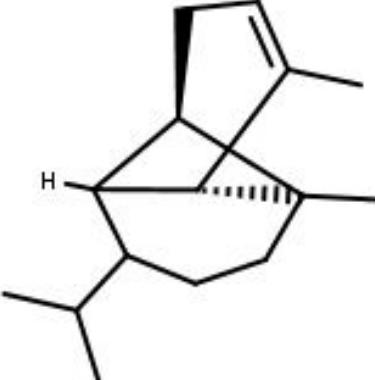
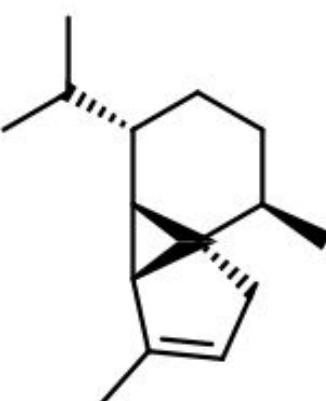
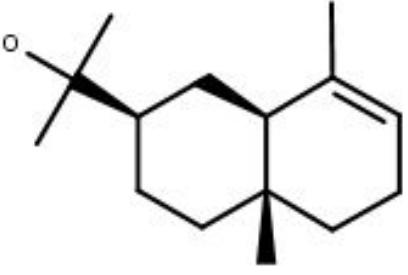
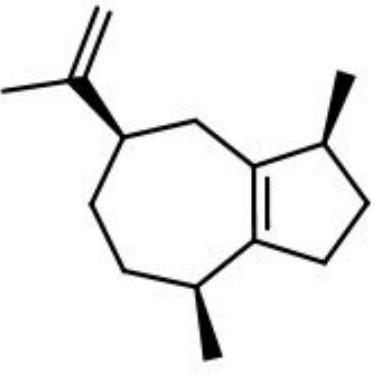
C99	11-Acetoxy-Delta- 9 - Tetrahydrocannabinolic acid A	
C100	Abnormal Cannabigerol	
C101	Acetaldehyde	

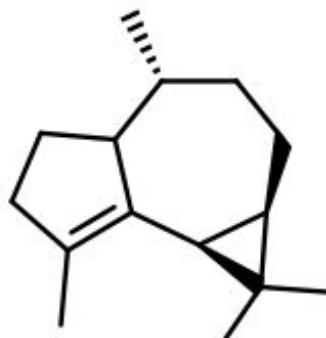
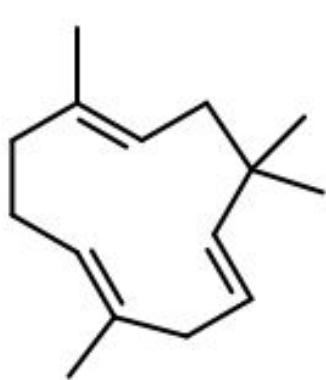
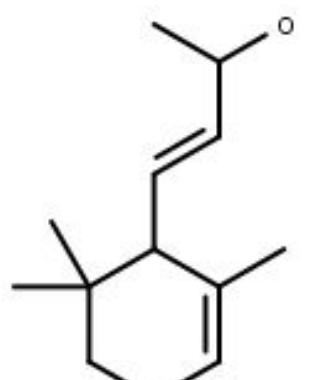
C102	Acetamide	
C103	Acetic acid	
C104	Acetone	
C105	Acetyl abnormal hydrocannabigerolquinol	
C106	Acetyl cannabigerolquinol	

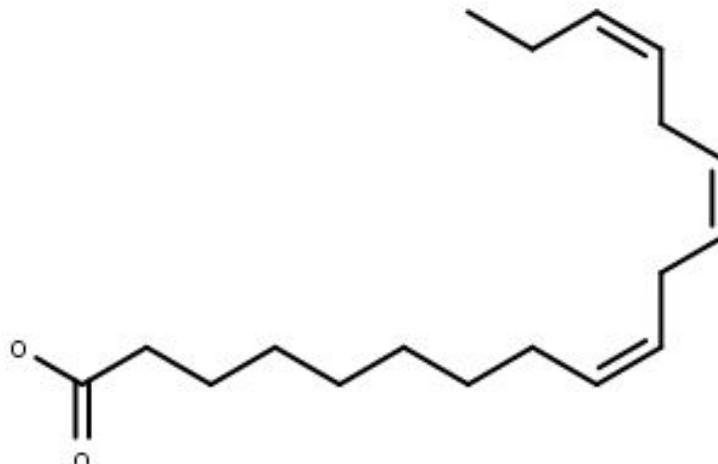
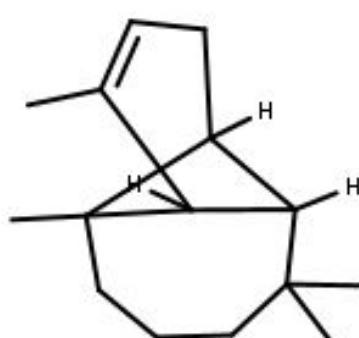
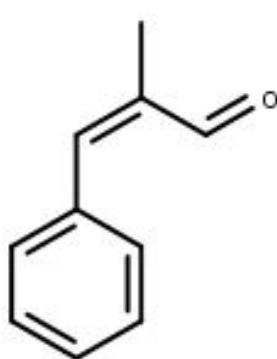
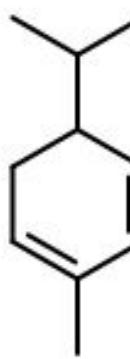
C107	Acrolein	
C108	Acetophenone	
C109	Alloaromadendrene	
C110	Alpha-Bisabolol	

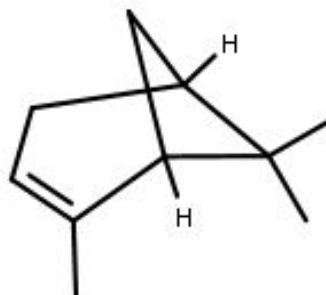
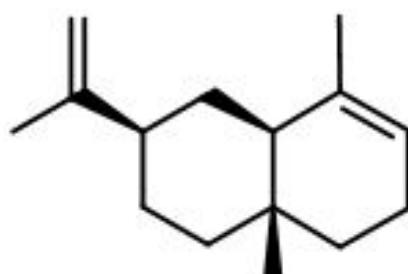
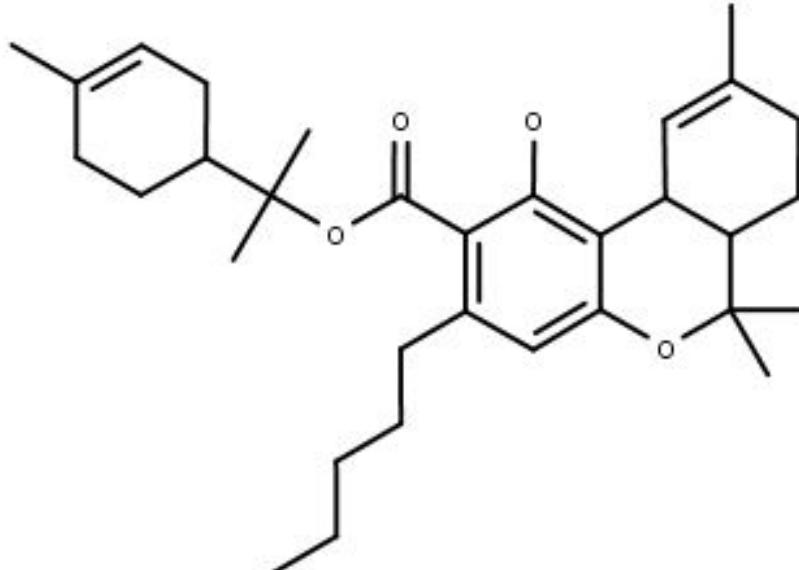
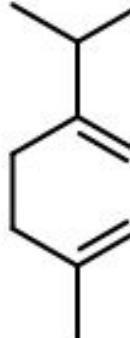
C111	α -Bulnescene	
C112	α -Cadinene	
C113	α -Cadinyl Delta-9-tetrahydrocannabinolate	

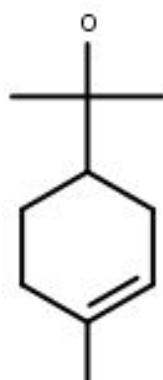
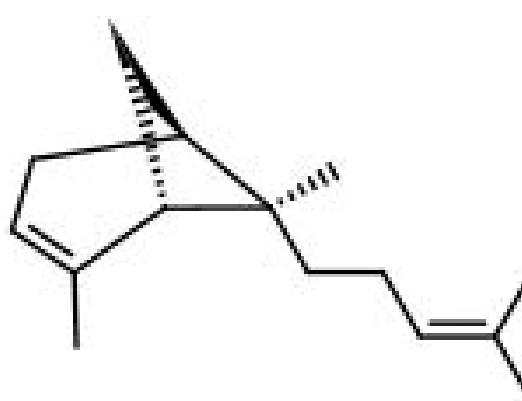
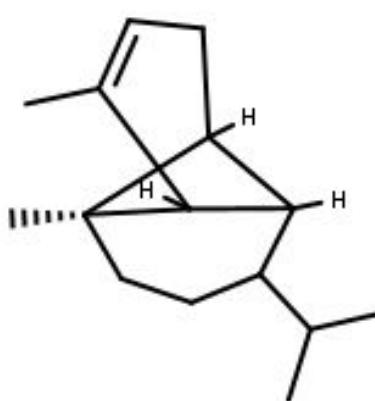
C114	Alpha-Cannabispiranol	
C115	Alpha-Cedrene	
C116	Alpha-Cis-Bergamotene	

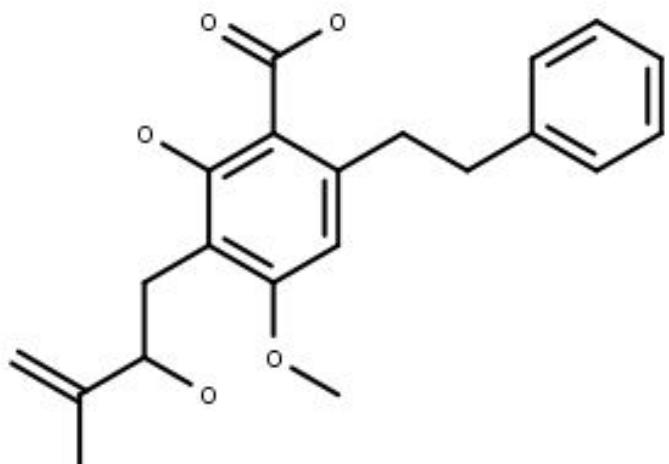
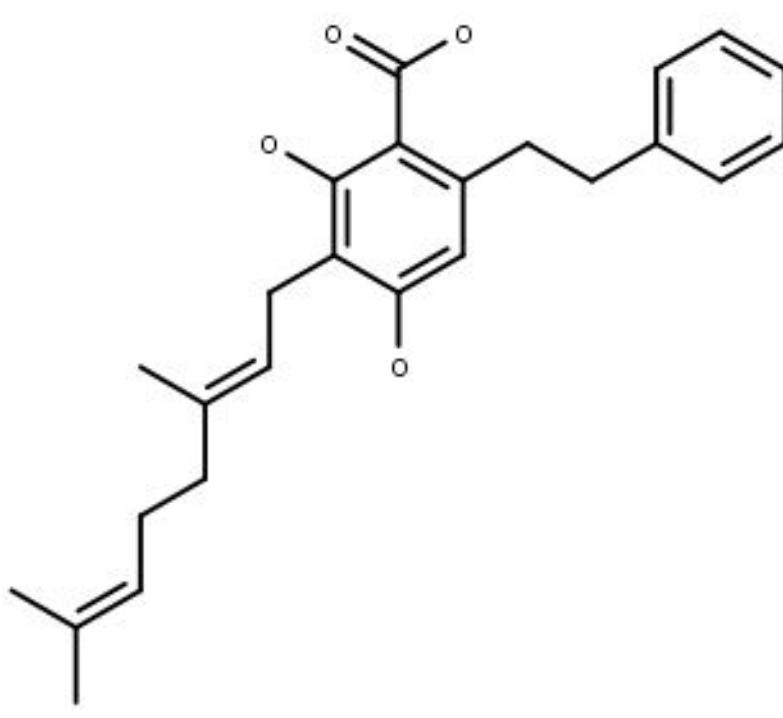
C117	Alpha- Copaene	
C118	Alpha-Cubebene	
C119	Alpha-Eudesmol	
C120	Alpha-Guaiene	

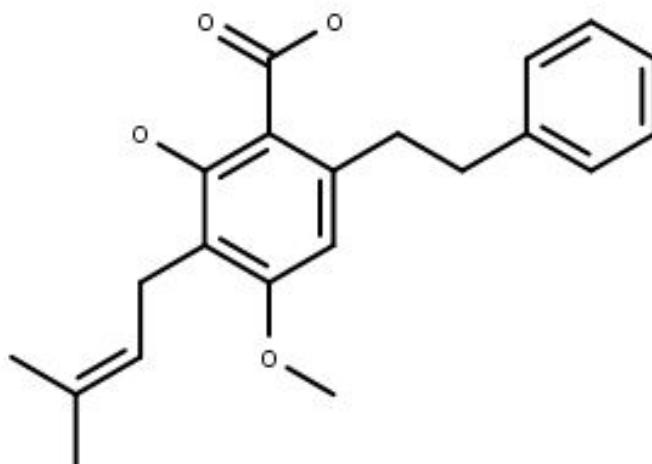
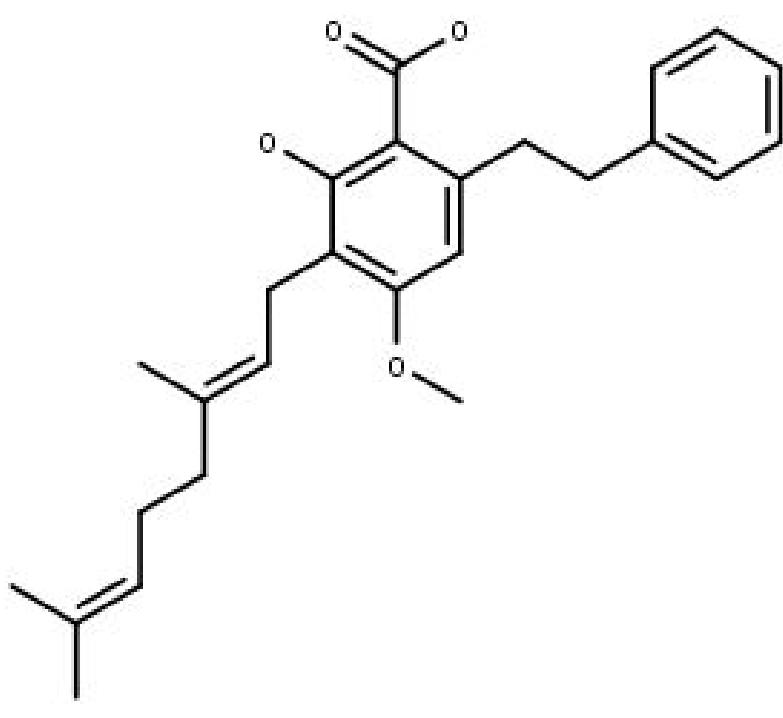
C121	Alpha-Gurjunene	
C122	Alpha-Humulene	
C123	Alpha-Ionol	

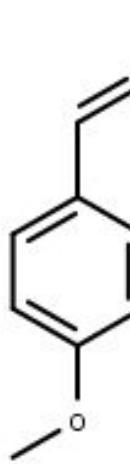
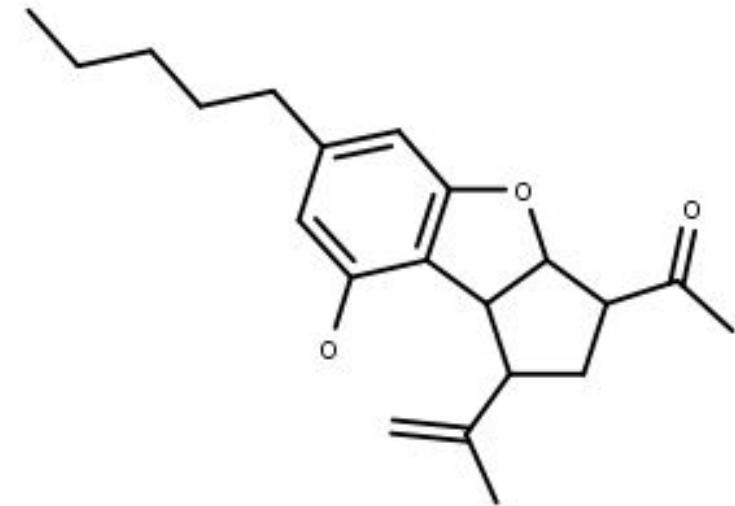
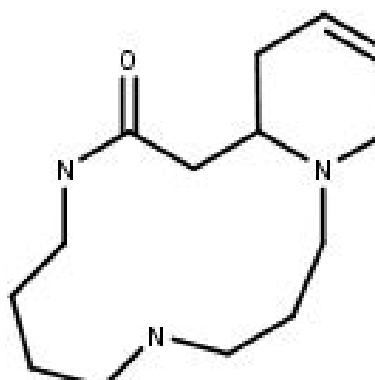
C124	Alpa-Linilenic acid	
C125	Alpha-Longipinene	
C126	Alpha-Methyl-Cinnamaldehyde	
C127	Alpha-Phellandrene	

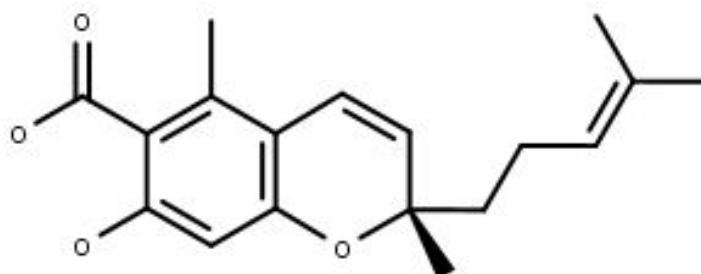
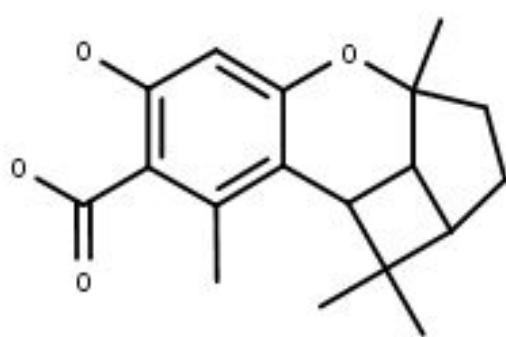
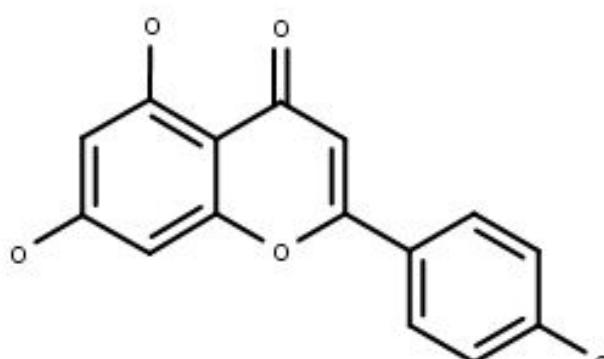
C128	Alpha-Pinene	
C129	Alpha-Selinene	
C130	Alpha-Terpinyl Delta-9-tetrahydrocannabinolate	
C131	Alpha-Terpinene	

C132	Alpha-Terpineol	
C133	Alpha-Thujene	
C134	Alpha-Trans-Bergamotene	
C135	Alpha-Ylangene	

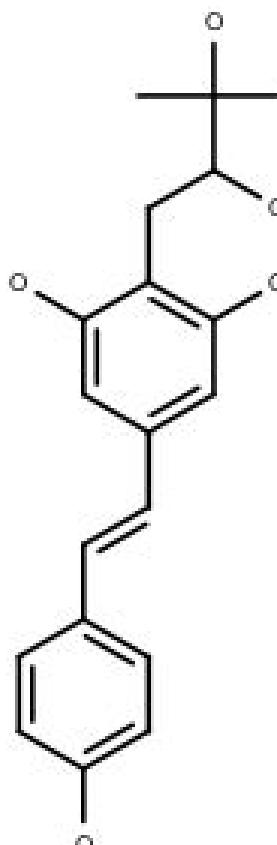
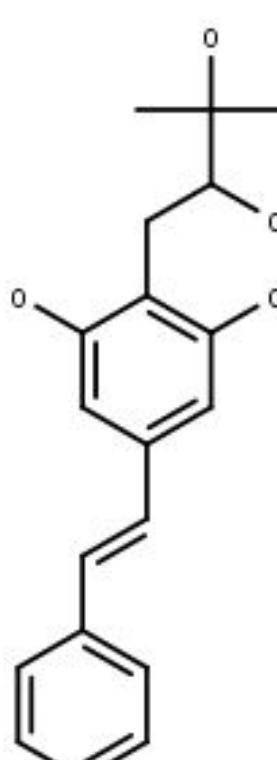
C136	Amorfrutin-3	
C137	Amorfrutin-4	

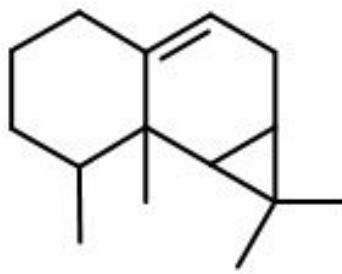
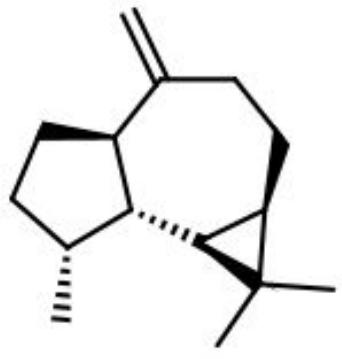
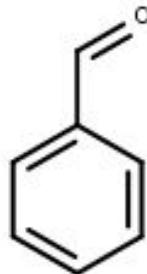
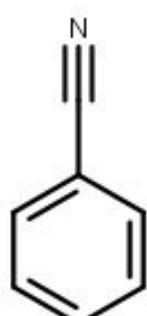
C138	Amorfrutin-A	
C139	Amorfrutin-B	

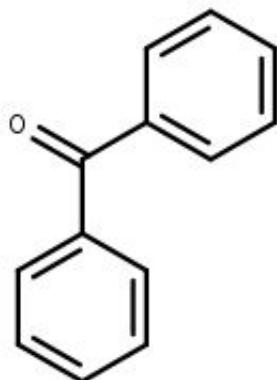
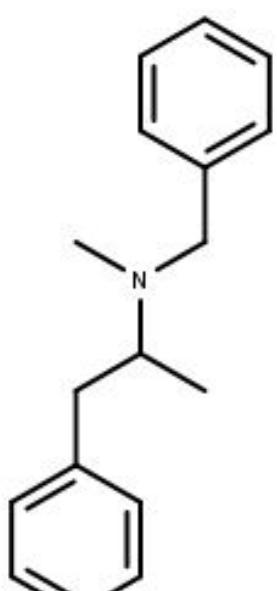
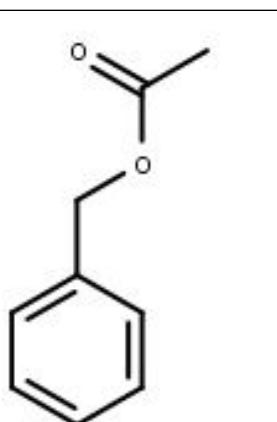
C140	Anethole	
C141	Anhydrocannabimovone	
C142	Anhydrocannabisativine	

C143	Anthopogochromenic acid	
C144	Anthopogocyclolic acid	
C145	Apigenin	

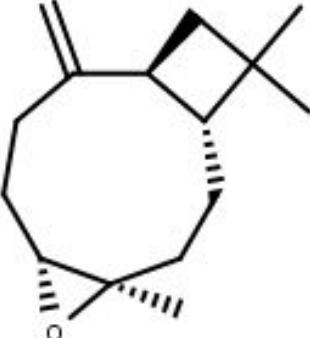
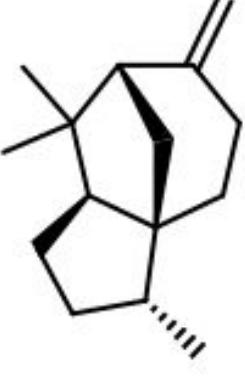
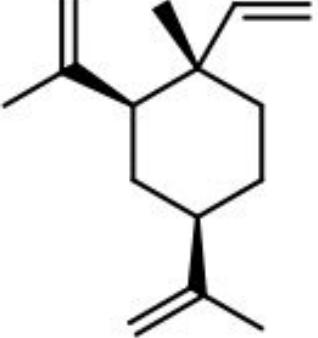
C146	Arachidin-3	
C147	Araphyn-1	

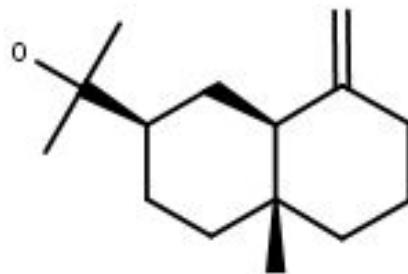
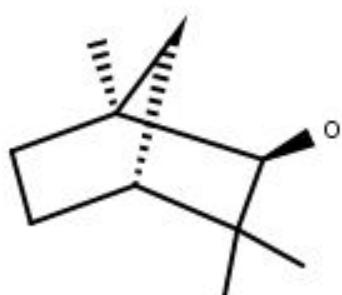
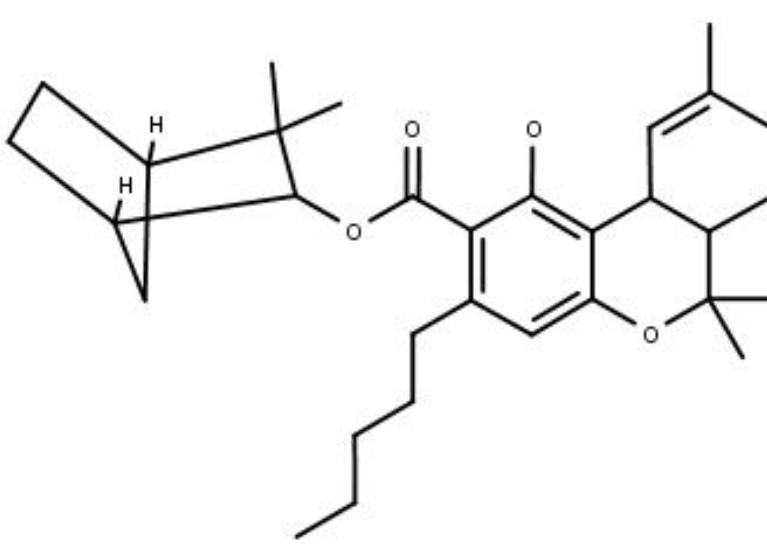
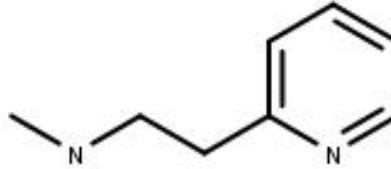
C148	Araphyn-3	
C149	Araphyn-4	

C150	Aristolene	
C151	Aromadendrene	
C152	Benzaldehyde	
C153	Benzonitrile	

C154	Benzophenone	
C155	Benzphetamine	
C156	Benzyl acetate	

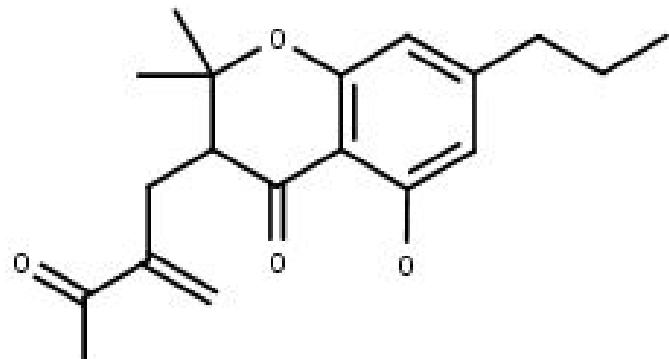
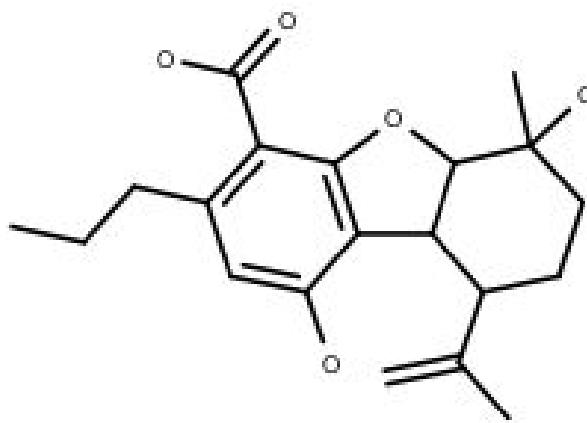
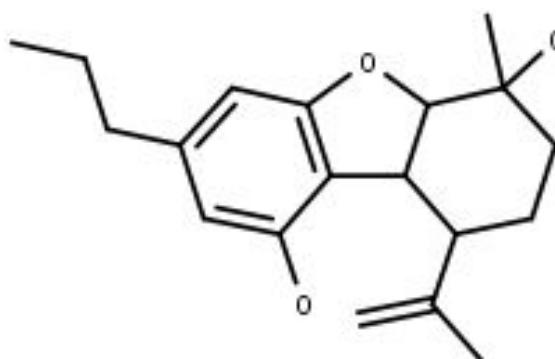
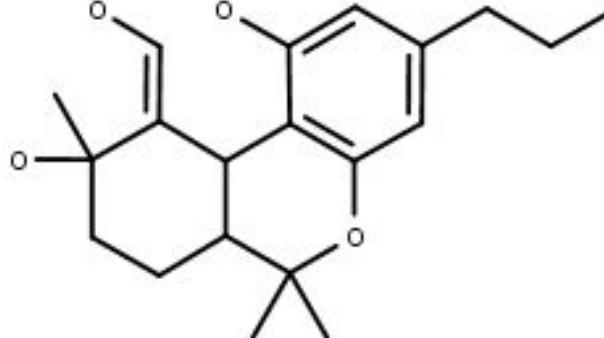
C157	Benzyl Alcohol	
C158	Benzyl formate	
C159	Benzyl Nitrile	
C160	Beta-Cannabispiranol	

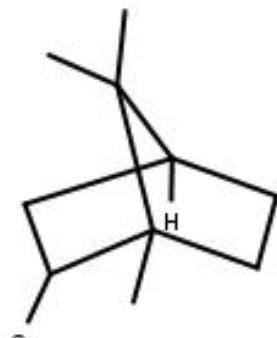
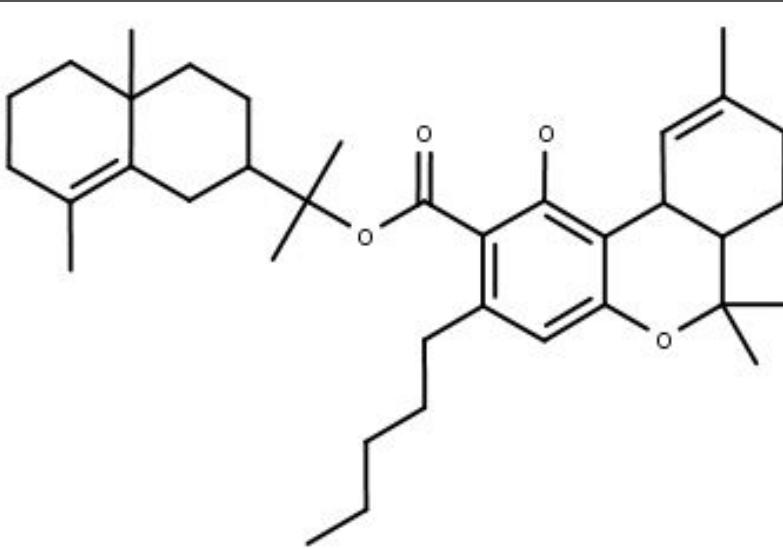
C161	Beta-Caryophyllene oxide	
C162	Beta-Caryophyllene	
C163	Beta-Cedrene	
C164	Beta-Elemene	

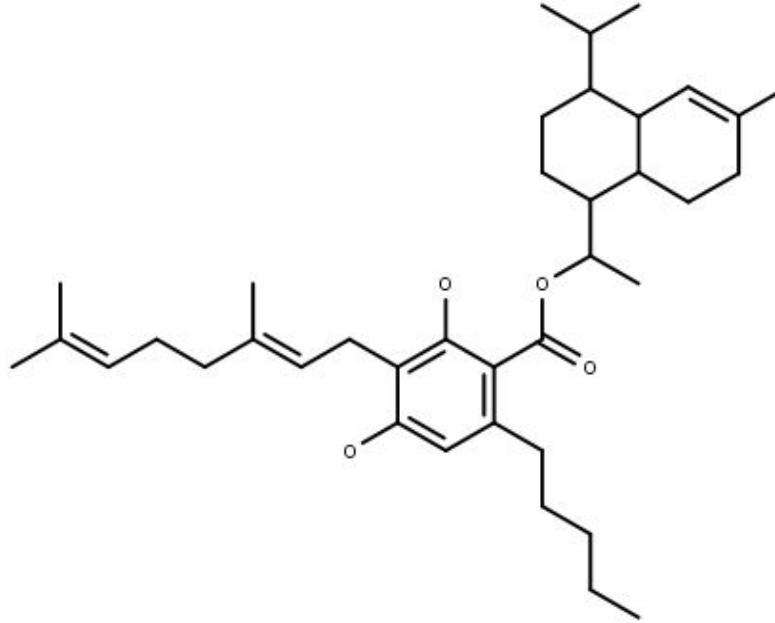
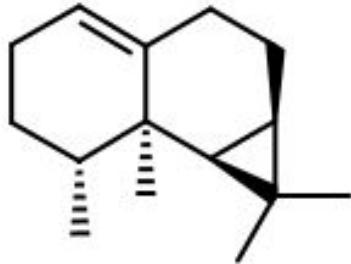
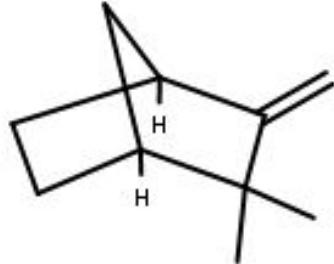
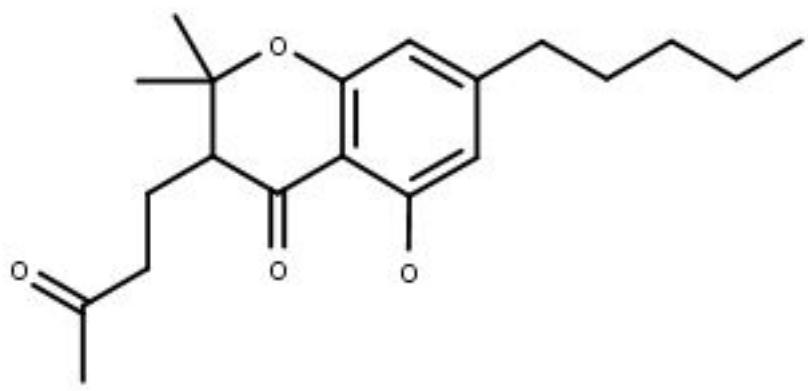
C165	Beta-Eudesmol	
C166	Beta-fenchol (Beta-Fenchyl Alcohol)	
C167	Beta-Fenchyl-Delta-9-tetrahydrocannabinolate	
C168	Betahistidine	

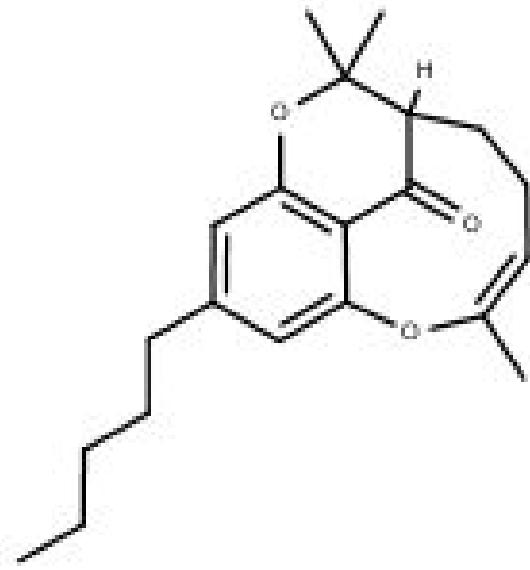
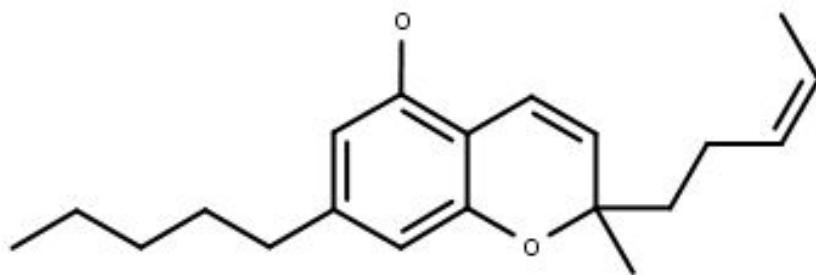
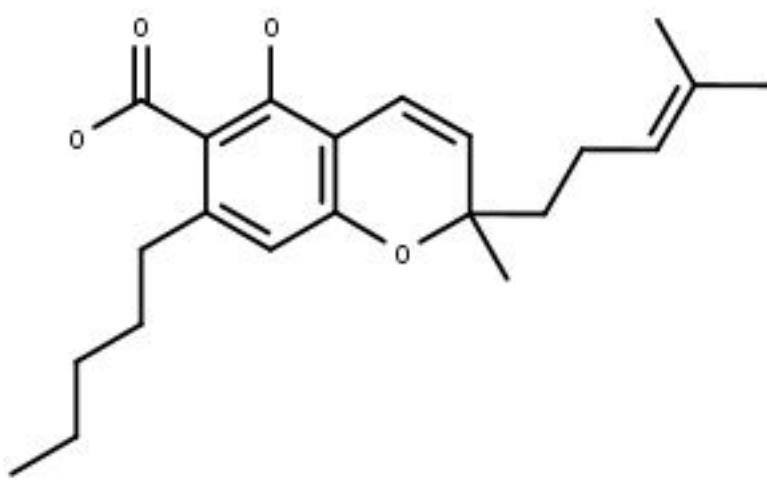
C169	Beta-Irone	
C170	Beta-phellandrene	
C171	Beta-Pinene	
C172	Beta-Selinene	

C173	β -sitosteryl-3-O- β -D-glucopyranoside-2'-O-palmitate	<p>The structure shows a branched 26-carbon palmitoyl chain (C173) attached to the C2' position of a glucose moiety. The glucose is attached to the C3 position of a sitosterol molecule. The palmitoyl chain has a terminal methyl group and a double-bonded carbonyl group.</p>
C174	Betazole	<p>The structure is a 1,2-dihydroimidazole derivative. It consists of a five-membered imidazole ring fused to a four-membered pyrrolidine ring. The nitrogen atoms are labeled 'N'.</p>

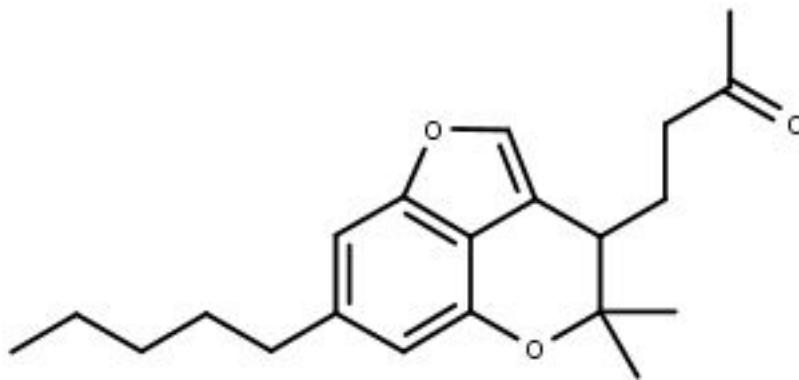
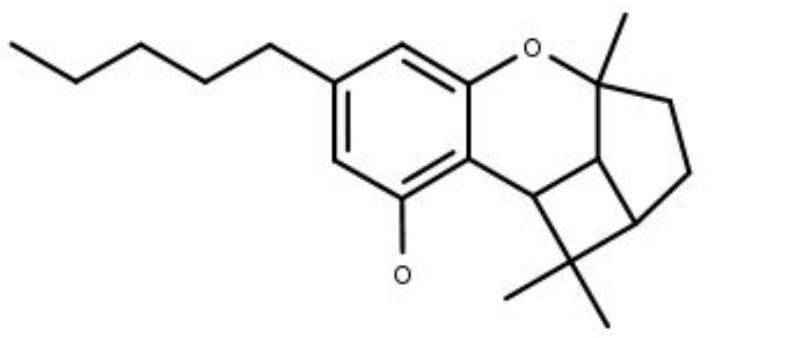
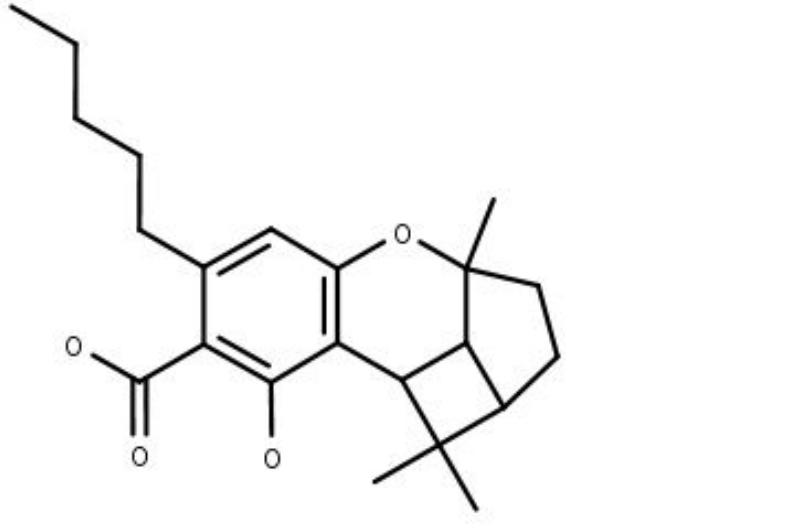
C175	Bis-nor-cannabichromanone	
C176	Bis-nor-cannabielsoic acid B	
C177	Bis-nor-cannabielsoin	
C178	Bis-nor-cannabitriol	

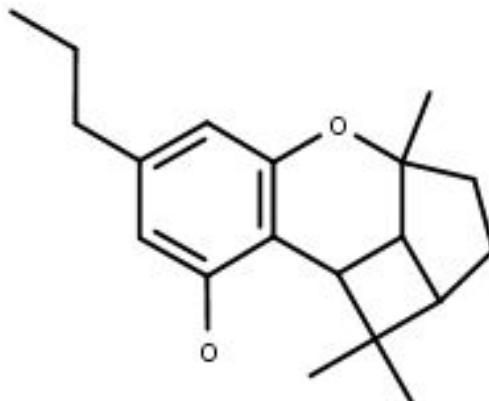
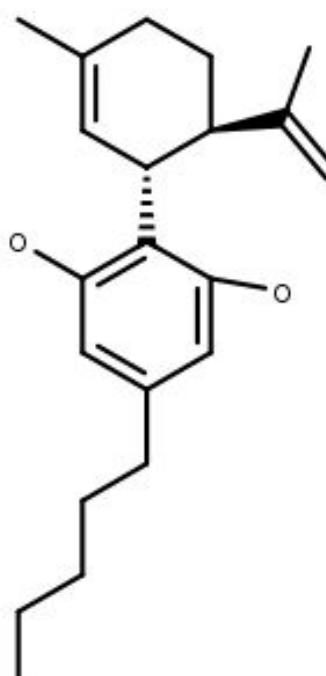
C179	Borneol	
C180	Bornyl Delta-9-tetrahydrocannabinolate	
C181	Butane	
C182	Butyl formate	

C183	Gamma-Cadinyl Cannabigerolate	
C184	Calarene	
C185	Camphene	
C186	Cannabichromanone (CBCF)	

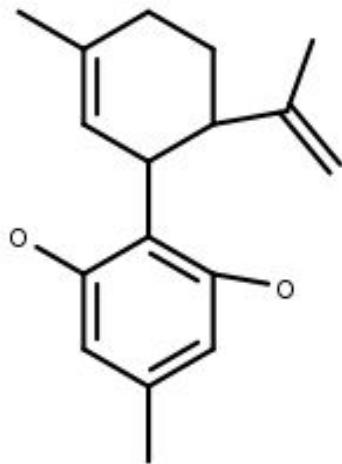
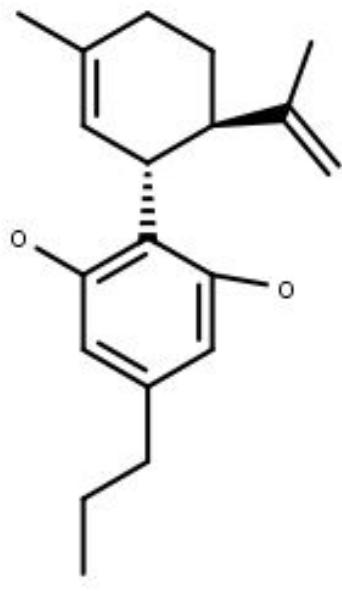
C187	Cannabichromonaonone D	
C188	Cannabichromene (CBC)	
C189	Cannabichromenic acid (CBCA)	

C190	Cannabichromevarin (CBCV)	
C191	Cannabichromevarinic acid (CBCVA)	
C192	Cannabicitran	

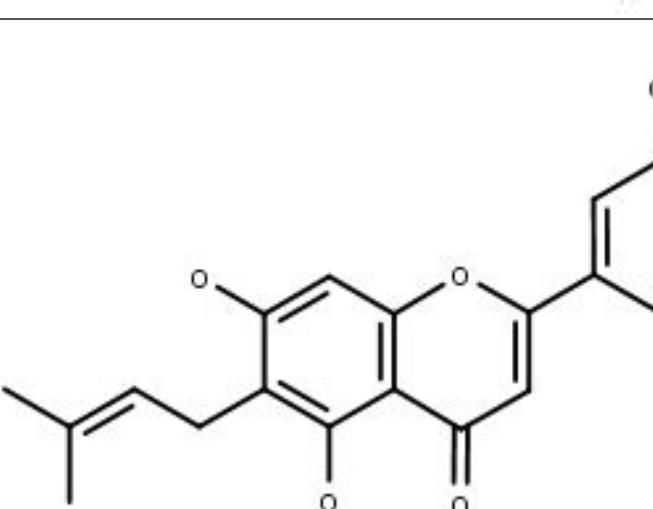
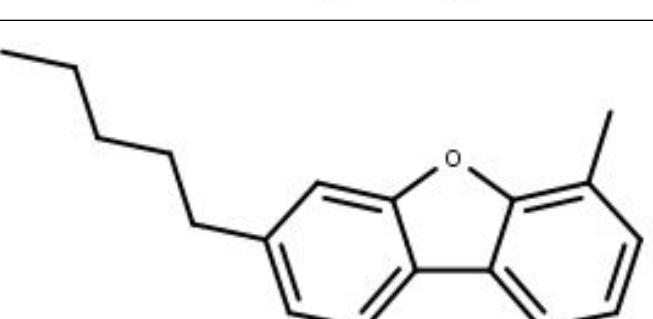
C193	Cannabicaumaronone	
C194	Cannabicyclol (CBL)	
C195	Cannabicyclolic acid (CBLA)	

C196	Cannabicyclovarin (CBLV)	
C197	Cannabidiol (CBD)	

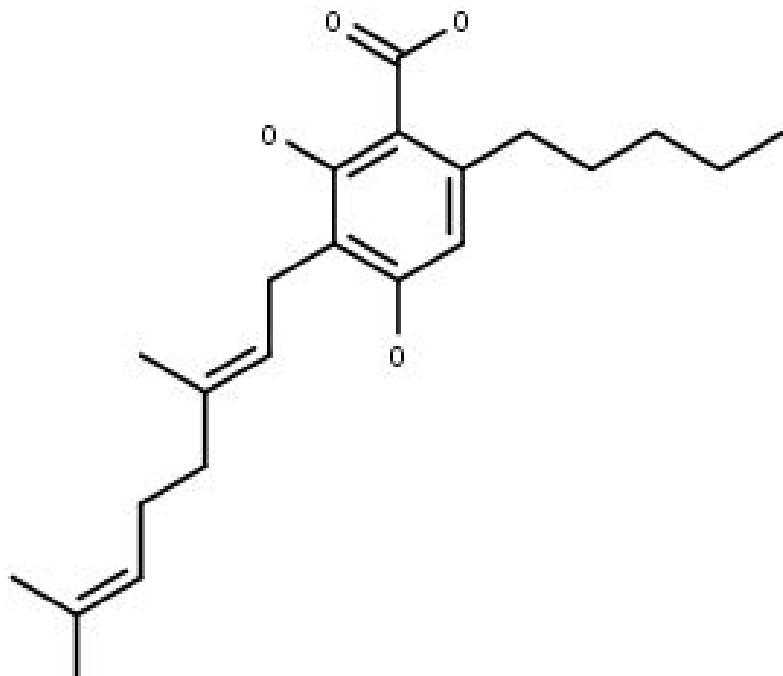
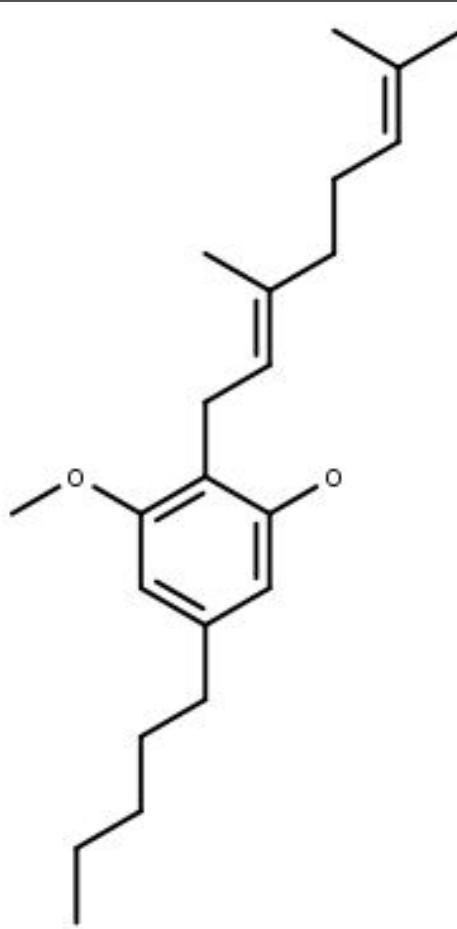
C198	Cannabidiolic acid (CBDA)	
C199	Cannabidiol monomethylether (CBDM)	

C200	Cannabidiol (CBD-C1)	
C201	Cannabidivarin (CBDV)	

C202	Cannabidivarinic acid (CBDVA)	
C203	Cannabielsoic acid B (CBEA-B)	
C204	Cannabielsoic acid A (CBEA-A)	

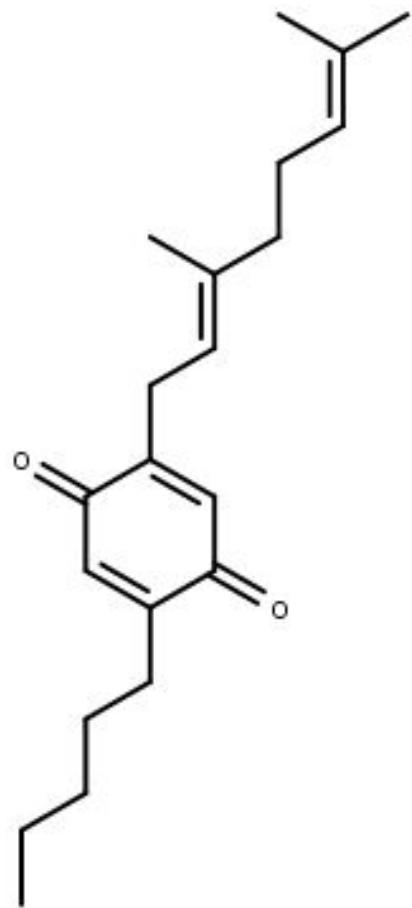
C205	Cannabielsoin (CBE)	
C206	Cannabiflavin B	
C207	Cannabifuran (CBF)	

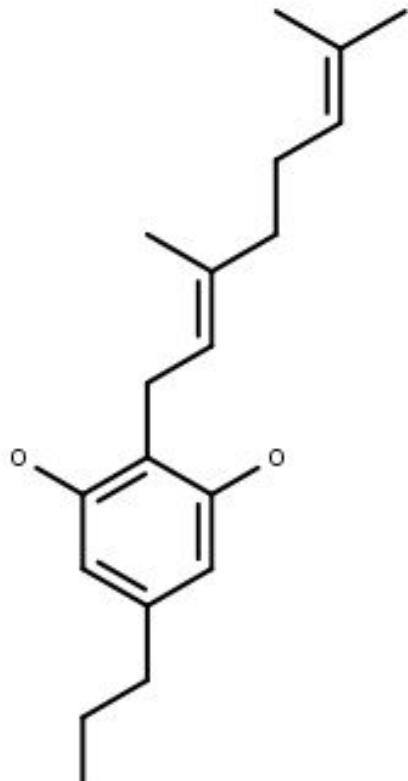
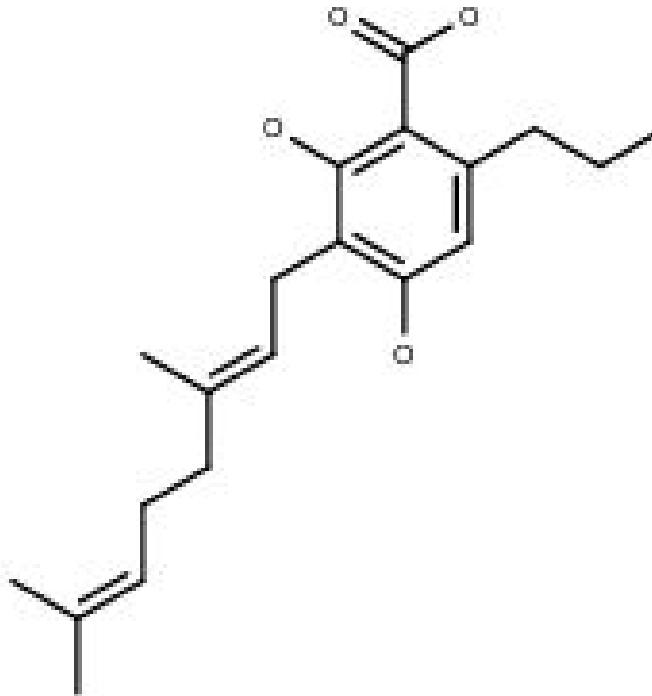
C208	Cannabigerol (CBG)	
C209	Cannabigerolic acid monomethylether (CBGAM)	

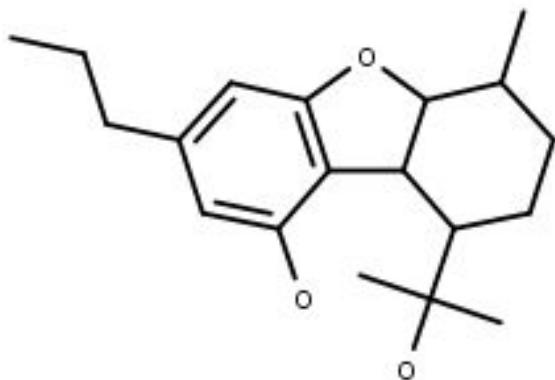
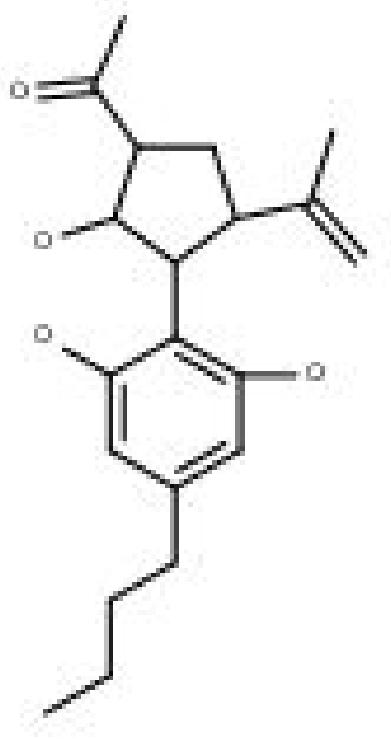
C210	Cannabigerolic acid (CBGA)	
C211	Cannabigerol monomethylether (CBGM)	

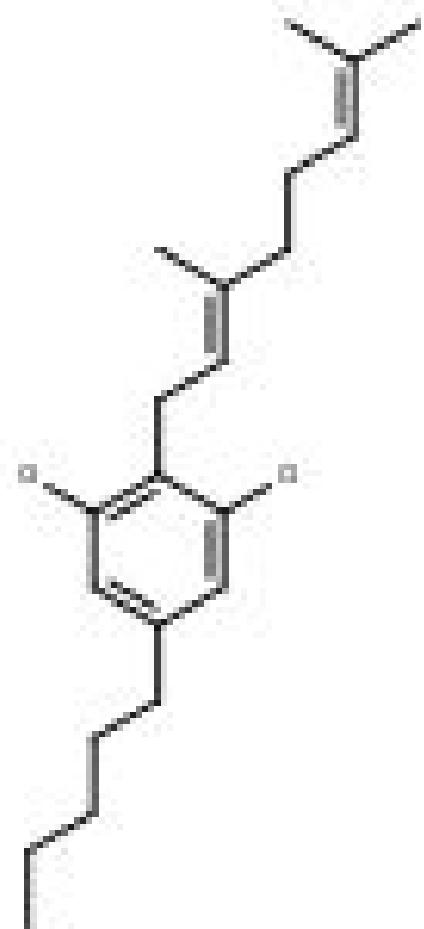
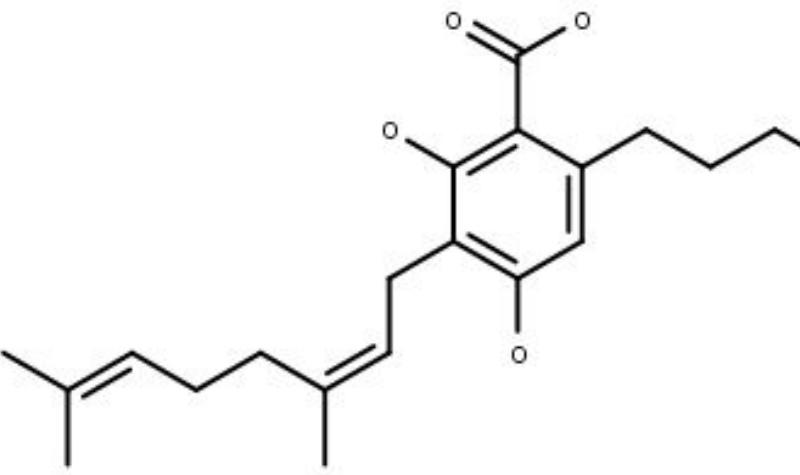
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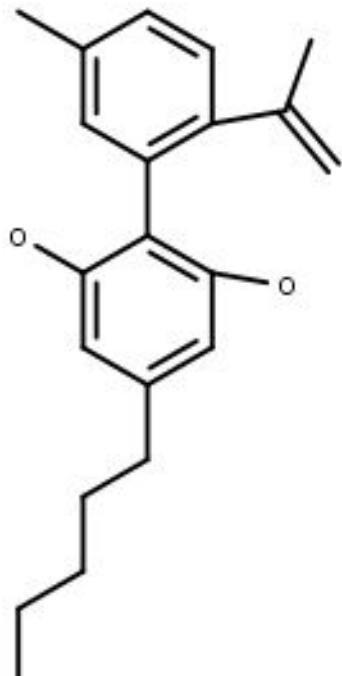
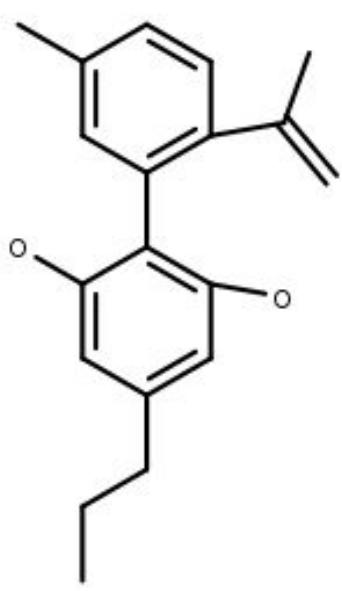
Cannabigerolquinone



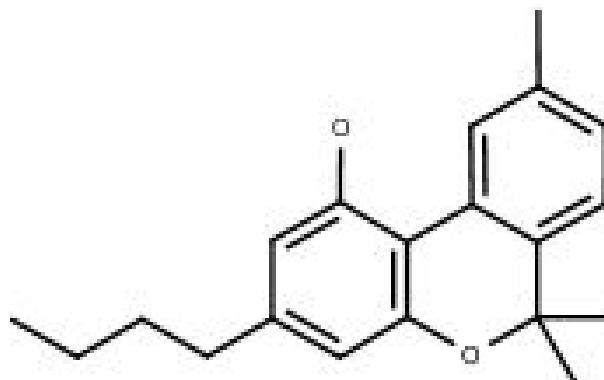
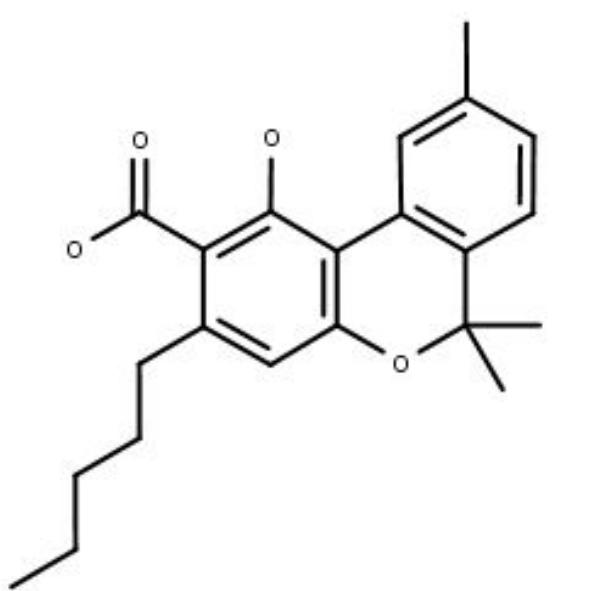
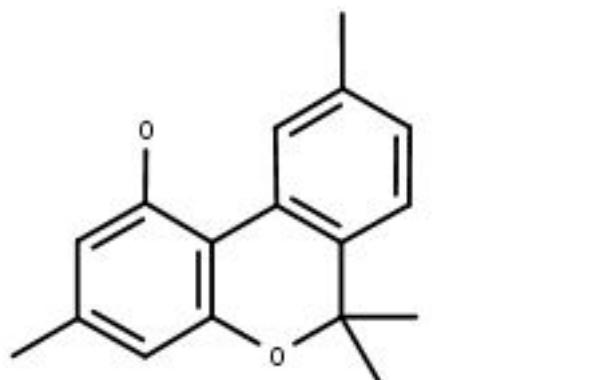
C213	Cannabigerovarin (CBGV)	
C214	Cannabigerovarinic acid (CBGVA)	

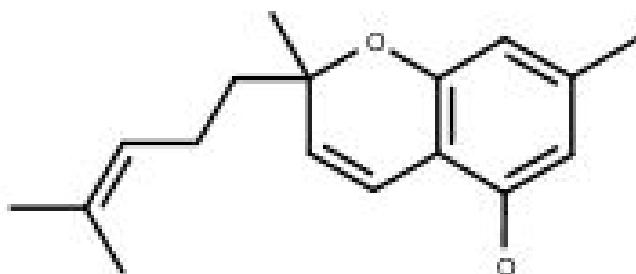
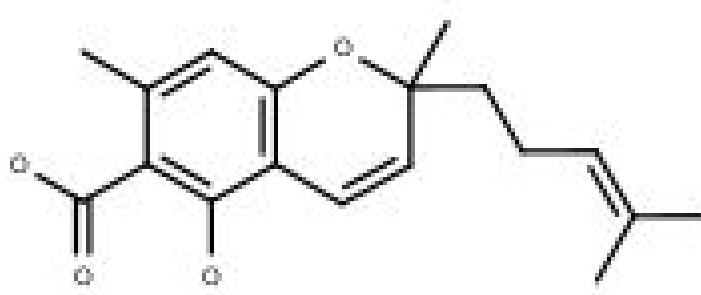
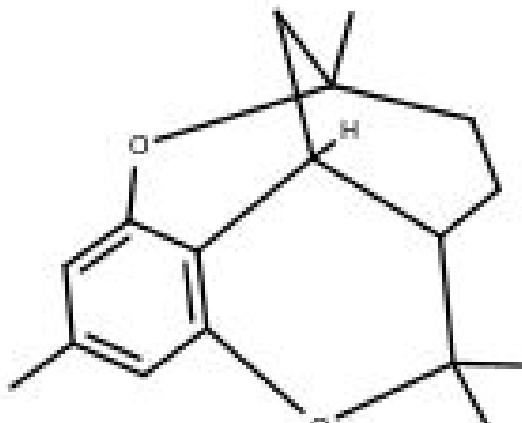
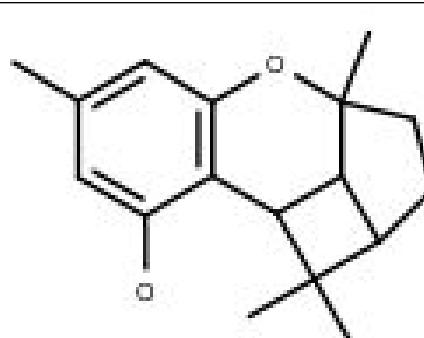
C215	Cannabiglendol	 The chemical structure of Cannabiglendol is a tricyclic diterpenoid. It features a central bicyclic core with a ketone group at position 2 and a methylene group at position 3. Attached to the core is a substituted cyclohexene ring with a methyl group at position 1 and a 2-methylpropyl side chain at position 4. A carbonyl group is located at the junction of the two rings.
C216	Cannabimovone	 The chemical structure of Cannabimovone is a tricyclic diterpenoid. It consists of a tricyclic core with a ketone group at position 2 and a methylene group at position 3. A phenyl ring is attached to the core at position 1. A 2-methylpropyl side chain is present at position 4. A carbonyl group is located at the junction of the core and the side chain.

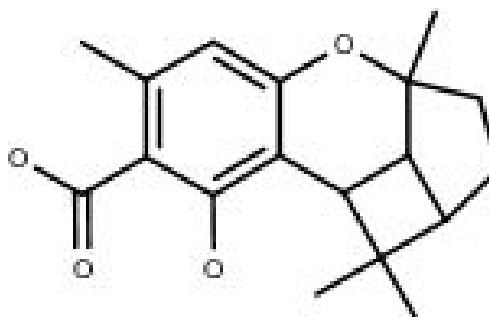
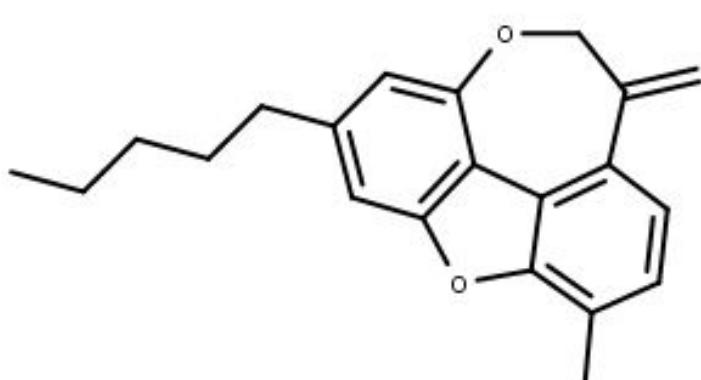
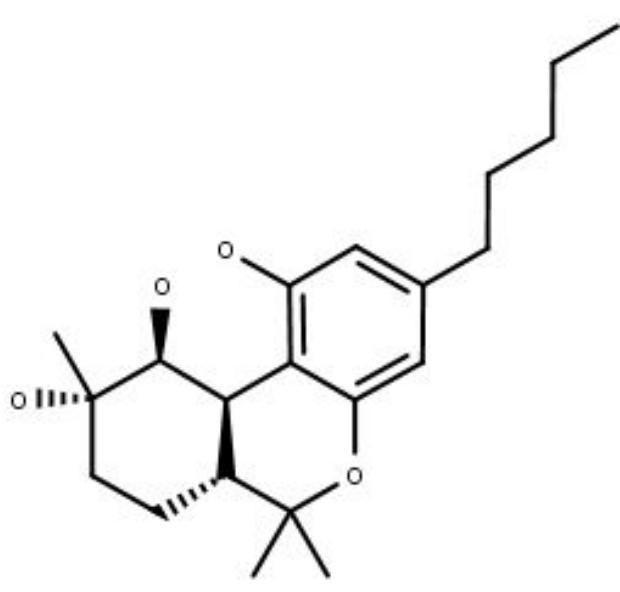
C217	Cannabinerol	 The chemical structure of Cannabinerol (C21H32) is shown. It features a central cyclohexene ring substituted with two isopropyl groups at the 1 and 4 positions. A long, branched hydrocarbon chain is attached to the 2-position of the ring. The chain consists of a six-carbon segment with a double bond between the third and fourth carbons, followed by a three-carbon segment with a double bond between the first and second carbons, and finally a five-carbon terminal chain.
C218	Cannabinerolic acid	 The chemical structure of Cannabinerolic acid (C21H30O4) is shown. It features a central cyclohexene ring substituted with two isopropyl groups at the 1 and 4 positions. A long, branched hydrocarbon chain is attached to the 2-position of the ring. The chain consists of a six-carbon segment with a double bond between the third and fourth carbons, followed by a three-carbon segment with a double bond between the first and second carbons, and finally a five-carbon terminal chain. The carboxylic acid group is located at the 3-position of the cyclohexene ring.

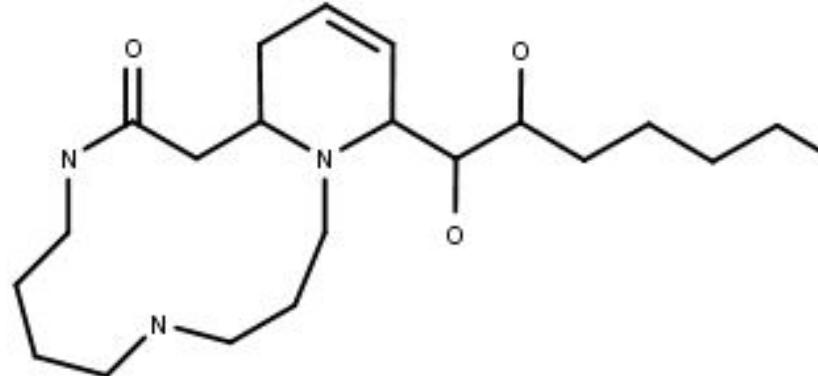
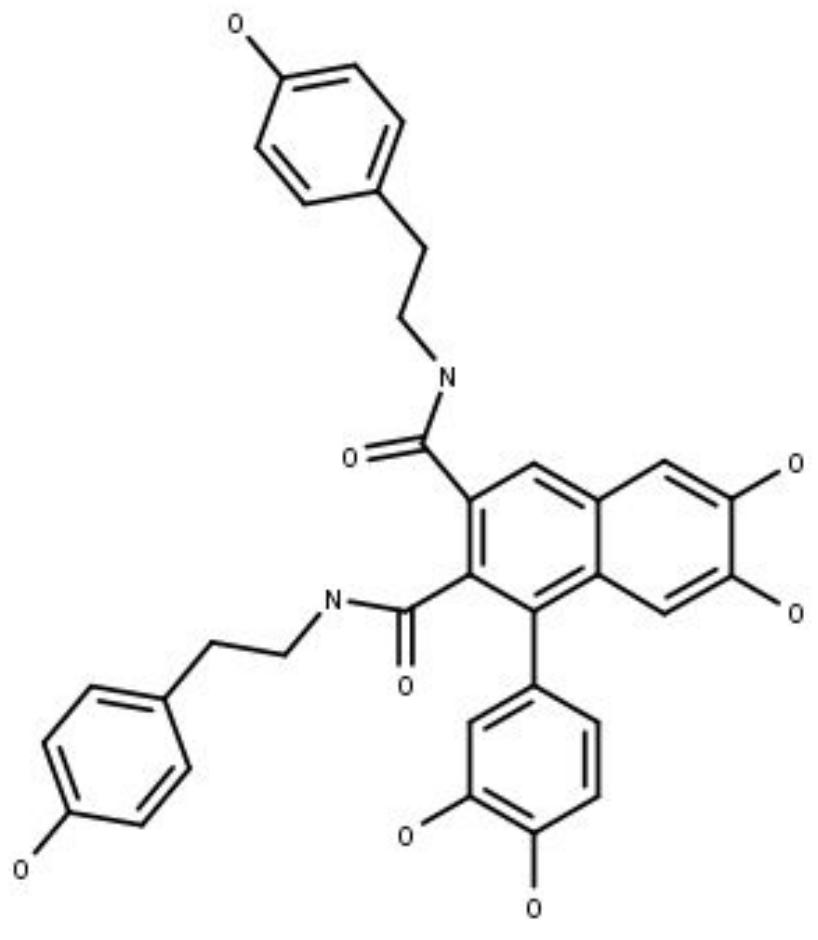
C219	Cannabinodiol (CBND)	
C220	Cannabinodivarin (CBVD)	

C221	Cannabinol methylether (CBNM)	
C222	Cannabinol (CBN)	
C223	Cannabinol-C2 (CBN-C2)	

C224	Cannabinol-C4 (CBN-C4)	
C225	Cannabinolic acid (CBNA)	
C226	Cannabiorcol (CBN-C1)	

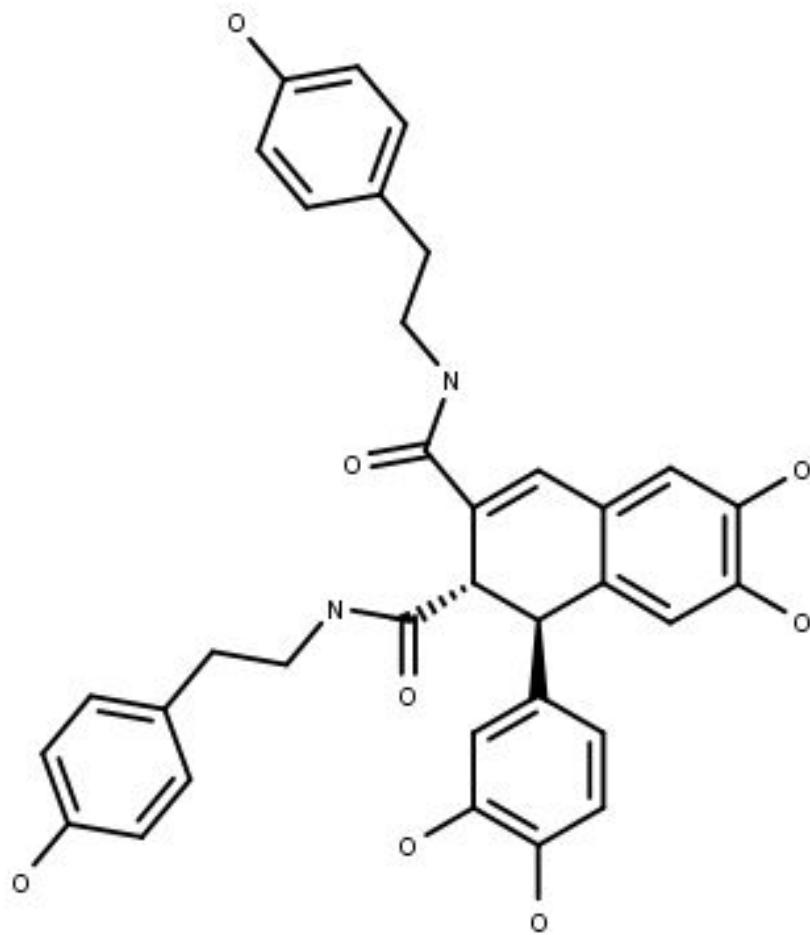
C227	Cannabiorcicchromene	
C228	Cannabiorcicchromenic acid	
C229	Cannabiorcicitran	
C230	Cannabiorcyclool	

C231	Cannabiorcyclolic acid	
C232	Cannabioxepane	
C233	Cannabiripsol (CBR)	

C234	Cannabissativine	 The chemical structure of Cannabissativine is a complex molecule. It features a tricyclic core consisting of a pyridine ring fused to a piperazine ring, which is further fused to a cyclohexene ring. A long, branched hydrocarbon chain is attached to the cyclohexene ring. The chain starts with a methylene group, followed by a carbonyl group (C=O), then another methylene group, and finally a branched chain of four carbon atoms.
C235	Cannabisin-A	 The chemical structure of Cannabisin-A is a tricyclic compound. It consists of a central indole ring system substituted with two phenyl groups at the 3 and 7 positions. Each phenyl group is further substituted with a methoxy group (-OCH ₃). The indole ring is also substituted with a nitrogen atom that is part of a pyrazine ring. This pyrazine ring is connected to a chain that extends to the right, ending in a carbonyl group (C=O).

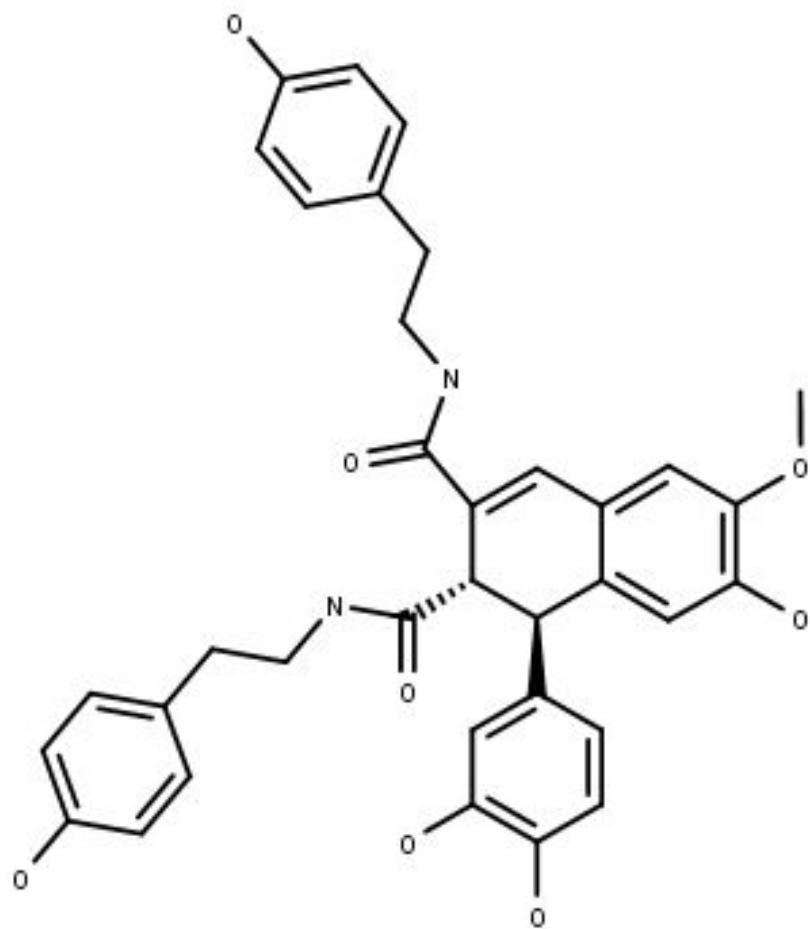
C236

Cannabisin-B

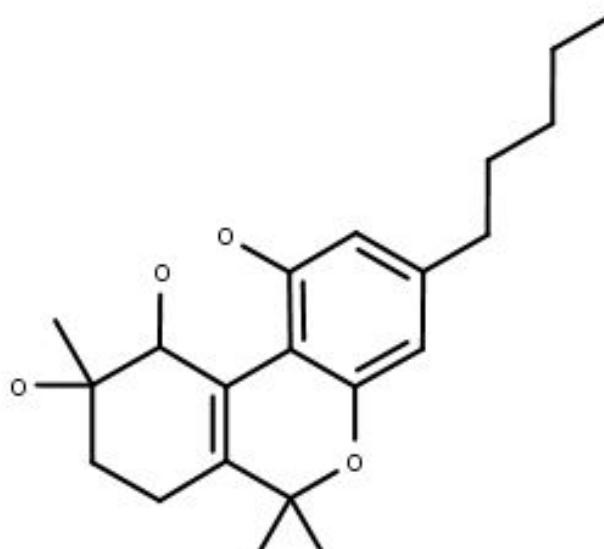
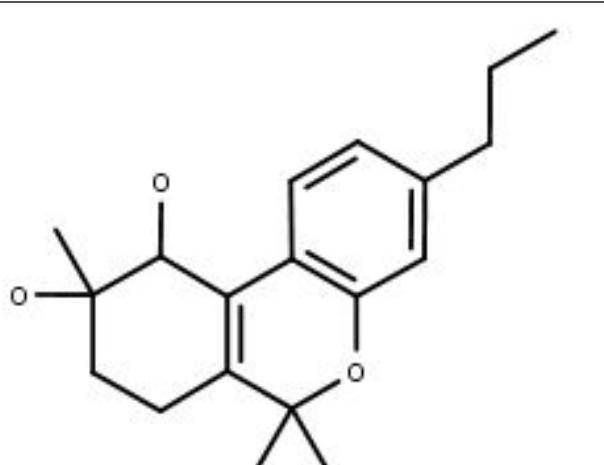
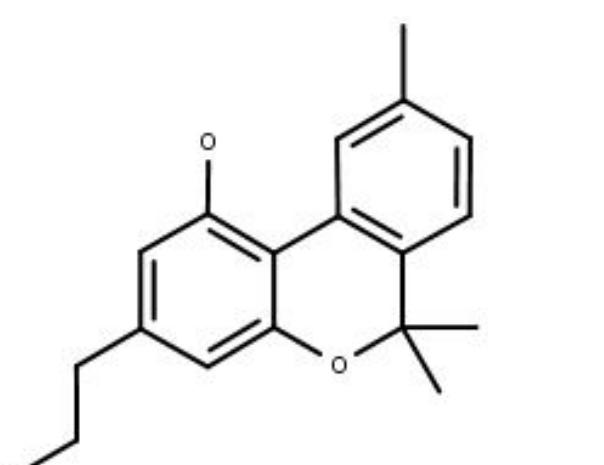


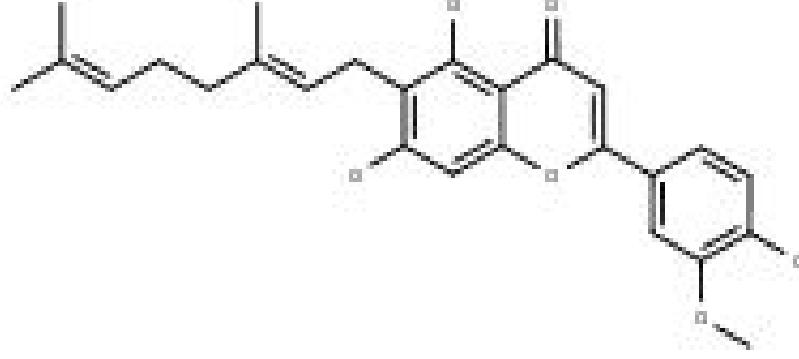
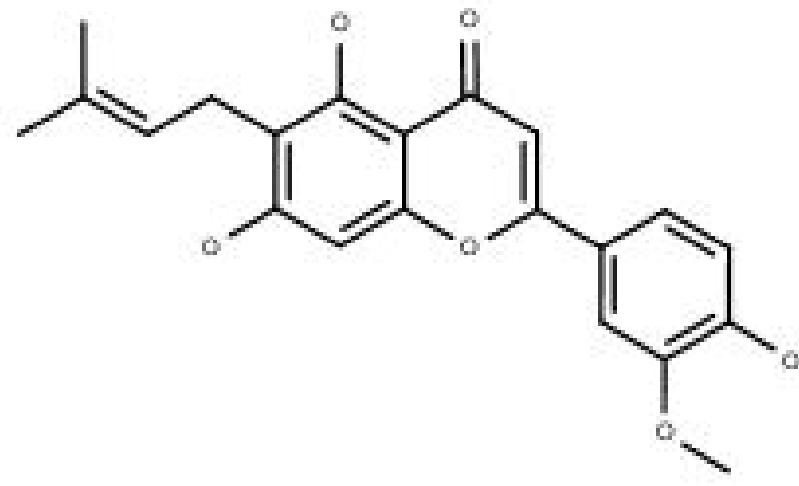
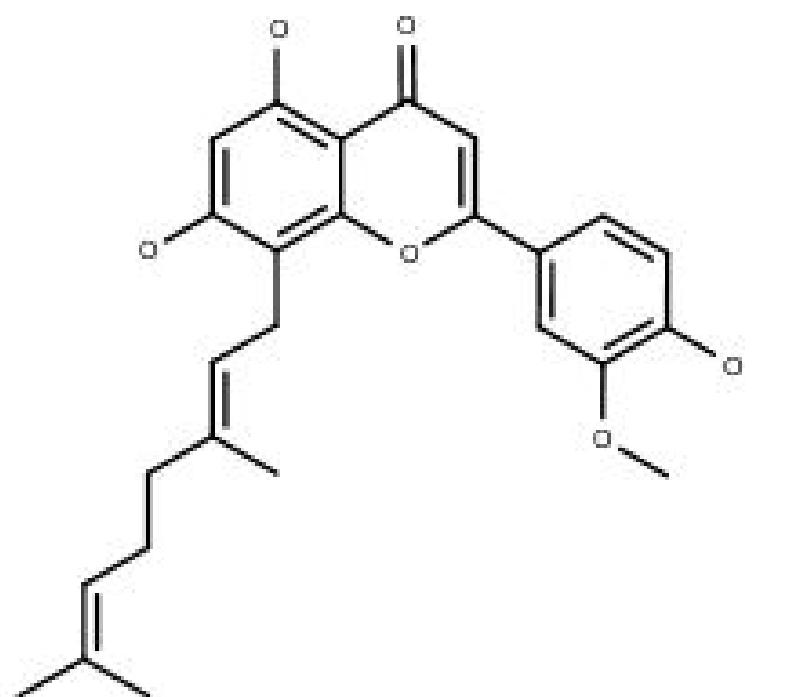
C237

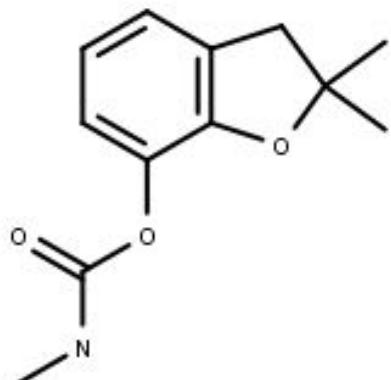
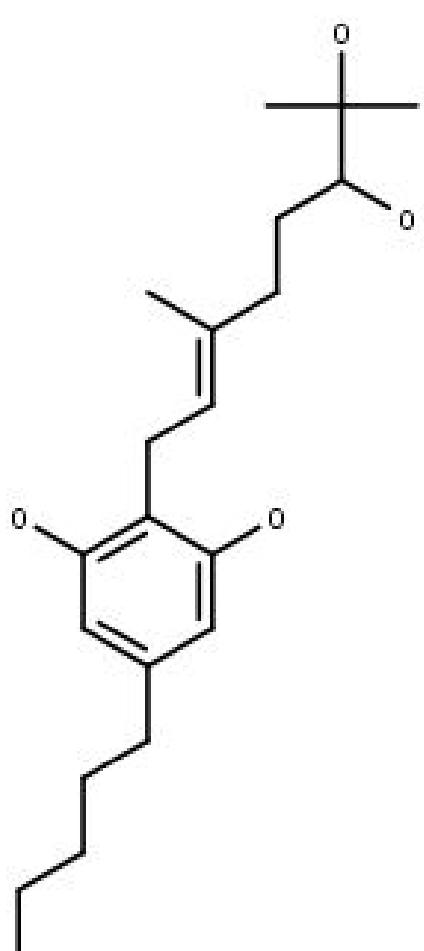
Cannabisin-C

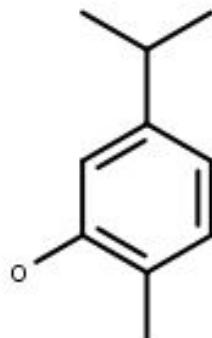
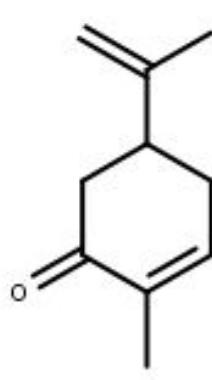
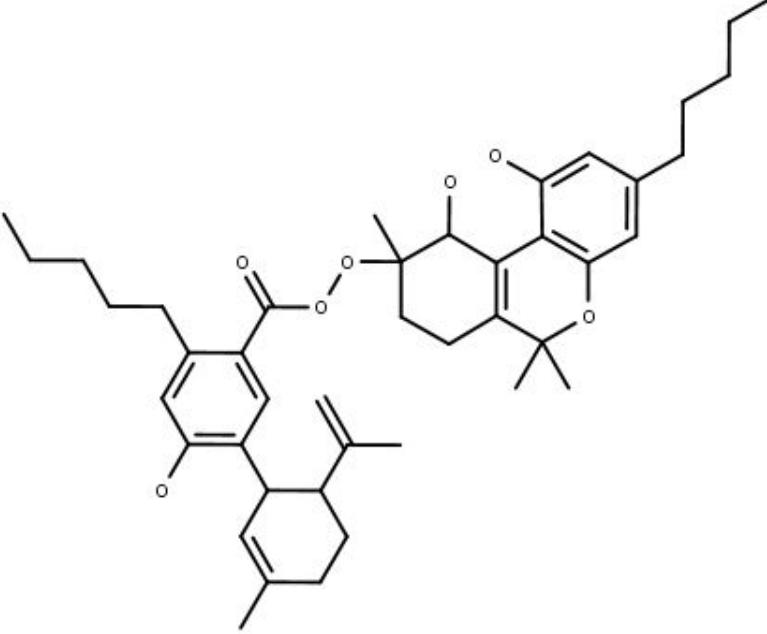


C238	Cannabisin-D	<p>Chemical structure of Cannabisin-D:</p> <p>It consists of a tricyclic core. A phenyl ring is attached to one carbon of a cyclohexene ring, which is fused to a cyclopentenone ring. This cyclopentenone ring is further fused to a 2H-chromene ring. Two amide groups are present: one connecting the cyclohexene ring to the chromene ring, and another connecting the cyclopentenone ring to the chromene ring. A biphenyl group is also part of the structure.</p>
C239	Cannabispirone	<p>Chemical structure of Cannabispirone:</p> <p>It consists of a tricyclic core. A benzodioxole ring is fused to a cyclopentenone ring, which is further fused to a cyclohexane ring. The cyclohexane ring has a ketone group at one of its vertices.</p>

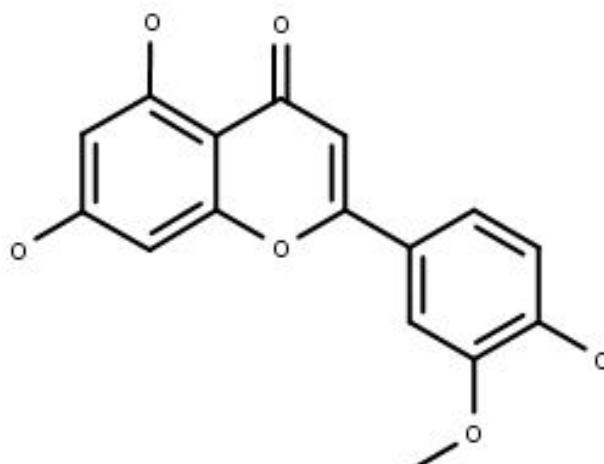
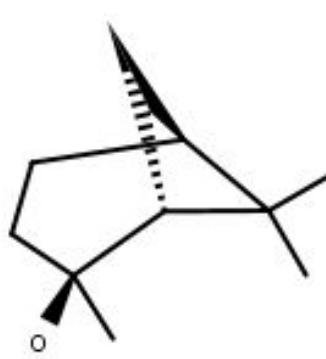
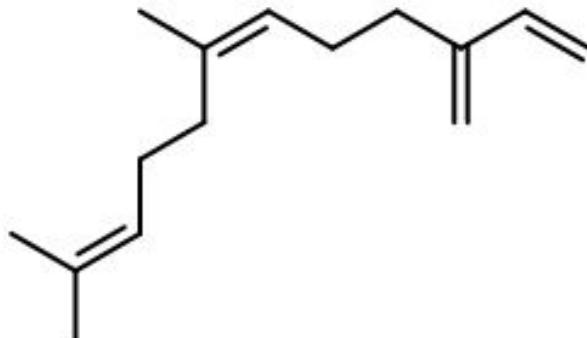
C240	Cannabitriol (CBT)	 The chemical structure of Cannabitriol (CBT) is a tricyclic diterpenoid. It features a central cyclohexanone ring fused to a cyclohexene ring, which is further fused to a benzene ring. The benzene ring has two methoxy groups (-OCH ₃) at positions 2 and 6. A long, branched hydrocarbon side chain is attached to the cyclohexene ring at position 3.
C241	Cannabitriolvarin (CBTV)	 The chemical structure of Cannabitriolvarin (CBTV) is similar to Cannabitriol (CBT), but it lacks the methoxy groups (-OCH ₃) at the 2 and 6 positions of the benzene ring. It features a central cyclohexanone ring fused to a cyclohexene ring, which is further fused to a benzene ring. A long, branched hydrocarbon side chain is attached to the cyclohexene ring at position 3.
C242	Cannabivarin (CBV)	 The chemical structure of Cannabivarin (CBV) is a tricyclic diterpenoid. It features a central cyclohexanone ring fused to a cyclohexene ring, which is further fused to a benzene ring. The benzene ring has one methoxy group (-OCH ₃) at position 2 and one isopropylidene group (-CH=CH-C(CH ₃) ₂) at position 6. A long, branched hydrocarbon side chain is attached to the cyclohexene ring at position 3.

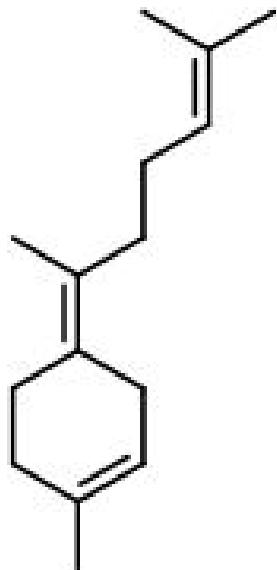
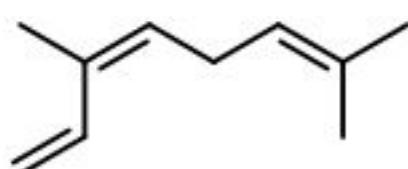
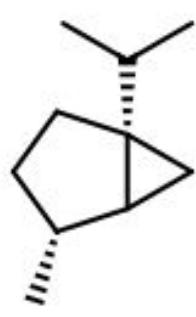
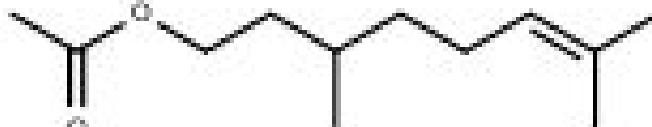
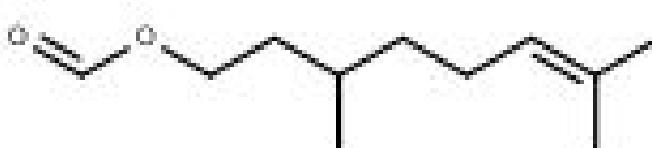
C243	Cannflavin A	
C244	Cannflavin B	
C245	Cannflavin C	

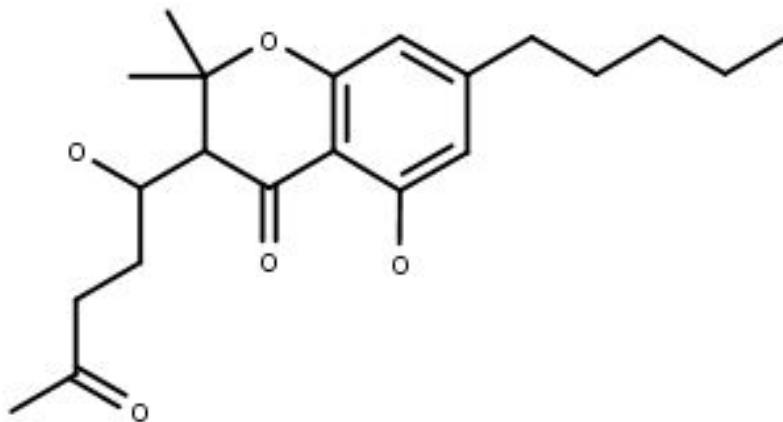
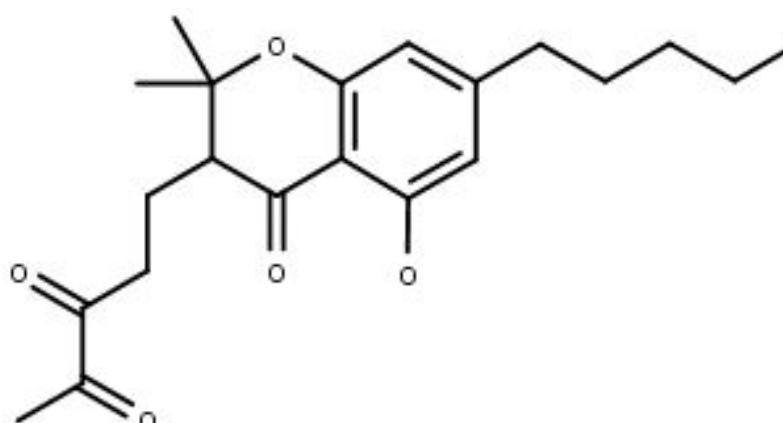
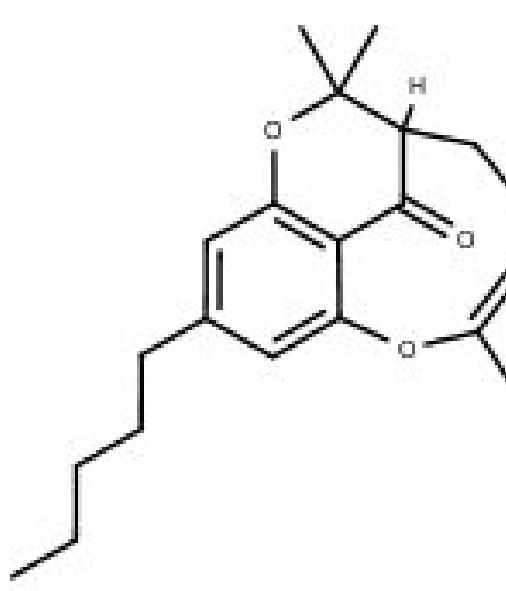
C246	Carbofuran	 The chemical structure of Carbofuran is shown. It consists of a furan ring system where the 2-position is substituted with a methyl group (-CH ₃) and the 5-position is substituted with a carbamoyl group (-CONMe ₂). The furan ring is five-membered with double bonds between the 1 and 2 positions, and between the 4 and 5 positions.
C247	Carmagerol	 The chemical structure of Carmagerol is shown. It features a central cyclopentenone ring fused to a cyclohexene ring. The cyclopentenone ring has a methyl group at position 2 and a 2-methylprop-1-enyl group at position 3. The cyclohexene ring has a 2-methylprop-1-enyl group at position 2 and a 2,2-dimethylprop-1-enyl group at position 3. Both rings have a double bond between the 4 and 5 positions.

C248	Carvacrol	
C249	Carvone	
C250	CBDA-THC ester	

C251	Cedryl acetate	
C252	Cetyl Alcohol	
C253	Chiricanine B	
C254	Chlorocannabiorcicchromenic acid	

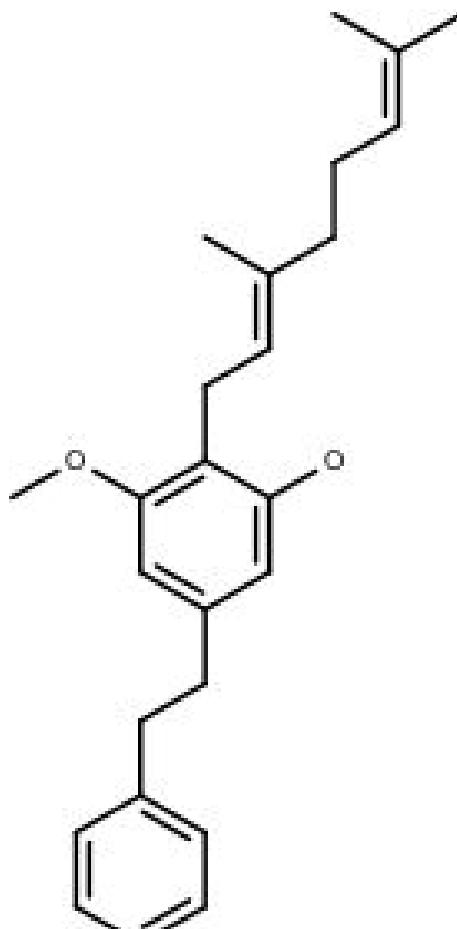
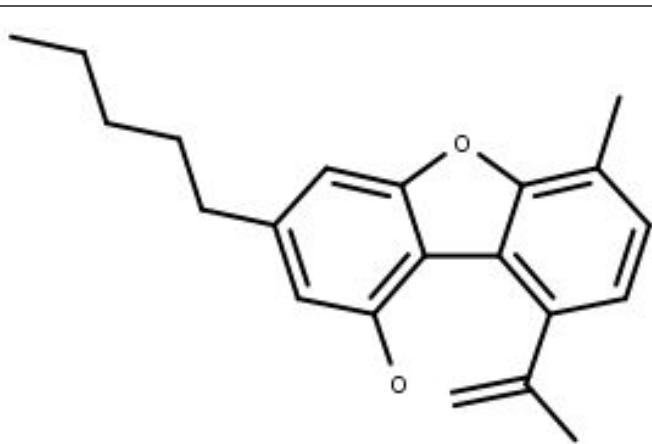
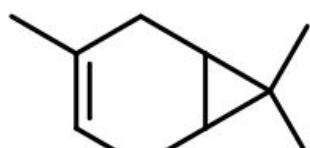
C255	Chrysoeriol	
C256	cis-2-Pinanol	
C257	cis-Beta-Farnesene	

C258	cis-Gamma-Bisabolene	
C259	cis-Ocimene	
C260	cis-Sabinene Hydrate	
C261	Citronellyl acetate	
C262	Citronelloformate	

C263	Compound-2	
C264	Compound-3	
C265	compound-4	

C266	Confluentin	
C267	Cumene	
C268	Cuminaldehyde	
C269	Daurichromenic acid	

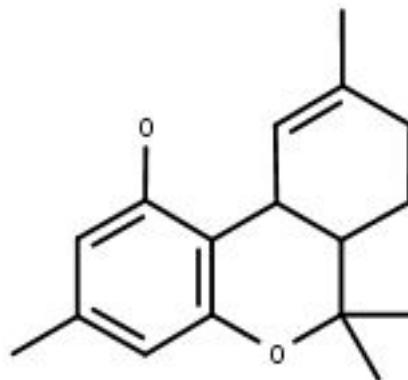
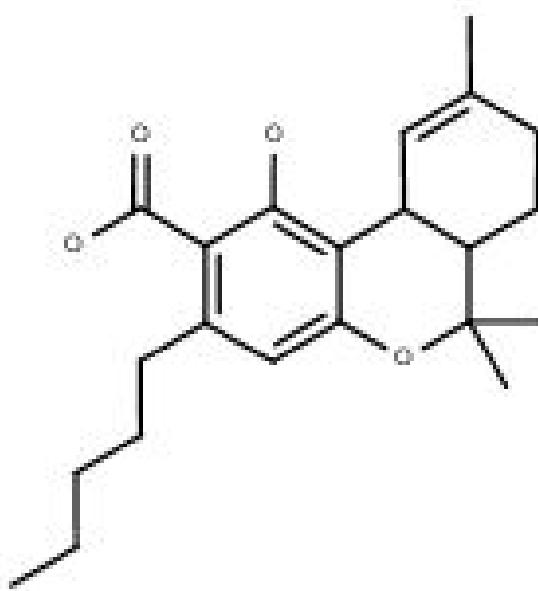
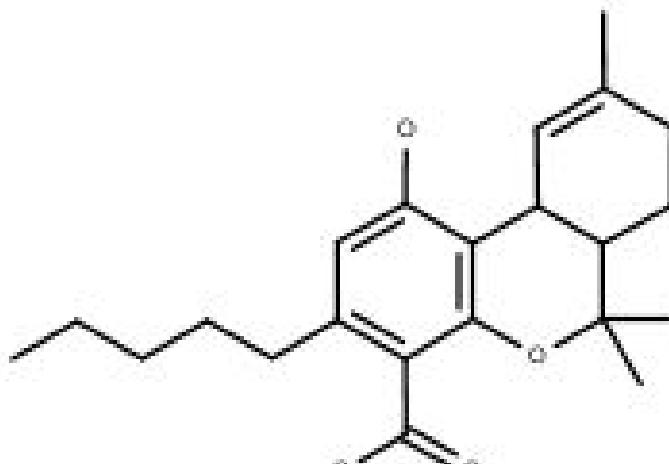
C270	Delta-9-tetrahydrocannabiorcolic acid (THCA-C1)	
C271	Decanal	
C272	Decarboxyamorfrutin A	

C273	Decarboxyamorfrutin B	
C274	Dehydrocannabifuran (DCBF)	
C275	Delta-3-Carene	

C276	Delta-7-cis-Isotetrahydrocannabivarin	
C277	Delta-7-trans-Isotetrahydrocannabinol	
C278	Delta-8-tetrahydrocannabinol ($\Delta 8$ -THC)	

C279	Delta-8-tetrahydrocannabinolic acid (Δ^8 -THCA)	
C280	Delta-9-cis-tetrahydrocannabivarin	

C281	Delta-9-nor-tetrahydrocannabinolic acid	
C282	Delta-9-nor-tetrahydrocannabinol	
C283	Delta-9-Tetrahydrocannabinol-C4	

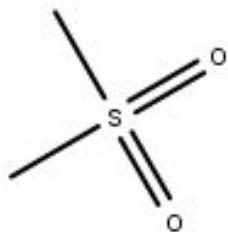
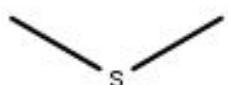
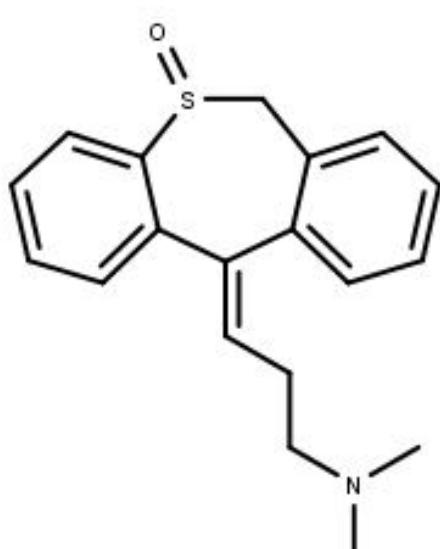
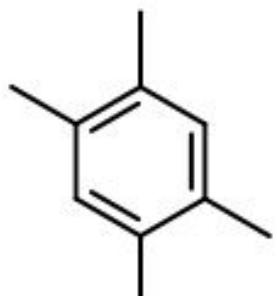
C284	Delta-9-tetrahydrocannabiorcol (THC-C1)	
C285	Delta-9-tetrahydrocannabinolic acid A (THCA-A)	
C286	Delta-9-tetrahydrocannabinolic acid B (THCA-B)	

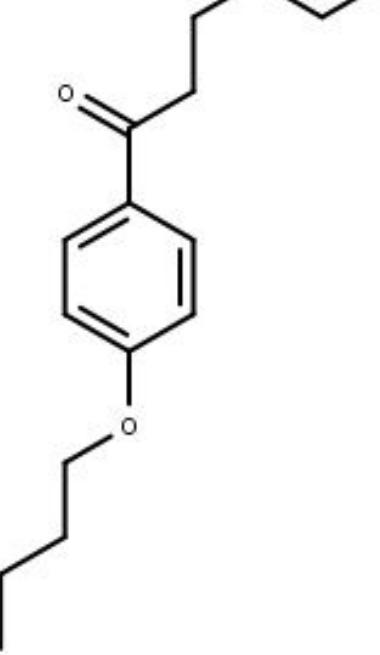
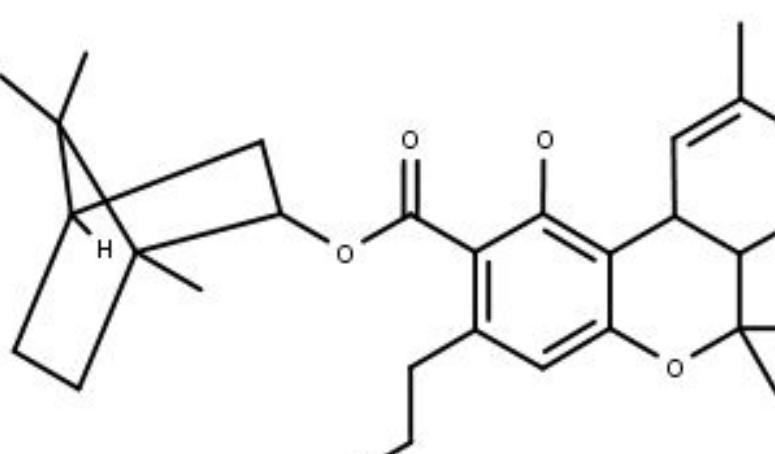
C287	Delta-9-tetrahydrocannabinolic acid-C4 (THCA-C4)	
C288	Delta-Cadinene	
C289	Demethylamorfrutin A	

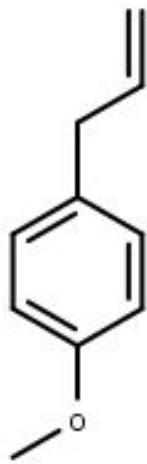
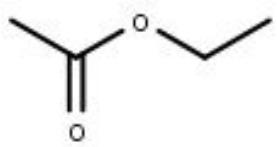
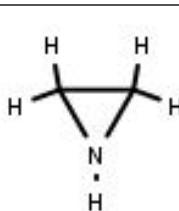
C290	Demethyldecarboxyamorfrutin A	
C291	Deprenyl O-methyl cannabigerolic acid	
C292	Desmodianone A	

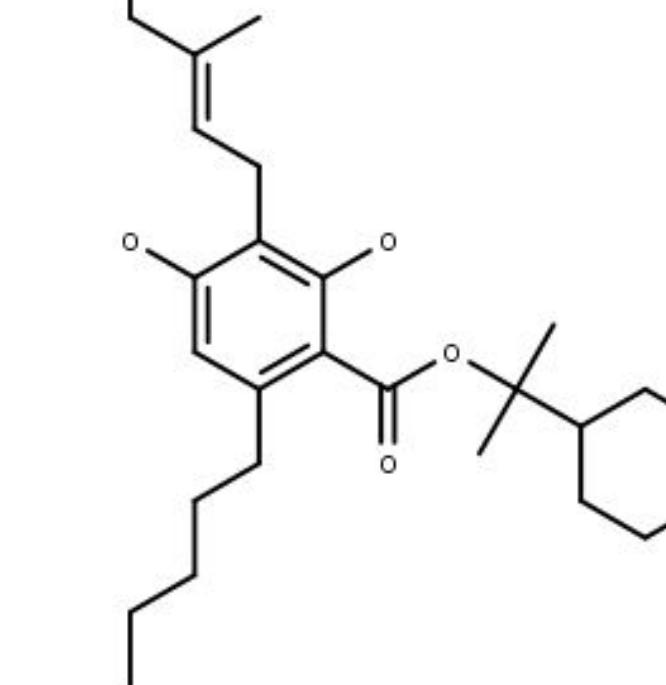
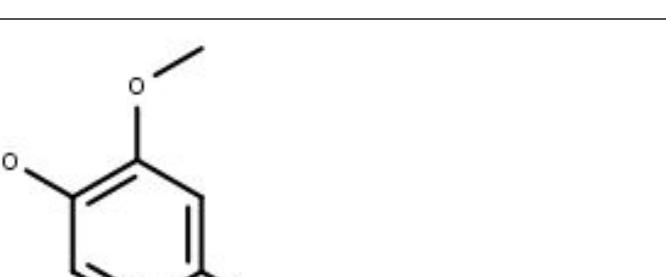
C293	Desmodianone C	
C294	Desmodianone D	
C295	Desmodianone E	

C296	Diacetone alcohol	
C297	Dibutyl phthalate	
C298	Diethyl Phthalate	
C299	Dimethylbenzylcarbinyl acetate	

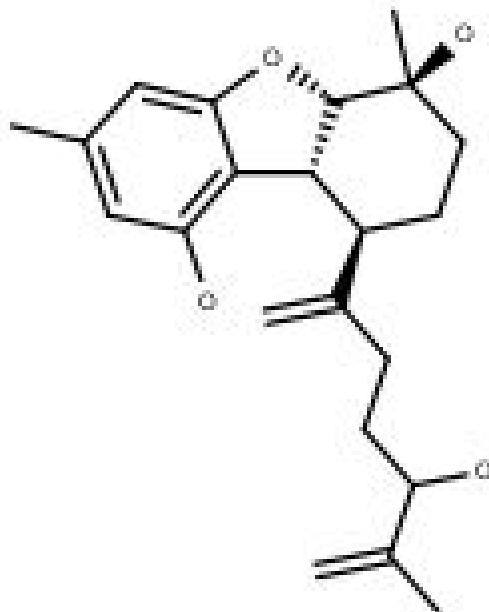
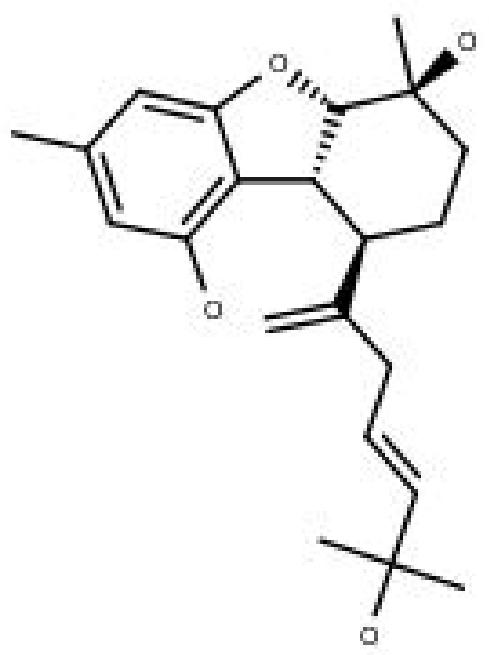
C300	Dimethylsulfone	
C301	Dimethylsulfide	
C302	Dodecane	
C303	Dothiepin Sulfoxide	
C304	Durene	

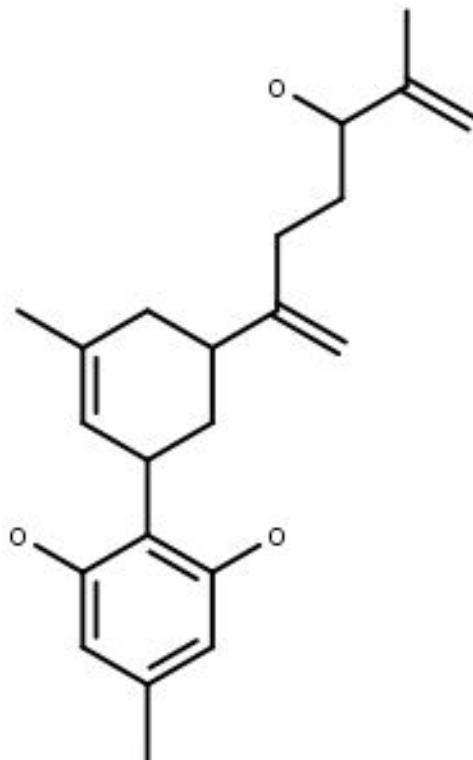
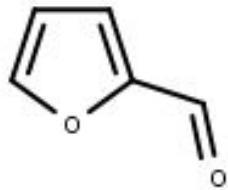
C305	Dyclocaine	
C306	epi-Bornyl Delta-9-tetrahydrocannabinolate	

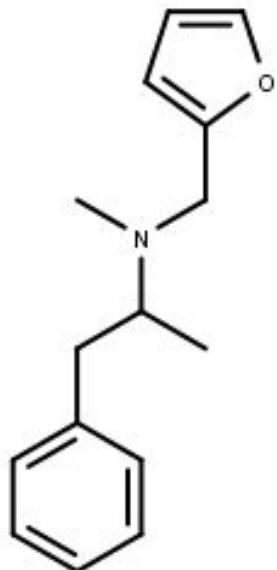
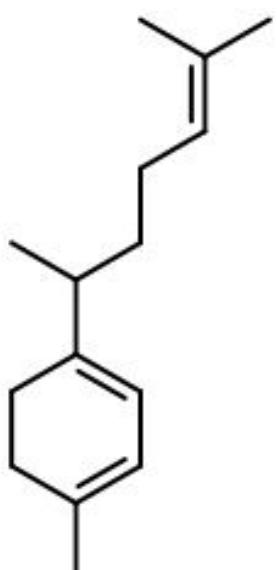
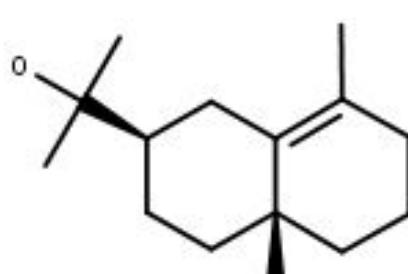
C307	Estragole	
C308	Ethylacetate	
C309	Ethylenediamine	
C310	Ethylene oxide	
C311	Ethylenimine	

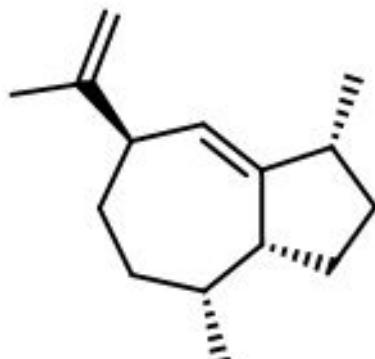
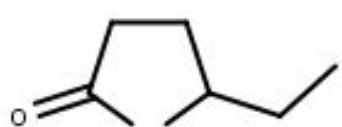
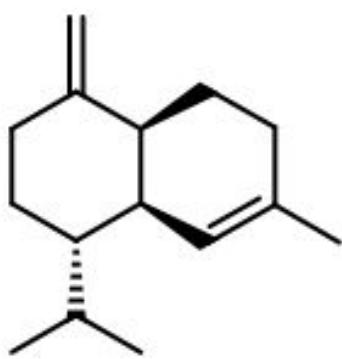
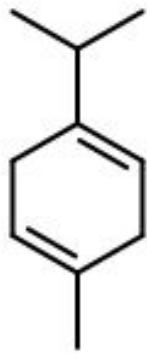
C312	Eudesmyl-Cannabigerolate	 The chemical structure of Eudesmyl-Cannabigerolate is shown. It features a complex polycyclic system. On the left, there is a trisubstituted cyclohexene ring with two methyl groups and a prop-1-enyl group. This is connected via a chain of three carbons to a trisubstituted cyclohexene ring with two methyl groups and a prop-1-enyl group. This second chain is further connected via a chain of three carbons to a central trisubstituted cyclohexene ring. This central ring has a prop-1-enyl group at one position and a carboxylic acid ester side chain at another. The ester side chain consists of a methylene group attached to a carbonyl group, which is in turn attached to a tert-butyl group.
C313	Eugenol	 The chemical structure of Eugenol is shown. It consists of a benzene ring substituted with a prop-1-enyl group at the para position and a methyl group at the ortho position.

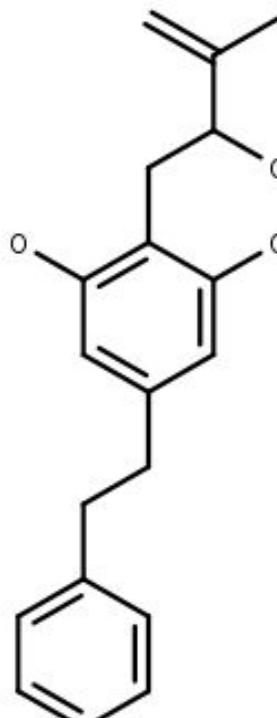
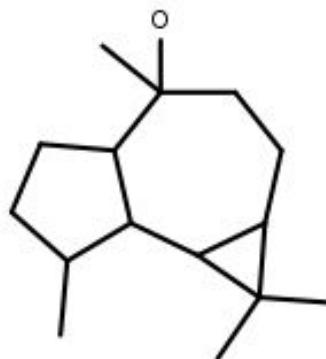
C314	Eugenyl acetate	
C315	Fenchone	
C316	Fenchyl Alcohol	

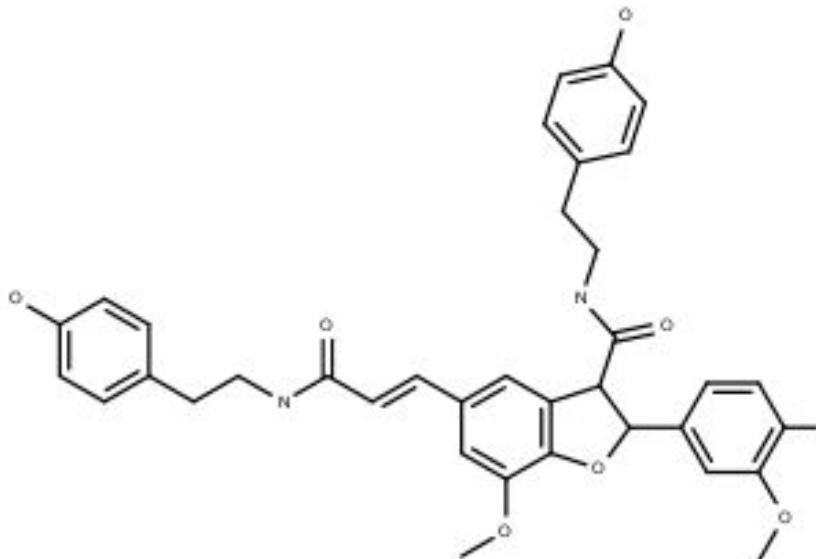
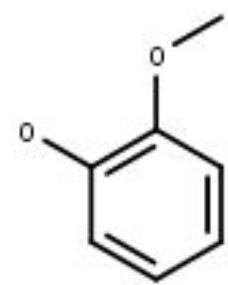
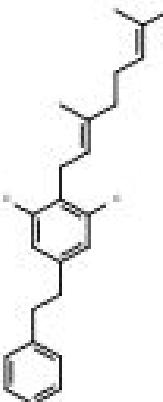
C317	Ferruginene A	 The chemical structure of Ferruginene A is a tricyclic diterpenoid. It features a trisubstituted cyclohexene ring fused to a bicyclo[2.2.1]hept-5-ene system. The molecule contains several oxygenated groups, including two hydroxyl groups (one axial, one equatorial) at C-10, a carbonyl group at C-11, and a ketone group at C-12. Stereochemistry is indicated by wedged and dashed bonds.
C318	Ferruginene B	 The chemical structure of Ferruginene B is very similar to Ferruginene A, differing only in the substitution pattern at the C-10 position. While Ferruginene A has two hydroxyl groups at C-10, Ferruginene B has a hydroxyl group (axial) and a methyl group (equatorial) at C-10. The rest of the structure, including the fused rings and the side chain, is identical to Ferruginene A.

C319	Ferruginene C	
C320	Formic acid	
C321	Furfural	

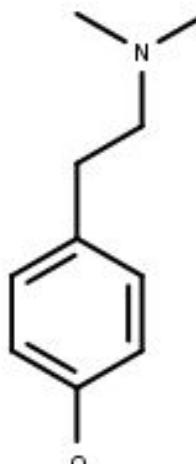
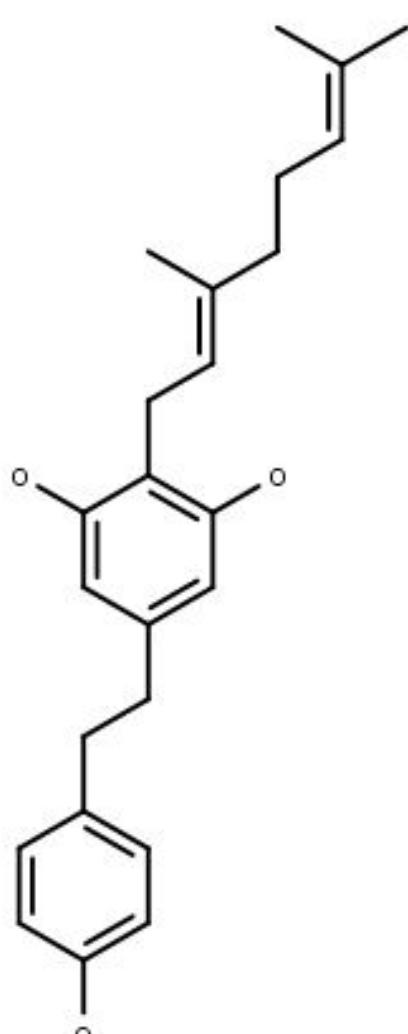
C322	Furfurylmethylamphetamine	
C323	Gamma-curcumene	
C324	Gamma-eudesmol	

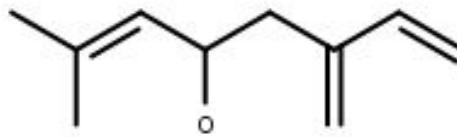
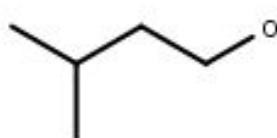
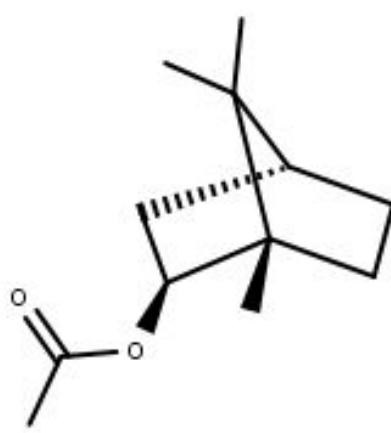
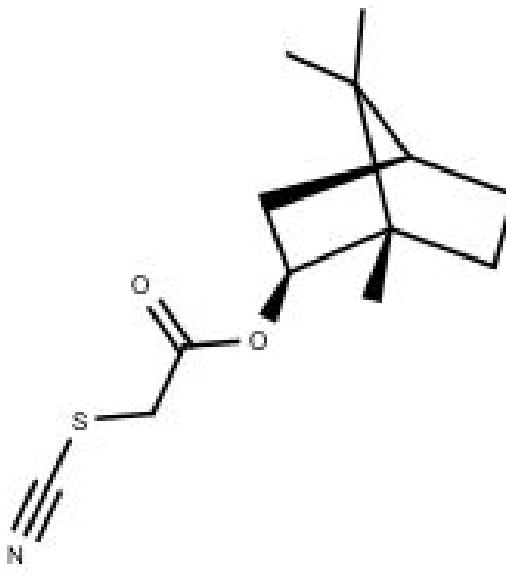
C325	Gamma-Gurjunene	
C326	Gamma-Hexalactone	
C327	Gamma-Muurolene	
C328	Gamma-Terpinene	

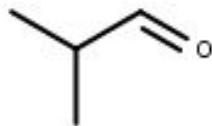
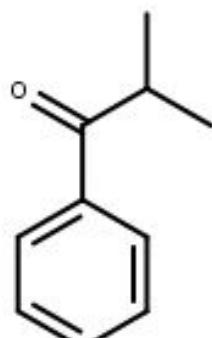
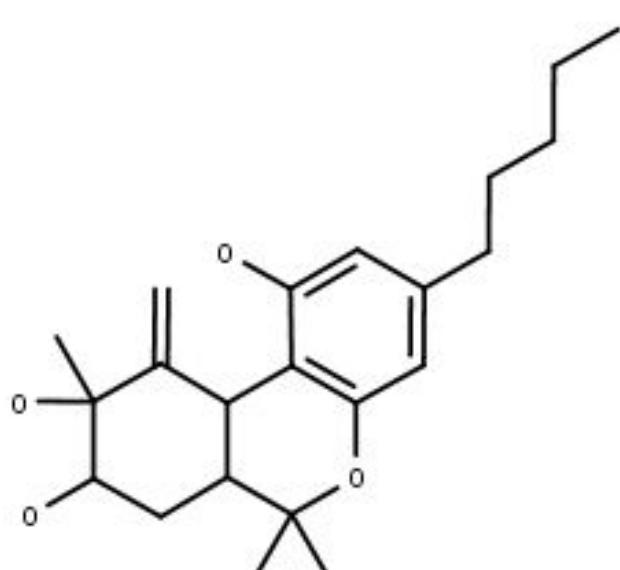
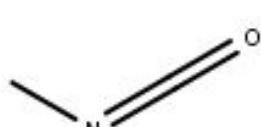
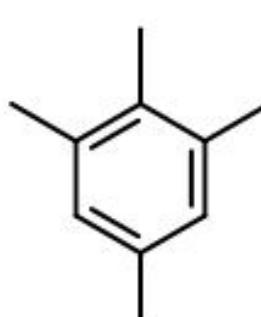
C329	Glepidotin C	
C330	Globulol	

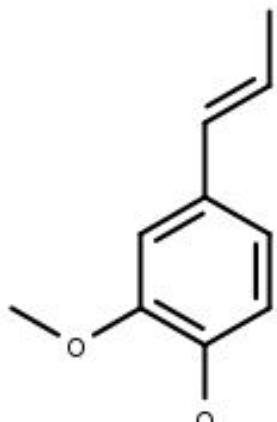
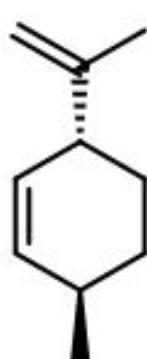
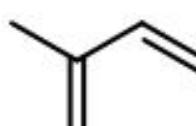
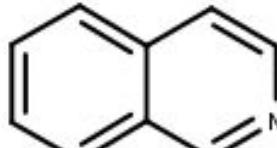
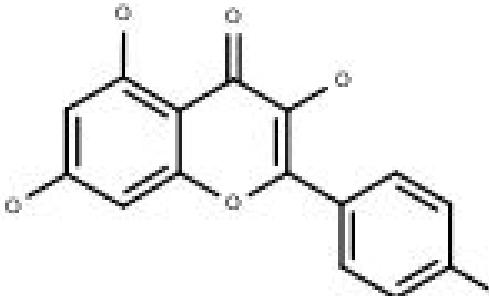
C331	Grossamide	
C332	Guajol	
C333	Heli-Cannabigenol	
C334	Heptanal	
C335	Hexadecane	

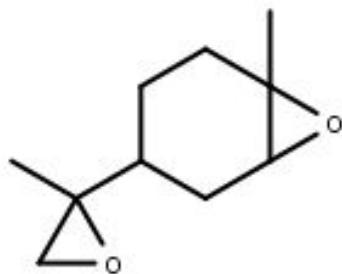
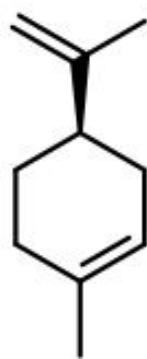
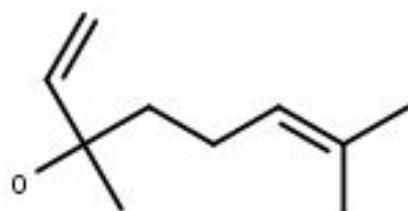
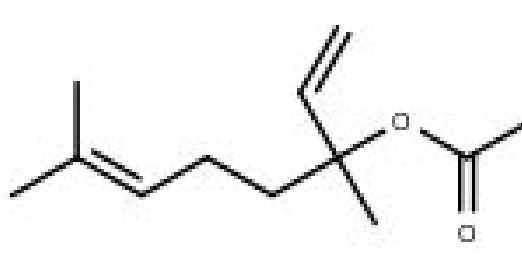
C336	Hexahydrocannabinol	
C337	Hexanal	
C338	Hexanoic acid, methyl ester	
C339	Hexanoic acid, propyl ester	
C340	Hexestrol	

C341	Hordenine	
C342	Hydroxy Heli-Cannabigerol	

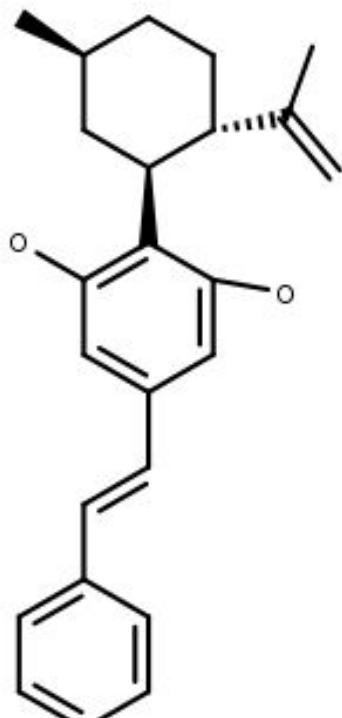
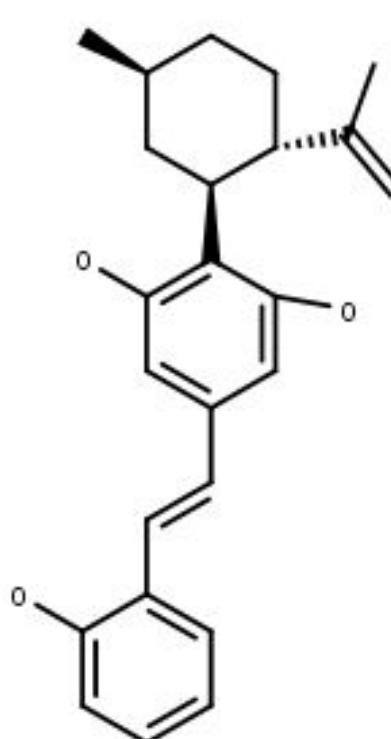
C343	Ipsdienol	
C344	Isoamyl alcohol	
C345	Isobornyl acetate	
C346	Isobornyl thiocyanoacetate	
C347	Isobutane	

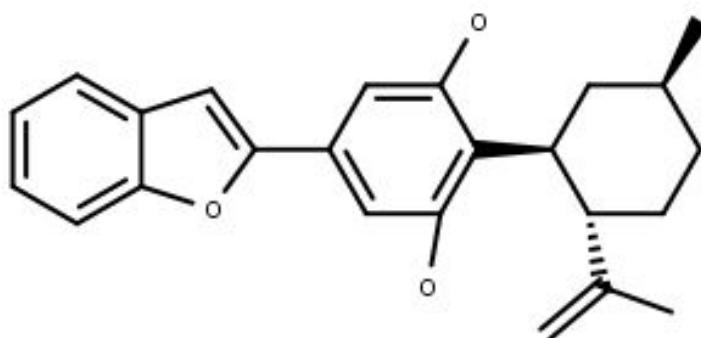
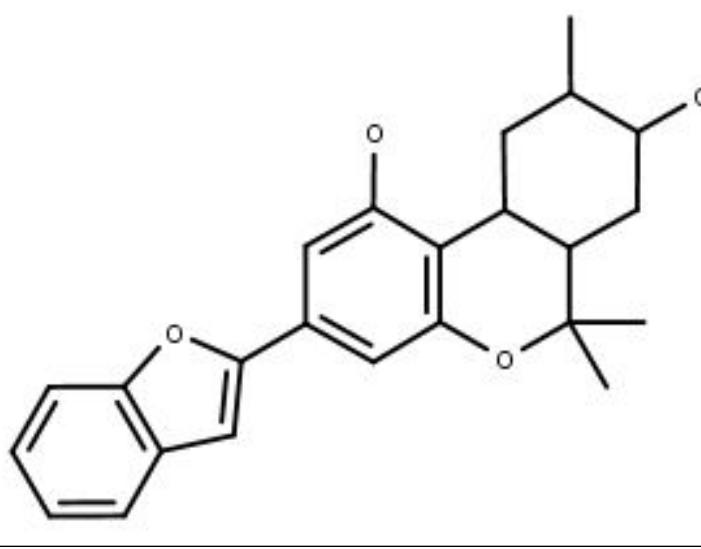
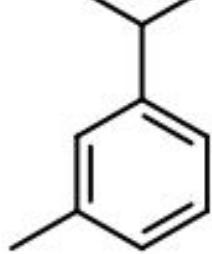
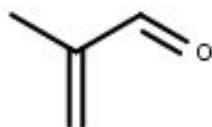
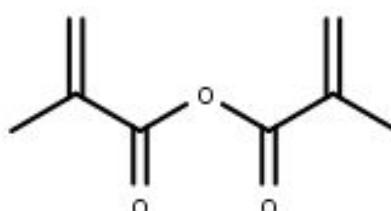
C348	Isobutyraldehyde	
C349	Isobutyrophenone	
C350	Isocannabidiol	
C351	Isocyanatomethane	
C352	Isodurene	

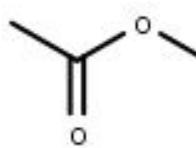
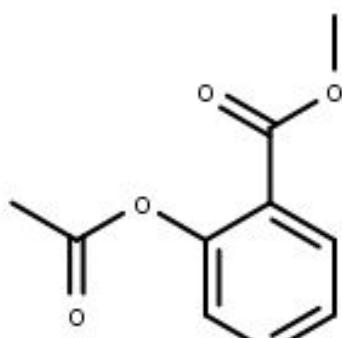
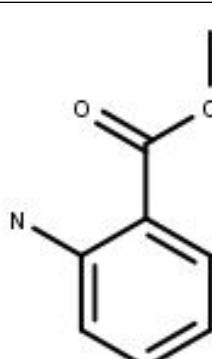
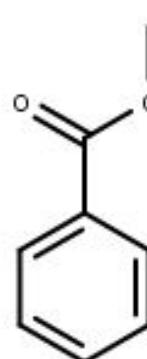
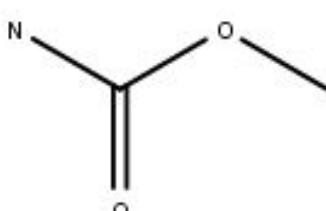
C353	Isoeugenol	
C354	Isolimonene	
C355	Isoprene	
C356	Isoquinoline	
C357	Kaempferol	

C358	Limonene oxide	
C359	Limonene	
C360	Linalool	
C361	Linalyl acetate	

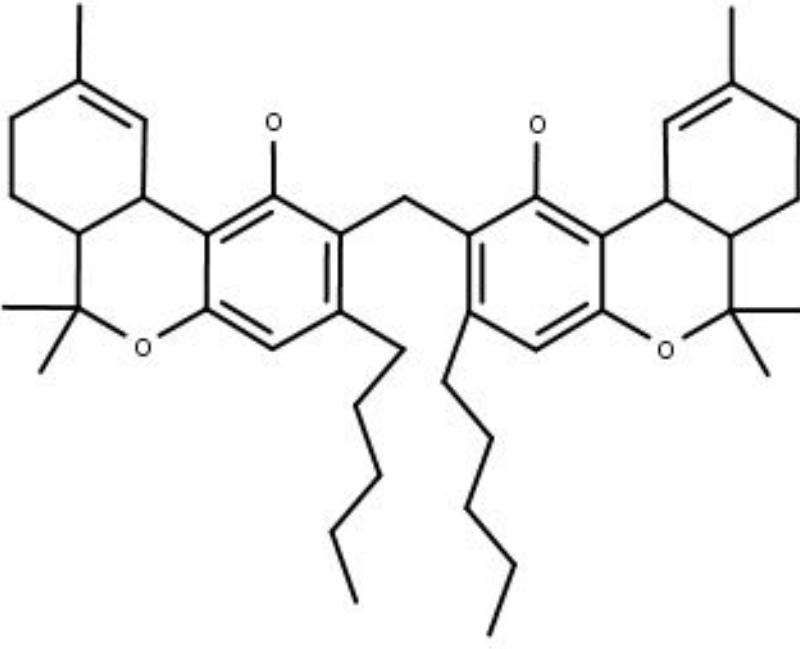
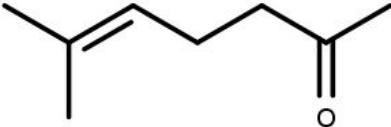
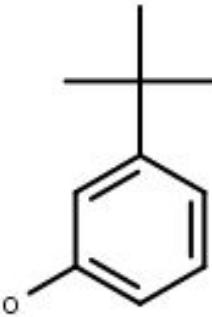
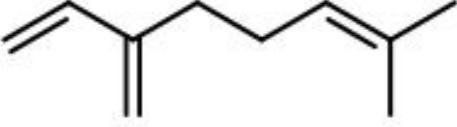
C362	Linoleic acid	<p>Chemical structure of Linoleic acid: A 16-carbon chain with two cis double bonds at positions 9 and 12, and a terminal carboxylic acid group.</p>
C363	Longifolene	<p>Chemical structure of Longifolene: A bicyclic diterpenoid with a decalin core, a cyclohexene ring fused to one of the decalin rings, and a methyl group on the cyclohexene ring.</p>
C364	Luteolin	<p>Chemical structure of Luteolin: A tricyclic flavonoid with a 2',3'-cyclic chalcone core, two 4'-hydroxyphenyl groups, and two 3-hydroxyphenyl groups.</p>

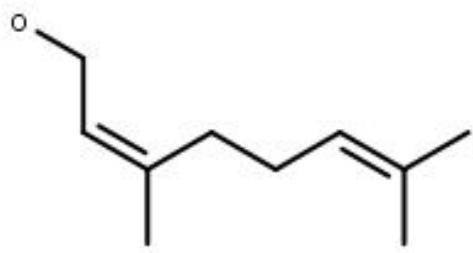
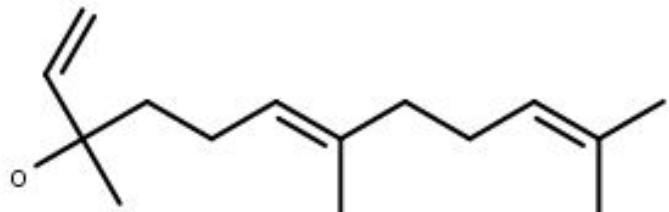
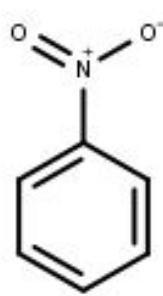
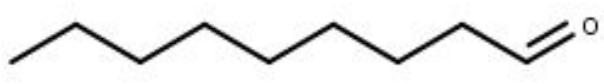
C365	Machaeridiol A	 The chemical structure of Machaeridiol A consists of a cyclohexane ring substituted with a methyl group at the 2-position and a chiral center at the 3-position. The chiral center is bonded to a phenylpropenyl group, a methoxy group, and two other groups. An acetyl group is attached to the cyclohexane ring at the 4-position.
C366	Machaeridiol B	 The chemical structure of Machaeridiol B is similar to Machaeridiol A, but it features a different substituent on the phenylpropenyl group. Instead of a methoxy group, it has a phenoxy group (a phenyl ring attached to an oxygen atom).

C367	Machaeridiol C	
C368	Machaeridiol D	
C369	m-Cymene	
C370	Methacrolein	
C371	Methacrylic anhydride	

C372	Methyl acetate	
C373	Methyl acetylsalicylate	
C374	Methyl anthranilate	
C375	Methyl Benzoate	
C376	Methyl carbamate	

C377	Methyl heptadienone	
C378	Methyl heptanoate	
C379	Methyl Hydrazine	
C380	Methyl isoeugenol	
C381	Methyl Salicylate	
C382	Methyl valerate	

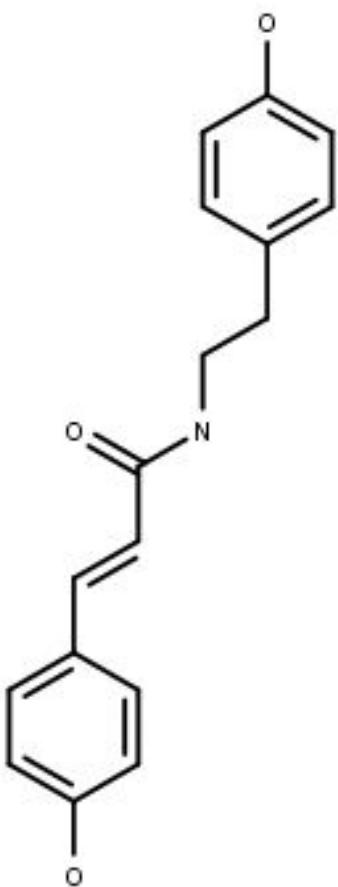
C383	Methylene Chloride	
C384	Methylen-bis-Delta-9-tetrahydrocannabinol	
C385	Methylisohexenyl ketone	
C386	m-Tert-Butyl Phenol	
C387	Myrcene	

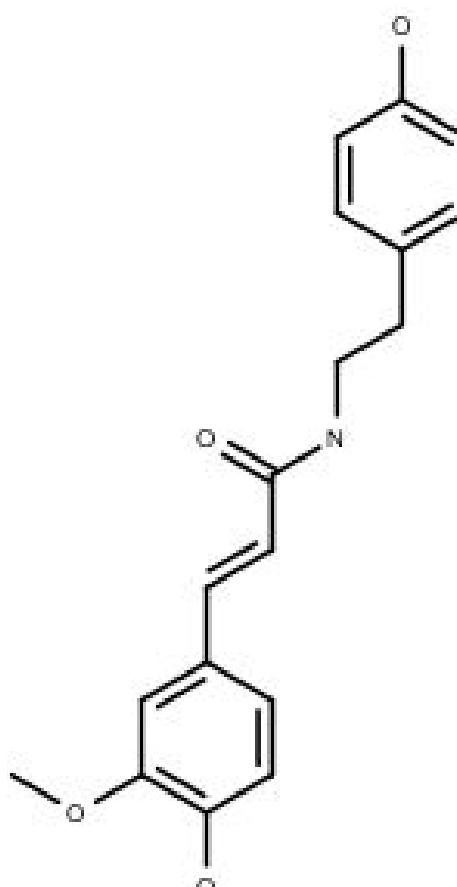
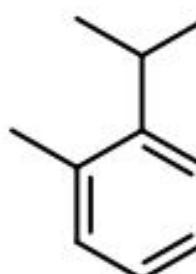
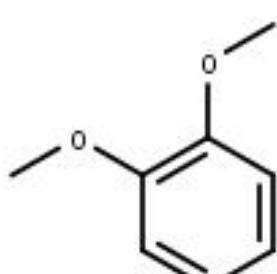
C388	Nerol	
C389	Nerolidol	
C390	Nitrobenzene	
C391	Nonanal	
C392	Nonane	

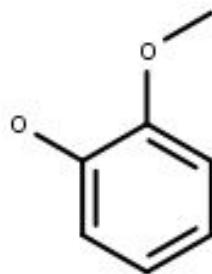
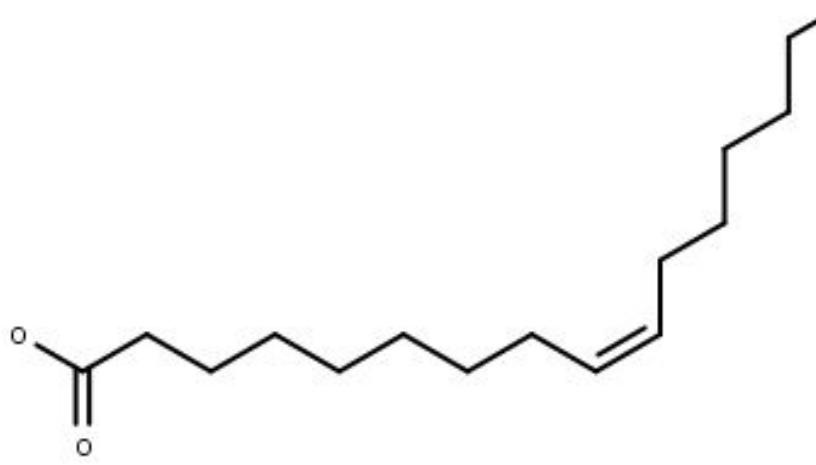
C393	nor-Cannabidiol	
C394	nor-Cannabinol	
C395	nor-Cannabivarin	

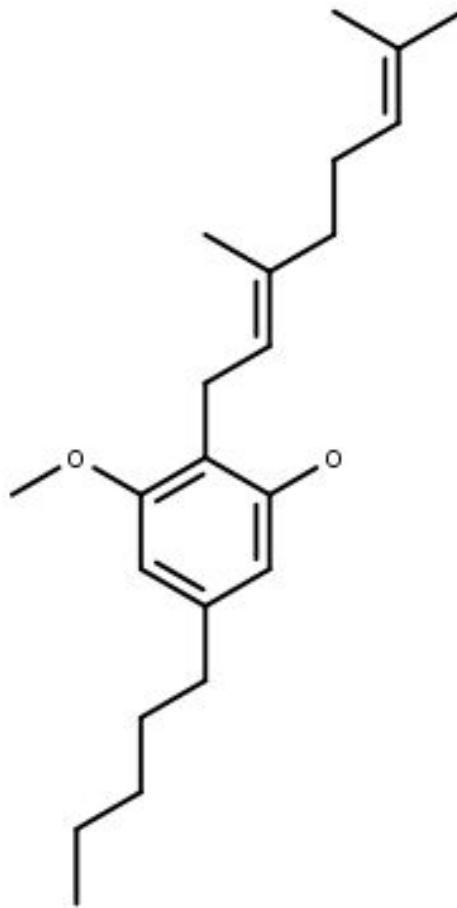
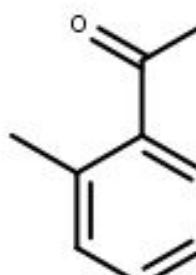
C396

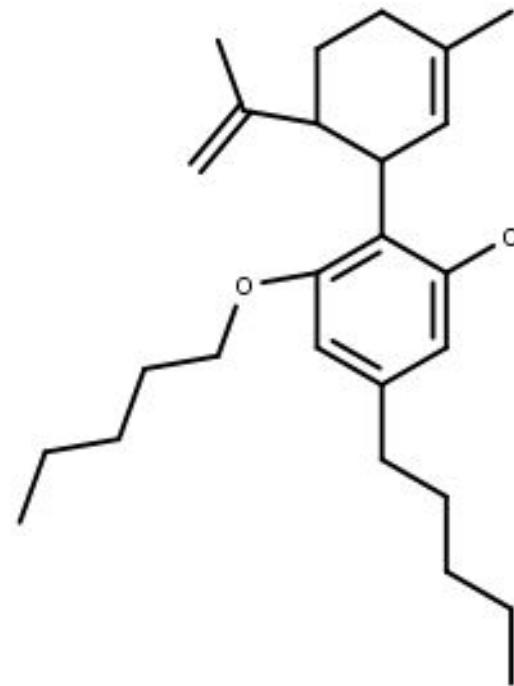
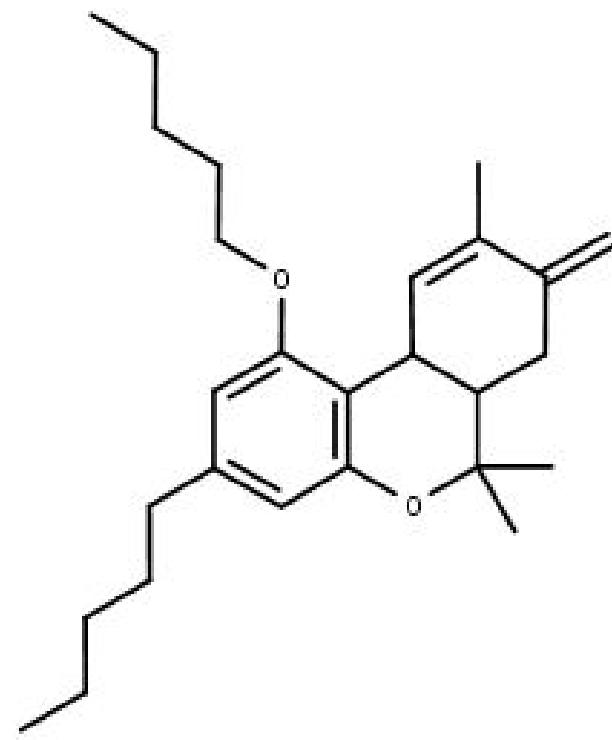
N-p-Coumaroyltyramine

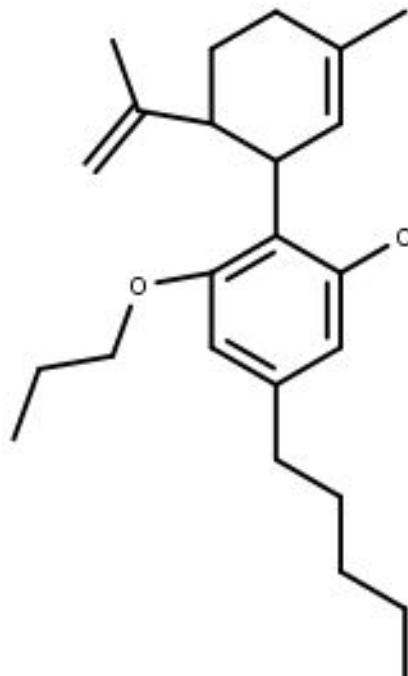
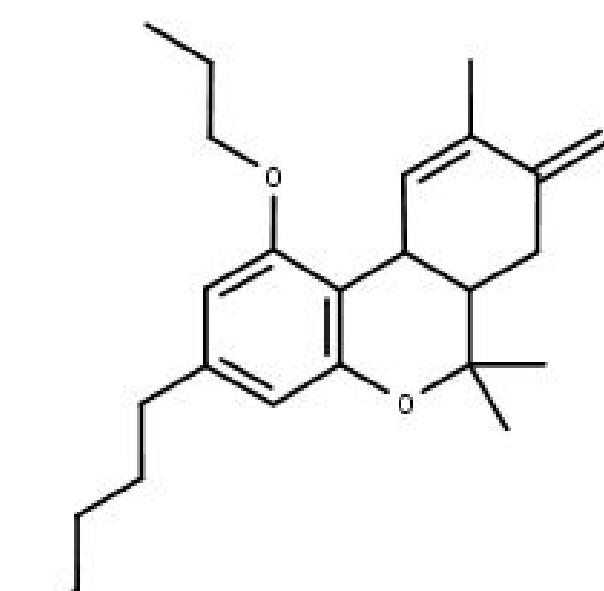


C397	N-trans-feruloyltyramine	 The chemical structure of N-trans-feruloyltyramine is shown. It consists of a tyramine molecule (4-hydroxy-N-methylphenylalanine) where the amine group (-NH ₂) is replaced by a trans-feruloyl group (-CH=CH-C(=O)-CH ₂ -C ₆ H ₃ (OH)(OCH ₃) ₂).
C398	Octanal	 The chemical structure of Octanal is shown. It is a straight-chain aldehyde with eight carbon atoms: CH ₃ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CHO.
C399	o-Cymene	 The chemical structure of o-Cymene is shown. It is a benzene ring with two methyl groups at the ortho positions (positions 1 and 2).
C400	o-Dimethyl Hydroquinone	 The chemical structure of o-Dimethyl Hydroquinone is shown. It is a benzene ring with a hydroxyl group at position 1 and two methyl groups at position 2.

C401	O-Guaiacol	
C402	Oleic acid	

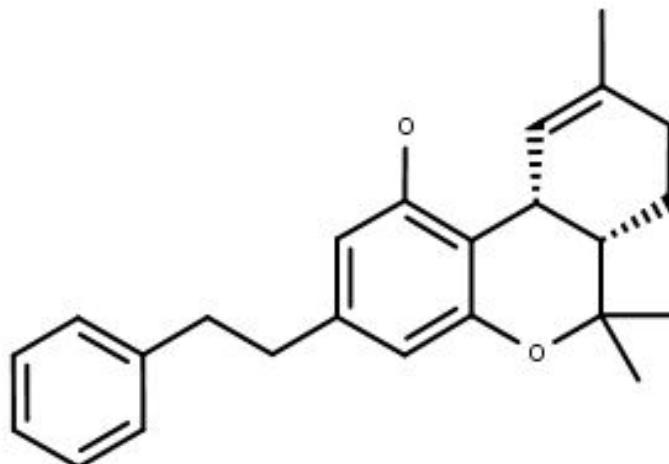
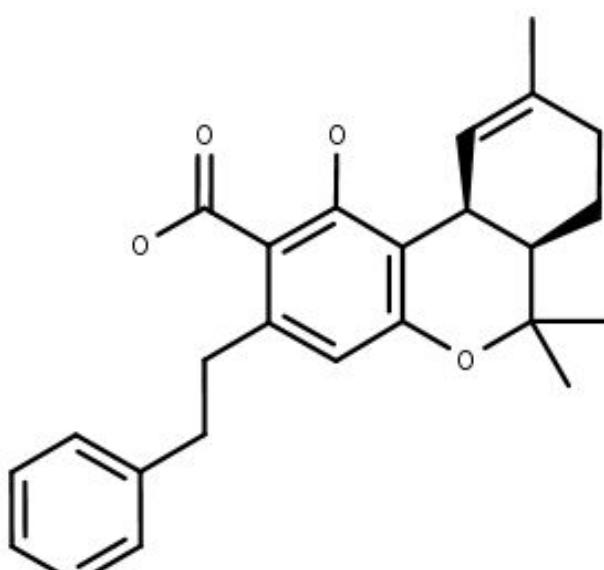
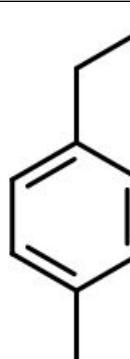
C403	O-Methyl Cannabigerol	 The chemical structure of O-Methyl Cannabigerol is shown. It features a central cyclohexene ring substituted with a methoxy group (-OCH ₃) at the 2-position and a carbonyl group (=O) at the 6-position. A long, branched hydrocarbon chain is attached to the 3-position of the ring. The chain consists of a pentyl group (-CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₃), followed by a trans double bond between the 4th and 5th carbons, and a final isopropylidene group (=C(CH ₃) ₂) at the 6th carbon.
C404	O-Methyl Acetophenone	 The chemical structure of O-Methyl Acetophenone is shown. It consists of a benzene ring substituted with a methyl group (-CH ₃) at the 1-position and a carbonyl group (=O-C(=O)-) at the 2-position.

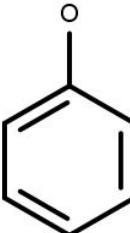
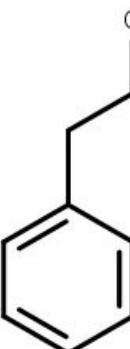
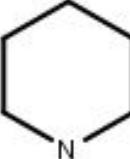
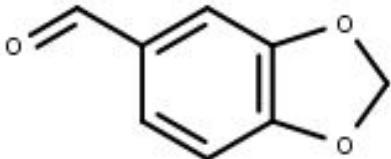
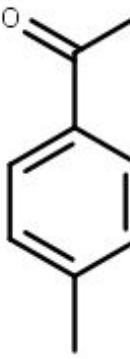
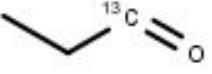
C405	O-Pentyl-cannabidiol	 The chemical structure of O-Pentyl-cannabidiol features a pentyl group attached to the C13 position of a cannabidiol molecule. The pentyl group is a five-carbon chain. The cannabidiol core consists of a central cyclohexene ring fused with a cyclobutene ring. The C13 position is substituted with a pentyl group, and the C15 position is substituted with a methyl group.
C406	O-Pentyl-Delta-9-tetrahydrocannabinol	 The chemical structure of O-Pentyl-Delta-9-tetrahydrocannabinol features a pentyl group attached to the C13 position of a tetrahydrocannabinol molecule. The pentyl group is a five-carbon chain. The tetrahydrocannabinol core consists of a central cyclohexene ring fused with a cyclobutene ring. The C13 position is substituted with a pentyl group, and the C15 position is substituted with a methyl group.

C407	O-Propyl-cannabidiol	 The chemical structure of O-Propyl-cannabidiol is shown. It features a central cyclohexene ring substituted at the 2-position with a 2-methylpropyl group (isopropylidene) and at the 3-position with a 2-propenyl group (prop-1-enyl). Attached to the 3-position is a 2-methylphenyl ring, which is further substituted at the para position with a prop-1-enyl group and at the meta position with a propoxy group (-O-CH2-CH3).
C408	O-Propyl-Delta-9-tetrahydrocannabinol	 The chemical structure of O-Propyl-Delta-9-tetrahydrocannabinol is shown. It consists of a tricyclic core (cannabinol skeleton) with a 2-propenyl group at the C-10 position. Attached to the C-10 position is a 2-methylphenyl ring, which is substituted at the para position with a propoxy group (-O-CH2-CH3) and at the meta position with a 2-propenyl group (prop-1-enyl). A long-chain propyl side chain is attached to the C-1 position.

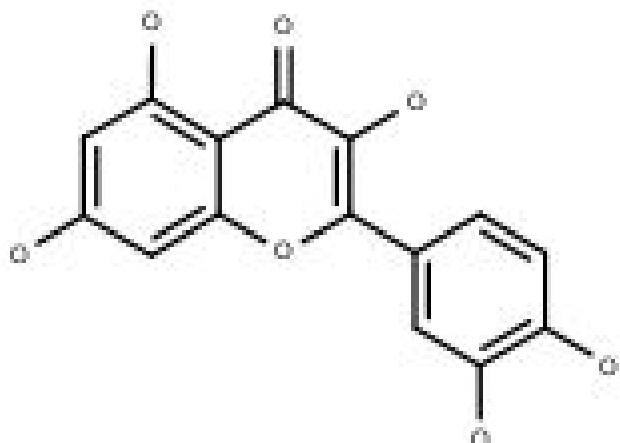
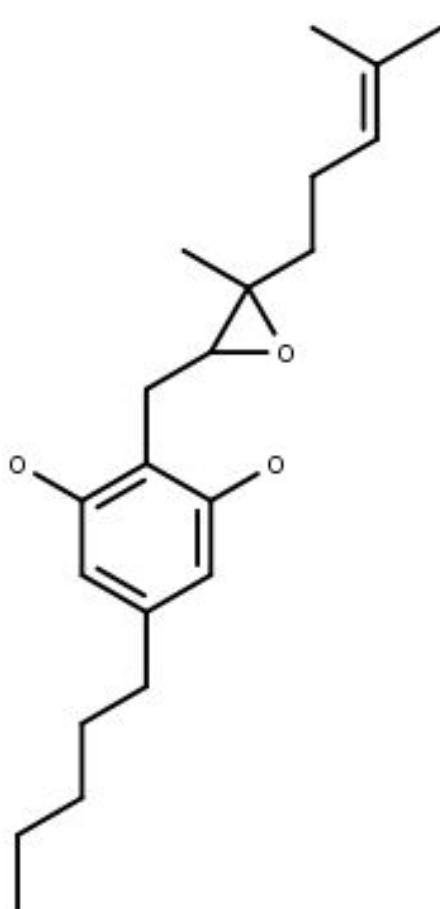
C409	Orientin	
C410	O-Xylene	
C411	P-Acetanisole	
C412	P-Aminotoluene	

C413	P-Cymene	
C414	Pentadecane	
C415	Pentamethylbenzene	
C416	Pentanal	
C417	Perillaldehyde	

C418	Perrottetinene	
C419	Perrottetinenic acid	
C420	P-ethyl Toulene	

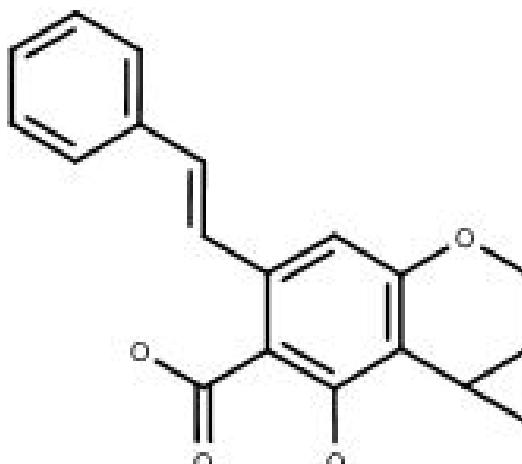
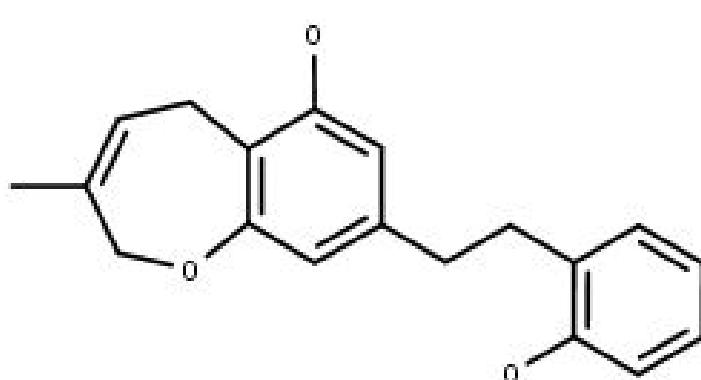
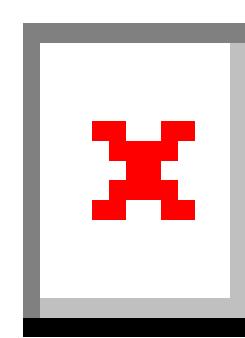
C421	Phenol	
C422	Phenylethyl alcohol	
C423	Piperidine	
C424	Piperonal	
C425	P-Methyl Acetophenone	
C426	Propanal	

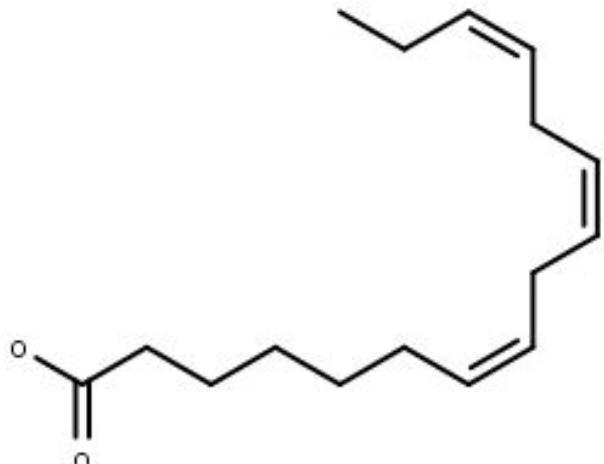
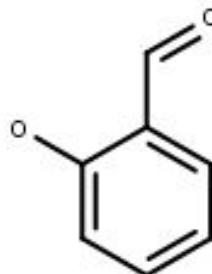
C427	Propofol	
C428	Propanoic acid,anhydride	
C429	Propylamine	
C430	Propylene Glycol	
C431	P-Tert-Butylphenol	
C432	P-Xylene	

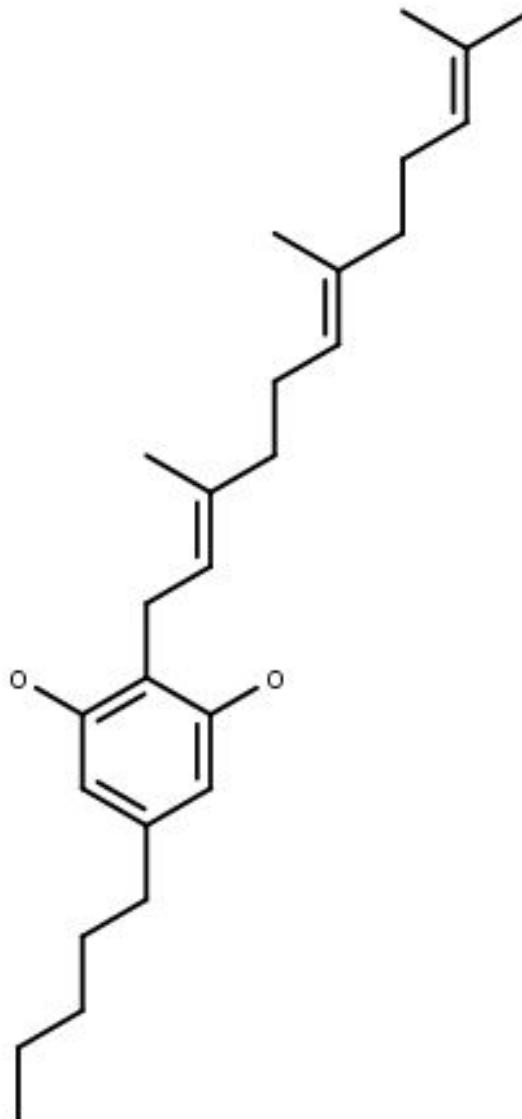
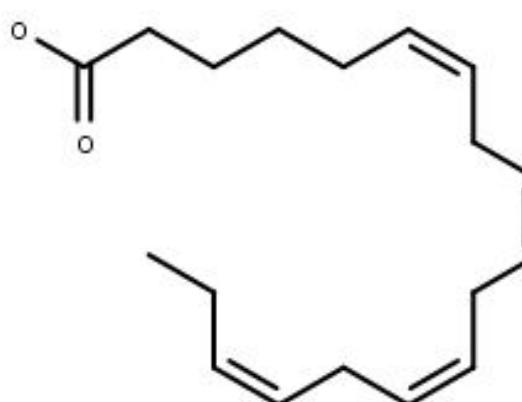
C433	Quercetin	 The chemical structure of Quercetin is shown. It consists of a central 3,5-dihydroxy-2H-1,4-benzodioxole-7-one ring system. This core is substituted at the 3 and 5 positions with hydroxyl groups (-OH). At the 7 position, there is a methoxyl group (-OCH3) and a 4-hydroxyphenyl ring attached via a methylene bridge. The 4-hydroxyphenyl ring has a hydroxyl group (-OH) at its para position.
C434	rac-6'-Epoxycannbigerol	 The chemical structure of rac-6'-Epoxycannbigerol is shown. It features a cannabigerol (CBG) skeleton, which is a tricyclic diterpenoid. The molecule includes a phytol side chain (a branched, hydrocarbon tail) attached to the CBG core. A key feature is a epoxide group (an oxygen atom bridging two carbons) located on the phytol side chain, specifically at the C6' position relative to the CBG core.

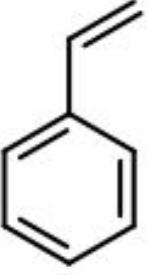
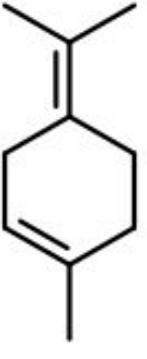
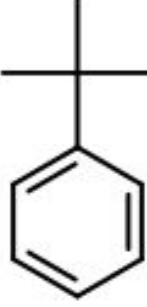
C435	rac-6'-Epoxycannbigerolic acid	
C436	Radulanin A	

C437	Radulanin H	
C438	Radulanin I	
C439	Radulanin J	

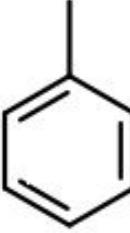
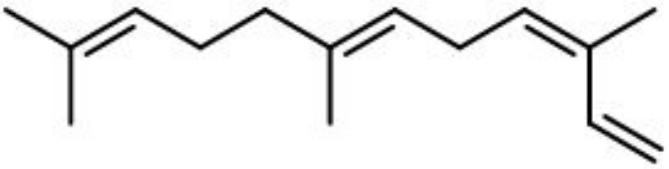
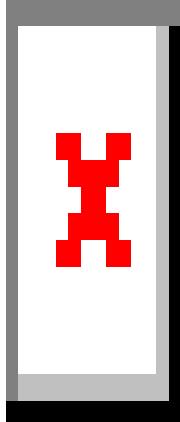
C440	Radulanin K	
C441	Radulanin L	
C442	Rhododaurichromanic A	

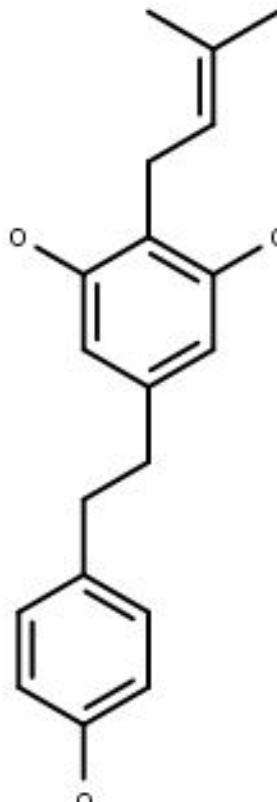
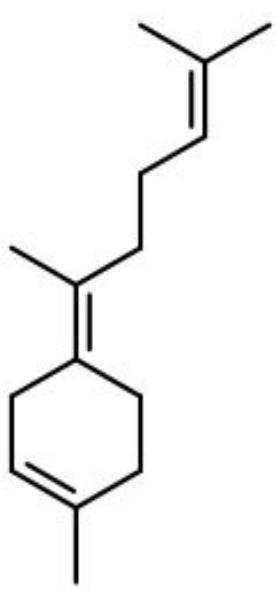
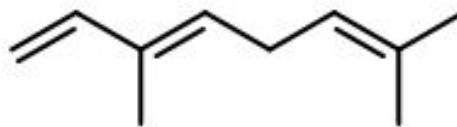
C443	Roughanic acid	
C444	Sabinene	
C445	Salicylaldehyde	
C446	Sativene	

C447	Sesquicannabigerol	 The chemical structure of Sesquicannabigerol is shown. It features a central pentyl chain with two double bonds at positions 2 and 4. At the 1-position, there is a phenyl ring substituted with two acetyl groups (-COCH ₃). The 5-position of the phenyl ring has a methyl group.
C448	Stearidonic acid	 The chemical structure of Stearidonic acid is shown. It consists of a cyclohexene ring with a double bond at the 2-position. Attached to the 1-position is a propyl chain, and attached to the 3-position is a pentadienyl chain.

C449	Styrene	
C450	Tert-butyl alcohol	
C451	Terpinolene	
C452	tert-butyl-benzene	

C453	Tetrahydrocannabinol epoxide	
C454	Tetrahydrozoline	
C455	Thymol	

C456	Toluene	
C457	Trans-alpha-farnesene	
C458	Trans-Archidin-1	

C459	Trans-Archipin-2	
C460	Trans-gamma-bisabolene	
C461	Trans-ocimene	

C462	Tridecane	
C463	Tyramine	
C464	Undecane	
C465	Valencene	
C466	Verbenone	

C467	Vitexin	
C468	N-trans-caffeooyltyramine	