

Supporting information to

CBD, a precursor of THC in e-cigarettes

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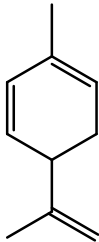
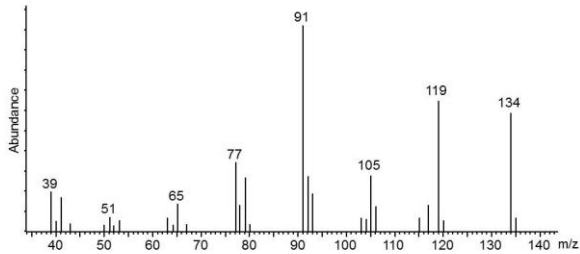
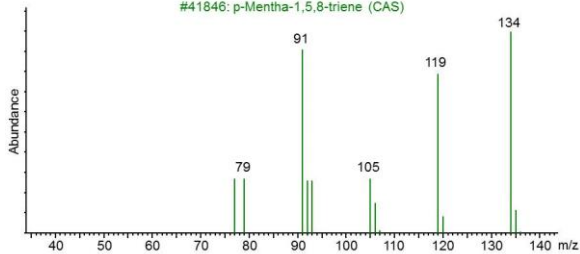
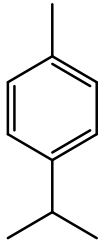
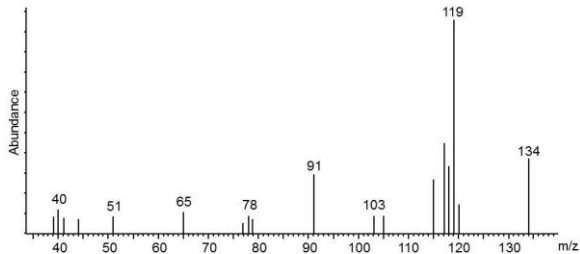
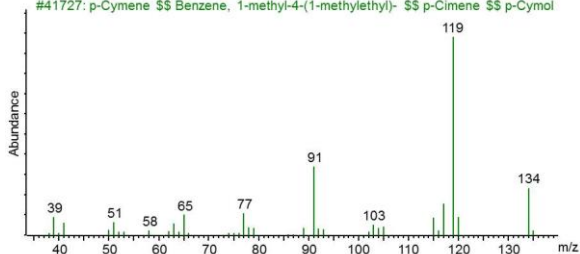
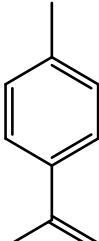
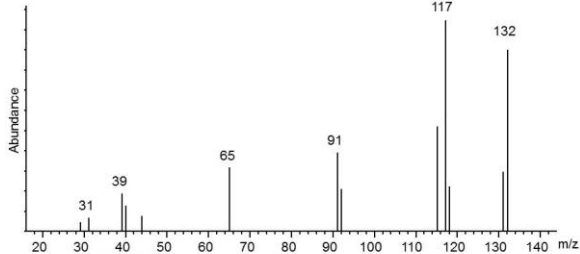
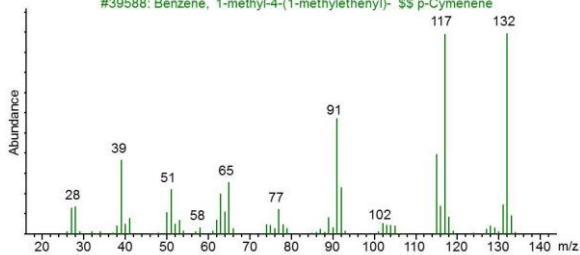
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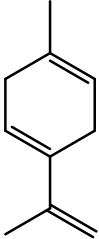
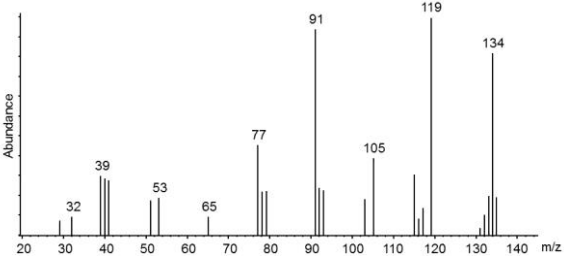
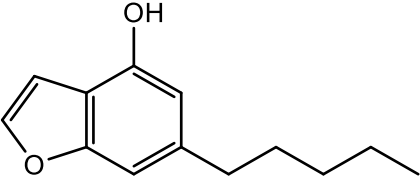
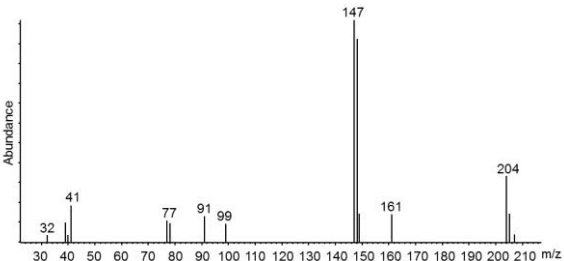
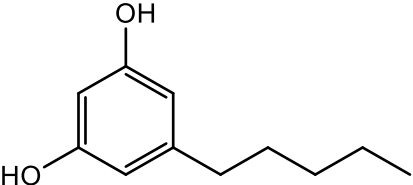
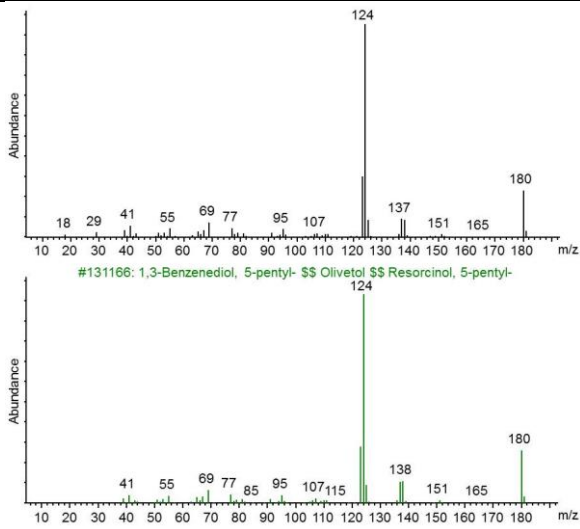
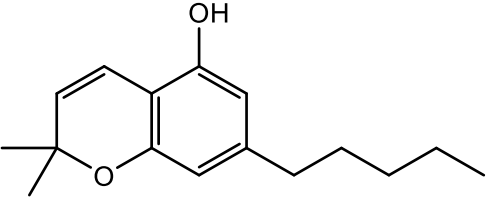
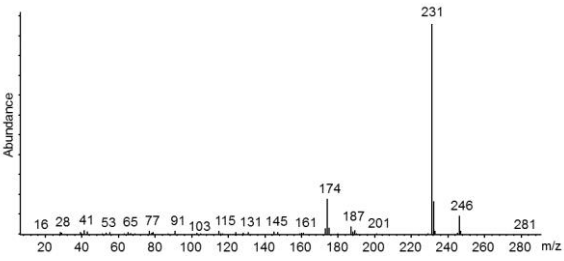
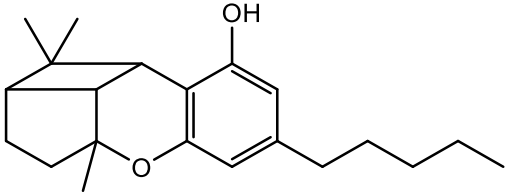
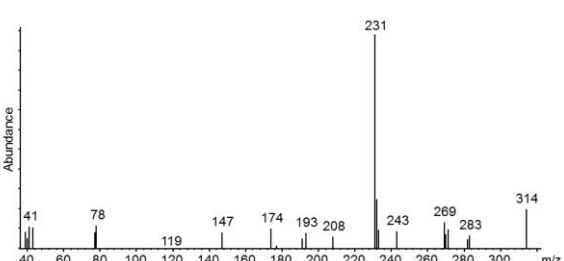
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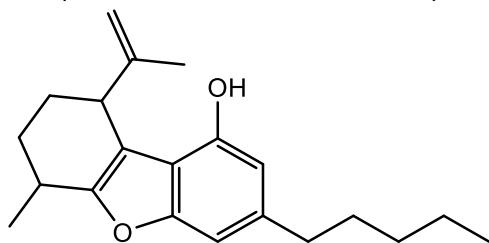
Table S1. EI mass spectra of the detected CBD decomposition products. Library mass spectra for comparison are also indicated in the cases of the identified components.

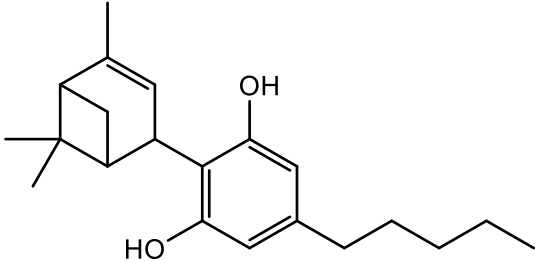
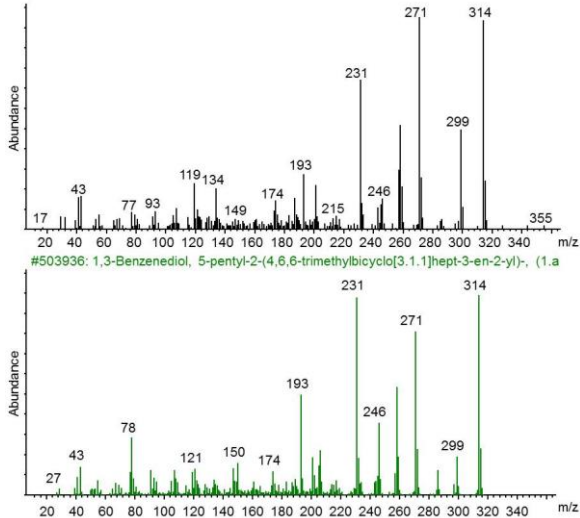
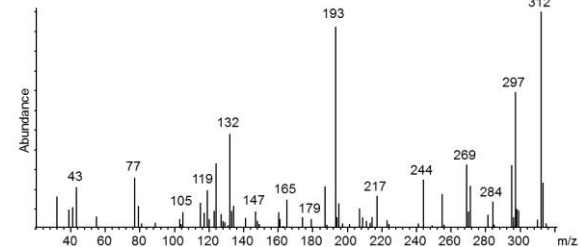
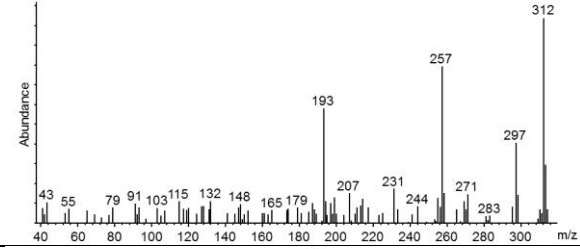
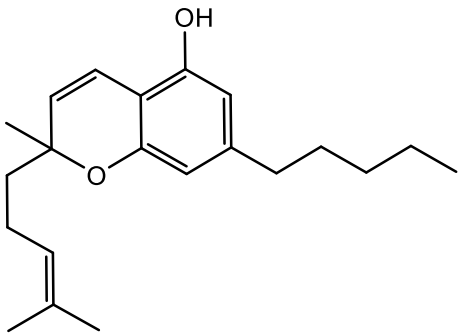
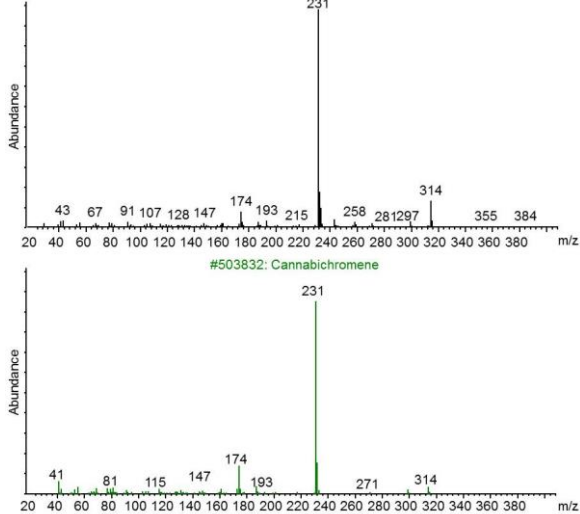
#	Compound	t _R (min)	Mw (g/mol)	EI mass spectra
1	Unidentified monoterpene	11.62	134	
2	<i>p</i>-Mentha-1,3,8-triene	12.76	134	

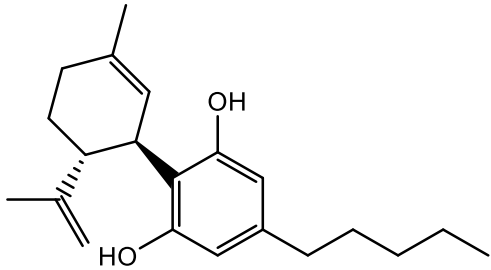
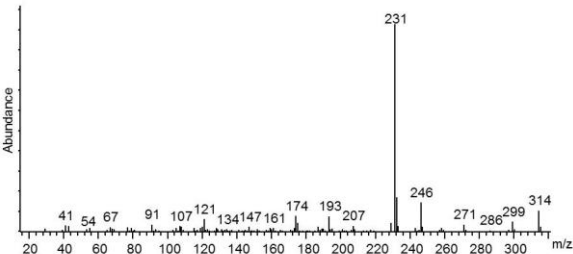
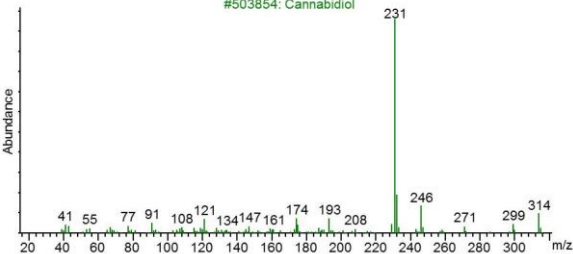
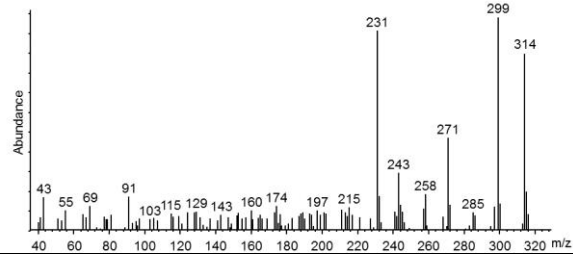
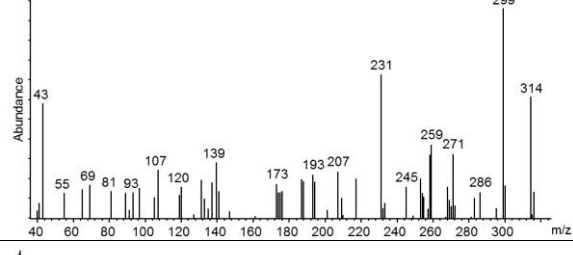
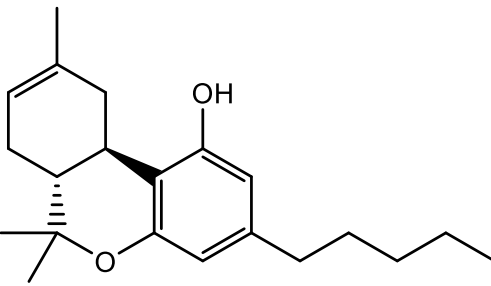
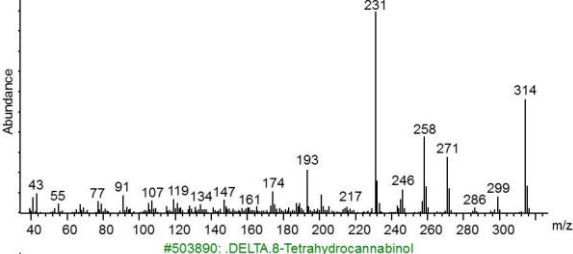
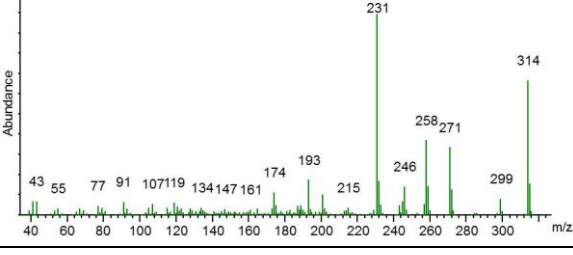
#	Compound	t_R (min)	Mw (g/mol)	El mass spectra
3	<i>p</i>-Mentha-1,5,8-triene 	13.17	134	 #41846: <i>p</i>-Mentha-1,5,8-triene (CAS) 
4	<i>p</i>-Cymene 	13.32	134	 #41727: <i>p</i>-Cymene \$\$ Benzene, 1-methyl-4-(1-methylethyl)- \$\$ <i>p</i>-Cimene \$\$ <i>p</i>-Cymol 
5	<i>p</i>-Cymenene 	14.83	132	 #39588: Benzene, 1-methyl-4-(1-methylethenyl)- \$\$ <i>p</i>-Cymenene 

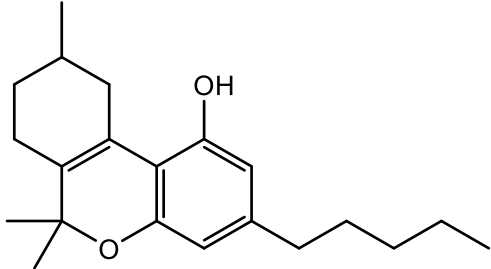
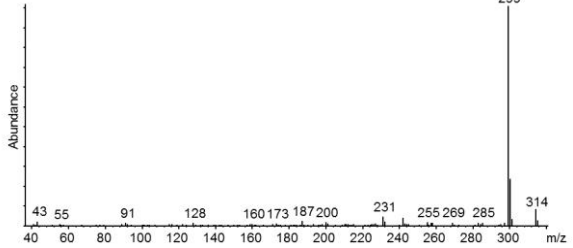
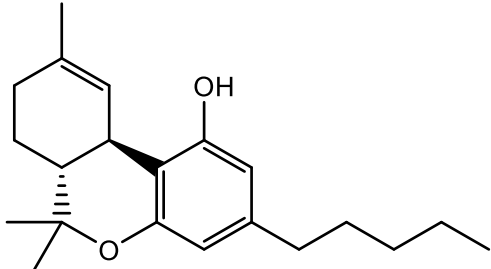
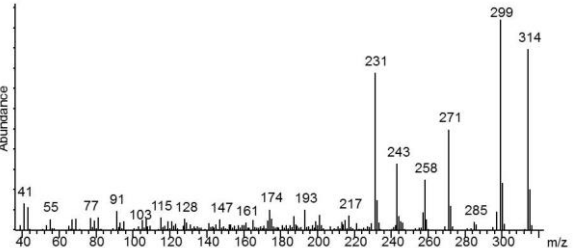
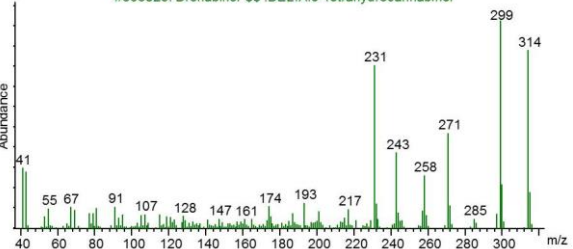
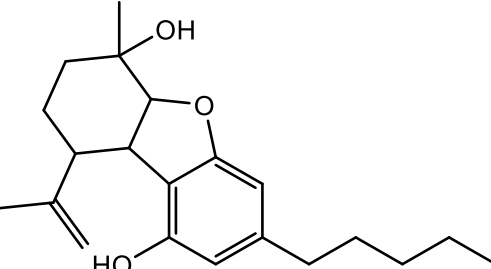
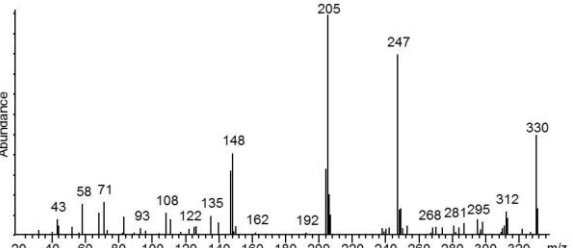
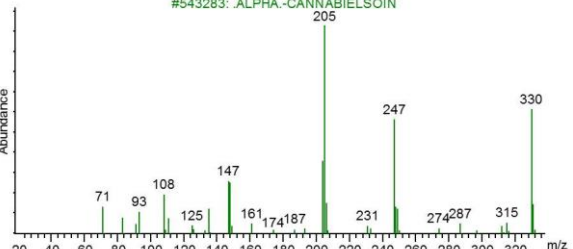
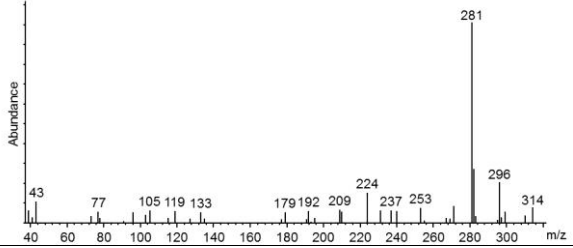
#	Compound	t_R (min)	Mw (g/mol)	El mass spectra
6	<i>p</i> -Mentha-1,4,8-triene 	14.92	134	
7	6-Pentylbenzofuran-4-ol (identification based on Ref.25 and Ref.29) 	25.99	204	
8	Olivetol 	26.43	180	
9	2,2-Dimethyl-7-pentyl-2 <i>H</i> -chromen-5-ol (identification based on Ref.25) 	27.21	246	
10	Cannabicyclol (identification based on Ref.26) 	29.74	314	

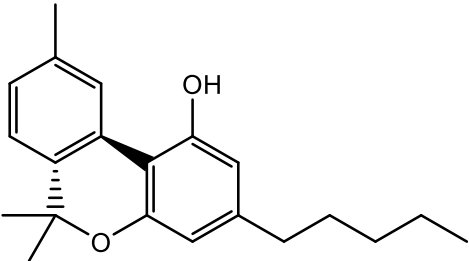
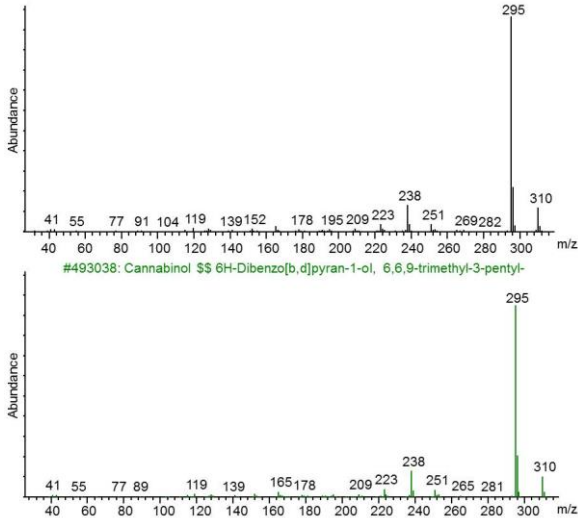
#	Compound	t _R (min)	Mw (g/mol)	El mass spectra
11	Unidentified	29.83	314	
12	Unidentified A	29.98	312	
13	Unidentified	30.08	314	
14	6-Methyl-3-pentyl-9-(propan-2-ylidene)- 5a,6,7,8,9,9a-hexahydrodibenzo[b,d]- furan-1-ol (identification based on Ref. 27)	30.28	314	
15	Unidentified	30.45	312	



#	Compound	t _R (min)	Mw (g/mol)	El mass spectra
16	5-Pentyl-2-(4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-yl)benzene-1,3-diol 	30.51	314	 #503936: 1,3-Benzenediol, 5-pentyl-2-(4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-yl)-, (1a)
17	Unidentified	30.54	312	
18	Unidentified B	30.61	312	
19	Cannabichromene 	30.73	314	 #503832: Cannabichromene

#	Compound	t_R (min)	Mw (g/mol)	El mass spectra
20	CBD 	30.81	314	 #503854: Cannabidiol 
21	Unidentified C	31.10	314	
22	Unidentified D	31.15	314	
23	Δ^8-THC 	31.25	314	 #503890: DELTA,8-Tetrahydrocannabinol 

#	Compound	t _R (min)	M _w (g/mol)	El mass spectra
24	$\Delta^{6a,10a}$ -THC (identification based on Ref. 28) 	31.39	314	
25	Δ^9 -THC 	31.48	314	 
26	Cannabielsoin 	31.50	330	 
27	Unidentified E*	31.81	314	

#	Compound	t _R (min)	M _w (g/mol)	El mass spectra
28	Cannabinol  The chemical structure of Cannabinol (C₂₁H₃₂O₃) is shown. It consists of a dibenzopyran core. The pyran ring has a hydroxyl group at position 1 and a pentyl group at position 3. The pyran oxygen is connected to a quaternary carbon which is also bonded to two methyl groups and a propyl group. The benzene ring fused to the pyran has a methyl group at position 6.	32.41	310	 Mass spectrum of Cannabinol. The x-axis represents the mass-to-charge ratio (m/z) from 40 to 320, and the y-axis represents relative abundance. The base peak is at m/z 295. Other significant peaks are labeled at m/z 41, 55, 77, 91, 104, 119, 139, 152, 178, 195, 209, 223, 238, 251, 269, 282, and 310. #493038: Cannabinol \$ 6H-Dibenzo[b,d]pyran-1-ol, 6,6,9-trimethyl-3-pentyl-