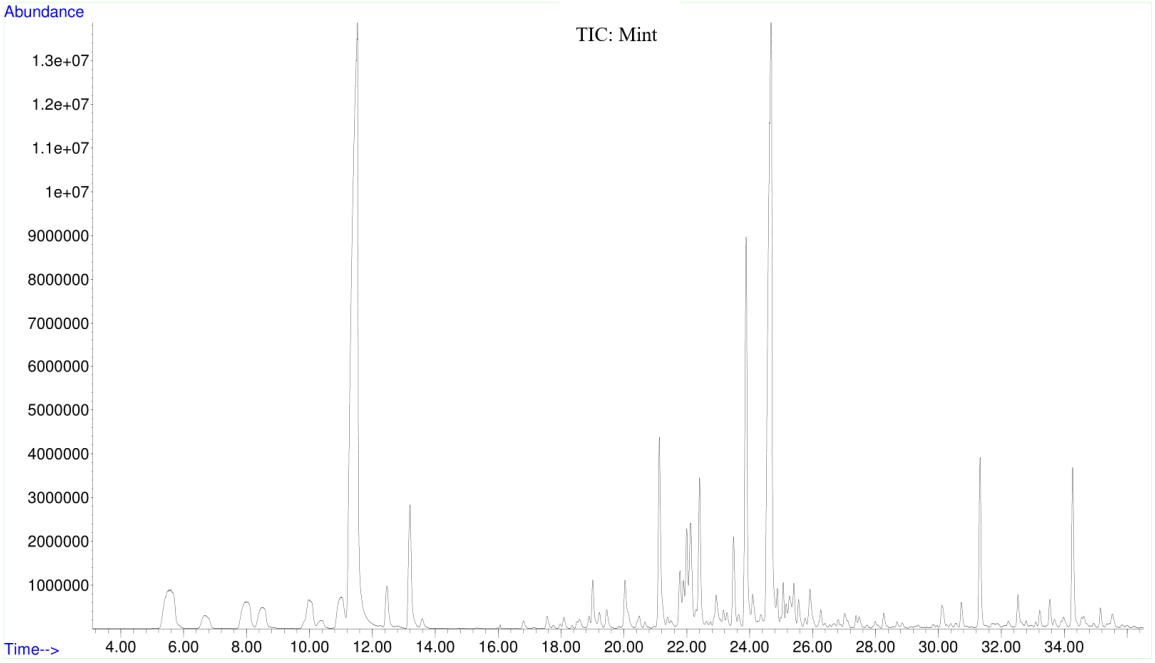
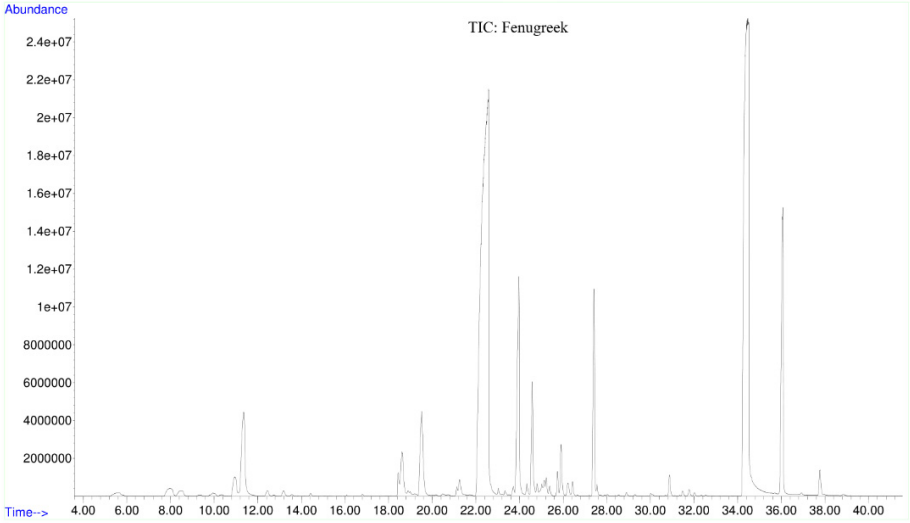
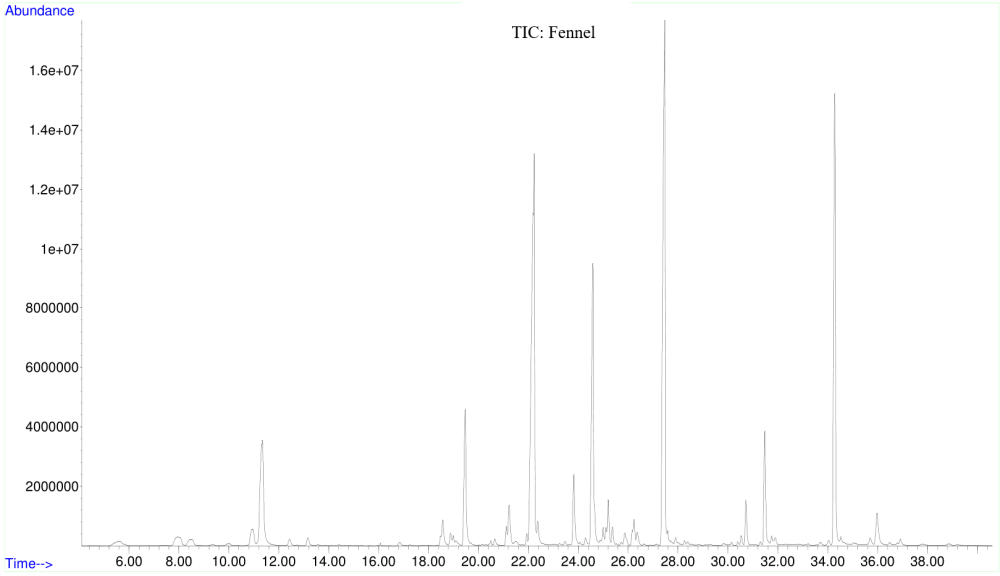
Supplementary Materials

LC-MS/MS and GC-MS Identification of Metabolites from the Selected Herbs and Spices, Their Antioxidant, Anti-diabetic Potential, and Chemometric Analysis




Abundance
TIC: Fenugreek
2.4e+07
2.2e+07
2e+07
1.8e+07
1.6e+07
1.4e+07
1.2e+07
1e+07
8000000
6000000
4000000
2000000
Time-->
4.00 6.00 8.00 10.00 12.00 14.00 16.00 18.00 20.00 22.00 24.00 26.00 28.00 30.00 32.00 34.00 36.00 38.00 40.00


Abundance
TIC: Fennel
1.6e+07
1.4e+07
1.2e+07
1e+07
8000000
6000000
4000000
2000000
Time-->
6.00 8.00 10.00 12.00 14.00 16.00 18.00 20.00 22.00 24.00 26.00 28.00 30.00 32.00 34.00 36.00 38.00

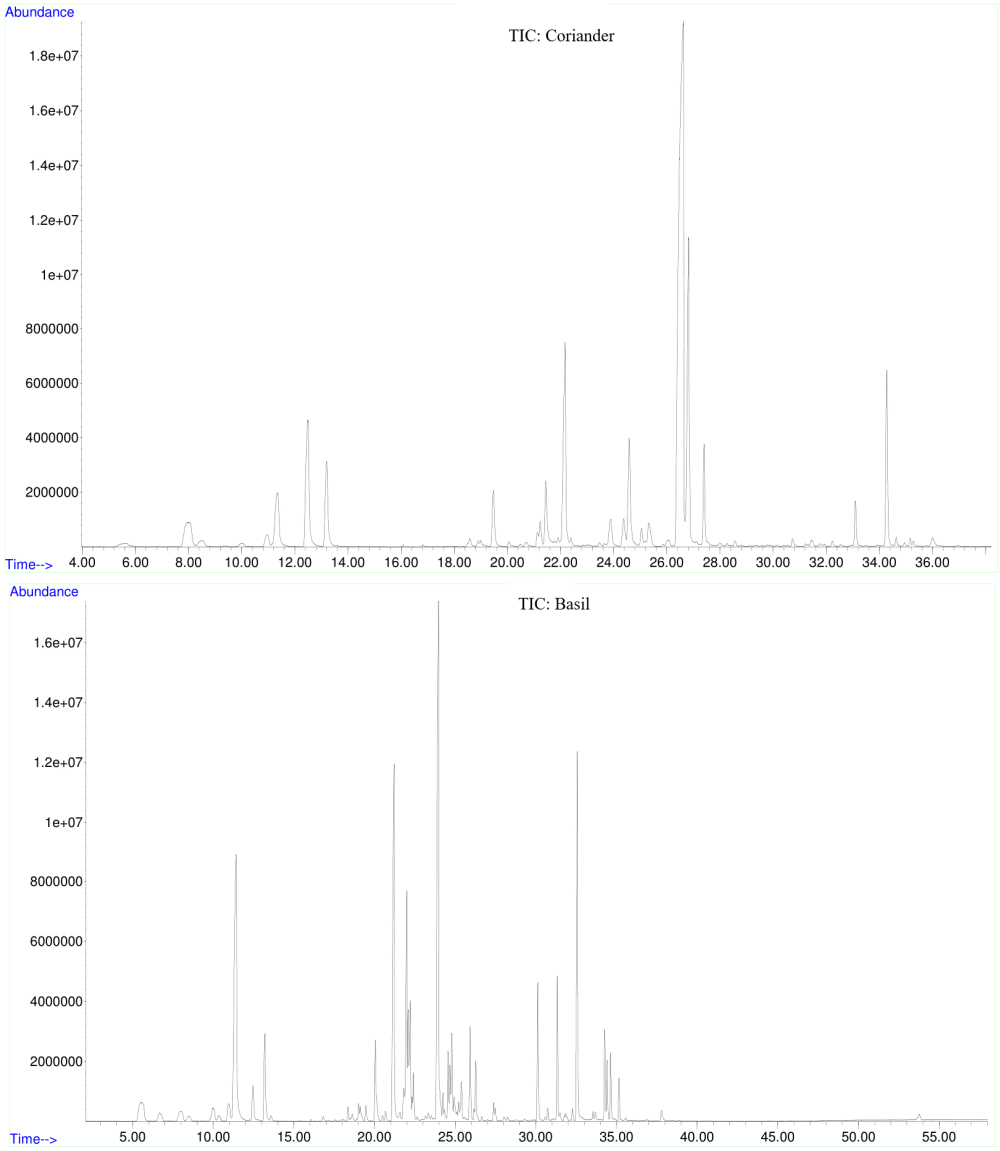
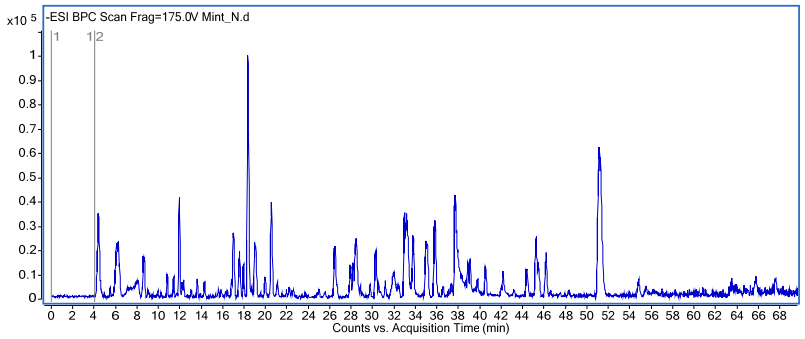
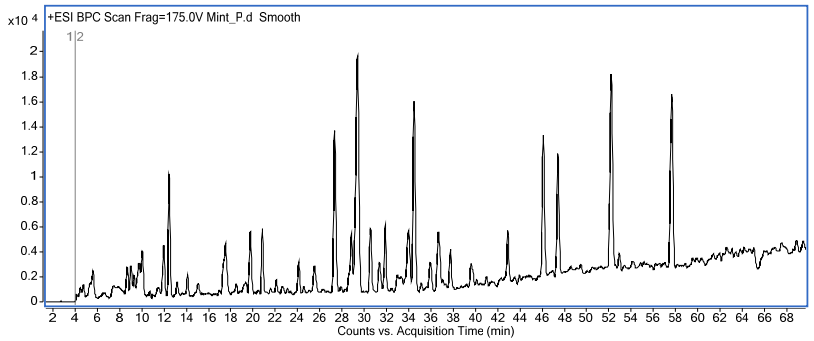
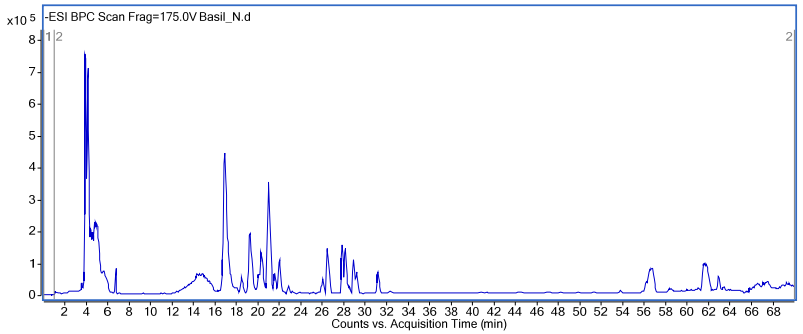
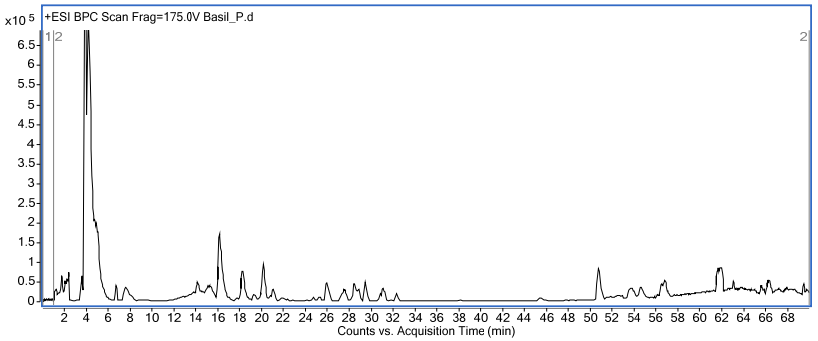


Figure S1. Total Ion Chromatograms (TIC) of fenugreek, mint, coriander, fennel, and basil using GC-MS are presented.


-ESI BPC Scan Frag=175.0V Mint_N.d
x10 5
Counts vs. Acquisition Time (min)


+ESI BPC Scan Frag=175.0V Mint_P.d Smooth
x10 4
Counts vs. Acquisition Time (min)


-ESI BPC Scan Frag=175.0V Basil_N.d
x10 5
Counts vs. Acquisition Time (min)


+ESI BPC Scan Frag=175.0V Basil_P.d
x10 5
Counts vs. Acquisition Time (min)

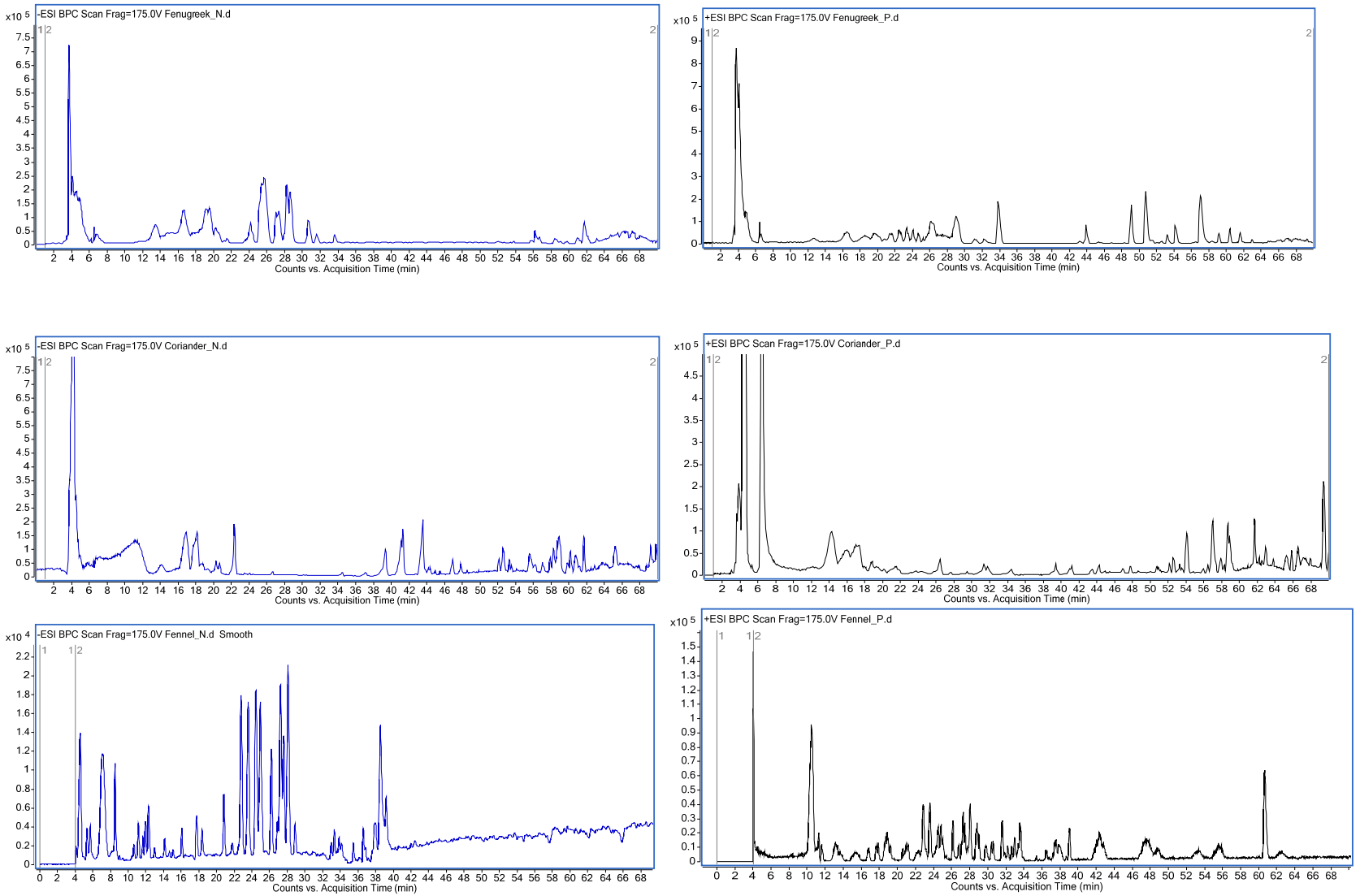


Figure S2. Base peak chromatograms (BPC) of mint, fennel, basil, coriander, and fenugreek in positive and negative modes

Table S1. Quantification/Semi quantification of abundant phenolic compounds (µg/g)

No.	Compounds	Mint	Basil	Fennel	Coriander	Fenugreek
1	Rosmarinic Acid	416.16 ± 19.13	307.27 ± 21.56	16.49 ± 2.04		43.63 ± 5.41
2	3-*p*-Coumaroylquinic acid			9.24 ± 0.08	23.43 ± 1.19	
3	3-Sinapoylquinic acid	114.73 ± 2.41	107.34 ± 4.98	8.93 ± 0.30		12.26 ± 1.06
4	5-Feruloylquinic acid		80.20 ± 5.11			
5	*p*-Coumaric acid	30.96 ± 0.24	144.63 ± 4.72	30.63 ± 0.12	22.43 ± 1.07	32.97 ± 0.23
6	*p*-Hydroxybenzoic acid		124.83 ± 15.83	73.39 ± 5.74		
7	Gallic Acid		74.46 ± 4.56	7.09 ± 0.06	17.03 ± 2.13	72.14 ± 1.50
9	Caffeic acid	157.82 ± 8.62	107.43 ± 12.93	52.25 ± 5.11	37.45 ± 3.31	11.66 ± 0.58
10	Chicoric acid	19.65 ± 1.43	17.21 ± 1.06			74.03 ± 2.25
11	Chlorogenic acid	38.76 ± 4.32	384.07 ± 12.39	29.07 ± 0.98	113.07 ± 11.09	147.52 ± 17.41
12	Cinnamic acid	22.40 ± 1.68	36.87 ± 3.20		14.08 ± 1.24	125.13 ± 13.81
13	Protocatechuic acid	35.47 ± 0.98	102.08 ± 11.43	43.57 ± 1.63		178.70 ± 19.34
14	Ferulic acid	30.77 ± 3.36	91.31 ± 2.56	15.92 ± 0.38	34.63 ± 3.17	
15	Diosmin	14.04 ± 0.47	45.17 ± 2.96	10.64 ± 0.46		31.46 ± 3.62
16	Catechin	74.03 ± 6.72	39.90 ± 1.26			36.06 ± 2.62
17	Epicatechin gallate		17.41 ± 1.73			
18	Kaempferol-3-glucoside		19.09 ± 0.83	2.59 ± 0.18		
19	Procyanidin B2	229.31 ± 11.52			11.05 ± 2.04	44.15 ± 2.87
20	Rosmanol	26.52 ± 0.88	16.45 ± 6.03			
21	Umbelliferone	52.41 ± 4.62	102.63 ± 24.94			
22	Sagerinic acid	402.63 ± 16.81	113.31 ± 9.29			
23	Carnosic acid	47.05 ± 3.27	71.29 ± 2.92	9.54 ± 0.40		
24	Carnosol	32.64 ± 2.39	92.25 ± 3.65			
25	Coumarin	52.49 ± 0.36	13.43 ± 0.97			110.51 ± 5.07
26	Syringic acid	44.82 ± 3.83	14.91 ± 0.62			
27	Gallocatechin	430.61 ± 19.62	25.03 ± 2.41			
28	Pyrogallol	10.56 ± 0.45		19.16 ± 0.47	24.52 ± 4.36	17.93 ± 0.77

Table S2. GC-MS analysis of culinary spices and herbs for volatile compounds (Peak area %)

No.	Target compounds	MF	RT	LRI	Mint	Fennel	Fenugreek	Coriander	Basil
1	α-Pinene	$C_{10}H_{16}$	5.614	1014	0.35	0.74	3.05	8.78	
2	β-Pinene	$C_{10}H_{16}$	8.036	1094	0.51		1.16		
3	β-Phellandrene	$C_{10}H_{16}$	8.526	1110	0.55	1.04		0.27	0.25
4	D-Limonene	$C_{10}H_{16}$	10.980	1186	1.1	1.7	3.43	4.01	
5	Estragole	$C_{10}H_{12}O$	11.355	1197		3.06			14.03
6	Eucalyptol	$C_{10}H_{18}O$	11.355	1197	3.39	11.1	1.46	4.69	11.97
7	γ-Terpinene	$C_{10}H_{16}$	12.492	1233	0.16		8.56	5.76	1.26
8	o-Cymene	$C_{10}H_{14}$	13.272	1258	0.18	0.48	2.23	3.43	2.81
9	Menthol	$C_{10}H_{20}O$	16.906	1319	24.07	0.51	2.43		
10	Acetic acid	$C_2H_4O_2$	18.524	1440	0.31	0.36	5.61	0.17	
11	Citral	$C_{10}H_{16}O$	18.542	1675	15.03				
12	α-Cubebene	$C_{15}H_{24}$	18.637	1444	1.1			0.41	0.13
13	(+)-2-Carene	$C_{10}H_{16}$	18.948	1456					1.31
14	p-Menth-8-en-1-ol	$C_{10}H_{18}O$	19.062	1460				0.13	0.01
15	α-Copaene	$C_{15}H_{24}$	19.570	1479	3.04	14.29		4.71	0.45
16	Camphor	$C_{10}H_{16}O$	20.025	1496			5.73	5.04	2.35
17	(+)-2-Bornanone	$C_{10}H_{16}O$	20.047	1504					2.57
18	Benzaldehyde	C_7H_6O	20.228	1504			3.02	0.25	
19	Linalool	$C_{10}H_{18}O$	21.276	1547	1.25	1.03	18.35	42.22	27.68
20	Terpinen-4-ol	$C_{10}H_{18}O$	22.413	1594				0.95	1.04
21	Caryophyllene	$C_{15}H_{24}$	22.477	1597	1.61	11.63	0.68	0.39	2.28
22	Cis-muurola-3,5-diene	$C_{15}H_{24}$	23.037	1621	0.09				
23	Humulene	$C_{15}H_{24}$	23.892	1658	2.77			2.02	4.22
24	(E)-Methyl cinnamate	$C_{15}H_{24}$	23.892	1658	5.77			2.02	14.22
25	γ-Muurolene	$C_{15}H_{24}$	24.376	1680	0.2				1.07
26	p-Menthone	$C_{10}H_{18}O$	24.403	1680	16.03				
27	β-curcumene	$C_{15}H_{24}$	24.418	1681			1.87		
28	1,6-Cyclodecadiene	$C_{10}H_{16}$	24.882	1702	0.14				
29	Octadecanal	$C_{18}H_{36}O$	24.915	1703		0.14			
30	1-Cyclohexene-1-carboxaldehyde	$C_7H_{10}O$	25.085	1711			1.74		

31	β-Bisabolene	$C_{15}H_{24}$	25.306	1721	1.17		0.79	0.54	
32	10s,11s-Himachala-3(12),4-diene	$C_{15}H_{24}$	25.372	1724					
33	D-Carvone	$C_{10}H_{14}O$	25.441	1727	0.12	0.56		0.62	0.86
34	α-Farnesene	$C_{15}H_{24}$	25.822	1745	0.37			0.53	
35	Anethole	$C_{10}H_{12}O$	27.534	1823	1.95	30.65	6.33	1.52	0.12
36	Geraniol	$C_{10}H_{18}O$	28.093	1848				2.36	0.04
37	Safrole	$C_{10}H_{10}O_2$	28.459	1864				0.15	
38	Benzyl alcohol	C_7H_8O	28.591	1870				0.13	
39	Caryophyllene oxide	$C_{15}H_{24}O$	30.761	1968	0.46			0.56	2.24
40	Methyleugenol	$C_{11}H_{14}O_2$	31.353	1995				0.51	5.16
41	Benzaldehyde, 4-methoxy-	$C_8H_8O_2$	31.511	2002	0.09	5.22		0.28	0.09
42	Cinnamaldehyde, (E)-	C_9H_8O	31.800	2015	0.12				0.11
43	p-Cymen-7-ol	$C_{10}H_{14}O$	33.139	2075			0.37		
44	Acetic acid, cinnamyl ester	$C_{11}H_{12}O_2$	34.021	2115				0.55	
45	Eugenol	$C_{10}H_{12}O_2$	34.309	2128	2.5	17.87	16.08	1.56	11.41
46	Thymol	$C_{10}H_{14}O$	34.63	2144	1.01				1.37
47	1,3-Benzodioxole	$C_7H_6O_2$	36.124	2210				0.2	
48	2-Propen-1-ol	C_3H_6O	36.655	2234				0.76	
49	2-Propenal	C_3H_4O	40.544	2409				2.5	

Linear retention index (LRI), molecular formula (MF), retention time (RT)

Table S3. The calculated binding energies of selected compounds

No.	Compounds	Binding energy (Kcal/mol)	Glide energy
1	Punicafolin	-12.16	−71.48
2	Rutin	-11.14	−69.71
3	Acarbose	-10.65	−58.26
4	Procyanidin B2	-10.05	−56.13
5	Punicalagin	-9.95	-72.90
6	Myricitrin	-9.59	63.23
7	3-Feruloylquinic acid	-9.32	59.38
8	Taxifolin	-9.13	-62.84
9	Diosmin	-8.77	−54.35
10	Chlorogenic acid	-8.17	−58.68
11	Quercetin-3-*O*-arabinoside	-7.59	51.48
12	Naringin	-7.58	-55.25
13	3-*p*-Coumaroylquinic acid	-7.38	-46.44
14	Myricetin	-6.92	-43.43
15	Apigenin 8-C-glucoside	-6.44	-40.31
16	Quercetin	-6.41	-39.43
17	Kaempferol	-6.01	-33.74
18	Ellagic acid	-5.94	-24.60
19	Carnosic acid	-5.91	-32.63
20	Isorhamnetin	-5.68	31.91
21	Luteolin	-5.67	-36.15
22	Hesperetin	-5.47	-25.08
23	(-)-Epicatechin	-5.36	31.65
24	Gallic acid	-5.10	-30.17
25	Protocatechuic acid	-4.96	-29.81
29	3-*O*-Sinapoylquinic acid	-4.91	30.62
26	Isorhamnetin	-4.89	-34.55
27	Caffeic acid	-4.87	-30.58
28	Pyrogallol	-4.80	-23.12
30	*p*-Hydroxybenzoic acid	-4.30	22.92
31	*p*-coumaric acid	-3.80	21.38
32	Cinnamic acid	-3.04	19.21