

Supplementary Materials

Table S1. Values of descriptors selected in SMLR and UFS-SMLR models.

Sr. No.	Compound	HNar	GATS2v	DISPe	Mor32e	Mp	IDM	DISPm	Mor22v	Mor28e
1	Gallic acid	1.565	1.177	0.065	−0.351	0.640	5.878	2.477	−0.025	0.126
2	Gentisic acid	1.610	1.168	0.374	−0.304	0.650	5.624	6.421	−0.073	−0.093
3	Protocatechuic acid	1.610	1.168	0.210	−0.253	0.650	5.606	4.129	−0.032	−0.068
4	Salicylic acid	1.667	1.157	0.464	−0.151	0.670	5.339	6.808	−0.035	−0.130
5	Syringic acid	1.615	0.668	0.066	−0.155	0.630	6.341	1.995	−0.072	−0.228
6	Vanillic acid	1.636	0.859	0.144	−0.168	0.640	5.867	4.871	−0.046	−0.117
7	2,4-Dihydroxybenzoic acid	1.610	1.168	0.238	−0.212	0.650	5.613	3.879	−0.082	−0.048
8	3-Methoxybenzoic acid	1.692	0.850	0.306	−0.090	0.650	5.603	5.865	−0.038	−0.151
9	4-Hydroxybenzoic acid	1.667	1.157	0.186	−0.231	0.670	5.306	3.998	−0.058	−0.031
10	Caffeic acid	1.660	1.205	0.160	−0.301	0.660	6.060	2.939	−0.009	−0.161
11	Chlorogenic acid	1.676	1.278	0.264	−0.488	0.630	7.975	2.307	−0.015	−0.421
12	Ferulic acid	1.680	0.946	0.287	−0.114	0.650	6.286	6.828	−0.047	−0.283
13	<i>m</i> -Coumaric acid	1.714	1.196	0.336	−0.226	0.670	5.825	5.429	−0.020	−0.078
14	<i>o</i> -Coumaric acid	1.714	1.196	0.499	−0.245	0.670	5.835	6.865	−0.091	−0.062
15	<i>p</i> -Coumaric acid	1.714	1.196	0.272	−0.256	0.670	5.810	3.809	−0.066	−0.030
16	Sinapic acid	1.655	0.773	0.210	−0.112	0.640	6.701	5.944	−0.080	−0.267
17	<i>trans</i> -Cinnamic acid	1.784	1.186	0.504	−0.170	0.680	5.560	6.354	0.011	−0.147
18	Dihydrocaffeic acid	1.660	1.259	0.205	−0.397	0.640	6.060	2.890	0.042	−0.169
19	Homovanillic acid	1.660	0.960	0.168	−0.196	0.640	6.085	5.035	−0.082	−0.016
20	DOPAC	1.636	1.222	0.040	−0.394	0.640	5.842	0.416	−0.086	−0.071
21	4-hydroxyphenylacetic acid	1.692	1.207	0.255	−0.343	0.650	5.569	2.793	−0.077	0.105
22	Ellagic acid	1.833	0.869	0.001	−0.135	0.710	7.684	0.027	0.138	0.164
23	Vanillin	1.692	0.817	0.099	−0.115	0.650	5.607	4.086	−0.055	−0.109
24	Tyrosol	1.765	1.169	0.077	−0.201	0.640	5.283	4.618	−0.008	−0.145

Table S1. *Cont.*

Sr. No.	Compound	HNar	GATS2v	DISPe	Mor32e	Mp	IDM	DISPm	Mor22v	Mor28e
25	Apigenin	1.875	1.061	0.220	−0.501	0.700	7.347	3.675	−0.141	0.158
26	Chrysin	1.932	1.057	0.458	−0.347	0.710	7.208	6.346	−0.093	−0.003
27	Luteolin	1.826	1.064	0.141	−0.481	0.690	7.493	2.822	−0.150	−0.047
28	Luteolin-7- <i>O</i> -glucoside	1.811	1.131	0.115	−0.605	0.650	8.709	5.401	−0.072	−0.209
29	Kaempferide	1.833	0.901	0.377	−0.350	0.680	7.626	8.482	−0.138	−0.259
30	Myricetin	1.747	1.070	0.149	−0.596	0.680	7.774	2.566	−0.108	0.157
31	Quercetin	1.784	1.067	0.133	−0.680	0.690	7.641	3.152	−0.111	−0.095
32	Rutin	1.779	1.165	0.135	−0.631	0.630	9.590	6.790	−0.115	0.182
33	Hesperidin	1.804	1.116	0.168	−0.148	0.620	9.554	5.027	−0.174	−0.440
34	Isosakuranetin	1.881	0.949	0.345	−0.387	0.670	7.478	8.139	−0.100	−0.306
35	Naringenin	1.875	1.094	0.204	−0.652	0.680	7.347	3.722	−0.207	−0.069
36	(+)-Catechin	1.826	1.137	0.115	−0.405	0.660	7.495	1.878	0.001	−0.557
37	(−)-Epicatechin	1.826	1.137	0.082	−0.315	0.660	7.495	1.225	−0.014	−0.364
38	Genistein	1.875	0.996	0.169	−0.623	0.700	7.347	2.274	−0.178	−0.062
39	(+)-Taxifolin	1.784	1.111	0.096	−0.359	0.670	7.641	2.375	−0.047	−0.177