

Supplementary Table. Evaluated/Investigated parent compounds with highest concentration

#	CAS	NAME	SMILES	STRUCTURE
1	331-39-5	3,4 – dihydroxycinnamic acid <i>Caffeic acid</i>	<chem>OC(=O)C=Cc1ccc(O)c(O)c1</chem>	
2	1135-24-6	(E)-3-(4-hydroxy-3-methoxyphenyl) prop-2-enoic acid <i>Ferulic acid</i>	<chem>COC1=C(C=CC(=C1)/C=C/C(=O)O)O</chem>	
3	69-72-7	2-Hydroxybenzoic acid <i>Salicylic acid</i>	<chem>OC(=O)c1ccccc1O</chem>	
4	480-19-3	3-Methylquercetin <i>Isorhamnetin</i>	<chem>COc1cc(ccc1O)C1Oc2cc(O)c(O)c2C(=O)C=1O</chem>	
5	520-36-5	5,7-dihydroxy-2-(4-hydroxyphenyl) chromen-4-one <i>Apigenin</i>	<chem>Oc1ccc(cc1)C1Oc2cc(O)cc(O)c2C(=O)C=1</chem>	
6	520-18-3	3,5,7-trihydroxy-2-(4-hydroxyphenyl) chromen-4-one <i>Kaempferol</i>	<chem>Oc1ccc(cc1)C1Oc2cc(O)cc(O)c2C(=O)C=1O</chem>	
7	327-97-9	(1S,4R,5R)-3-{{[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy}-1,4,5-trihydroxycyclohexanecarboxylic acid <i>Chlorogenic acid</i>	<chem>O[C@]1C[C@](O)(C[C@](OC(=O)C=Cc2ccc(O)c(O)c2)[C@]1O)C(O)=O</chem>	
8	61276-17-3	[(2R,3R,4R,5R,6R)-6-[2-(3,4-dihydroxyphenyl) ethoxy]-5-hydroxy-2-(hydroxymethyl)-4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-3-yl] (E)-3-(3,4-dihydroxyphenyl) prop-2-enoate <i>Verbascoside</i>	<chem>C[C@]1O[C@](O[C@]2[C@](O)[C@](O)C[C@]2OC(=O)C=Cc3ccc(O)c(O)c3)O[C@](C)[C@]2OC(=O)C=Cc4ccc(O)c(O)c4[C@](O)[C@](O)[C@]1O</chem>	
9	490-79-9	2,5-dihydroxybenzoic acid <i>Gentisic acid</i>	<chem>OC(=O)c1cc(O)ccc1O</chem>	
10	530-57-4	3,5-Dimethoxy-4-hydroxybenzoic acid <i>Syringic acid</i>	<chem>COc1cc(cc(OC)c1O)C(=O)O</chem>	