

Supplementary material

ID	Ingredient name	Formula	CAS	Canonical SMILES	Mass	Adducts
		a			error	r
BSZ J1	3-Dehydrotrametenolic acid	C30H4 6O3	2922 0- 16-4	<chem>CC(=CCCC(C1CCC2(C1(CC=C3C2=CCC4C3(CCC(C4(C)C)O)C)C)C(=O)O)C</chem>	0.2	+H
BSZ J2	BidentatosideI	C47H7 0O20- 19	3308 08- 27-0	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)C6C7C(C(C(O6)C(=O)O)O)OC(C(O7)OCC(=O)O)(C(=O)O)O)C)C)C2</chem>	1.3	-H
BSZ J3	Chikusetsusaponin iva	C42H6 6O14	5141 5- 02-2	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)OC6C(C(C(C(O6)C(=O)O)O)O)O)C)C)C2C1)C)C(=O)OC7C(C(C(C(O7</chem>	0.5	-H
BSZ J4	Ginsenoside Ro	C48H7 6O19	3436 7- 04-9	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)OC6C(C(C(C(O6)C(=O)O)O)O)OC7C(C(C(C(O7)CO)O)O)O)C)C)C2C</chem>	0.1	-H
BSZ J5	Paeonilactone B	C10H1 2O4	9875 1- 78-1	<chem>CC1(CC2C(CC1=O)C(=C)C(=O)O2)O</chem>	1.3	+H
BSZ J6	Asperosaponin VI	C47H7 6O18	3952 4- 08-8	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)CO)OC6C(C(C(CO6)O)O)O)C)C)C2C1)C)C(=O)OC7C(C(C(C(O7)COC8</chem>	0	+H, +Na
BSZ J7	Sucrose	C12H2 2O11	57- 50-1	<chem>C(C1C(C(C(C(O1)OC2(C(C(C(O2)CO)O)O)CO)O)O)O)O</chem>	1.9	-H
BSZ J8	Paeonilactone C	C17H1 8O6	9875 1- 77-0	<chem>CC1(CC2C(CC1=O)C(C(=O)O2)COC(=O)C3=CC=CC=C3)O</chem>	1.6	+H
BSZ J9	Adenosine	C10H1 3N5O4	58- 61-7	<chem>C1=NC(=C2C(=N1)N(C=N2)C3C(C(C(O3)CO)O)O)N</chem>	1.5	+H
BSZ J10	Geniposidic acid	C16H2 2O10	2774 1-	<chem>C1C=C(C2C1C(=COC2OC3C(C(C(C(O3)CO)O)O)O)C(=O)O)CO</chem>	0.9	-H

			01-1					
BSZ J11	Narirutin	C27H3 2O14	1425 9- 46-2	CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=CC(=C4C(=O)CC(OC4=C3)C5=CC=C(C(C=C5)O)O)O)O)O)O)O)O	1.6	-H		
BSZ J12	Gallic Acid	C7H6 O5	149- 91-7	C1=C(C=C(C(=C1O)O)O)C(=O)O	3.8	-H		
BSZ J13	Pachymic acid	C33H5 2O5	2907 0- 92-6	CC(C)C(=C)CCC(C1C(CC2(C1(CCC3=C2CCC4C3(CCC(C4(C)C)OC(=O)C)C)C)O)C(=O)O	0.8	-H		
BSZ J14	Adenine	C5H5 N5	73- 24-5	C1=NC2=NC=NC(=C2N1)N		+H		
BSZ J15	Quinic acid	C7H12 O6	77- 95-2	C1C(C(C(CC1(C(=O)O)O)O)O)O	3.2	-H		
BSZ J16	b-D-Glucopyranosiduronic acid,(3b)-17-carboxy-28-norolean-12-en-3-yl	C36H5 6O9	2602 0- 14-4	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)OC6C(C(C(C(O6)C(=O)O)O)O)C)C)C2C1)C)C(=O)O)C	1	-H		
BSZ J17	Albiflorin	C23H2 8O11	3901 1- 90-0	CC12CC(C3CC1(C3(C(=O)O2)COC(=O)C4=CC=CC=C4)OC5C(C(C(C(O5)CO)O)O)O)O	0.9	-H		
BSZ J18	Hesperidin	C28H3 4O15	520- 26-3	CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=CC(=C4C(=O)CC(OC4=C3)C5=CC(=C(C(C=C5)OC)O)O)O)O)O)O)O)O	0.4	-H		
BSZ J19	Stachyose	C24H4 2O21	1009 4- 58-3	C(C1C(C(C(C(O1)OCC2C(C(C(C(O2)OCC3C(C(C(C(O3)OC4(C(C(C(O4)CO)O)O)CO)O)O)O)O)O)O)O)O.O.O.O.O.O	1.1	-H		
BSZ J20	(+)-Pinoresinol O-β-D-glucopyranoside	C32H4 2O16	6925 1- 96-3	COC1=C(C=CC(=C1)C2C3COC(C3CO2)C4=CC(=C(C=C4)OC5C(C(C(C(O5)CO)O)O)O)OC)O	0.7	-H		
BSZ J21	Albiflorin	C23H2 8O11	3901 1- 90-0	CC12CC(C3CC1(C3(C(=O)O2)COC(=O)C4=CC=CC=C4)OC5C(C(C(C(O5)CO)O)O)O)O	-0.1	-H		
BSZ J22	Deacetylasperulosidic acid	C16H2 2O11	1425 9-	C1=C(C2C(C1O)C(=COC2OC3C(C(C(C(O3)CO)O)O)O)C(=O)O)CO	2.3	-H		

BSZ J23	Levistilide A	C24H2 8O4	55-3 8818	CCCC=C1C2=C(C3C(CC2)C4CCC35C(=C4)C(=O)OC5=CCCC)C(=O)O1	0.6	+H, +Na
			2-			
BSZ J24	pinusolidic acid	C10H1 2O3	33-6 4043	CC12CCCC(C1CCC(=C)C2CCC3=CCOC3=O)(C)C(=O)O	-1	+H
			3-			
BSZ J25	Shidasterone	C27H4 2O6	82-7 2636	CC1(CCC(O1)C(C)(C2CCC3(C2(CCC4C3=CC(=O)C5C4(CC(C(C5)O)O)C)C)O)O)C	-1.3	+H
			1-			
BSZ J26	Linolenic Acid	C18H3 0O2	67-1 463-	CCC=CCC=CCC=CCCCCCCCC(=O)O	0.4	+H
			40-1			
BSZ J27	Verbascose	C30H5 2O26	546- 62-3	C(C1C(C(C(C(O1)OCC2C(C(C(C(O2)OCC3C(C(C(C(O3)OCC4C(C(C(C(O4)OC5(C(C(C(O5)CO)O)O)CO)O)O)O)O)O)O)O)O)O)O)O)O)O	1	-H
BSZ J28	Raffinose	C18H3 2O16	512- 69-6	C(C1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3(C(C(C(O3)CO)O)O)CO)O)O)O)O)O)O)O	0.9	-H
BSZ J29	Dehydropachymic acid	C33H5 0O5	7701 2-	CC(C)C(=C)CCC(C1C(CC2(C1(CC=C3C2=CCC4C3(CCC(C4(C)C)OC(=O)C)C)C)O)C(=O)O	-0.4	-H
			31-8			
BSZ J30	1-methyl-2-[(Z)-tetradec-8-enyl]quinolin-4-one	C24H3 5NO	/	CCCCC=CCCCCCCCC1=CC(=O)C2=CC=CC=C2N1C	-3.8	+Na
BSZ J31	Berberine	C17H1 7N	2086 -83-	C1CN2CC3=CC=CC=C3CC2C4=CC=CC=C41	0.8	+H
			1			
BSZ J32	Manninotriose	C18H3 2O16	1338 2-	C(C1C(C(C(C(O1)OCC2C(C(C(C(O2)OCC(C(C(C(C=O)O)O)O)O)O)O)O)O)O)O)O	-9.4	+H, +Na
			86-0			
BSZ J33	Inokosterone	C27H4 4O7	1513 0-	CC(CCC(C(C)(C1CCC2(C1(CCC3C2=CC(=O)C4C3(CC(C(C4)O)O)C)C)O)O)O)CO	-0.7	+H
			85-5			
BSZ J34	threo-Guaiacylglycerol	C10H1 4O5	2739 1-	COC1=C(C=CC(=C1)C(C(CO)O)O)O	2.3	-H
			16-8			

BSZ J35	3,4-dihydroxycinnamic acid	C9H8 O4	331- 39-5	<chem>C1=CC(=C(C=C1C=CC(=O)O)O)O</chem>	4.2	-H
BSZ J36	3-O-Acetyl-16 α -hydroxytrametenolic acid	C32H5 O05	1682 93- 13-8	<chem>CC(=CCCC(C1C(CC2(C1(CCC3=C2CCC4C3(CCC(C4(C)C)OC(=O)C)C)C)O)C(=O)O)C</chem>	1.5	-H
BSZ J37	Tumulosic acid	C31H5 O04	508- 24-7	<chem>CC(C)C(=C)CCC(C1C(CC2(C1(CCC3=C2CCC4C3(CCC(C4(C)C)O)C)C)O)C(=O)O</chem>	0.6	-H
BSZ J38	Benzyl Alcohol	C7H8 O	100- 51-6	<chem>C1=CC=C(C=C1)CO</chem>	2.1	+H
BSZ J39	Paeonol	C9H10 O3	552- 41-0	<chem>CC(=O)C1=C(C=C(C=C1)OC)O</chem>	0.2	+H
BSZ J40	Betulinic Acid	C30H4 8O3	472- 15-1	<chem>CC(=C)C1CCC2(C1C3CCC4C5(CCC(C(C5CCC4(C3(CC2)C)C)(C)C)O)C)C(=O)O</chem>	0.2	-H
BSZ J41	Sinomenine	C21H2 1NO4	115- 53-7	<chem>CN1CCC23CC(=O)C(=CC2C1CC4=C3C(=C(C=C4)OC)O)OC</chem>	0	+H
BSZ J42	Poricoic Acid C	C31H4 6O4	/	<chem>CC(C)C(=C)CCC(C1CCC2(C1(CC=C3C2=CCC(C3(C)CCC(=O)O)C(=C)C)C)C)C(=O)O</chem>	0.4	-H
BSZ J43	(S)-7-(((2-O-6-Deoxy-alpha-L-mannopyranosyl)-beta-D-glucopyranosyl)oxy)-2,3-dihydro-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-4H-1-benzopyran-4-one	C28H3 4O15	1324 1- 33-3	<chem>CC1C(C(C(C(O1)OC2C(C(C(OC2OC3=CC(=C4C(=O)CC(OC4=C3)C5=CC(=C(C=C5)OC)O)O)CO)O)O)O)O</chem>	5.9	+Na
BSZ J44	Pinoresinol	C20H2 2O6	487- 36-5	<chem>COC1=C(C=CC(=C1)C2C3COC(C3CO2)C4=CC(=C(C=C4)O)OC)O</chem>	0.2	-H
BSZ J45	Ursolic Acid	C30H4 8O3	77- 52-1	<chem>CC1CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)O)C)C)C2C1C)C)C(=O)O</chem>	1.5	-H
BSZ J46	Dehydrotumulosic acid	C31H4 8O4	6754 -16- 1	<chem>CC(C)C(=C)CCC(C1C(CC2(C1(CC=C3C2=CCC4C3(CCC(C4(C)C)O)C)C)O)C(=O)O</chem>	0.1	-H
BSZ J47	Rhapontisterone B	C27H4 4O7	6989 75-	<chem>CC12CCC3C(=CC(=O)C4C3(CC(C(C4)O)O)C)C1(CCC2C(C)(C(CCC(C)(C)O)O)O)O</chem>	-0.3	+H

Index	Compound	Formula	Mass	SMILES	Δ <i>m/z</i>	Charge
BSZ J48	Hederagenin	C ₃₀ H ₄₈ O ₄	465-99-6	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)CO)O)C)C)C2C1)C)C(=O)O)C	-0.5	-H
BSZ J49	alpha-Spinasterol	C ₂₉ H ₄₈ O	481-18-5	CCC(C=CC(C)C1CCC2C1(CCC3C2=CCC4C3(CCC(C4)O)C)C)C(C)C	-1.3	+H
BSZ J50	Evodiamine	C ₁₉ H ₁₇ N ₃ O	518-17-2	CN1C2C3=C(C(CN2C(=O)C4=CC=CC=C41)C5=CC=CC=C5N3	-8.3	+Na
BSZ J51	Poricoic acid F	C ₃₁ H ₄₆ O ₅	1375-51-38-3	CC(C)C(=C)CCC(C1C(CC2(C1(CC=C3C2=CCC(C3(C)CCC(=O)O)C(=C)C)C)C)O)C(=O)O	0.6	-H
BSZ J52	Emodin	C ₁₅ H ₁₀ O ₅	518-82-1	CC1=CC2=C(C(=C1)O)C(=O)C3=C(C2=O)C=C(C(=C3O)O	0.2	-H
BSZ J53	Eucommin A	C ₂₇ H ₃₄ O ₁₂	9963-3-12-2	COC1=CC(=CC(=C1OC2C(C(C(C(O2)CO)O)O)OC)C3C4COC(C4CO3)C5=CC(=C(C(=C5)O)OC	0.2	+H
BSZ J54	Buddlejasaponin IVb	C ₄₈ H ₇₈ O ₁₈	1525-80-79-5	CC1C(C(C(C(O1)OC2CCC3(C(C2(C)CO)CCC4(C3C=CC5=C6CC(CCC6(C(CC54C)O)CO)(C)C)C)C)OC7C(C(C(C(O7)CO)O)O)OC8C(C(C(C(O8)CO)O)O)O)O	-1.1	+H, +Na
BSZ J55	Naringin	C ₂₇ H ₃₄ O ₁₄	1023-6-47-2	CC1C(C(C(C(O1)OC2C(C(C(OC2OC3=CC(=C4C(=O)CC(OC4=C3)C5=CC=C(C(=C5)O)O)CO)O)O)O)O)O	2.3	+H
BSZ J56	Gentisic acid	C ₇ H ₆ O ₄	490-79-9	C1=CC(=C(C(=C1O)C(=O)O)O	0.1	+H
BSZ J57	8-Hydroxypinoresinol 4'-Glucoside	C ₂₆ H ₃₄ O ₁₂	1025-82-69-4	COC1=C(C=CC(=C1)C2C3COC(C3(CO2)O)C4=CC(=C(C(=C4)O)OC)OC5C(C(C(C(O5)CO)O)O)O	-1.1	-H
BSZ J58	pethyl hydroxybenzene	C ₈ H ₁₀ O	123-07-9	CCC1=CC=C(C(=C1)O	-1.2	+H
BSZ J59	Oleanolic acid 28-O-β-D-glucopyranoside	C ₃₆ H ₅₈ O ₈	1416-2-53-9	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)O)C)C)C2C1)C)C(=O)OC6C(C(C(C(O6)CO)O)O)O)C	-2.6	+H
BSZ J60	(-)-Syringaresinol-4-O-beta-D-glucopyranoside	C ₂₈ H ₃₆ O ₁₃	/	COC1=CC(=CC(=C1O)OC)C2C3COC(C3CO2)C4=CC(=C(C(=C4)OC)OC5C(C(C(C(O5)CO)O)O)O)OC	-3.6	-H

BSZ J61	(+)-Medioresinol	C21H2 4O7	4095 7- 99-1	<chem>COC1=CC(=CC(=C1O)OC)C2C3COC(C3CO2)C4=CC(=C(C=C4)O)OC</chem>	-0.9	+H
BSZ J62	Pyrogallol	C6H6 O3	87- 66-1	<chem>C1=CC(=C(C(=C1)O)O)O</chem>	0.8	+H
BSZ J63	beta-Bisabolene	C15H2 4	495- 61-4	<chem>CC1=CCC(CC1)C(=C)CCC=C(C)C</chem>	-0.4	+H
BSZ J64	1-Hydroxypinoresinol 1-O-glucoside	C20H2 2O7	8149 5- 71-8	<chem>COC1=C(C=CC(=C1)C2C3COC(C3(CO2)OC4C(C(C(C(O4)CO)O)O)O)C5=CC(=C(C=C5)O)OC)O</chem>	-3.2	-H
BSZ J65	Asperosaponin VI	C47H7 6O18	3952 4- 08-8	<chem>CC1(CCC2(CCCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)CO)OC6C(C(C(CO6)O)O)O)C)C)C2C1)C)C(=O)OC7C(C(C(C(O7)COC8</chem>	1.9	+H, +Na
BSZ J66	kaobraside	/	/	<chem>COC1=CC(O)=CC(OC)=C1C</chem>	7.9	+Na
BSZ J67	Achyranthoside C	C47H7 2O20	1680 09- 90-3	<chem>CC1(CCC2(CCCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)OC6C(C(C(C(O6)C(=O)O)O)OC(C(C(=O)O)O)OCC(=O)O)O)C)C)C2C</chem>	-2	+H
BSZ J68	dehydrodiconiferyl alcohol 4,γ'-di-O-β-D-glucopyranoside	C32H4 2O16	1097 92- 90-7	<chem>COC1=C(O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)C=CC(C)=C1</chem>	-0.8	-H
BSZ J69	Nicotinic acid	C6H5 NO2	59- 67-6	<chem>C1=CC(=CN=C1)C(=O)O</chem>	1	+H
BSZ J70	Benzoic Acid	C7H6 O2	65- 85-0	<chem>C1=CC=C(C=C1)C(=O)O</chem>	2.6	-H
BSZ J71	(-)-Catechin	C15H1 4O6	1882 9- 70-4	<chem>C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O</chem>	1.7	-H
BSZ J72	Poricoic Acid B	C30H4 4O5	1375 51- 39-4	<chem>CC(=CCCC(C1C(CC2(C1(CC=C3C2=CCC(C3(C)CCC(=O)O)C(=C)C)C)O)C(=O)O)C</chem>	-3.2	+H

BSZ J73	Lactiflorin	C23H2 6O10	1361 049- 59-3	<chem>CC12C3(CC4C3(C(O1)CC4=O)COC(=O)C5=CC=CC=C5)OC6C(O2)C(C(C(O6)CO)O)O</chem>	5.6	+H
BSZ J74	Syringaresinol	C22H2 6O8	487- 35-4	<chem>COC1=CC(=CC(=C1O)OC)C2C3COC(C3CO2)C4=CC(=C(C(=C4)OC)O)OC</chem>	0.7	-H
BSZ J75	9H-Pyrido[3,4-B]indole	C11H8 N2	244- 63-3	<chem>C1=CC=C2C(=C1)C3=C(N2)C=NC=C3</chem>	4.7	+H
BSZ J76	[(z)(1S,5R)-β-pinen-10-yl-β-vicianoside]	C21H3 4O10		<chem>CC1[C@H]2C[C@@H]1\C(CC2)=C/OC1OC(COC2OCC(O)C(O)C2O)C(O)C(O)C1O</chem>	1.3	-H
BSZ J77	4-(Methylamino)benzoic acid	C8H9 NO2	1054 1- 83-0	<chem>CNC1=CC=C(C=C1)C(=O)O</chem>	-8.5	+H
BSZ J78	[(+)-medioresinol-di-O-β-D-glucopyranoside]	C33H4 4O17	8814 2- 63-6	<chem>COC1=CC(=CC(=C1OC2C(C(C(C(O2)CO)O)O)O)OC)C3C4COC(C4CO3)C5=CC(=C(C(=C5)OC6C(C(C(C(O6)CO)O)O)O)OC</chem>	-2.1	-H
BSZ J79	[2-(methylamino)phenyl]-(1,3,4,9-tetrahydropyrido[3,4-b]indol-2-yl)methanone	C19H1 9N3O	/	<chem>CNC1=CC=CC=C1C(=O)N2CCC3=C(C2)NC4=CC=CC=C34</chem>	-9.3	+Na
BSZ J80	apocynin	C9H10 O3	498- 02-2	<chem>CC(=O)C1=CC(=C(C=C1)O)OC</chem>	2.7	-H
BSZ J81	3-(3,4-Dihydroxyphenyl)propionic acid	C9H10 O4	1078 -61- 1	<chem>C1=CC(=C(C=C1CCC(=O)O)O)O</chem>	-0.5	+H
BSZ J82	2',4'-Dihydroxyacetophenone	C8H8 O3	89- 84-9	<chem>CC(=O)C1=C(C=C(C=C1)O)O</chem>	-2.6	+H
BSZ J83	Azelaic Acid	C9H16 O4	123- 99-9	<chem>C(CCCC(=O)O)CCCC(=O)O</chem>	2.1	-H
BSZ J84	Liriodendrin	C34H4 6O18	573- 44-4	<chem>COC1=CC(=CC(=C1OC2C(C(C(C(O2)CO)O)O)O)OC)C3C4COC(C4CO3)C5=CC(=C(C(=C5)OC)OC6C(C(C(C(O6)CO)O)O)O)OC</chem>	1.1	+Na , +H
BSZ J85	Stearic Acid	C18H3 6O2	57- 11-4	<chem>CCCCCCCCCCCCCCCCCCCC(=O)O</chem>	0.8	-H
BSZ J86	Guaiacol	C7H8 O2	90- 05-1	<chem>COC1=CC=CC=C1O</chem>	3.5	-H

BSZ J87	Paeonilactone A	C10H14O4	9875-1-79-2	<chem>CC1C2CCC(=O)C(CC2OC1=O)(C)O</chem>	1.9	-H
BSZ J88	beta-Cadinene	C15H24	523-47-7	<chem>CC1=CCCC2C(C1)C(CC=C2C)C(C)C</chem>	-2	+H, +Na
BSZ J89	30-Norhederagenin	C29H44O4	1176-54-06-5	<chem>CC12CCC(C(C1CCC3(C2CC=C4C3(CCC5(C4CC(=C)CC5)C(=O)O)C)C)(C)CO)O</chem>	1.7	-H
BSZ J90	Poricoic Acid A	C31H46O5	1375-51-38-3	<chem>CC(C)C(=C)CCC(C1C(CC2(C1(CC=C3C2=CCC(C3(C)CCC(=O)O)C(=C)C)C)C)O)C(=O)O</chem>	-0.7	-H
BSZ J91	poricoic acid AM	C32H48O5	1512-00-92-9	<chem>CC(C)C(=C)CCC(C1C(CC2(C1(CC=C3C2=CCC(C3(C)CCC(=O)OC)C(=C)C)C)C)O)C(=O)O</chem>	-0.5	-H
BSZ J92	Phenol	C6H6O	108-95-2	<chem>C1=CC=C(C=C1)O</chem>	0.9	+H
BSZ J93	3-Dimethylallyl-4-methoxy-2-quinolone	C15H17NO2	7282-19-1	<chem>CC(=CCC1=C(C2=CC=CC=C2NC1=O)OC)C</chem>	-6.6	+Na
BSZ J94	Catalpol	C15H22O10	2415-24-9	<chem>C1=COC(C2C1C(C3C2(O3)CO)O)OC4C(C(C(C(O4)CO)O)O)O</chem>	0.4	-H
BSZ J95	OCTACOSANOIC ACID	C28H56O2	506-48-9	<chem>CCCCCCCCCCCCCCCCCCCCCCCCCC(=O)O</chem>	4.1	+H
BSZ J96	inokosterone	C27H44O8	1513-0-85-5	<chem>CC(CCC(C(C)(C1CCC2(C1(CCC3C2=CC(=O)C4C3(CC(C(C4)O)O)C)C)O)O)O)CO</chem>	-1.1	+H
BSZ J97	Catechol	C6H6O2	120-80-9	<chem>C1=CC=C(C(=C1)O)O</chem>	1	+H, +Na
BSZ J98	Kaempferol	C15H10O6	520-18-3	<chem>C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C(=C3O2)O)O)O)O</chem>	0.5	+H

BSZ J99	Higenamine	C16H1 7NO3	5843 -65- 2	C1CNC(C2=CC(=C(C=C21)O)O)CC3=CC=C(C=C3)O	-1.4	+H
BSZ J100	Isoevodiamine	C18H1 5N3O	5986 3- 00-2	CN1C2C3=C(CCN2C(=O)C4=CC=CC=C41)C5=CC=CC=C5N3	-7.4	+Na , +H
BSZ J101	Butylated Hydroxytoluene	C15H2 4O	128- 37-0	CC1=CC(=C(C(=C1)C(C)(C)C)O)C(C)(C)C	-1.5	+H
BSZ J102	D(-)-Tartaric acid	C4H6 O6	526- 83-0	C(C(C(=O)O)O)(C(=O)O)O	3.8	-H
BSZ J103	1-(7-hydroxy-5-methoxy-2,2-dimethyl-2H-chromen-6-yl)ethan-1-one	C14H1 6O4	529- 70-4	CC(=O)C1=C(C2=C(C=C1O)OC(C=C2)(C)C)OC	7.3	+Na
BSZ J104	(2R)-2-[(1R,2R,3aR,5aR,7S,9aS,11aR)-2,7-bis(acetyloxy)-3a,6,6,9a,11a-pentamethyl-1H,2H,3H,3aH,4H,5H,5aH,6H,7H,8H,9H,9aH,10H,11H,11aH-cyclopenta[a]phenanthren-1-yl]-6-methyl-5-methylideneheptanoic acid	C35H5 4O6	/	[H][C@]1([C@@H](CCC(=C)C(C)C)C(O)=O)[C@@H](C[C@@]2(C)C3=C(CC[C@]12C)[C@@]1(C)CC[C@H](OC(C)=O)C(C)(C)[C@]1([H])CC3)OC(C)=O	1.2	-H
BSZ J105	(6Z,9Z)-6-methylpentadeca-6,9-dien-2-one	C14H2 4O2	/	[H]\C(CCCCC)=C(/[H])C\C([H])=C(\C)CCCC(C)=O	9.5	+Na
BSZ J106	3'-ethyl-3-methylidene-6,7-dihydro-3H-spiro[2-benzofuran-1,1'-cyclopropane]	C12H1 4O2	/	CCC1CC11OC(=C)C2=C1CCC=C2	0.8	+H
BSZ J107	(1R,2R,4R)-4-{4-[(1S,3aR,4S,6aR)-4-{4-[(1S,2S)-2-(4-{[(2S,4S,5S)-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-3-methoxyphenyl)-1,2-	C43H5 6O21	/	[H][C@]12CO[C@H](C3=CC(OC)=C(O[C@H](O)[C@@H](O)C4=CC(OC)=C(O[C@H]5C[C@H](O)[C@H](O)C(CO)O5)C=C4)C(OC)=C3)[C@@]1([H])CO[C@@H]2C1=CC(OC)=C(O[C@@H]2CC(CO)[C@@H](O)[C@@H](O)C2O)C=C1	-3.2	-H

dihydroxyethoxy]-3,5-
dimethoxyphenyl}-
hexahydrofuro[3,4-c]furan-1-yl]-
2-methoxyphenoxy}-6-
(hydroxymethyl)cyclohexane-
1,2,3-triol
