Supplementary material

Supplementary Table 1. A list of 181 plant bioactives and their metabolites selected as candidates for the multiplatform analysis classified based on their chemical or metabolite class.

Carotenoids
Lutein
Lycopene
Zeaxanthin
β-Carotene
β-Cryptoxanthin
Phytosterols
Brassicasterol
Campesterol
Stigmasterol
β-Sitosterol
Phenolic acids
2-Hydroxycinnamic acid
5-Feruloylquinic acid
Caffeic acid
Chlorogenic acid
p-Coumaric acid
Ellagic acid
Ferulic acid
Gallic acid
Homovanillic acid
Protocatechuic acid
Rosmarinic acid
Sinapic acid
Vanillic acid
Veratric acid
Verbascoside
Flavonoids
(−)-Epicatechin
(−)-Epigallocatechin 3-*O*-gallate
8-Prenylnaringenin
Apigenin
Apigenin 7-*O*-glucoside
Cyanidin
Cyanidin 3-*O*-glucoside
Cyanidin 3-*O*-rutinoside
Daidzein
Delphinidin
Dihydrogenistein

Diosmetin
Eriodictyol
Genistein
Hesperetin
Homoeriodictyol
Homoorientin
Isoliquiritigenin
Isoquercitrin
Isorhamnetin
Isosakuranetin
Kaempferol
Luteolin
Malvidin 3-*O*-glucoside
Myricetin
Naringenin
Naringin
Nobiletin
Phloretin
Procyanidin A2
Procyanidin B1
Procyanidin B2
Procyanidin B4
Quercetin
Silybin
Sinensetin
Tangeretin
Taxifolin
Vitexin
Xanthohumol

Other polyphenols

(+)-lariciresinol
5-heptadecylresorcinol (AR17:0)
5-pentacosylresorcinol (AR25:0)
α-Tocopherol
Curcumin
Hydroxytyrosol
Resveratrol
Vanillin

Glucuronides

3'-Methylcyanidin 3-glucuronide
4-Hydroxybenzoic acid 4-*O*-glucuronide
Apigenin 7-glucuronide
Caffeic acid 3-*O*-β-D-glucuronide
cis-Resveratrol 3-*O*-β-D-glucuronide
cis-Resveratrol 4'-*O*-β-D-glucuronide
Curcumin 4-*O*-β-D-glucuronide

Cyanidin 3-glucuronide
Daidzein 4’-β-D-glucuronide
Daidzein 7-β-D-glucuronide
Daidzein diglucuronide
Diosmetin 3'-*O*-β-D-glucuronide
Epicatechin 3-*O*-glucuronide
Genistein 4’-β-D-glucuronide
Genistein 7-β-D-glucuronide
Genistein diglucuronide
Hesperetin 3'-*O*-β-D-glucuronide
Hesperetin 7,3'-di-*O*-β-D-glucuronide
Hesperetin 7-*O*-β-D-glucuronide
Isorhamnetin 3-*O*-glucuronide
Isorhamnetin 4'-*O*-glucuronide
Isovanillic acid 3-*O*-glucuronide
Kaempferol 3-*O*-β-D-glucuronide
Luteolin 7-*O*-β-D-glucuronide
Myricetin 3'-*O*-glucuronide
Naringenin 4'-*O*-β-D-glucuronide
Naringenin 7-*O*-β-D-glucuronide
Protocatechuic acid 4-*O*-glucuronide
Quercetin 3'-*O*-β-D-glucuronide
Quercetin 5,7-diglucuronide
Quercetin 7-*O*-β-D-glucuronide
trans-Resveratrol 3-*O*-β-D-glucuronide
trans-Resveratrol 4'-*O*-β-D-glucuronide
Vanillic acid 4-*O*-glucuronide

Sulfates

1-Methylpyrogallol 3-O-sulfate
2-Methylpyrogallol 1-O-sulfate
3,4-Dihydroxybenzoic acid 3-*O*-sulfate
3,4-Dihydroxybenzoic acid 4-*O*-sulfate
3'-O-Methyl-(-)-epicatechin 5-*O*-sulfate
3'-O-Methyl-(-)-epicatechin 7-*O*-sulfate
4-Hydroxybenzoic acid 4-O-sulfate
4-Methylcatechol 1-O-sulfate
4-Methylcatechol 2-O-sulfate
4-O-Methylgallic acid 3-O-sulfate
Benzoic acid sulfate
Caffeic acid 3-O-sulfate
Caffeic acid 4-O-sulfate
Catechol *O*-sulfate
Daidzein 4' sulfate
Epicatechin 3-*O*-sulfate
Genistein 7-sulfate
Isoferulic acid 3-*O*-sulfate

Isoquercitrin 4'-*O*-sulfate
Isorhamnetin 3-*O*-sulfate
Isovanillic acid 3-*O*-sulfate
Kaempferol 3-*O*-sulfate
Myricetin 3'-*O*-sulfate
Protocatechuic acid 3-O-sulfate
Protocatechuic acid 4-O-sulfate
Pyrogallol 2-*O*-sulfate
Quercetin 3'-*O*-sulfate
Quercetin 4'-*O*-sulfate
Quercetin disulfate
Silybin 20-*O*-sulfate
Silybin 7,20-di-*O*-sulfate
Taxifolin 4'-*O*-sulfate
Vanillic acid 4-*O*-sulfate

Sulfates and glucuronides

3'-Methylcyanidin 3-glucuronide-5-glucoside-4'-sulfate
Daidzein 7-β-D-glucuronide 4’-Sulfate
Genistein 7-sulfate 4’-β-D-glucuronide
Genistein 7-β-D-glucuronide 4’-sulfate

Microbial metabolites

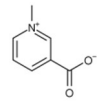
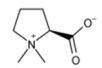
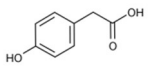
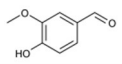
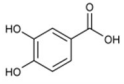
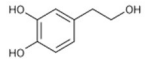
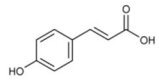
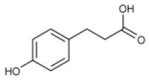
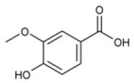
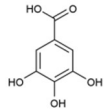
3,4-Dihydroxybenzoic acid
3,4-Dihydroxyphenylacetic acid
3,4-Dihydroxyphenylpropionic acid
3,4-Dimethoxybenzoic acid
3-Hydroxybenzoic acid
3-Hydroxyphenylacetic acid
3-Hydroxyphenylpropionic acid
3-Phenylpropionic acid
4-Coumaric acid
4-Hydroxybenzoic acid
4-Hydroxyphenylacetic acid
4-Hydroxyphenylpropionic acid
4-Methylcatechol
Benzoic acid
Dihydrocaffeic acid
Dihydrodaidzein
Enterodiol
Enterolactone
Equol
Equol 4'-sulfate
Equol 7-β-D-glucuronide
Hippuric acid
O-Desmethylangolensin
Protocatechuic acid

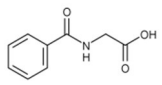
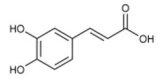
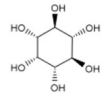
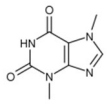
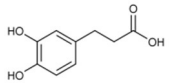
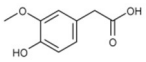
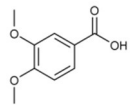
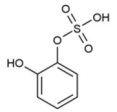
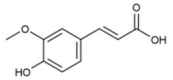
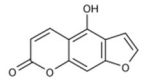
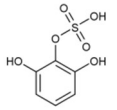
Urolithin A
Urolithin A 3-glucuronide
Urolithin A 8-glucuronide
Urolithin B
Urolithin B 3-*O*-glucuronide
Urolithin C
Urolithin D

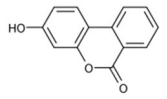
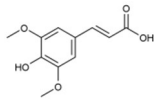
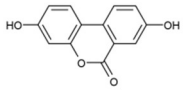
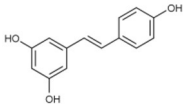
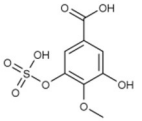
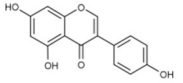
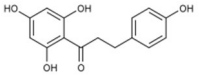
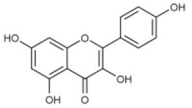
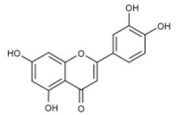
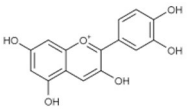
Other compounds

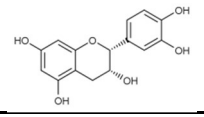
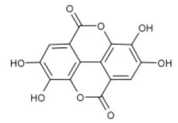
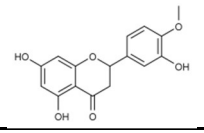
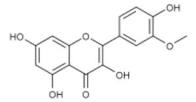
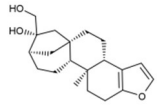
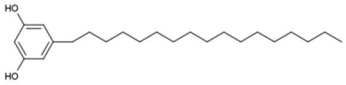
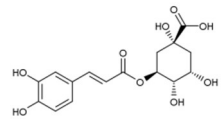
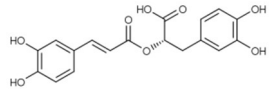
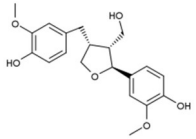
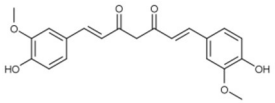
Bergaptol
Cafestol
myo-Inositol
Stachydrine
Theobromine
Trigonelline
Ursolic acid

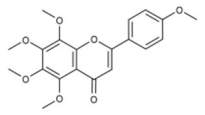
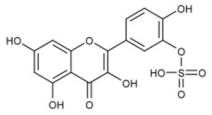
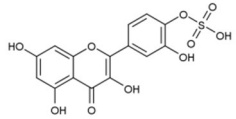
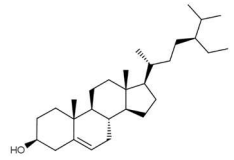
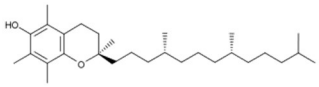
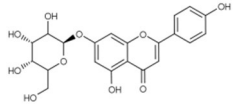
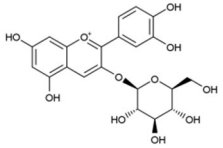
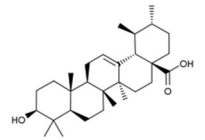
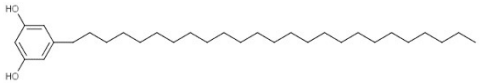
Supplementary Table 2. Chemical standards analysed in the multiplatform test. Concentration in the stock solution other than 10 mM: * 5 mM, † 1 mM, ‡ 0.5 mM, § 50 ppm

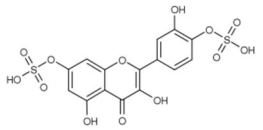
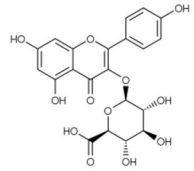
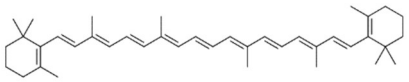
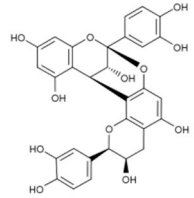
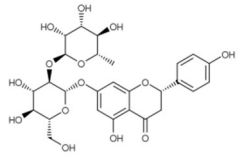
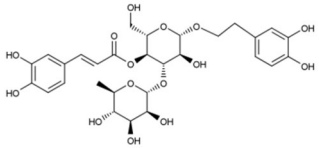
Compound	PhytoHub ID	Class	Formula	M_0 [Da]	log *P* (calc.)	Supplier	Mix	Structure
trigonelline	PHUB001378	betaine	$C_7H_7NO_2$	137.0477	−3.30	Extrasynthese	A	
stachydrine (proline betaine)	PHUB000844	betaine	$C_7H_{13}NO_2$	143.0946	−2.24	Extrasynthese	A	
4-hydroxyphenylacetic acid	PHUB000543	microbial metabolite	$C_8H_8O_3$	152.0473	0.93	Aldrich	A	
vanillin	PHUB000645	other phenolic	$C_8H_8O_3$	152.0473	1.31	Sigma-Aldrich	A	
protocatechuic acid	PHUB000310	phenolic acid	$C_7H_6O_4$	154.0266	1.32	Sigma	A	
hydroxytyrosol	PHUB001321	other phenolic	$C_8H_{10}O_3$	154.0630	0.13	Extrasynthese	B	
p-coumaric acid	PHUB000590	phenolic acid	$C_9H_8O_3$	164.0473	1.74	Sigma	A	
3-(4-hydroxyphenyl)-propionic acid	PHUB001072	microbial metabolite	$C_9H_{10}O_3$	166.0630	1.15	Fluka	A	
vanillic acid	PHUB000316	phenolic acid	$C_8H_8O_4$	168.0423	1.70	Sigma	A	
gallic acid	PHUB000303	phenolic acid	$C_7H_6O_5$	170.0215	1.17	Sigma (G73849	A	

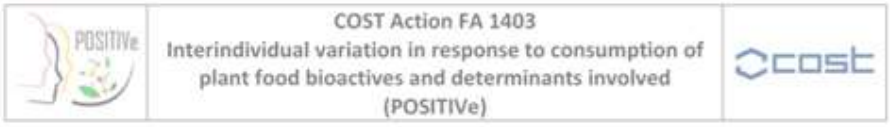
hippuric acid	PHUB001174	phenolic acid	$C_9H_9NO_3$	179.0582	0.23	Sigma (112003)	A	
caffeic acid	PHUB000574	phenolic acid	$C_9H_8O_4$	180.0423	1.67	Sigma (C0625)	A	
myo-inositol	PHUB001870	sugar alcohol	$C_6H_{12}O_6$	180.0634	−2.59	Merck	A	
theobromine	PHUB000790	alkaloid	$C_7H_8N_4O_2$	180.0650	−0.46	Extrasynthese	A	
dihydrocaffeic acid	PHUB000604	microbial metabolite	$C_9H_{10}O_4$	182.0579	1.04	Sigma	A	
homovanillic acid	PHUB000617	phenolic acid	$C_9H_{10}O_4$	182.0579	1.02	Extrasynthese	B	
veratric acid	PHUB001218	phenolic acid	$C_9H_{10}O_4$	182.0579	1.52	Aldrich	A	
catechol *O*-sulfate	PHUB001352	sulfate	$C_6H_6O_5S$	189.9936	−0.81	*synthesised in-house*	B†	
ferulic acid	PHUB000608	phenolic acid	$C_{10}H_{10}O_4$	194.0579	1.58	Aldrich (128708)	A	
bergaptol	PHUB000259	other phenolic	$C_{11}H_6O_4$	202.0270	1.86	Extrasynthese	B*	
pyrogallol 2-*O*-sulfate	PHUB001416	sulfate	$C_6H_6O_6S$	205.9885	−0.66	*synthesised in-house*	A	

urolithin B	PHUB001394	microbial metabolite	$C_{13}H_8O_3$	212.0473	2.65	Villapharma Research S.L.	B	
sinapic acid	PHUB000638	phenolic acid	$C_{11}H_{12}O_5$	224.0685	1.63	Sigma	A[†]	
urolithin A	PHUB001391	microbial metabolite	$C_{13}H_8O_4$	228.0423	2.16	Villapharma Research S.L.	B	
resveratrol	PHUB000324	other phenolic	$C_{14}H_{12}O_3$	228.0786	2.57	Sigma	A	
4-*O*-methylgallic acid 3-*O*-sulfate	PHUB001873	sulfate	$C_8H_8O_8S$	263.9940	−0.53	*synthesised in-house*	A	
genistein	PHUB000225	flavonoid	$C_{15}H_{10}O_5$	270.0528	3.04	Extrasynthese	B	
phloretin	PHUB001344	other phenolic	$C_{15}H_{14}O_5$	274.0841	2.23	Extrasynthese	B	
kaempferol	PHUB000672	flavonoid	$C_{15}H_{10}O_6$	286.0477	1.99	Extrasynthese	B	
luteolin	PHUB000892	flavonoid	$C_{15}H_{10}O_6$	286.0477	2.73	Fluka	B*	
cyanidin	PHUB000483	flavonoid	$C_{15}H_{11}O_6^+$	287.0556	2.41	n/a	B	

(−)-epicatechin	PHUB000262	flavonoid	$C_{15}H_{14}O_6$	290.0790	1.02	Sigma	B	
ellagic acid	PHUB000298	phenolic acid	$C_{14}H_6O_8$	302.0063	1.59	Sigma	A[§]	
hesperetin	PHUB000380	flavonoid	$C_{16}H_{14}O_6$	302.0790	2.52	Sigma	A	
isorhamnetin	PHUB000662	flavonoid	$C_{16}H_{12}O_7$	316.0583	1.96	Extrasynthese	B[‡]	
cafestol	PHUB000006	terpenoid	$C_{20}H_{28}O_3$	316.2038	3.04	MP Biomedicals	A	
5-heptadecylresorcinol (AR17:0)	PHUB000554	alkylresorcinol	$C_{23}H_{40}O_2$	348.3028	8.79	ReseaChem	B	
chlorogenic acid	PHUB000585	phenolic acid	$C_{16}H_{18}O_9$	354.0950	0.17	Aldrich (C3878)	A	
rosmarinic acid	PHUB000634	phenolic acid	$C_{18}H_{16}O_8$	360.0845	2.57	Extrasynthese	A	
(+)-lariciresinol	PHUB001390	lignan	$C_{20}H_{24}O_6$	360.1573	2.16	ArboNova	A	
curcumin	PHUB001408	other phenolic	$C_{21}H_{20}O_6$	368.1260	3.62	Sigma	B*	

tangeretin	PHUB000907	flavonoid	$C_{20}H_{20}O_7$	372.1210	2.88	Extrasynthese	B	
quercetin 3'-*O*-sulfate	PHUB001316	sulfate	$C_{15}H_{10}O_{10}S$	381.9995	0.65	*synthesised in-house*[29]	A†	
quercetin 4'-*O*-sulfate	PHUB001871	sulfate	$C_{15}H_{10}O_{10}S$	381.9995	0.70	*synthesised in-house*[29]	A†	
β-sitosterol	PHUB000479	steroid	$C_{29}H_{50}O$	414.3862	7.27	Sigma	C	
α-tocopherol	PHUB001872	other phenolic	$C_{29}H_{50}O_2$	430.3811	8.84	Sigma	A	
apigenin 7-*O*-glucoside	PHUB000865	flavonoid	$C_{21}H_{20}O_{10}$	432.1056	0.68	HWI Analytik	B*	
cyanidin 3-*O*-glucoside	PHUB000503	flavonoid	$C_{21}H_{21}O_{11}^+$	448.1006	0.98	Extrasynthese	B	
ursolic acid	PHUB000190	terpenoid	$C_{30}H_{48}O_3$	456.3603	6.35	Aldrich	A	
5-pentacosylresorcinol (AR25:0)	PHUB000560	alkylresorcinol	$C_{31}H_{56}O_2$	460.4280	10.4	ReseaChem	B*	

quercetin disulfate	PHUB001874	sulfate	$C_{15}H_{10}O_{13}S_2$	461.9563	−0.34	*a mixture of isomers synthesised in-house*[29]	B‡	
kaempferol 3-glucuronide	PHUB001318	glucuronide	$C_{21}H_{18}O_{12}$	462.0798	1.40	Extrasynthese	A	
β-carotene	PHUB000350	terpenoid	$C_{40}H_{56}$	536.4382	9.72	Extrasynthese	C	
procyanidin A2	PHUB000275	flavonoid	$C_{30}H_{24}O_{12}$	576.1268	2.43	Extrasynthese	A	
naringin	PHUB000389	flavonoid	$C_{27}H_{32}O_{14}$	580.1792	−0.24	Sigma	A	
verbascoside	PHUB000646	phenolic acid	$C_{29}H_{36}O_{15}$	624.2054	1.09	Extrasynthese	A	



Contents

Supplementary Figure 1. The contents of the standard operating procedure (SOP) sent to each participating platform.