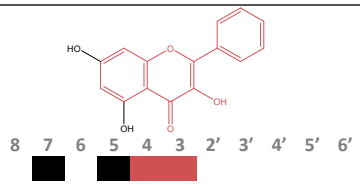
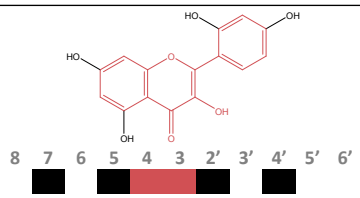
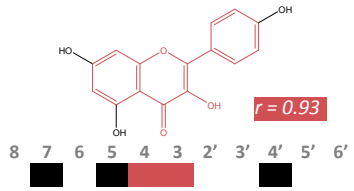
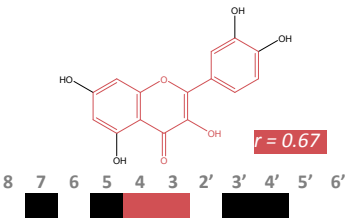
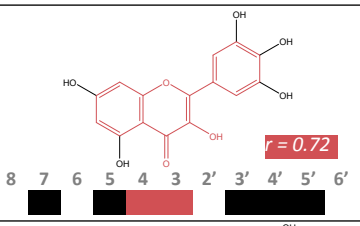
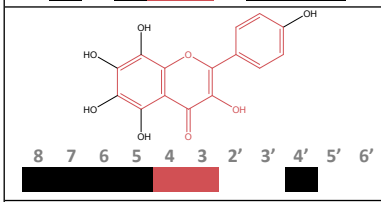
Electronic Supplementary Material (ESI) for Food & Function.

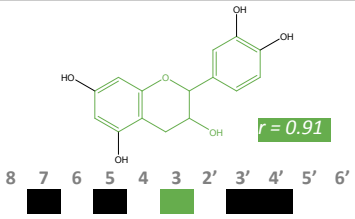
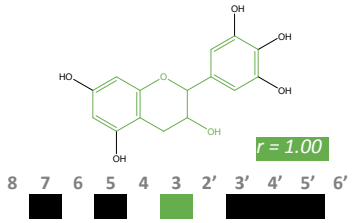
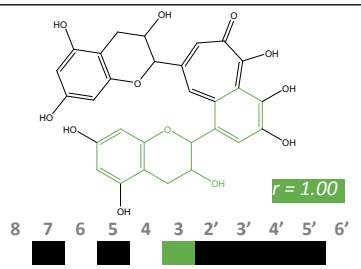
Supplementary Table 1: Flavonol compounds reported in the United States Department of Agriculture (USDA) and Phenol-Explorer (PE) databases

Aglycone structure[1]	Compounds reported in USDA	Compounds reported in PE
		Galangin*; Methylgalangin
		Morin*
	Kaempferol*	Kaempferol*; Kaempferol 3,7,4'-O-triglucoside; Kaempferol 3,7-O-diglucoside; Kaempferol 3-O-(2''-rhamnosyl-6''-acetyl-galactoside) 7-O-rhamnoside; Kaempferol 3-O-(2''-rhamnosyl-galactoside) 7-O-rhamnoside; Kaempferol 3-O-(6''-malonyl-glucoside) ; Kaempferol 7-O-glucoside; Kaempferol 3-O-(6''-acetyl-galactoside) 7-O-rhamnoside; Kaempferol 3-O-xylosyl-rutinoside; Kaempferol3-O-rutinoside; Kaempferol 3-O-acetyl-glucoside; Kaempferol 3-O-galactoside; Kaempferol 3-O-galactoside 7-O-rhamnoside; Kaempferol 3-O-glucoside; Kaempferol 3-O-glucosyl-rhamnosyl-galactoside; Kaempferol 3-O-sophoroside; Kaempferol 3-O-glucosyl-rhamnosyl-glucoside; Kaempferol 3-O-glucuronide; Kaempferol 3-O-rhamnoside; Kaempferol 3-O-rhamnosyl-rhamnosyl-glucoside; Kaempferol 3-O-sophoroside 7-O-glucoside; Kaempferol 3-O-xylosyl-glucoside; Kaempferide.
	Quercetin*; Isorhamnetin	Quercetin*; Quercetin 3,4'-O-diglucoside; Quercetin 3-O-(6''-malonyl-glucoside); Quercetin 3-O-(6''-malonyl-glucoside) 7-O-glucoside; Quercetin 7,4'-O-diglucoside; Quercetin 3-O-(6''-acetyl-galactoside) 7-O-rhamnoside; 3,7-Dimethylquercetin; Quercetin 3-O-acetyl-rhamnoside; Quercetin 3-O-xylosyl-rutinoside; Quercetin 3-O-galactoside; Quercetin 3-O-galactoside 7-O-rhamnoside; Quercetin 3-O-glucoside; Quercetin 3-O-glucosyl-rhamnosyl-galactoside; Quercetin 3-O-glucosyl-rhamnosyl-glucoside; Quercetin 3-O-glucosyl-xyloside; Quercetin 3-O-glucuronide; Quercetin 3-O-rhamnoside; Quercetin 4'-O-glucoside; Quercetin 3-O-rhamnosyl-galactoside; Quercetin 3-O-xylosyl-glucuronide; Quercetin 3-O-rhamnosyl-rhamnosyl-glucoside; Quercetin 3-O-rutinoside; Quercetin 3-O-sophoroside; Quercetin 3-O-xyloside; Quercetin 3-O-arabinoside; Isorhamnetin; Isorhamnetin 3-O-glucoside; Isorhamnetin 3-O-galactoside; Isorhamnetin 3-O-glucoside 7-O-rhamnoside; Isorhamnetin 3-O-glucuronide; Isorhamnetin 3-O-rutinoside; Isorhamnetin 4'-O-glucoside; Isorhamnetin 7-O-rhamnoside; Rhamnetin.
	Myricetin*	Myricetin*; Myricetin 3-O-arabinoside; Myricetin 3-O-galactoside; Myricetin 3-O-glucoside; Myricetin 3-O-rhamnoside; Myricetin 3-O-rutinoside.
		6,8-dihydroxykaempferol*
		3-Methoxynobiletin*

	3-Methoxysinensetin* ;5,3',4'-Trihydroxy-3-methoxy-6:7-methylenedioxyflavone 4'-O-glucuronide; 5,4'-Dihydroxy-3,3'-dimethoxy-6:7-methylenedioxyflavone 4'-O-glucuronide; Patuletin 3-O-(2''-feruloylglucosyl)(1->6)-[apiosyl(1->2)]-glucoside; Patuletin 3-O-glucosyl-(1->6)-[apiosyl(1->2)]-glucoside; Jaceidin 4'-O-glucuronide; Spinacetin 3-O-(2"-feruloylglucosyl)(1->6)-[apiosyl(1->2)]-glucoside; Spinacetin 3-O-(2"-p-coumaroylglucosyl)(1->6)-[apiosyl(1->2)]-glucoside; Spinacetin 3-O-glucosyl-(1->6)-glucoside; Spinacetin 3-O-glucosyl-(1->6)-[apiosyl(1->2)]-glucoside.

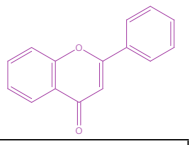
*[1] Characterising structure based on the compound, with the smallest functional groups, that is reported in either database. For brevity and clarity, structures are drawn in a 2-dimensional plane. Coloured squares represent carbons on the flavan nucleus to which functional groups are attached. * Indicates characterising compound. r: pearson correlation coefficient, P < 0.01.*

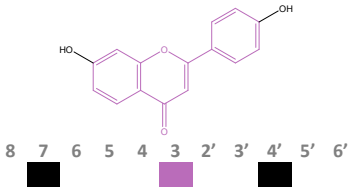
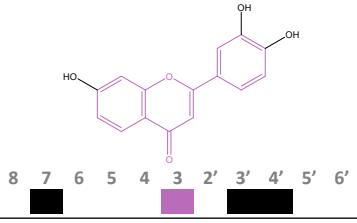
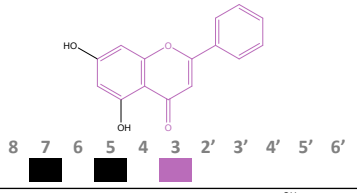
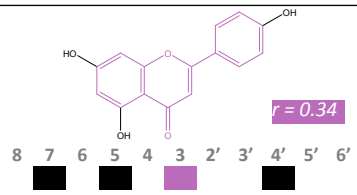
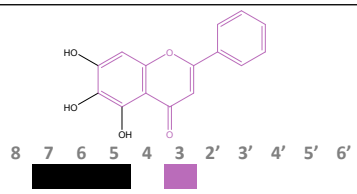
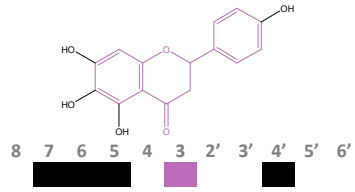
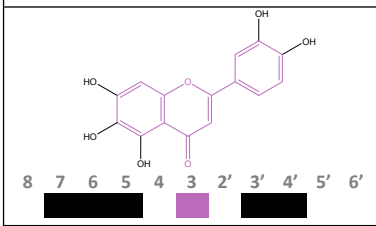
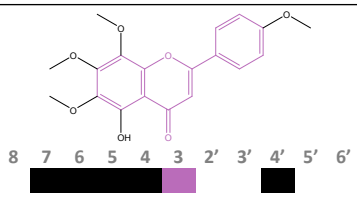
Supplementary Table 2: Flavanol compounds reported in the United States Department of Agriculture (USDA) and Phenol-Explorer (PE) databases

Aglycone structure[1]	Compounds reported in USDA	Compounds reported in PE
	(-)-epicatechin*; (+)-catechin*.	(-)-epicatechin*; (-)-epicatechin 3-O-gallate; (+)-catechin*; (+)-catechin 3-O-gallate; (+)-catechin 3-O-glucose.
	(-)-epigallocatechin*; (-)-epigallocatechin 3-gallate; (+)-gallocatechin*.	(-)-epigallocatechin*; (-)-epigallocatechin 3-O-gallate; (+)-gallocatechin*; (+)-gallocatechin 3-O-gallate.
	Theaflavin*; Theaflavin-3,3'-digallate; Theaflavin-3-gallate; Theaflavin-3'-gallate.	Theaflavin*; Theaflavin 3,3'-O-digallate; Theaflavin 3'-O-gallate; Theaflavin 3-O-gallate.
r = 0.75 **Polymeric compounds**	Dimers; Trimmers; 4-6mers; 7-10mers; Polymers; Thearubigins	02 mers; Procyanidin dimer B1; Procyanidin dimer B2; Procyanidin dimer B3; Procyanidin dimer B4; Procyanidin dimer B5; Procyanidin dimer B7; Prodelphinidin dimer B3; 03 mers; Procyanidin trimer C1; Procyanidin trimer C2; Procyanidin trimer EEC; Procyanidin trimer T2; Prodelphinidin trimer C-GC-C; Prodelphinidin trimer GC-C-C; Prodelphinidin trimer GC-GC-C; 04-06 mers; 07-10 mers; Polymers (>10 mers); (-)-epicatechin-(2a-7)(4a-8)-epicatechin 3-O-galactoside; Cinnamtannin A2.

[1] *Characterising structure based on the compound, with the smallest functional groups, that is reported in either database. For brevity and clarity, structures are drawn in a 2-dimensional plane. Coloured squares represent carbons on the flavan nucleus to which functional groups are attached.* * *Indicates characterising compound. r: pearson correlation coefficient, P < 0.01.*

Supplementary Table 3: Flavone compounds reported in the United States Department of Agriculture (USDA) and Phenol-Explorer (PE) databases

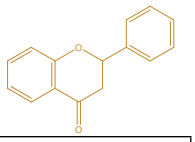


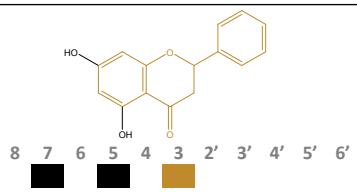
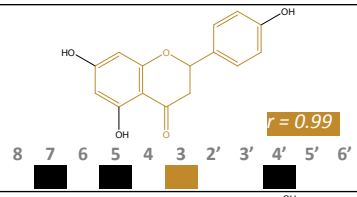
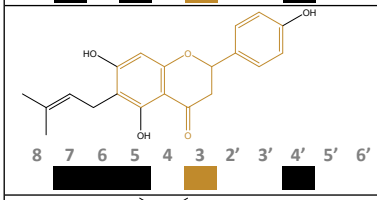
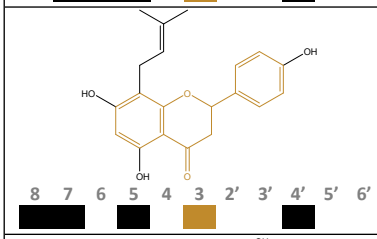
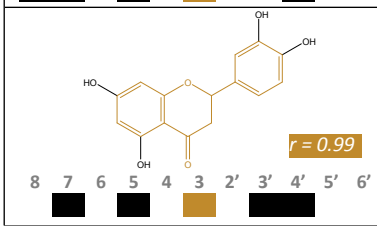
Aglycone structure[1]	Compounds reported in USDA	Compounds reported in PE
		7,4'-Dihydroxyflavone*
		7,3',4'-Trihydroxyflavone*; Geraldone.
		Chrysin*
	Apigenin*	Apigenin*; Apigenin 7-O-(6''-malonyl-apiosyl-glucoside); Apigenin 7-O-apiosyl-glucoside; Apigenin 7-O-diglucuronide; Apigenin 7-O-glucoside; Apigenin 7-O-glucuronide; Rhoifolin; Rhoifolin 4'-O-glucoside; Isorhoifolin.
	Luteolin*	Luteolin*; Luteolin 7-O-(2-apiosyl-6-malonyl)-glucoside; Luteolin 7-O-(2-apiosyl-glucoside); Luteolin 7-O-diglucuronide; Luteolin 7-O-glucoside; Luteolin 7-O-glucuronide; Luteolin 7-O-malonyl-glucoside; Luteolin 7-O-rutinoside; Pebrellin; Diosmin; Chrysoeriol 7-O-glucoside; Chrysoeriol 7-O-apiosyl-glucoside; Chrysoeriol 7-O-(6''-malonyl-glucoside); Chrysoeriol 7-O-(6''-malonyl-apiosyl-glucoside); Neodiosmin.
		Baicalein*
		Scutellarein*; Tetramethylscutellarein; Cirsimaritin; Apigenin 6-C-glucoside; Hispidulin.
		6-Hydroxyluteolin*; 6-Hydroxyluteolin 7-O-rhamnoside; Luteolin 6-C-glucoside; Nepetin; Cirsilineol; Sinensetin; Eupatorin; Jaceosidin.
		Gardenin B*; Apigenin 6,8-di-C-glucoside; Apigenin arabinoside-glucoside; Apigenin galactoside-arabinoside; Tangeretin.

5,6-Dihydroxy-7,8,3',4'-tetramethoxyflavone*; Nobiletin.

*[1] Characterising structure based on the compound, with the smallest functional groups, that is reported in either database. For brevity and clarity, structures are drawn in a 2-dimensional plane. Coloured squares represent carbons on the flavan nucleus to which functional groups are attached. * Indicates characterising compound. r: pearson correlation coefficient, P < 0.01.*

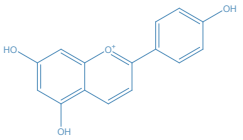
Supplementary Table 4: Flavanone compounds reported in the United States Department of Agriculture (USDA) and Phenol-Explorer (PE) databases

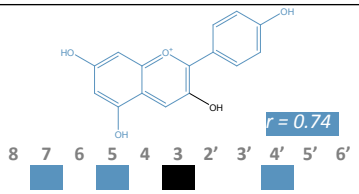
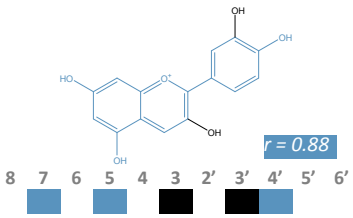
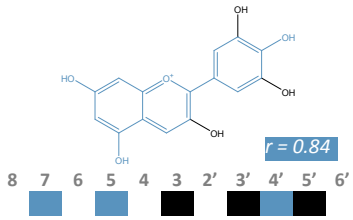


Aglycone structure[1]	Compounds reported in USDA	Compounds reported in PE
		Pinocembrin
	Naringenin	Naringenin; Naringenin 7-O-glucoside; Naringin; Naringin 4'-O-glucoside; Naringin 6'-malonate; Narirutin; Narirutin 4'-O-glucoside; Sakuranetin; Didymin; Poncirin.
		6-Prenylnaringenin*; 6-Geranylnaringenin.
		8-Prenylnaringenin*; Isoxanthohumol.
	Eriodictyol*; Hesperetin	Eriodictyol*; Eriodictyol 7-O-glucoside; Eriocitrin; Neoeriocitrin; Hesperetin; Hesperidin; Neohesperidin.

*[1] Characterising structure based on the compound, with the smallest functional groups, that is reported in either database. For brevity and clarity, structures are drawn in a 2-dimensional plane. Coloured squares represent carbons on the flavan nucleus to which functional groups are attached. * Indicates characterising compound. r: pearson correlation coefficient, $P < 0.01$.*

Supplementary Table 5: Anthocyanidin compounds reported in the United States Department of Agriculture (USDA) and Phenol-Explorer (PE) databases



Aglycone structure[1]	Compounds reported in USDA	Compounds reported in PE
	Pelargonidin*	Pelargonidin*; Pelargonidin 3,5-O-diglucoside; Pelargonidin 3-O-sambubioside; Pelargonidin 3-O-(6''-malonyl-glucoside); Pelargonidin 3-O-(6''-succinyl-glucoside); Pelargonidin 3-O-arabinoside; Pelargonidin 3-O-galactoside; Pelargonidin 3-O-glucoside; Pelargonidin 3-O-glucosyl-rutinoside; Pelargonidin 3-O-rutinoside; Pelargonidin 3-O-sophoroside.
	Cyanidin*; Peonidin	Cyanidin*; Cyanidin 3,5-O-diglucoside; Cyanidin 3-O-(6''-acetyl-galactoside); Cyanidin 3-O-(6''-acetyl-glucoside); Cyanidin 3-O-(6''-caffeoyl-glucoside); Cyanidin 3-O-(6''-dioxalyl-glucoside); Cyanidin 3-O-galactoside; Cyanidin 3-O-(6''-malonyl-3''-glucosyl-glucoside) ; Cyanidin 3-O-xylosyl-rutinoside; Cyanidin 3-O-(6''-malonyl-glucoside); Cyanidin 3-O-(6''-p-coumaroyl-glucoside); Cyanidin 3-O-(6''-succinyl-glucoside); Cyanidin 3-O-arabinoside; Cyanidin 3-O-glucosyl-rutinoside; Cyanidin 3-O-rutinoside; Cyanidin 3-O-glucoside; Cyanidin 3-O-sambubioside; Cyanidin 3-O-sambubiosyl 5-O-glucoside; Cyanidin 3-O-sophoroside; Cyanidin 3-O-xyloside; Peonidin; Peonidin 3-O-(6''-acetyl-galactoside); Peonidin 3-O-(6''-acetyl-glucoside); Peonidin 3-O-(6''-malonyl-glucoside); Peonidin 3-O-(6''-p-coumaroyl-glucoside); Peonidin 3-O-arabinoside; Peonidin 3-O-galactoside; Peonidin 3-O-glucoside; Peonidin 3-O-rutinoside.
	Delphinidin*; Malvidin; Petunidin	Delphinidin 3,5-O-diglucoside; Delphinidin 3-O-(6''-acetyl-galactoside); Delphinidin 3-O-(6''-acetyl-glucoside); Delphinidin 3-O-(6''-malonyl-glucoside); Delphinidin 3-O-(6''-p-coumaroyl-glucoside); Delphinidin 3-O-sambubioside; Delphinidin 3-O-feruloyl-glucoside; Delphinidin 3-O-galactoside; Delphinidin 3-O-glucoside; Delphinidin 3-O-glucosyl-glucoside; Delphinidin 3-O-rutinoside; Delphinidin 3-O-xyloside; Delphinidin 3-O-arabinoside; Malvidin 3,5-O-diglucoside; Malvidin 3-O-(6''-acetyl-galactoside); Malvidin 3-O-(6''-acetyl-glucoside); Malvidin 3-O-(6''-caffeoyl-glucoside); Malvidin 3-O-(6''-p-coumaroyl-glucoside); Malvidin 3-O-arabinoside; Malvidin 3-O-galactoside; Malvidin 3-O-glucoside; Petunidin 3,5-O-diglucoside; Petunidin 3-O-(6''-acetyl-galactoside); Petunidin 3-O-(6''-acetyl-glucoside); Petunidin 3-O-(6''-p-coumaroyl-glucoside); Petunidin 3-O-arabinoside; Petunidin 3-O-galactoside; Petunidin 3-O-glucoside; Petunidin 3-O-rhamnoside; Petunidin 3-O-rutinoside.
		Vitisin A*; Pigment A; Pinotin A.

[1] *Characterising structure based on the compound, with the smallest functional groups, that is reported in either database. For brevity and clarity, structures are drawn in a 2-dimensional plane. Coloured squares represent carbons on the flavan nucleus to which functional groups are attached.* ** Indicates characterising compound. r: pearson correlation coefficient, $P < 0.01$.*