molecules

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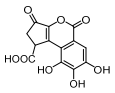
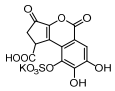
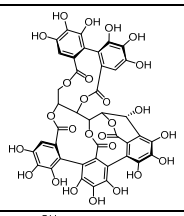
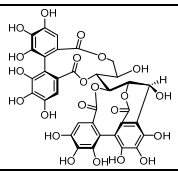
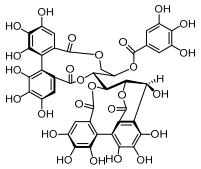
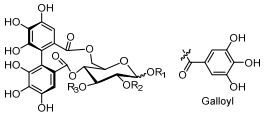
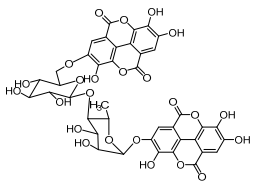
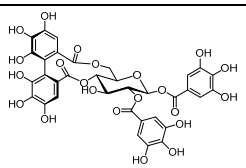
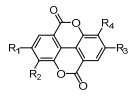
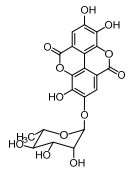
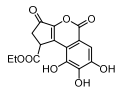
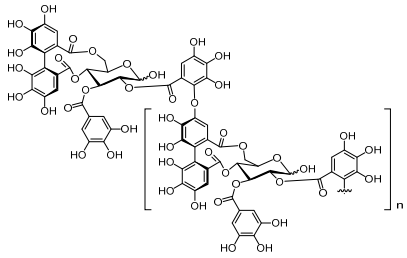
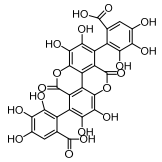
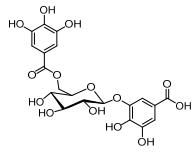
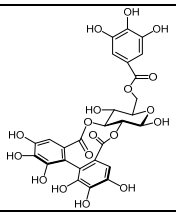
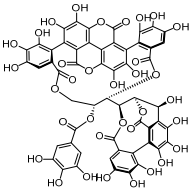
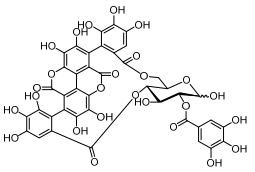
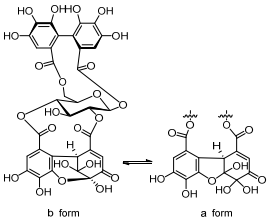
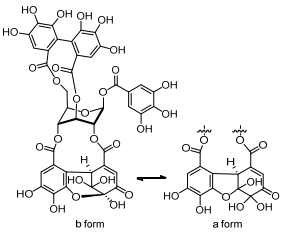
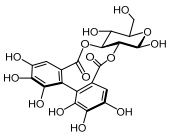
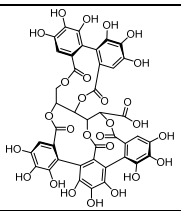
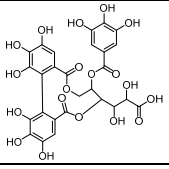
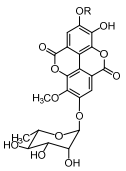
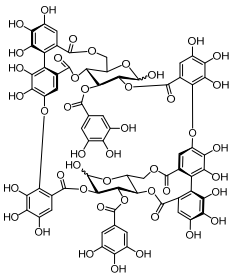
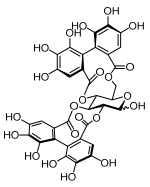
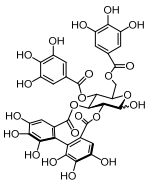
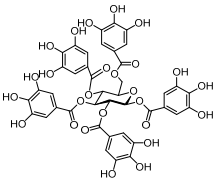
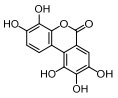
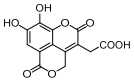
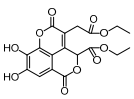
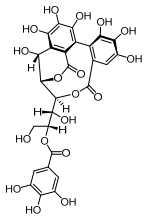
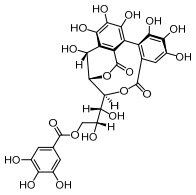
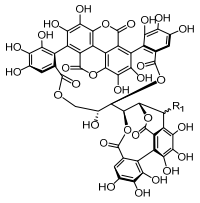
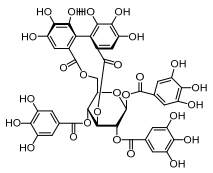
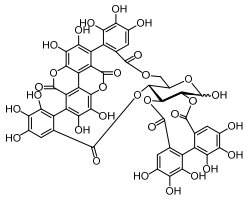
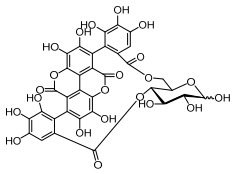
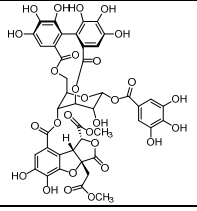
Table S1. Phytochemicals identified from different pomegranate tissues. The chemical structures, molecular formulas, and molecular weights of the phytochemicals are shown. The analytical methods, tissues of identification, and representative references are also indicated. CAS, chemical abstracts service; DAD, diode array detection; ESR, electron spin resonance; FD, fluorescence detection; FID, flame ionization detection; ID, identification method; IR, infrared spectroscopy; MP, melting point; MS, mass spectrometry; MW, molecular weight; NMR, nuclear magnetic resonance; TLC, thin layer chromatography.

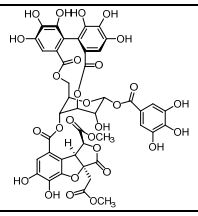
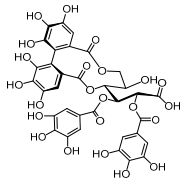
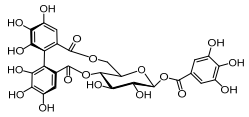
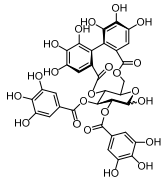
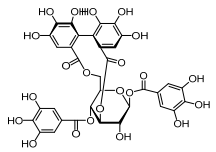
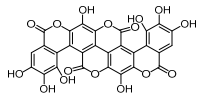
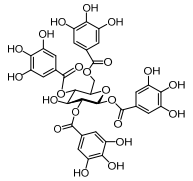
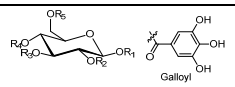
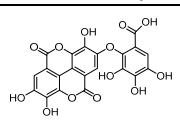
Name	Structure	Formula	MW	ID	Tissue	References
Ellagitannins, gallotannins and derivatives						
Brevifolin		$C_{12}H_8O_6$	248.1900	NMR	Leaf	[1]
Brevifolin carboxylic acid		$C_{13}H_8O_8$	292.1990	NMR	Leaf, flower, heartwood	[1-3]
Brevifolin carboxylic acid 10-monopotassium sulphate		$C_{13}H_7KO_{11}S$	410.3463	NMR	Leaf	[4]
Castalagin		$C_{41}H_{26}O_{26}$	934.6330	NMR	Stem bark	[5]
Casuariin		$C_{34}H_{24}O_{22}$	784.5440	NMR	Stem bark	[5]
Casuarinin		$C_{41}H_{28}O_{26}$	936.6490	NMR	Peel, stem bark	[5, 6]
						
Corilagin	R_1 = Galloyl (β-configuration), R_2 = R_3 = H	$C_{27}H_{22}O_{18}$	634.4550	NMR	Peel, leaf	[6, 7]
Isocorilagin	R_1 = Galloyl (α-configuration), R_2 = R_3 = H	$C_{27}H_{22}O_{18}$	634.4550	NMR	Flower	[8]
Hippomanin A	R_2 = Galloyl, R_1 = R_3 = H	$C_{27}H_{22}O_{18}$	634.4550	IR	Flower	[2]
Gemin D	R_1 = R_2 = H, R_3 = Galloyl	$C_{27}H_{22}O_{18}$	634.4550	IR	Flower	[2]
Diellagic acid rhamnosyl(1→4) glucopyranoside		$C_{40}H_{30}O_{24}$	894.6560	NMR	Heartwood	[9]
1,2-Di-*O*-galloyl-4,6-*O*-(*S*)-hexahydroxydiphenoyl β-D-glucopyranoside		$C_{34}H_{26}O_{22}$	786.5600	MS	Flower	[10]

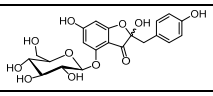
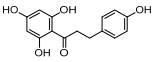
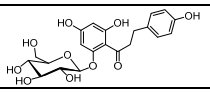
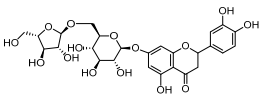
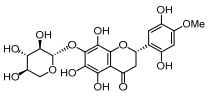
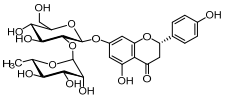
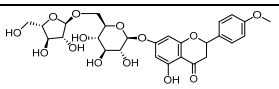
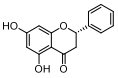
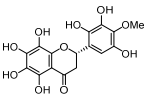
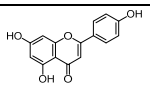
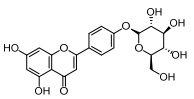
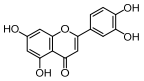
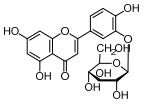
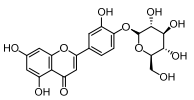
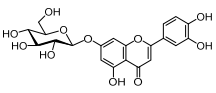
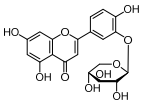
						
Ellagic acid	$R_1 = R_2 = R_3 = R_4 = OH$	$C_{14}H_6O_8$	302.1940	NMR MS	Peel, flower, leaf	[1, 11, 12]
3,3′-Di-*O*-methylellagic acid	$R_1 = R_3 = OH$, $R_2 = R_4 = OCH_3$	$C_{16}H_{10}O_8$	330.2480	IR	Seed	[13]
3,3′,4′-Tri-*O*-methylellagic acid	$R_1 = OH$, $R_2 = R_3 = R_4 = OCH_3$	$C_{17}H_{12}O_8$	344.2750	IR	Seed	[13]
3-*O*-methylellagic acid	$R_2 = OCH_3$, $R_1 = R_3 = R_4 = OH$	$C_{15}H_8O_8$	316.2210	NMR	Heartwood	[3]
4,4′-Di-*O*-methylellagic acid	$R_1 = R_3 = OCH_3$, $R_2 = R_4 = OH$	$C_{16}H_{10}O_8$	330.2480	NMR	Heartwood	[3]
3′-*O*-methyl-3,4-methylenedioxy-ellagic acid	R_1-$R_2 = OCH_2O$, $R_3 = OH$, $R_4 = OCH_3$	$C_{16}H_8O_8$	328.2320	NMR	Heartwood	[14]
Eschweilenol C (Ellagic acid 4-*O*-α-L-rhamnopyranoside)		$C_{20}H_{16}O_{12}$	448.3360	NMR	Heartwood	[14]
Ethyl brevifolincarboxylate		$C_{15}H_{12}O_8$	320.2530	IR	Flower	[12]
						
Eucalbanin B	n = 1	$C_{68}H_{50}O_{44}$	1571.1040	NMR	Aril	[15]
Eucarpanin T_1	n = 2	$C_{102}H_{74}O_{66}$	2355.6480	NMR	Aril	[15]
Pomegraniin A	n = 3	$C_{136}H_{98}O_{88}$	3140.1920	NMR	Aril	[15]
Pomegraniin B	n = 4	$C_{170}H_{122}O_{110}$	3924.7360	NMR	Aril	[15]
Gallagic acid		$C_{28}H_{14}O_{18}$	638.4020	MS	Peel	[11]
Gallic acid 3-*O*-β-D-(6′-*O*-galloyl)-glucopyranoside		$C_{20}H_{20}O_{14}$	484.3660	IR	Flower	[2]

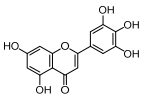
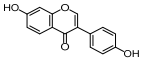
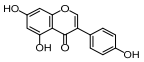
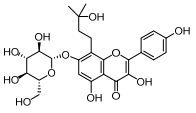
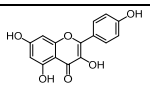
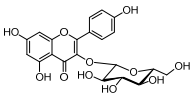
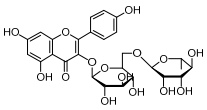
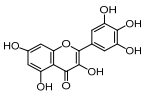
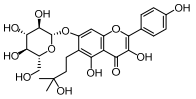
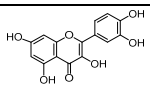
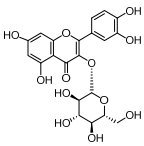
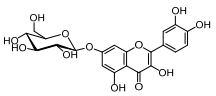
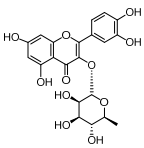
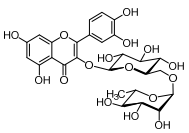
6-*O*-galloyl-2,3-(*S*)-hexahydroxydiphenoyl-D-glucose		$C_{27}H_{22}O_{18}$	634.4550	NMR MS	Stem bark, juice	[16, 17]
5-Galloylpunicacortein D		$C_{55}H_{32}O_{34}$	1236.8270	NMR	Heartwood	[9]
2-*O*-galloylpunicalin (2-*O*-galloyl-4,6-(*S*,*S*)-gallagyl-D-glucose)		$C_{41}H_{26}O_{26}$	934.6330	NMR	Heartwood, stem bark	[9, 16]
Granatin A		$C_{34}H_{24}O_{23}$	800.5430	NMR	Fruit, leaf	[7, 18]
Granatin B		$C_{41}H_{28}O_{27}$	952.6480	NMR	Fruit, leaf	[7, 18]
2,3-(*S*)-hexahydroxydiphenoyl-D-glucose		$C_{20}H_{18}O_{14}$	482.3500	NMR MS	Stem bark, juice	[16, 17]
Lagerstannin B		$C_{41}H_{26}O_{27}$	950.6320	MS	Peel	[19]
Lagerstannin C		$C_{27}H_{22}O_{19}$	650.4540	MS	Juice	[17]

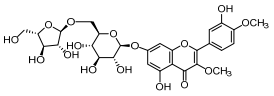
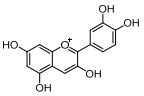
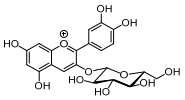
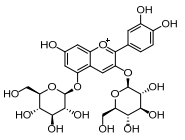
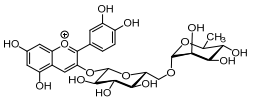
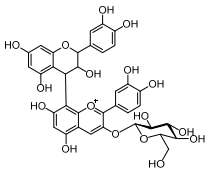
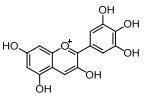
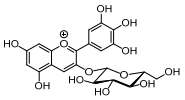
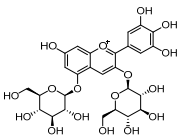
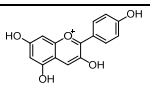
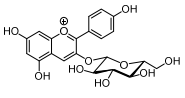
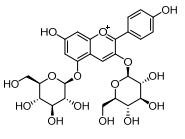
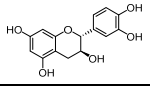
3-*O*-methylellagic acid 4-*O*-α-L-rhamnopyranoside	 R = H	$C_{21}H_{18}O_{12}$	462.3630	NMR	Heartwood	[3]
3,4'-*O*-dimethylellagic acid 4-*O*-α-L-rhamnopyranoside	R = CH_3	$C_{22}H_{20}O_{12}$	476.3900	NMR	Heartwood	[3]
Oenothein B		$C_{68}H_{48}O_{44}$	1569.0880	NMR	Aril	[15]
Pedunculagin I		$C_{34}H_{24}O_{22}$	784.5440	NMR MS	Peel, stem bark	[16, 17]
Pedunculagin II		$C_{34}H_{26}O_{22}$	786.5600	MS	Juice	[17]
1,2,3,4,6-Penta-*O*-galloyl-β-D-glucose		$C_{41}H_{32}O_{26}$	940.6810	NMR	Leaf	[7]
3,4,8,9,10-Pentahydroxydibenzo[*b*,*d*]pyran-6-one (Urolithin M-5)		$C_{13}H_8O_7$	276.2000	NMR	Leaf	[1]
Phyllanthusiin E		$C_{13}H_8O_8$	292.1990	NMR	Flower	[12]
Pomegranatate		$C_{18}H_{16}O_{10}$	392.3160	NMR	Flower	[12]

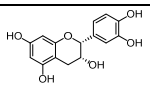
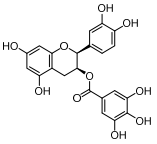
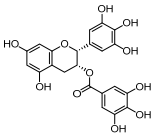
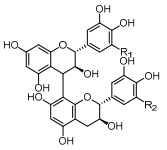
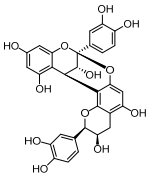
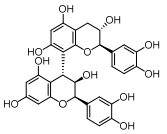
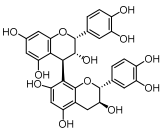
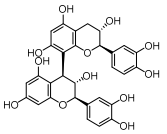
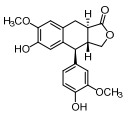
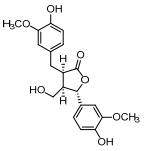
Punicacortein A		$C_{27}H_{22}O_{18}$	634.4550	NMR	Stem bark	[5]
Punicacortein B		$C_{27}H_{22}O_{18}$	634.4550	NMR	Stem bark	[5]
Punicacortein C Punicacortein D	 R_1 = α-OH R_1 = β-OH	$C_{48}H_{28}O_{30}$ $C_{48}H_{28}O_{30}$	1084.7220 1084.7220	NMR NMR	Stem bark, peel Stem bark	[5, 15] [5]
Punicafolin		$C_{41}H_{30}O_{26}$	938.6650	NMR	Leaf	[7]
Punicalagin A Punicalagin B	 α-OH β-OH	$C_{48}H_{28}O_{30}$	1084.7220	NMR MS	Peel, stem bark, aril, juice, root	[11, 15, 16, 19, 20]
Punicalin		$C_{34}H_{22}O_{22}$	782.5280	NMR MS	Peel, stem bark, aril, juice, heartwood	[9, 11, 15, 16, 19]
Punicatannin A		$C_{43}H_{34}O_{28}$	998.7170	NMR	Flower	[8]

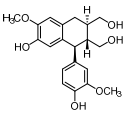
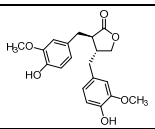
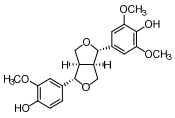
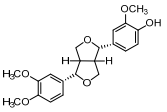
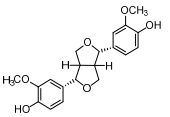
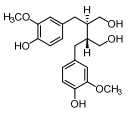
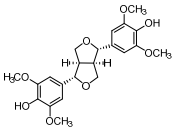
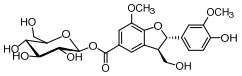
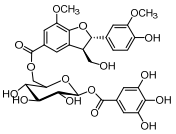
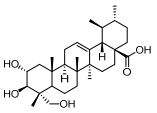
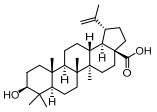
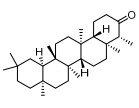
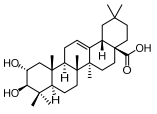
Punicatannin B		$C_{43}H_{34}O_{28}$	998.7170	NMR	Flower	[8]
Punigluconin		$C_{34}H_{26}O_{23}$	802.5590	NMR	Stem bark	[5]
Strictinin [1-*O*-galloyl-4,6-(*S*) - hexahydroxydiphenoyl-D-glucose]		$C_{27}H_{22}O_{18}$	634.4550	NMR	Leaf	[7]
Tellimagrandin I		$C_{34}H_{26}O_{22}$	786.5600	NMR	Peel	[6]
Tercatain [1,4-Di-*O*-galloyl-3,6-(*R*)- hexahydroxydiphenoyl-β-glucopyranose]		$C_{34}H_{26}O_{22}$	786.5600	NMR	Leaf	[4]
Terminalin (Gallagyl dilactone)		$C_{28}H_{10}O_{16}$	602.3720	NMR	Stem bark	[16]
1,2,4,6-Tetra-*O*-galloyl-β-D-glucose		$C_{34}H_{28}O_{22}$	788.5760	NMR	Leaf	[7]
						
1,2,3-Tri-*O*-galloyl-β-glucopyranose	$R_1 = R_2 = R_3 =$ Galloyl, $R_4 = R_5 = H$	$C_{27}H_{24}O_{18}$	636.4710	NMR	Leaf	[1]
1,2,4-Tri-*O*-galloyl-β-glucopyranose	$R_1 = R_2 = R_4 =$ Galloyl, $R_3 = R_5 = H$	$C_{27}H_{24}O_{18}$	636.4710	NMR	Leaf	[4]
1,2,6-Tri-*O*-galloyl-β-glucopyranose	$R_1 = R_2 = R_5 =$ Galloyl, $R_3 = R_4 = H$	$C_{27}H_{24}O_{18}$	636.4710	NMR MS	Leaf, flower	[1, 10]
1,3,4-Tri-*O*-galloyl-β-glucopyranose	$R_1 = R_3 = R_4 =$ Galloyl, $R_2 = R_5 = H$	$C_{27}H_{24}O_{18}$	636.4710	NMR	Leaf	[4]
1,4,6-Tri-*O*-galloyl-β-glucopyranose	$R_1 = R_4 = R_5 =$ Galloyl, $R_2 = R_3 = H$	$C_{27}H_{24}O_{18}$	636.4710	NMR	Leaf	[1]
3,4,6-Tri-*O*-galloyl-β-glucopyranose	$R_3 = R_4 = R_5 =$ Galloyl, $R_1 = R_2 = H$	$C_{27}H_{24}O_{18}$	636.4710	IR	Flower	[2]
Valoneic acid dilactone		$C_{21}H_{10}O_{13}$	470.2980	MS	Juice, peel	[19]

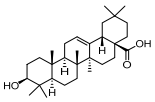
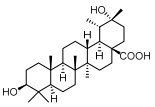
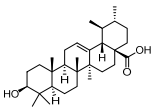
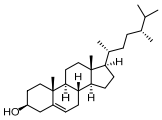
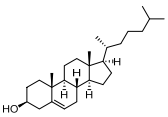
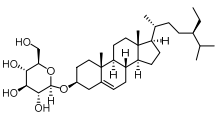
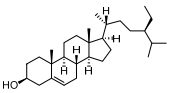
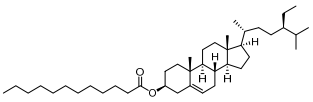
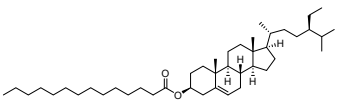
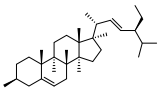
Flavonoids						
Hovetrichoside C		$C_{21}H_{22}O_{11}$	450.3960	IR	Flower	[2]
Phloretin		$C_{15}H_{14}O_5$	274.2720	MS	Juice	[21]
Phlorizin		$C_{21}H_{24}O_{10}$	436.4130	IR	Flower	[2]
Eriodictyol-7-*O*-α-L-arabinofuranosyl (1-6)-β-D-glucoside		$C_{26}H_{30}O_{15}$	582.5110	NMR	Stem bark	[22]
Granatumflavanyl xyloside		$C_{21}H_{22}O_{13}$	482.3940	NMR	Flower	[23]
Naringin (Naringenin-7-*O*-rhamnoglucoside)		$C_{27}H_{32}O_{14}$	580.5390	DAD	Peel	[24]
Naringenin-4'methyl ether 7-*O*-α-L-arabinofuranosyl(1-6)-β-D-glucoside		$C_{27}H_{32}O_{14}$	580.5390	NMR	Stem bark	[22]
Pinocembrin		$C_{15}H_{12}O_4$	256.2570	MS	Juice	[21]
Punicaflavanol		$C_{16}H_{14}O_{10}$	366.2780	NMR	Flower	[23]
Apigenin		$C_{15}H_{10}O_5$	270.2400	DAD	Peel	[25]
Apigenin 4'-*O*-β-glucopyranoside		$C_{21}H_{20}O_{10}$	432.3810	NMR	Leaf	[26]
Luteolin		$C_{15}H_{10}O_6$	286.2390	NMR MS	Peel, flower	[10, 27]
Luteolin 3'-*O*-β-glucopyranoside		$C_{21}H_{20}O_{11}$	448.3800	NMR	Leaf	[26]
Luteolin 4'-*O*-β-glucopyranoside		$C_{21}H_{20}O_{11}$	448.3800	NMR	Leaf	[26]
Cynaroside (Luteolin 7-*O*-glycoside)		$C_{21}H_{20}O_{11}$	448.3800	MS	Peel	[28]
Luteolin 3'-*O*-β-xylopyranoside		$C_{20}H_{18}O_{10}$	418.3540	NMR	Leaf	[26]

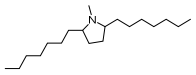
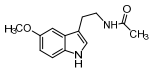
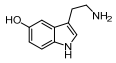
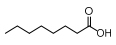
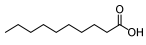
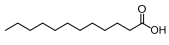
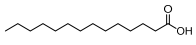
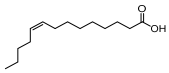
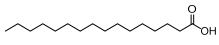
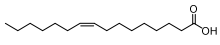
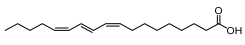
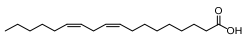
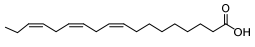
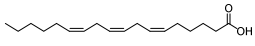
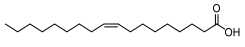
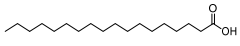
Tricetin		$C_{15}H_{10}O_7$	302.2380	MS NMR	Flower, peel	[10, 27]
Daidzein		$C_{15}H_{10}O_4$	254.2410	DAD	Seed	[29]
Genistein		$C_{15}H_{10}O_5$	270.2400	DAD	Seed	[29]
Amurensin (Noricaritin 7-β-D-glucopyranoside)		$C_{26}H_{30}O_{12}$	534.5140	MS	Juice	[30]
Kaempferol		$C_{15}H_{10}O_6$	286.2390	MS	Peel	[28]
Astragalin (Kaempferol 3-*O*-glucoside)		$C_{21}H_{20}O_{11}$	448.3800	MS	Peel	[31]
Kaempferol-3-*O*-rhamnoglucoside		$C_{21}H_{20}O_{10}$	432.3810	MS	Juice	[21]
Myricetin		$C_{15}H_{10}O_8$	318.2370	DAD	Peel	[25]
Phellatin		$C_{26}H_{30}O_{12}$	534.5140	MS	Juice	[30]
Quercetin		$C_{15}H_{10}O_7$	302.2380	DAD MS	Juice, leaf, seed, peel	[28, 32]
Hirsutrin (Quercetin-3-*O*-glucoside)		$C_{21}H_{20}O_{12}$	464.3790	MS	Peel	[31]
Quercimeritrin (Quercetin-7-*O*-glucoside)		$C_{21}H_{20}O_{12}$	464.3790	MS	Peel	[31]
Quercetin 3-*O*-rhamnoside		$C_{21}H_{20}O_{11}$	448.3800	MS	Peel	[31]
Rutin (Quercetin-3-*O*-rutinoside)		$C_{27}H_{30}O_{16}$	610.5210	DAD	Juice	[33]

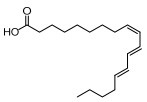
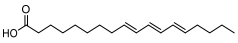
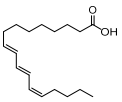
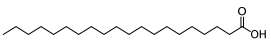
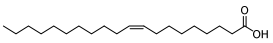
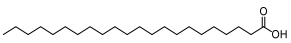
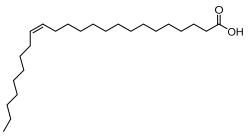
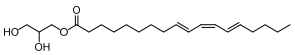
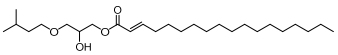
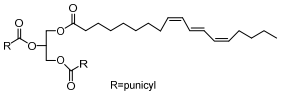
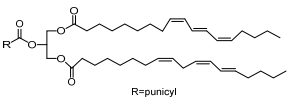
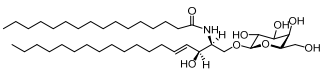
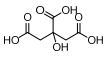
Quercetin-3,4'-dimethyl ether 7-*O*-α-L-arabinofuranosyl(1-6)-β-D-glucoside		$C_{28}H_{32}O_{16}$	624.5480	NMR	Stem bark	[34]
Cyanidin		$C_{15}H_{11}O_6^+$	287.2465	ESR	Juice	[35]
Chrysanthemin (Cyanidin-3-*O*-glucoside)		$C_{21}H_{21}O_{11}^+$	449.3875	MS	Juice	[30]
Cyanin (Cyanidin-3,5-di-*O*-glucoside)		$C_{27}H_{31}O_{16}^+$	611.5285	MS	Juice	[30]
Antirrhinin (Cyanidin-3-*O*-rutinoside)		$C_{27}H_{31}O_{15}^+$	595.5295	MS	Juice	[30]
Catechin-cyanidin-3-hexoside		$C_{36}H_{33}O_{17}^+$	737.1715	MS	Juice	[30]
Delphinidin		$C_{15}H_{11}O_7^+$	303.2455	ESR	Juice	[35]
Myrtillin (Delphinidin-3-*O*-glucoside)		$C_{21}H_{21}O_{12}^+$	465.3865	MS	Juice	[30]
Delphinidin-3,5-di-*O*-glucoside		$C_{27}H_{31}O_{17}^+$	627.5275	MS	Juice	[30]
Pelargonidin		$C_{15}H_{11}O_5^+$	271.2475	ESR	Juice	[35]
Callistephin (Pelargonidin-3-*O*-glucoside)		$C_{21}H_{21}O_{10}^+$	433.3885	MS	Juice	[30]
Pelargonin (Pelargonidin-3,5-di-*O*-glucoside)		$C_{27}H_{31}O_{15}^+$	595.5295	MS	Juice	[30]
Catechin		$C_{15}H_{14}O_6$	290.2710	MS DAD	Peel, juice, leaf	[21, 31, 32]

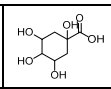
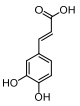
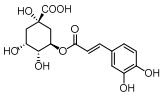
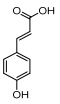
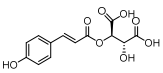
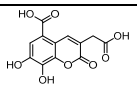
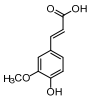
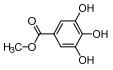
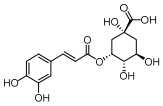
Epicatechin		$C_{15}H_{14}O_6$	290.2710	MS DAD	Peel, juice, leaf, seed	[21, 31, 32]
Epicatechin gallate		$C_{22}H_{18}O_{10}$	442.3760	MS	Peel	[31]
Epigallocatechin-3-*O*-gallate		$C_{22}H_{18}O_{11}$	458.3750	DAD	Fruit	[36]
						
Gallocatechin-(4→8)-catechin	R_1 = OH, R_2 = H	$C_{30}H_{26}O_{13}$	594.5250	MS	Peel	[37]
Gallocatechin-(4→8)-gallocatechin	R_1 = OH, R_2 = OH	$C_{30}H_{26}O_{14}$	610.5240	MS	Peel	[37]
Catechin-(4→8)-gallocatechin	R_1 = H, R_2 = OH	$C_{30}H_{26}O_{13}$	594.5250	MS	Peel	[37]
Procyanidin A2		$C_{30}H_{24}O_{12}$	576.5100	MS	Peel	[31]
Procyanidin B1		$C_{30}H_{26}O_{12}$	578.5260	MS	Peel	[31]
Procyanidin B2		$C_{30}H_{26}O_{12}$	578.5260	MS	Peel	[31]
Procyanidin B3		$C_{30}H_{26}O_{12}$	578.5260	MS	Peel	[31]
Lignans						
Conidendrin		$C_{20}H_{20}O_6$	356.3740	MS	Juice	[38]
Isohydroxymatairesinol		$C_{20}H_{22}O_7$	374.3890	MS	Peel	[38]

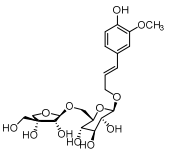
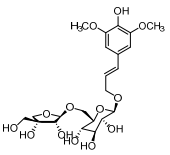
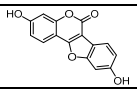
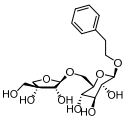
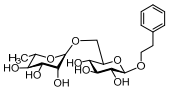
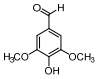
Isolariciresinol		$C_{20}H_{24}O_6$	360.4060	MS	Juice, peel	[38]
Matairesinol		$C_{20}H_{22}O_6$	358.3900	MS	Wood knot	[39]
Medioresinol		$C_{21}H_{24}O_7$	388.4160	MS	Juice, wood knot, seed	[39]
Phylligenin		$C_{21}H_{24}O_6$	372.4170	MS	Peel	[38]
Pinoresinol		$C_{20}H_{22}O_6$	358.3900	MS	Juice	[21]
Secoisolariciresinol		$C_{20}H_{26}O_6$	362.4220	MS	Peel, juice	[38]
Syringaresinol		$C_{22}H_{26}O_8$	418.4420	MS	Juice, wood knot, peel, seed	[39]
Pomegralignan		$C_{24}H_{28}O_{12}$	508.4760	NMR	Aril, peel	[15]
Punicatannin C		$C_{31}H_{32}O_{16}$	660.5810	NMR	Flower	[2]
Triterpenoids and phytosterols						
Asiatic acid		$C_{30}H_{48}O_5$	488.7090	MS	Flower	[10]
Betulinic acid (Betulic acid)		$C_{30}H_{48}O_3$	456.7110	MP	Leaf	[40]
Friedooleanan-3-one (Friedelin)		$C_{30}H_{50}O$	426.7290	IR	Stem and root bark	[41]
Maslinic acid		$C_{30}H_{48}O_4$	472.7100	MS	Flower	[10]

Oleanolic acid		$C_{30}H_{48}O_3$	456.7110	MS	Flower	[10]
Punicanolic acid		$C_{30}H_{50}O_4$	474.7260	DAD NMR	Flower, peel	[10, 27]
Ursolic acid		$C_{30}H_{48}O_3$	456.7110	MS	Flower	[10]
Campesterol		$C_{28}H_{48}O$	400.6910	MS	Seed	[42]
Cholesterol		$C_{27}H_{46}O$	386.6640	MS	Seed	[42]
Daucosterol		$C_{35}H_{60}O_6$	576.8590	MS	Seed, flower	[12, 13]
β-Sitosterol		$C_{29}H_{50}O$	414.7180	MS DAD	Seed, flower	[10, 42]
β-Sitosterol laurate		$C_{41}H_{72}O_2$	597.0250	NMR	Peel	[27]
β-Sitosterol myristate		$C_{43}H_{76}O_2$	625.0790	NMR	Peel	[27]
Stigmasterol		$C_{29}H_{48}O$	412.7020	MS	Seed	[42]
Alkaloids and indolamines						
N-(2',5'-dihydroxyphenyl)pyridinium chloride		$C_{11}H_{10}ClNO_2$	223.6560	NMR	Leaf	[26]
Hygrine		$C_8H_{15}NO$	141.2140	MS	Root bark	[43]
Norhygrine		$C_7H_{13}NO$	127.1870	MS	Root bark	[43]
Pelletierine		$C_8H_{15}NO$	141.2140	MS	Stem and root bark	[43]
N-methylpelletierine		$C_9H_{17}NO$	155.2410	MS	Stem and root bark	[43]
Norpseudopelletierine		$C_8H_{13}NO$	139.1980	MS	Stem and root bark	[43]
Pseudopelletierine		$C_9H_{15}NO$	153.2250	MS	Stem and root bark	[43]

2-(2'-Hydroxypropyl)-Δ^1piperideine		$C_8H_{15}NO$	141.2140	MS	Root bark	[43]
2-(2'-Propenyl)-Δ^1piperideine		$C_8H_{13}N$	123.1990	MS	Root bark	[43]
Punigratane (2,5-Diheptyl-*N*-methylpyrrolidine)		$C_{19}H_{39}N$	281.5280	NMR	Peel	[44]
Sedridine		$C_8H_{17}NO$	143.2300	MS	Root bark	[43]
Melatonin		$C_{13}H_{16}N_2O_2$	232.2830	MS	Fruit extract	[45]
Serotonin		$C_{10}H_{12}N_2O$	176.2190	FD	Fruit extract	[45]
Tryptamine		$C_{10}H_{12}N_2$	160.2200	FD	Fruit extract	[45]
Fatty acids and lipids						
Caproic acid (Hexanoic acid)		$C_6H_{12}O_2$	116.1600	MS	Juice	[46]
Caprylic acid (Octanoic acid)		$C_8H_{16}O_2$	144.2140	MS	Juice	[47]
Capric acid (Decanoic acid)		$C_{10}H_{20}O_2$	172.2680	MS	Juice	[47]
Lauric acid (Dodecanoic acid)		$C_{12}H_{24}O_2$	200.3220	FID	Seed	[48]
Myristic acid (Tetradecanoic acid)		$C_{14}H_{28}O_2$	228.3760	FID	Seed, fruit	[32]
Myristoleic acid (9-*cis*-Tetradecanoic acid)		$C_{14}H_{26}O_2$	226.3600	FID	Seed	[48]
Palmitic acid (Hexadecanoic acid)		$C_{16}H_{32}O_2$	256.4300	FID	Seed, fruit	[32, 49]
Palmitoleic acid (Hexadec-9-enoic acid)		$C_{16}H_{30}O_2$	254.4140	FID	Seed, fruit	[32]
Punicic acid (9*Z*, 11*E*, 13*Z*-octadecatrienoic acid)		$C_{18}H_{30}O_2$	278.4360	FID	Seed	[49]
Linoleic acid (*cis*, *cis*-9,12-Octadecadienoic acid)		$C_{18}H_{32}O_2$	280.4520	FID	Seed, fruit	[32, 49]
α-Linolenic acid (All-*cis*-9,12,15-octadecatrienoic acid)		$C_{18}H_{30}O_2$	278.4360	FID	Seed, fruit	[32]
γ-Linolenic acid (All-*cis*-6,9,12-octadecatrienoic acid)		$C_{18}H_{30}O_2$	278.4360	FID	Seed, fruit	[32]
Oleic acid (9*Z*-octadecenoic acid)		$C_{18}H_{34}O_2$	282.4680	MS FID	Seed, fruit	[32, 50]
Stearic acid (Octadecanoic acid)		$C_{18}H_{36}O_2$	284.4840	MS FID	Seed, fruit	[32, 50]

α-Eleostearic acid (9*Z*, 11*E*, 13*E*-octadecatrienoic acid)		$C_{18}H_{30}O_2$	278.4360	MS	Seed	[51]
β-Eleostearic acid (9*E*, 11*E*, 13*E*-octadecatrienoic acid)		$C_{18}H_{30}O_2$	278.4360	MS	Seed	[51]
Catalpic acid (9*E*, 11*E*, 13*Z*-octadecatrienoic acid)		$C_{18}H_{30}O_2$	278.4360	MS	Seed	[51]
Arachidic acid (Eicosanoic acid)		$C_{20}H_{40}O_2$	312.5380	MS FID	Seed, fruit	[32, 50]
Gadoleic acid (9*Z*-icosenoic acid)		$C_{20}H_{38}O_2$	310.5220	MS	Seed	[51]
Behenic acid (Docosanoic acid)		$C_{22}H_{44}O_2$	340.5920	MS	Seed	[51]
Nervonic acid (*cis*-15-Tetracosenoic acid)		$C_{24}H_{46}O_2$	366.6300	FID	Seed, fruit	[32]
1-*O*-9*E*,11*Z*,13*E*-octadecatrienoyl glycerol		$C_{21}H_{36}O_4$	352.5150	NMR	Seed, peel	[27, 50]
1-*O*-isopentyl-3-*O*-octadec-2-enoyl glycerol		$C_{26}H_{50}O_4$	426.6820	NMR MS	Seed, peel	[27, 50]
Tri-*O*-punicylglycerol		$C_{57}H_{92}O_6$	873.3570	NMR	Seed	[52]
Di-*O*-punicyl-*O*-octadeca-8*Z*, 11*Z*, 13*E*-trienylglycerol		$C_{57}H_{92}O_6$	873.3570	NMR	Seed	[52]
N-palmitoyl cerebroside		$C_{40}H_{77}NO_8$	700.0550	TLC FID	Seed	[53]
Organic acids and phenolic acids						
Ascorbic acid		$C_6H_8O_6$	176.1240	DAD	Leaf, peel, seed, juice	[32]
Citric acid		$C_6H_8O_7$	192.1230	MS DAD	Juice, leaf, peel, seed	[21, 32]
Fumaric acid		$C_4H_4O_4$	116.0720	DAD	Juice	[54]
L-malic acid		$C_4H_6O_5$	134.0870	MS DAD	Juice, leaf, peel, seed	[21, 32]
Oxalic acid		$C_2H_2O_4$	90.0340	DAD	Juice, leaf, peel, seed	[32, 55]

Quinic acid		$C_7H_{12}O_6$	192.1670	DAD	Juice	[33]
Succinic acid		$C_4H_6O_4$	118.0880	DAD	Juice, leaf, peel, seed	[32, 55]
Tartaric acid		$C_4H_6O_6$	150.0860	DAD	Juice	[55]
Caffeic acid		$C_9H_8O_4$	180.1590	DAD	Peel, juice, seed, leaf	[32, 33]
Chlorogenic acid		$C_{16}H_{18}O_9$	354.3110	MS	Juice	[19]
Cinnamic acid		$C_9H_8O_2$	148.1610	DAD	Juice	[33]
O-Coumaric acid		$C_9H_8O_3$	164.1600	DAD	Juice	[33]
p-Coumaric acid		$C_9H_8O_3$	164.1600	MS DAD	Peel, juice, seed, leaf	[19, 31, 32]
Cis-p-Coumaric acid		$C_9H_8O_3$	164.1600	MS	Peel	[31]
Coutaric acid		$C_{13}H_{12}O_8$	296.2310	MS	Peel	[31]
7,8-Dihydroxy-3-carboxymethylcoumarin-5-carboxylic acid		$C_{12}H_8O_8$	280.1880	NMR	Flower	[2]
Ferulic acid		$C_{10}H_{10}O_4$	194.1860	MS DAD	Juice, seed, peel, leaf	[17, 32]
Gallic acid		$C_7H_6O_5$	170.1200	MS	Peel, juice, flower	[17, 19, 23]
Methyl gallate		$C_8H_8O_5$	184.1470	MS	Heartwood	[14]
Neochlorogenic acid (5-*O*-caffeoylquinic acid)		$C_{16}H_{18}O_9$	354.3110	MS	Peel, juice	[19, 31]
Protocatechuic acid		$C_7H_6O_4$	154.1210	MS	Peel, juice	[19, 31]

Vanillic acid		$C_8H_8O_4$	168.1480	MS	Peel, juice	[17, 31]
Coniferyl 9-*O*-[*β*-D-apiofuranosyl(1→6)]-*O*-*β*-D-glucopyranoside		$C_{21}H_{30}O_{12}$	474.4590	NMR	Seed	[13]
Sinapyl 9-*O*-[*β*-D-apiofuranosyl(1→6)]-*O*-*β*-D-glucopyranoside		$C_{22}H_{32}O_{13}$	504.4850	NMR	Seed	[13]
Other compounds						
Catechol		$C_6H_6O_2$	110.1120	DAD	Juice	[33]
Coumestrol		$C_{15}H_8O_5$	268.2240	DAD	Seed	[29]
Icariside D1		$C_{19}H_{28}O_{10}$	416.4230	MS	Seed	[13]
Phenylethylrutinoside		$C_{20}H_{30}O_{10}$	430.4500	MS	Seed	[13]
Syringaldehyde		$C_9H_{10}O_4$	182.1750	MS	Juice	[21]

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