SUPPLEMENTARY INFORMATION

Chlorogenic acids and the acyl-quinic acids: discovery, biosynthesis, bioavailability and bioactivity

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Supplementary Table 1. Trivial names associated with acyl-quinic acids and the associated systematic name using IUPAC numbering.[a1]

Trivial Name	Origin	Current Interpretation with IUPAC numbering	Notes
Band 510	Sondheimer (1958)[2]	4-*O*-Caffeoylquinic acid	
Burkinabins	Ouattara *et al.* (2004)[3]	Divanilloylquinic acids	
Castusic acid	Kirmizibekmev and Demir (2016)[4]	4-*p*-Hydroxybenzoyl-5-*O*-caffeoylquinic acid	
Chlorogen acid/chlorogenic acid	Payen (1846)[5,6]	5-*O*-Caffeoylquinic acid	The original isolate subsequently described as 3-caffeoylquinic acid and now known as 5-caffeoylquinic acid IUPAC
Chlorogenic acids			Used in the plural to denote the extended family of structurally related compounds
Cryptochlorogenic acid	Unknown	4-*O*-Caffeoylquinic acid	
Cynarin(e)	Panizzi *et al*. (1954)[7,8]	1,3-O-Dicaffeoylquinic acid	Rapidly formed from 1,5-I-dicaffeoylquinic acid in aqueous media
Dactylifric acid	Maier *et al*. (1964)[9]	5-*O*-Caffeoylshikimic acid	
Dattelic acid	Wada *et al*. (1988)[10]	5-*O*-Caffeoylshikimic acid	
Hauschild's substance	Hauschild (1935)[11]	3-Caffeoylquinic-1,5-γ-lactone	Rapidly formed from 1,5-dicaffeoylquinic acid in aqueous media
Irbic acid	Antognoni *et al.* (2011)[12]	3,5-*O*-Dicaffeoyl-4-*O*-malonoyl-quinic acid	This name was applied first to a compound isolated from cultured cells of *Centella asiatica* but subsequently found in the whole plant.[13,14] This compound had been known from at least 2007.[15]
Isochlorogenic acid	Barnes *et al*. (1950)[16]	A mixture of at least three dicaffeoylquinic acids	Originally described as 5-*O*-caffeoylquinic acid using non-IUPAC numbering, contaminated with the associated lactone. Prefix 'iso' used to indicate 'isomer'.
Isochlorogenic acid a, b and c, or A, B and C	Scarpati and Guiso (1964)[17] Corse *et al*. (1965)[18]	Coffee bean dicaffeoylquinic acids	The two research groups used the descriptors a, b and c, or A, B and C, differently and it is thus very difficult to tell which letter applies to which regio-isomer in later usage. As originally published A = c = 3,4-*O*-diCQA, and C = b = 3,5-*O*-diCQA IUPAC. Logically B = a = 4,5-*O*-diCQA IUPAC but there remains an unexplained difference in specific rotation of the two isolates.[17]

Macranthoin F and G	Chen *et al*. (1994)[19]	Methyl-4,5-*O*-dicaffeoylquinate and methyl 3,5-dicaffeoylquinate, respectively	Note that the term 'macranthoin' refers to constituents of *Lonicera macranthoides* regardless of whether or not they are chlorogenic acids.
Mumeic acid	Nakamura *et al*. (2013)[20]	4-Benzoyl-5-*O*-caffeoylquinic acid	
n-Chlorogenic acid	Maier and Grimsehl (1982)[21]	5-*O*-Caffeoylquinic acid	Prefix '*n*' used to distinguish 5-*O*-caffeoylquinic acid from total chlorogenic acids
Neochlorogenic acid	Corse (1953)[22]	3-*O*-Caffeoylquinic acid	Neochlorogenic acid
Origanine A–C	Liu *et al*. (2012)[23]	Derivatives of 1,3,4,5- and 1,3,5,6-tetra-carboxy-shikimic acid	Reported in *Origanum vulgare* L. Biosynthetic origin unknown and possibly different from (–)-quinic and (–)-shikimic acids.
Pistafolins	Hou *et al*. (2000)[24]	Galloylquinic acid depsides	Term applied to some galloylquinic acids of *Pistacia lentiscus*
Podospermic acid	Zidorn *et al*. (2005)[25]	1,3,5-*O*-tri-dihydrocaffeoylquinic acids	Some close relatives, such as di-dihydrocaffeoyl-feruloylquinic acids, may also be included in the trivial name.[26]
Pseudochlorogenic acid	Uritani and Miyano (1955)[27]	1-*O*-Caffeoylquinic acid	Probably the original isolate was a poorly defined mixture of caffeoylquinic and dicaffeoylquinic acids
Salicornate	Kim *et al.* (2011)[28]	Methyl-4-*O*-caffeoyl-3-dihydrocaffeoyl-quinate	
Theogallin	Roberts (1958)[29]	5-Galloylquinic acid	
Tuntungmadic acid	Chung *et al*. (2005)[30]	4-*O*-Dihydrocaffeoyl-5-*O*-caffeoylquinic acid	
Viarum acids	Wu *et al*. (2012)[31]	5-*O*-Caffeoyl-[4-(1β-[6-(5-*O*-caffeoyl) quinate]gluco-pyranosyl)]quinic acid and 3-*O*-malonyl-5-*O*-caffeoyl-[4-(1β-[6-(5-*O*-caffeoyl)-quinate]gluco-pyranosyl)]quinic acid	

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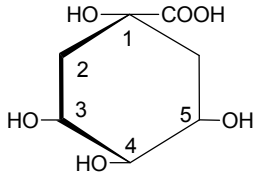
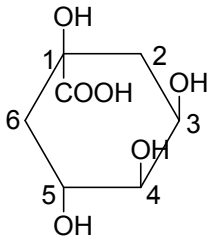
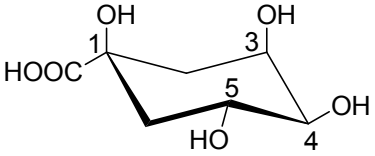
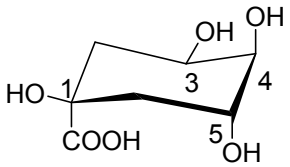
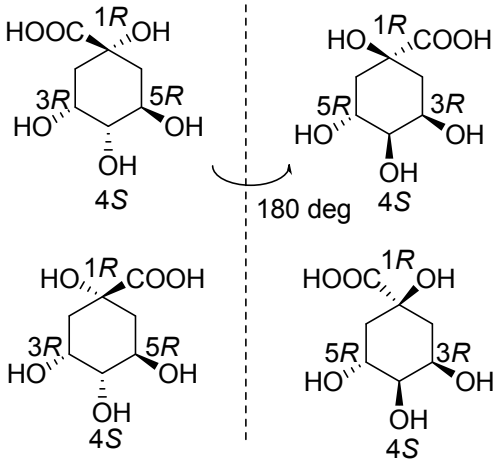
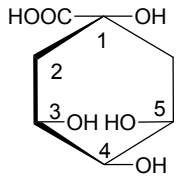
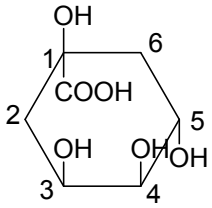
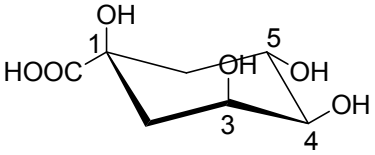
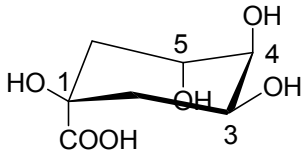
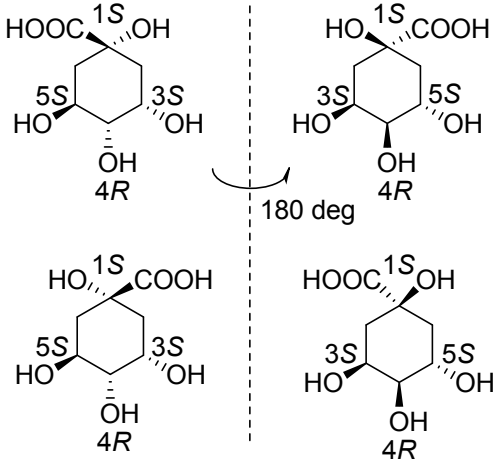
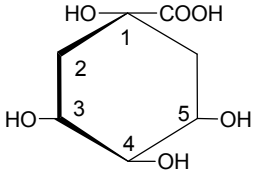
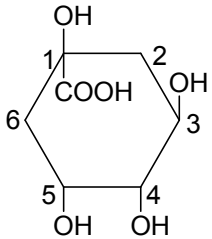
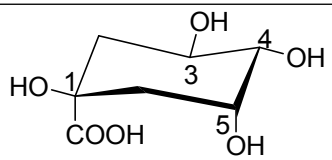
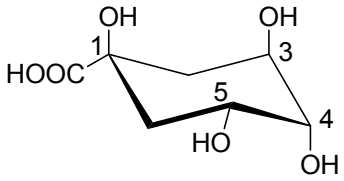
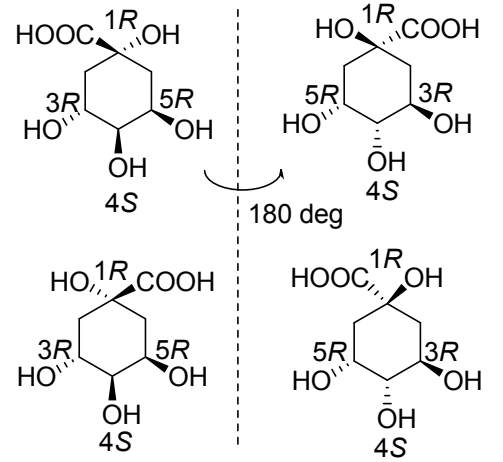
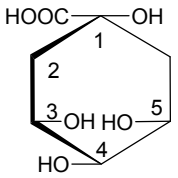
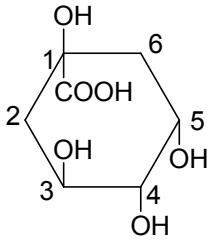
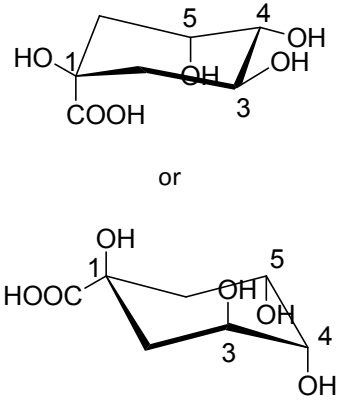
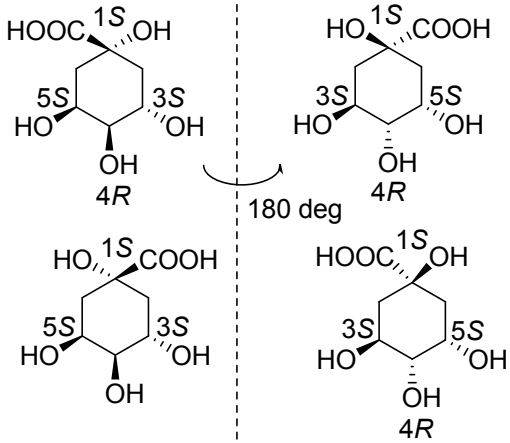
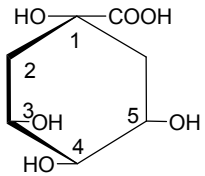
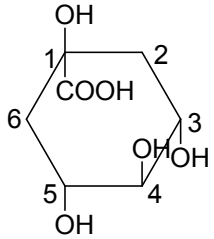
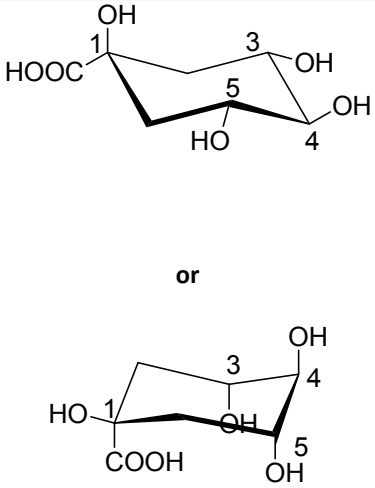
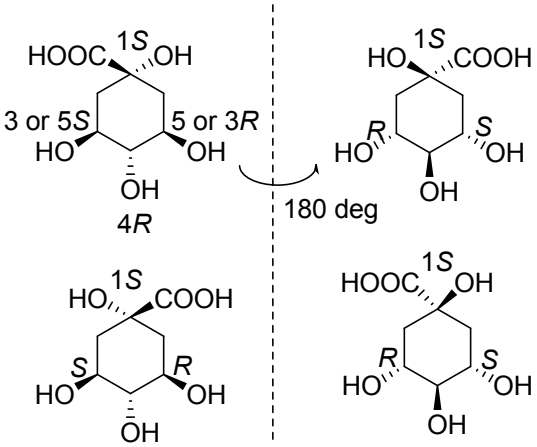
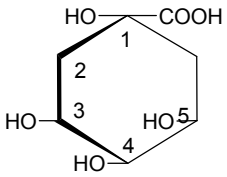
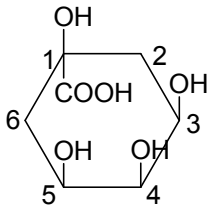
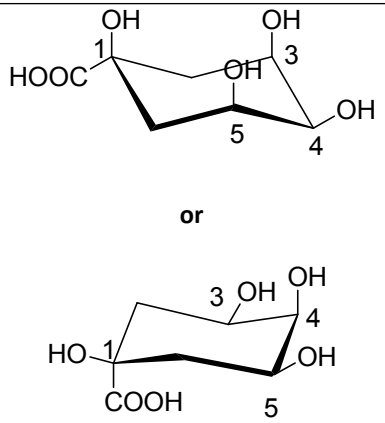
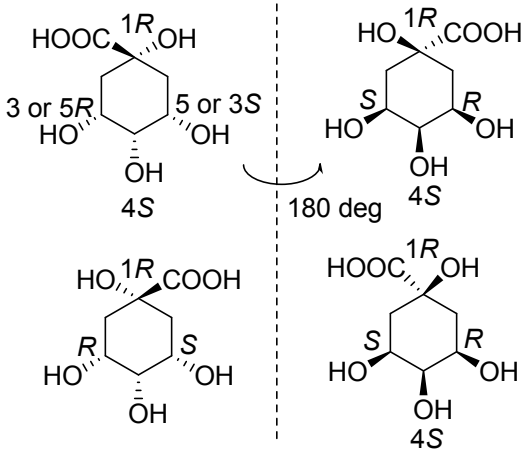
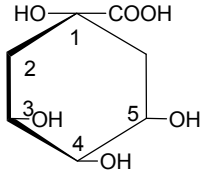
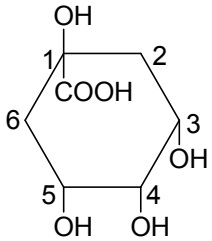
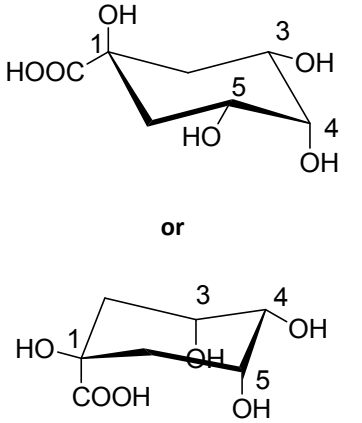
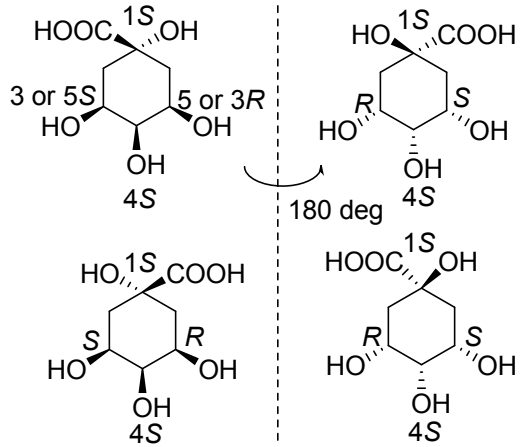
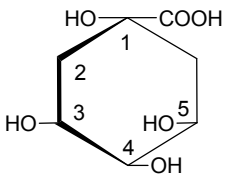
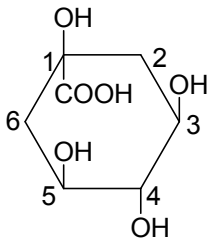
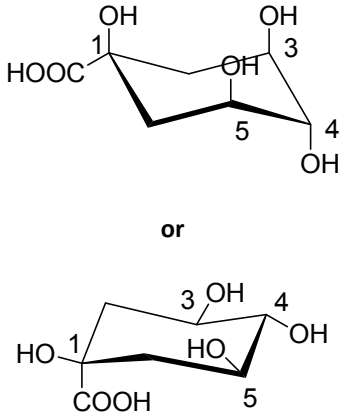
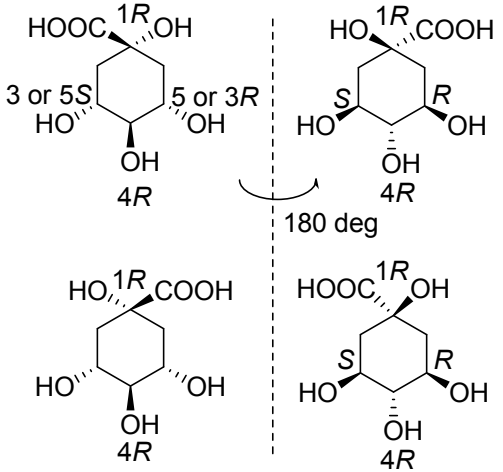
Supplementary Table S2 An unambiguous nomenclature for the acyl-quinic acids commonly known as chlorogenic acids.[a1]

Isomer	CIP[b] description and recommended description[1]	Fischer–Tollens structure	2D structure using the recommended convention	Conformers	2D structures for individual isomers drawn from four different perspectives
1L-(–)-quinic acid	1*R*, 3*R*, 4*S*, 5*R* *or* 3*R*, 5*R*-(1α, 3α, 4α, 5β)			 Upper structure with equatorial COOH and axial 4H as shown in Corse and Lundin.[33] The lower carboxy equatorial structure is preferred.[1] 	

1D-(+)-quinic acid	1*S*, 3*S*, 4*R*, 5*S* *or* 3*S*, 5*S*-(1α, 3α, 4α, 5β)			 Upper structure with equatorial COOH and axial 4H. The lower carboxy equatorial structure is preferred.[1] 	
1L-(–)-*epi*-quinic acid (derived from 1L-(–)-quinic acid by 4-OH inversion)	1*R*, 3*R*, 4*S*, 5*R* *or* 3*R*, 5*R*-(1α, 3α, 4β, 5β)			 Upper structure with equatorial COOH and axial 4H. The lower carboxy equatorial structure is preferred.[1] 	

1D-(+)-*epi*-quinic acid (derived from 1D-(+)-quinic acid by 4-OH inversion)	1*S*, 3*S*, 4*R*, 5*S* *or* 3*S*, 5*S*-(1α, 3α, 4β, 5β)			 Carboxy axial preferred.[1]	
***Muco*-quinic acid** (derived from 1L-(–)-quinic acid by 3-OH inversion) ***meso* form**	1*S*, 3*S*, 4*R*, 5*R* *or* 3*S*, 5*R* (1α, 3β, 4α, 5β)			 Carboxy equatorial preferred.[1]	

***Cis*-quinic acid** (derived from 1L-(–)-quinic acid by 5-OH inversion) ***meso* form**	1*R*, 3*R*, 4*S*, 5*S* *or* 3*R*, 5*S* (1α, 3α, 4α, 5α)			 **or** Carboxy axial preferred.[1]	
***Neo*-quinic acid** (derived from 1L-(–)-quinic acid by 3-OH and 4-OH inversion) ***meso* form**	1*S*, 3*S*, 4*S*, 5*R* *or* 3*S*, 5*R* (1α, 3β, 4β, 5β)			 **or** Carboxy axial preferred.[1]	

***Scyllo*-quinic acid** (derived from 1L-(–)-quinic acid by 4-OH and 5-OH inversion) **meso form**	1*R*, 3*R*, 4*R*, 5*S* *or* 3*R*, 5*S* (1α, 3α, 4β, 5α)			 Carboxy equatorial preferred.[1]	

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[b]CIP - Cahn-Ingold-Prelog[34]

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