Galloylated proanthocyanidins from shea (Vitellaria paradoxa) meal have potent anthelmintic activity against Ascaris suum

Article

Accepted Version

Equations for quantifying extractable and unextractable PA:

PA calculation of extractable PA (ePA) in whole meal:

$$ePA\ in\ g/100g\ of DW\ of\ whole\ shea\ meal = \left(\frac{extract\ yield\ g}{100\ g\ whole\ meal}\right) \times \left(\frac{PA\ g}{100\ g\ extract}\right)$$

PA calculation of unextractable PA (uPA) in whole meal:

$$uPA\ in\ g/100g\ of DW\ of\ whole\ shea\ meal = \left(\frac{residue\ yield\ g}{100\ g\ whole\ meal}\right) \times \left(\frac{PA\ g}{100\ g\ extract}\right)$$

Equations for characterising PA compositions:

Thiolysis degrades PA and yields a 'global average' flavanol composition in the PA mixtures (Figure S1; Gea et al 2011):

The mean degree of polymerisation (mDP) is calculated as follows:

$$\text{mDP} = \frac{\text{Amount of extension and terminal flavanol units [mole]}}{\text{Amount of terminal flavanol units [mole]}}$$

The percentage of procyanidins (PC) within PA is calculated as follows:

$$\%\ \text{PC} = \frac{\text{C} + \text{EC} + \text{Cg} + \text{ECg units [mole]}}{\text{Total flavanols in PA [mole]}}\ x\ 100$$

The percentage of prodelphinidins (PD) within PA is calculated as follows:

$$\%\ \text{PD} = 100\ \% - \%\ \text{PC}$$

The percentage of *cis* flavan-3-ols within PA is calculated as follows:

$$\%\ cis = \frac{\text{EC} + \text{ECg} + \text{EGC} + \text{EGCg units [moles]}}{\text{Total flavanols in PA [mole]}}\ x\ 100$$

The percentage of trans flavan-3-ols within PA is calculated as follows:

$$\%\ trans = 100\ \% - \%\ cis$$

C = catechin, EC = epicatechin, EGC = epigallocatechin, Xg = flavan-3-ol gallate

Figure S1: Thiolytic degradation of galloylated and non-galloylated proanthocyanidins

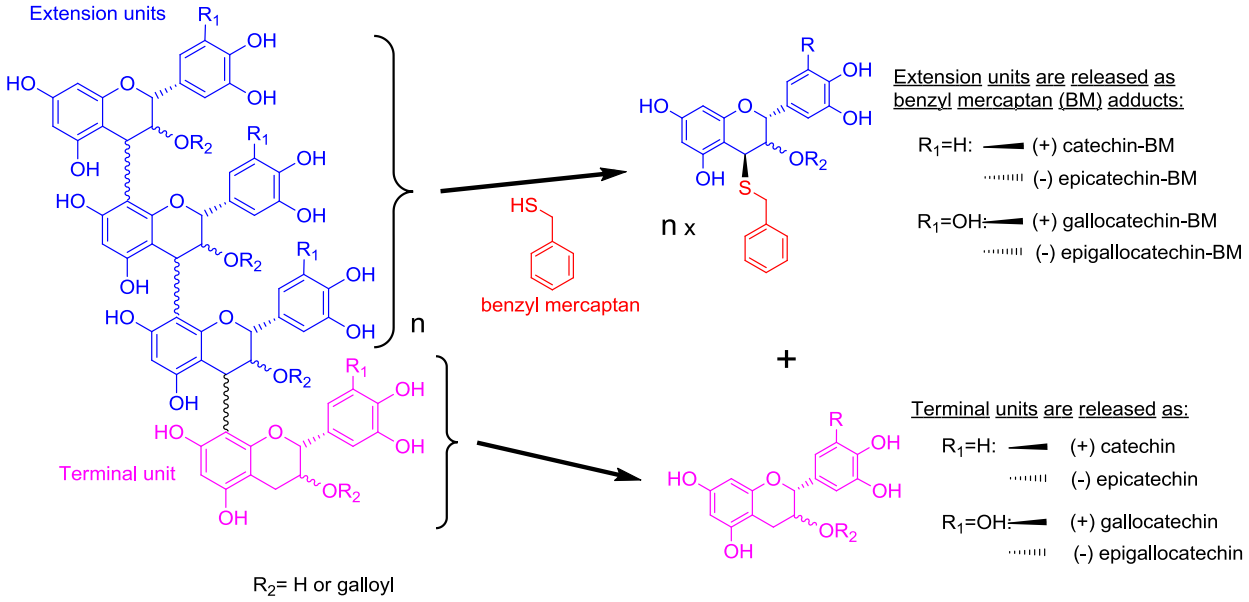

Table S1: Flavan-3-ol composition of proanthocyanidins in shea meal as terminal and extension units (relative molar percentages; SD in parentheses; n = 3).). Data are presented so that terminal units add up to 100% and extension units add up to 100%.

	Terminal units (%)						**Extension units (%)**							
Proanthocyanidins	GC	EGC	GCg	EGCg	C	ECg	GC	EGC	GCg	EGCg	C	EC	Cg	ECg
Total PA	5.3	21.1	10.2	41.4	6.1	15.8	31.2	16.3	5.9	14.5	5.0	20.1	0.7	6.3
	(0.5)	(3.6)	(0.3)	(7.1)	(1.9)	(1.9)	(0.7)	(1.0)	(0.2)	(0.6)	(0.1)	(0.5)	(0.1)	(0.3)
Extractable PA	26.1	22.2	7.7	30.9	5.8	7.4	26.5	15.7	7.5	19.2	4.6	18.0	0.7	7.7
	(0.7)	(1.9)	(0.2)	(0.8)	(0.3)	(0.1)	(0.5)	(0.4)	(0.1)	(0.3)	(0.1)	(0.3)	(0.1)	(0.1)
Unextractable PA	5.9	13.3	9.0	49.6	5.5	16.7	29.1	15.5	5.3	15.1	5.2	22.1	0.6	7.2
	(0.2)	(0.9)	(0.2)	(0.7)	(0.6)	(0.6)	(0.8)	(0.4)	(0.1)	(0.4)	(0.1)	(0.6)	(0.1)	(0.2)

Table S2: Composition of flavan-3-ol terminal and extension units in three proanthocyanidin fractions (relative molar percentages; SD in parentheses; n = 3). Data are presented so that terminal units add up to 100% and extension units add up to 100%.

	Terminal units (%)						**Extension units (%)**							
Shea meal	GC	EGC	GCg	EGCg	C	ECg	GC	EGC	GCg	EGCg	C	EC	Cg	ECg
F1-fraction	36.1	24.2	3.4	23.9	7.6	4.8	20.3	27.1	7.2	12.8	6.8	20.5	0.7	4.6
	(0.2)	(0.1)	(0.1)	(0.2)	(0.1)	(0.1)	(2.3)	(4.1)	(1.2)	(0.2)	(0.1)	(0.4)	(0.1)	(0.1)
F2-fraction	17.0	10.4	15.6	40.4	4.5	12.1	27.3	12.3	8.1	21.2	4.6	16.6	1.1	8.7
	(0.3)	(0.1)	(0.1)	(0.2)	(0.1)	(0.1)	(0.2)	(0.4)	(0.1)	(0.2)	(0.1)	(0.1)	(0.1)	(0.1)
F3-fraction	18.8	12.2	15.1	40.6	5.7	7.7	13.7	33.3	3.4	20.8	4.4	14.9	0.7	8.7
	(1.2)	(0.5)	(0.8)	(2.1)	(0.3)	(4.7)	(5.6)	(2.6)	(0.2)	(1.4)	(0.2)	(0.9)	(0.1)	(0.6)

Table S3: 2D NMR (HSQC) chemical shifts (□ ppm) of the proanthocyanidin F2-fraction (DMSO-d_6/pyridine-d_5, 500 MHz).

Assignments*	^{1}H	^{13}C
2	5.25; 5.53	75.57; 67.83
3	4.02	71.19
4	4.83	35.91
6/8	6.00	95.98
2' PD/6' PD	6.57	106.01
2' PC	7.06	114.87
5' PC	6.75	114.87
6' PC	6.77	117.59
Gallic acid (2H)	7.03	108.97

* See Figure 1 for hydrogen and carbon numbers.