Intestinal anti-inflammatory effects of artichoke pectin and modified pectin fractions in dextran sulfate sodium model of mice colitis. Artificial neural network modelling of inflammatory markers

Carlos Sabater[a], Jose Alberto Molina-Tijeras[b], Teresa Vezza[b], Nieves Corzo[a], Antonia Montilla[a]*, Pilar Utrilla[b]

[a]Instituto de Investigación en Ciencias de la Alimentación CIAL, (CSIC-UAM) CEI (UAM + CSIC), C/ Nicolás Cabrera, 9, E-28049 Madrid (Spain).

[b]Departamento de Farmacología, Centro de Investigaciones Biomédicas en Red – Enfermedades Hepáticas y Digestivas (CIBER-EHD), Centro de Investigación Biomédica, Universidad de Granada, Granada, Spain

*Author to whom correspondence should be addressed:

C/ Nicolás Cabrera 9,

E-28049 Madrid (Spain).

Tel: +34 910017952

E-mail: a.montilla@csic.es

SUPPLEMENTARY TABLE CAPTIONS:

Table S1. Clinical parameters considered to determine the Disease Activity Index (DAI) in healthy, DSS treated and DSS + pectins treated mice groups.

Table S2. Monomeric composition of citrus (**CP**) and artichoke pectin **(AP)** and modified artichoke pectin fractions used in this study: **APwA**: modified artichoke pectin without arabinose, **APwG**: modified artichoke pectin without galactose, **GalA**: galacturonic acid, **Xyl**: xylose, **Ara**: arabinose, **Rha**: rhamnose, **Fru**: fructose, **Gal**: galactose, **Man**: mannose, **Glc**: glucose.

Table S3. Molecular weight (M_w) distribution of citrus (**CP**) and artichoke pectin (**AP**) and modified artichoke pectin fractions used in this study. **APwA**: modified artichoke pectin without arabinose, **APwG**: modified artichoke pectin without galactose.

Table S4. Train, cross-validation, test rates and kappa values for all artificial neural network (ANN) models developed to study characteristic expression profiles of cytokine and intestinal proteins in studied groups of mice. **DSS**: dextran sulfate sodium, **CP**: citrus pectin control, **AP**: artichoke pectin, **APwA**: modified artichoke pectin without arabinose, **APwG**: modified artichoke pectin without galactose.

Table S1. Clinical parameters considered to determine the Disease Activity Index (DAI) in healthy, DSS treated and DSS + pectins treated mice groups.

Bleeding	**Stool consistency**	**Weight loss (WL, %)**	**Value assigned according to WL**
0: normal	**0**: normal	0	0
1: presence of blood	**1**: moderate soft stools	1 - 4	1
2: moderate bleeding	**2**: soft stools	5 – 9	2
3: moderately high bleeding	**3**: soft stools and diarrhea	10 – 19	3
4: abundant bleeding	**4**: diarrhea	> 20	4

Table S2. Monomeric composition of citrus (**CP**) and artichoke pectin **(AP)** and modified artichoke pectin fractions used in this study: **APwA**: modified artichoke pectin without arabinose, **APwG**: modified artichoke pectin without galactose, **GalA**: galacturonic acid, **Xyl**: xylose, **Ara**: arabinose, **Rha**: rhamnose, **Fru**: fructose, **Gal**: galactose, **Man**: mannose, **Glc**: glucose.

Sample	Monomeric composition (% total identified monosaccharides)								Degree of branching Rha/GalA	Linearity pectin backbone GalA/(Rha+Ara+Gal)	Extent of branching (Ara+Gal)Rha	Degree of methyl-esterification (%)
	GalA	Xyl	Ara	Rha	Fru	Gal	Man	Glc				
CP*	75.51^{a,b} (0.54)	2.51^{a} (0.02)	3.18^{c} (0.01)	4.52^{a,b} (0.05)	-	11.10^{a} (0.10)	0.30^{b} (0.00)	0.98^{c} (0.01)	0.060^{a} (0.00)	4.02^{a} (0.01)	3.16^{b} (0.03)	71.0^{a} (1.4)
AP	68.68^{b} (1.23)	0.53^{c} (0.19)	15.92^{a} (0.03)	3.25^{b} (0.18)	0.55^{a} (0.07)	6.38^{b} (0.57)	1.35^{a} (0.09)	3.33^{b} (0.42)	0.047^{a} (0.003)	2.69^{a} (0.13)	6.86^{a} (0.20)	19.5^{b} (0.0)
APwA	76.04^{a,b} (3.45)	0.17^{c} (0.05)	1.38^{c} (0.16)	6.32^{a} (0.93)	<0.10^{b} (0.00)	9.69^{a} (1.35)	0.47^{b} (0.11)	5.93^{a} (0.84)	0.083^{a} (0.016)	4.43^{a} (0.82)	1.75^{d} (0.02)	24.0^{b} (1.9)
APwG	77.26^{a} (1.66)	1.52^{b} (0.22)	12.57^{b} (0.88)	4.93^{a,b} (0.49)	<0.10^{b} (0.00)	0.62^{c} (0.05)	0.30^{b} (0.03)	2.80^{b,c} (0.01)	0.064^{a} (0.008)	4.28^{a} (0.43)	2.68^{c} (0.08)	24.3^{b} (0.9)

*Data obtained from Pacheco et al. (2018).

^{a,b,c,d} Statistically significant differences between pectins.

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	CP	**AP**	**APwA**	**APwG**
M_w of each fragment [abundance, %]	547 ± 11 kDa [100 ± 0%]	660 ± 0 kDa [28.5 ± 0.2%]	542 ± 12 kDa [41.7 ± 1.3%]	605 ± 15 kDa [31.0 ± 0.8%]
		105 ± 3 kDa [36.6 ± 0.1%]	63 ± 3 kDa [58.3 ± 1.3%]	74 ± 8 kDa [39.5 ± 2.4%]
		4.8 ± 1.2 kDa [34.9 ± 0.2%]		5.1 ± 0.5 kDa [29.5 ± 1.6%]

Table S4. Train, cross-validation, test rates and kappa values for all artificial neural network (ANN) models developed to study characteristic expression profiles of cytokine and intestinal proteins in studied groups of mice. **DSS**: dextran sulfate sodium, **CP**: citrus pectin control, **AP**: artichoke pectin, **APwA**: modified artichoke pectin without arabinose, **APwG**: modified artichoke pectin without galactose.

Parameter	ANN-1 (Healthy control)	DSS treatment				
		ANN-2 (Control)	ANN-3 (+ CP)	ANN-4 (+ AP)	ANN-5 (+ APwA)	ANN-6 (+ APwG)
Train rate (%)	100	100	100	100	100	100
Cross-validation rate (%)	100	100	97.5	95.5	92.6	98.0
Test rate (%)	100	94.7	94.1	94.4	94.4	100
Kappa	1.00	0.94	0.94	0.85	0.82	0.98
Sensitivity	100	100	100	90.0	100	100
Specificity	100	94.1	93.3	100	93.3	100
Balanced accuracy	100	97.1	96.7	95.0	96.7	100

Reference of electronic supplementary information (ESI):

6. M. T. Pacheco, T. Vezza, P. Diez-Echave, P. Utrilla, M. Villamiel and F. J. Moreno, Anti-inflammatory bowel effect of industrial orange by-products in DSS-treated mice, *Food Funct.,* 2018, **9**, 4888-4896.