Supplementary Materials

Xylooligosaccharides from corn cobs alleviates loperamide-induced constipation in mice via modulation of gut microbiota and SCFAs metabolism

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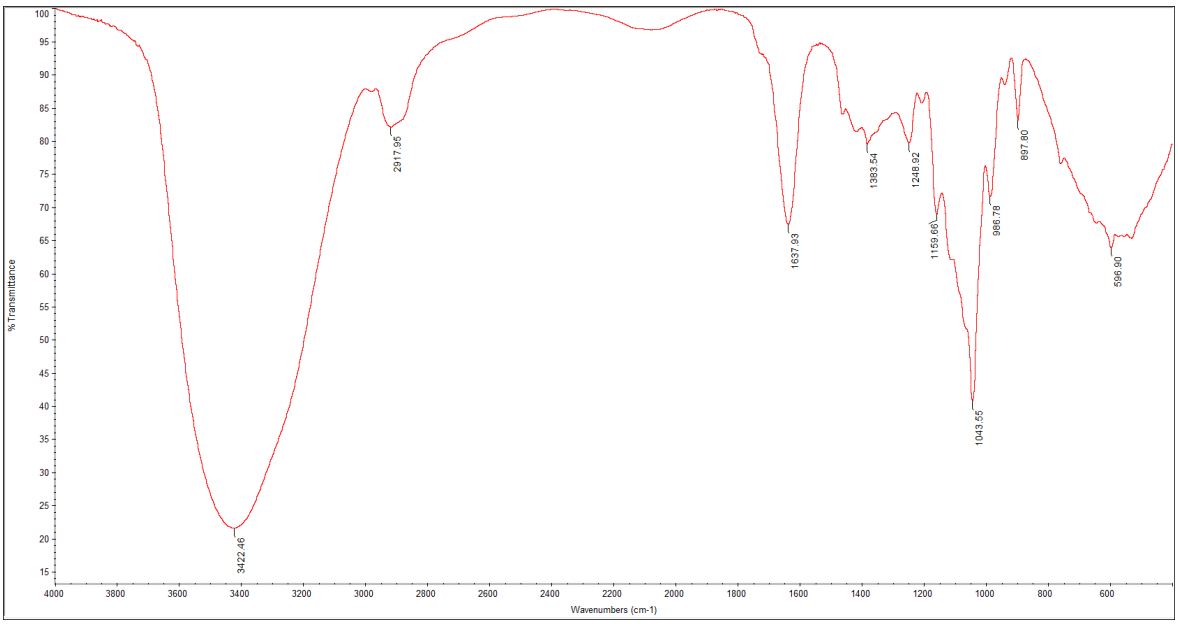
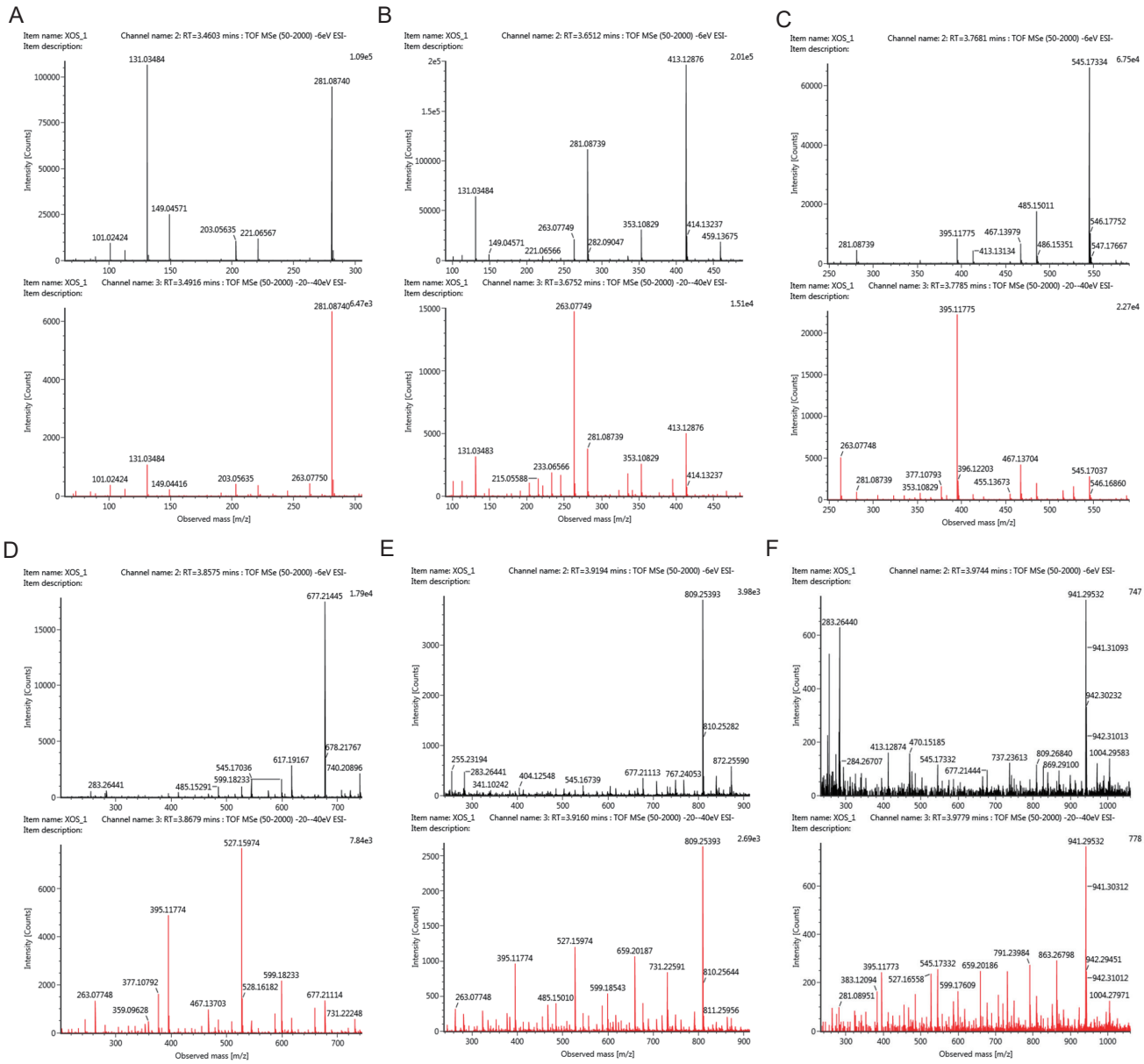


Fig. S1. The FT-IR spectrum of XOS.



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24 **Fig. S2.**The negative mass spectrum of XOS DP 2-7 (A-F).

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Table S1. The fragment ions of XOS produced by UHPLC-HDMS^{E}

RT	DP	[M-H]$^-$	Glycosidic bond cleavages ions	Cross-ring cleavage ions
15.287	2	281.08740	C_1 (*m/z* 149.04571) Y_1 (*m/z* 149.04571)	$^{0,2}A_2$ (*m/z* 221.06567)
13.193	3	413.12876	C_2 (*m/z* 281.08739) C_1 (*m/z* 149.04571) Y_2 (*m/z* 281.08739) Y_1 (*m/z* 149.04571)	$^{0,2}A_3$ (*m/z* 353.10829) $^{0,2}A_2$ (*m/z* 221.06566) $^{0,2}A_3$-H_2O (*m/z* 335.10453) $^{0,2}A_2$-H_2O (*m/z* 207.06325)
11.792	4	545.17334	C_3 (*m/z* 413.13134) C_2 (*m/z* 281.08739) Y_3 (*m/z* 413.13134) Y_2 (*m/z* 281.08739)	$^{0,2}A_4$ (*m/z* 485.15011) $^{0,2}A_3$ (*m/z* 353.10829) $^{0,2}A_4$-H_2O (*m/z* 467.13979) $^{0,2}A_3$-H_2O (*m/z* 335.10453)
10.830	5	677.21445	C_4 (*m/z* 545.17036) C_3 (*m/z* 413.12876) C_2 (*m/z* 281.08740) Y_4 (*m/z* 545.17036) Y_3 (*m/z* 413.12876) Y_2 (*m/z* 281.08740)	$^{0,2}A_5$ (*m/z* 617.19167) $^{0,2}A_4$ (*m/z* 485.15291) $^{0,2}A_3$ (*m/z* 353.10829) $^{0,2}A_5$-H_2O (*m/z* 599.18223) $^{0,2}A_4$-H_2O (*m/z* 467.13979) $^{0,2}A_3$-H_2O (*m/z* 335.10453)
10.267	6	809.25394	C_5 (*m/z* 677.21113) C_4 (*m/z* 545.16739) C_3 (*m/z* 413.12876) C_2 (*m/z* 281.08740) Y_5 (*m/z* 677.21113) Y_4 (*m/z* 545.16739) Y_3 (*m/z* 413.12876) Y_2 (*m/z* 281.08740)	$^{0,2}A_6$ (*m/z* 749.24672) $^{0,2}A_5$ (*m/z* 617.19445) $^{0,2}A_4$ (*m/z* 485.15011) $^{0,2}A_3$ (*m/z* 353.10829) $^{0,2}A_5$-H_2O (*m/z* 599.18543) $^{0,2}A_4$-H_2O (*m/z* 467.14413)
8.837	7	941.29532	C_6 (*m/z* 809.25394) C_5 (*m/z* 677.21444) C_4 (*m/z* 545.17332) C_3 (*m/z* 413.12874) C_2 (*m/z* 281.08951) Y_6 (*m/z* 809.25394) Y_5 (*m/z* 677.21444) Y_4 (*m/z* 545.17332) Y_3 (*m/z* 413.12874) Y_2 (*m/z* 281.08951)	$^{0,2}A_7$ (*m/z* 881.28752) $^{0,2}A_6$ (*m/z* 749.22679) $^{0,2}A_5$ (*m/z* 617.20143) $^{0,2}A_4$ (*m/z* 485.15011) $^{0,2}A_7$-H_2O (*m/z* 863.26798) $^{0,2}A_6$-H_2O (*m/z* 731.22351) $^{0,2}A_5$-H_2O (*m/z* 599.18543)

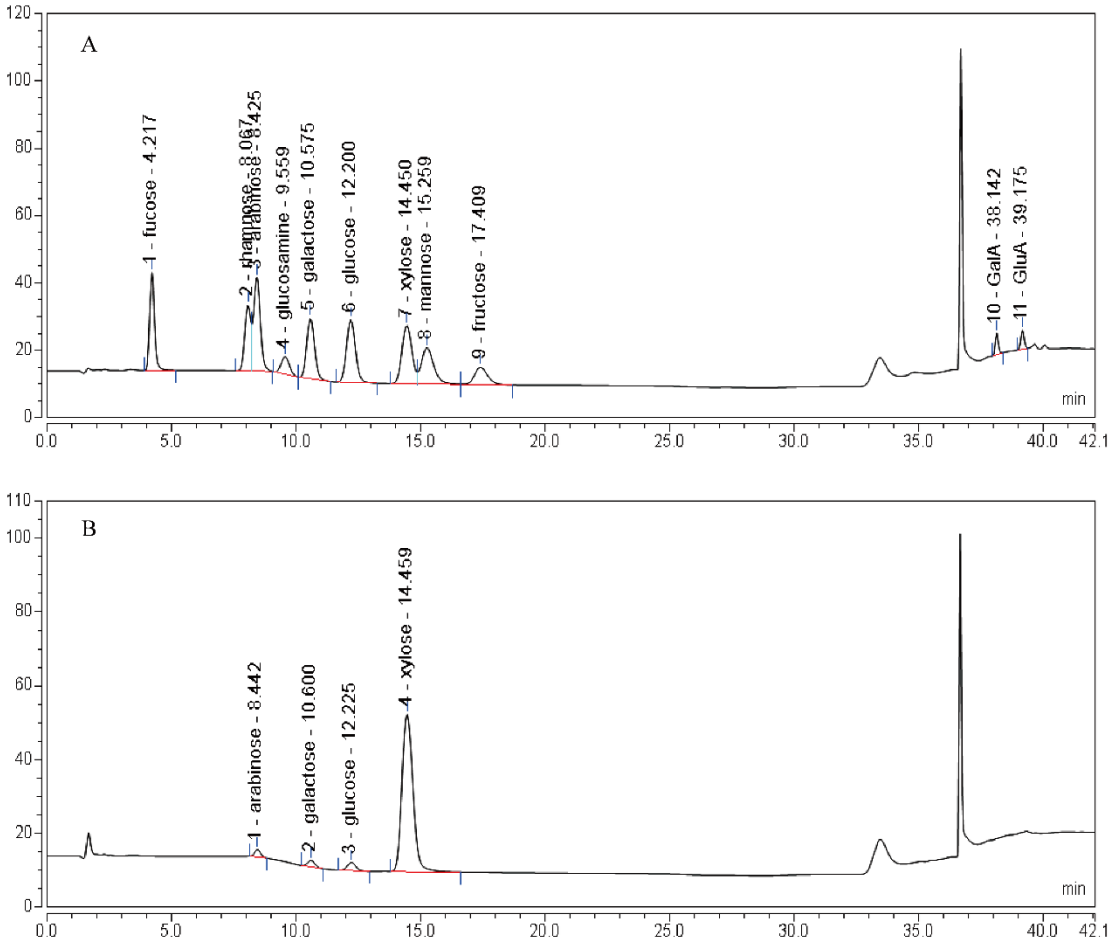

Fig. S3. The standard monosaccharide (A) and the monosaccharide composition analysis of XOS (B).

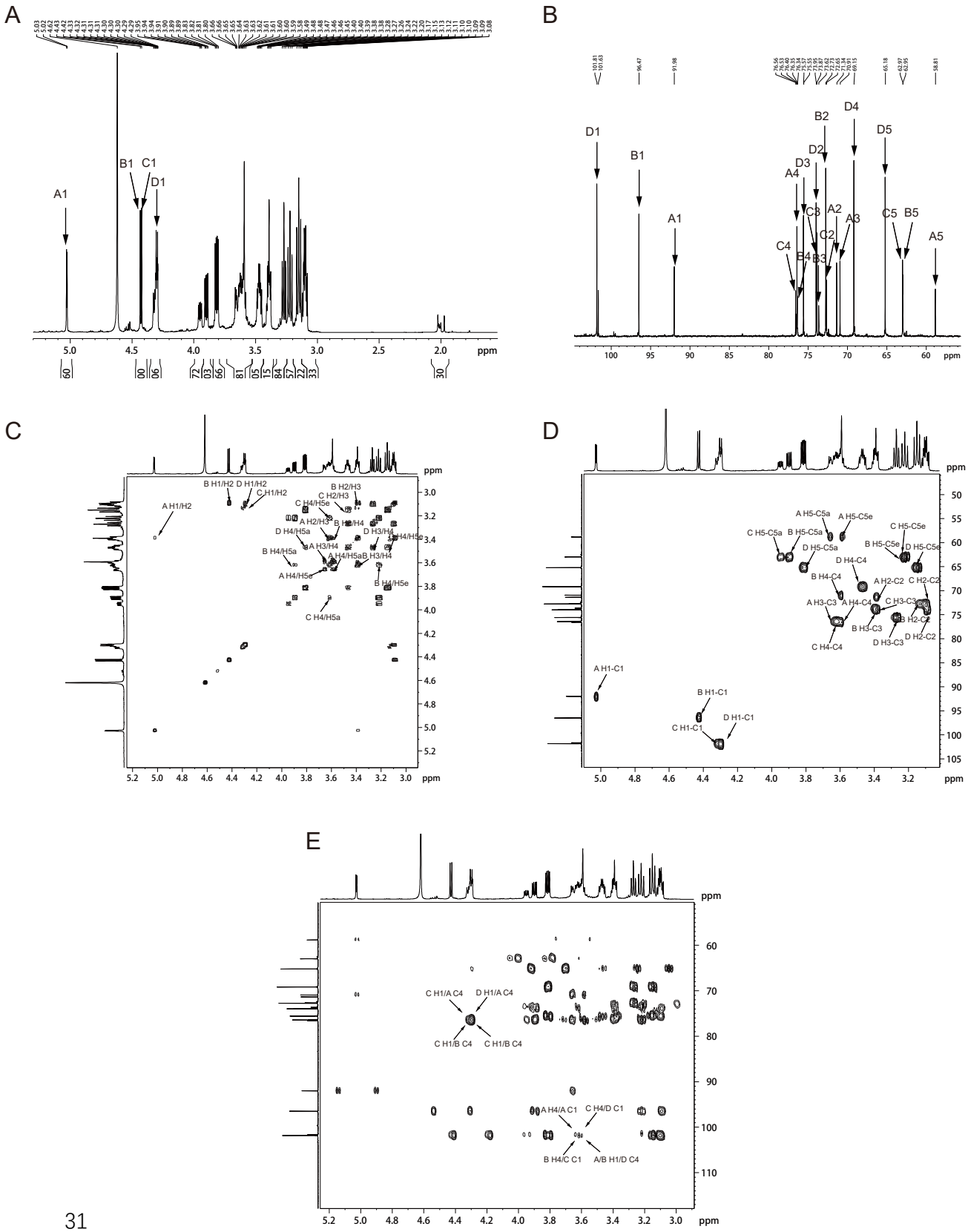

Fig. S4. ^{1}H NMR (A), ^{13}C NMR (B), ^{1}H-^{1}H correlation spectroscopy COSY (C), ^{1}H-^{13}C heteronuclear single quantum coherence spectroscopy HSQC (D) and ^{1}H-^{13}C heteronuclear multiple bond correlation spectroscopy (HMBC) (E) spectra of XOS.

Table S2. The ^{1}H NMR and ^{13}C NMR signal assignments of XOS.

Sequence residues		H1	H2	H3	H4	H5e， H5a	
		C1	C2	C3	C4	C5	
A	→4)-α-Xyl	5.03	3.38	3.61	3.63	3.59	3.65
		91.98	71.34	70.91	76.35	58.81	
B	→4)-β-Xyl	4.43	3.09	3.40	3.60	3.24	3.89
		96.47	72.73	73.62	76.34	62.97	
C	→4)-β-Xyl-(1→	4.32	3.13	3.39	3.62	3.22	3.90
		101.63	72.65	73.95	76.56	62.95	
D	β-Xyl-(1→	4.30	3.10	3.27	3.48	3.14	3.82
		101.81	73.87	75.57	69.15	65.18	

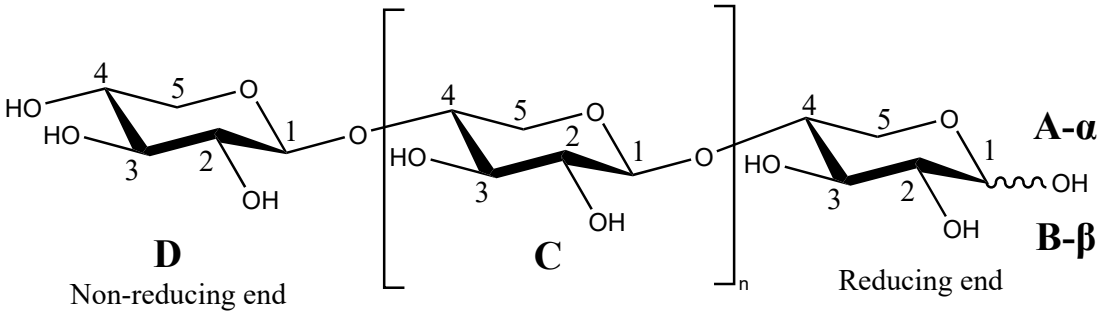

Fig. S5. The structure of XOS from corn cobs.