Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Molecular scale behavior of xylan during solvent-controlled extraction and precipitation

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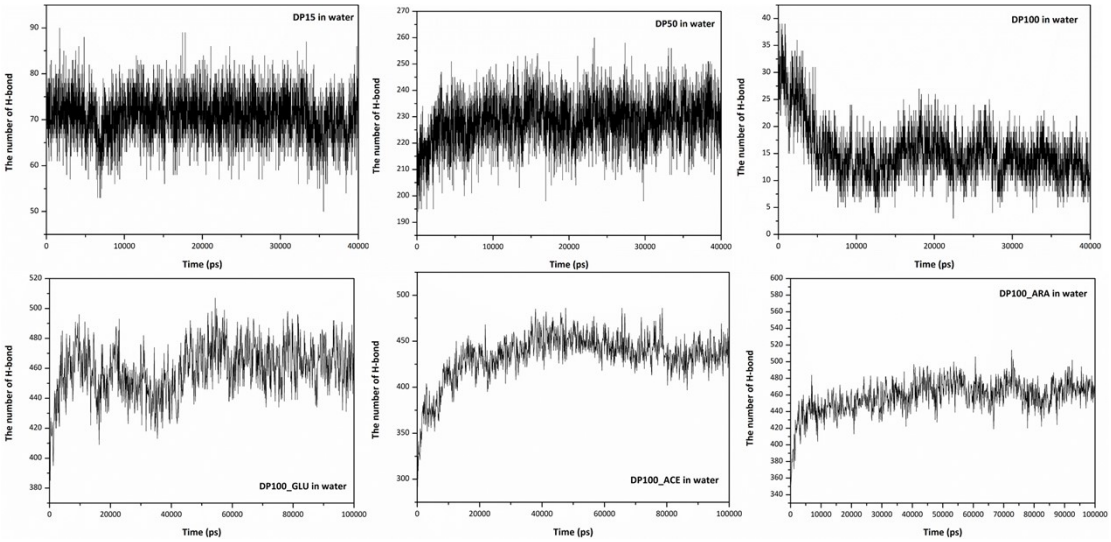

Figure S1. The number of H-bond between xylan (DP15, DP50, DP100, DP100_GLU, DP100_ACE, and DP100_ARA) and water

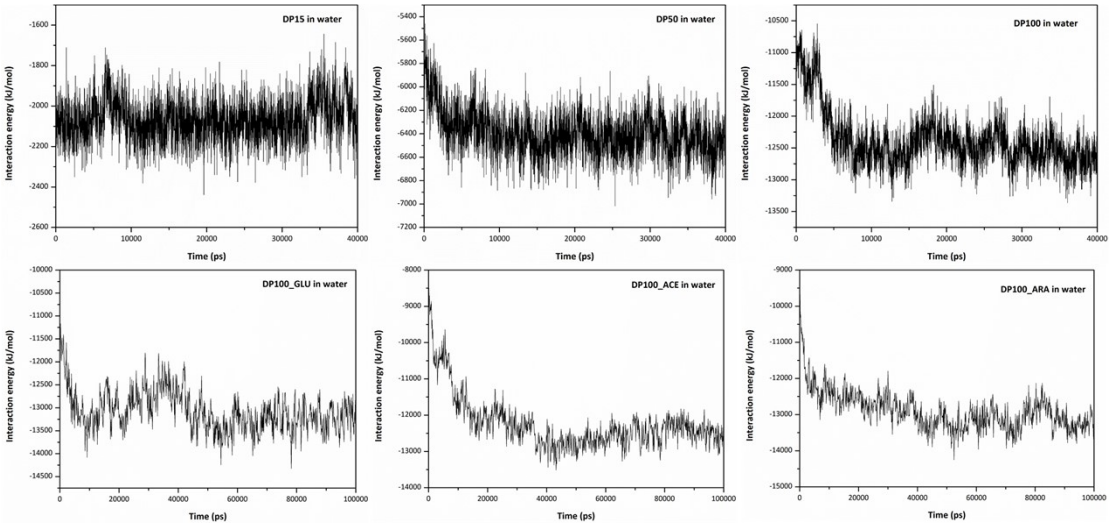

Figure S2. The interaction energy between xylan (DP15, DP50, DP100, DP100_GLU, DP100_ACE, and DP100_ARA) and water

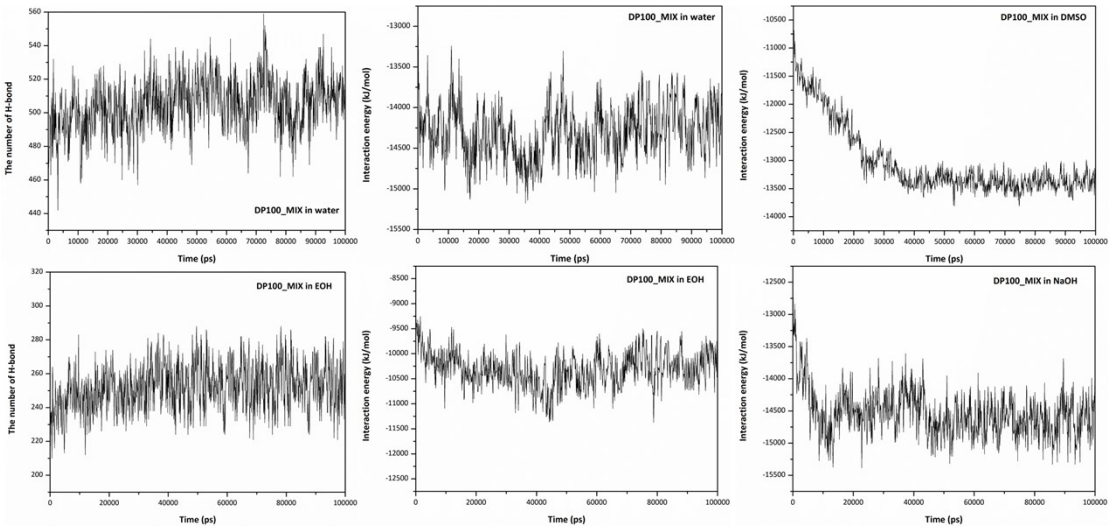

Figure S3. The interaction energy and the number of H-bond between xylan (DP100_MIX) and solvent (water, ethanol, DMSO, and NaOH solution)

Table S1 The number of hydrogen bond and interaction energy of DP15 and DP100_MIX in water and ethanol

		DP15		**DP100_MIX**	
		In water	In ethanol	In water	In ethanol
Interaction energy (kJ/mol)	3Xylan-3Xylan	-12887±112	-13521±148	-85789±742	-87982±679
	3Xylan-solvent	-6259.4±31.1	-4407.7±24.7	-43794±289	-31983±194
	Xylan①-Xylan①	-4268.1±36.0	-4400.5±17.8	-28858±155	-29162±171
	Xylan①-Xylan②	-1.4±0.2	-55.4±4.2	0	-0.003±5E-4
	Xylan①-Xylan③	-3.5±0.6	-66.8±8.7	0	-0.05±0.003
	Xylan②-Xylan②	-4269.2±15.3	-4385.6±29.5	-28625±208	-29549±214
	Xylan②-Xylan③	-11.8±0.8	-195.4±5.6	0	-105.5±3.8
	Xylan③-Xylan③	-4271.1±35.7	-4367.0±29.4	-28306±164	-29167±123
Hydrogen bond	3Xylan-3Xylan	5.6±0.1	25.2±1.4	55.6±6.4	160.5±7.6
	3Xylan-solvent	216.3±8.6	102.1±2.6	1513.6±20.1	761.6±10.7
	Xylan①-Xylan①	1.8±0.2	7.1±0.4	19.1±1.5	54.3±6.3
	Xylan①-Xylan②	0.004±7E-4	1.3±0.2	0	0
	Xylan①-Xylan③	0.09±0.004	1.5±0.1	0	0
	Xylan②-Xylan②	1.8±0.1	6.5±0.5	18.2±1.5	51.4±3.5
	Xylan②-Xylan③	0.2±0.01	3.4±0.4	0	2.9±0.5
	Xylan③-	1.7±0.1	5.5±0.6	18.4±1.0	52.0±4.5

Xylan③

Table S2 Force-field parameters for all species

Species	Atom	q (e)	ε (kJ/mol)	σ (nm)	Source
Na^+	Na	1	0.132754039	0.262815122	DOI: 10.1021/ct500918t[1]
Hydronium	H	0.32	0.50208	0.302905564168	CHARMM36 force field
	O	-1.32	0.192464	0.0400013524445	

[1] Pengfei Li, Lin Frank Song, and Kenneth M. Merz, Jr. Systematic Parameterization of Monovalent Ions Employing the Nonbonded Model. J. Chem. Theory Comput. 2015, 11, 4, 1645–1657. DOI: 10.1021/ct500918t