Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY INFORMATION

Screening ionic liquids for dissolving hemicellulose by COSMO-RS based on the selective model

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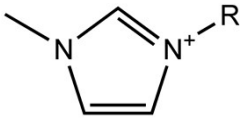
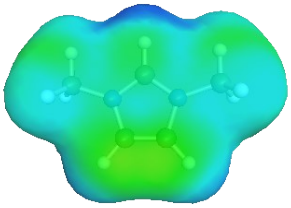
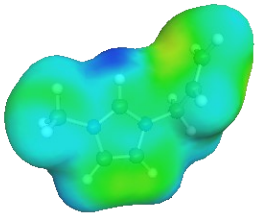
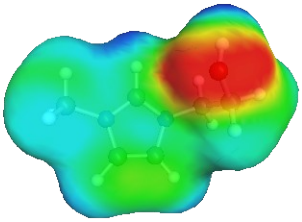
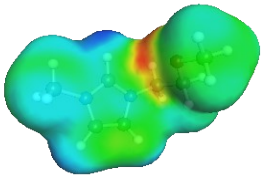
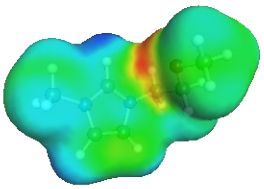
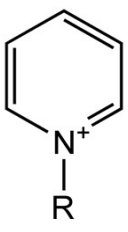
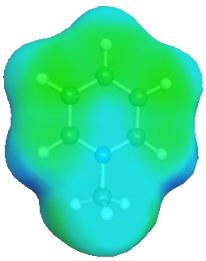
Table S1. The molecular model and conformation of hemicellulose and ions

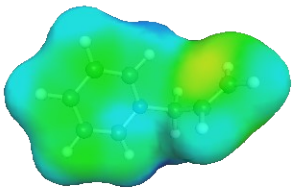
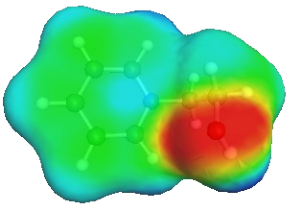
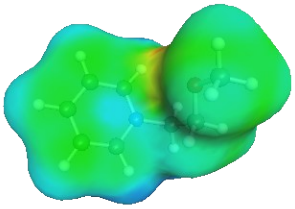
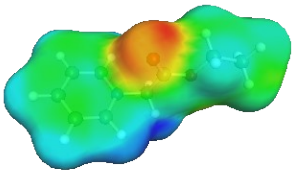
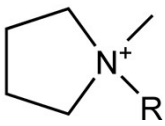
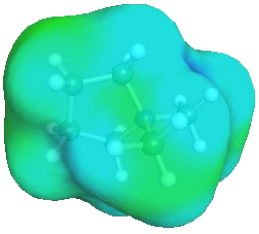
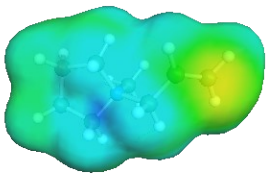
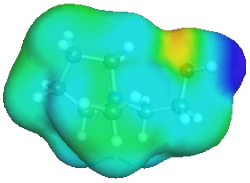
Table S2. R^2, RSS and Optimization time of the six hemicellulose models

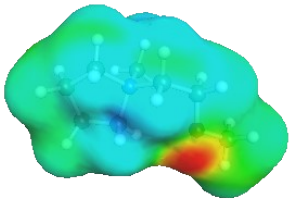
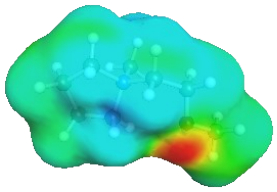
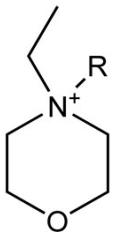
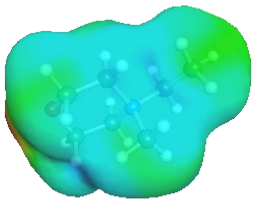
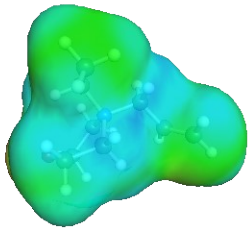
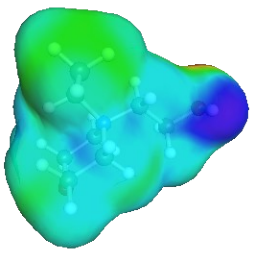
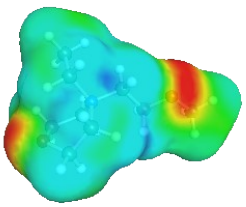
Table S3. The R^2 of the integral area and lnγ of 38 kind anions in four intervals considered

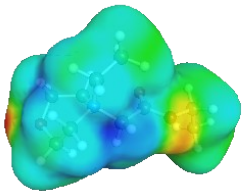
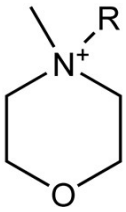
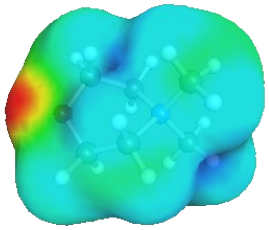
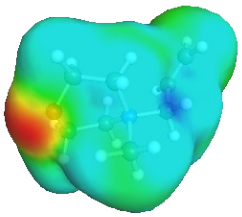
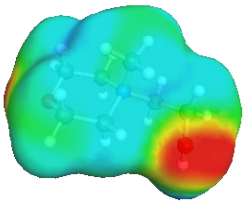
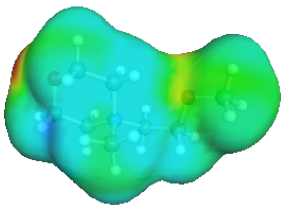
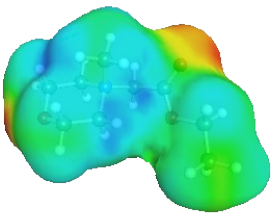
Figure S1. σ-profile curves of hemicellulose and 38 anions.

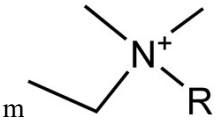
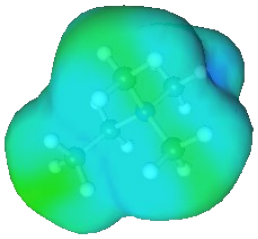
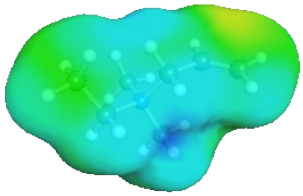
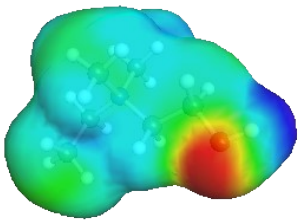
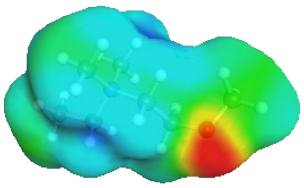
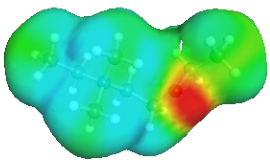
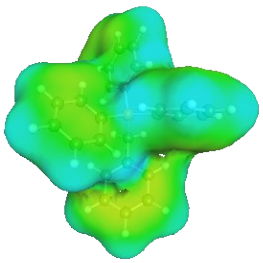
Table S1. The molecular model and conformation of hemicellulose and ions used in this work

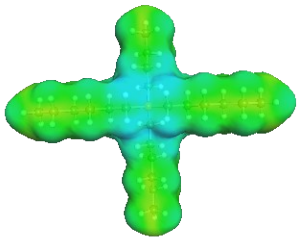
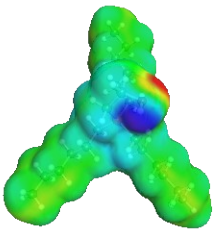
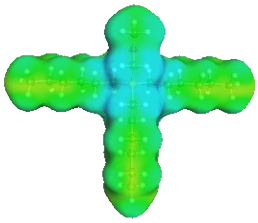
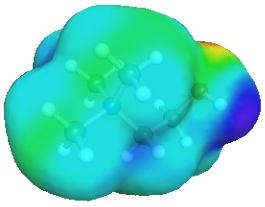
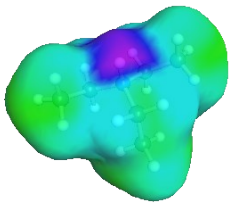
No.	Name of cation	Acronym	Conformation
1-5	1-R-3-Methylimidazolium 	1: [Mmim], R=methyl	
		2: [Amim], R=allyl	
		3: [HOEtmim], R=2-hydroxylethyl	
		4: [EtOMmim], R=2-methoxyethyl	
		5: [EOEmim], R=2-ethoxy-2oxoethyl	
6-10	N-R-Pyridinium 	6: [Mpy], R=methyl	

No.	Name of cation	Acronym	Conformation
		7: [Apy], R=allyl	
		8: [HOEtpy], R=2-hydroxylethyl	
		9: [EtOMpy], R=2-methoxyethyl	
		10: [EOEpy], R=2-ethoxy-2oxoethyl	
11-15	1R-1-Methylpyrrolidinium 	11: [Mpy], R=methyl	
		12: [Apy], R=allyl	
		13: [HOEtpy], R=2-hydroxylethyl	

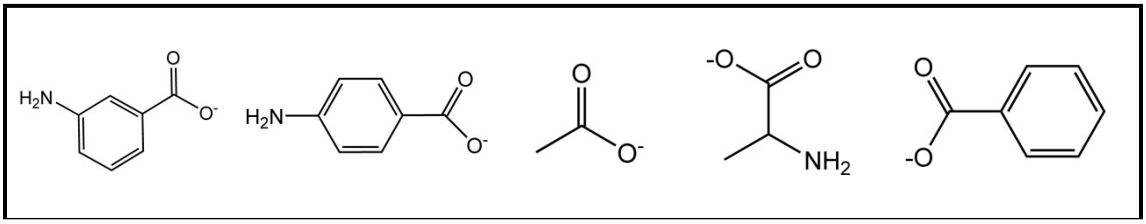
No.	Name of cation	Acronym	Conformation
		14: [EtOMpy], R=2-methoxyethyl	
		15: [EOEpy], R=2-ethoxy-2oxoethyl	
16-20	4-R-4-Ethylmorpholinium 	16: [Memor], R=methyl	
		17: [Aemor], R=allyl	
		18: [HOEtemor], R=2-hydroxylethyl	
		19: [EtOMemor], R=2-methoxyethyl	

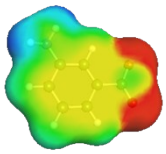
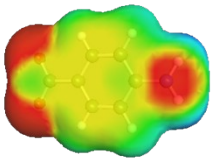
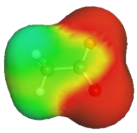
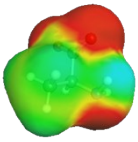
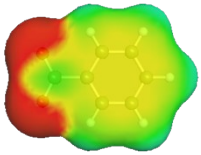
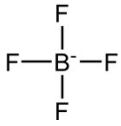
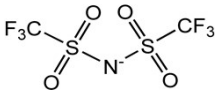
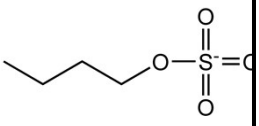
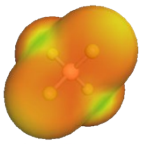
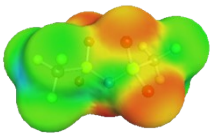
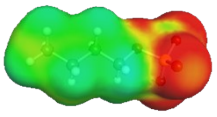
No.	Name of cation	Acronym	Conformation
		20:[EOEemor], R=2-ethoxy-2oxoethyl	
21-25	4-R-4-Methylmorpholinium 	21: [Mmmor], R=methyl	
		22: [Ammor], R=allyl	
		23: [HOEtmmor], R=2-hydroxylethyl	
		24: [EtOMmmor], R=2-methoxyethyl	
		25:[EOEmmor], R=2-ethoxy-2oxoethyl	

No.	Name of cation	Acronym	Conformation
26-30	R-ethyl-dimethylammonium 	26: [Medmam], R=methyl	
		27: [Aedmam], R=allyl	
		28:[HOEtedmam], R=2-hydroxylethyl	
		29:[EtOMedmam], R=2-methoxyethyl	
		30:[EOEedmam], R=2-ethoxy-2oxoethyl	
31	Benzyl-triphenyl-phosphonium	[Bentpho]	

No.	Name of cation	Acronym	Conformation
32	Butyl-trihexyl-phosphonium	[Butpho]	
33	Trihexyl(2-hydroxyethyl)phosphonium	[Thhpho]	
34	Trihexyl(methoxymethyl)-phosphonium	[Thmompho]	
35	Choline	[Choline]	
36	Triethylamine	[Triam]	

The conformation of anions studied in this work



				
1.[Oabc]$^-$	2.[Pabc]$^-$	3.[Ac]$^-$	4.[Ala]$^-$	5.[BEN]$^-$
		Br^-	Cl^-	
				
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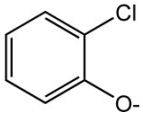	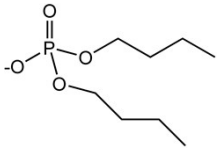	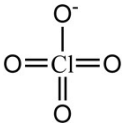	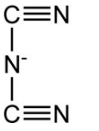	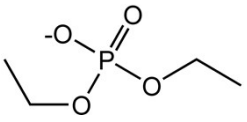
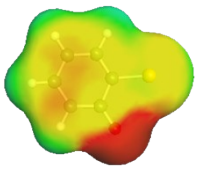	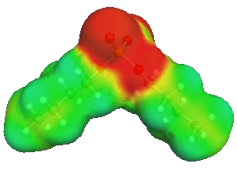	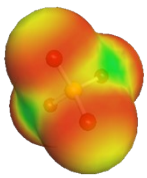	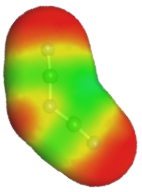	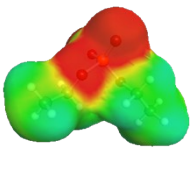
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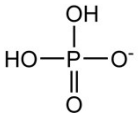	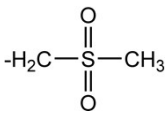	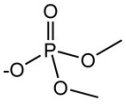	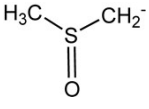	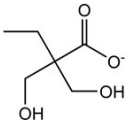

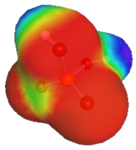	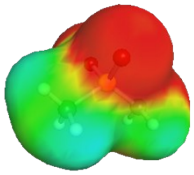	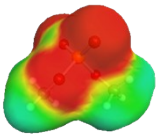	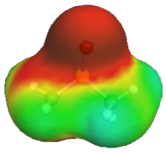	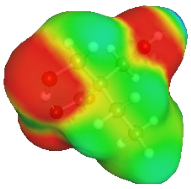
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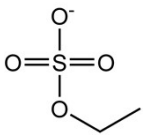	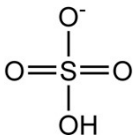	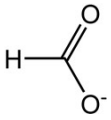	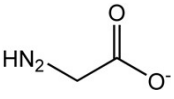	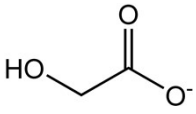
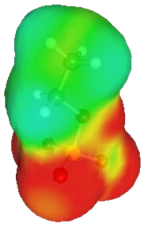	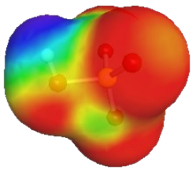	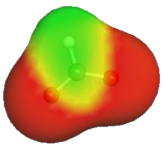	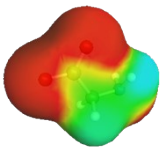	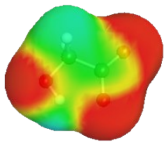
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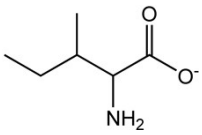
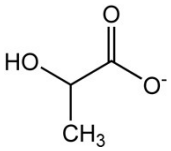
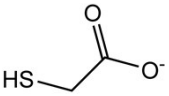
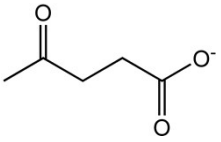
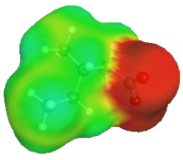
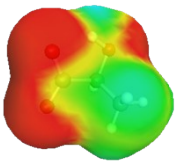
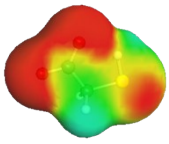
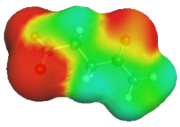
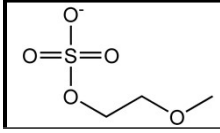
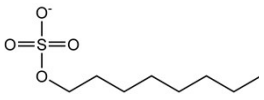
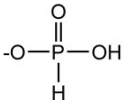
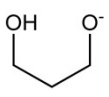
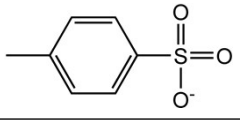
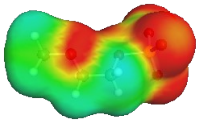
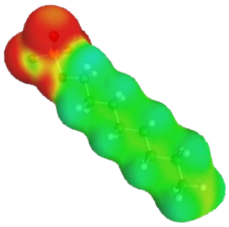
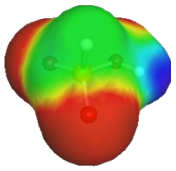
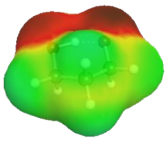
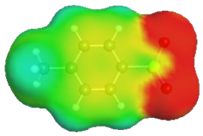
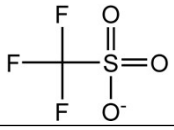
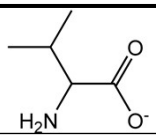
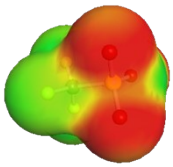
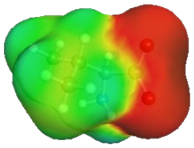
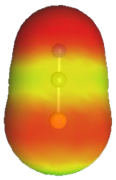
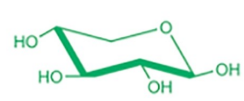
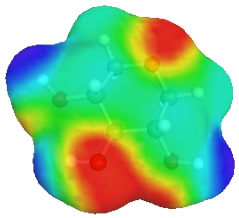
		I$^-$		
				
26.[Isoec]$^-$	27.[EtHOCOO]$^-$	28.[I]$^-$	29.[MeHSCOO]	30.[lev]$^-$
				

				
31.[MeOEtSO4]$^-$	32.[$OcSO_4$]$^-$	33.[Pho]$^-$	34.[Pdo]$^-$	35.[Tos]$^-$
				
				
36.[Otf]$^-$	37.[Val]$^-$	38.[SCN]$^-$		

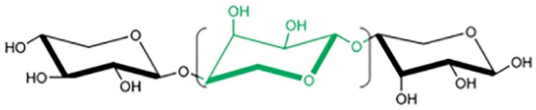
The conformation of hemicellulose models studied in this work

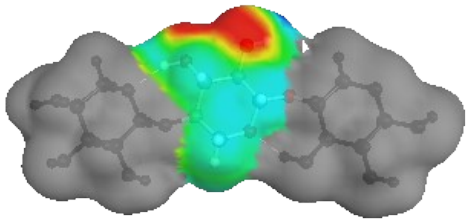
Model 1



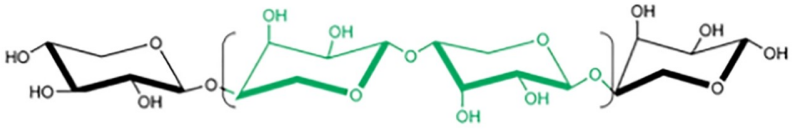


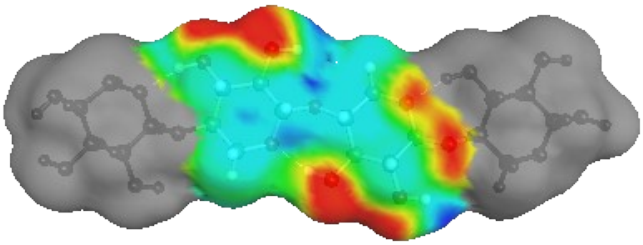
Model 2



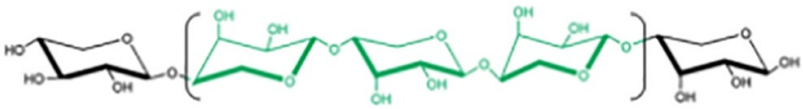


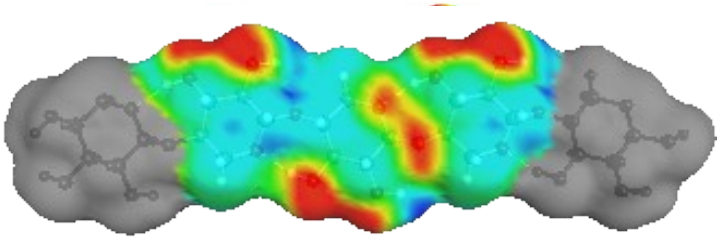
Model 3





Model 4





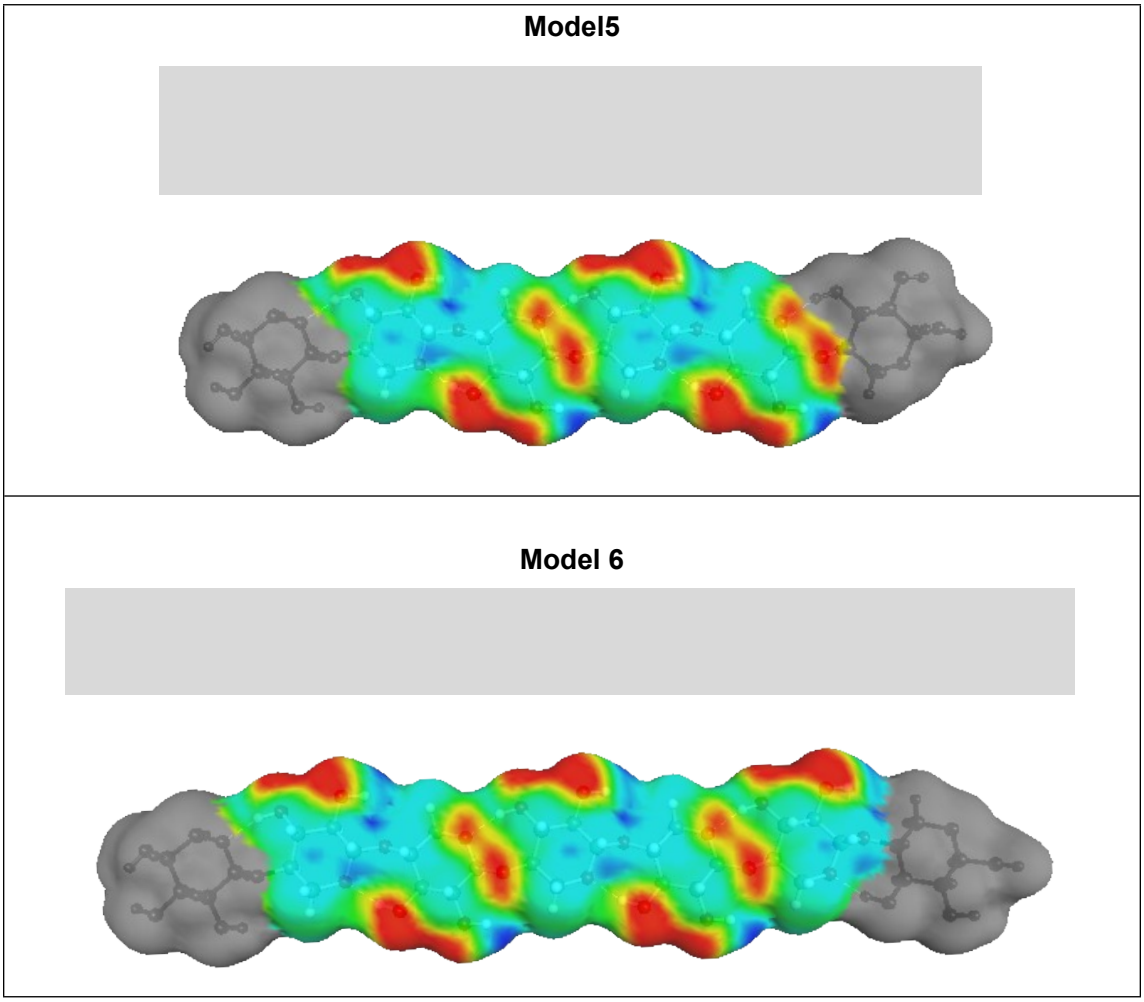


Table S2. R^2, RSS and Optimization time of the six hemicellulose models

	Model 1	Model 2	Model 3	Model 4	Model 5	Model 6
R^2	0.162	0.648	0.824	0.827	0.828	0.828
RSS	15.43	0.09	0.20	0.51	0.96	1.57
Optimization time(min)	6	56	176	434	678	790

Table S3. The R^2 of the integral area and lnγ of 38 kind anions in four intervals considered.

Region	+0.015~+0.021	**+0.016~+0.021**	+0.015~+0.022	+0.016~+0.022
R^2	0.703	**0.779**	0.622	0.630

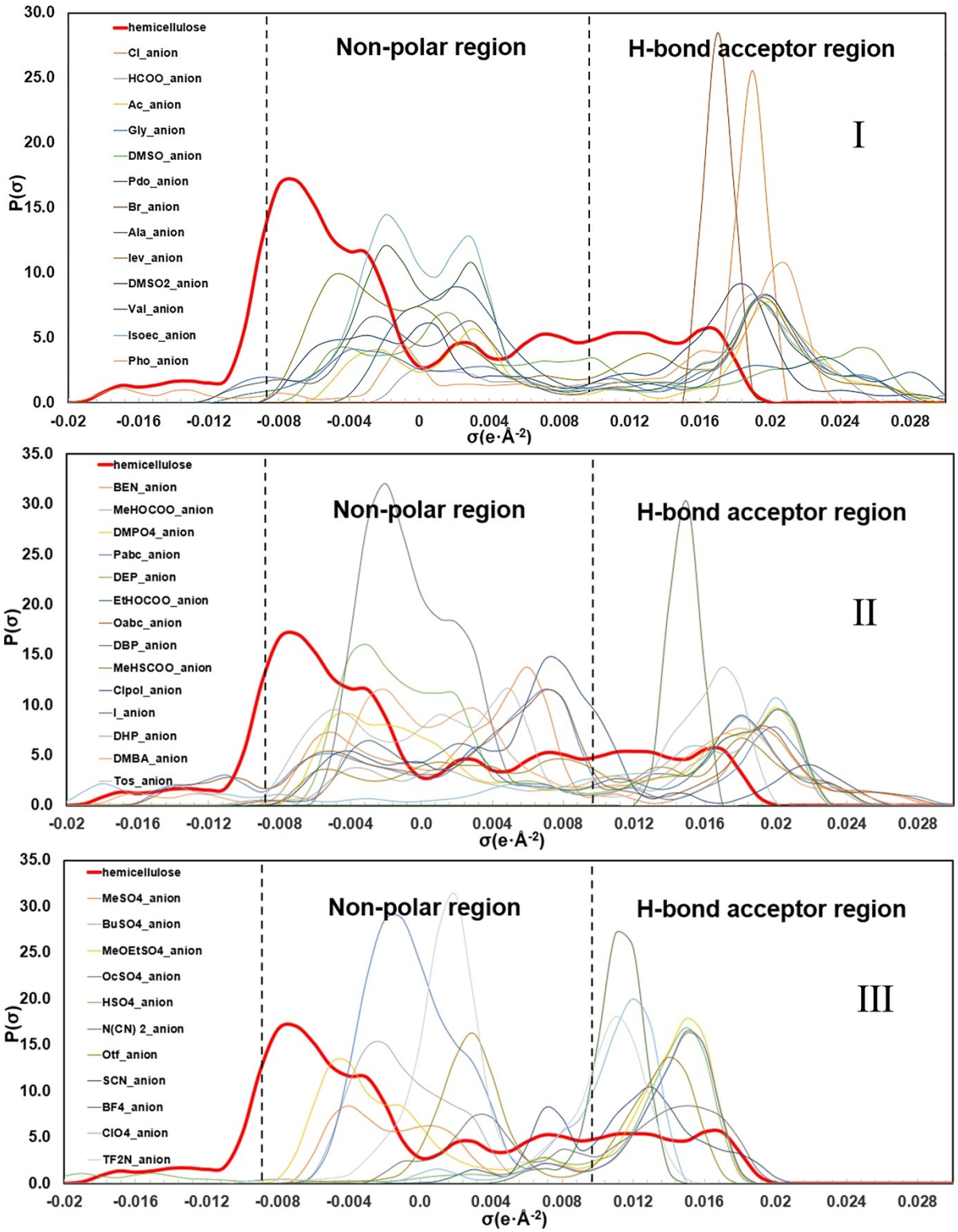


Figure S1. σ-profile curves of hemicellulose and 38 anions. The red curve is the σ-profile of the hemicellulose model. The anions are divided into three groups according to the order of activity coefficients.