

Biosourced 1,2,3-Triazolium Chiral Ionic Liquids derived from Isosorbide

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Supporting information (New Journal of Chemistry)

Table S1. Solubility of 1,2,3-triazolium-Based Ionic Liquids **17-24** and their 1,2,3-triazole precursors **15,16**

Entry	H ₂ O	Hexane	MeOH	EtOAc	Acetone	Et ₂ O	THF	CH ₂ Cl ₂	CHCl ₃	CH ₃ CN	PhCH ₃	DMF	DMSO
15	++	-	++	++	++	-	++	++	++	++	-	++	++
16	++	-	++	++	++	-	++	++	++	++	-	++	++
17	++	-	++	~	++	-	-	++	++	++	-	++	++
18	++	-	++	~	++	-	-	++	++	++	-	++	++
19	++	-	++	-	++	-	-	++	++	++	-	++	++
20	++	-	++	-	++	-	-	++	++	++	-	++	++
21	++	-	++	-	++	-	-	++	++	++	-	++	++
22	++	-	++	-	++	-	-	++	++	++	-	++	++
23	++	-	++	-	++	-	-	++	++	++	-	++	++
24	++	-	++	-	++	-	-	++	++	++	-	++	++

“++” indicates solubility at 10 mg.mL⁻¹, “+” indicates solubility at 1 mg.mL⁻¹, “~” indicates partial solubility at 0.1 mg.mL⁻¹, while “-” indicates no detectable solubility even at 0.1 mg.mL⁻¹.

Entry	15	16	17	18	19	20	21	22	23	24
fragment	[M+H] ⁺	[M+H] ⁺	[M+2I] ⁻	[M+2I] ⁻	[M+2BF ₄] ⁻	[M+2PF ₆] ⁻	[M+2NTf ₂] ⁻	[M+2BF ₄] ⁻	[M+2PF ₆] ⁻	[M+2NTf ₂] ⁻
Calcd	240.1343	240.1343	507.9600	507.9600	428.1573	544.0794	813.9856	428.1573	544.0794	813.9856
Found	240.1335	240.1340	507.9605	507.9604	428.1570	544.0802	813.9858	428.1579	544.0797	813.9861

[a] negative mode ESI-HRMS [M+2X]⁻; [b] positive mode ESI-HRMS [M+H]⁺.

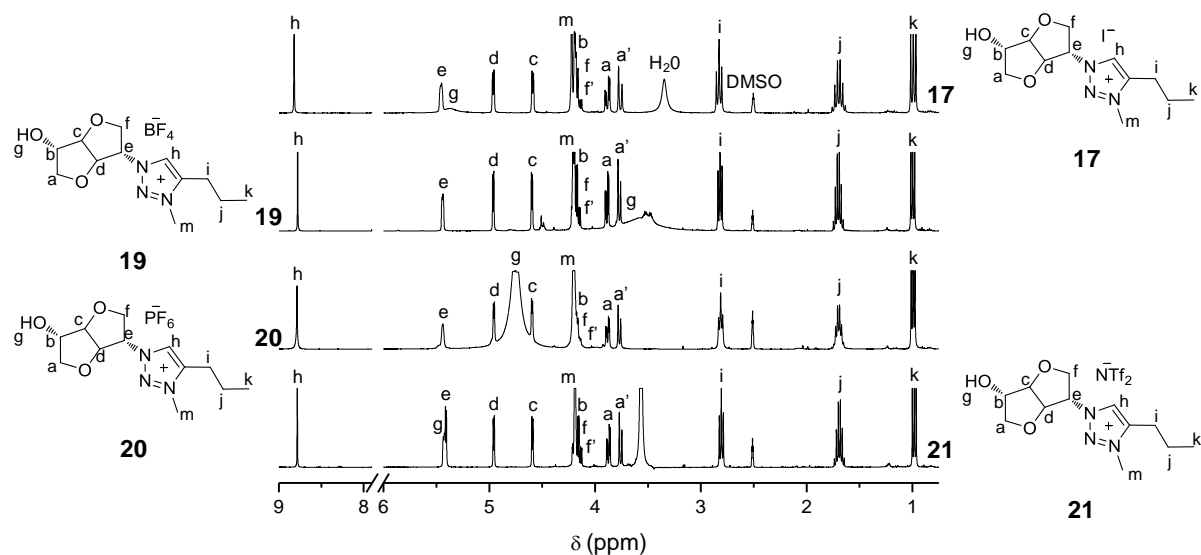


Figure S1. ¹H NMR (DMSO-*d*₆, 25 °C) of biosourced 1,2,3-triazoliums **17**, **19**-**21**.

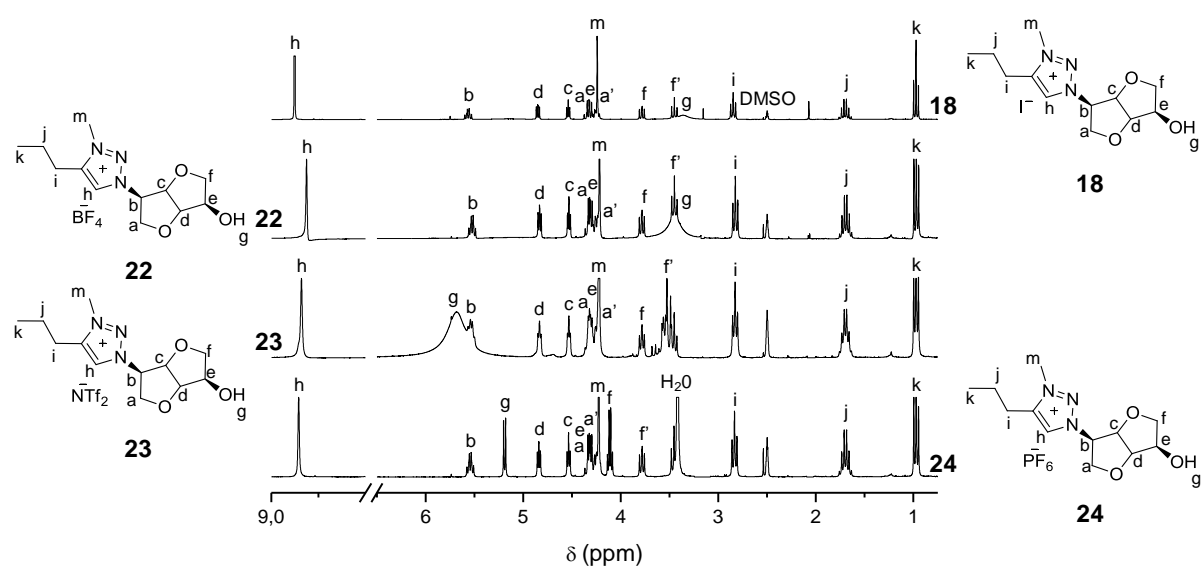


Figure S2. ¹H NMR (DMSO-*d*₆, 25 °C) of biosourced 1,2,3-triazoliums **18**, **22**-**24**.

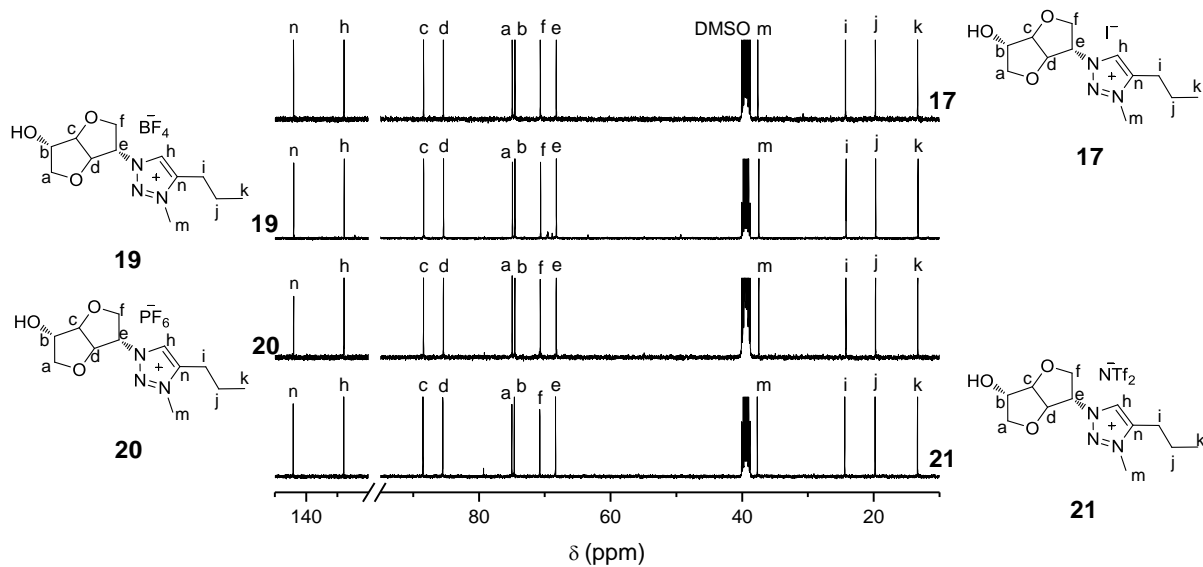


Figure S3. ^{13}C NMR (DMSO- d_6 , 25 °C) of biosourced 1,2,3-triazoliums **17**, **19**-**21**.

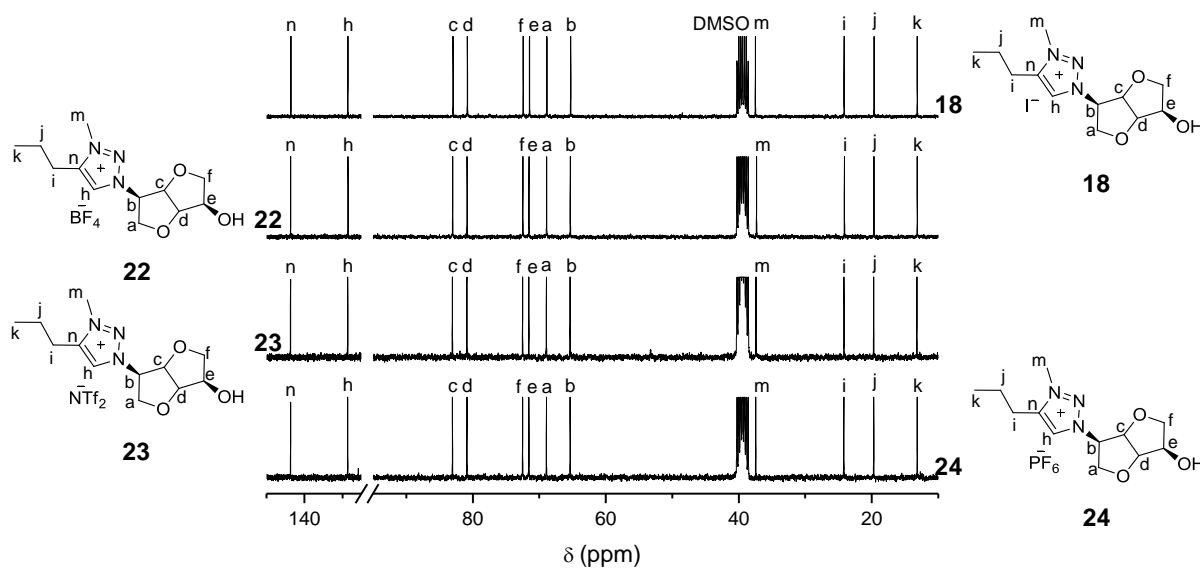
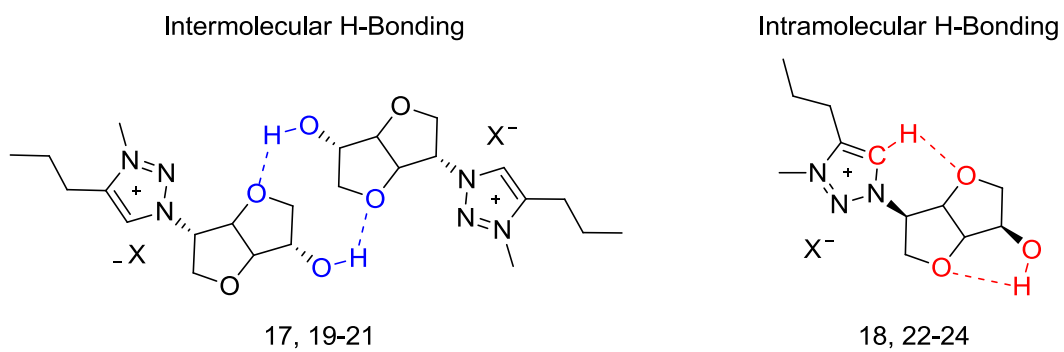


Figure S4. ^{13}C NMR (DMSO- d_6 , 25 °C) of biosourced 1,2,3-triazoliums **18**, **22**-**24**.



Scheme S1. Difference in *H*-bonding between the isoidide (**17,19-21**) and isomannide (**18,22-24**) series.