

## **Supporting Materials**

### **Experimental and In Silico Comparative Study of Physicochemical Properties and Antimicrobial Activity of Carboxylate Ionic Liquids**

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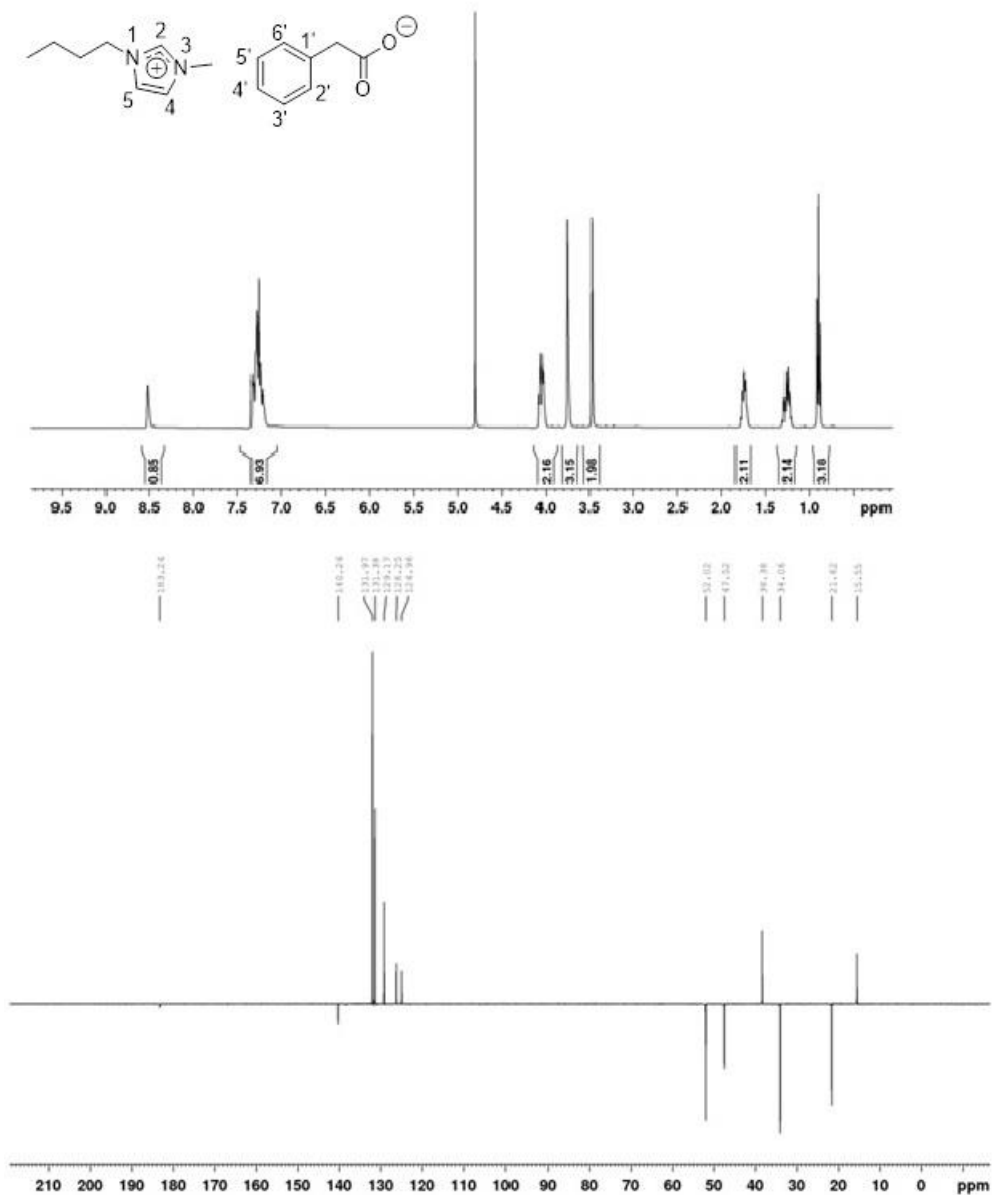
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**Table S1.** Provenance and purity of the samples

Chemical name	Source	Mass fraction purity	Purification method
1-butyl-3-methylimidazolium chloride	Sigma Aldrich	98% <sup>**</sup>	None
Phenylacetic acid	Sigma Aldrich	99% <sup>**</sup>	None
Benzoic acid	Sigma Aldrich	$\geq 99.5\%$ <sup>**</sup>	None
4-methoxyphenylacetic acid	Sigma Aldrich	99% <sup>**</sup>	None
Methanol	J.T. Baker	$> 99\%$ <sup>**</sup>	None
1-butyl-3-methylimidazolium phenylacetate	Synthesis	$\geq 98\%$ <sup>*</sup>	Rotary evaporation followed by vacuum
1-butyl-3-methylimidazolium benzoate	Synthesis	$\geq 98\%$ <sup>*</sup>	Rotary evaporation followed by vacuum
1-butyl-3-methylimidazolium 4-methoxyphenylacetate	Synthesis	$\geq 98\%$ <sup>*</sup>	Rotary evaporation followed by vacuum

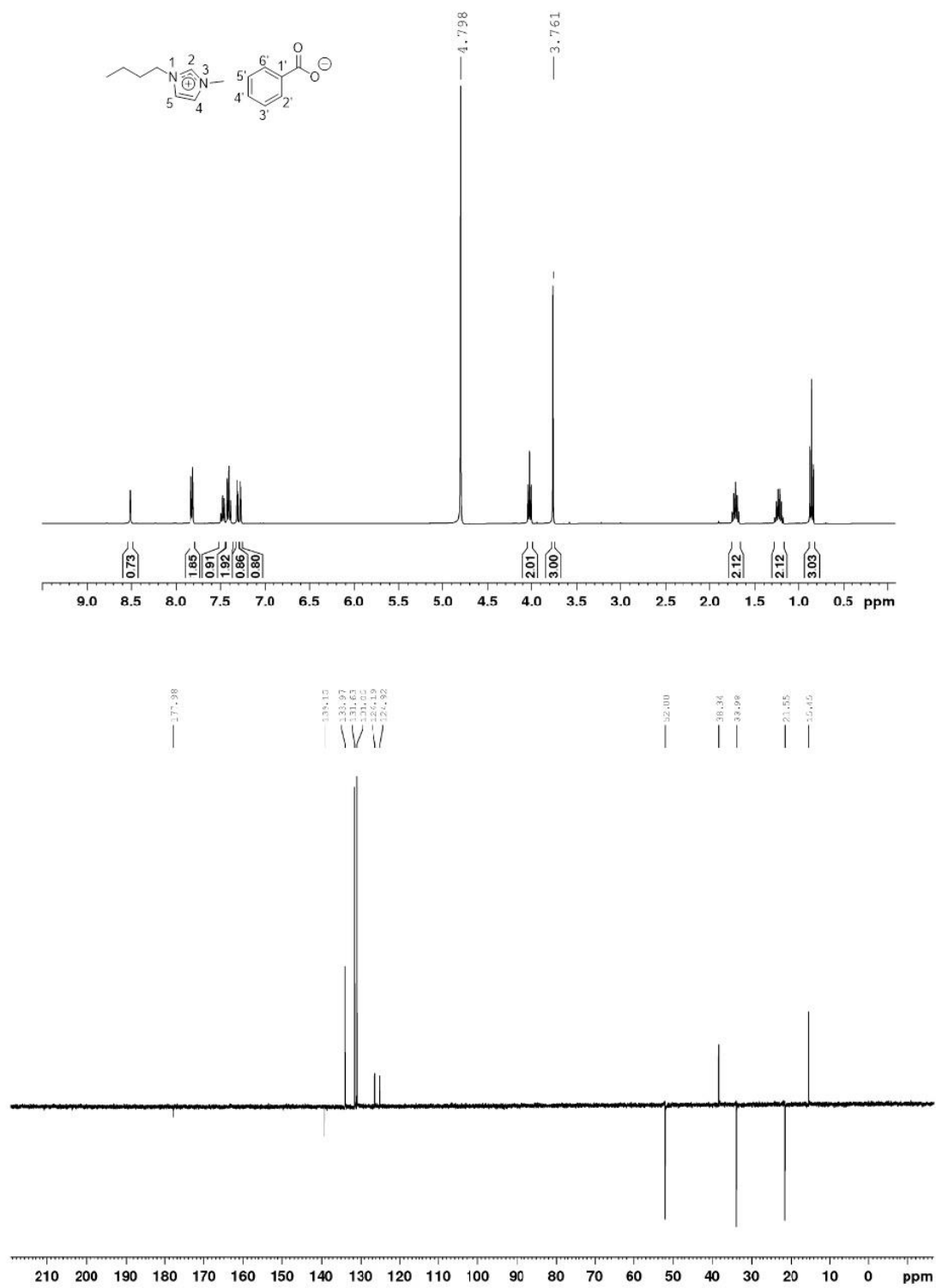
<sup>\*</sup>Determined by NMR measurements.<sup>\*\*</sup>Provided by the supplier.



**Figure S1.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of [Bmim][Phe]

**<sup>1</sup>H NMR** spectrum (D<sub>2</sub>O): 8.52 (s, 1H, H-2); 7.16-7.37 (m, 7H, H-3', H-5', H-2', H-6', H-4', H-4, H-5); 4.05 (t, 2H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 3.75 (s, 3H, NCH<sub>3</sub>); 3.47 (s, 2H, CH<sub>2</sub>CO<sub>2</sub><sup>-</sup>); 1.75 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 1.26 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 0.89 (t, 3H, *J* = 7.1 Hz, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>).

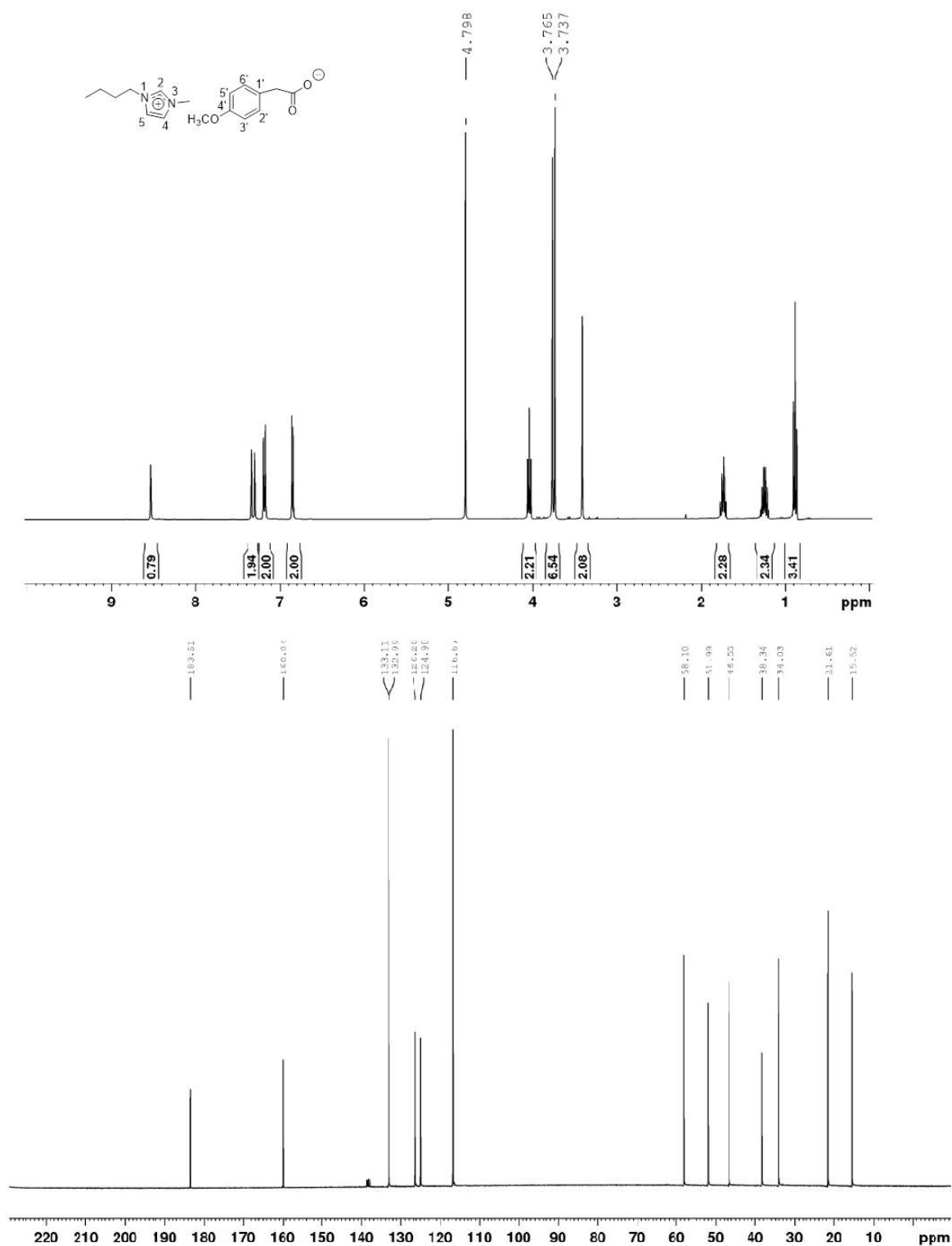
**<sup>13</sup>C NMR** spectrum (D<sub>2</sub>O): 183.24 (C=O); 140.24 (C-1'); 138.40 (t, *J*<sub>2,D</sub> = 33.6 Hz, C-2); 131.97 (C-2' and C-6'); 131.38 (C-3' and C-5'); 129.17 (C-4'); 126.25 (C-4); 124.96 (C-5); 52.02 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 47.52 (CH<sub>2</sub>CO<sub>2</sub><sup>-</sup>); 38.38 (NCH<sub>3</sub>); 34.06 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 21.62 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 15.55 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>).



**Figure S2.**  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra of [Bmim][Ben]

**<sup>1</sup>H NMR** spectrum (D<sub>2</sub>O): 8.51, (s, 1H, H-2); 7.37-7.85 (m, 5H, Ph-H); 7.16 (t, 1H, *J* = 1.8 Hz, H-5); 7.14 (t, 1H, *J* = 1.8 Hz, H-4); 4.02 (t, 2H, *J* = 7.3 Hz, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 3.76 (s, 3H, NCH<sub>3</sub>); 1.71 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 1.22 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 0.86 (t, 3H, *J* = 7.6 Hz, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>).

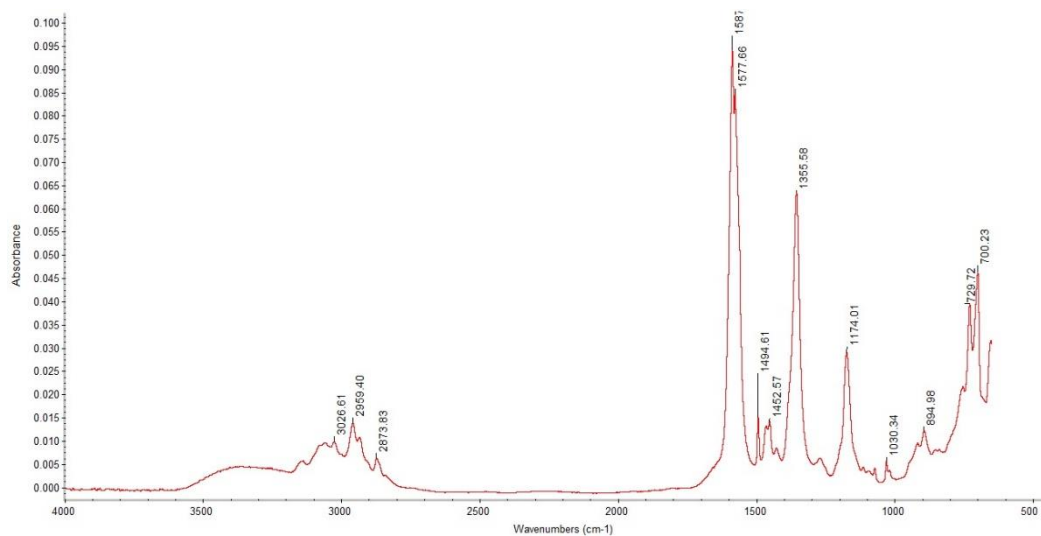
**<sup>13</sup>C NMR** spectrum (D<sub>2</sub>O): 177.98 (C=O); 139.15 (C-1'); 138.36 (t, *J*<sub>2,D</sub> = 33.6 Hz, C-2); 133.97 (C-4'); 131.63 (C-2' and C-6'); 131.05 (C-3' and C-5'); 126.19 (C-4); 124.92 (C-5); 52.00 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 38.34 (NCH<sub>3</sub>); 33.98 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 21.55 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 15.45 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>).



**Figure S3.**  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra of [Bmim][CH<sub>3</sub>OPhe]

**<sup>1</sup>H NMR** spectrum (D<sub>2</sub>O): 8.53 (s, 1H, H-2); 7.34 (t, 1H, *J* = 1.8 Hz, H-5); 7.30 (t, 1H, *J* = 1.8 Hz, H-4); 7.18 (d, 2H, *J* = 8.6 Hz, H-2' and H-6'); 6.85 (d, 2H, *J* = 8.6 Hz, H-3' and H-5'); 3.85 (t, 2H, *J* = 7.1 Hz, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 3.76 (s, 3H, NCH<sub>3</sub>); 3.74 (s, 3H, OCH<sub>3</sub>); 3.41 (s, 2H, CH<sub>2</sub>CO<sub>2</sub><sup>-</sup>); 1.74 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 1.25 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 0.88 (t, 3H, *J* = 7.1 Hz, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>).

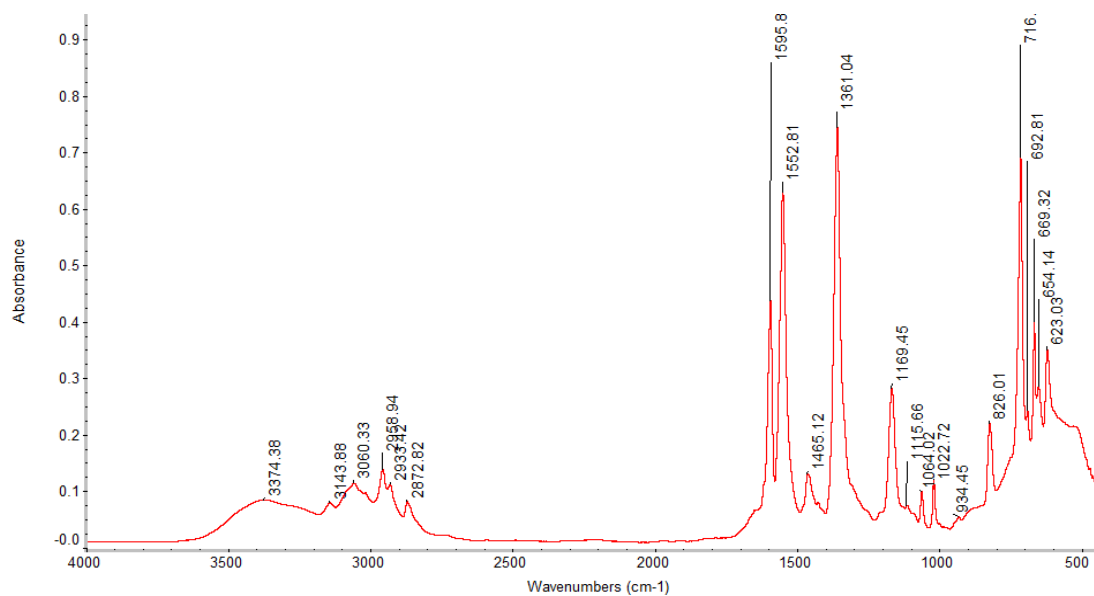
**<sup>13</sup>C NMR** spectrum (D<sub>2</sub>O): 183.51 (C=O); 160.04 (C-4'); 138.19 (t, *J*<sub>2,D</sub> = 33.6 Hz, C-2); 133.11 (C-2' and C-6'); 132.99 (C-1'); 126.20 (C-4); 124.90 (C-5); 116.67 (C-3' and C-5'); 58.10 (OCH<sub>3</sub>); 51.99 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 46.55 (CH<sub>2</sub>CO<sub>2</sub><sup>-</sup>); 38.34 (NCH<sub>3</sub>); 34.03 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 21.61 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>); 15.52 (NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>).



**Figure S4.** FTIR spectra of [Bmim][Phe]

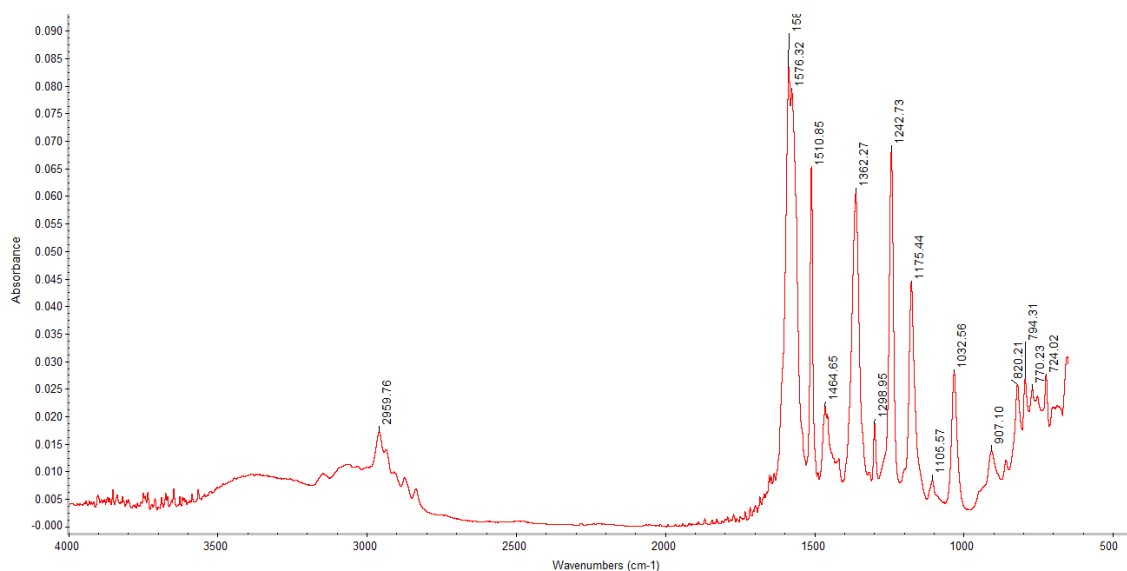
3026 (sym. stretching vibration of N-CH<sub>3</sub>); 2959 (sym. stretching vibration –CH<sub>3</sub> group bound to N); 1577 (sym. stretching vibration of the acetate ion, COO<sup>-</sup> group of phenylacetate); 1355 (rocking vibration H-C-H of butyl group); 1174 (bending vibration of imidazolium ring); 700 (in-plane bending vibration of monosubstituted aromatic ring).





**Figure S5.** FTIR spectra of [Bmim][Ben]

2958 (sym. stretching vibration  $\text{—CH}_3$  group bound to N); 1552 (asym. vibration of substituted benzoate); 1361 (rocking vibration H-C-H of butyl group); 1169 (bending vibration of imidazolium ring); 716 (in-plane bending vibration of monosubstituted aromatic ring).

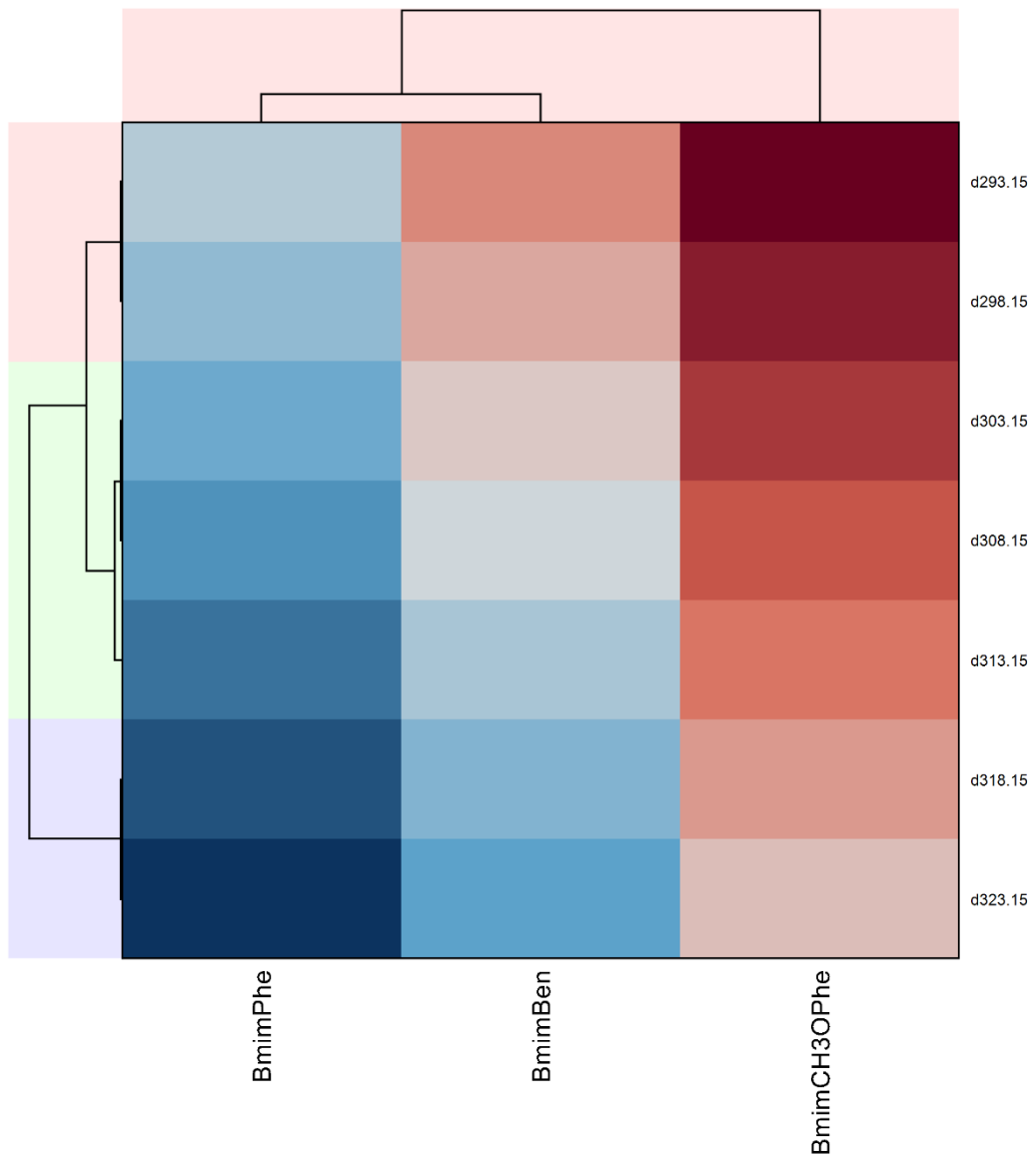


**Figure S6.** FTIR spectra of [Bmim][CH<sub>3</sub>OPhe]

IR (neat): 2959 (sym. stretching vibration –CH<sub>3</sub> group bound to N), 1580 (sym. stretching vibration of the acetate ion, COO<sup>-</sup> group of phenylacetate); 1362 (rocking vibration H-C-H of butyl group); 1242 (stretching vibration of aromatic ethers, aryl-O); 1175 (bending vibration of imidazolium ring); 1105 (stretching vibration of alkyl-substituted ether, C-O); 770 (vibration of para disubstituted aromatic ring).

S7a)

Clustered Heat Map



1.085

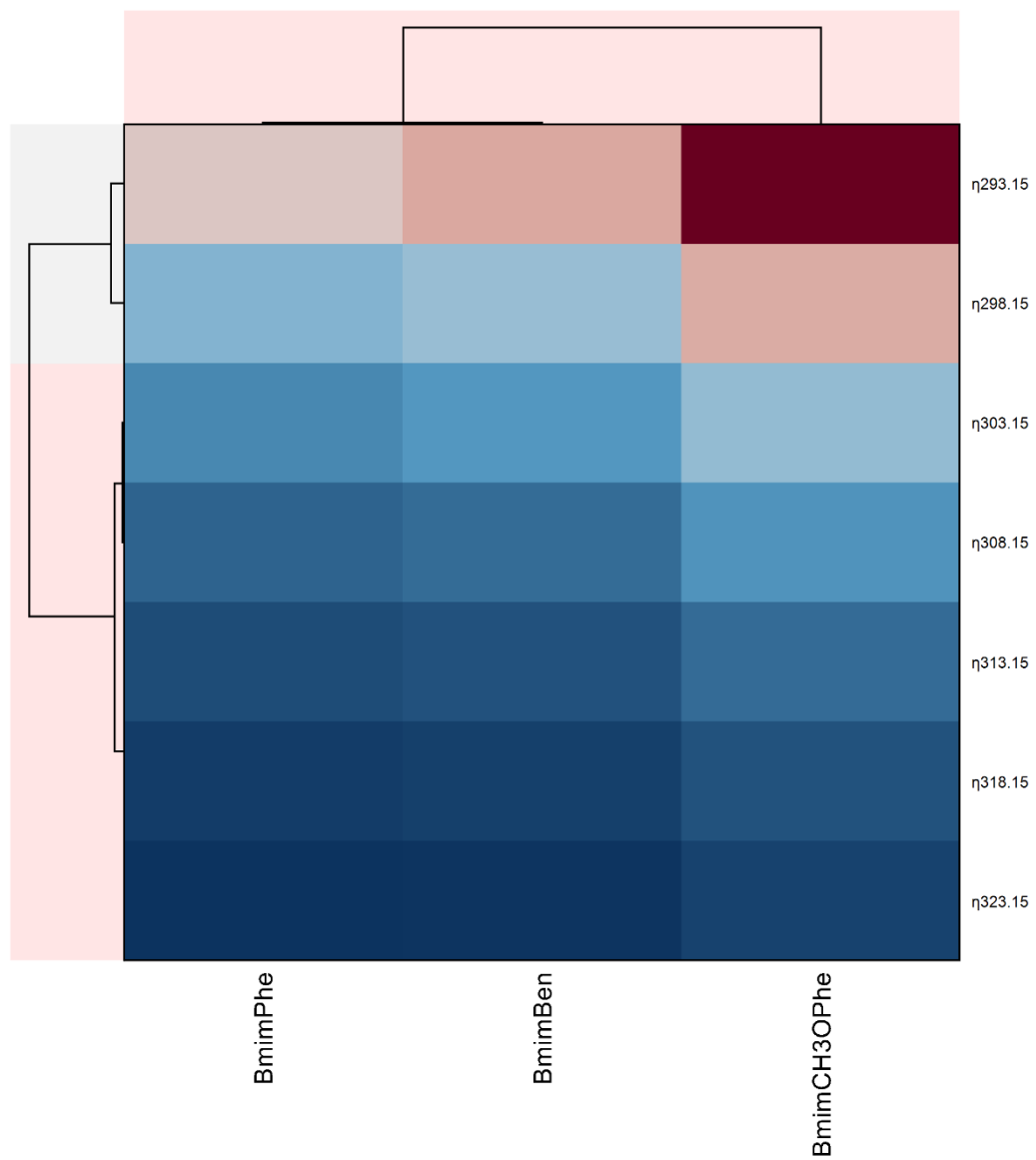
1.100

1.115

Data Value

S7b)

Clustered Heat Map



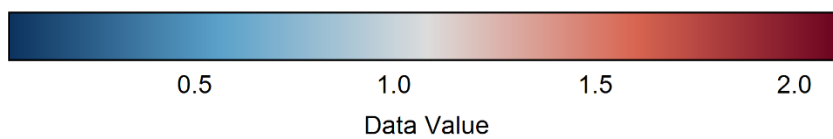
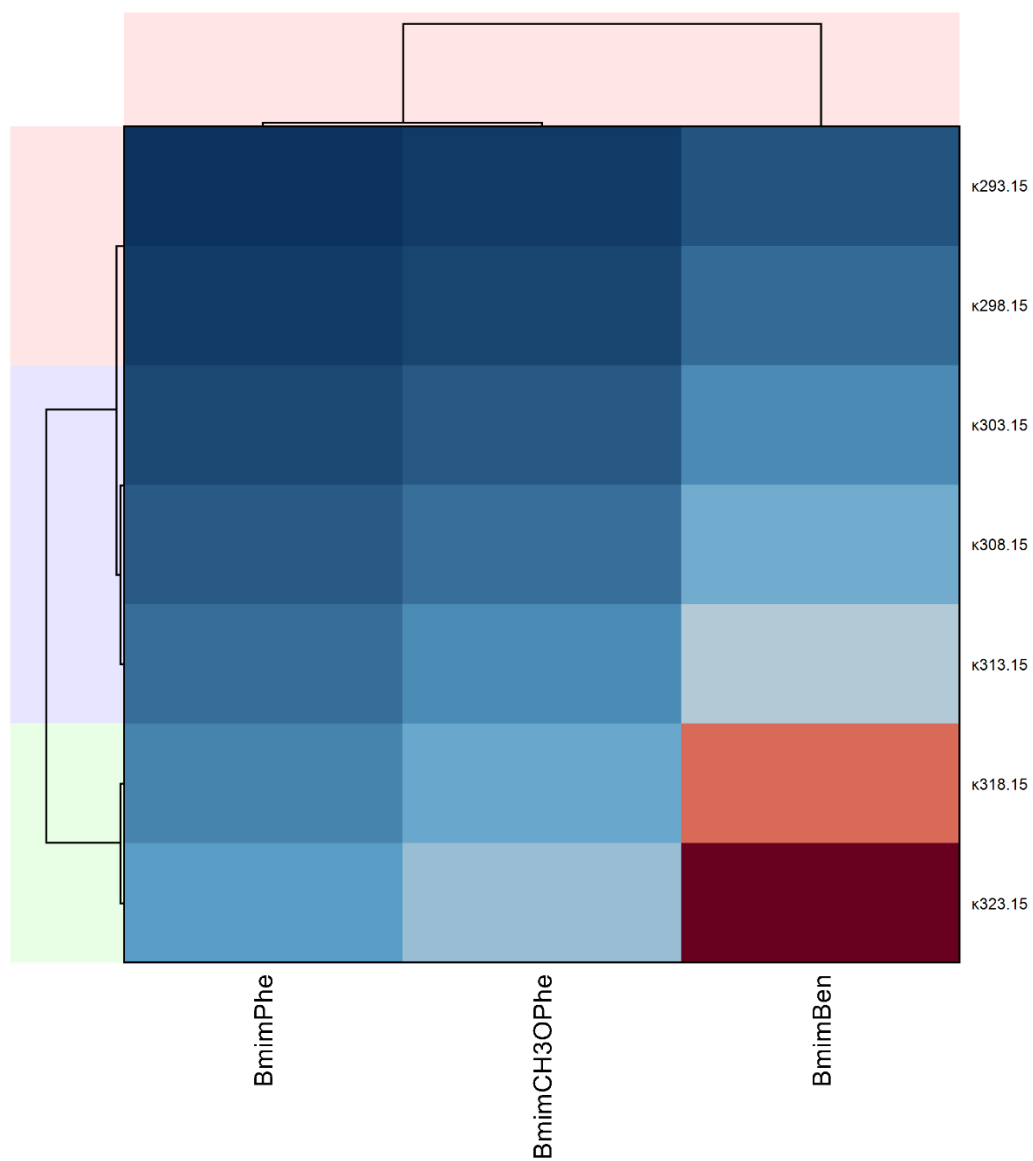
500

1000

Data Value

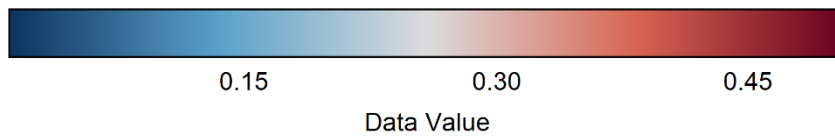
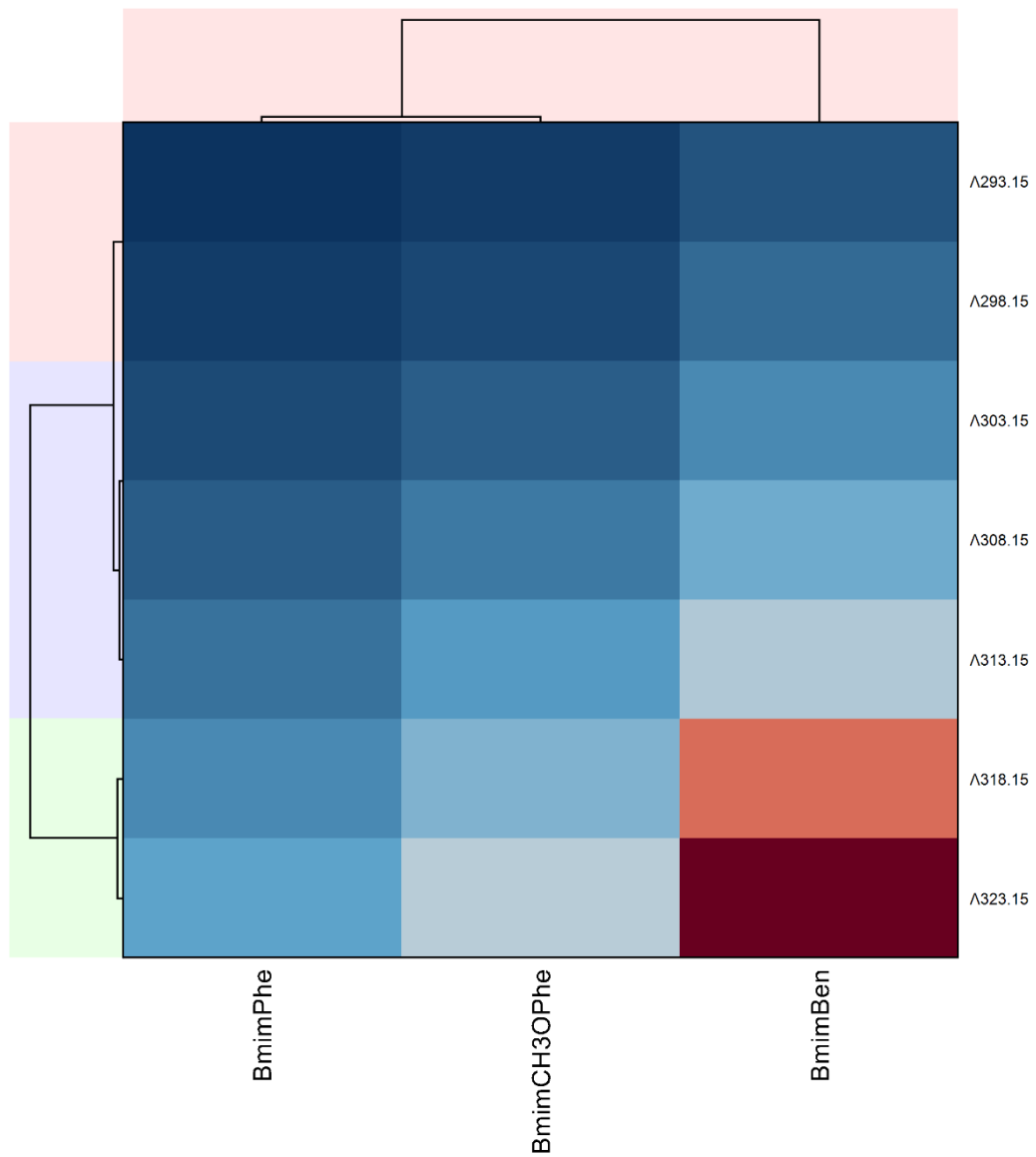
S7c)

Clustered Heat Map



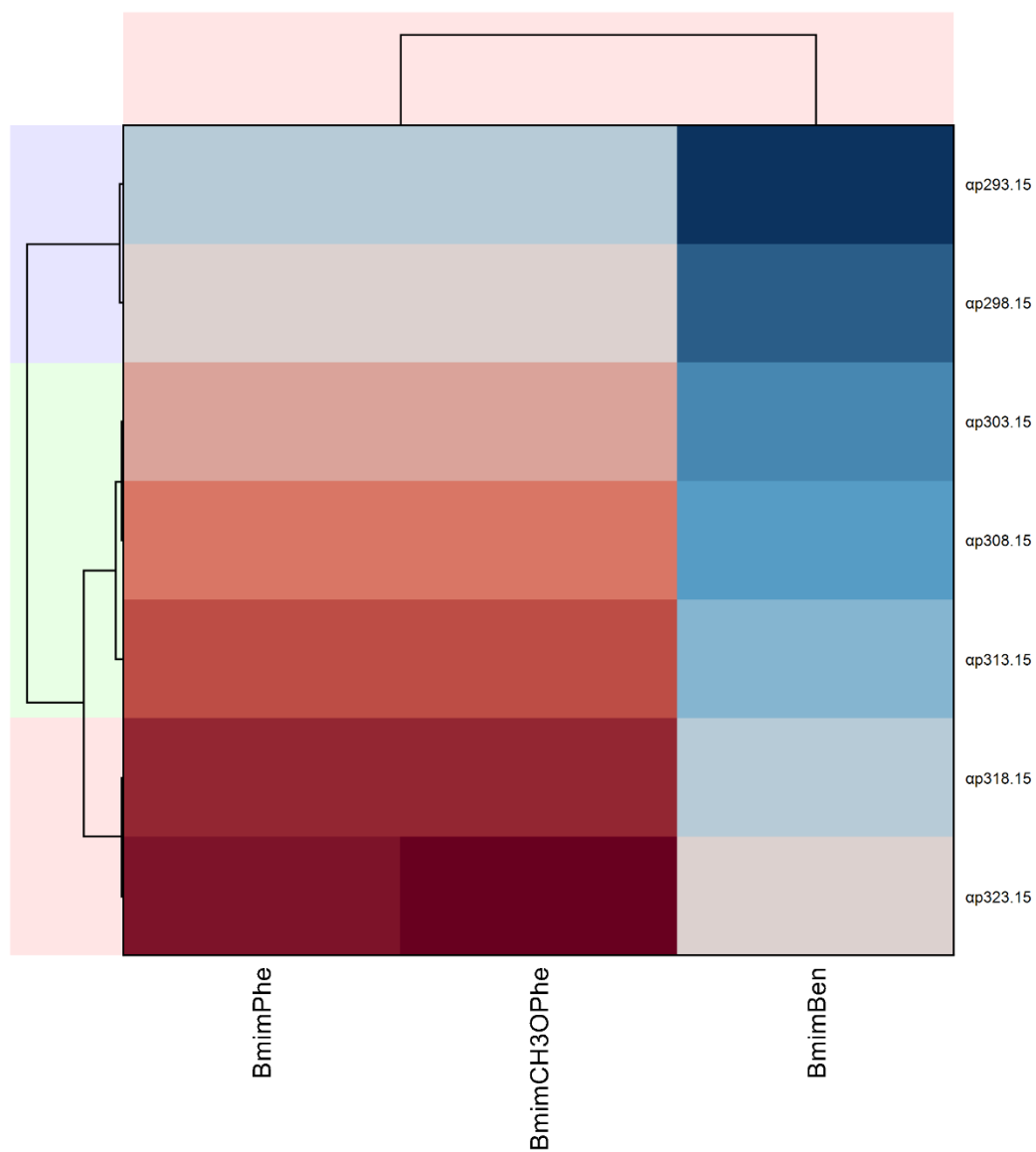
S7d)

Clustered Heat Map



S7e)

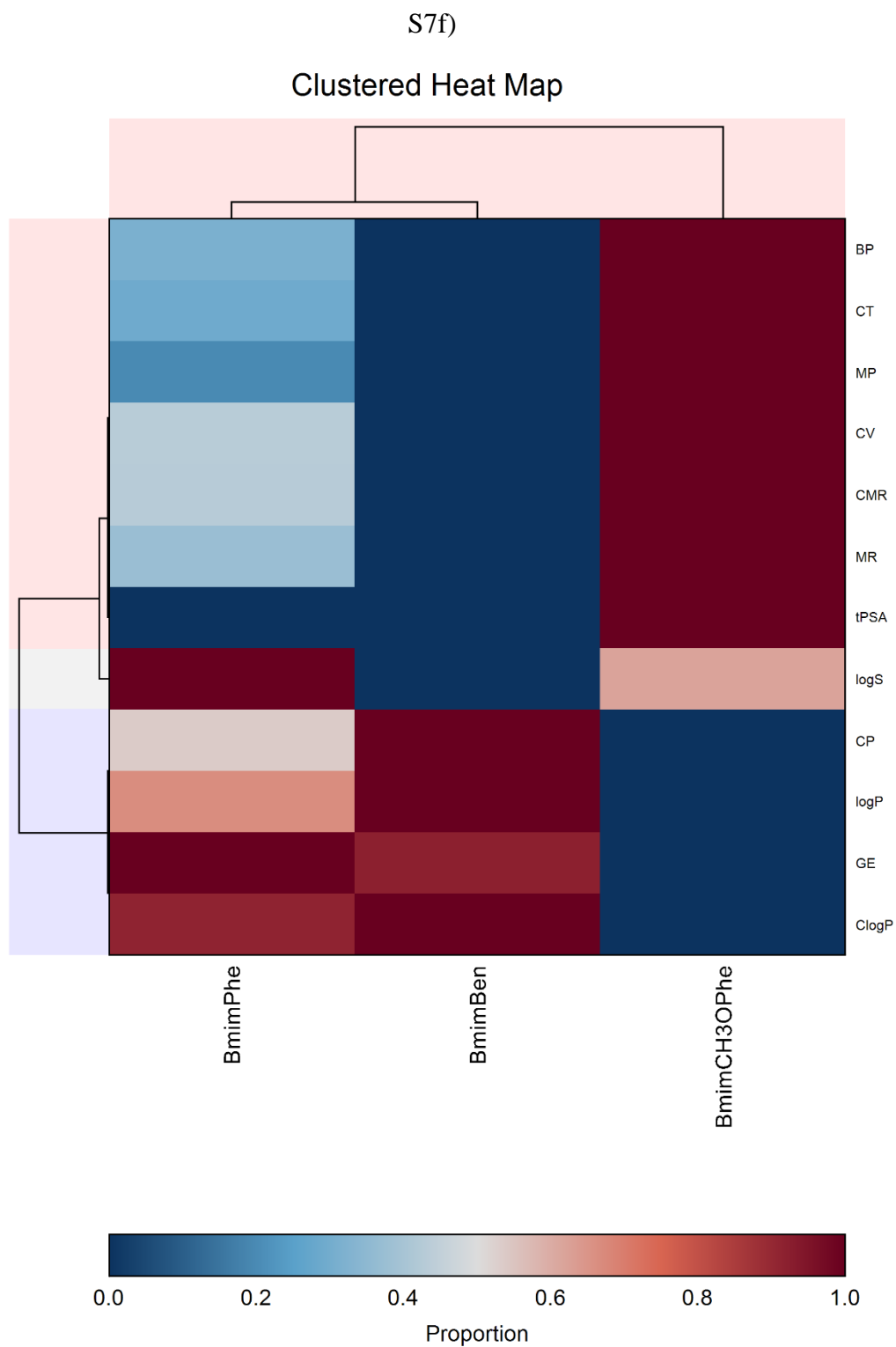
### Clustered Heat Map



6.075

6.150

Data Value

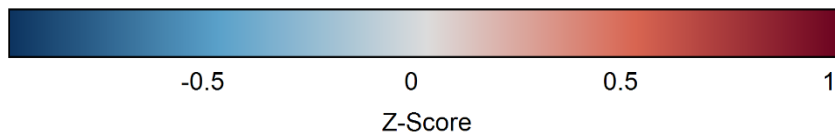
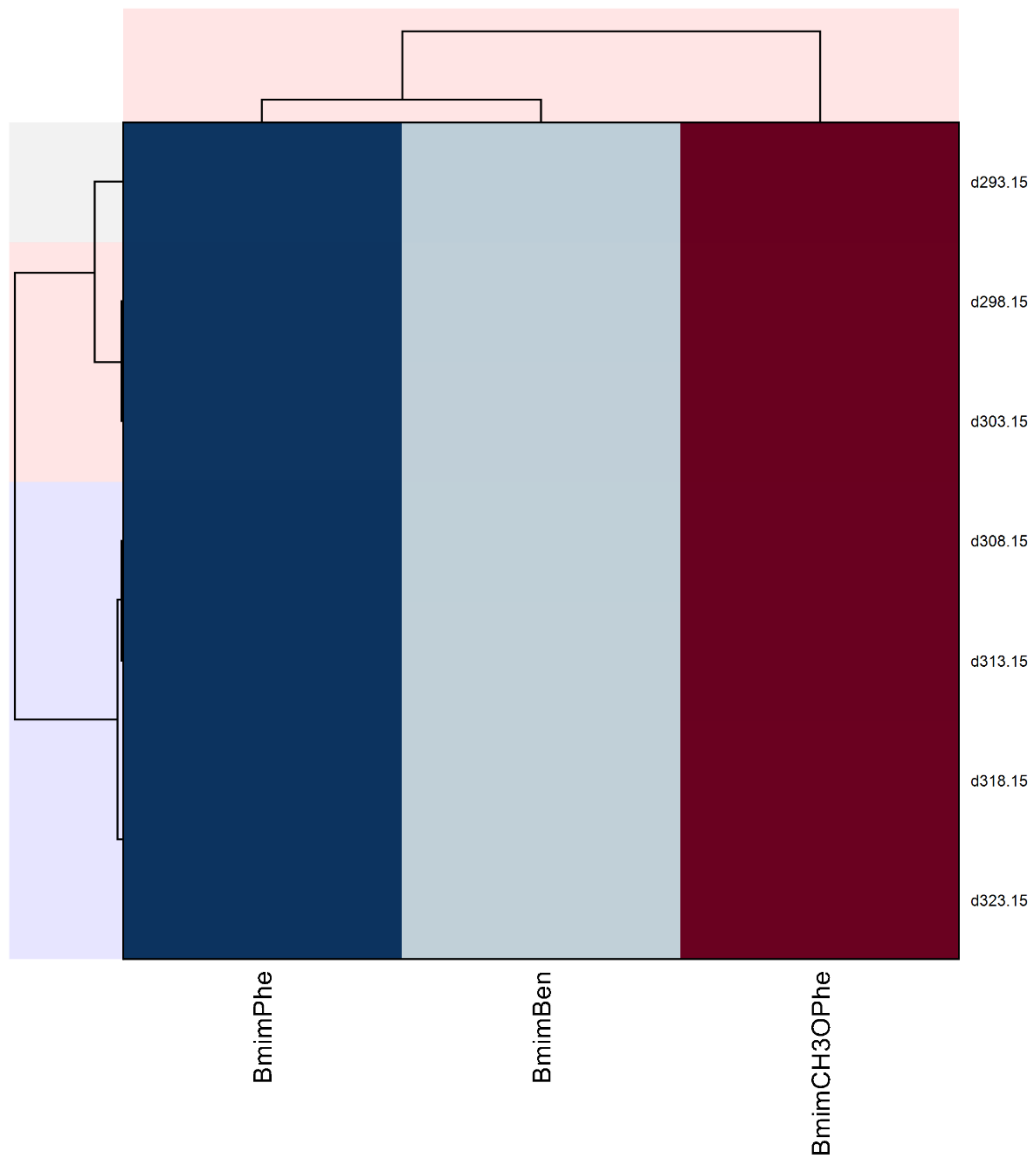


**Figure S7.** The results of HCA of ILs are based on a) density, b) viscosity, c) electrical conductivity, d) molar conductivity, e) thermal expansion coefficient, and f) in silico physicochemical properties.



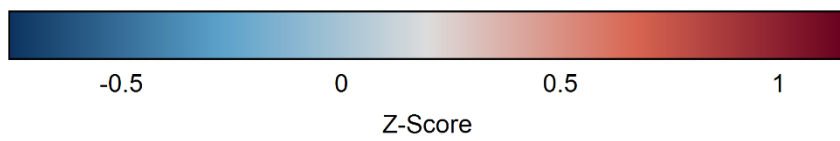
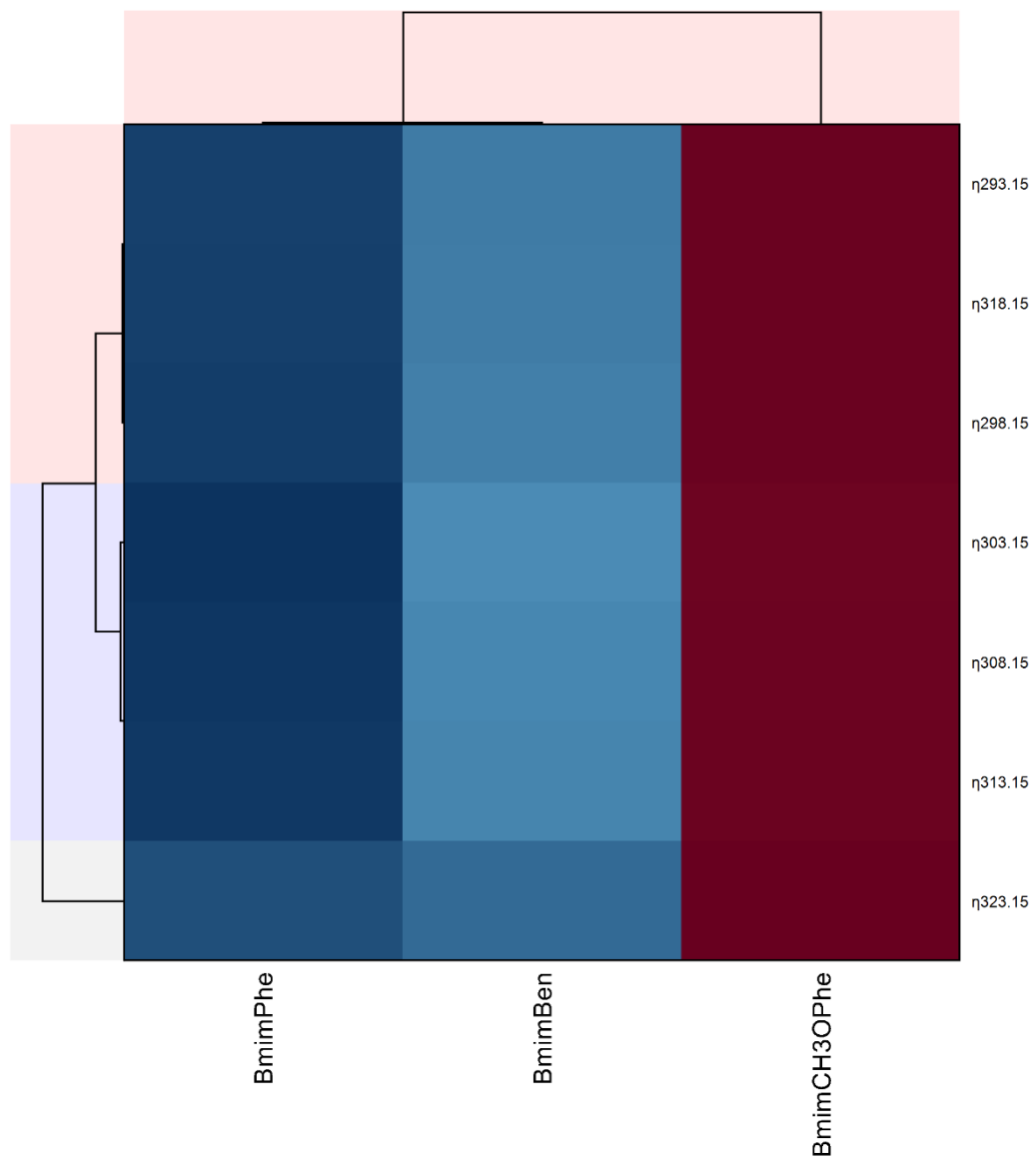
S8a)

Clustered Heat Map



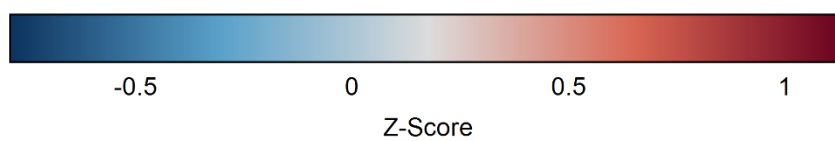
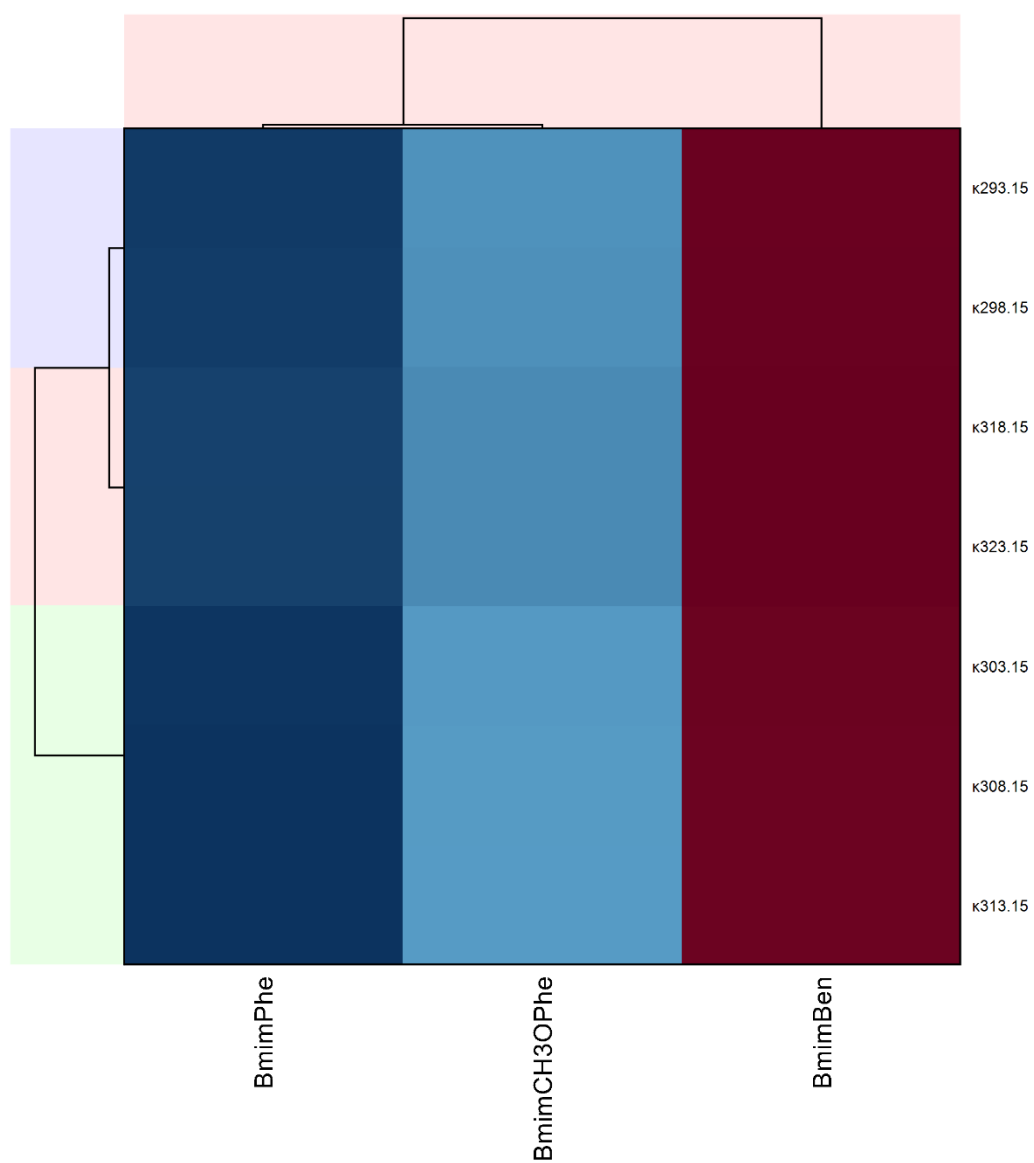
S8b)

Clustered Heat Map



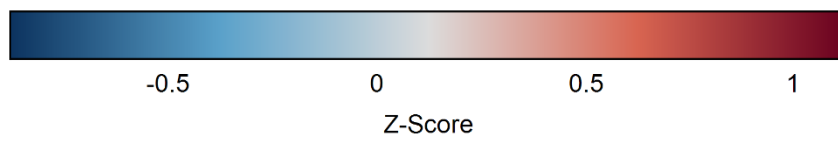
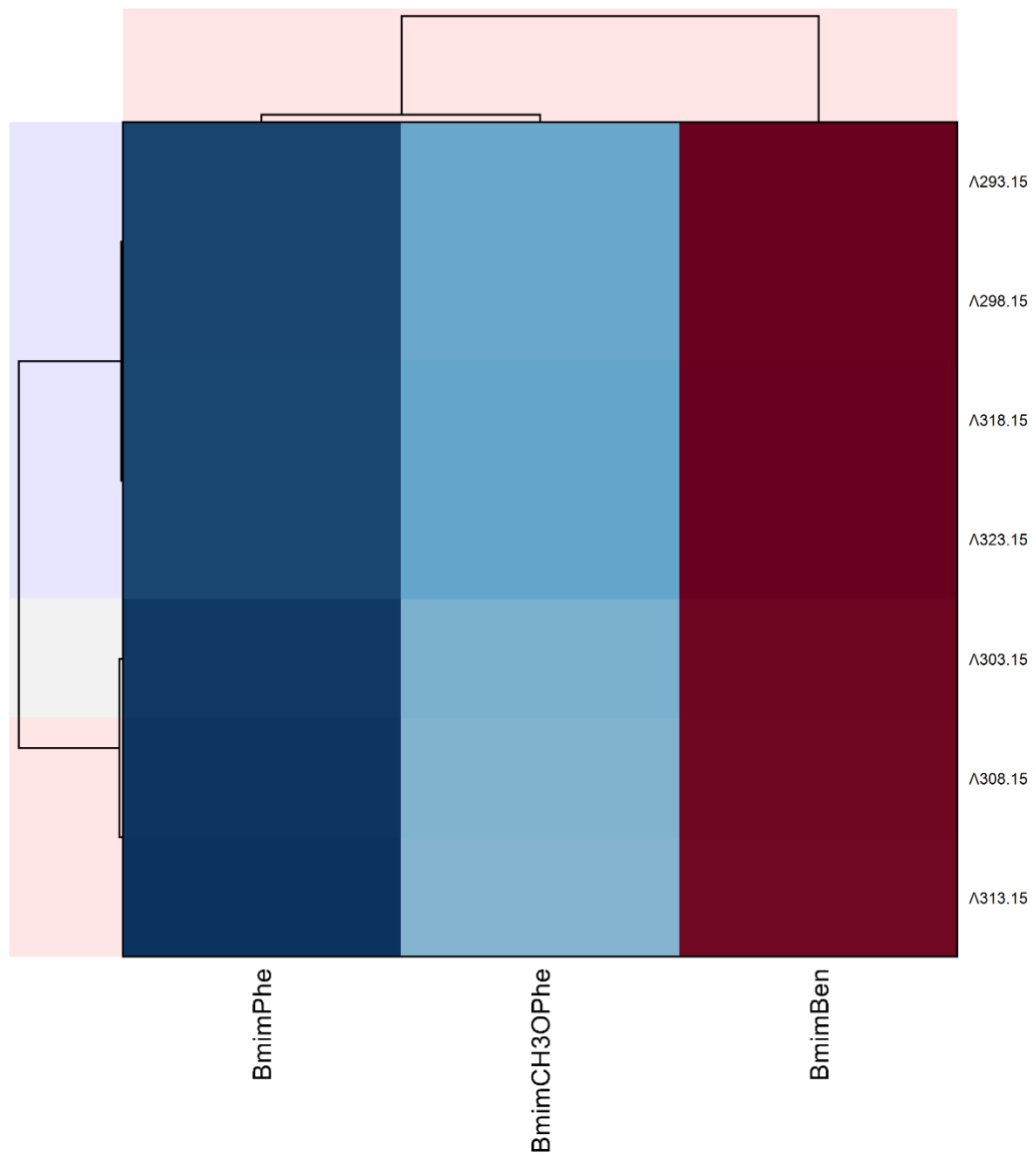
S8c)

Clustered Heat Map



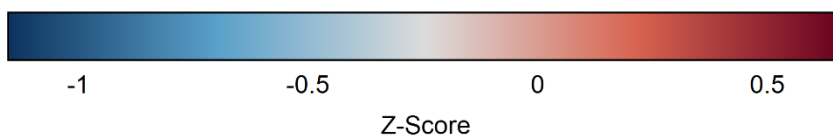
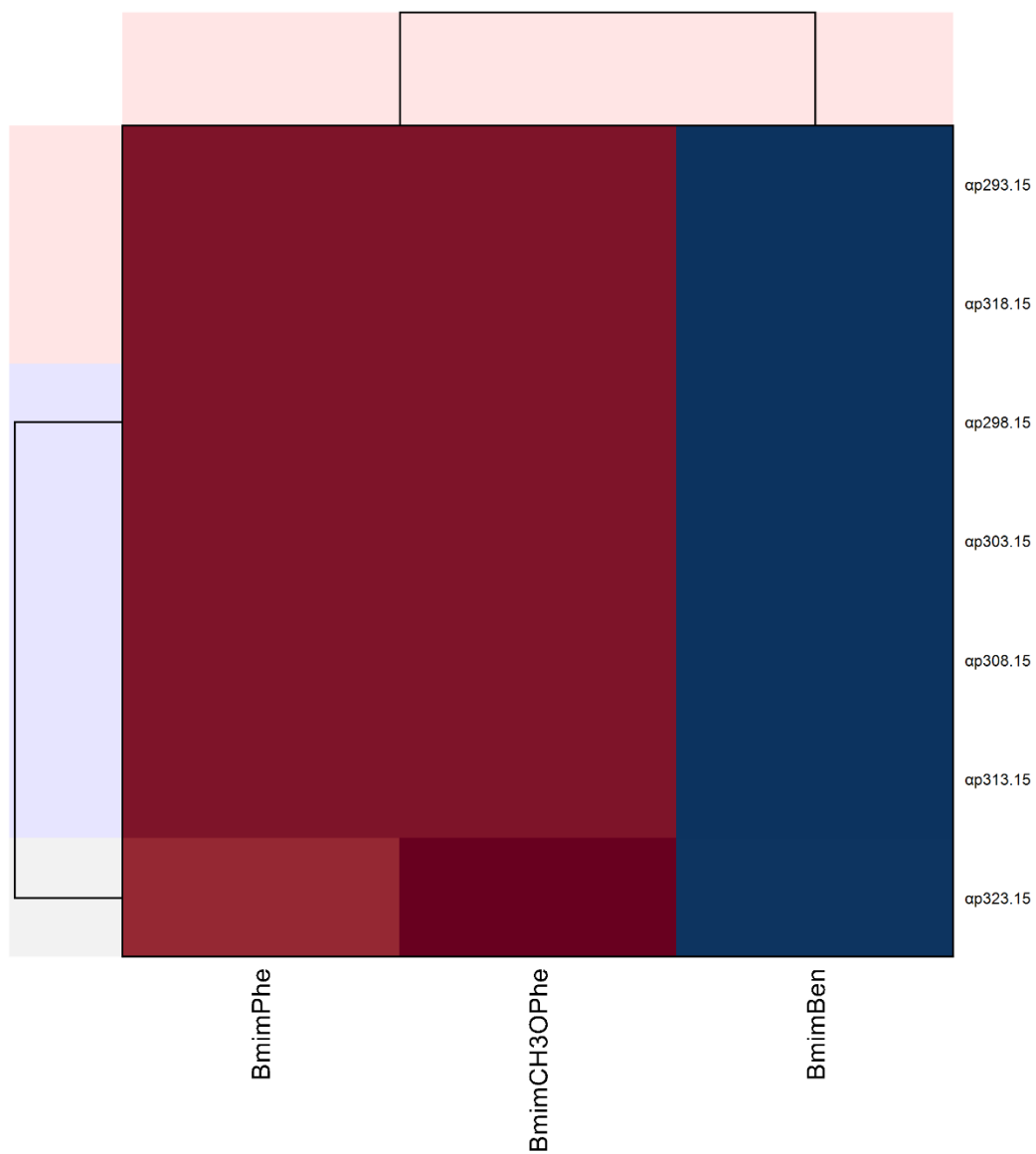
S8d)

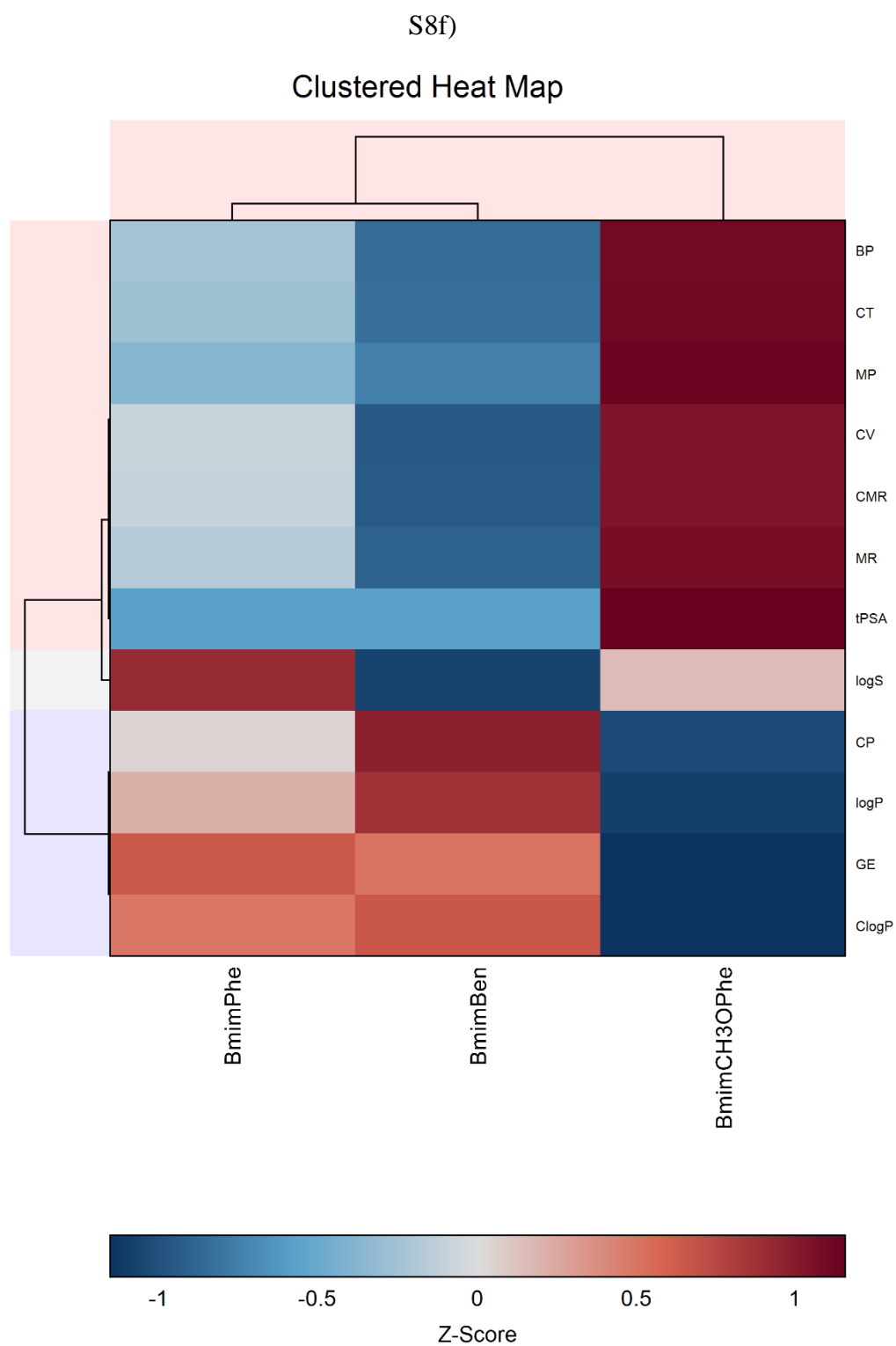
Clustered Heat Map



S8e)

Clustered Heat Map





**Figure S8.** The results of HCA of ILs based on scaled data using Z-scores of a) density, b) viscosity, c) electrical conductivity, d) molar conductivity, e) thermal expansion coefficient, and f) *in silico* physicochemical properties.