Supporting Information

Correlation between lipophilicity of newly synthesized ionic liquids and selected *Fusarium* genus growth rate

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Table S1. Provenance and purity of the chemicals.

| Chemical name         | Provenance          | CAS Number | Purification method | Mass fraction purity |
|----------------------|---------------------|------------|---------------------|----------------------|
| 2-methylpyridine     | Alfa Aesar          | 109-06-8   | -                   | $\omega \geq 0.98$   |
| 3-methylpyridine     | Acros Organics      | 108-99-6   | -                   | $\omega \geq 0.99$   |
| 4-methylpyridine     | Acros Organics      | 108-89-4   | -                   | $\omega \geq 0.99$   |
| 3-chloro-1-propanol  | Aldrich             | 627-30-5   | -                   | $\omega \geq 0.98$   |
| 1-bromobutane        | Sigma Aldrich       | 109-65-9   | -                   | $\omega \geq 0.99$   |
| Toluene              | Sigma Aldrich       | 108-88-3   | -                   | $\omega \geq 0.995$  |
| Ethyl-acetate        | Sigma Aldrich       | 141-78-6   | -                   | $\omega \geq 0.99$   |
| $\text{P}_2\text{O}_5^a$ | Sigma Aldrich     | 1314-56-3  | -                   | $\omega \geq 0.99$   |
| Amberlite IRN 78     | Supelco             | 11128-95-3 | -                   | -                    |
| (RS)-Mandelic acid   | Sigma Aldrich       | 90-64-2    | -                   | $\omega \geq 0.99$   |
| Caffeic acid         | Sigma Aldrich       | 331-39-5   | -                   | $\omega \geq 0.98$   |
| trans-Cinnamic acid  | Sigma Aldrich       | 140-10-3   | -                   | $\omega \geq 0.99$   |

$^a\text{P}_2\text{O}_5$ = phosphorus pentoxide
| Abbreviation     | Name                                         | Structure | Purity<sup>*</sup> |
|------------------|----------------------------------------------|-----------|-------------------|
| [C<sub>4</sub>-2mpyc][Br] | 1-butyl-2-methylpycolinium bromide            | ![Structure](image1.png) | 0.95              |
| [C<sub>4</sub>-3mpyc][Br] | 1-butyl-3-methylpycolinium bromide            | ![Structure](image2.png) | 0.96              |
| [C<sub>4</sub>-4mpyc][Br] | 1-butyl-4-methylpycolinium bromide            | ![Structure](image3.png) | 0.96              |
| [OHC<sub>3</sub>-2mpyc][Cl] | 1-(3-hydroxypropyl)-2-methylpycolinium chloride | ![Structure](image4.png) | 0.97              |
| [OHC<sub>3</sub>-3mpyc][Cl] | 1-(3-hydroxypropyl)-3-methylpycolinium chloride | ![Structure](image5.png) | 0.96              |
| [OHC<sub>3</sub>-4mpyc][Cl] | 1-(3-hydroxypropyl)-4-methylpycolinium chloride | ![Structure](image6.png) | 0.97              |
| [OHC<sub>3</sub>-2mpyc][Cin] | 1-(3-hydroxypropyl)-2-methylpycolinium cinnamate | ![Structure](image7.png) | 0.94              |
| [OHC<sub>3</sub>-3mpyc][Cin] | 1-(3-hydroxypropyl)-3-methylpycolinium cinnamate | ![Structure](image8.png) | 0.95              |
| [OHC<sub>3</sub>-4mpyc][Cin] | 1-(3-hydroxypropyl)-4-methylpycolinium cinnamate | ![Structure](image9.png) | 0.94              |
| [OHC<sub>3</sub>-2mpyc][Man] | 1-(3-hydroxypropyl)-2-methylpycolinium mandelate | ![Structure](image10.png) | 0.96              |
| Formula                  | Structure                                      | pKᵢ  |
|-------------------------|------------------------------------------------|-------|
| [OHC₃⁻₃mpyc][Man]       | ![Structure](image1)                            | 0.95  |
| [OHC₃⁻⁴mpyc][Man]       | ![Structure](image2)                            | 0.93  |
| [OHC₃⁻²mpyc][Caff]      | ![Structure](image3)                            | 0.92  |
| [OHC₃⁻³mpyc][Caff]      | ![Structure](image4)                            | 0.93  |
| [OHC₃⁻⁴mpyc][Caff]      | ![Structure](image5)                            | 0.92  |
| [bmim][Cl]              | ![Structure](image6)                            |       |
| [bmim][Cin]             | ![Structure](image7)                            | 0.96  |
| [bmim][Man]             | ![Structure](image8)                            | 0.97  |
| [bmim][Caff]            | ![Structure](image9)                            | 0.95  |
| [OHC₃mim][Cl]           | ![Structure](image10)                           | 0.98  |
| [OHC₃mim][Cin]          | ![Structure](image11)                           | 0.95  |
| [OHC₃mim][Man]          | ![Structure](image12)                           | 0.96  |
| [OHC₃mim][Caff]         | ![Structure](image13)                           | 0.94  |
*Obtained from NMR spectra
Figure S1. $^1$H and $^{13}$C NMR spectra for synthesized [C$_4$-2mpyc][Br]

$^1$H NMR (D$_2$O): 2.22 (m, 2H, CH$_2$-2'), 2.91 (s, 3H, CH$_3$), 3.75 (t, 3H, CH$_3$), 4.70 (t, 2H, $J_{1',2'} = 7.2$ Hz, CH$_2$-1'), 7.96 (dd, 1H, $J_{5',6'} = 6.1$ Hz, $J_{5,6} = 8.0$ Hz H-5), 8.40 (d, 1H, $J_{4,5} = 8.0$ Hz, H-4), 8.80 (d, 1H, $J_{5,6} = 6.1$ Hz, H-6)

$^{13}$C NMR (D$_2$O): 22.41 (CH$_3$), 34.13 (CH$_2$-2'), 58.42 (CH$_3$), 60.77 (CH$_2$-1'), 128.53 (C-5); 133.12 (C-3); 144.62 (C-6); 147.81 (C-2); 149.41 (C-4)
Figure S2. IR spectra of [C₄-2mpic][Br]

3020 (CH ring sym. stretching), 2958 (asym. stretching CH₃), 2933 and 2873 (sym. stretching CH₃), 1574 (aromatic C-C stretching), 1485 (rocking CH₃), 1167 (wagging CH₂), 797 (out of plane bending vibrations of ring)
Figure S3. MS spectra of [C₄-2mpyc][Br]
Figure S4. $^1$H and $^{13}$C NMR spectra for synthesized [C$_4$-3mpyc][Br]

$^1$H NMR (D$_2$O): 2.27 (m, 2H, $CH_2$-2'), 2.58 (s, 3H, $CH_3$), 3.70 (t, 3H, $CH_3$), 4.71 (t, 2H, $J_{1',2'} = 7.2$ Hz, $CH_2$-1'), 7.98 (dd, 1H, $J_{5',6'} = 6.1$ Hz, $J_{5,6} = 8.0$ Hz H-5), 8.40 (d, 1H, $J_{4,5} = 8.0$ Hz, H-4), 8.71 (d, 1H, $J_{5,6} = 6.1$ Hz, H-6), 8.77 (s, 1H, H-2)
$^{13}$C NMR (D$_2$O): 20.57 (CH$_3$), 35.55 (CH$_2$-2'), 60.63 (CH$_3$), 61.67 (CH$_2$-1'), 130.35 (C-5), 142.84 (C-3), 144.40 (C-6), 146.82 (C-2), 149.01 (C-4)

![Figure S5: IR spectra of [C$_4$-3mpic][Br]](image)

3010 (CH ring sym. stretching), 2957 (asym. stretching CH$_3$), 2931 and 2871 (sym. stretching CH$_3$), 1584 (aromatic C-C stretching), 1503 (rocking CH$_3$), 1154 (wagging CH$_2$), 808 (out of plane bending vibrations of ring)
Figure S6. MS spectra of [C₄-3mpyc][Br]
Figure S7. $^1$H and $^{13}$C NMR spectra for synthesized [C$_4$-4mpic][Br]

$^1$H NMR (D$_2$O): 2.25 ($m$, 2H, CH$_2$-2'), 2.67 ($s$, 3H, CH$_3$), 3.68 ($t$, 3H, CH$_3$), 4.67 ($t$, 2H, J$_{1',2'}$ = 7.3 Hz, CH$_2$-1'), 7.91 (d, 1H, $J = 6.3$ Hz, H-3 and H-5), 8.69 (d, 1H, $J = 6.3$ Hz, H-2 and H-6)
$^{13}$C NMR (D$_2$O): 24.20 (CH$_3$), 35.42 (CH$_2$-2'), 60.62 (CH$_3$), 60.95 (CH$_2$-1'), 131.55 (C3 and C-5), 146.14 (C-2 and C-6), 163.00 (C-4)

**Figure S8.** IR spectra of [C$_4$-4mpic][Br]

3018 (CH ring sym. stretching), 2961 (asym. stretching CH$_3$), 2935 and 2873 (sym. stretching CH$_3$), 1564 (aromatic C-C stretching), 1472 (rocking CH$_3$), 1174 (wagging CH$_2$), 833 (out of plane bending vibrations of ring)
Figure S9. MS spectra of [C₄-4mpyc][Br]
Figure S10. \(^1\)H and \(^{13}\)C NMR spectra for synthesized [OHC\(_3\)-2mpyc][Cl]

\(^1\)H NMR (D\(_2\)O): 2.22 (m, 2H, CH\(_2\)-2'), 2.91 (s, 3H, CH\(_3\)), 3.75 (t, 2H, \(J\_2,3\'\) = 6.0 Hz, CH\(_2\)OH), 4.70 (t, 2H, \(J\_1,2\) = 7.2 Hz, CH\(_2\)-1'), 7.96 (dd, 1H, \(J\_5,6\) = 8.0 Hz \(H-5\)), 8.40 (d, 1H, \(J\_4,5\) = 8.0 Hz, H-4), 8.80 (d, 1H, \(J\_5,6\) = 6.1 Hz, H-6)
$^{13}$C NMR (D$_2$O): 22.41 (CH$_3$), 34.13 (CH$_2$-2'), 58.42 (HOCH$_2$), 60.77 (CH$_2$-1'), 128.53 (C-5); 133.12 (C-3); 144.62 (C-6); 147.81 (C-2); 149.41 (C-4)

Figure S11. IR spectra of [OHC$_3$-2mpyc][Cl]

3265 (OH stretching); 3037 (CH sym. stretching); 2848 (sym. vibrations of CO-H); 1630 (OH bending); 1577 (aromatic C-C stretching); 1481 (rocking CH$_3$); 1301 and 1239 and 1239 (C$_{aromatic}$ - C$_{alifatic}$ or C-CH$_3$ stretching vibrations); 1167 and 1282 (wagging CH$_2$ (hydroxypropile)); 1063 (skeletal vibrations of the ring); 928 (out-of-plane bending vibrations CH (ring)).
Figure S12. MS spectra of [OHC₃-2mpyc][Cl]
**Figure S13.** $^1$H and $^{13}$C NMR spectra for synthesized [OHC$_3$-3mpyc][Cl]

$^1$H NMR (D$_2$O): 2.27 (m, 2H, $CH_2{}^2$-2'), 2.58 (s, 3H, $CH_3{}$), 3.70 (t, 2H, $J_{1',2'} = 6.0$ Hz, $CH_2{}$OH), 4.71 (t, 2H, $J_{1,2} = 7.2$ Hz, $CH_2{}$-1'), 7.98 (dd, 1H, $J_{5',6'} = 6.1$ Hz, $J_{5,6} = 8.0$ Hz H-5), 8.40 (d, 1H, $J_{4,5} = 8.0$ Hz, H-4), 8.71 (d, 1H, $J_{5,6} = 6.1$ Hz, H-6), 8.77 (s, 1H, H-2)
$^{13}$C NMR (D$_2$O): 20.57 (CH$_3$), 35.55 (CH$_2$-2'), 60.63 (HOCH$_2$), 61.67 (CH$_2$-1'), 130.35 (C-5), 142.84 (C-3), 144.40 (C-6), 146.82 (C-2), 149.01 (C-4)

Figure S14. FTIR spectra of [OHC$_3$-3mpyc][Cl]

3032 (CH sym. stretching); 2849 (sym. vibrations of CO-H); 2941 (sym. and asym. vibrations of CH$_3$ group); 1633 (OH bending); 1590 (aromatic C-C stretching); 1482 (rocking CH$_3$); 1320 and 1249 (C$_{aromatic}$-C$_{alifatic}$ or C-CH$_3$ stretching vibrations); 1152 and 1282 (wagging CH$_2$ (hydroxypropile)); 1053 (skeletal vibrations of the ring); 827 (out-of-plane bending vibrations CH (ring)).
Figure S15. MS spectra of [OHC₃₃mpyc][Cl]
Figure S16. $^1$H and $^{13}$C NMR spectra for synthesized [OHC$_3$-4mpyc][Cl]

$^1$H NMR (D$_2$O): 2.25 (m, 2H, CH$_2$-2'), 2.67 (s, 3H, CH$_3$), 3.68 (t, 2H, $J_{2',3'} = 6.1$ Hz, CH$_2$OH), 4.67 (t, 2H, $J_{1',2'} = 7.3$ Hz, CH$_2$-1'), 7.91 (d, 1H, $J = 6.3$ Hz, H-3 and H-5), 8.69 (d, 1H, $J = 6.3$ Hz, H-2 and H-6)
\[^{13}\text{C} \text{NMR} \ (\text{D}_2\text{O}): 24.20 \ (\text{CH}_3), \ 35.42 \ (\text{CH}_2-2'), \ 60.62 \ (\text{HOCH}_2), \ 60.95 \ (\text{CH}_2-1'), \ 131.55 \ (\text{C}3 \text{ and C-5)}, \ 146.14 \ (\text{C}-2 \text{ and C-6)}, \ 163.00 \ (\text{C}-4)\]

![Figure S17. FTIR spectra of [OHC\textsubscript{3}-4mpyc][Cl]](image_url)

3012 (CH sym. stretching); 2941 (sym. vibrations of CO-H); 1633 (OH bending); 1571 (aromatic C-C stretching); 1473 (rocking CH\textsubscript{3}); 1312 and 1238 (C\textsubscript{aromatic}-C\textsubscript{aliphatic} or C\textsubscript{CH\textsubscript{3}} stretching vibrations); 1171 and 1282 (wagging CH\textsubscript{2} (hydroxypropyle)); 1049 (skeletal vibrations of the ring); 827 (out-of-plane bending vibrations CH (ring)).
Figure S18. MS spectra of [OHC$_3$-4mpyc][Cl]
Figure S19. $^1$H and $^{13}$C NMR spectra for synthesized [OHC$_3$-2mpyc][Cin]

$^1$H NMR (D$_2$O): 2.22 (m, 2H, CH$_2$-2'), 2.94 (s, 3H, CH$_3$), 3.78 (t, 2H, J$_{2,3'}$ = 6.0 Hz, CH$_2$OH), 4.70 (t, 2H, J$_{1,2}$ = 7.2 Hz, CH$_2$-1'), 7.14, 7.21 and 7.26 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.96 (dd, 1H, J$_{5,6}$ = 6.1 Hz, J$_{5,6}$ = 8.0 Hz, H-5), 8.44 (d, 1H, J$_{4,5}$ = 8.0 Hz, H-4), 8.92 (d, 1H, J$_{5,6}$ = 6.1 Hz, H-6)

$^{13}$C NMR (D$_2$O): 22.41 (CH$_3$), 34.13 (CH$_2$-2'), 59.42 (HOCH$_2$), 61.77 (CH$_2$-1'), 129.63 (C-5); 133.12 (C-3); 135.24 (C-6); 135.99 (C-7), 136.81 (C-8); 144.62 (C-6); 147.51 (C-2); 148.93 (C-4); 150.66 (C-9) and 179.01 (COO)
Figure S20. FTIR spectra of [OHC$_3$-2mpic] [Cin]

3215 (stretching OH), 1635 (skeletal vibration of cinnamate ring); 1556 (C-C in plane bending, cinnamate anion); 1429 and 1365 (C-N stretching); 1173 and 1059 (C=O stretching); 981 (CH wagging); 881 (in plane bending CC); 775 (C-O wagging)
Figure S21. MS spectra of [OHC$_3$-2mpyc][Cin]
Figure S22. $^1$H and $^{13}$C NMR spectra for synthesized [OHC$_3$-3mpyc][Cin]

$^1$H NMR (D$_2$O): 2.33 (m, 2H, CH$_2$-2'), 2.63 (s, 3H, CH$_3$), 3.70 (t, 2H, $J_{2',3'}$ = 6.0 Hz, CH$_2$OH), 4.71 (t, 2H, $J_{1',2'}$ = 7.2 Hz, CH$_2$-1'), 7.21, 7.26 and 7.32 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.98 (dd, 1H, $J_{5',6'}$ = 6.1 Hz, $J_{5,6}$ = 8.0 Hz H-5), 8.42 (d, 1H, $J_{4.5}$ = 8.0 Hz, H-4), 8.83 (d, 1H, $J_{5,6}$ = 6.1 Hz, H-6), 8.91 (s, 1H, H-2)
$^{13}$C NMR (D$_2$O): 21.63 (CH$_3$), 35.78 (CH$_2$-2'), 60.71 (HOCH$_2$), 61.67 (CH$_2$-1'), 131.35 (C-5), 135.11 (C-6); 135.62 (C-7), 136.24 (C-8); 144.84 (C-3), 147.40 (C-6), 148.82 (C-2), 149.51 (C-4); 150.23 (C-9) and 178.96 (COO$^-$)

Figure S23. FTIR spectra of [OHC$_3$-3mpic] [Cin]

3172 (stretching OH), 1619 (skeletal vibration of cinnamate ring); 1531 (C-C in plane bending, cinnamate anion); 1419 and 1355 (C-N stretching); 1173 and 1056 (C=O stretching); 978 (CH wagging); 876 (in plane bending CC); 732 (C-O wagging)
Figure S24. MS spectra of [OHC$_3$-3mpyc][Cin]
Figure S25. $^1$H and $^{13}$C NMR spectra for synthesized [OHC$_3$-4mpyc][Cin]

$^1$H NMR (D$_2$O): 2.25 ($m$, 2H, CH$_2$-2'), 2.67 ($s$, 3H, CH$_3$), 3.68 ($t$, 2H, $J_{2,3}$ = 6.1 Hz, CH$_2$OH), 4.67 ($t$, 2H, $J_{1,2}$ = 7.3 Hz, CH$_2$-1'), 7.08, 7.14 and 7.21 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.91 ($d$, 1H, $J$ = 6.3 Hz, H-3 and H-5), 8.69 ($d$, 1H, $J$ = 6.3 Hz, H-2 and H-6)

$^{13}$C NMR (D$_2$O): 24.20 (CH$_3$), 35.42 (CH$_2$-2'), 60.62 (HOCH$_2$), 60.95 (CH$_2$-1'), 131.55 (C3 and C-5), 135.81 (C-6); 136.47 (C-7), 137.22 (C-8); 146.14 (C-2 and C-6), 163.00 (C-4); 165.21 (C-9) and 183.22 (COO-)

Figure S25. $^1$H and $^{13}$C NMR spectra for synthesized [OHC$_3$-4mpyc][Cin]

$^1$H NMR (D$_2$O): 2.25 ($m$, 2H, CH$_2$-2'), 2.67 ($s$, 3H, CH$_3$), 3.68 ($t$, 2H, $J_{2,3}$ = 6.1 Hz, CH$_2$OH), 4.67 ($t$, 2H, $J_{1,2}$ = 7.3 Hz, CH$_2$-1'), 7.08, 7.14 and 7.21 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.91 ($d$, 1H, $J$ = 6.3 Hz, H-3 and H-5), 8.69 ($d$, 1H, $J$ = 6.3 Hz, H-2 and H-6)

$^{13}$C NMR (D$_2$O): 24.20 (CH$_3$), 35.42 (CH$_2$-2'), 60.62 (HOCH$_2$), 60.95 (CH$_2$-1'), 131.55 (C3 and C-5), 135.81 (C-6); 136.47 (C-7), 137.22 (C-8); 146.14 (C-2 and C-6), 163.00 (C-4); 165.21 (C-9) and 183.22 (COO-)
Figure S26. FTIR spectra of [OHC$_3$-4mpyc] [Cin]

3151 (stretching OH), 1623 (sceletal vibration of cinnamate ring); 1518 (C=C in plane bending, cinnamate anion); 1422 and 1359 (C-N stretching); 1173 and 1056 (C=O stretching); 976 (CH wagging); 877 (in plane bending CC); 731 (C-O wagging)
Figure S27. MS spectra of [OHC$_3$-4mpyc][Cin]
Figure S28. $^1$H and $^{13}$C NMR spectra for [OHC$_3$-2mpyc][Man]

$^1$H NMR (D$_2$O): 2.18 ($m$, 2H, CH$_2$-2'), 2.90 ($s$, 3H, CH$_3$), 3.75 ($t$, 2H, $J_{2',3'} = 6.0$ Hz, CH$_2$OH), 4.70 ($t$, 2H, $J_{1',2'} = 7.2$ Hz, CH$_2$-1'), 5.13 (C-OH); 7.18, 7.22 and 7.26 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.96 (dd, 1H, $J_{5',6'} = 6.1$ Hz, $J_{5,6} = 8.0$ Hz H-5), 8.40 ($d$, 1H, $J_{4,5} = 8.0$ Hz, H-4), 8.80 ($d$, 1H, $J_{5,6} = 6.1$ Hz, H-6)

$^{13}$C NMR (D$_2$O): 22.41 (CH$_3$), 34.13 (CH$_2$-2'), 58.42 (HOCH$_2$), 60.77 (CH$_2$-1'), 77.63 (C-OH); 128.53 (C-5); 133.12 (C-3); 135.24 (C-6); 135.99 (C-7), 136.81 (C-8); 144.62 (C-6); 147.81 (C-2); 149.41 (C-4); 150.66 (C-9) and 179.22 (COO$^-$)
Figure S29. FTIR spectra of [OHC$_3$-2mpic] [Man]

3268 (OH stretching), 3037 (CH sym. stretching), 2848 (sym. vibrations CO-H), 1605 (ring deformation mandelate), 1514 (C-C in plane bending, mandelate anion), 1485 (rocking CH$_3$), 1452 and 1353 (C-N stretching), 1172 and 1053 (C=O stretching), 931 (CH wagging), 734 (C-O wagging)
Figure S30. MS spectra of \([\text{OHC}_3\text{-2mpyc}][\text{Man}]\)
**Figure S31.** $^1$H and $^{13}$C NMR spectra for [OHC$_3$-3mpyc][Man]

$^1$H NMR (D$_2$O): 2.27 (m, 2H, CH$_2$-2'), 2.58 (s, 3H, CH$_3$), 3.70 (t, 2H, $J_{2',3'} = 6.0$ Hz, CH$_2$OH), 4.71 (t, 2H, $J_{1',2'} = 7.2$ Hz, CH$_2$-1'), 5.23 (C-OH); 7.21, 7.26 and 7.32 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.98 (dd, 1H, $J_{5',6'} = 6.1$ Hz, $J_{5,6} = 8.0$ Hz H-5), 8.40 (d, 1H, $J_{4,5} = 8.0$ Hz, H-4), 8.71 (d, 1H, $J_{5,6} = 6.1$ Hz, H-6), 8.77 (s, 1H, H-2)
Figure S32. FTIR spectra of [OHC$_3$-3mpyc][Man]

3266 (OH stretching), 3037 (CH sym. stretching), 2846 (sym. vibrations of CO-H), 1604 (ring deformation mandelate), 1505 (C-C in plane bending, mandelate anion), 1353 (C-N stretching), 1181 and 1052 (C=O stretching), 930 (CH wagging), 736 (C-O wagging)
Figure S33. MS spectra of [OHC₃-3mpyc][Man]
Figure S34. $^1$H and $^{13}$C NMR spectra for [OHC$_3$-4mpyc][Man]

$^1$H NMR (D$_2$O): 2.25 ($m$, 2H, CH$_2$-2'), 2.67 ($s$, 3H, CH$_3$), 3.68 ($t$, 2H, $J_{2',3'}$ = 6.1 Hz, CH$_2$OH), 4.67 ($t$, 2H, $J$ = 7.3 Hz, CH$_2$-1'), 5.11 (C-OH); 7.08, 7.14 and 7.21 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.91 ($d$, 1H, $J$ = 6.3 Hz, H-3 and H-5), 8.69 ($d$, 1H, $J$ = 6.3 Hz, H-2 and H-6)

$^{13}$C NMR (D$_2$O): 24.20 (CH$_3$), 35.42 (CH$_2$-2'), 60.62 (HOCH$_2$), 60.95 (CH$_2$-1'), 76.91 (C-OH); 131.55 (C3 and C-5), 135.81 (C-6); 136.47 (C-7), 137.22 (C-8); 146.14 (C-2 and C-6), 163.00 (C-4); 165.21 (C-9) and 183.22 (COO$^-$)
Figure S35. FTIR spectra of [OHC_{3-4mpic}][Man]

3268 (OH stretching), 2840 (sym. vibrations of CO-H), 1597 (aromatic C-C stretching), 1518 (C-C in plane bending, mandelate anion), 1473 and 1354 (C-N stretching), 1191 and 1053 (C-O stretching), 932 (CH wagging), 826 (out of plane bending vibrations CH (ring)), 736 (C-O wagging)
Figure S36. MS spectra of [OHC₃-4mpyc][Man]
Figure S37. $^1$H and $^{13}$C NMR spectra for [OHC$_3$-2mpyc][Caff]

$^1$H NMR (D$_2$O): 2.24 (m, 2H, CH$_2$-2'), 2.94 (s, 3H, CH$_3$), 3.81 (t, 2H, $J_{2',3'} = 6.0$ Hz, CH$_2$OH), 4.70 (t, 2H, $J_{1',2'} = 7.2$ Hz, CH$_2$-1'), 5.29 (s, 2H, C-OH); 7.19, 7.25 and 7.31 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 8.21 (dd, 1H, $J_{5',6} = 6.1$ Hz, $J_{5,6} = 8.0$ Hz H-5), 8.59 (d, 1H, $J_{4,5} = 8.0$ Hz, H-4), 8.92 (d, 1H, $J_{5,6} = 6.1$ Hz, H-6)
Figure S38. FTIR spectra of [OHC$_3$-2mpyc][Caff]

3211 (stretching OH), 1469 (sceletal vibration of caffete ring), 1404 and 1319 (C-N stretching), 1222 and 1196 (stretching OH group); 1141 and 1069 (C-O stretching); 966 (CH wagging); 707 (C-O wagging)
Figure S39. MS spectra of [OHC$_3$-2mpyc][Caff]
Figure S40. $^1$H and $^{13}$C NMR spectra for [OHC$_3$-3mpyc][Caff]

$^1$H NMR (D$_2$O): 2.28 ($m$, 2H, CH$_2$-2), 2.62 (s, 3H, CH$_3$), 3.74 ($t$, 2H, $J_{2,3'} = 6.0$ Hz, CH$_2$OH), 4.71 ($t$, 2H, $J_{1,2'} = 7.2$ Hz, CH$_2$-1'), 5.49 (d, 2H, C-OH); 7.25, 7.29 and 7.32 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 8.03 (dd, 1H, $J_{5,6} = 6.1$ Hz, $J_{5,6} = 8.0$ Hz H-5), 8.49 (d, 1H, $J_{4,5} = 8.0$ Hz, H-4), 8.71 (d, 1H, $J_{5,6} = 6.1$ Hz, H-6), 8.82 (s, 1H, H-2)

$^{13}$C NMR (D$_2$O): 20.54 (CH$_3$), 35.51 (CH$_2$-2), 60.84 (HOCH$_2$), 61.73 (CH$_2$-1'), 76.99 (C-OH); 130.35 (C-5), 135.94 (C-6); 136.62 (C-7), 137.24 (C-8); 143.96 (C-3), 144.51 (C-6), 146.82 (C-2), 149.01 (C-4); 153.23 (C-9) and 179.22 (COO$^-$)
Figure S41. FTIR spectra of [OHC$_3$-3mpyc][Caff]

3202 (stretching OH), 1461 (sceletal vibration of caffeate ring), 1402 and 1322 (C-N stretching), 1201 and 1176 (stretching OH group); 1133 and 1052 (C-O stretching); 969 (CH wagging); 712 (C-O wagging)
**Figure S42.** MS spectra of [OHC$_3$-3mpyc][Caff]

| m/z  | Absolute Intensity | Relative Intensity |
|------|--------------------|--------------------|
| 104.10 | 2000000            | 100.00             |
| 105.15 | 6103809            | 30.52              |
| 137.05 | 2589522            | 12.95              |
| 148.10 | 19879035           | 99.40              |
| 149.20 | 2150284            | 10.75              |
| 152.05 | 19374720           | 96.87              |
| 153.10 | 20000000           | 100.00             |
| 154.15 | 3125046            | 15.63              |
| 159.00 | 1792430            | 8.96               |
| 192.15 | 2659051            | 13.30              |
Figure S43. $^1$H and $^{13}$C NMR spectra for [OHC$_3$-4mpyc][Caff]

$^1$H NMR (D$_2$O): 2.20 (m, 2H, CH$_2$-2'), 2.69 (s, 3H, CH$_3$), 3.74 (t, 2H, $J_{2,3'}$ = 6.1 Hz, CH$_2$OH), 4.67 (t, 2H, $J_{1,2'}$ = 7.3 Hz, CH$_2$-1'), 5.49 (d, 2H, C=OH); 7.18, 7.24 and 7.33 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.91 (d, 1H, $J$ = 6.3 Hz, H-3 and H-5), 8.71 (d, 1H, $J$ = 6.3 Hz, H-2 and H-6).

$^{13}$C NMR (D$_2$O): 24.20 (CH$_3$), 35.96 (CH$_2$-2'), 61.62 (HOCH$_2$), 61.95 (CH$_2$-1'), 76.91 (C-OH); 131.55 (C3 and C-5), 135.94 (C-6); 136.65 (C-7), 137.22 (C-8); 146.14 (C-2 and C-6), 162.41 (C-4); 166.21 (C-9) and 181.02 (COO$^-$)
Figure S44. FTIR spectra of [OHC₃₋₄mpyc][Caff]

3154 (stretching OH), 1482 (skeletal vibration of caffeate ring), 1398 and 1301 (C-N stretching), 1194 and 1155 (stretching OH group); 1102 and 1051 (C-O stretching); 971 (CH wagging); 710 (C-O wagging)
**Figure S45.** MS spectra of [OHC$_3$-4mpyc][Caff]
Figure S46. $^1$H and $^{13}$C NMR spectra for [bmim][Cin]

$^1$H NMR (D$_2$O): 2.31 ($m$. 2H. NCH$_2$CH$_2$CH$_2$: 3.86 ($t$. 2H. J=6.1 Hz. NCH$_2$CH$_2$CH$_2$: 3.96 (s. 3H. CH$_3$); 4.31 ($t$. 2H. J=7.1 Hz. NCH$_2$CH$_2$CH$_2$: 7.31, 7.38 and 7.41 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.61 and 7.67 (2xs. 2H. H-4 and H-5); 8.97 (s. 1H. H-2).

$^{13}$C NMR (D$_2$O): 31.44 (NCH$_2$CH$_2$CH$_2$: 35.94 (CH$_3$); 46.79 (NCH$_2$CH$_2$CH$_2$: 57.86 (NCH$_2$CH$_2$CH$_2$: 124.34 i 125.65 (C-4 i C-5); 129.65 (C-6); 130.21 (C-7), 130.86 (C-8); 135.11 (d. C-2); 141.73 (C-9) and 174.05 (COO$^-$)
Figure S47. FTIR spectra of [bmim][Cin]

3216 (N-H streching); 2949 (asym. stretching CH₃), 2871 (sym. stretching CH₃), 1506 (in plane vibrations of imidazolium ring), 1491(sceletal vibration of cinnamate), 1447 and 1362 (C-N stretching), 1218 (stretching OH group); 1161 and 1068 (C-O stretching); 959 (CH wagging); 771 (C-O wagging)
**Figure S48.** MS spectra of [bmim][Cin]
Figure S49. $^1$H and $^{13}$C NMR spectra for [bmim][Man]

$^1$H NMR (D$_2$O): $^1$H NMR (D$_2$O): 2.11 (m. 2H. NCH$_2$CH$_2$CH$_3$); 3.67 (t. 2H. J=6.1 Hz. NCH$_2$CH$_2$H$_2$CH$_3$); 3.96 (s. 3H. CH$_3$); 4.34 (t. 2H. J=7.1 Hz. NCH$_2$CH$_2$CH$_2$CH$_3$); 5.26 (NCH$_2$CH$_2$CH$_2$CH$_3$); 7.29, 7.38 and 7.41 (2xs. 5H. H-6, H-7, H-8, H-9, H-10); 7.51 and 7.52 (2xs. 2H. H-4 and H-5); 8.91 (s. 1H. H-2).

$^{13}$C NMR (D$_2$O): 31.22 (NCH$_2$CH$_2$CH$_2$CH$_3$); 35.81 (CH$_3$); 46.79 (NCH$_2$CH$_2$CH$_2$ CH$_3$); 57.93 (NCH$_2$CH$_2$CH$_2$CH$_3$); 77.44 (NCH$_2$CH$_2$CH$_2$CH$_3$); 122.34 i 123.65 (C-4 i C-5); 129.05 (C-6); 130.21 (C-7), 130.56 (C-8); 136.02 (d. C-2); 142.73 (C-9) and 176.01 (COO$^-$)
Figure S50. FTIR spectra of [bmim][Man]

3189 (N-H stretching); 2965 (asym. stretching CH₃), 2877 (sym. stretching CH₃), 1609 (ring deformation mandelate), 1577 (in plane vibration imidazolium ring), 1444 and 1351 (C-N stretching); 1169 and 1036 (C-O stretching); 926 (CH wagging); 741 (C-O wagging)
Figure S51. MS spectra of [bmim][Man]
Figure S52. $^1$H and $^{13}$C NMR spectra for [bmim][Caff]

$^1$H NMR (D$_2$O): $^1$H NMR (D$_2$O): 2.09 (m. 2H. NCH$_2$CH$_2$CH$_2$CH$_3$); 3.71 (t. 3H. J=6.1 Hz. NCH$_2$CH$_2$CH$_2$CH$_3$); 3.82 (s. 3H. CH$_3$); 4.31 (t. 2H. J=7.1 Hz. NCH$_2$CH$_2$CH$_2$CH$_3$); 5.29 (s. 3H, NCH$_2$CH$_2$CH$_2$CH$_3$); 7.29, 7.38 and 7.40 (2xs. 5H, H-6, H-7, H-8, H-9, H-10); 7.54 and 7.58 (2xs. 2H. H-4 and H-5); 8.82 (s. 1H. H-2).
Figure S53. FTIR spectra of [bmim][Caff]

3198 (N-H stretching); 2976 (asym. stretching CH$_3$), 2894 (sym. stretching CH$_3$), 1501 (in plane vibrations of imidazolium ring), 1434 (skeletal vibration of caffeate ring), 1445 and 1362 (C-N stretching), 1218 and 1183 (stretching OH group); 1151 and 1062 (C-O stretching); 961 (CH wagging); 704 (C-O wagging)
Figure S54. MS spectra of [bmim][Caff]
Figure S55. $^1$H and $^{13}$C NMR spectra for [OHC$_3$ mim][Cin]

$^1$H NMR (D$_2$O): 2.31 (m. 2H. NCH$_2$CH$_2$OH); 3.83 (t. 2H. J=6.1 Hz. NCH$_2$CH$_2$CH$_2$OH); 3.96 (s. 3H. CH$_3$); 4.31 (t. 2H. J=7.1 Hz. NCH$_2$CH$_2$CH$_2$OH); 7.29, 7.38 and 7.41 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.61 and 7.67 (2xs. 2H. H-4 and H-5); 8.93 (s. 1H. H-2).

$^{13}$C NMR (D$_2$O): 31.44 (NCH$_2$CH$_2$CH$_2$OH); 35.94 (CH$_3$); 46.79 (NCH$_2$CH$_2$CH$_2$OH); 57.93 (NCH$_2$CH$_2$CH$_2$OH); 124.34 i 125.65 (C-4 i C-5); 129.65 (C-6); 130.21 (C-7), 130.86 (C-8); 136.11 (d. C-2); 142.73 (C-9) and 177.05 (COO$^-$)
Figure S56. FTIR spectra of [OHC₃mim][Cin]

3079 (stretching OH), 2946 (asym. stretching CH₃), 2845 (sym. stretching CH₃), 1555 (in plane vibrations of imidazolium ring), 1494 (skeletal vibration of cinnamate), 1447 and 1362 (C-N stretching), 1165 and 1072 (C-O stretching); 956 (CH wagging); 774 (C-O wagging)
Figure S57. MS spectra of \([\text{OHC}_3\text{mim}][\text{Cin}]\)
Figure S58. $^1$H and $^{13}$C NMR spectra for [OHC$_3$mim][Man]

$^1$H NMR (D$_2$O): $^1$H NMR (D$_2$O): 2.16 (m, 2H, NCH$_2$CH$_2$OH); 3.67 (t, 2H, J=6.1 Hz, NCH$_2$CH$_2$OH); 3.96 (s, 3H, CH$_3$); 4.36 (t, 2H, J=7.1 Hz, NCH$_2$CH$_2$OH); 5.26 (C-OH); 7.29, 7.38 and 7.41 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.51 and 7.57 (2xs, 2H, H-4 and H-5); 8.82 (s, 1H, H-2).

$^{13}$C NMR (D$_2$O): 31.49 (NCH$_2$CH$_2$OH); 35.81 (CH$_3$); 46.79 (NCH$_2$CH$_2$OH); 57.93 (NCH$_2$CH$_2$OH); 75.44 (C-OH); 122.34 i 123.65 (C-4 i C-5); 129.05 (C-6); 130.21 (C-7), 130.86 (C-8); 136.11 (d, C-2); 142.73 (C-9) and 176.01 (COO$^-$)
Figure S59. FTIR spectra of [OHC₃mim][Man]

3204 (stretching vibration OH from mandelate), 3086 (stretching OH), 2954 (asym. stretching CH₃), 1606 (ring deformation mandelate), 1572 (in plane vibration imidazolium ring), 1451 and 1352 (C-N stretching); 1165 and 1053 (C-O stretching); 928 (CH wagging); 735 (C-O wagging)
Figure S60. MS spectra of [OHC₃mim][Man]
Figure S61. $^1$H and $^{13}$C NMR spectra for [OHC$_3$mim][Caff]

$^1$H NMR (D$_2$O): $^1$H NMR (D$_2$O): 2.19 (m, 2H, NCH$_2$CH$_2$CH$_2$OH); 3.71 (t, 2H, J=6.1 Hz, NCH$_2$CH$_2$CH$_2$OH); 3.89 (s, 3H, CH$_3$); 4.39 (t, 2H, J=7.1 Hz, NCH$_2$CH$_2$CH$_2$OH); 5.29 (s, 2H, C-OH); 7.29, 7.38 and 7.41 (2xs, 5H, H-6, H-7, H-8, H-9, H-10); 7.54 and 7.59 (2xs, 2H, H-4 and H-5); 8.86 (s, 1H, H-2).

$^{13}$C NMR (D$_2$O): 31.82 (NCH$_2$CH$_2$CH$_2$OH); 36.22 (CH$_3$); 46.75 (NCH$_2$CH$_2$CH$_2$OH); 57.93 (NCH$_2$CH$_2$CH$_2$OH); 75.73 and 77.29 (C-12 and C-13); 122.34 and 123.65 (C-4 and C-5); 131.25 (C-6); 132.28 (C-7), 133.46 (C-8); 136.11 (d, C-2); 142.73 (C-9) and 179.81 (COO$^-$)
Figure S62. FTIR spectra of [OHC₃mim][Caff]

3126 (stretching OH), 2945 (asym. stretching CH₃), 2849 (sym. stretching CH₃), 1533 (in plane vibrations of imidazolium ring), 1442 (sceletal vibration of caffeate ring), 1401 and 1318 (C-N stretching), 1224 and 1189 (stretching OH group); 1144 and 1069 (C-O stretching); 962 (CH wagging); 705 (C-O wagging)
**Figure S63.** MS spectra of [OHC$_3$mim][Caff]