

Supporting Information

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

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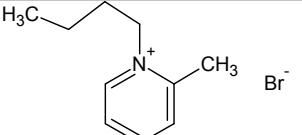
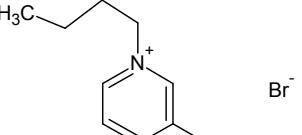
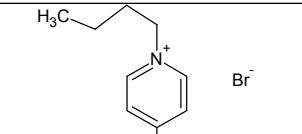
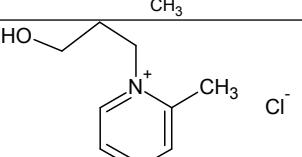
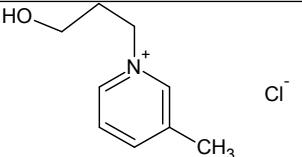
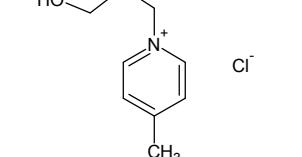
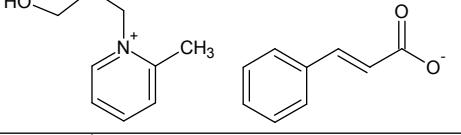
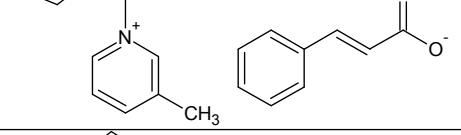
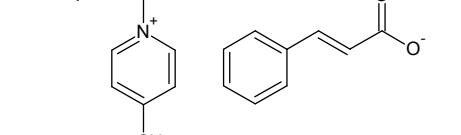
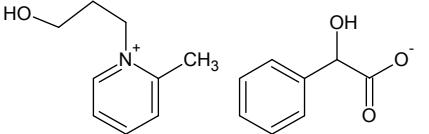
*Corresponding Author: Tel: +381 21 485 2751; Fax: +381 21 454 065; E-mail: aleksandar.tot@dh.uns.ac.rs

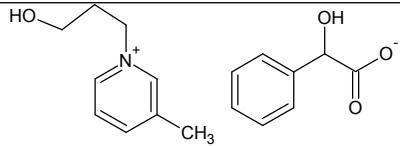
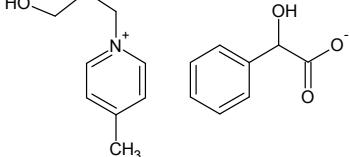
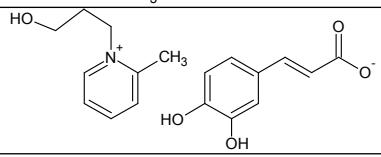
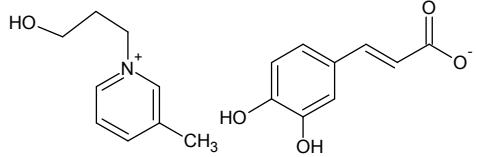
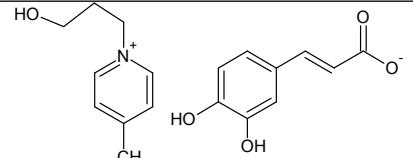
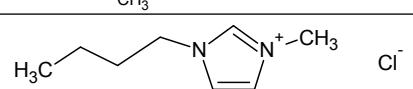
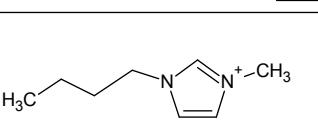
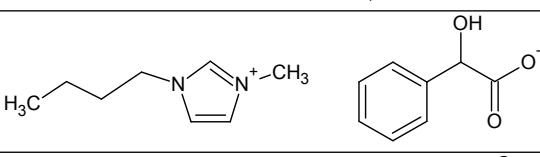
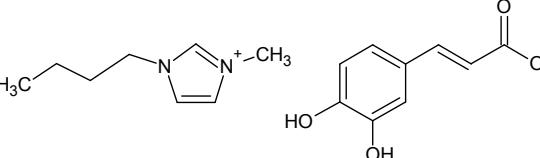
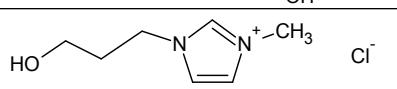
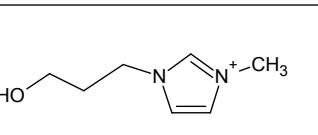
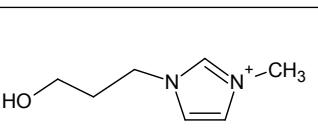
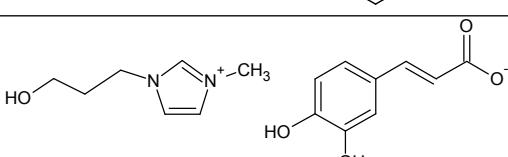
Table S1. Provenance and purity of the chemicals.

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	-	$\omega \geq 0.99$
$\text{P}_2\text{O}_5^{\text{a}}$	Sigma Aldrich	1314-56-3	-	$\omega \geq 0.99$
Amberlite IRN 78	Supelco	11128-95-3	-	-
(<i>RS</i>)-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 P_2O_5 = phosphorus pentoxide

Table S2. Structures of investigated ILs

Abbreviation	Name	Structure	Purity*
[C ₄ -2mpyc][Br]	1-butyl-2-methylpycolinium bromide		0.95
[C ₄ -3mpyc][Br]	1-butyl-3-methylpycolinium bromide		0.96
[C ₄ -4mpyc][Br]	1-butyl-4-methylpycolinium bromide		0.96
[OHC ₃ -2mpyc][Cl]	1-(3-hydroxypropyl)-2-methylpycolinium chloride		0.97
[OHC ₃ -3mpyc][Cl]	1-(3-hydroxypropyl)-3-methylpycolinium chloride		0.96
[OHC ₃ -4mpyc][Cl]	1-(3-hydroxypropyl)-4-methylpycolinium chloride		0.97
[OHC ₃ -2mpyc][Cin]	1-(3-hydroxypropyl)-2-methylpycolinium cinnamate		0.94
[OHC ₃ -3mpyc][Cin]	1-(3-hydroxypropyl)-3-methylpycolinium cinnamate		0.95
[OHC ₃ -4mpyc][Cin]	1-(3-hydroxypropyl)-4-methylpycolinium cinnamate		0.94
[OHC ₃ -2mpyc][Man]	1-(3-hydroxypropyl)-2-methylpycolinium mandelate		0.96

[OHC ₃ -3mpyc][Man]	1-(3-hydroxypropyl)-3-methylpycolinium mandelate		0.95
[OHC ₃ -4mpyc][Man]	1-(3-hydroxypropyl)-4-methylpycolinium mandelate		0.93
[OHC ₃ -2mpyc][Caff]	1-(3-hydroxypropyl)-2-methylpycolinium caffete		0.92
[OHC ₃ -3mpyc][Caff]	1-(3-hydroxypropyl)-3-methylpycolinium caffete		0.93
[OHC ₃ -4mpyc][Caff]	1-(3-hydroxypropyl)-4-methylpycolinium caffete		0.92
[bmim][Cl]	1-butyl-3-methylimidazolium chloride		
[bmim][Cin]	1-butyl-3-methylimidazolium cinnamate		0.96
[bmim][Man]	1-butyl-3-methylimidazolium mandelate		0.97
[bmim][Caff]	1-butyl-3-methylimidazolium caffete		0.95
[OHC ₃ mim][Cl]	1-(3-hydroxypropyl)-3-methylimidazolium chloride		0.98
[OHC ₃ mim][Cin]	1-(3-hydroxypropyl)-3-methylimidazolium cinnamate		0.95
[OHC ₃ mim][Man]	1-(3-hydroxypropyl)-3-methylimidazolium mandelate		0.96
[OHC ₃ mim][Caff]	1-(3-hydroxypropyl)-3-methylimidazolium caffete		0.94

*Obtained from NMR spectra

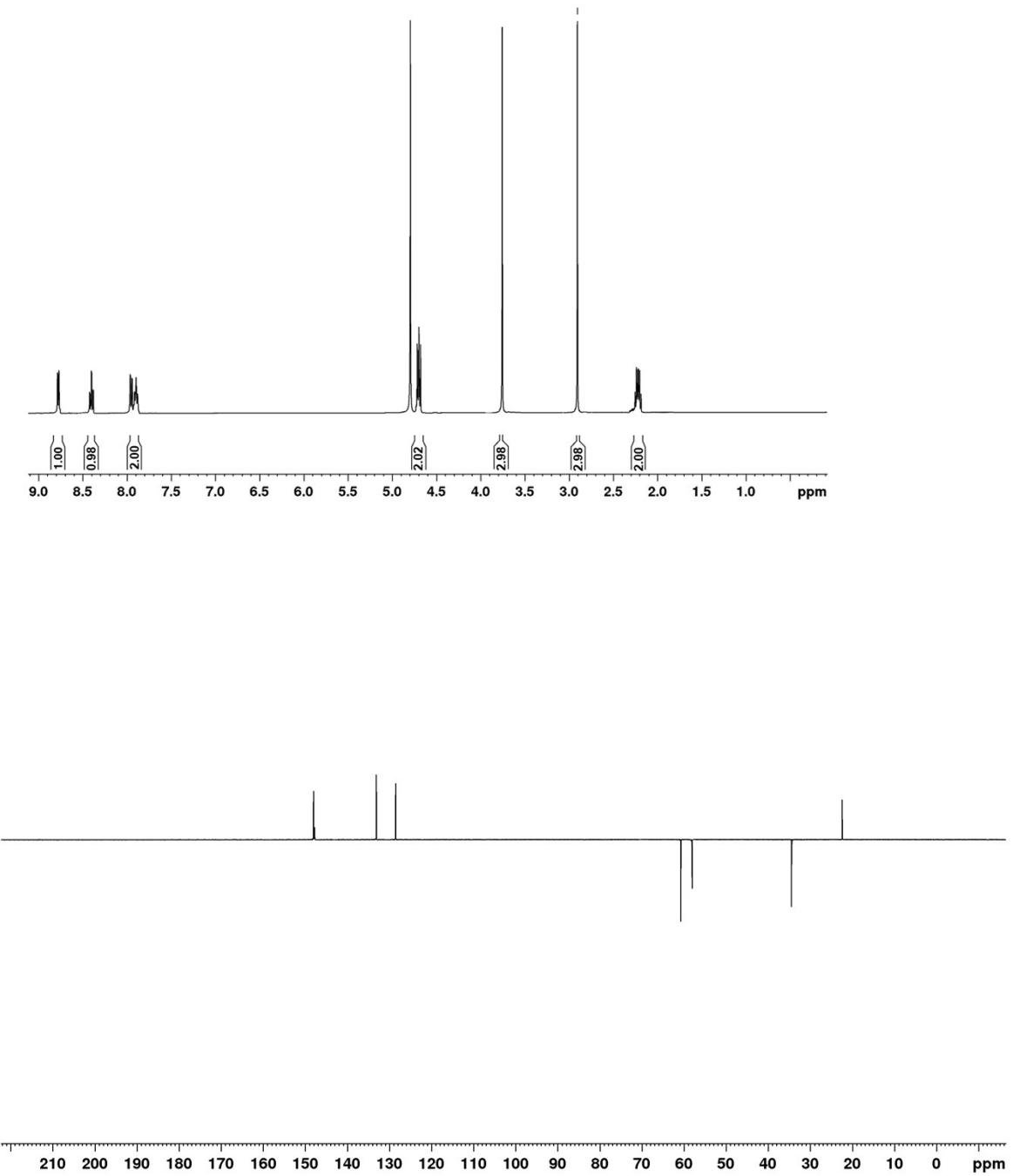


Figure S1. ^1H and ^{13}C NMR spectra for synthesized $[C_4\text{-}2\text{mpyc}]\text{[Br]}$

^1H NMR (D_2O): 2.22 (*m*, 2H, $\text{CH}_2\text{-2}'$), 2.91 (*s*, 3H, CH_3), 3.75 (*t*, 3H, CH_3), 4.70 (*t*, 2H, $J_{1',2'} = 7.2$ Hz, $\text{CH}_2\text{-1}'$), 7.96 (dd, 1H, $J_{5,6} = 6.1$ Hz, $J_{5,6} = 8.0$ Hz $H\text{-5}$), 8.40 (*d*, 1H, $J_{4,5} = 8.0$ Hz, $H\text{-4}$), 8.80 (*d*, 1H, $J_{5,6} = 6.1$ Hz, $H\text{-6}$)

^{13}C NMR (D_2O): 22.41 (CH_3), 34.13 ($\text{CH}_2\text{-2}'$), 58.42 (CH_3), 60.77 ($\text{CH}_2\text{-1}'$), 128.53 (C-5); 133.12 (C-3); 144.62 (C-6); 147.81 (C-2); 149.41 (C-4)

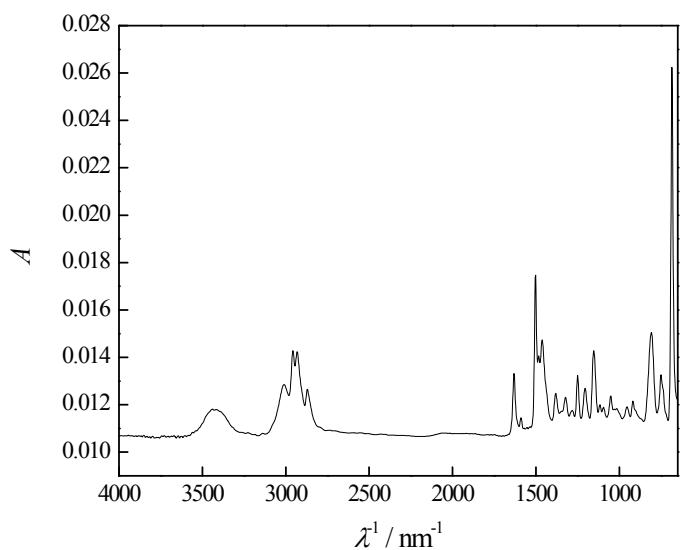


Figure S2. IR spectra of $[\text{C}_4\text{-2mpic}]\text{[Br]}$

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)

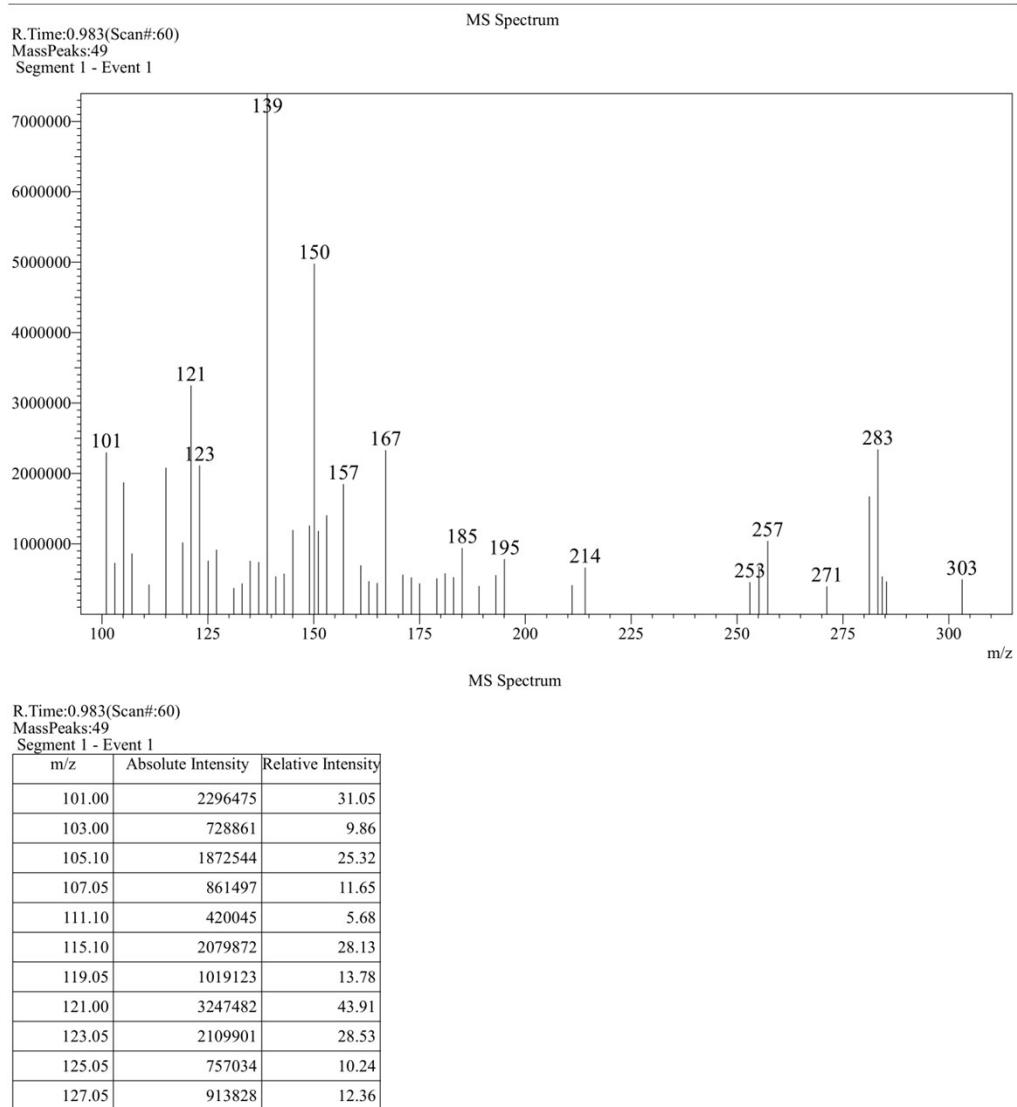


Figure S3. MS spectra of [C₄-2mpyc][Br]

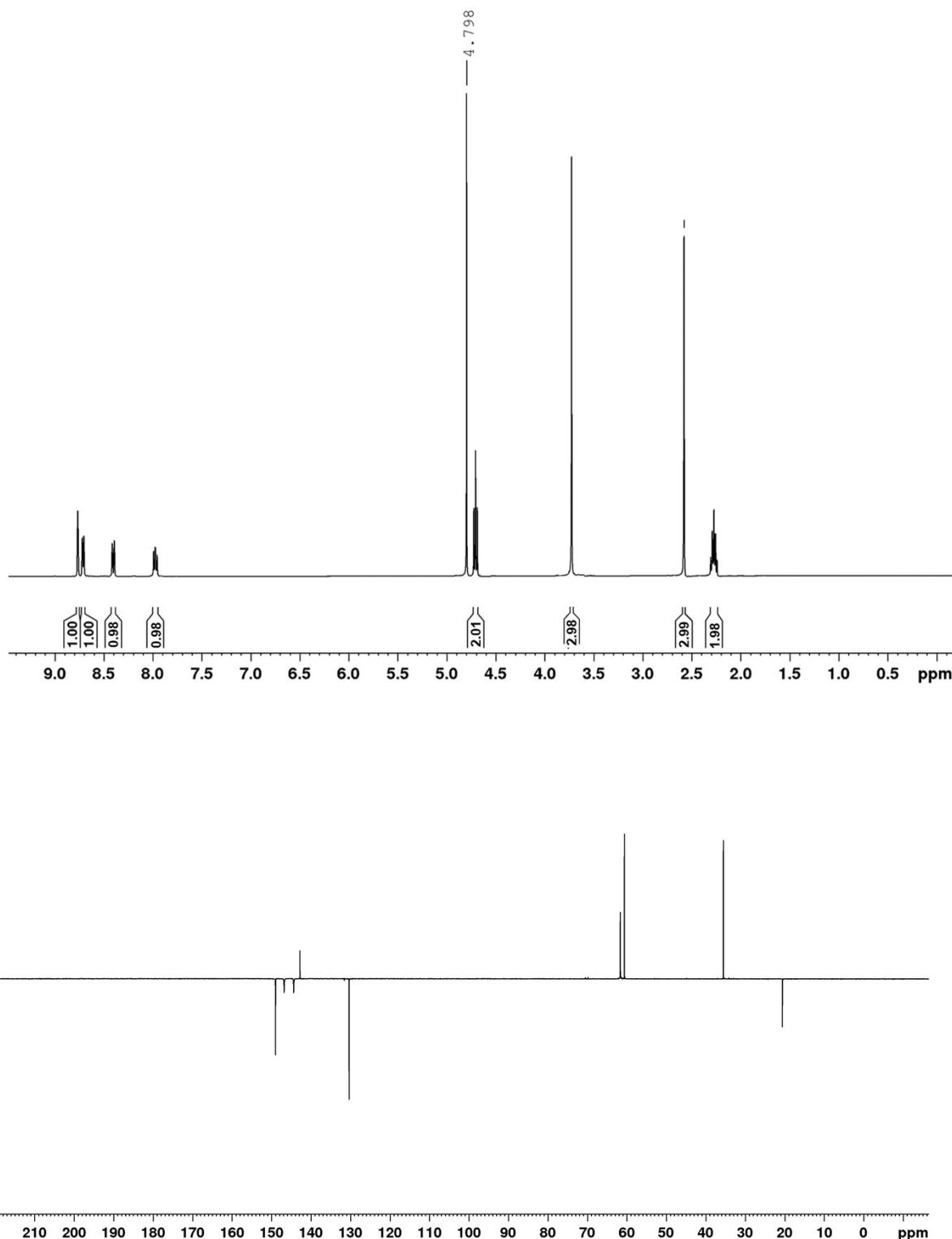


Figure S4. ^1H and ^{13}C NMR spectra for synthesized [C₄-3mpyc][Br]

¹H NMR (D₂O): 2.27 (*m*, 2H, CH₂-2'), 2.58 (*s*, 3H, CH₃), 3.70 (*t*, 3H, CH₃), 4.71 (*t*, 2H, *J*_{1',2'} = 7.2 Hz, CH₂-1'), 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_2O): 20.57 (CH_3), 35.55 ($\text{CH}_2\text{-}2'$), 60.63 (CH_3), 61.67 ($\text{CH}_2\text{-}1'$), 130.35 (C-5), 142.84 (C-3), 144.40 (C-6), 146.82 (C-2), 149.01 (C-4)

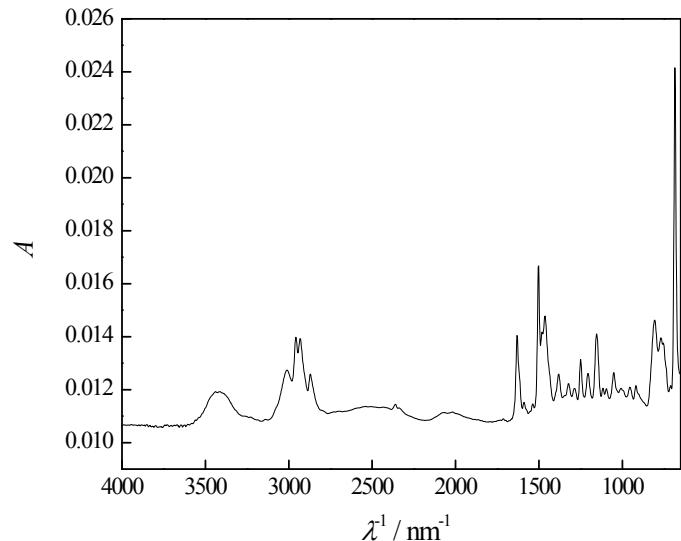
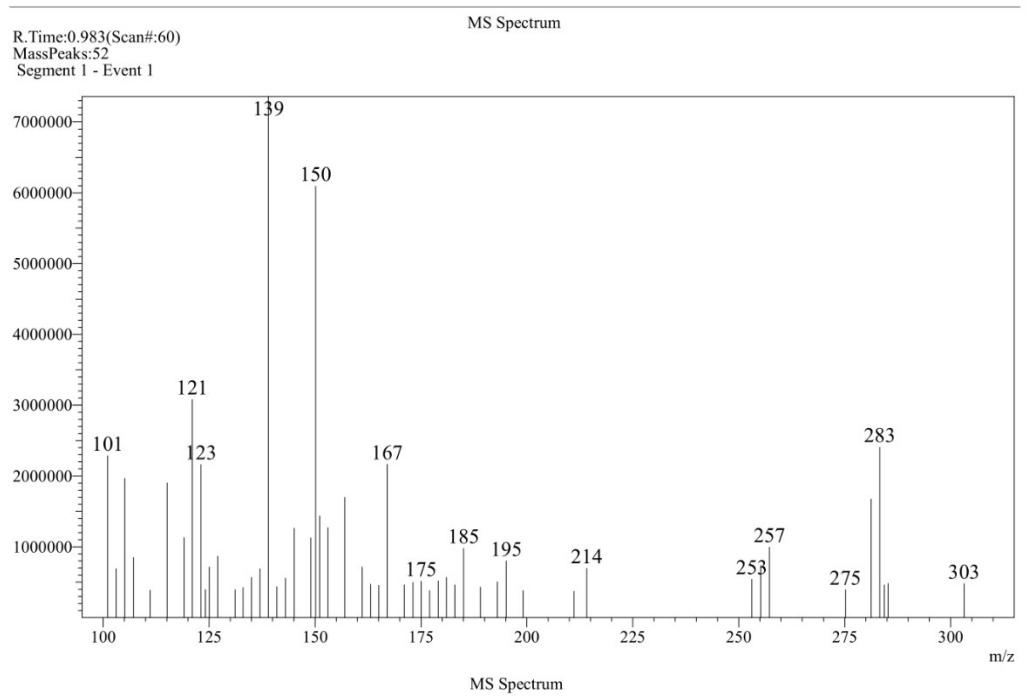


Figure S5. IR spectra of $[\text{C}_4\text{-}3\text{mpic}]\text{[Br]}$

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)



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Segment 1 - Event 1

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105.10	1966026	26.71
107.10	848199	11.52
111.05	388396	5.28
115.10	1902504	25.85
119.05	1132047	15.38
121.05	3077662	41.81
123.05	2163224	29.39
124.10	393752	5.35
125.05	715243	9.72

Figure S6. MS spectra of [C₄-3mpyc][Br]

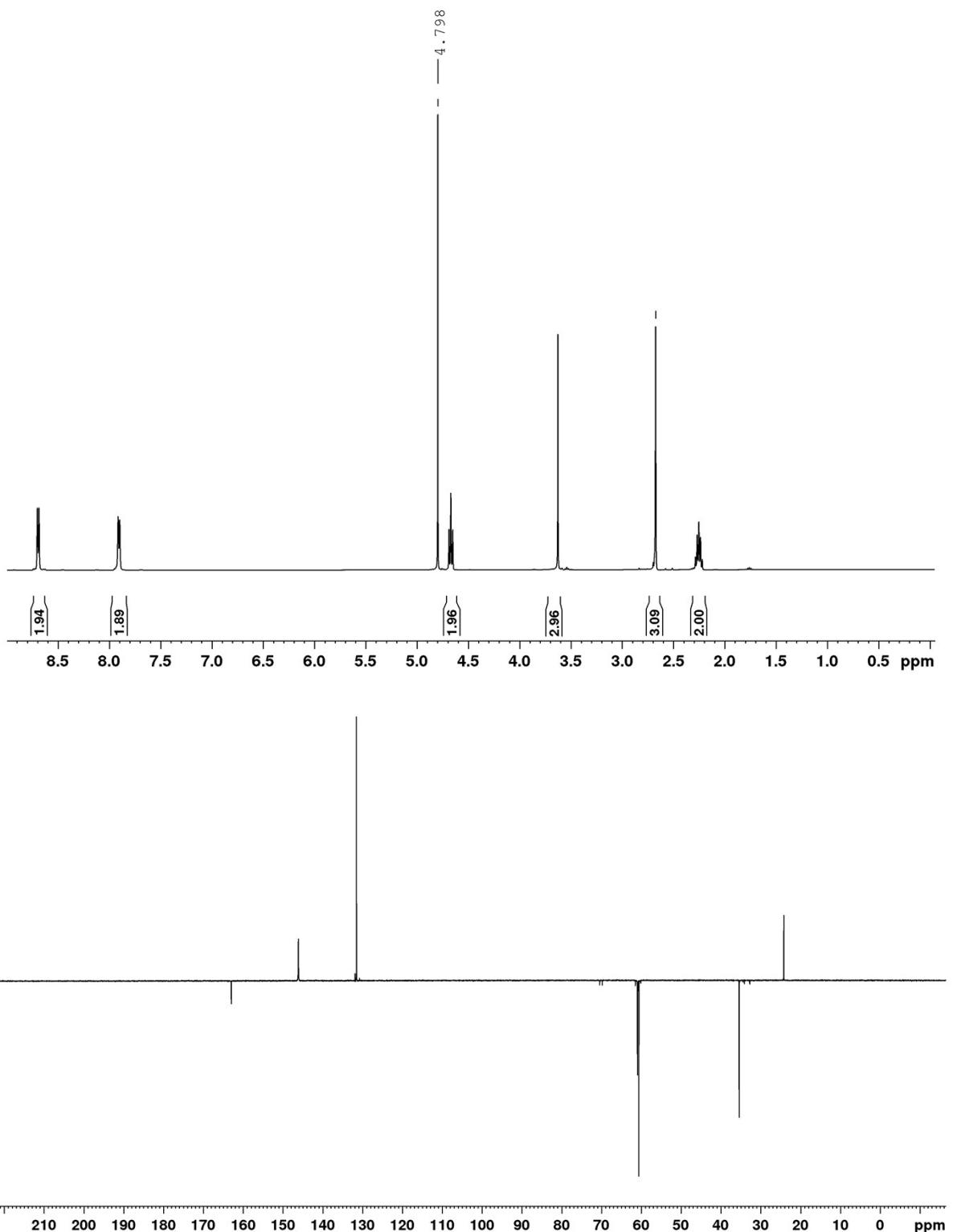


Figure S7. ^1H and ^{13}C NMR spectra for synthesized $[C_4\text{-}4\text{mpic}][\text{Br}]$

^1H NMR (D_2O): 2.25 (*m*, 2H, $\text{CH}_2\text{-}2'$), 2.67 (*s*, 3H, CH_3), 3.68 (*t*, 3H, CH_3), 4.67 (*t*, 2H, $J_{1',2'} = 7.3$ Hz, $\text{CH}_2\text{-}1'$), 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_2O): 24.20 (CH_3), 35.42 ($\text{CH}_2\text{-}2'$), 60.62 (CH_3), 60.95 ($\text{CH}_2\text{-}1'$), 131.55 (C3 and C-5), 146.14 (C-2 and C-6), 163.00 (C-4)

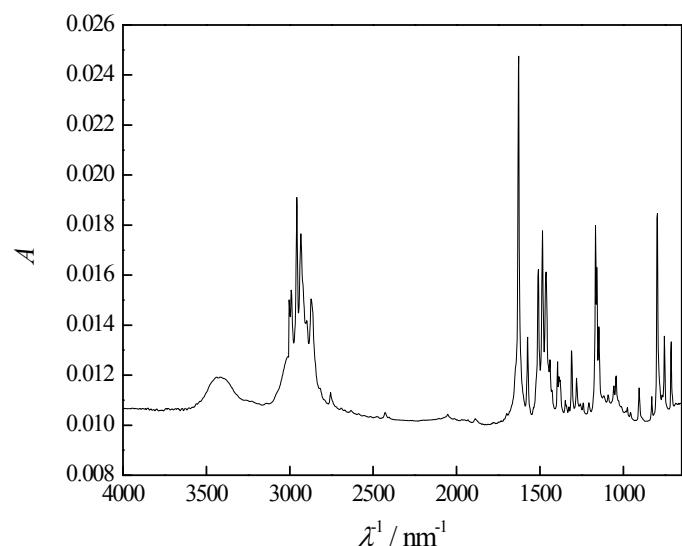


Figure S8. IR spectra of $[\text{C}_4\text{-4mpic}][\text{Br}]$

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]

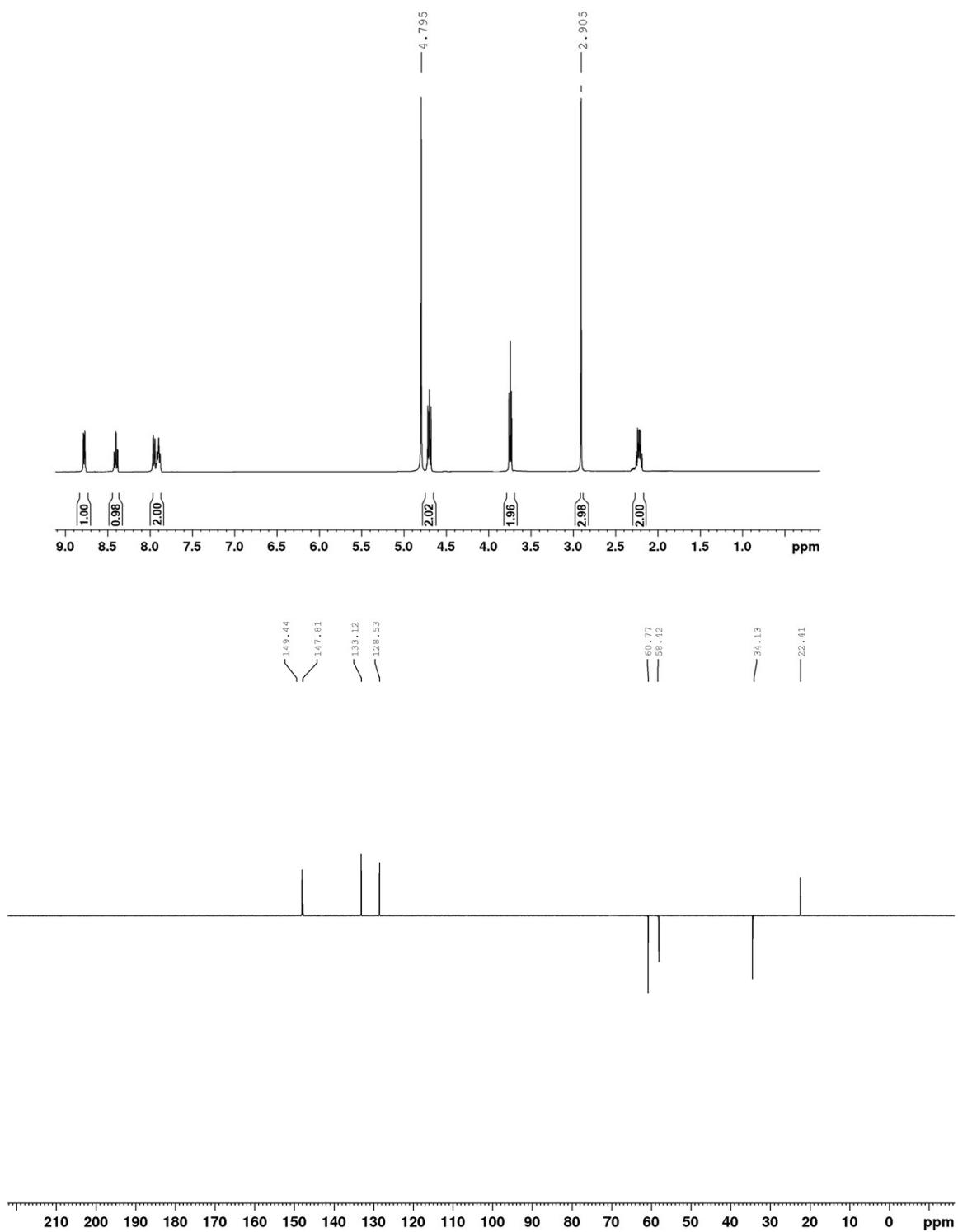


Figure S10. ^1H and ^{13}C NMR spectra for synthesized $[\text{OHC}_3\text{-}2\text{mpyc}]\text{[Cl]}$

^1H NMR (D_2O): 2.22 (*m*, 2H, $\text{CH}_2\text{-}2'$), 2.91 (*s*, 3H, CH_3), 3.75 (*t*, 2H, $J_{2',3'} = 6.0$ Hz, CH_2OH), 4.70 (*t*, 2H, $J_{1',2'} = 7.2$ Hz, $\text{CH}_2\text{-}1'$), 7.96 (dd, 1H, $J_{5',6'} = 6.1$ Hz, $J_{5',6'} = 8.0$ Hz $H\text{-}5$), 8.40 (*d*, 1H, $J_{4,5} = 8.0$ Hz, H-4), 8.80 (*d*, 1H, $J_{5,6} = 6.1$ Hz, H-6)

¹³C NMR (D₂O): 22.41 (CH₃), 34.13 (CH₂-2'), 58.42 (HOCH₂), 60.77 (CH₂-1'), 128.53 (C-5); 133.12 (C-3); 144.62 (C-6); 147.81 (C-2); 149.41 (C-4)

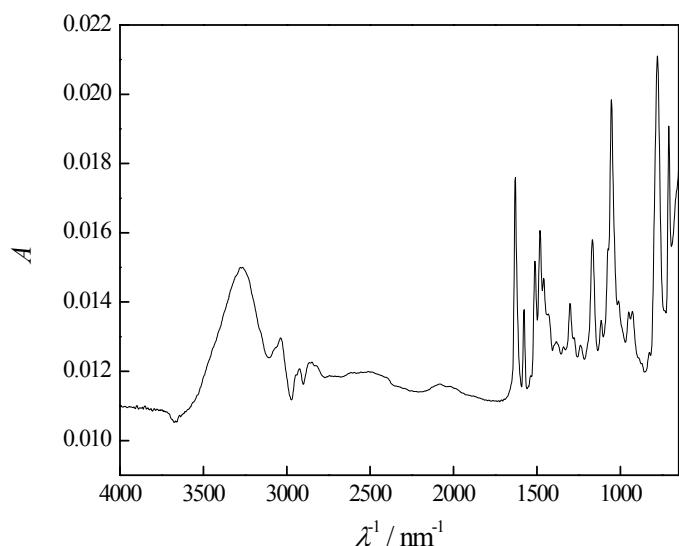


Figure S11. IR spectra of [OHC₃-2mpyc][Cl]

3265 (OH stretching); 3037 (CH sym. stretching); 2848 (sym. vibrations of CO-H); 1630 (OH bending); 1577 (aromatic C-C stretching); 1481 (rocking CH₃); 1301 and 1239 and 1239 (C_{aromatic}-C_{alifatic} or C-CH₃ stretching vibrations); 1167 and 1282 (wagging CH₂ (hydroxypropile)); 1063 (skeletal vibrations of the ring); 928 (out-of-plane bending vibrations CH (ring)).

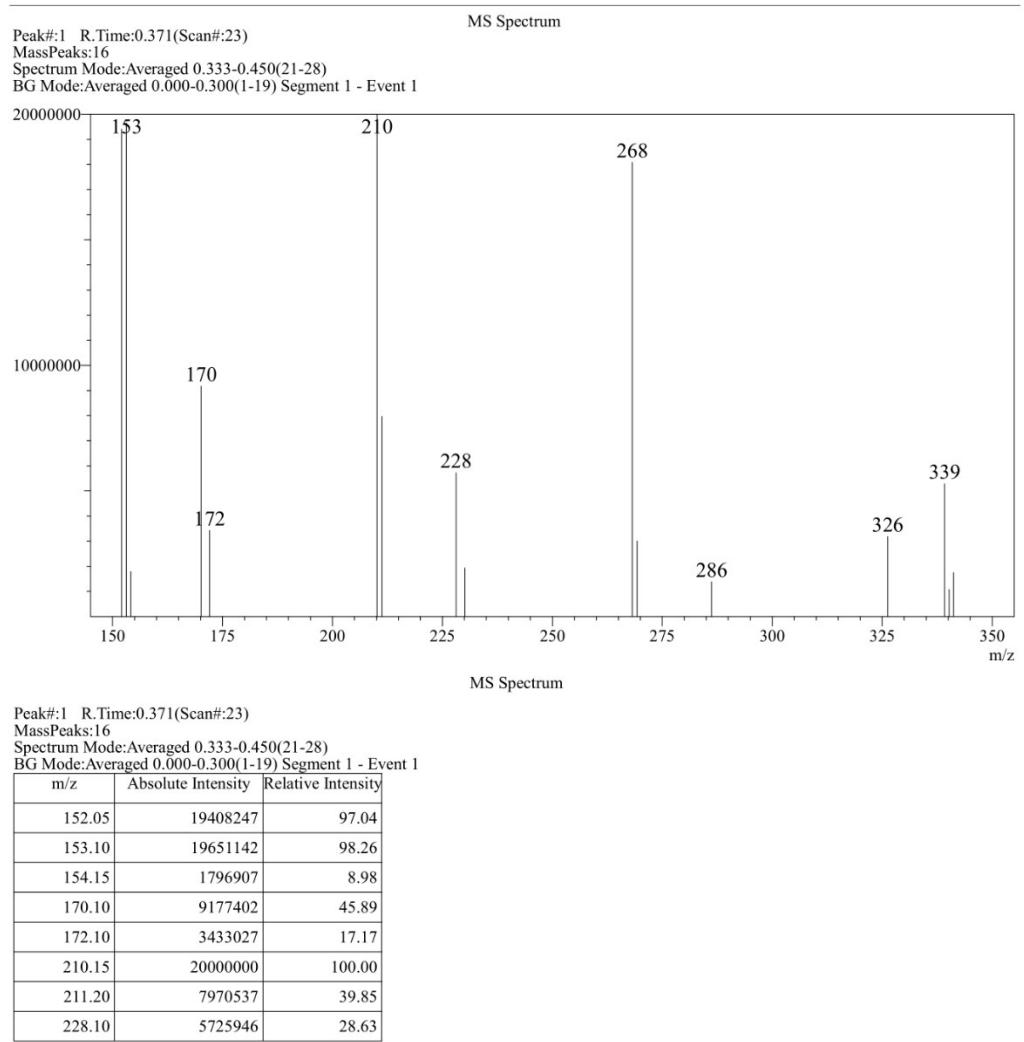


Figure S12. MS spectra of [OHC₃-2mpyc][Cl]

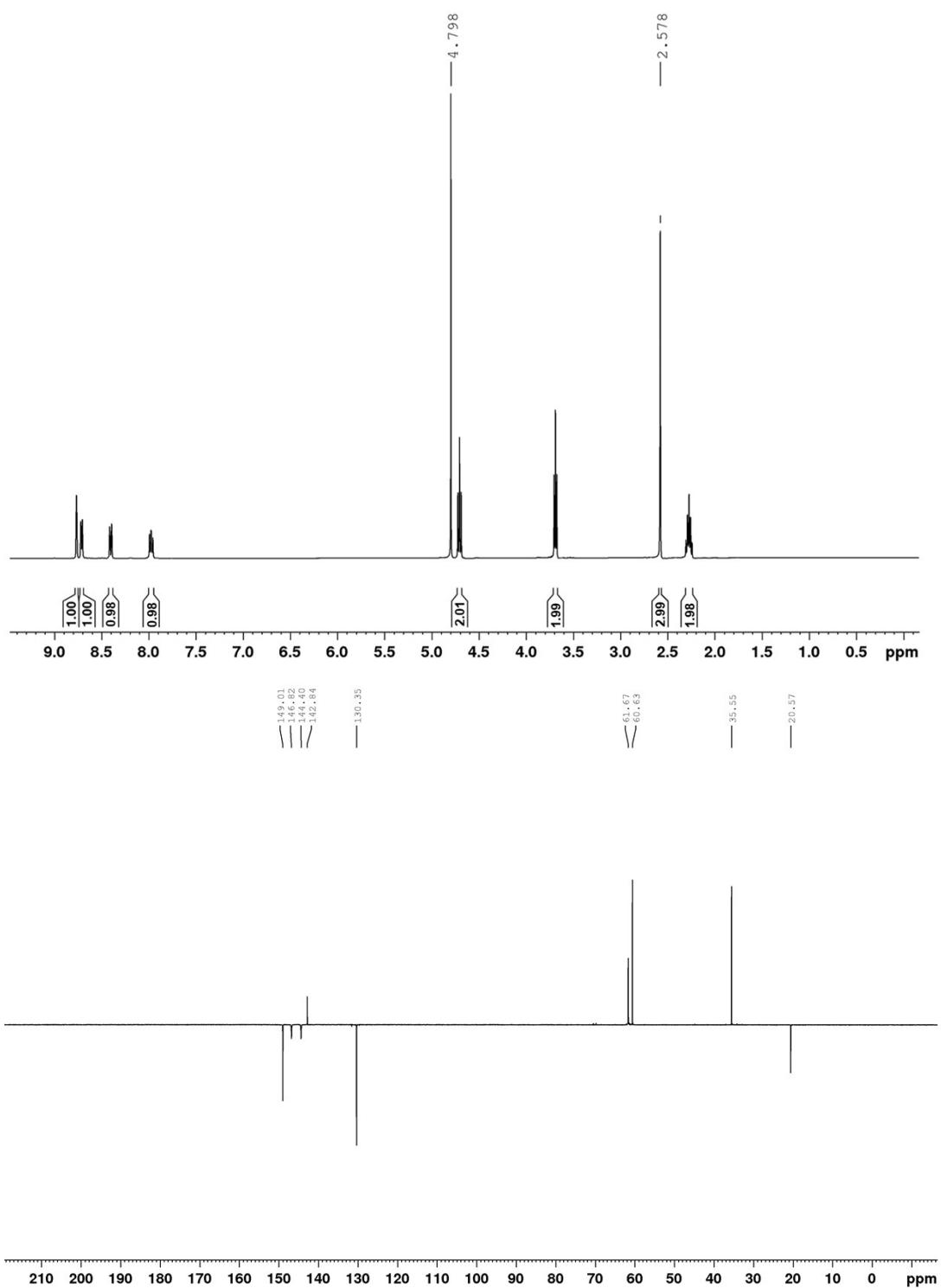


Figure S13. ^1H and ^{13}C NMR spectra for synthesized $[OHC_3\text{-}3mpyc][Cl]$

^1H NMR (D_2O): 2.27 (*m*, 2H, CH₂-2'), 2.58 (*s*, 3H, CH₃), 3.70 (*t*, 2H, $J_{2',3'} = 6.0$ Hz, CH₂OH), 4.71 (*t*, 2H, $J_{1',2'} = 7.2$ Hz, CH₂-1'), 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_2O): 20.57 (CH_3), 35.55 ($\text{CH}_2\text{-}2'$), 60.63 (HOCH_2), 61.67 ($\text{CH}_2\text{-}1'$), 130.35 (C-5), 142.84 (C-3), 144.40 (C-6), 146.82 (C-2), 149.01 (C-4)

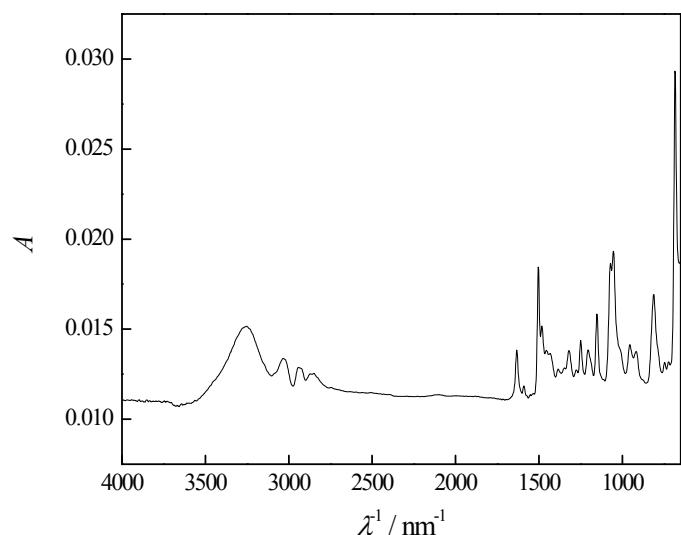


Figure S14. FTIR spectra of $[\text{OHC}_3\text{-}3\text{mpyc}][\text{Cl}]$

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 ($\text{C}_{\text{aromatic}}\text{-C}_{\text{alifatic}}$ 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)).

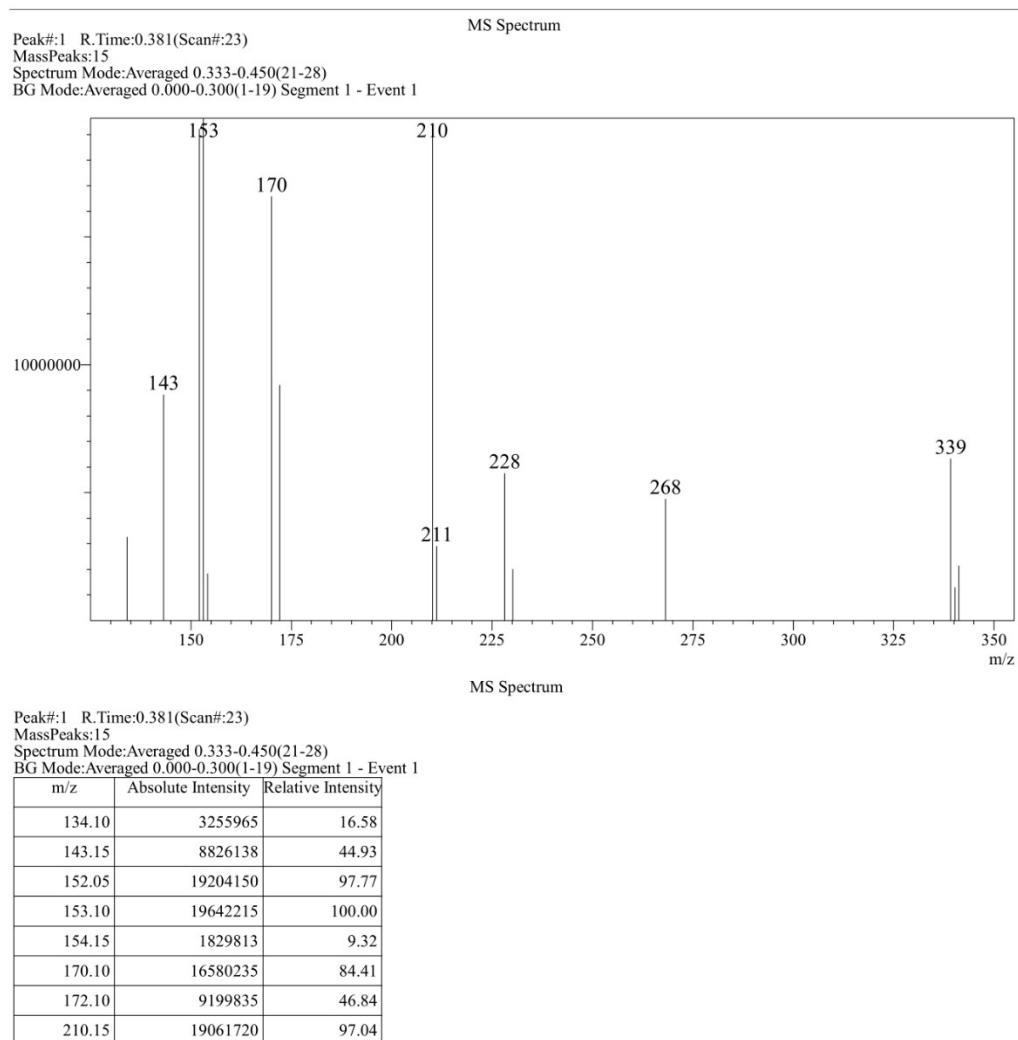


Figure S15. MS spectra of [OHC₃-3mpyc][Cl]

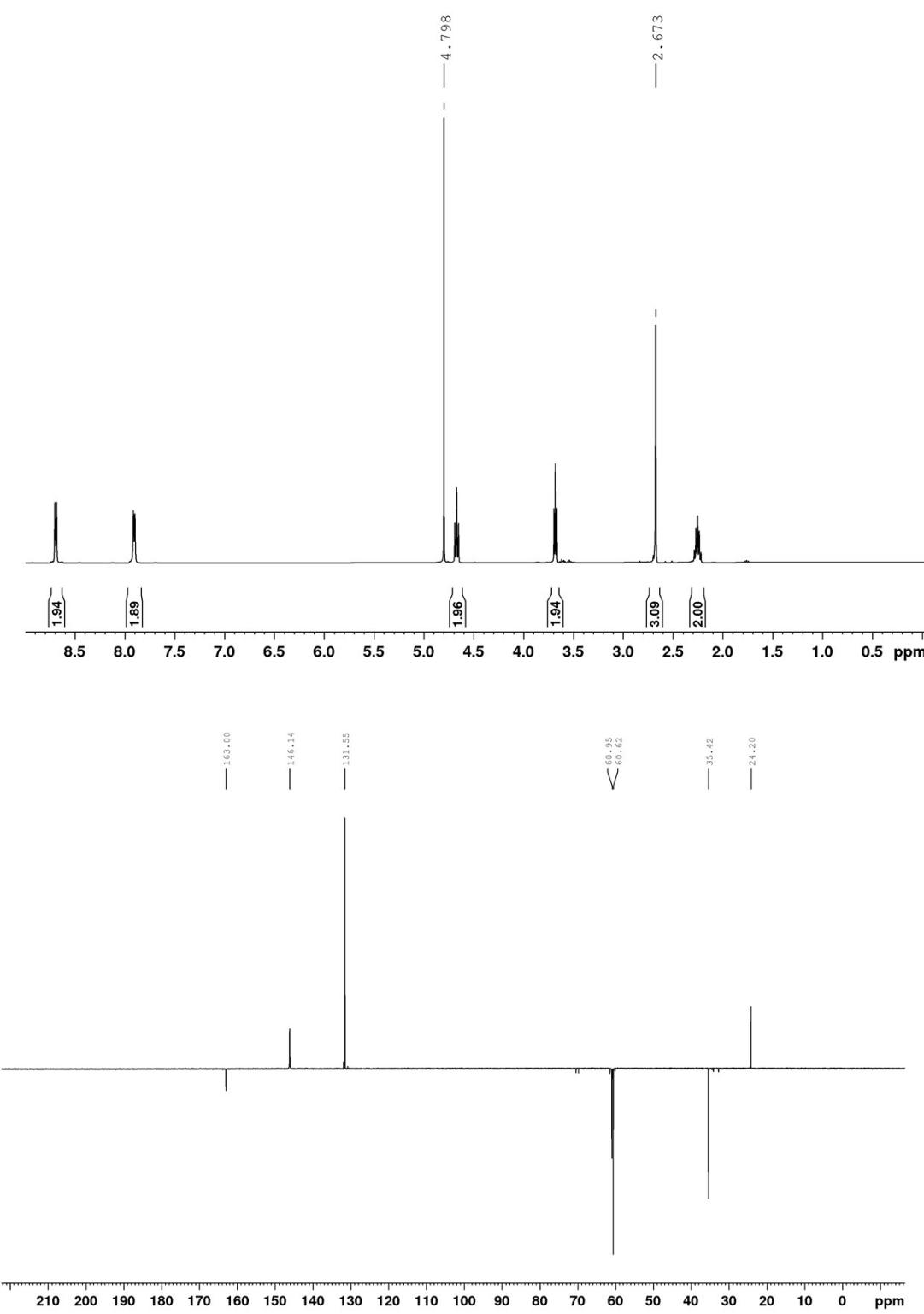


Figure S16. ^1H and ^{13}C NMR spectra for synthesized $[OHC_3\text{-}4\text{mpyc}][Cl]$

^1H NMR (D_2O): 2.25 (*m*, 2H, $CH_2\text{-}2'$), 2.67 (*s*, 3H, CH_3), 3.68 (*t*, 2H, $J_{2',3'} = 6.1$ Hz, $CH_2\text{OH}$), 4.67 (*t*, 2H, $J_{1',2'} = 7.3$ Hz, $CH_2\text{-}1'$), 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)

¹³C NMR (D_2O): 24.20 (CH_3), 35.42 (CH_2-2'), 60.62 ($HOCH_2$), 60.95 (CH_2-1'), 131.55 (C3 and C-5), 146.14 (C-2 and C-6), 163.00 (C-4)

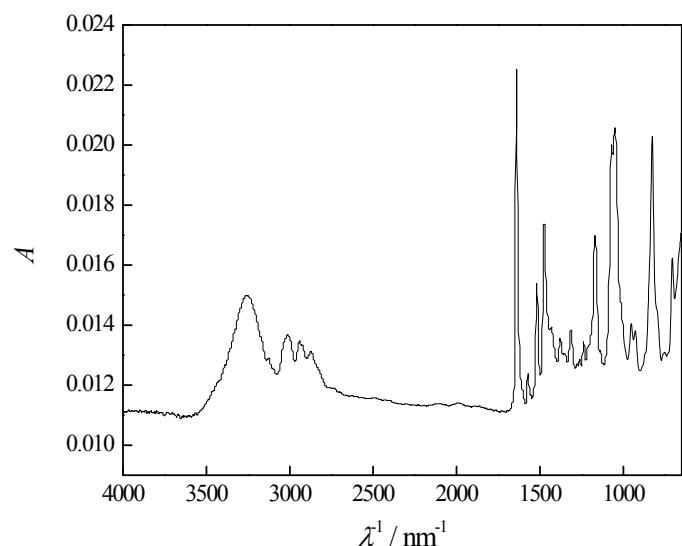


Figure S17. FTIR spectra of $[OHC_3\text{-}4mpyc][Cl]$

3012 (CH sym. stretching); 2941 (sym. vibrations of CO-H); 1633 (OH bending); 1571 (aromatic C-C stretching); 1473 (rocking CH_3); 1312 and 1238 ($C_{\text{aromatic}}\text{-}C_{\text{aliphatic}}$ or C- CH_3 stretching vibrations); 1171 and 1282 (wagging CH_2 (hydroxypropile)); 1049 (skeletal vibrations of the ring); 827 (out-of-plane bending vibrations CH (ring)).

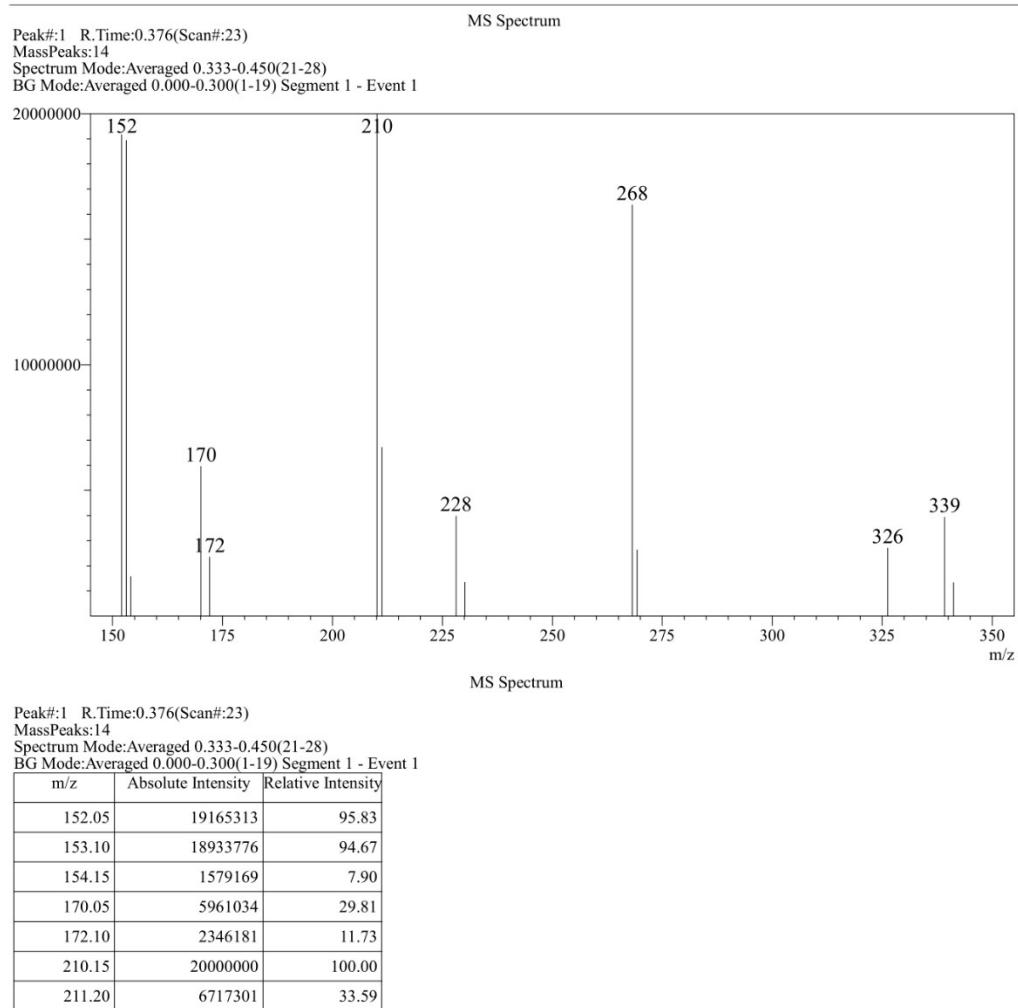


Figure S18. MS spectra of [OHC₃-4mpyc][Cl]

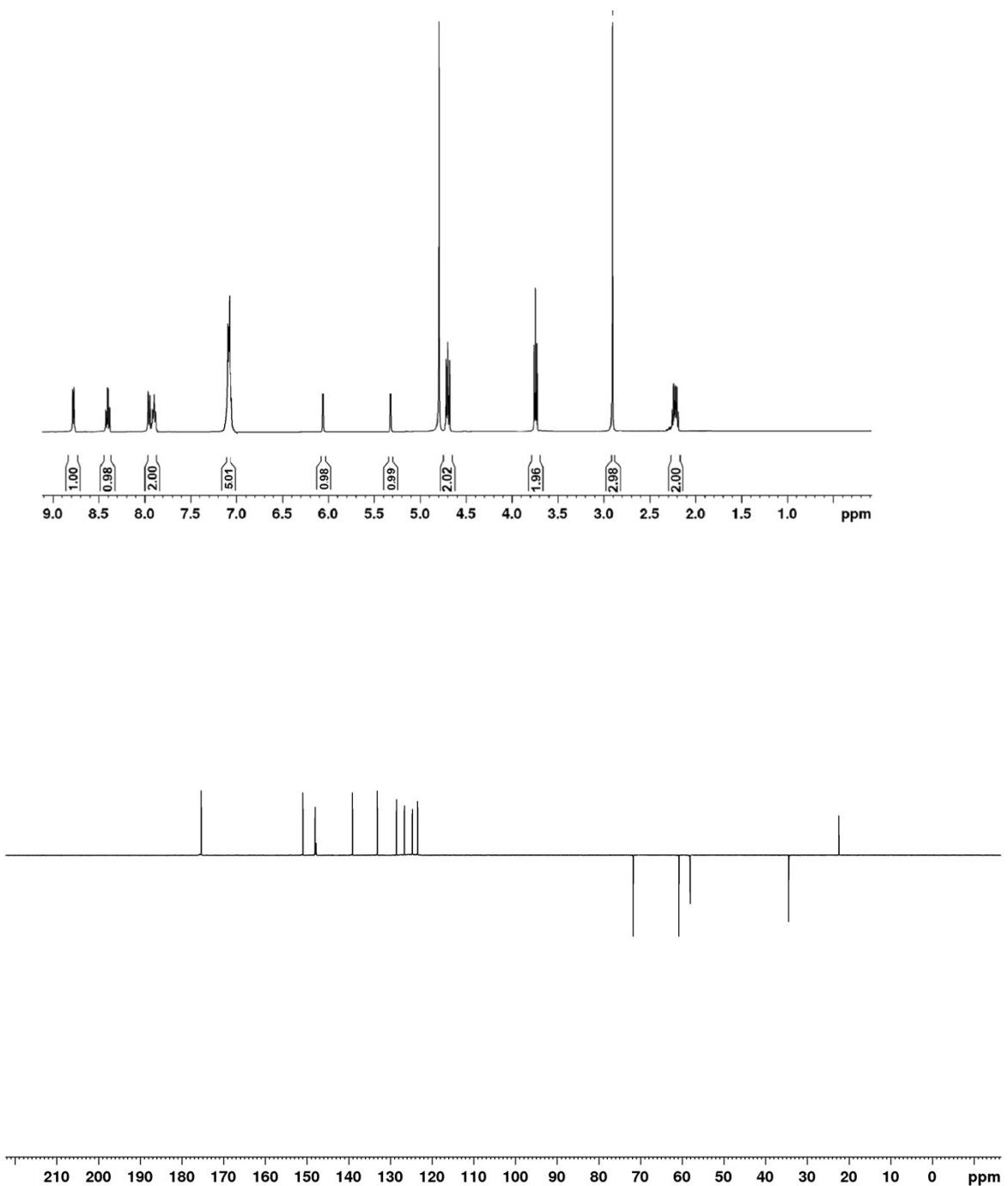


Figure S19. ^1H and ^{13}C NMR spectra for synthesized $[OHC_3\text{-}2mpyc][Cin]$

^1H NMR (D_2O): 2.22 (*m*, 2H, $CH_2\text{-}2'$), 2.94 (*s*, 3H, CH_3), 3.78 (*t*, 2H, $J_{2',3'} = 6.0$ Hz, $CH_2\text{OH}$), 4.70 (*t*, 2H, $J_{1',2'} = 7.2$ Hz, $CH_2\text{-}1'$), 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_2O): 22.41 (CH_3), 34.13 ($CH_2\text{-}2'$), 59.42 ($HOCH_2$), 61.77 ($CH_2\text{-}1'$), 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^-)

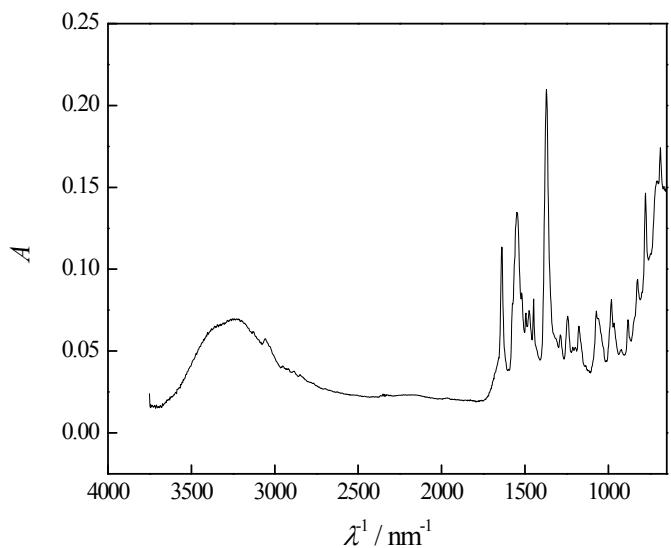
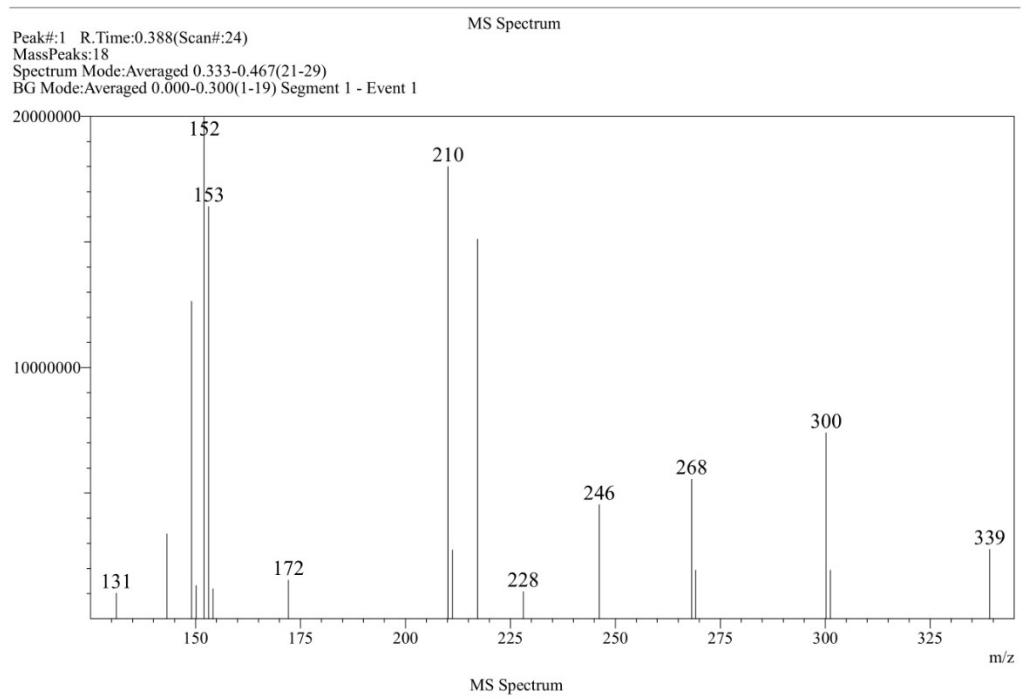


Figure S20. FTIR spectra of $[\text{OHC}_3\text{-}2\text{mpic}] \text{ [Cin]}$

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)



Peak#:1 R.Time:0.388(Scan#:24)
 MassPeaks:18
 Spectrum Mode:Averaged 0.333-0.467(21-29)
 BG Mode:Averaged 0.000-0.300(1-19) Segment 1 - Event 1

m/z	Absolute Intensity	Relative Intensity
131.10	1019381	5.10
143.15	3379728	16.90
149.05	12634396	63.17
150.10	1327198	6.64
152.05	20000000	100.00
153.10	16408110	82.04
154.15	1188618	5.94
172.15	1540713	7.70
210.15	18007233	90.04

Figure S21. MS spectra of [OHC₃-2mpyc][Cin]

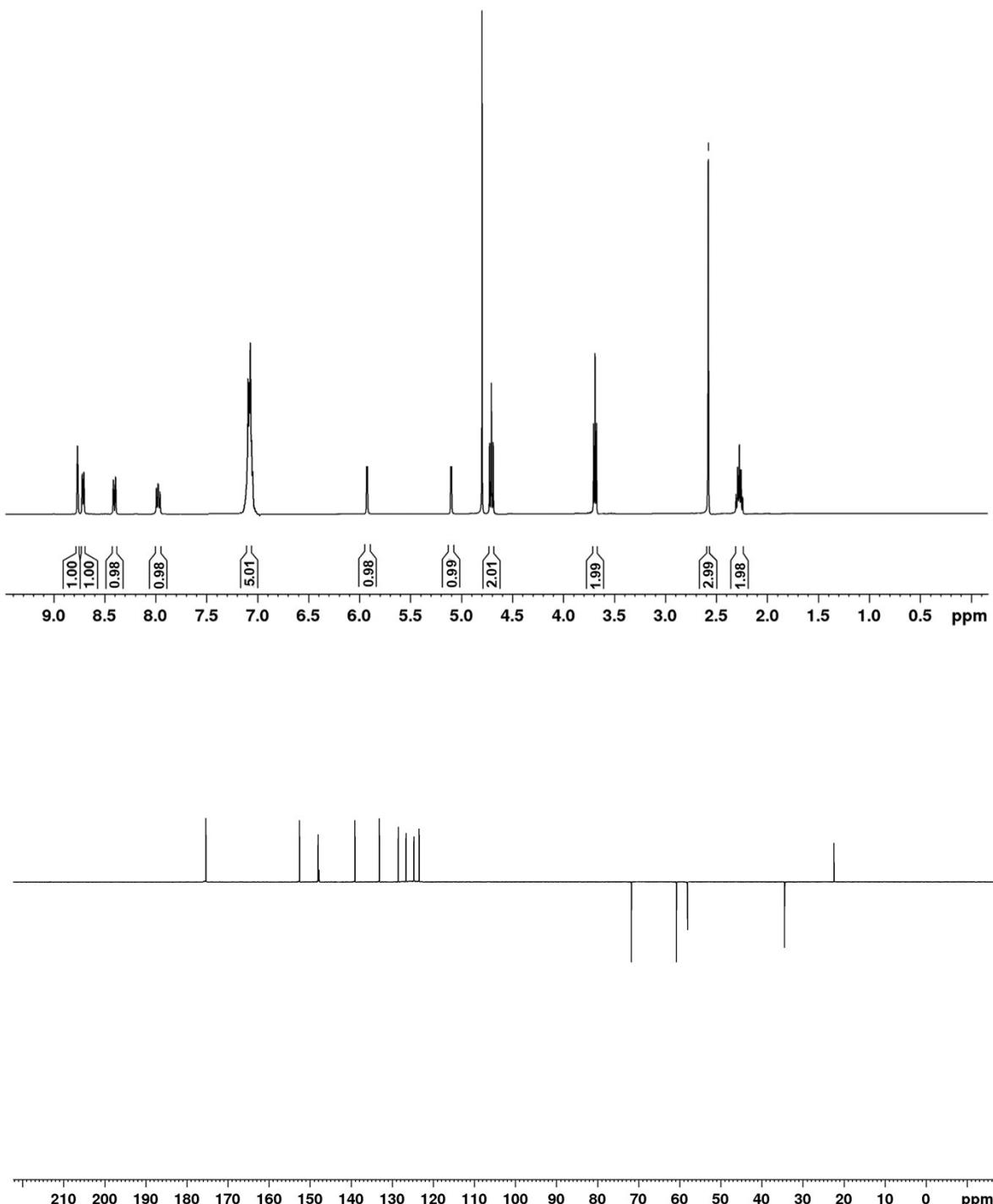


Figure S22. ^1H and ^{13}C NMR spectra for synthesized $[OHC_3\text{-}3mpyc][Cin]$

^1H NMR (D_2O): 2.33 (m , 2H, $CH_2\text{-}2'$), 2.63 (s , 3H, CH_3), 3.70 (t , 2H, $J_{2',3'} = 6.0$ Hz, $CH_2\text{OH}$), 4.71 (t , 2H, $J_{1',2'} = 7.2$ Hz, $CH_2\text{-}1'$), 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)

¹³C NMR (D₂O): 21.63 (CH₃), 35.78 (CH₂-2'), 60.71 (HOCH₂), 61.67 (CH₂-1'), 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⁻)

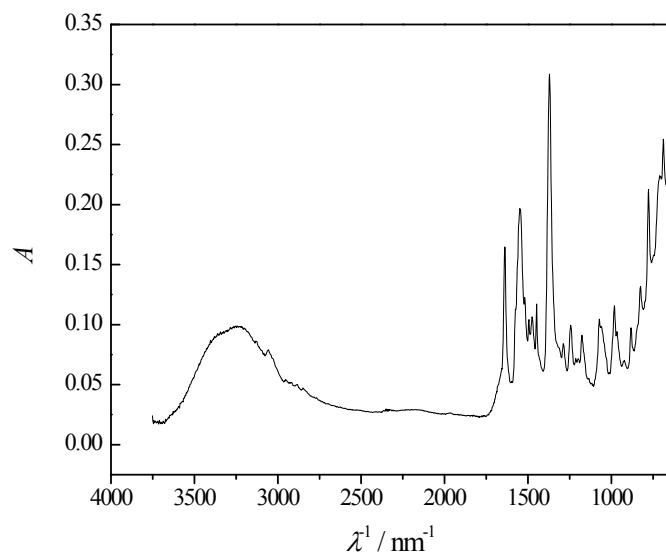
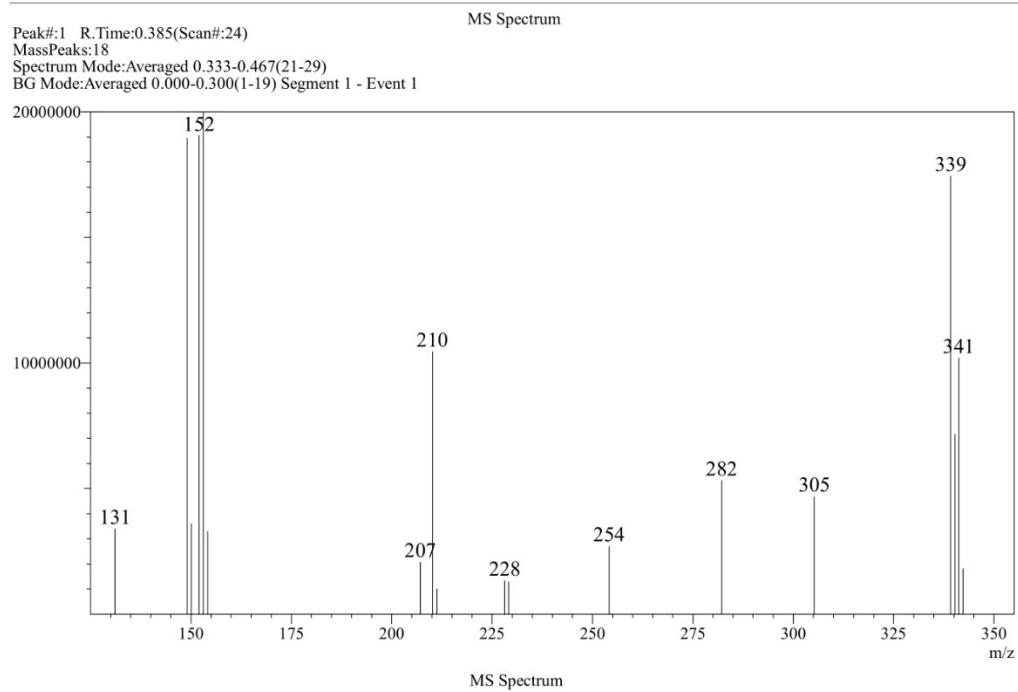


Figure S23. FTIR spectra of [OHC₃-3mpic] [Cin]

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)



Peak#:1 R.Time:0.385(Scan#:24)
 MassPeaks:18
 Spectrum Mode:Averaged 0.333-0.467(21-29)
 BG Mode:Averaged 0.000-0.300(1-19) Segment 1 - Event 1

m/z	Absolute Intensity	Relative Intensity
131.10	3389185	16.95
149.05	18952480	94.76
150.10	3603663	18.02
152.00	19065386	95.33
153.10	20000000	100.00
154.15	3301500	16.51
207.15	2067115	10.34
210.15	10451781	52.26
211.25	1005520	5.03

Figure S24. MS spectra of [OHC₃-3mpyc][Cin]

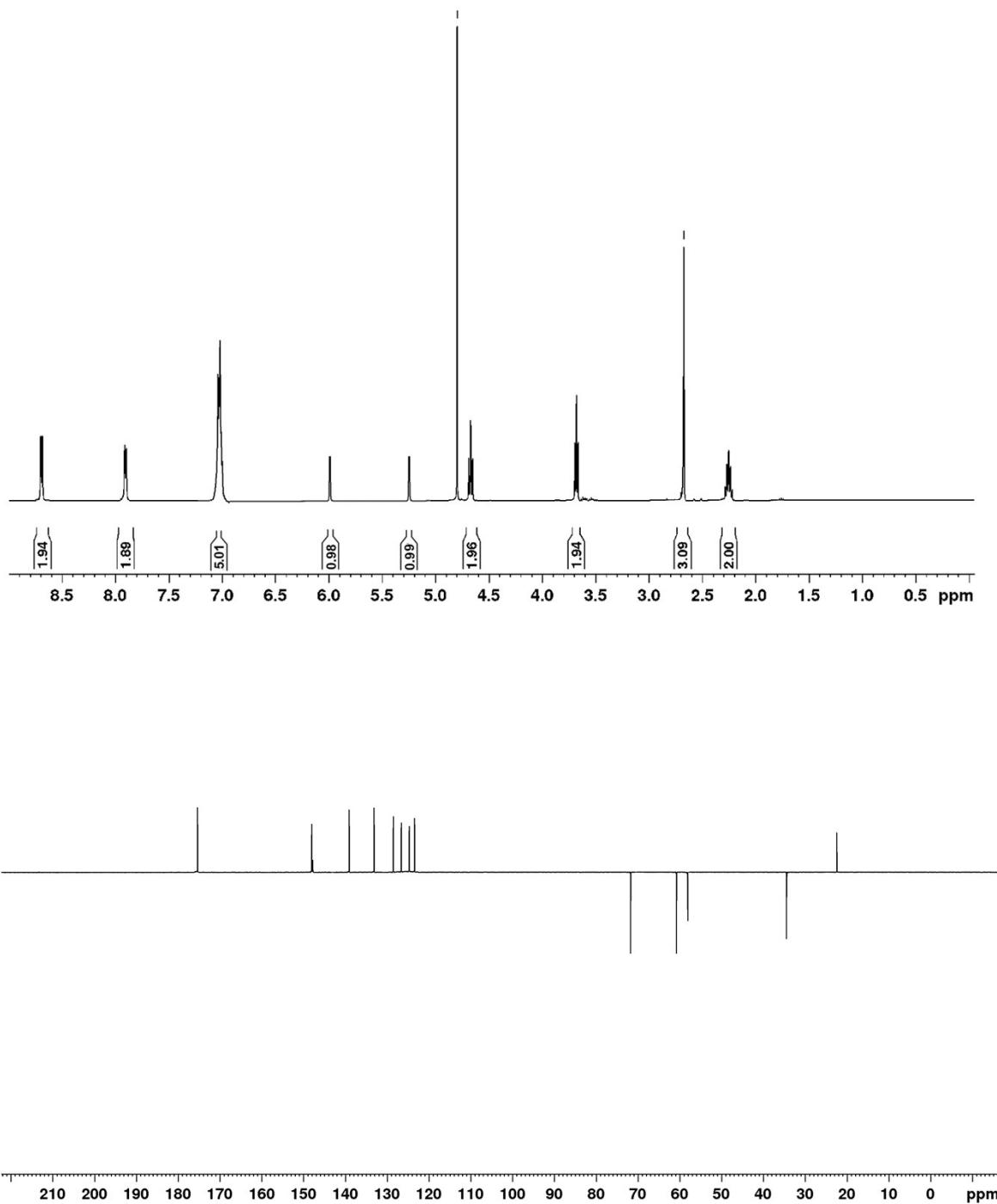


Figure S25. ¹H and ¹³C NMR spectra for synthesized [OHC₃-4mpyc][Cin]

¹H NMR (D₂O): 2.25 (*m*, 2H, CH₂-2'), 2.67 (*s*, 3H, CH₃), 3.68 (*t*, 2H, *J*_{2',3'} = 6.1 Hz, CH₂OH), 4.67 (*t*, 2H, *J*_{1',2'} = 7.3 Hz, CH₂-1'), 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)

¹³C NMR (D₂O): 24.20 (CH₃), 35.42 (CH₂-2'), 60.62 (HOCH₂), 60.95 (CH₂-1'), 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⁻)

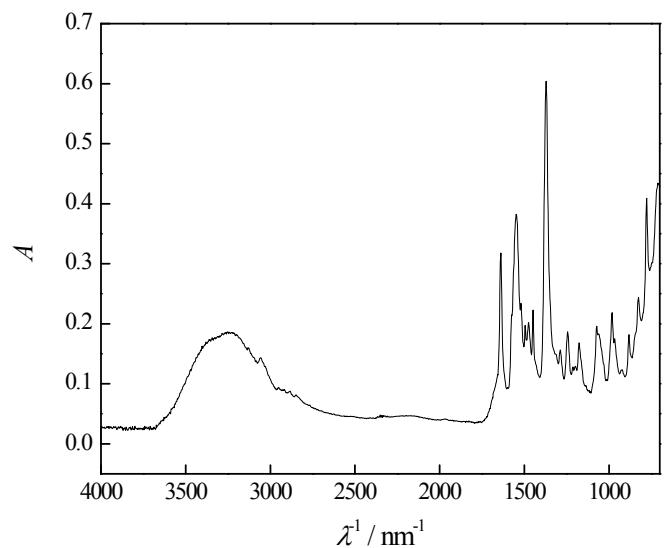


Figure S26. FTIR spectra of $[\text{OHC}_3\text{-4mpyc}] [\text{Cin}]$

3151 (stretching OH), 1623 (skeletal 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)

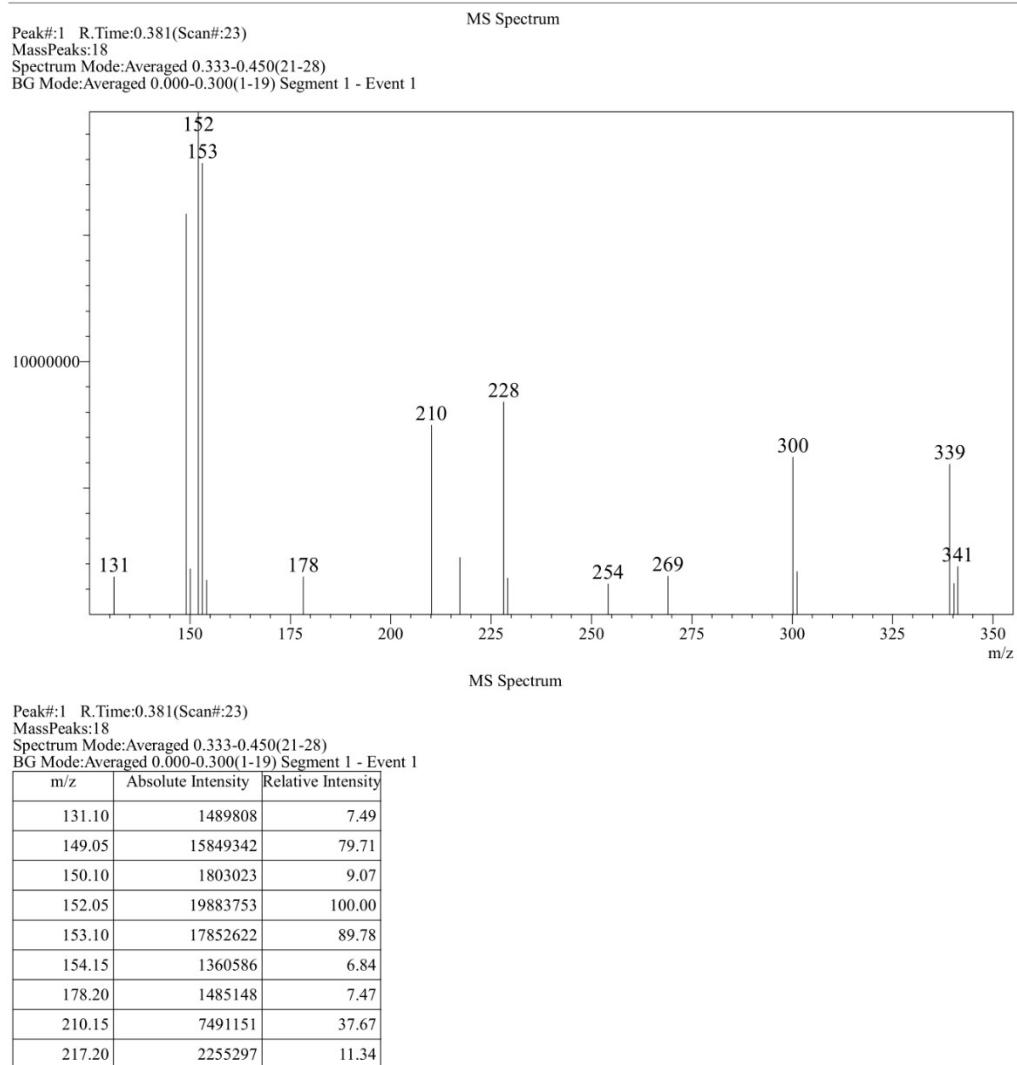


Figure S27. MS spectra of [OHC₃-4mpyc][Cin]

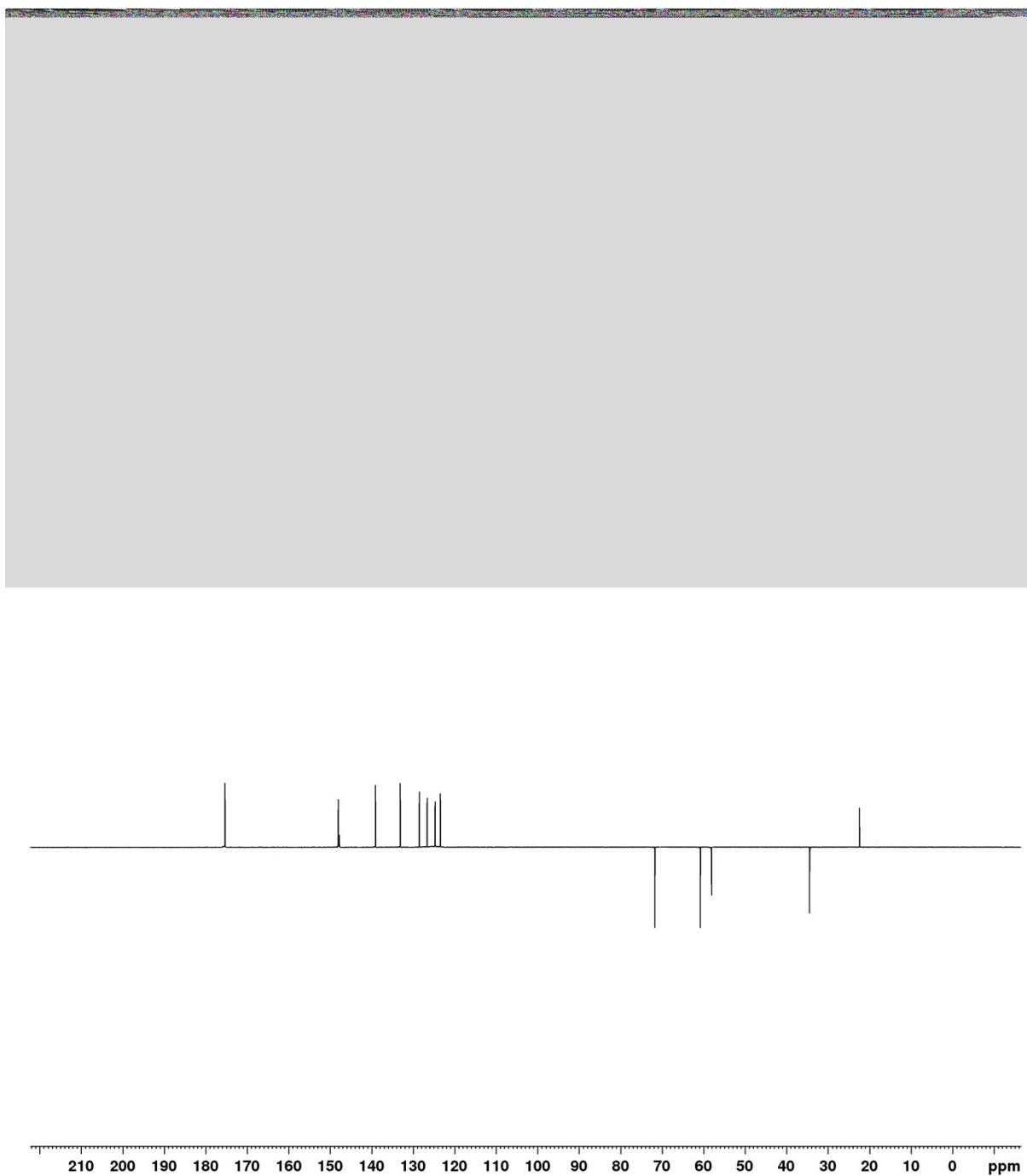


Figure S28. ^1H and ^{13}C NMR spectra for $[\text{OHC}_3\text{-2mpyc}][\text{Man}]$

^1H NMR (D_2O): 2.18 (*m*, 2H, $\text{CH}_2\text{-2}'$), 2.90 (*s*, 3H, CH_3), 3.75 (*t*, 2H, $J_{2',3'} = 6.0$ Hz, CH_2OH), 4.70 (*t*, 2H, $J_{1',2'} = 7.2$ Hz, $\text{CH}_2\text{-1}'$), 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 $H\text{-5}$), 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_2O): 22.41 (CH_3), 34.13 ($\text{CH}_2\text{-2}'$), 58.42 (HOCH_2), 60.77 ($\text{CH}_2\text{-1}'$), 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^-)

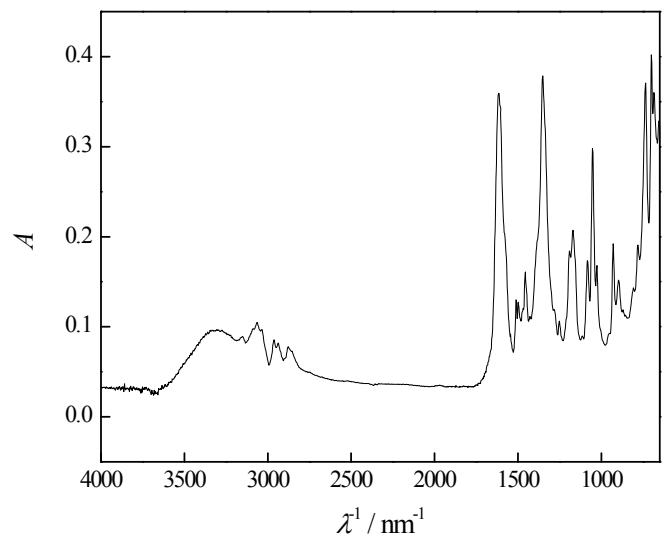


Figure S29. FTIR spectra of $[\text{OHC}_3\text{-2mpic}] [\text{Man}]$

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)

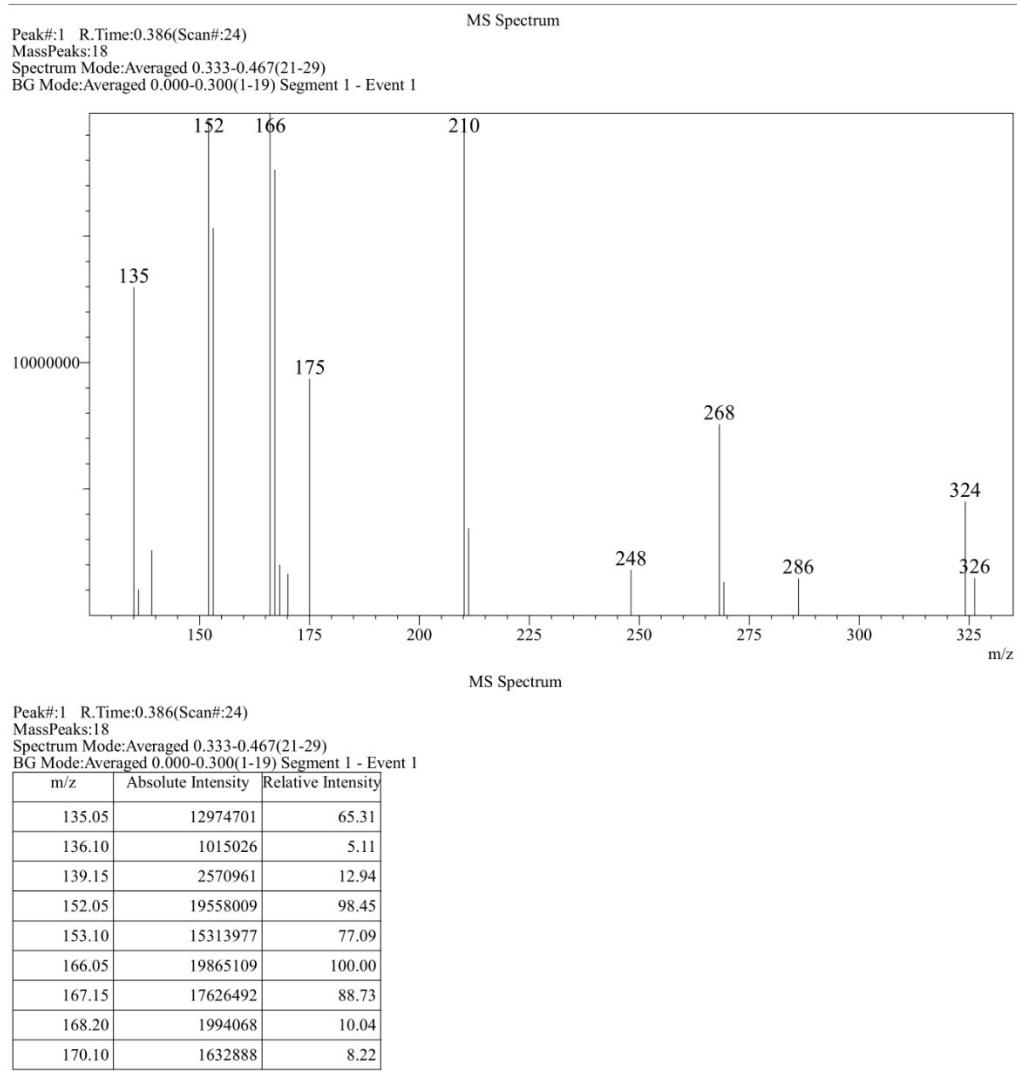


Figure S30. MS spectra of [OHC₃-2mpyc][Man]

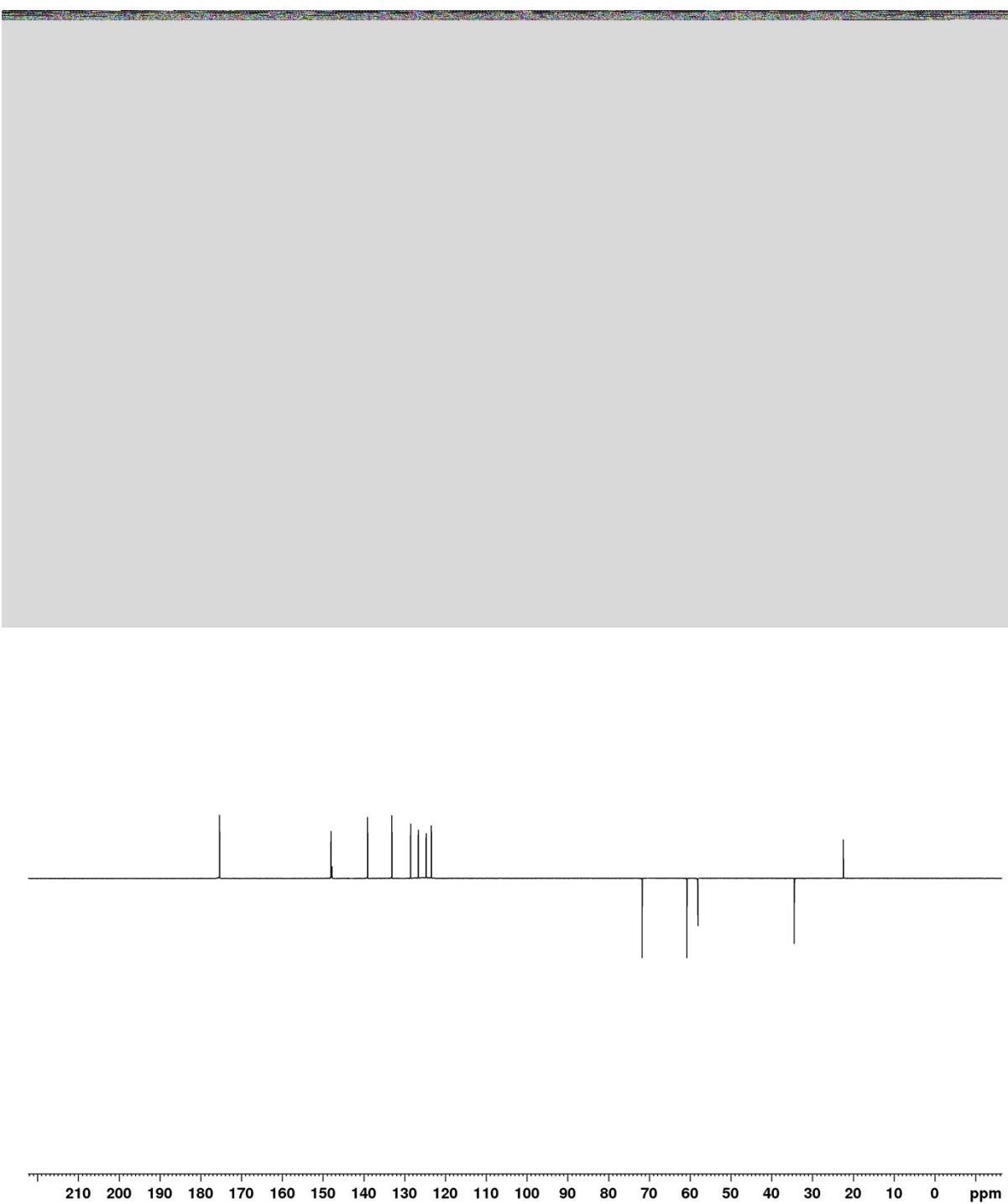


Figure S31. ^1H and ^{13}C NMR spectra for $[\text{OHC}_3\text{-3mpyc}][\text{Man}]$

^1H NMR (D_2O): 2.27 (*m*, 2H, $\text{CH}_2\text{-2}'$), 2.58 (*s*, 3H, CH_3), 3.70 (*t*, 2H, $J_{2',3'} = 6.0$ Hz, CH_2OH), 4.71 (*t*, 2H, $J_{1',2'} = 7.2$ Hz, $\text{CH}_2\text{-1}'$), 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)

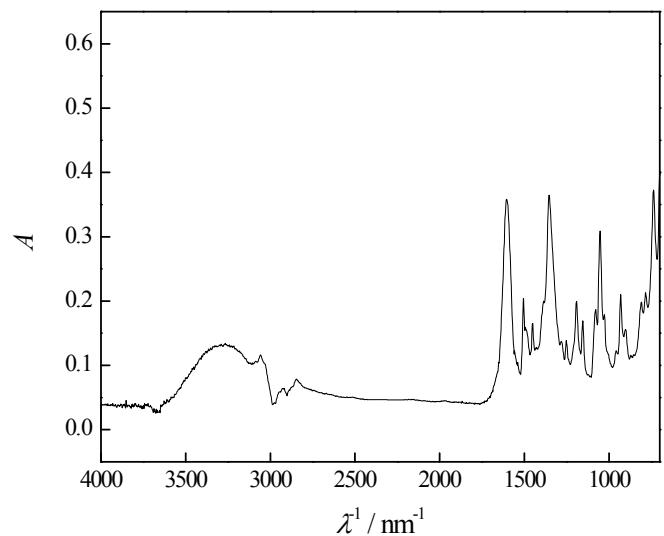


Figure S32. FTIR spectra of $[\text{OHC}_3\text{-3mpyc}][\text{Man}]$

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)

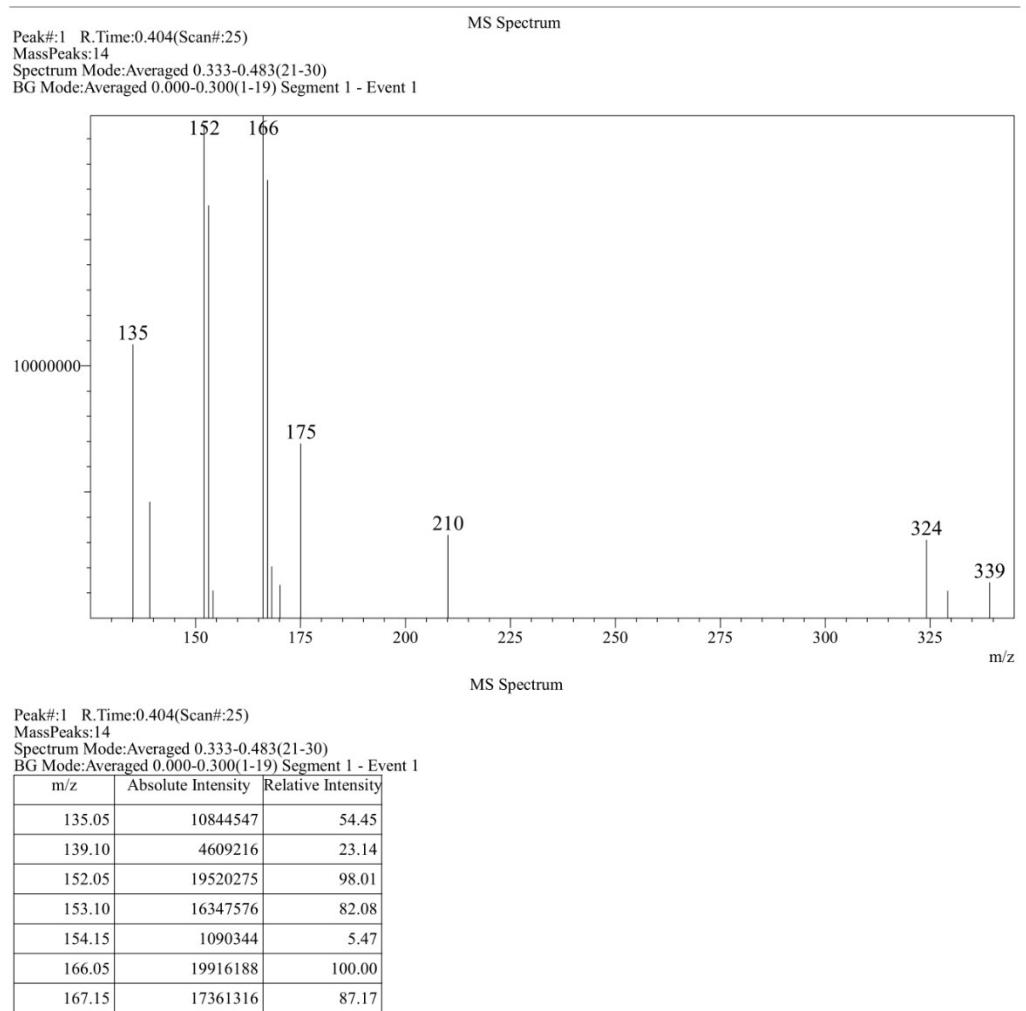


Figure S33. MS spectra of $[\text{OHC}_3\text{-3mpyc}][\text{Man}]$

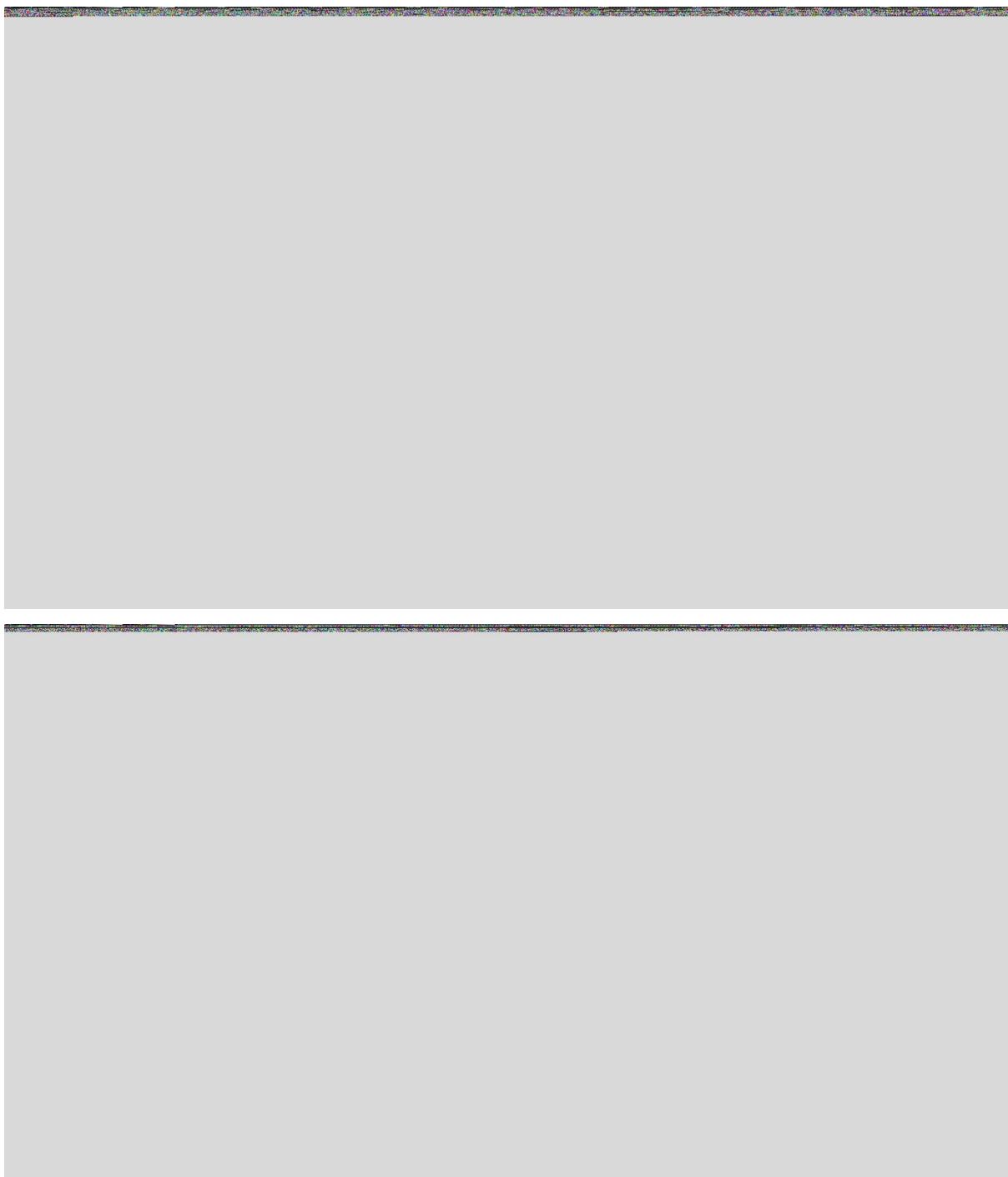


Figure S34. ¹H and ¹³C NMR spectra for [OHC₃-4mpyc][Man]

¹H NMR (D₂O): 2.25 (*m*, 2H, CH₂-2'), 2.67 (*s*, 3H, CH₃), 3.68 (*t*, 2H, *J*_{2',3'} = 6.1 Hz, CH₂OH), 4.67 (*t*, 2H, *J*_{1',2'} = 7.3 Hz, CH₂-1'), 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)

¹³C NMR (D₂O): 24.20 (CH₃), 35.42 (CH₂-2'), 60.62 (HOCH₂), 60.95 (CH₂-1'), 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⁻)

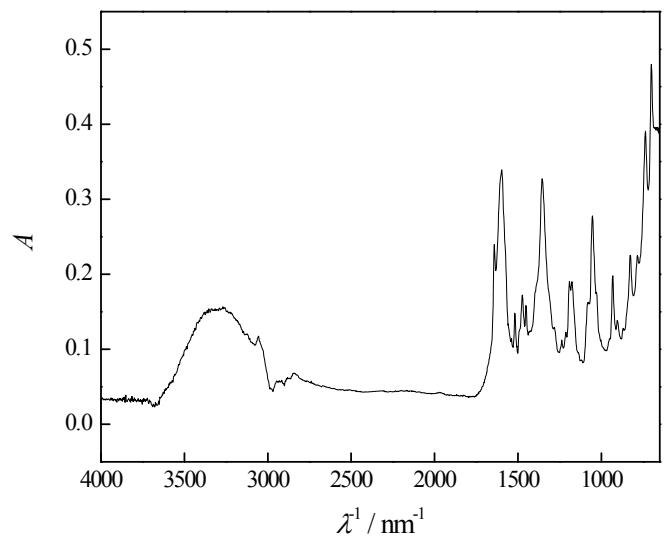


Figure S35. FTIR spectra of $[\text{OHC}_3\text{-4mpic}][\text{Man}]$

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)

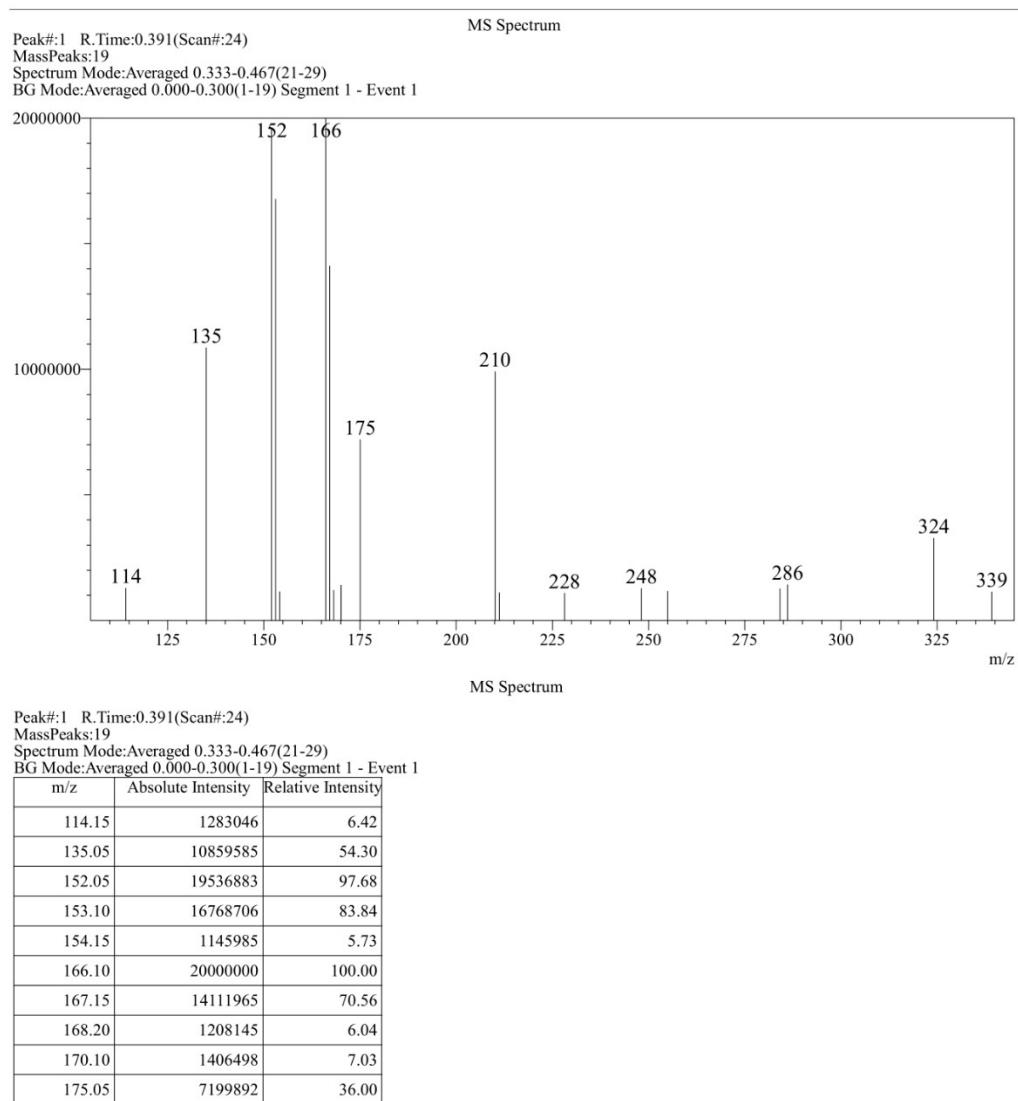


Figure S36. MS spectra of [OHC₃-4mpyc][Man]

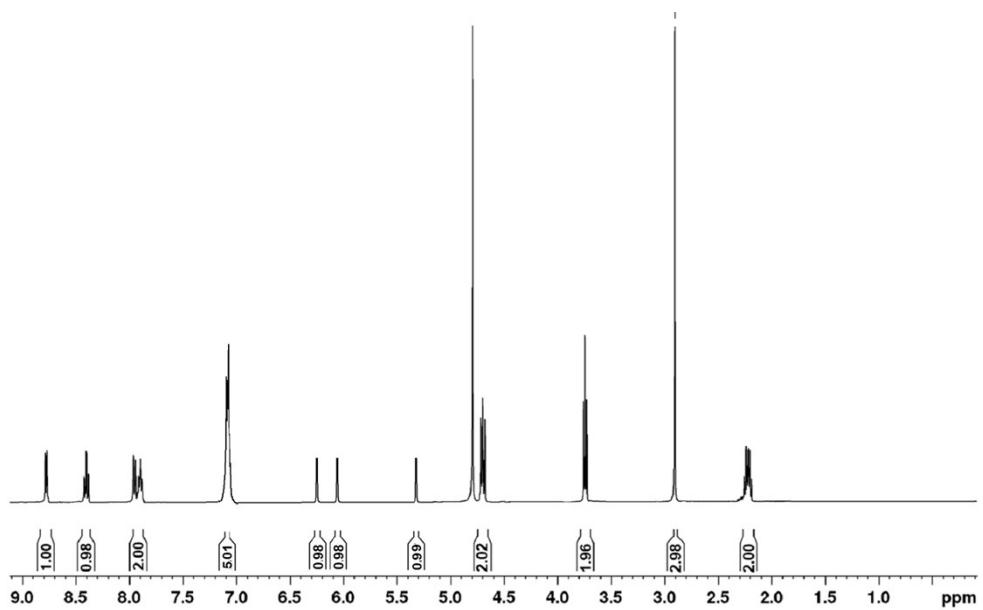


Figure S37. ¹H and ¹³C NMR spectra for [OHC₃-2mpyc][Caff]

¹H NMR (¹D₂O): 2.24 (*m*, 2H, CH₂-2'), 2.94 (*s*, 3H, CH₃), 3.81 (*t*, 2H, *J*_{2',3'} = 6.0 Hz, CH₂OH), 4.70 (*t*, 2H, *J*_{1',2'} = 7.2 Hz, CH₂-1'), 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)

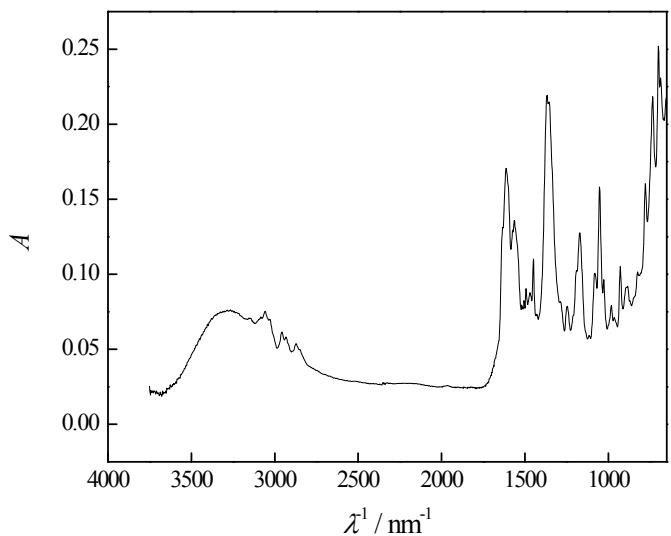
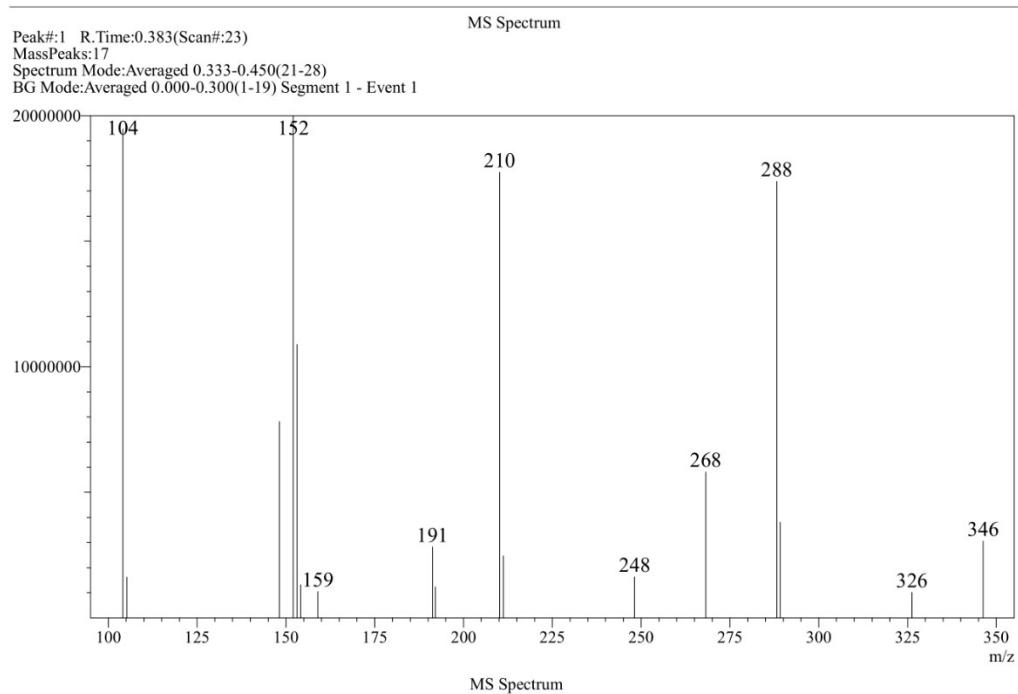


Figure S38. FTIR spectra of $[\text{OHC}_3\text{-2mpyc}][\text{Caff}]$

3211 (stretching OH), 1469 (skeletal vibration of caffeate 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)



Peak#:1 R.Time:0.383(Scan#:23)
 MassPeaks:17
 Spectrum Mode:Averaged 0.333-0.450(21-28)
 BG Mode:Averaged 0.000-0.300(1-19) Segment 1 - Event 1

m/z	Absolute Intensity	Relative Intensity
104.10	19464599	97.32
105.20	1627402	8.14
148.15	7820362	39.10
152.05	20000000	100.00
153.10	10890251	54.45
154.15	1326844	6.63
159.00	1049371	5.25
191.20	2832666	14.16
192.05	1235103	6.18

Figure S39. MS spectra of [OHC₃-2mpyc][Caff]

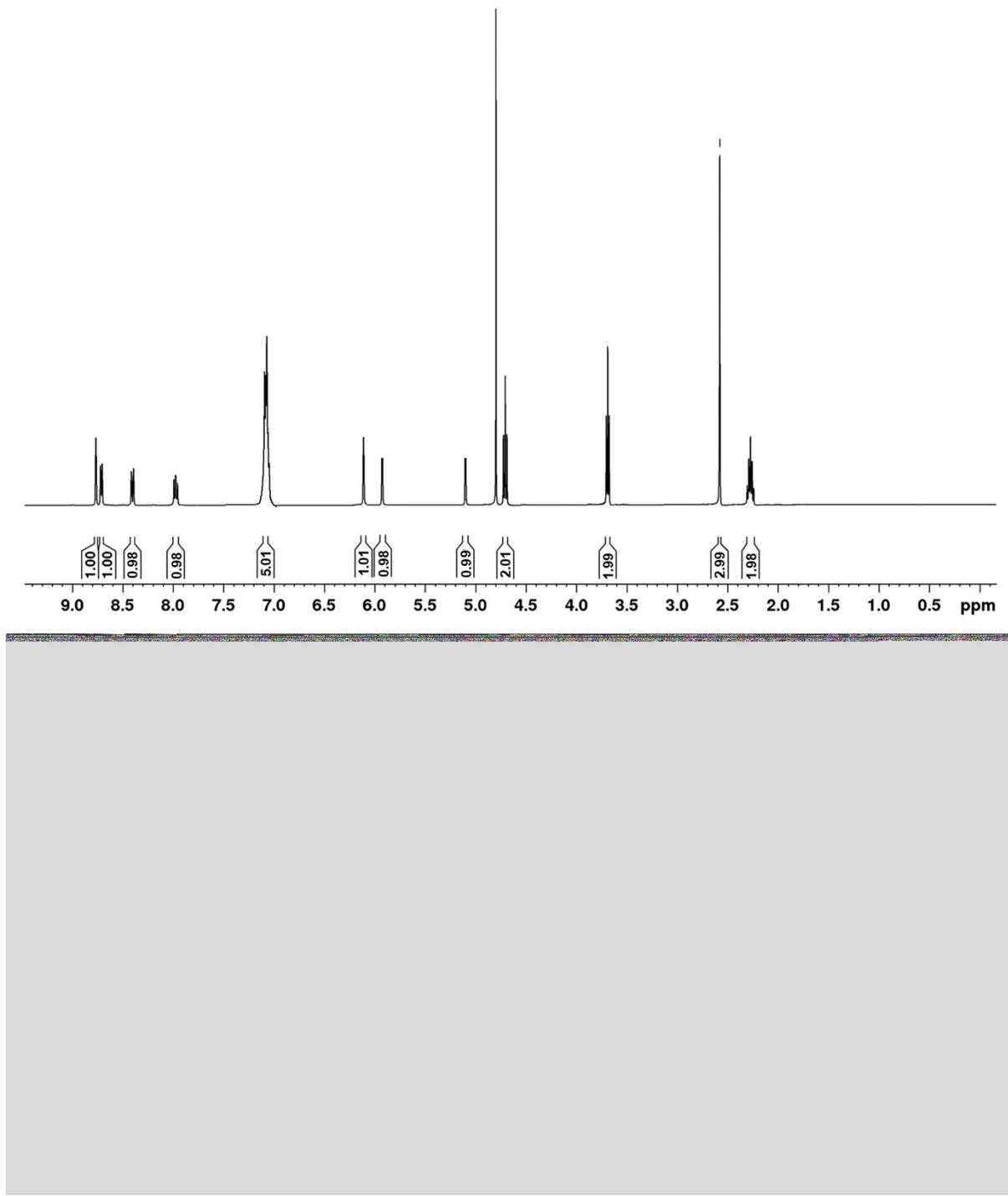


Figure S40. ^1H and ^{13}C NMR spectra for $[OHC_3\text{-}3\text{mpyc}][\text{Caff}]$

^1H NMR (D_2O): 2.28 (*m*, 2H, $CH_2\text{-}2'$), 2.62 (*s*, 3H, CH_3), 3.74 (*t*, 2H, $J_{2',3'} = 6.0$ Hz, $CH_2\text{OH}$), 4.71 (*t*, 2H, $J_{1',2'} = 7.2$ Hz, $CH_2\text{-}1'$), 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_2O): 20.54 (CH_3), 35.51 ($CH_2\text{-}2'$), 60.84 ($HOCH_2$), 61.73 ($CH_2\text{-}1'$), 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^-)

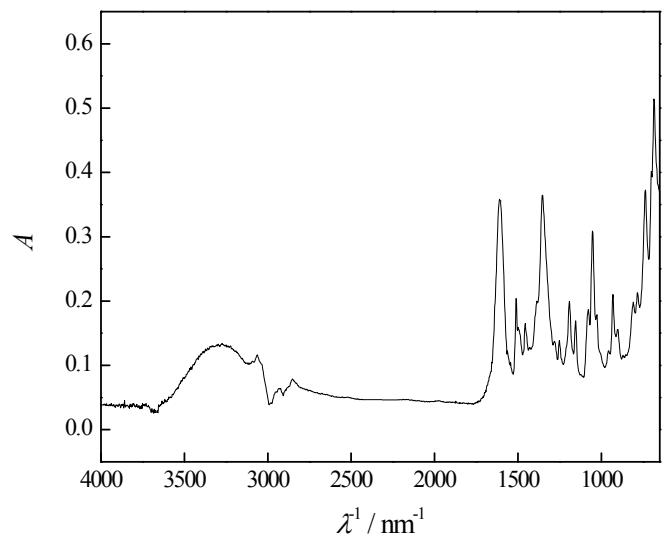


Figure S41. FTIR spectra of $[\text{OHC}_3\text{-3mpyc}][\text{Caff}]$

3202 (stretching OH), 1461 (skeletal 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)

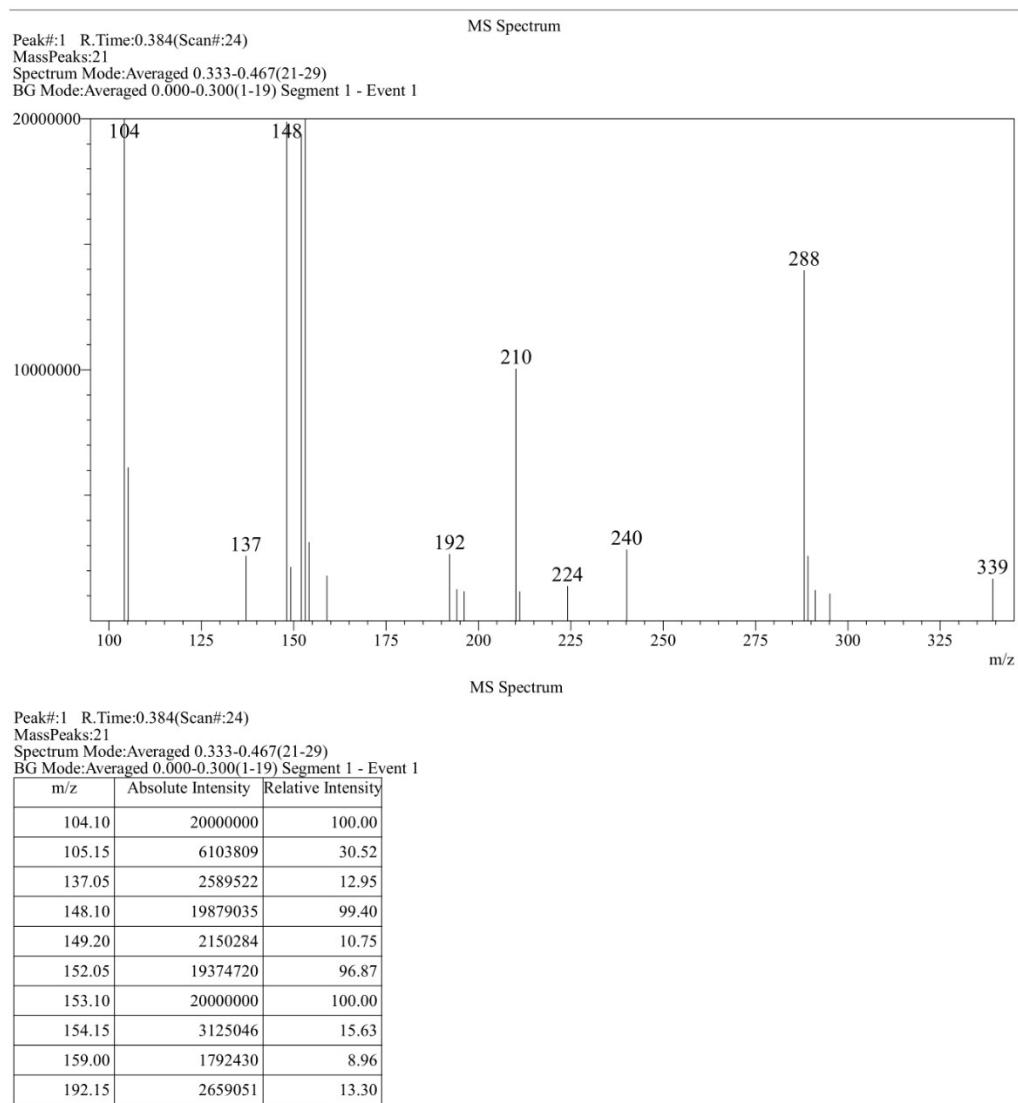


Figure S42. MS spectra of [OHC₃-3mpyc][Caff]

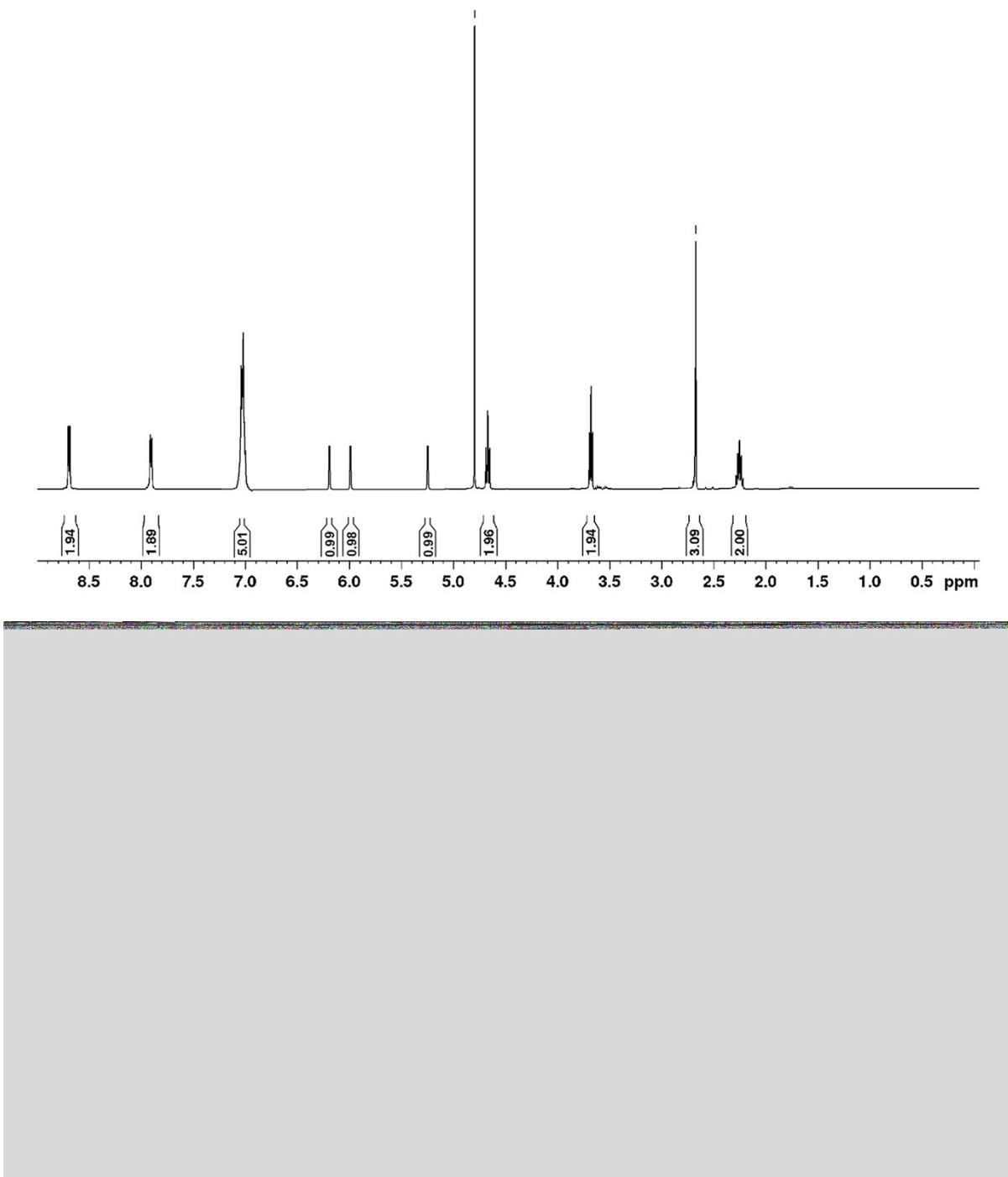


Figure S43. ^1H and ^{13}C NMR spectra for $[\text{OHC}_3\text{-4mpyc}][\text{Caff}]$

^1H NMR (D_2O): 2.20 (*m*, 2H, $\text{CH}_2\text{-2}'$), 2.69 (*s*, 3H, CH_3), 3.74 (*t*, 2H, $J_{2',3'} = 6.1$ Hz, CH_2OH), 4.67 (*t*, 2H, $J_{1',2'} = 7.3$ Hz, $\text{CH}_2\text{-1}'$), 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_2O): 24.20 (CH_3), 35.96 ($\text{CH}_2\text{-2}'$), 61.62 (HOCH_2), 61.95 ($\text{CH}_2\text{-1}'$), 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^-)

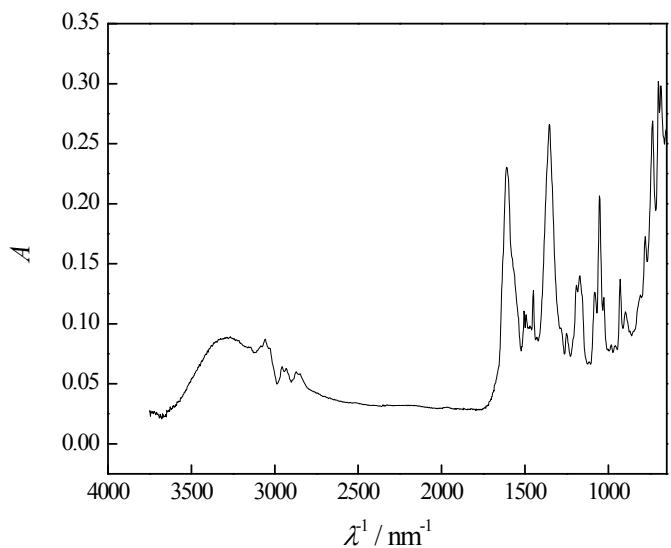


Figure S44. FTIR spectra of [OHC₃-4mpyc][Caff]

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)

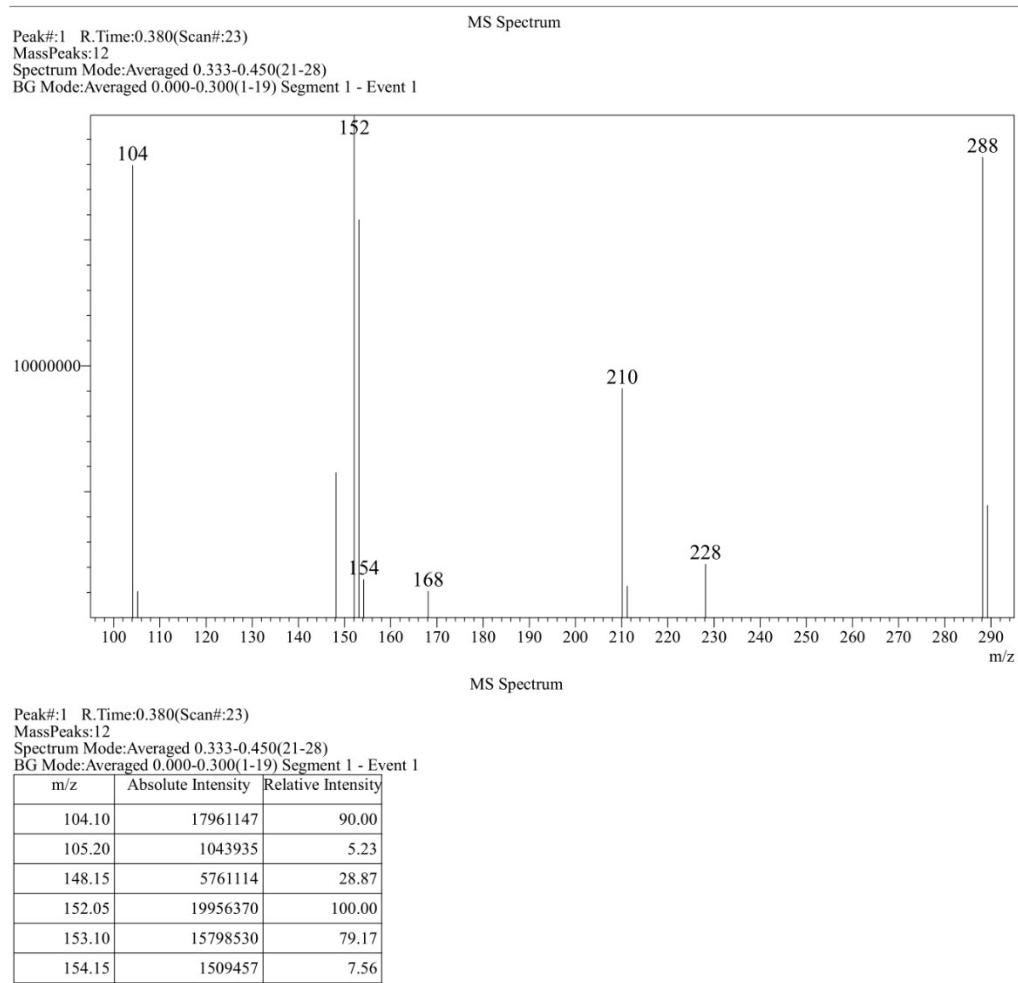


Figure S45. MS spectra of [OHC₃-4mpyc][Caff]

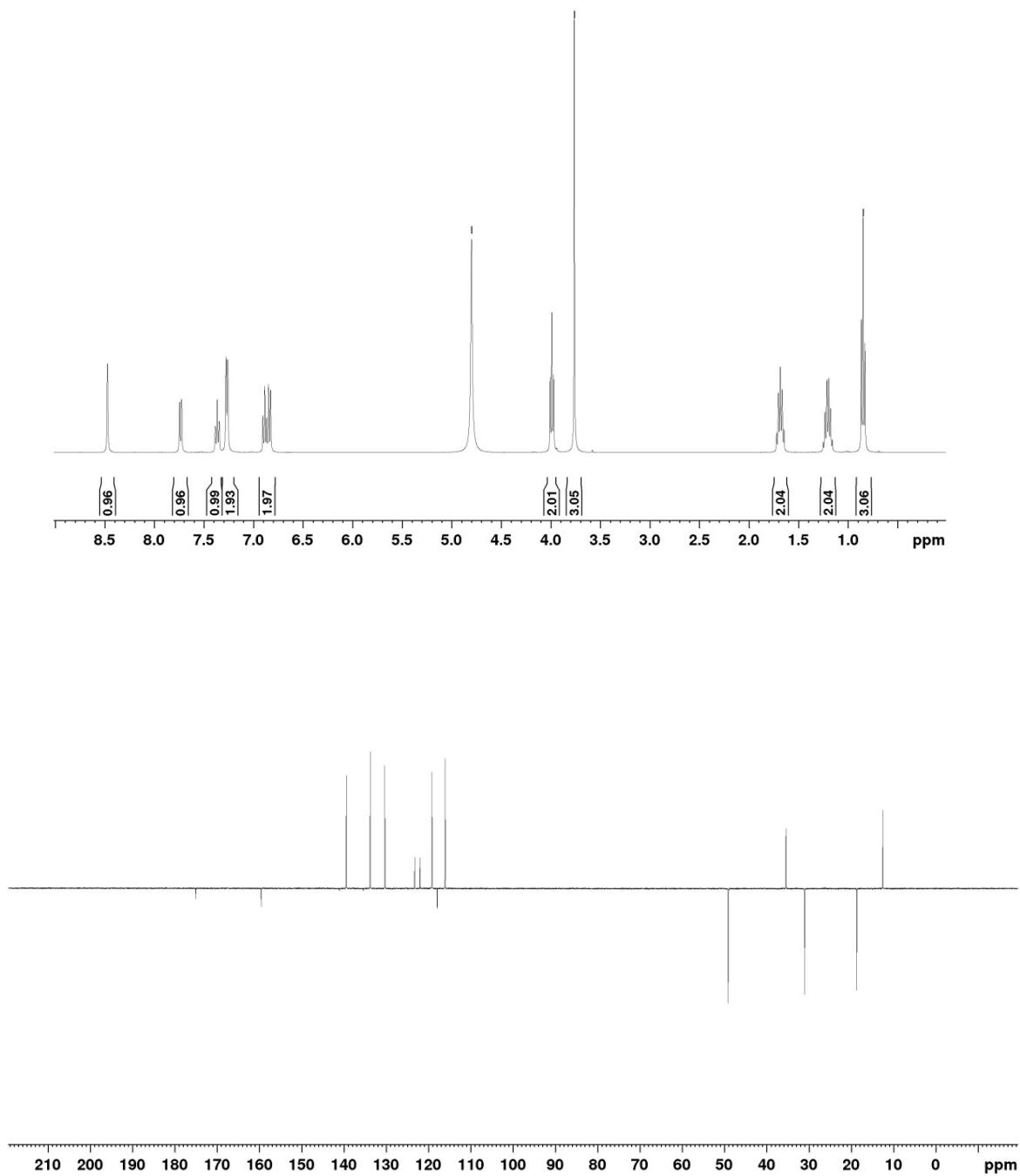


Figure S46. ^1H and ^{13}C NMR spectra for [bmim][Cin]

^1H NMR (D₂O): 2.31 (*m.* 2H. NCH₂CH₂CH₂CH₃); 3.86 (*t.* 2H. J=6.1 Hz. NCH₂CH₂CH₂CH₃); 3.96 (*s.* 3H. CH₃); 4.31 (*t.* 2H. J=7.1 Hz. NCH₂CH₂CH₂CH₃); 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 (D₂O): 31.44 (NCH₂CH₂CH₂CH₃); 35.94 (CH_3); 46.79 (NCH₂CH₂CH₂CH₃); 57.86 (NCH₂CH₂CH₂CH₃); 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⁻)

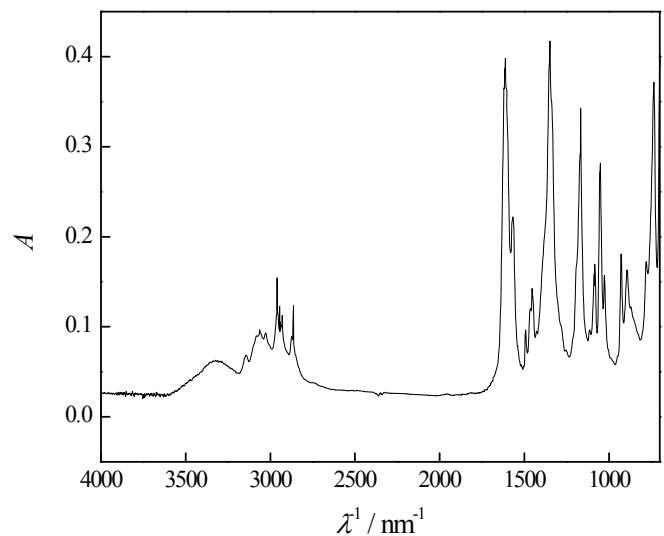


Figure S47. FTIR spectra of [bmim][Cin]

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)

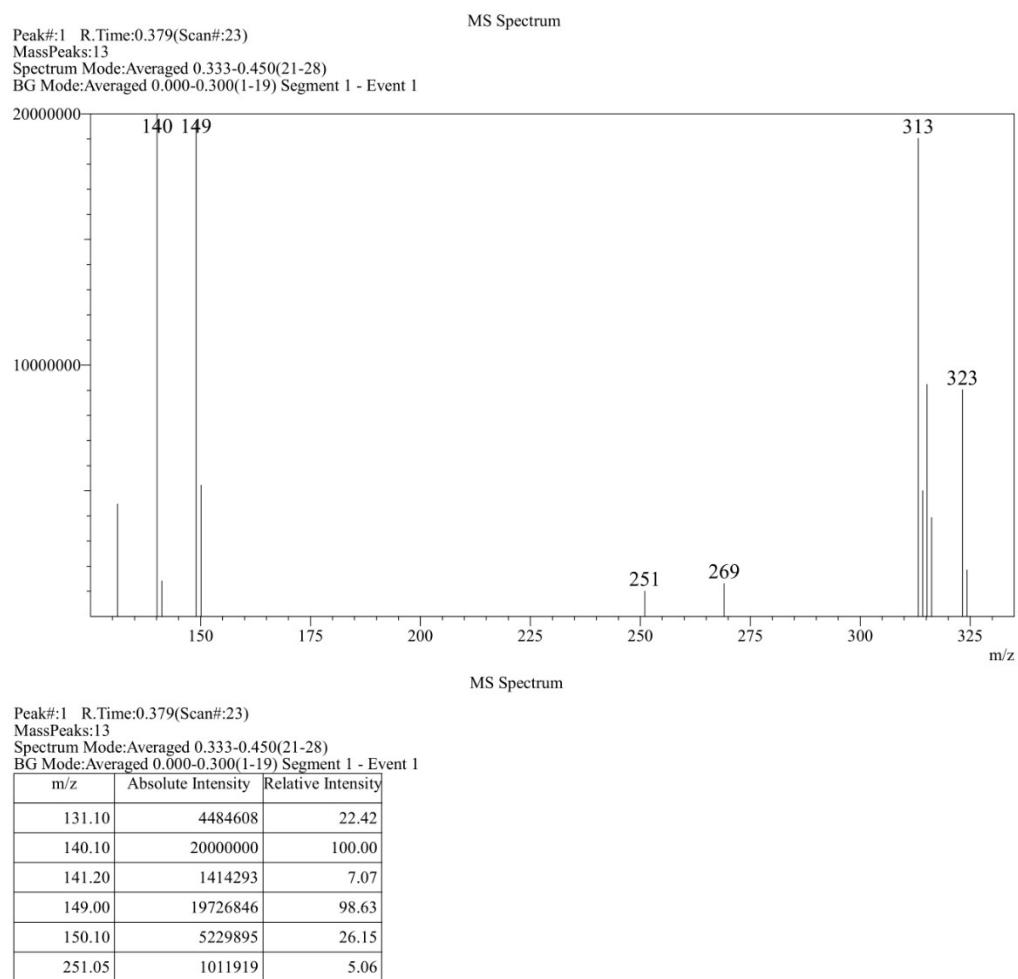


Figure S48. MS spectra of [bmim][Cin]

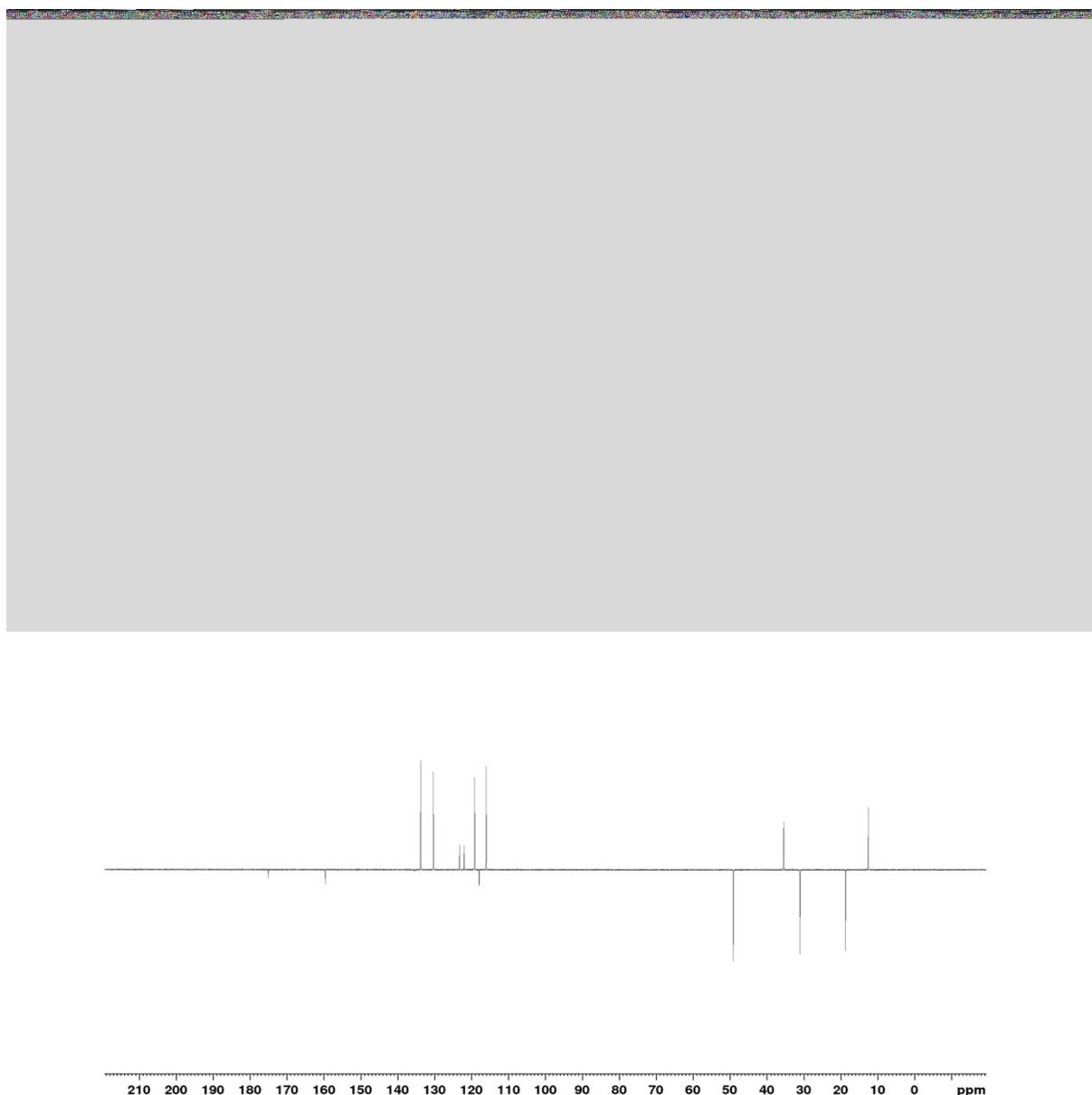


Figure S49. ^1H and ^{13}C NMR spectra for [bmim][Man]

^1H NMR (D_2O): ^1H NMR (D_2O): 2.11 (*m*. 2H. $\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$); 3.67 (*t*. 2H. $J=6.1$ Hz. $\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$); 3.96 (*s*. 3H. CH_3); 4.34 (*t*. 2H. $J=7.1$ Hz. $\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$); 5.26 ($\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$); 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_2O): 31.22 ($\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$); 35.81 (CH_3); 46.79 ($\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$); 57.93 ($\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$); 77.44 ($\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$); 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^-)

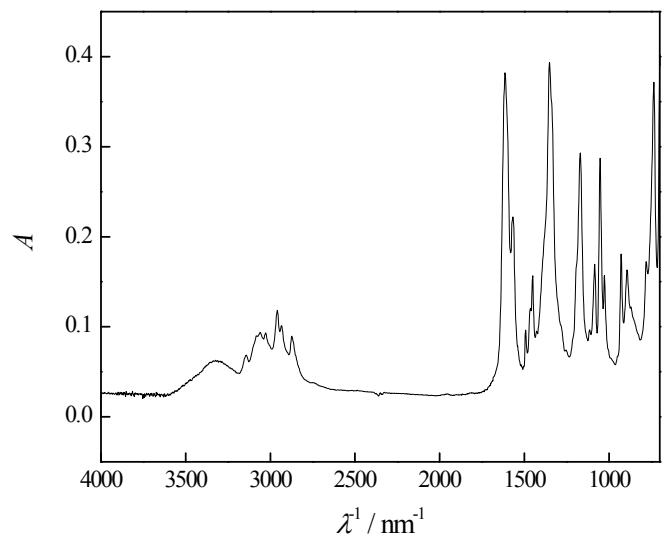


Figure S50. FTIR spectra of [bmim][Man]

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)

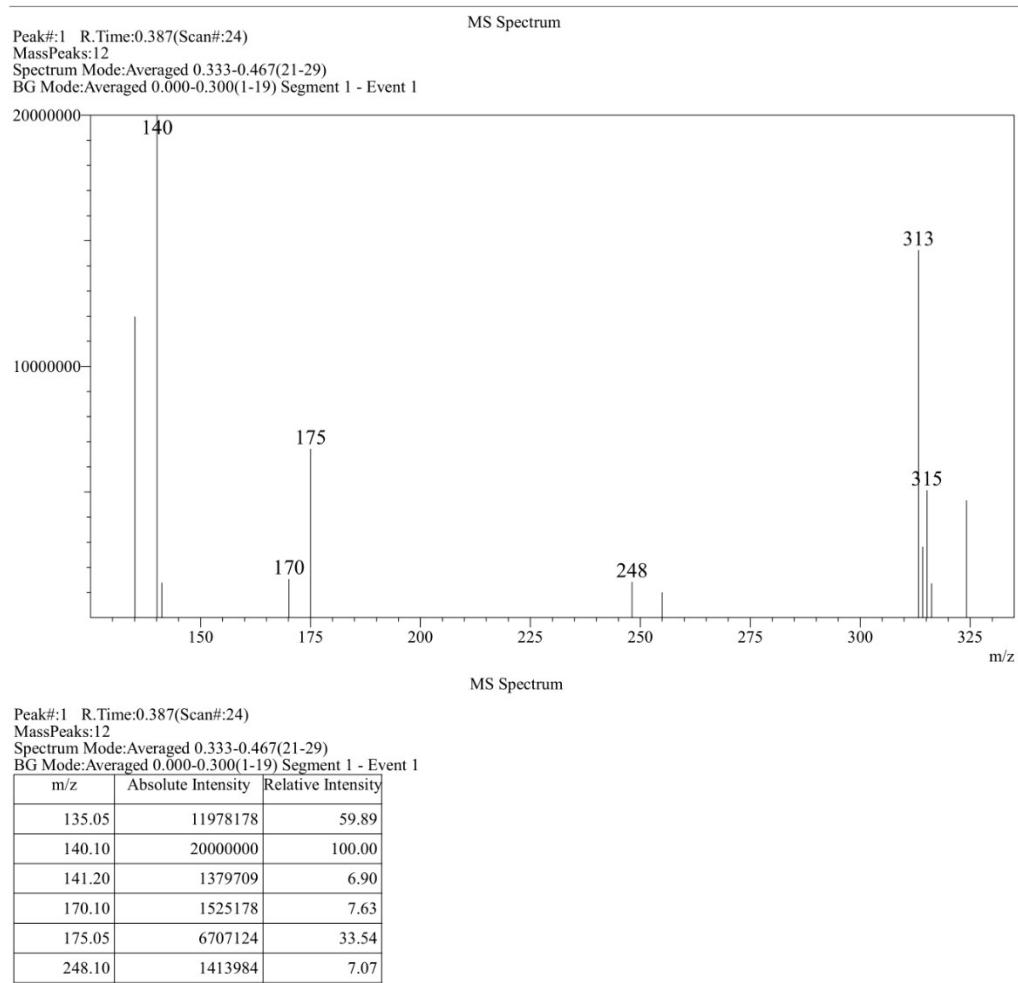


Figure S51. MS spectra of [bmim][Man]

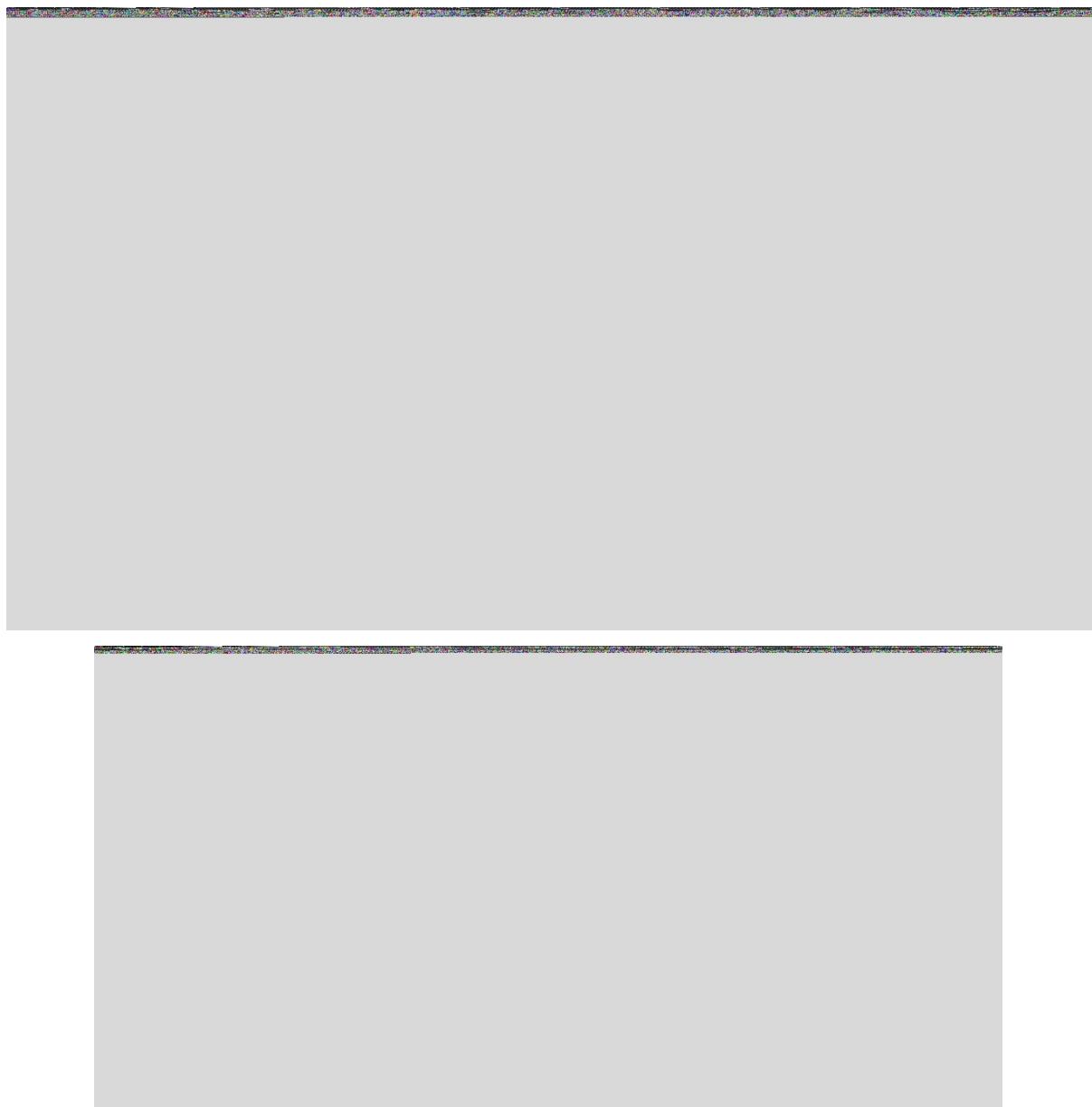


Figure S52. ¹H and ¹³C NMR spectra for [bmim][Caff]

¹H NMR (D₂O): ¹H NMR (D₂O): 2.09 (*m*. 2H. NCH₂CH₂CH₂CH₃); 3.71 (*t*. 3H. J=6.1 Hz. NCH₂CH₂CH₂CH₃); 3.82 (*s*. 3H. CH₃); 4.31(*t*. 2H. J=7.1 Hz. NCH₂CH₂CH₂CH₃); 5.29 (*s*, 3H, NCH₂CH₂CH₂CH₃); 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).

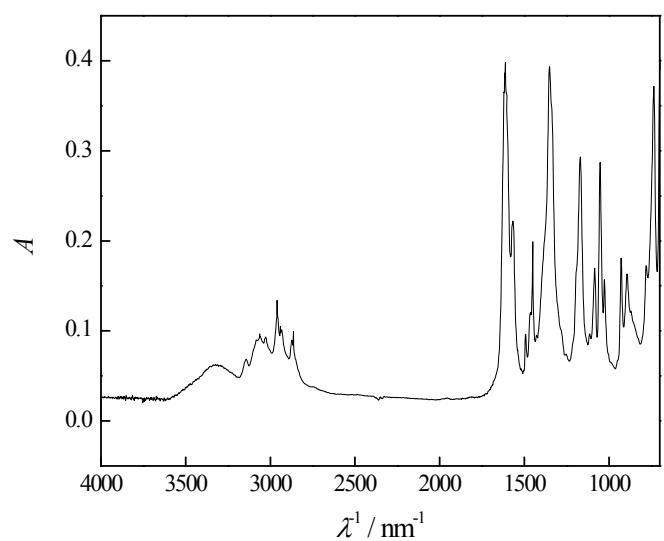
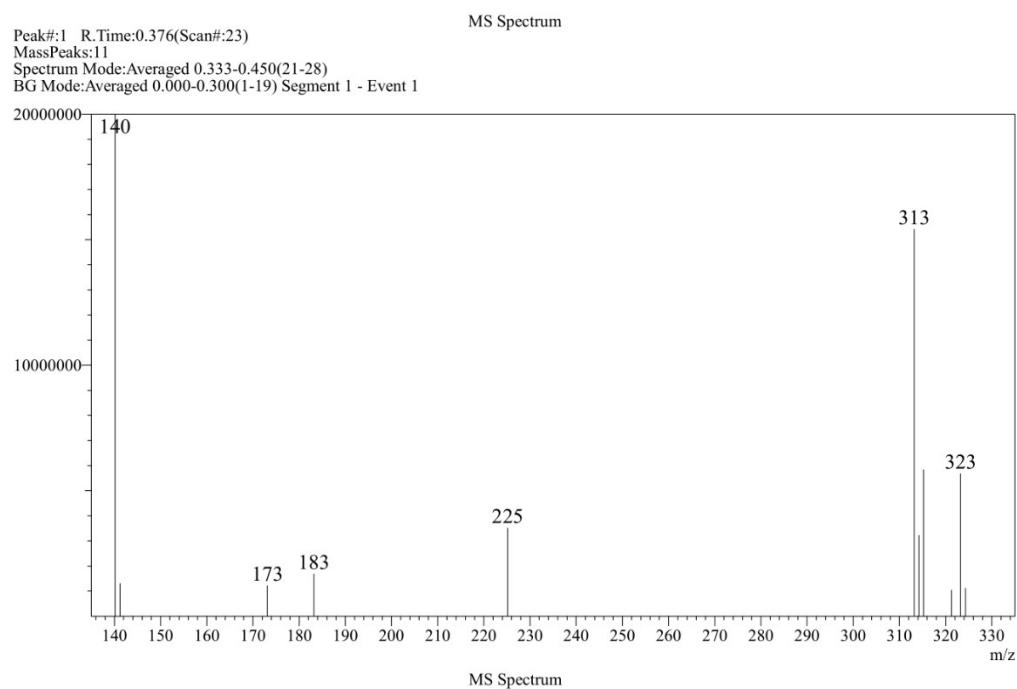


Figure S53. FTIR spectra of [bmim][Caff]

3198 (N-H streching); 2976 (asym. stretching CH₃), 2894 (sym. stretching CH₃), 1501 (in plane vibrations of imidazolium ring), 1434 (skeletal vibration of caffate 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)



Peak#:1 R.Time:0.376(Scan#:23)
 MassPeaks:11
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 BG Mode:Averaged 0.000-0.300(1-19) Segment 1 - Event 1

m/z	Absolute Intensity	Relative Intensity
140.10	20000000	100.00
141.20	1300361	6.50
173.10	1210078	6.05
183.20	1685438	8.43
225.15	3511997	17.56

Figure S54. MS spectra of [bmim][Caff]

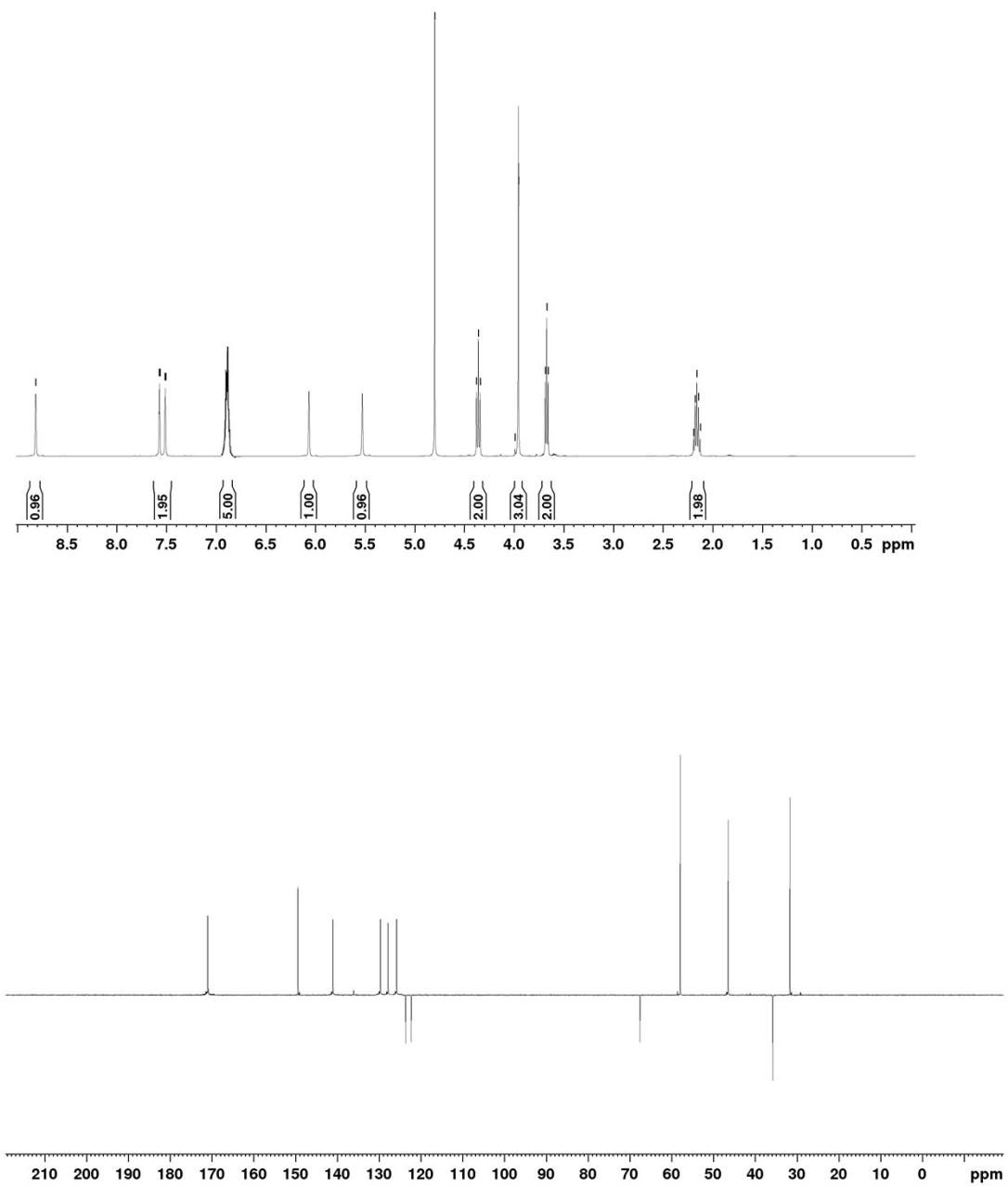


Figure S55. ^1H and ^{13}C NMR spectra for $[\text{OHC}_3\text{mim}][\text{Cin}]$

^1H NMR (D_2O): 2.31 (*m*. 2H. $\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 3.83 (*t*. 2H. $J=6.1$ Hz. $\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 3.96 (*s*. 3H. CH_3); 4.31 (*t*. 2H. $J=7.1$ Hz. $\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 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_2O): 31.44 ($\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 35.94 (CH_3); 46.79 ($\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 57.93 ($\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 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^-)

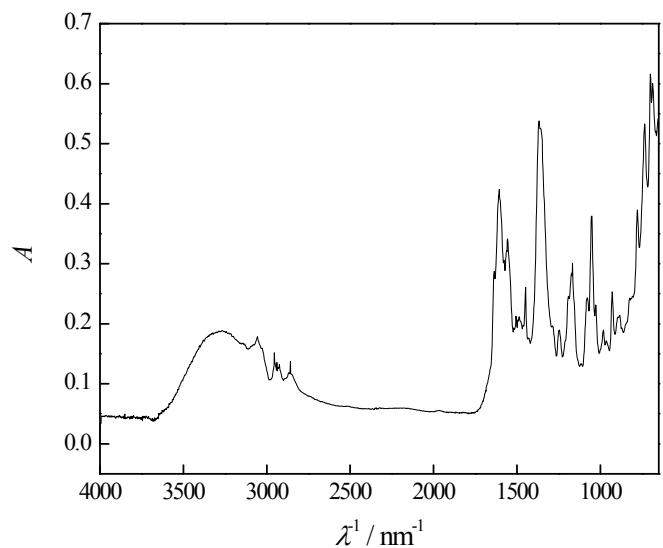


Figure S56. FTIR spectra of $[\text{OHC}_3\text{mim}][\text{Cin}]$

3079 (stretching OH), 2946 (asym. stretching CH_3), 2845 (sym. stretching CH_3), 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)

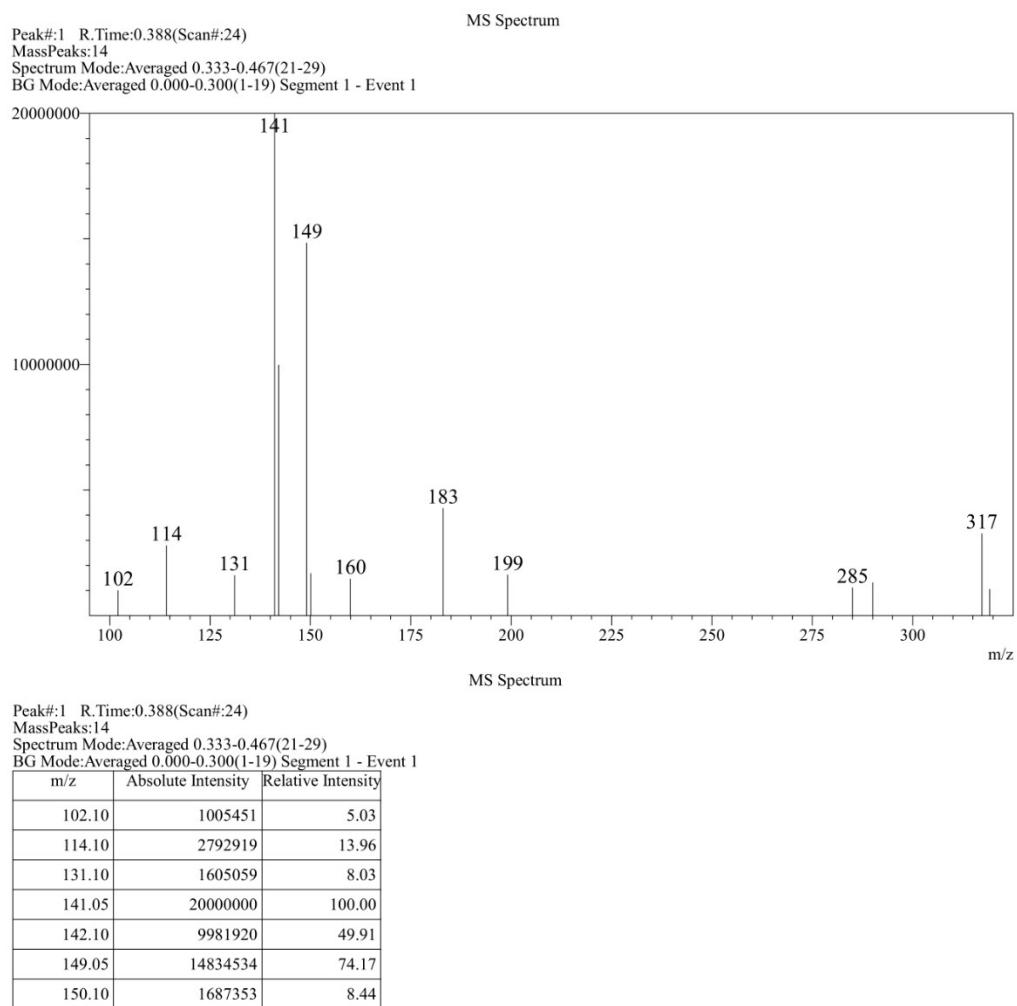


Figure S57. MS spectra of [OHC₃mim][Cin]

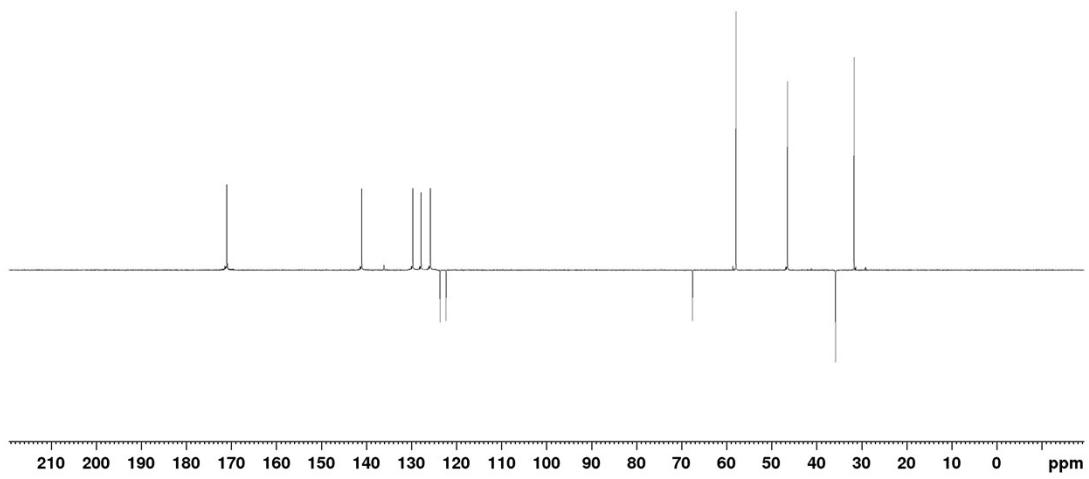


Figure S58. ^1H and ^{13}C NMR spectra for $[\text{OHC}_3\text{mim}][\text{Man}]$

^1H NMR (D_2O): ^1H NMR (D_2O): 2.16 (*m*. 2H. $\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 3.67 (*t*. 2H. $J=6.1$ Hz. $\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 3.96 (*s*. 3H. CH_3); 4.36 (*t*. 2H. $J=7.1$ Hz. $\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 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_2O): 31.49 ($\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 35.81 (CH_3); 46.79 ($\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 57.93 ($\text{NCH}_2\text{CH}_2\text{CH}_2\text{OH}$); 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^-)

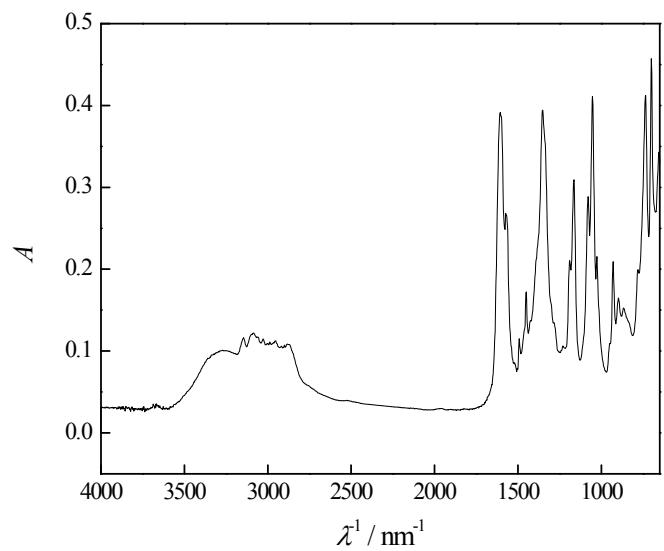
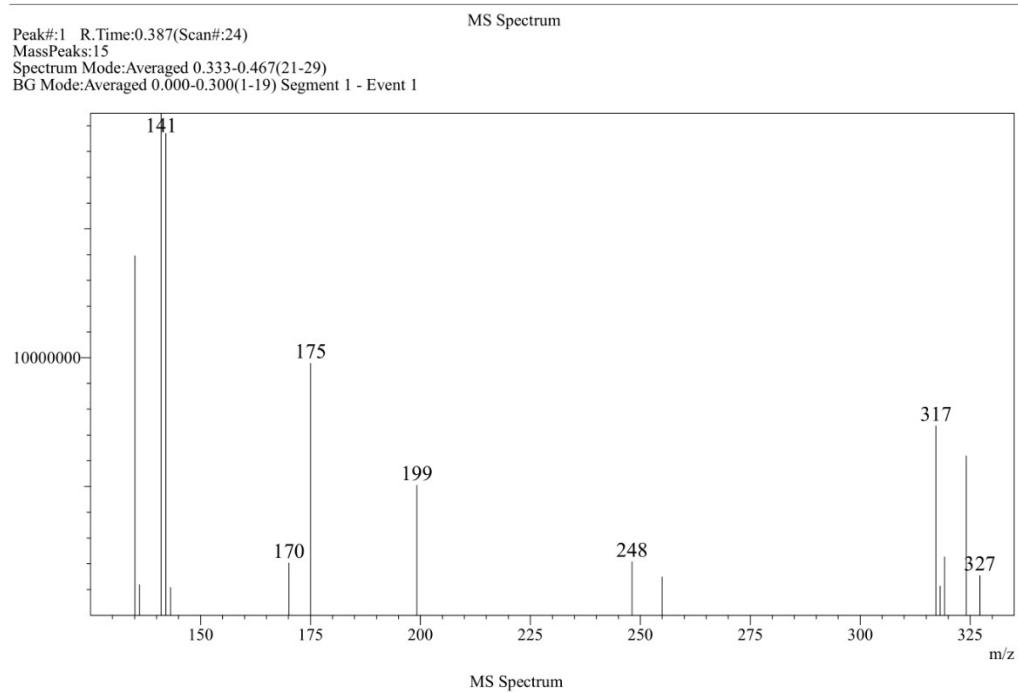


Figure S59. FTIR spectra of $[\text{OHC}_3\text{mim}][\text{Man}]$

3204 (stretching vibration OH from mandelate), 3086 (stretching OH), 2954 (asym. stretching CH_3), 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)



Peak#:1 R.Time:0.387(Scan#:24)
 MassPeaks:15
 Spectrum Mode:Averaged 0.333-0.467(21-29)
 BG Mode:Averaged 0.000-0.300(1-19) Segment 1 - Event 1

m/z	Absolute Intensity	Relative Intensity
135.05	13960292	71.63
136.10	1190379	6.11
141.00	19488990	100.00
142.10	18711759	96.01
143.20	1086124	5.57
170.10	2032978	10.43
175.05	9783340	50.20
199.15	5056877	25.95

Figure S60. MS spectra of [OHC₃mim][Man]

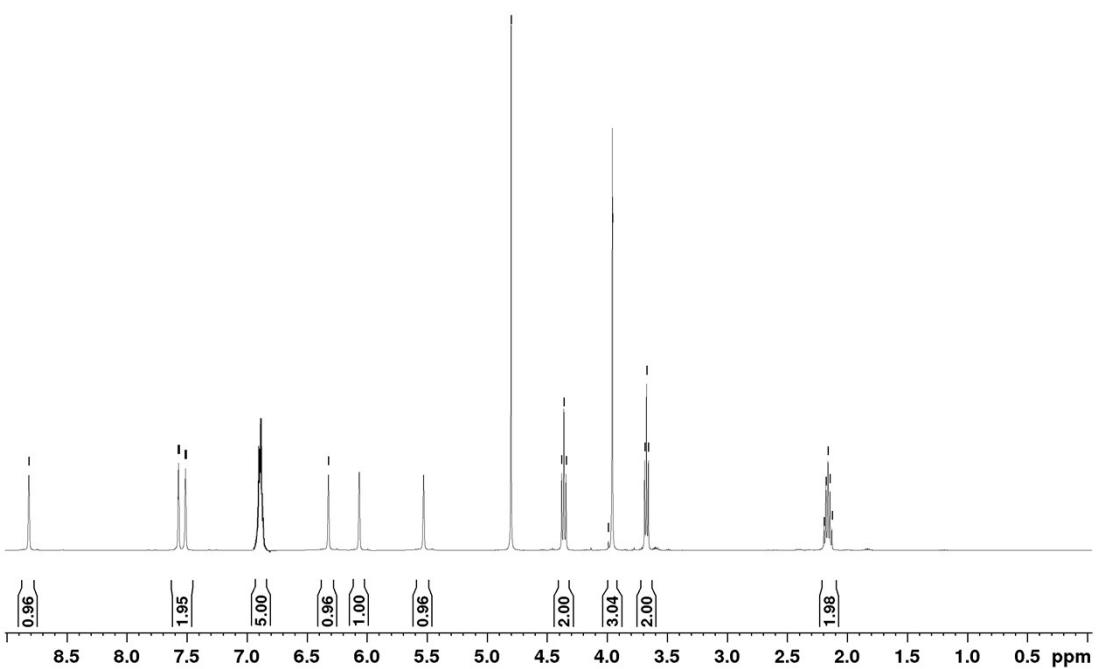


Figure S61. ¹H and ¹³C NMR spectra for [OHC₃mim][Caff]

¹H NMR (D₂O): ¹H NMR (D₂O): 2.19 (*m.* 2H. NCH₂CH₂CH₂OH); 3.71 (*t.* 2H. J=6.1 Hz. NCH₂CH₂CH₂OH); 3.89 (*s.* 3H. CH₃); 4.39 (*t.* 2H. J=7.1 Hz. NCH₂CH₂CH₂OH); 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).

¹³C NMR (D₂O): 31.82 (NCH₂CH₂CH₂OH); 36.22 (CH₃); 46.75 (NCH₂CH₂CH₂OH); 57.93 (NCH₂CH₂CH₂OH); 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⁻)

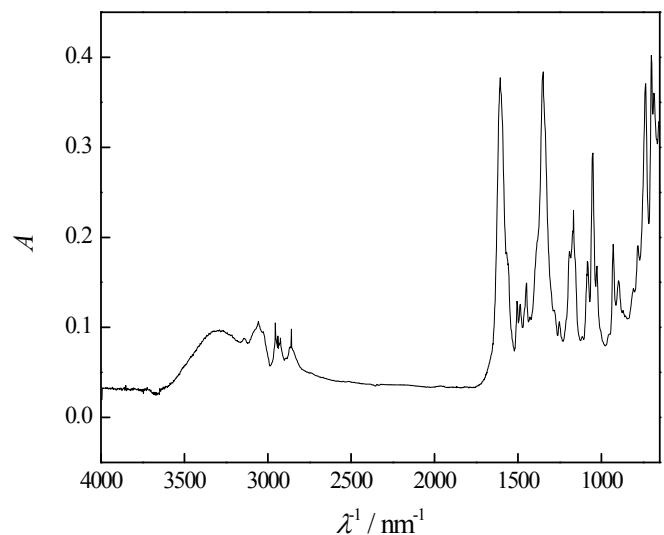


Figure S62. FTIR spectra of [OHC₃mim][Caff]

3126 (stretching OH), 2945 (asym. stretching CH₃), 2849 (sym. stretching CH₃), 1533 (in plane vibrations of imidazolium ring), 1442 (skeletal vibration of caffate 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)

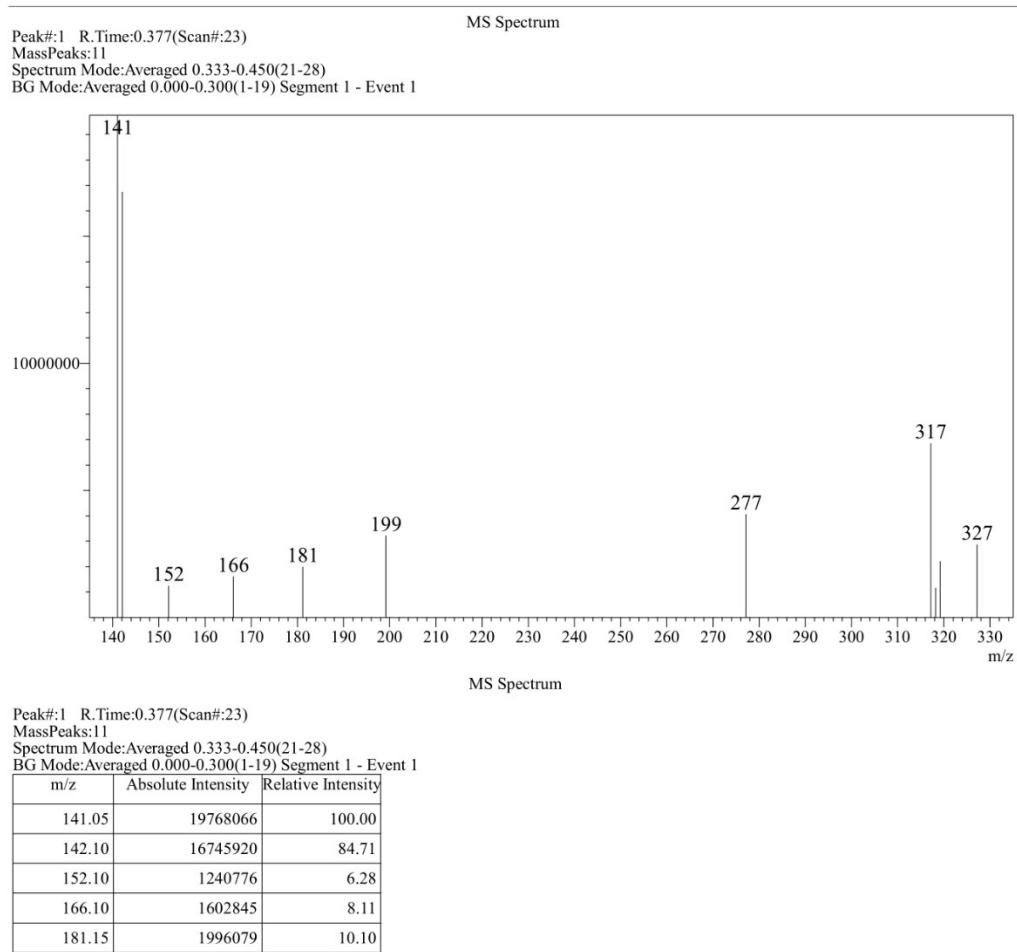


Figure S63. MS spectra of [OHC₃mim][Caff]