

**Dual function of Amino Acids Ionic Liquids (Bmim[AA]) on the Degradation of  
Organophosphorus Pesticide, Paraoxon®**

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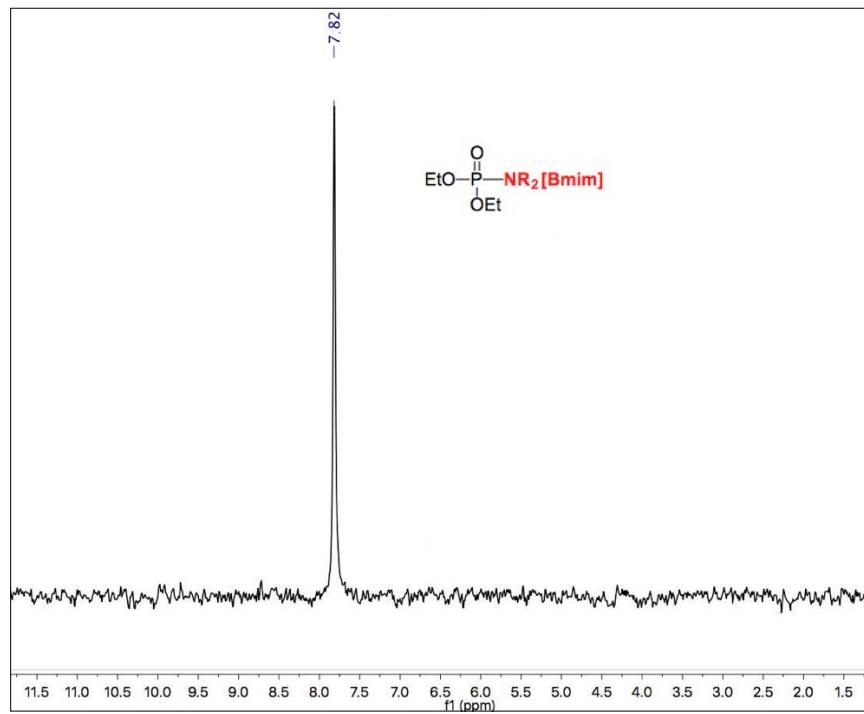
## Table of Contents

<b>Figure S1.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>2a</b> , obtained in the reaction of <i>O,O</i> -diethyl chlorophosphate with Bmim[Pro] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S2.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>2b</b> , obtained in the reaction of <i>O,O</i> -diethyl chlorophosphate with Bmim[Ala] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S3.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>2c</b> , obtained in the reaction of <i>O,O</i> -diethyl chlorophosphate with Bmim[Phe] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S4.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>2d</b> , obtained in the reaction of <i>O,O</i> -diethyl chlorophosphate with Bmim[Asp] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S5.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>2e</b> , obtained in the reaction of <i>O,O</i> -diethyl chlorophosphate with Bmim[Ser] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S6.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>2f</b> , obtained in the reaction of <i>O,O</i> -diethyl chlorophosphate with Bmim[Gly] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S7.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>2g</b> , obtained in the reaction of <i>O,O</i> -diethyl chlorophosphate with Bmim[Met] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S8.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>3</b> , obtained in the reaction <i>O,O</i> -diethyl chlorophosphate with NaOH in Bmim[Pro] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S9.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>3</b> , obtained in the reaction <i>O,O</i> -diethyl chlorophosphate with NaOH in Bmim[Ala] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S10.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>3</b> , obtained in the reaction <i>O,O</i> -diethyl chlorophosphate with NaOH in Bmim[Phe] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S11.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>3</b> , obtained in the reaction <i>O,O</i> -diethyl chlorophosphate with NaOH in Bmim[Asp] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S12.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>3</b> , obtained in the reaction <i>O,O</i> -diethyl chlorophosphate with NaOH in Bmim[Ser] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S13.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>3</b> , obtained in the reaction <i>O,O</i> -diethyl chlorophosphate with NaOH in Bmim[Gly] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S14.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>3</b> , obtained in the reaction <i>O,O</i> -diethyl chlorophosphate with NaOH in Bmim[Met] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S15.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>3</b> , obtained in the reaction <i>O,O</i> -diethyl chlorophosphate with NaOH in Bmim[Cys] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S16.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>3</b> , obtained in the reaction <i>O,O</i> -diethyl chlorophosphate with NaOH in Bmim[His] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S17.</b> Time-dependent UV-vis spectra of compound 6, obtained in the reaction of Paraoxon® in Bmim[Pro].
<b>Figure S18. (a)</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>4</b> in Bmim[Pro]. <b>(b)</b> $^1\text{H}$ -NMR spectrum (400MHz, DMSO) of compound <b>4</b> . <b>(c)</b> $^{13}\text{C}$ -NMR spectrum (400MHz, DMSO) of compound <b>4</b> .
<b>Figure S19.</b> Experimental plot of absorbance (at 420 nm) vs time for the reaction of Paraoxon in Bmim[Pro] at 2.50 $^{\circ}\text{C}$ .
<b>Figure S20.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>5a</b> , obtained in the reaction of O-ethyl 4-nitrophenyl phosphate monoester with Bmim[Pro].
<b>Figure S21.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>5b</b> , obtained in the reaction of O-ethyl 4-nitrophenyl phosphate monoester with Bmim[Ala] at 25.0 $^{\circ}\text{C}$ .

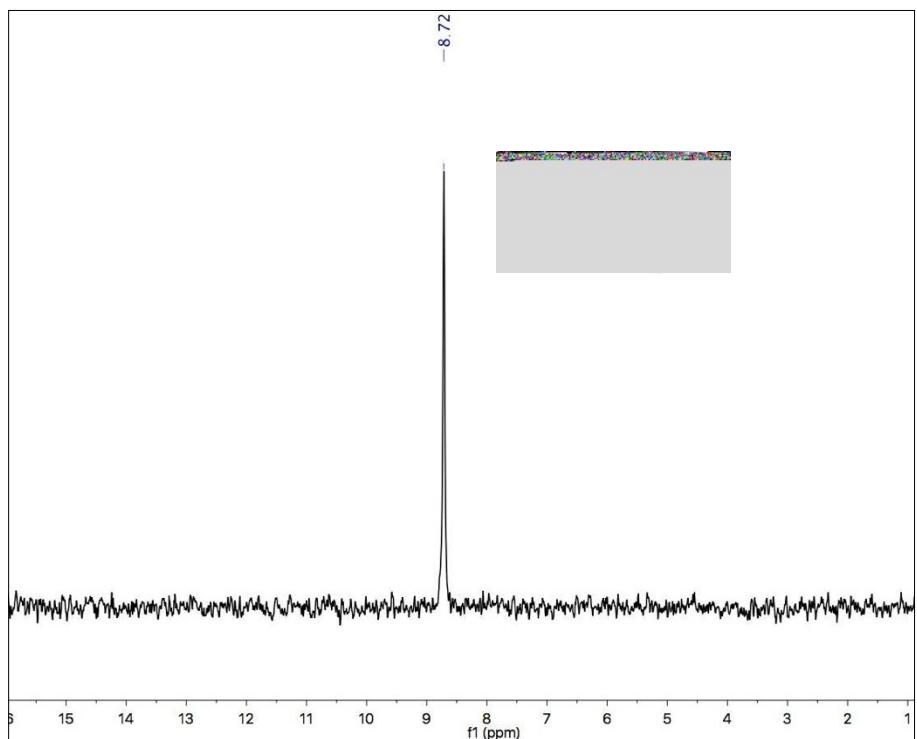
<b>Figure S22.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>5c</b> , obtained in the reaction of O-ethyl 4-nitrophenyl phosphate monoester with Bmim[Phe] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S23.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>5d</b> , obtained in the reaction of O-ethyl 4-nitrophenyl phosphate monoester with Bmim[Asp] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S24.</b> $^{31}\text{P}$ -NMR spectrum (400MHz) of compound <b>5e</b> , obtained in the reaction of O-ethyl 4-nitrophenyl phosphate monoester with Bmim[Ser] at 25.0 $^{\circ}\text{C}$ .
<b>Figure S25.</b> Stacked $^{31}\text{P}$ -NMR plot for the reaction of Paraoxón 0.015M in Bmim[Ala] at 25 $^{\circ}\text{C}$ .
<b>Figure S26.</b> Stacked $^{31}\text{P}$ -NMR plot for the reaction of Paraoxón 0.015M in Bmim[Phe] at 25 $^{\circ}\text{C}$ .
<b>Figure S27.</b> Stacked $^{31}\text{P}$ -NMR plot for the reaction of Paraoxón 0.015M in Bmim[Asp] at 25 $^{\circ}\text{C}$ .
<b>Figure S28.</b> Stacked $^{31}\text{P}$ -NMR plot for the reaction of Paraoxón 0.015M in Bmim[Ser] at 25 $^{\circ}\text{C}$ .
<b>Figure S29.</b> $^{31}\text{P}$ -NMR plot for the reaction of Paraoxón 0.015M in Bmim[Gly] at 25 $^{\circ}\text{C}$ .
<b>Figure S30.</b> $^{31}\text{P}$ -NMR plot for the reaction of Paraoxón 0.015M in Bmim[Met] at 25 $^{\circ}\text{C}$ .
<b>Figure S31.</b> Stacked $^{31}\text{P}$ -NMR plot for the reaction of Paraoxón 0.015M in Bmim[His] at 25 $^{\circ}\text{C}$ .
<b>Figure S32.</b> UV-vis spectra of compound <b>7i</b> (at 356 nm), obtained in the reaction of Paraoxon® in Bmim[Pro].
<b>Figure S33.</b> Set of dyes used for derive the Kamlet-Taft parameters; (a) Reichardts' dye (Reichardt's dye #30), (b) 4-nitroaniline (4N), (c) <i>N,N</i> -diethyl-4-nitroaniline (NN).
<b>Figure S34.</b> (a) $^1\text{H}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Ala], (b) $^{13}\text{C}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Ala]. (c) ESI-MS spectrum of [BMIM][Ala].
<b>Figure S35.</b> (a) $^1\text{H}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Pro], (b) $^{13}\text{C}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Pro]. (c) ESI-MS spectrum of [BMIM][Pro].
<b>Figure S36.</b> (a) $^1\text{H}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Phe], (b) $^{13}\text{C}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Phe]. (c) ESI-MS spectrum of [BMIM][Phe].
<b>Figure S37.</b> (a) $^1\text{H}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][His], (b) $^{13}\text{C}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][His]. (c) ESI-MS spectrum of [BMIM][His].
<b>Figure S38.</b> (a) $^1\text{H}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Cys], (b) $^{13}\text{C}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Cys]. (c) ESI-MS spectrum of [BMIM][Cys].
<b>Figure S39.</b> (a) $^1\text{H}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Ser], (b) $^{13}\text{C}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Ser]. (c) ESI-MS spectrum of [BMIM][Ser].
<b>Figure S40.</b> (a) $^1\text{H}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Gly], (b) $^{13}\text{C}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Gly]. (c) HRMS-ESI spectrum of [BMIM][Gly].
<b>Figure S41.</b> (a) $^1\text{H}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Met], (b) $^{13}\text{C}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Met]. (c) HRMS-ESI spectrum of [BMIM][Met].
<b>Figure S42.</b> (a) $^1\text{H}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Asp], (b) $^{13}\text{C}$ NMR spectrum (400MHz, DMSO-d <sub>6</sub> ) of [BMIM][Asp]. (c) HRMS-ESI spectrum of [BMIM][Asp].
<b>Figure S43.</b> Solvatochromic shift for each dye used: (—) <i>N,N</i> -diethyl-4-nitroaniline, (—) 4-nitroaniline and (—) Reichardt's dye #30 in (a)Bmim[Ala], (b) Bmim[Cys], (c)Bmim[His], (d)Bmim[Phe], (e)Bmim[Pro], (f)Bmim[Ser], (g)Bmim[Gly], (h)Bmim[Met] and (i)Bmim[Asp] at 25 $^{\circ}\text{C}$ .
<b>Table S1.</b> Relative product distribution (%) for the nucleophilic attack of each BMIM[AA] to Paraoxón.
<b>Table S2.</b> Molar amount of the different products at various time for the reaction of Paraoxon with Bmim[Pro] at 25.0 $^{\circ}\text{C}$ . These amounts were obtained by integration of the corresponding of $^{31}\text{P}$ -NMR spectra.
<b>Table S3.</b> Pseudo-First-Order Rate Constants ( $k_{\text{obsd}}$ )for the degradation of Paraoxon in the

BMIM[AA]s.

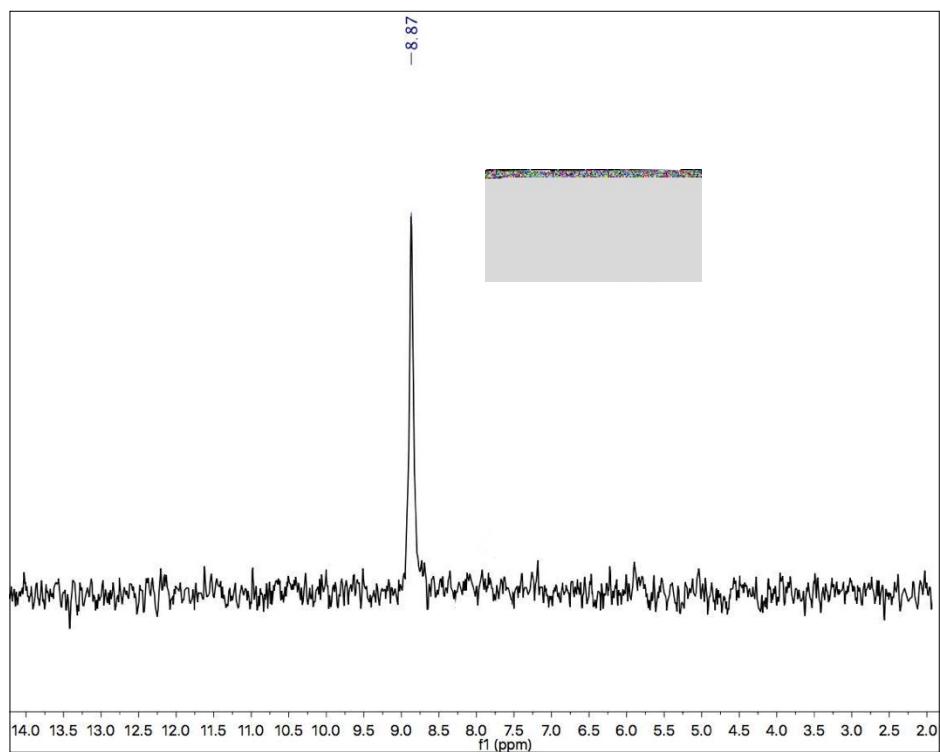
**Table S4.** Half-life ( $t_{1/2}$ ) for the degradation of Paraoxón® in Bmim[Ala] with different water amount added.



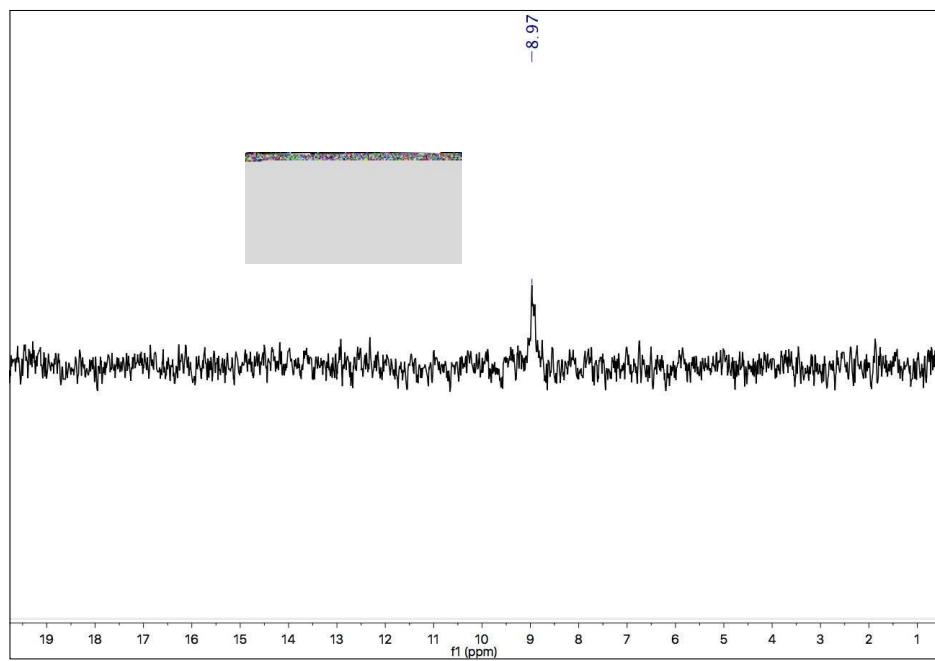
**Figure S1.**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **2a**, obtained in the reaction of *O,O*-diethyl chlorophosphate with Bmim[Pro] al 25.0 °C.



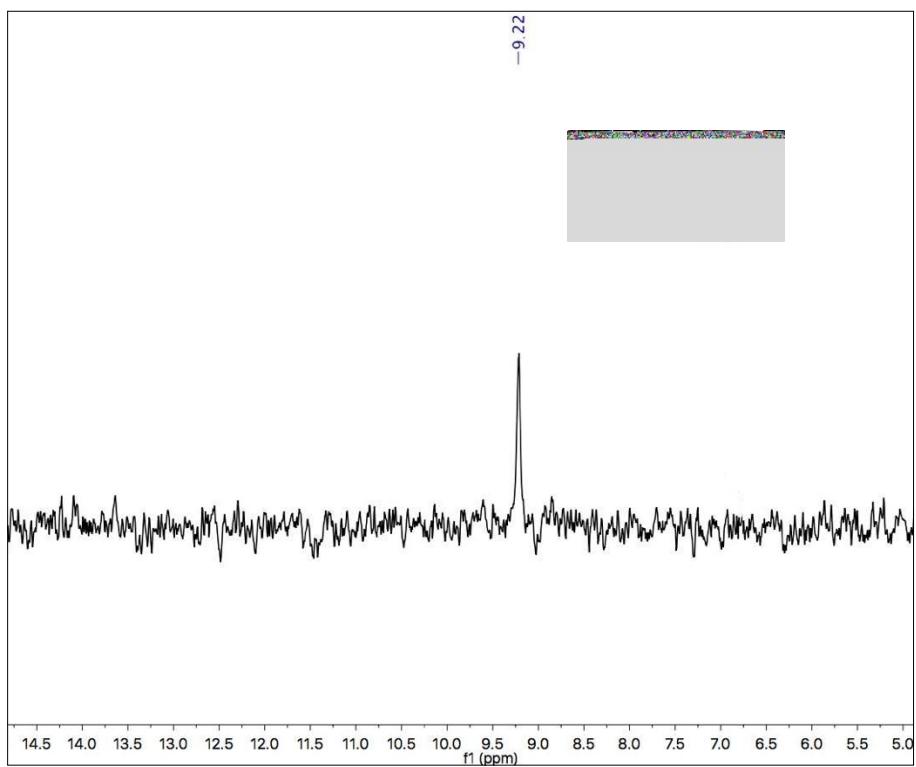
**Figure S2.**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **2b**, obtained in the reaction of *O,O*-diethyl chlorophosphate with Bmim[Ala] at 25.0 °C.



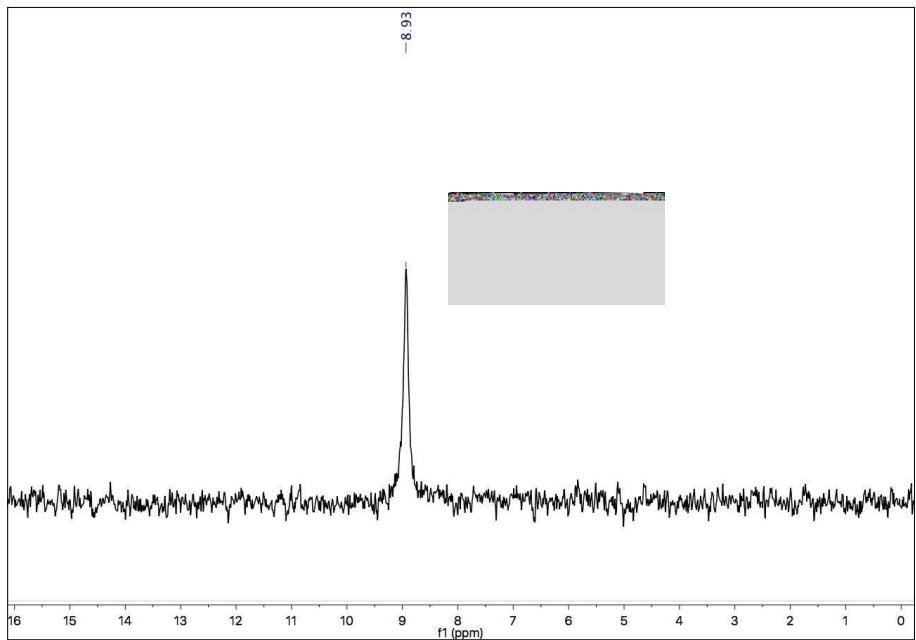
**Figure S3.**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **2c**, obtained in the reaction of *O,O*-diethyl chlorophosphate with Bmim[Phe] at 25.0  $^{\circ}\text{C}$ .



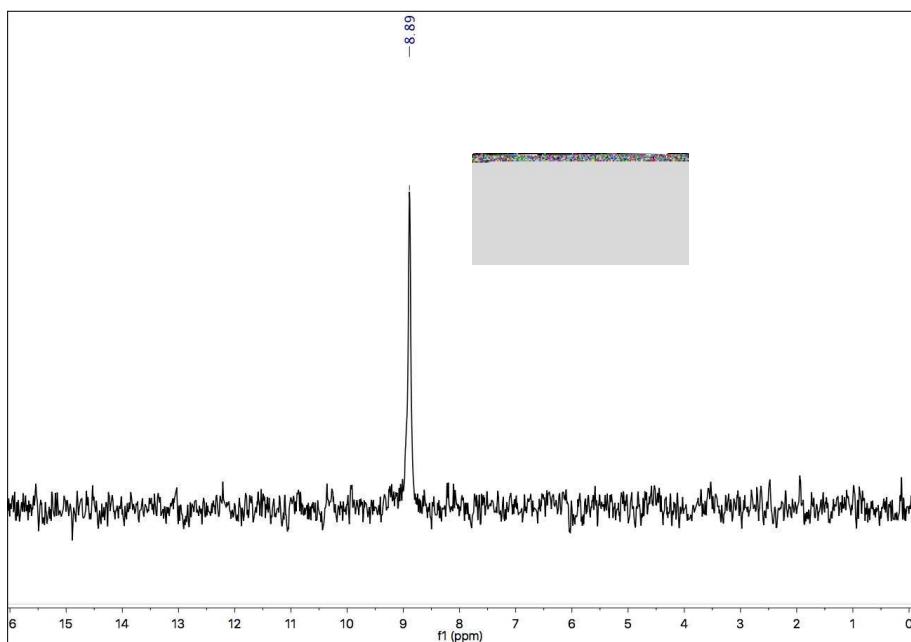
**Figure S4.**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **2d**, obtained in the reaction of *O,O*-diethyl chlorophosphate with Bmim[Asp] at 25.0  $^{\circ}\text{C}$ .



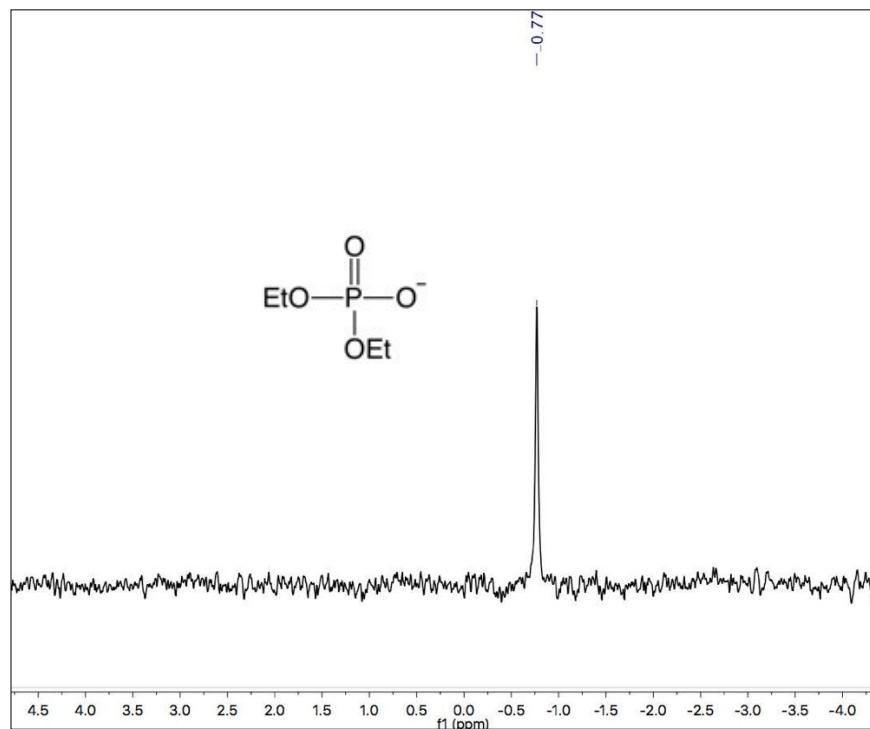
**Figure S5.** <sup>31</sup>P-NMR spectrum (400MHz) of compound **2e**, obtained in the reaction of *O,O*-diethyl chlorophosphate with Bmim[Ser] at 25.0°C.



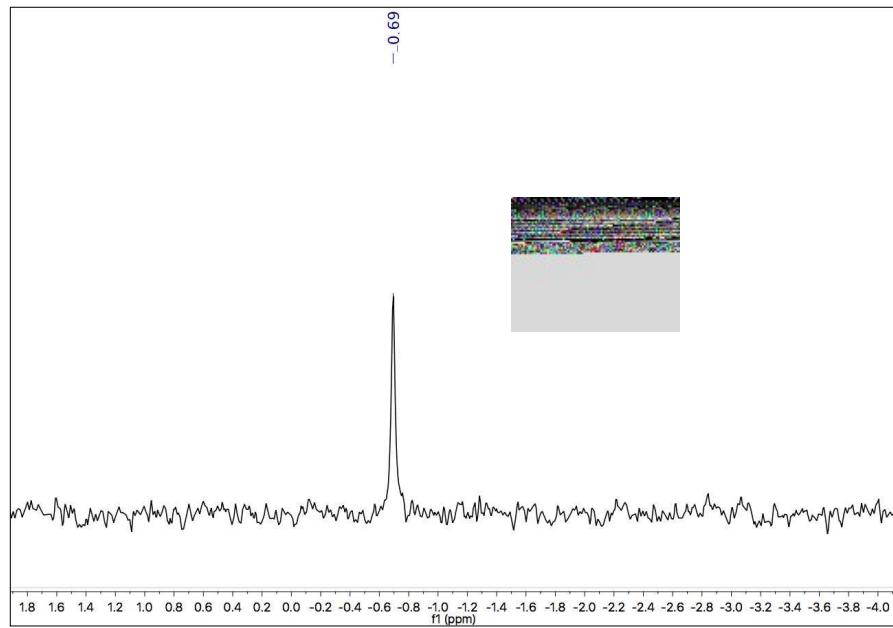
**Figure S6.** <sup>31</sup>P-NMR spectrum (400MHz) of compound **2f**, obtained in the reaction of *O,O*-diethyl chlorophosphate with Bmim[Gly] at 25.0 °C.



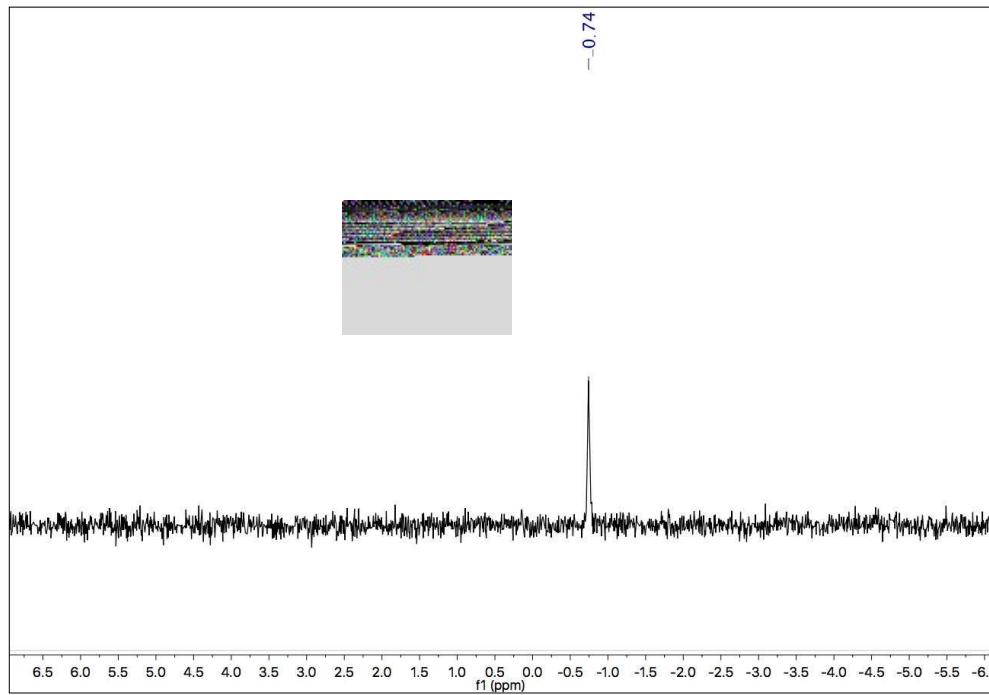
**Figure S7.** <sup>31</sup>P-NMR spectrum (400MHz) of compound **2g**, obtained in the reaction of *O,O*-diethyl chlorophosphate with Bmim[Met] at 25.0 °C.



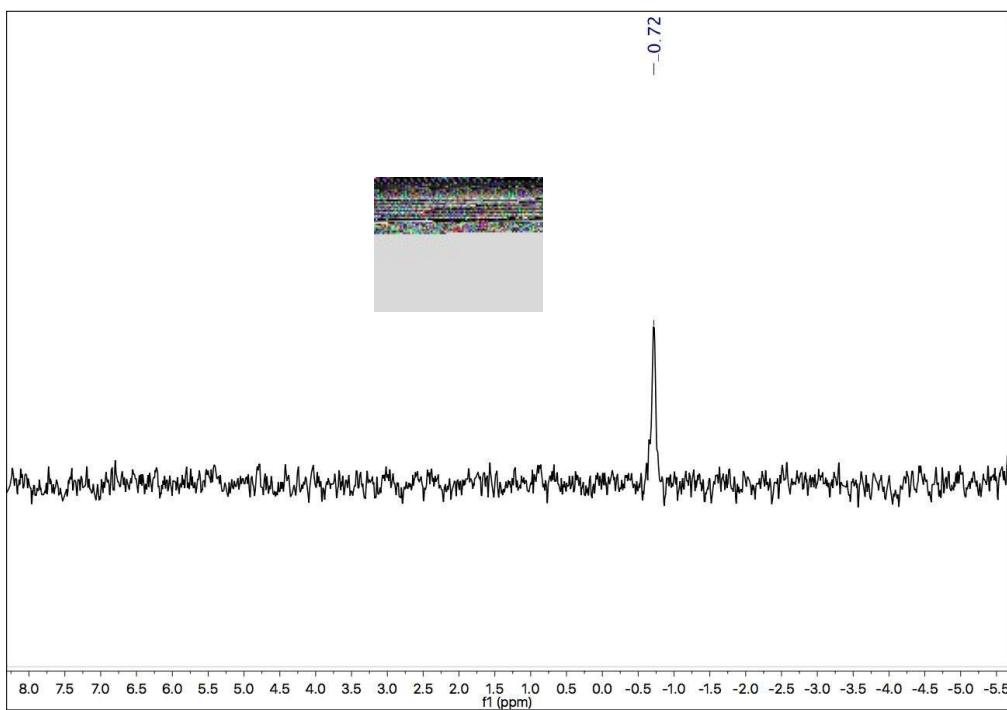
**Figure S8.** <sup>31</sup>P-NMR spectrum (400MHz) of compound **3**, obtained in the reaction *O,O*-diethyl chlorophosphate with NaOH in Bmim[Pro] at 25.0 °C.



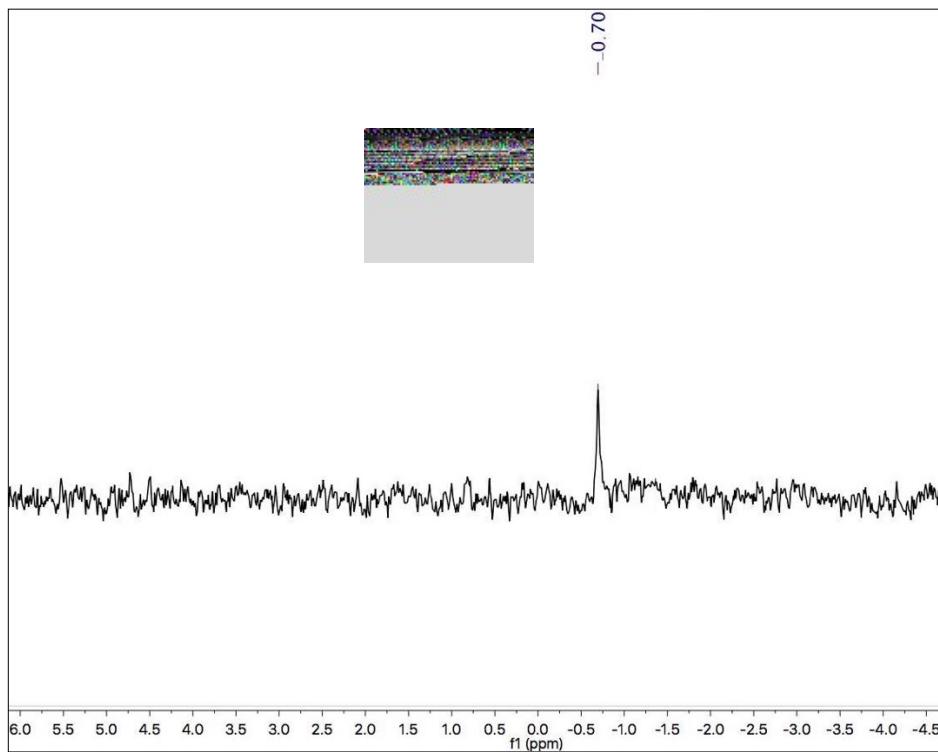
**Figure S9.**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **3**, obtained in the reaction *O,O*-diethyl chlorophosphate with NaOH in Bmim[Ala] at 25.0  $^{\circ}\text{C}$ .



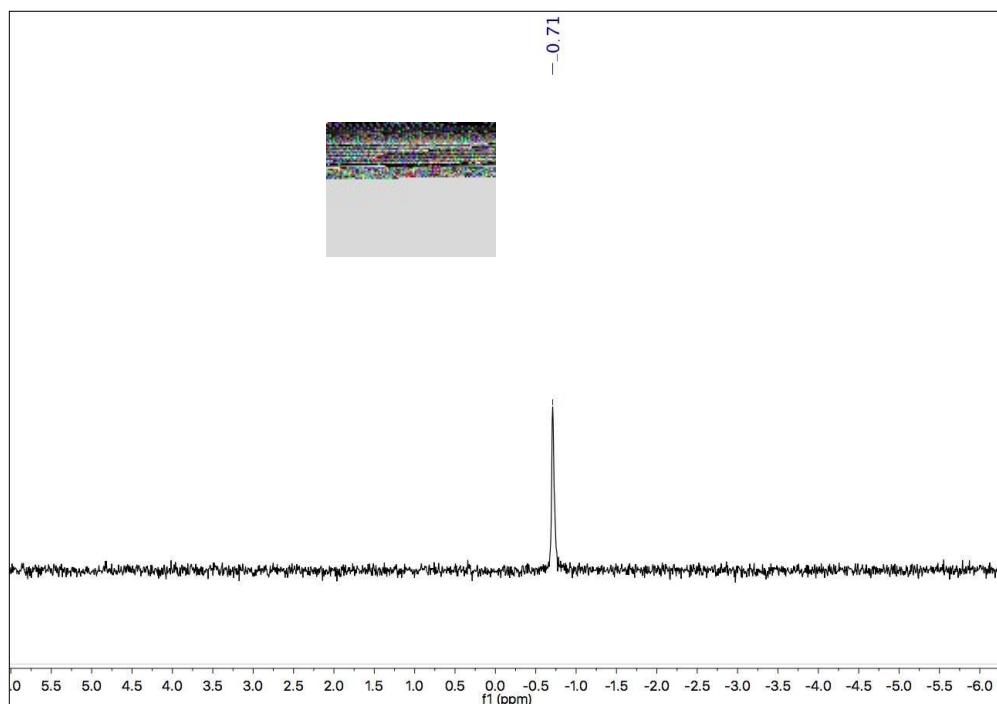
**Figure 10.**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **3**, obtained in the reaction *O,O*-diethyl chlorophosphate with NaOH in Bmim[Phe] at 25.0  $^{\circ}\text{C}$ .



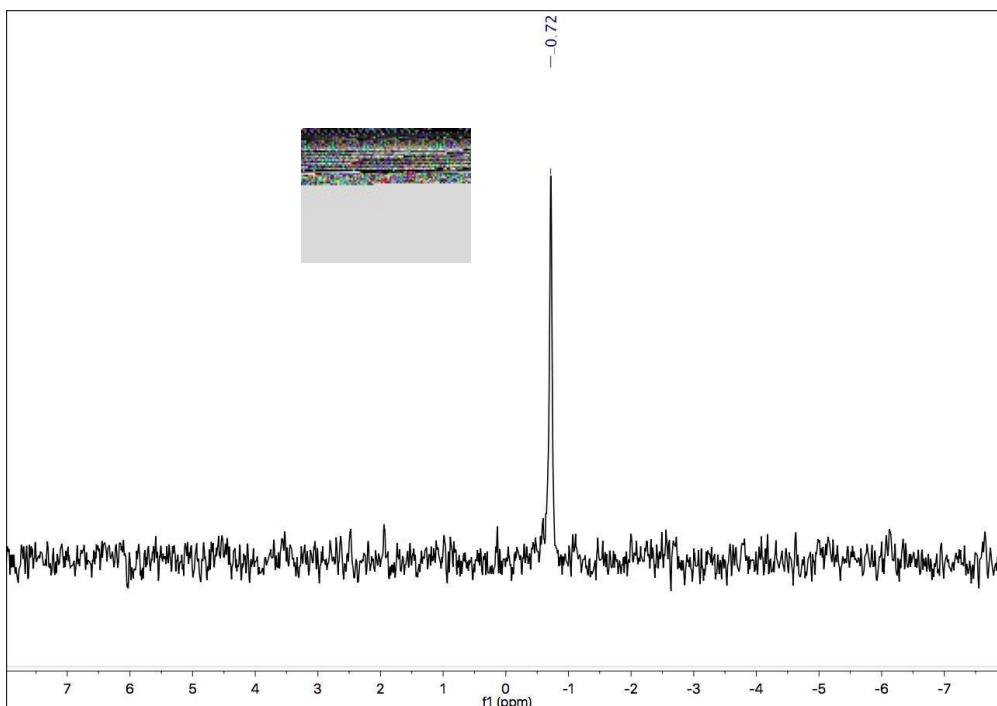
**Figure S11.**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **3**, obtained in the reaction  $O,O$ -diethyl chlorophosphate with NaOH in Bmim[Asp] at 25.0  $^{\circ}\text{C}$ .



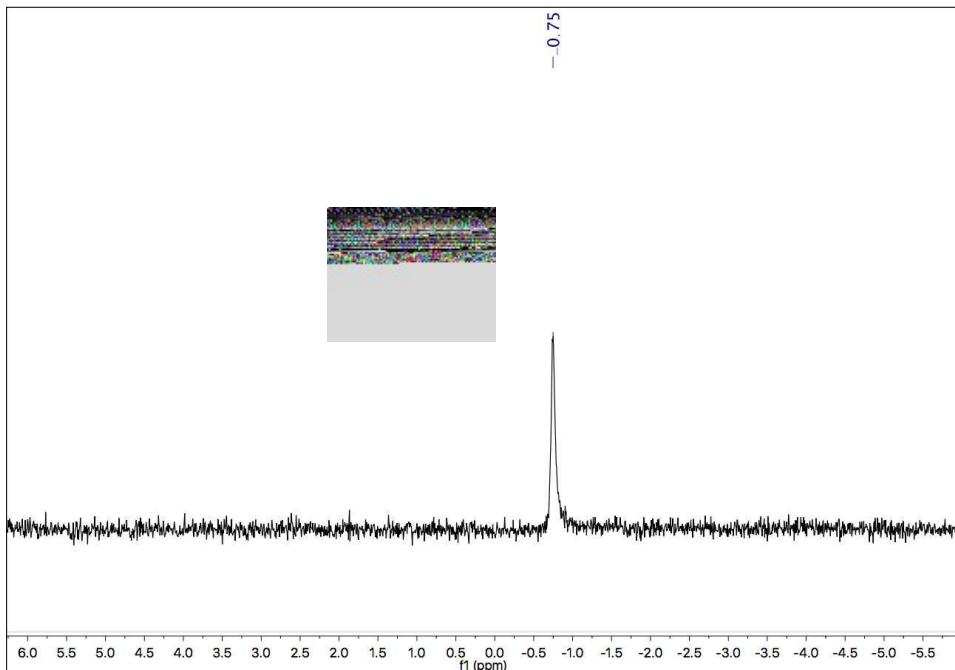
**Figure S12.**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **3**, obtained in the reaction  $O,O$ -diethyl chlorophosphate with NaOH in Bmim[Ser] at 25.0  $^{\circ}\text{C}$ .



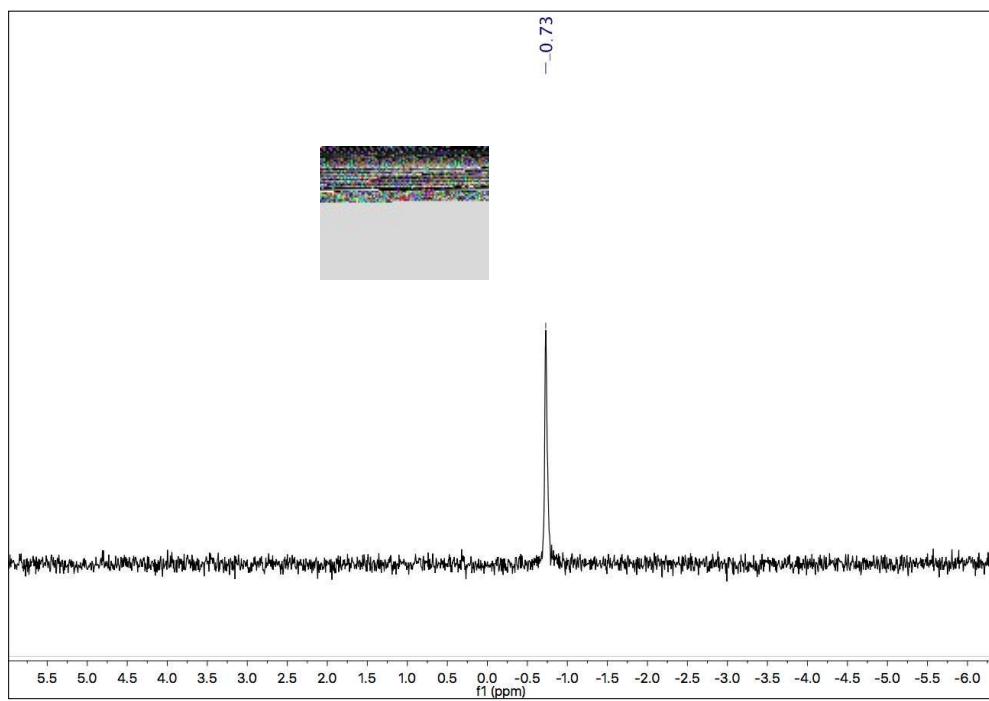
**Figure S13.** <sup>31</sup>P-NMR spectrum (400MHz) of compound **3**, obtained in the reaction *O,O*-diethyl chlorophosphate with NaOH in Bmim[Gly] at 25.0 °C.



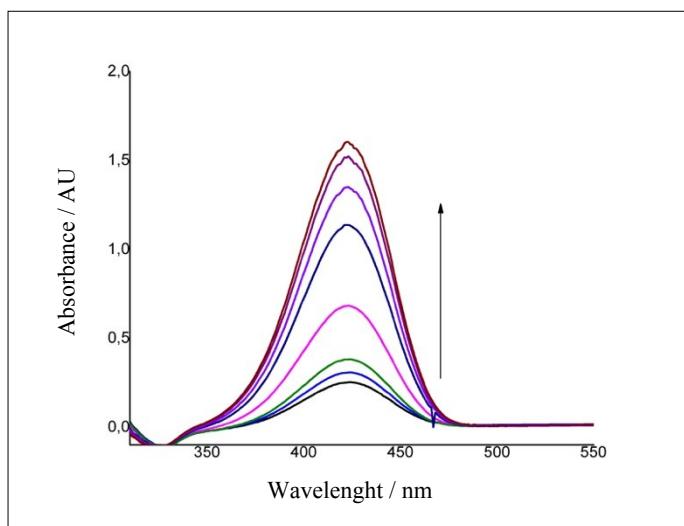
**Figure S14.** <sup>31</sup>P-NMR spectrum (400MHz) of compound **3**, obtained in the reaction *O,O*-diethyl chlorophosphate with NaOH in Bmim[Met] at 25.0 °C.



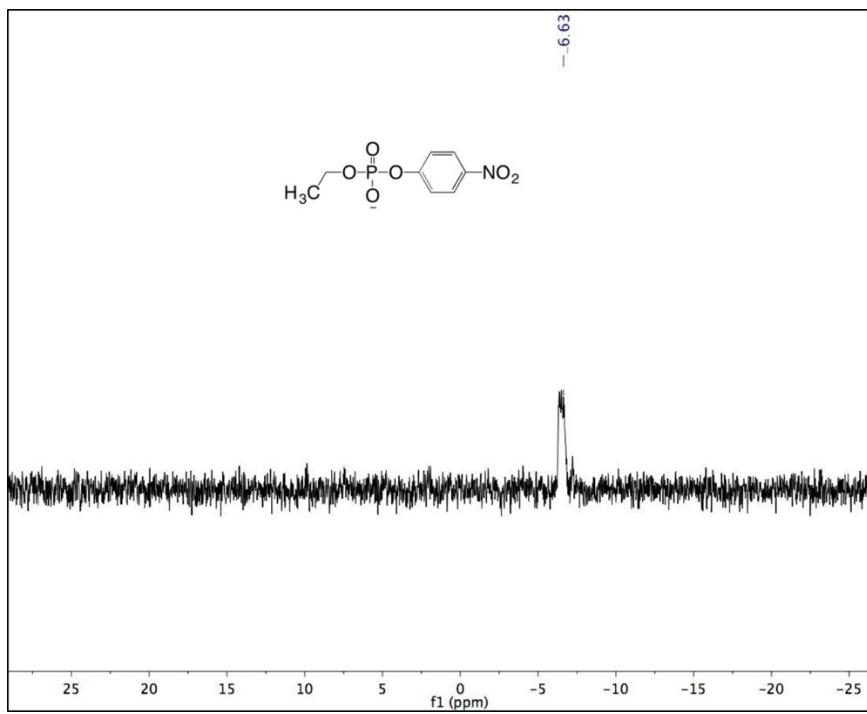
**Figure S15.**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **3**, obtained in the reaction *O,O*-diethyl chlorophosphate with NaOH in Bmim[Cys] at 25.0  $^{\circ}\text{C}$ .



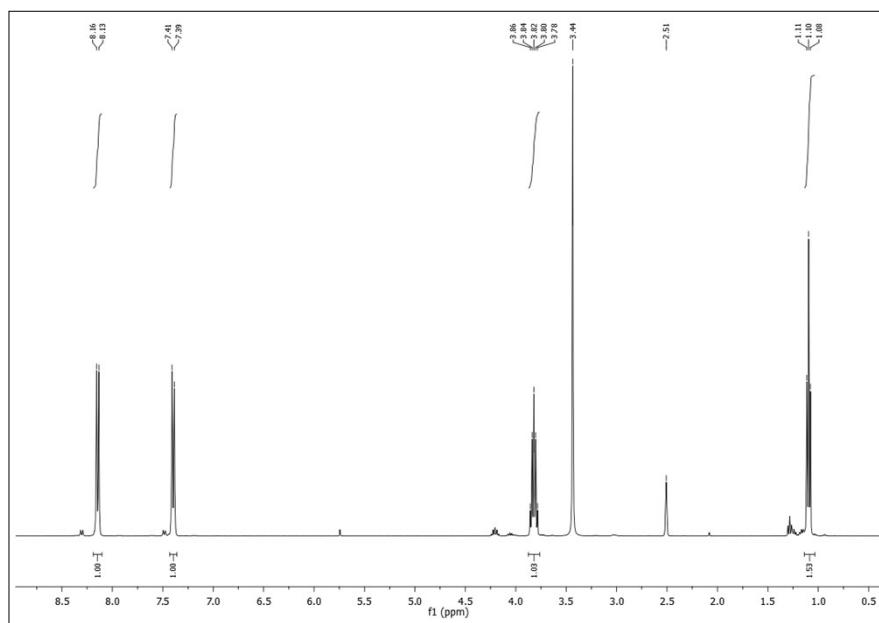
**Figure S16.**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **3**, obtained in the reaction *O,O*-diethyl chlorophosphate with NaOH in Bmim[His] at 25.0  $^{\circ}\text{C}$ .



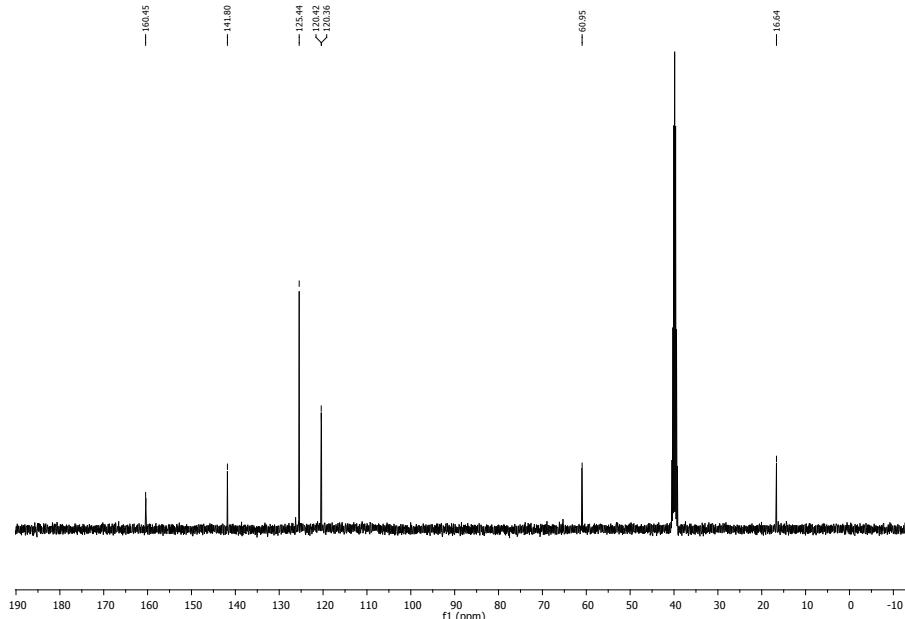
**Figure S17.** Time-dependent UV-vis spectra of compound **6** (at 420 nm), obtained in the reaction of Paraoxon® in Bmim[Pro].



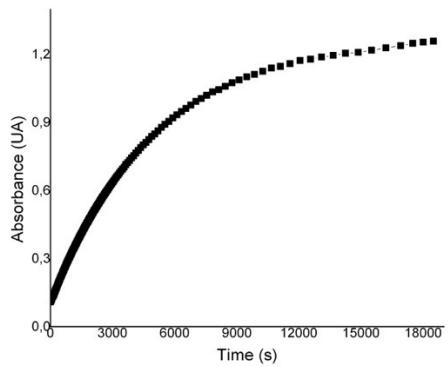
**Figure S18 (a).**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **4** in Bmim[Pro].



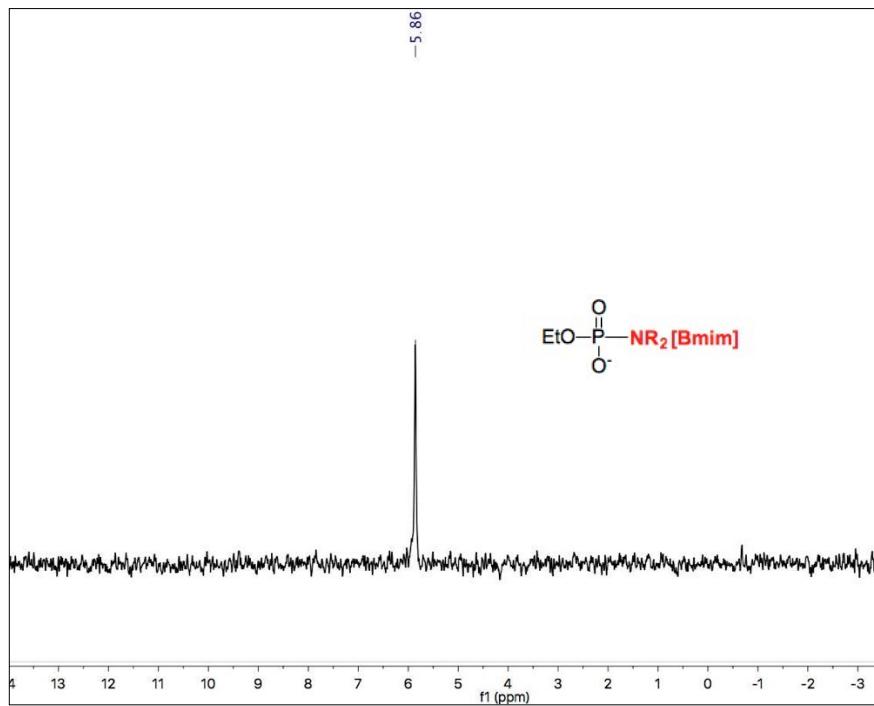
**Figure S18 (b).**  $^1\text{H}$ -NMR spectrum (400MHz, DMSO) of compound **4**.<sup>37</sup>



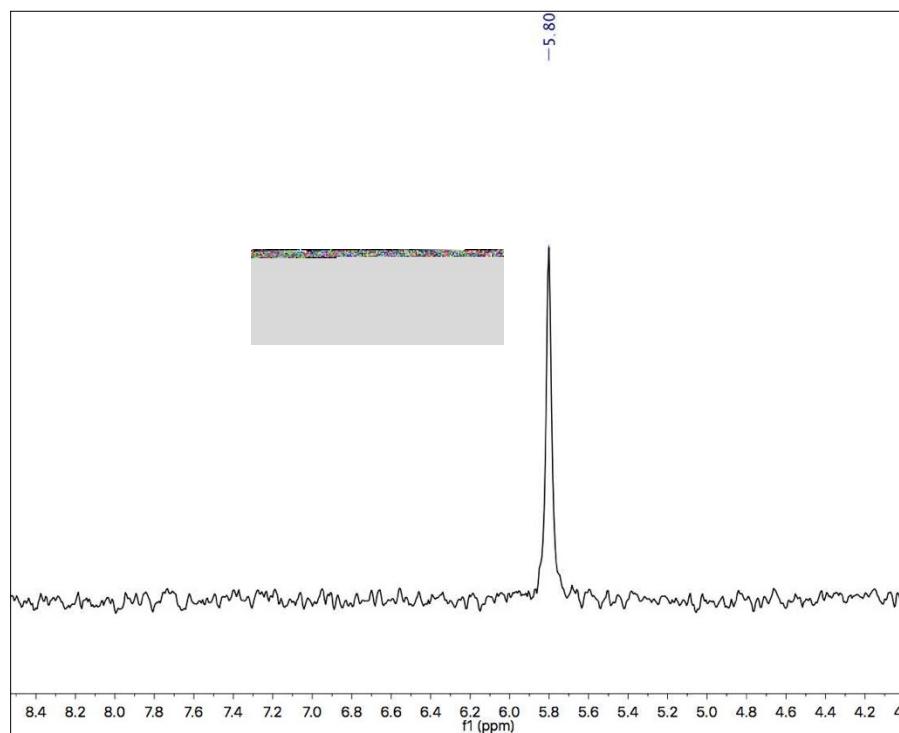
**Figure S18 (c).**  $^{13}\text{C}$ -NMR spectrum (400MHz, DMSO) of compound 4.<sup>37</sup>



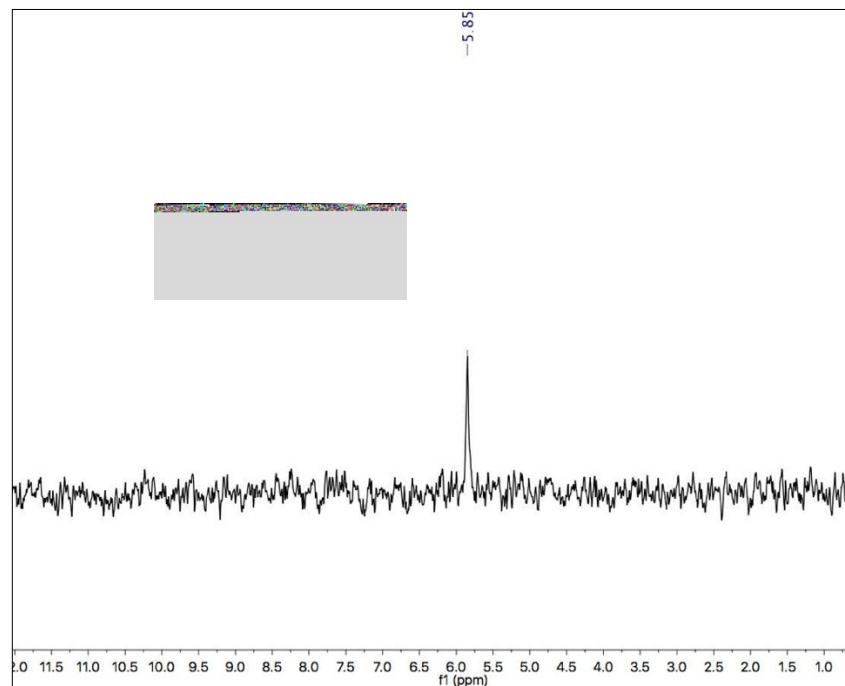
**Figure S19.** Experimental plot of absorbance (at 420 nm) vs time for the reaction of Paraoxon in Bmim[Pro] at 25.0 °C.



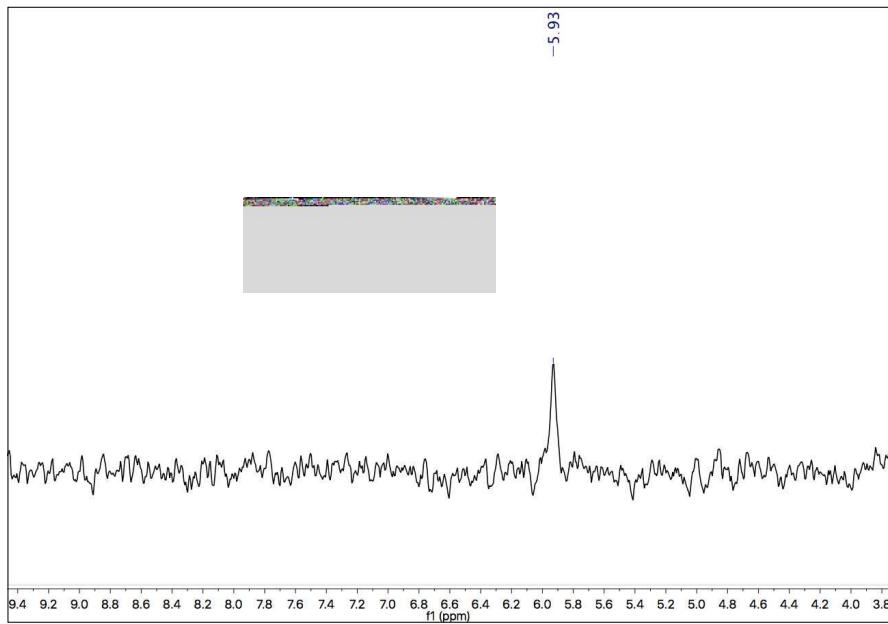
**Figure S20.**  $^{31}\text{P}$ -NMR spectrum (400MHz) of compound **5a**, obtained in the reaction of *O*-ethyl 4-nitrophenyl phosphate monoester with Bmim[Pro] at 25°C.



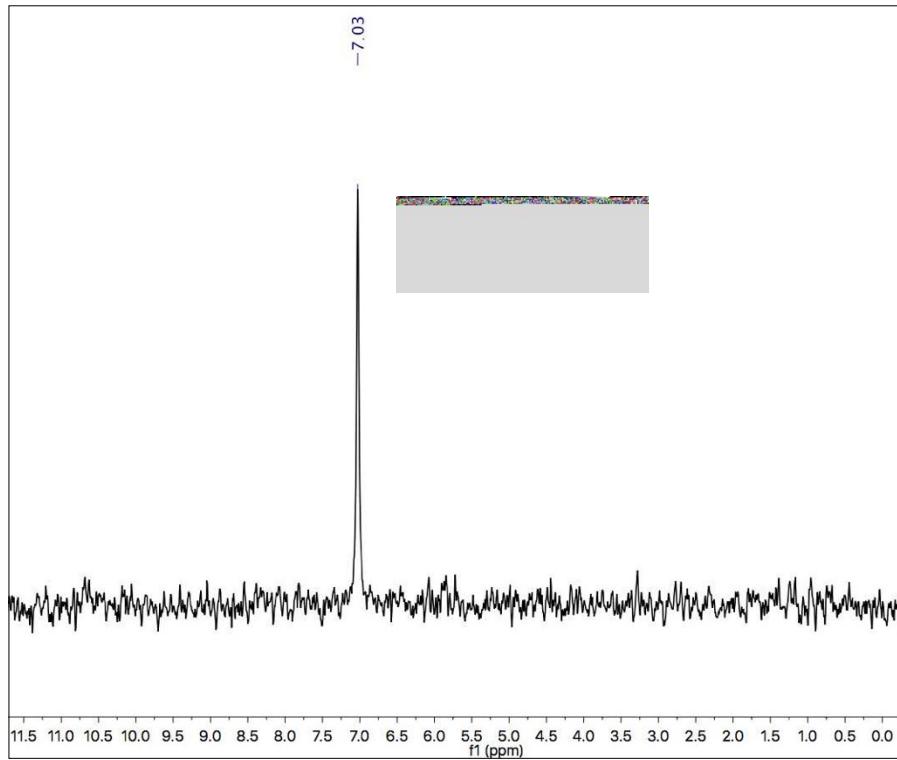
**Figure S21.** <sup>31</sup>P-NMR spectrum (400MHz) of compound **5b**, obtained in the reaction of *O*-ethyl 4-nitrophenyl phosphate monoester with Bmim[Ala] at 25.0 °C.



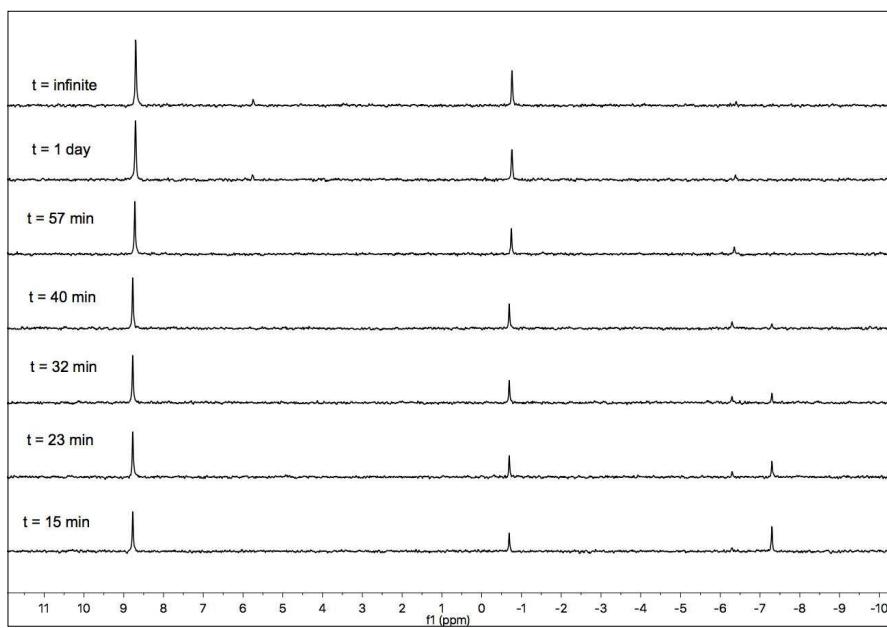
**Figure S22.** <sup>31</sup>P-NMR spectrum (400MHz) of compound **5c**, obtained in the reaction of *O*-ethyl 4-nitrophenyl phosphate monoester with Bmim[Phe] at 25.0 °C.



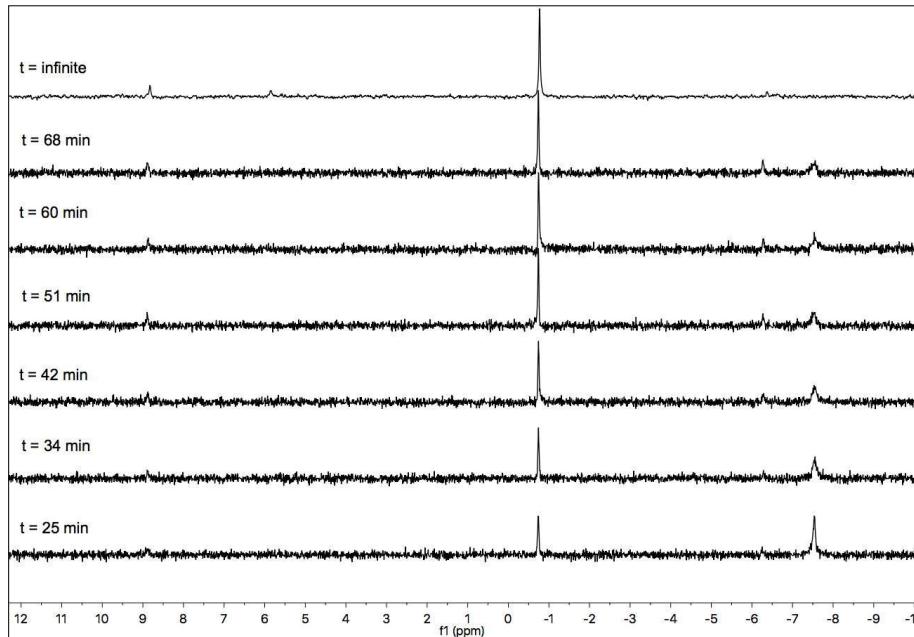
**Figure S23.** <sup>31</sup>P-NMR spectrum (400MHz) of compound **5d**, obtained in the reaction of *O*-ethyl 4-nitrophenyl phosphate monoester with Bmim[Asp] at 25.0 °C.



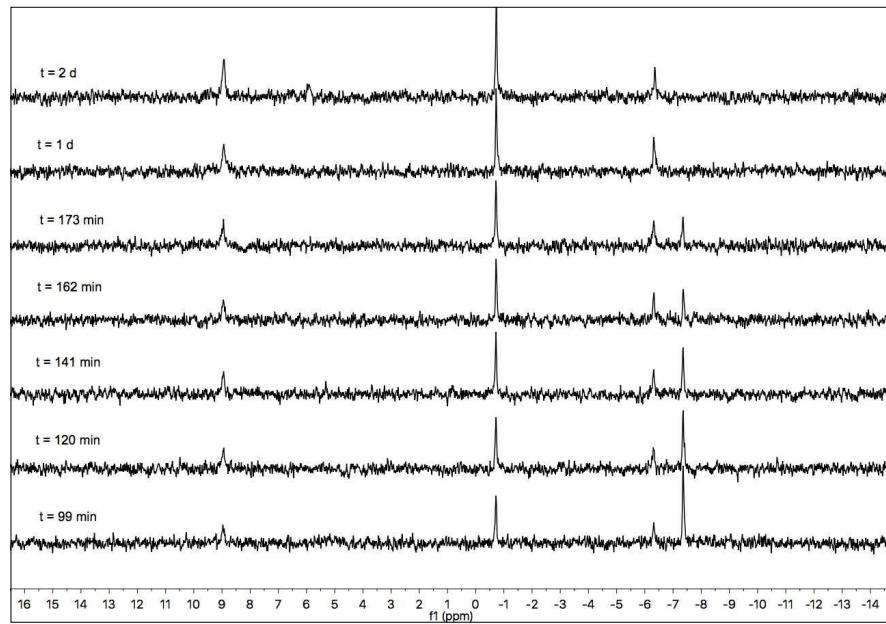
**Figure S24.** <sup>31</sup>P-NMR spectrum (400MHz) of compound **5e**, obtained in the reaction of *O*-ethyl 4-nitrophenyl phosphate monoester with Bmim[Ser] at 25.0 °C



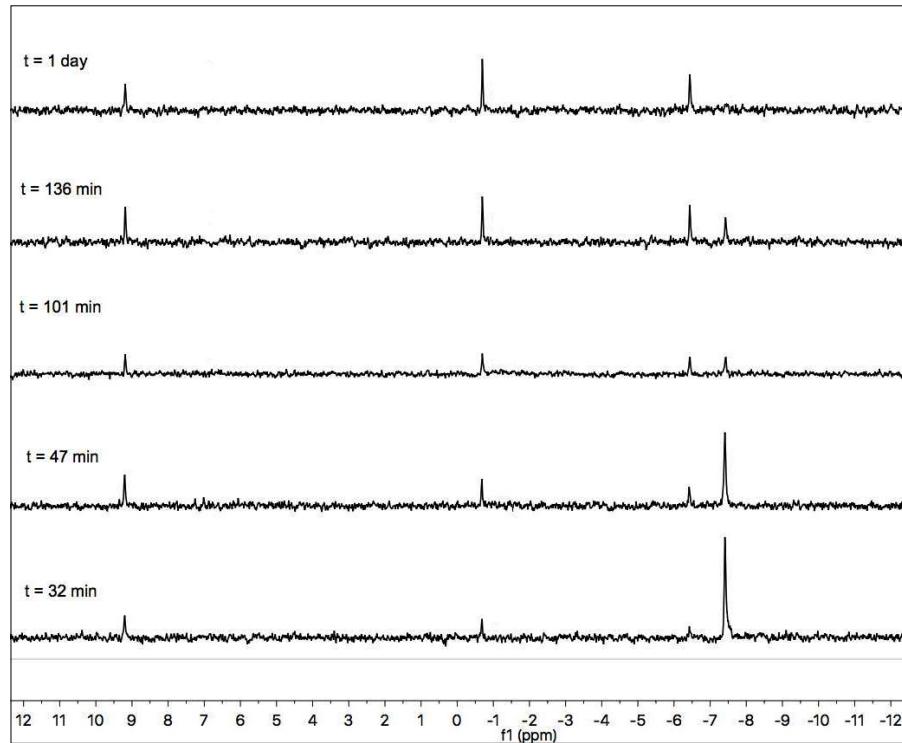
**Figure S25.** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of Paraoxon 0.015M in Bmim[Ala] at 25°C.



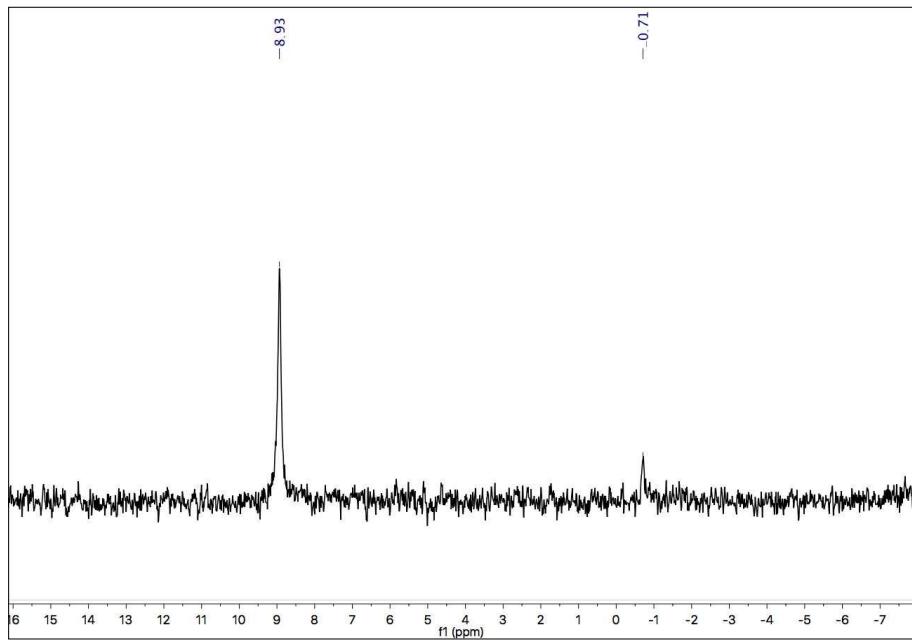
**Figure S26.** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of Paraoxon 0.015M in Bmim[Phe] at 25°C.



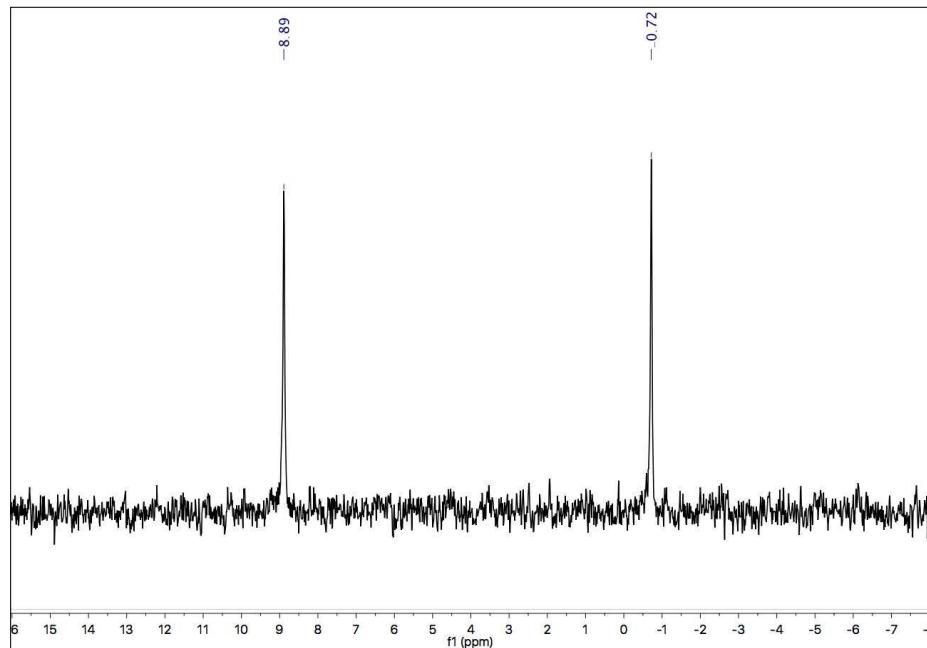
**Figure S27.** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of Paraoxon 0.015M in Bmim[Asp] at 25°C.



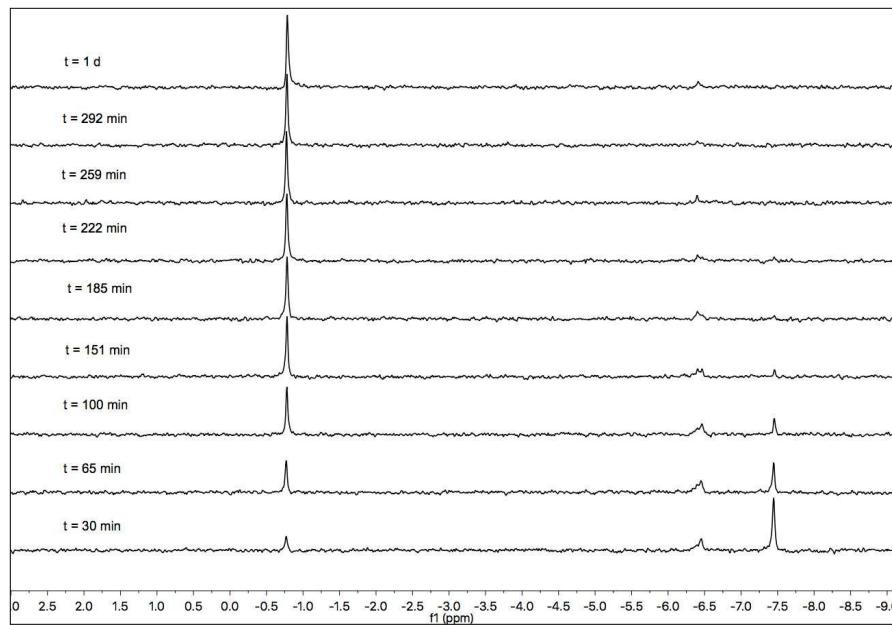
**Figure S28.** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of Paraoxon 0.015M in Bmim[Ser] at 25°C.



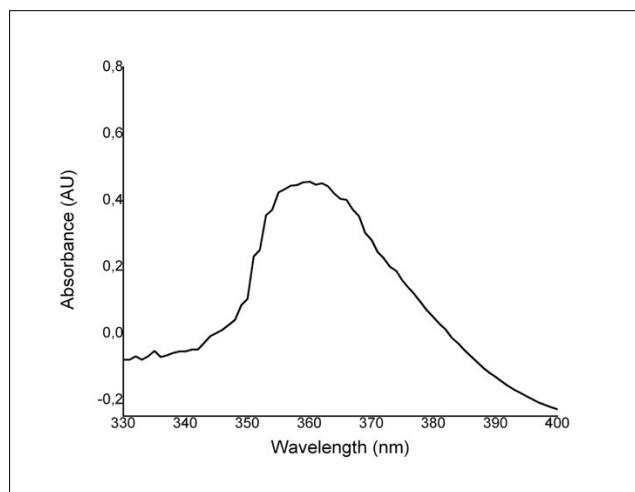
**Figure S29.**  $^{31}\text{P}$ -NMR plot for the reaction of Paraoxon 0.015M in Bmim[Gly] at 25°C.



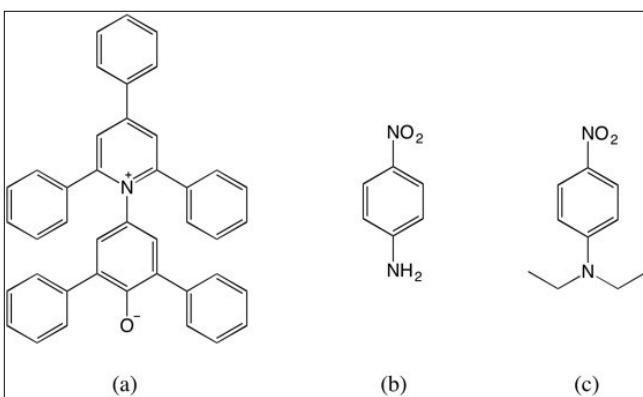
**Figure S30.**  $^{31}\text{P}$ -NMR plot for the reaction of Paraoxon 0.015M in Bmim[Met] at 25°C.



**Figure S31.** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of Paraoxon 0.015M in Bmim[His] at 25°C.

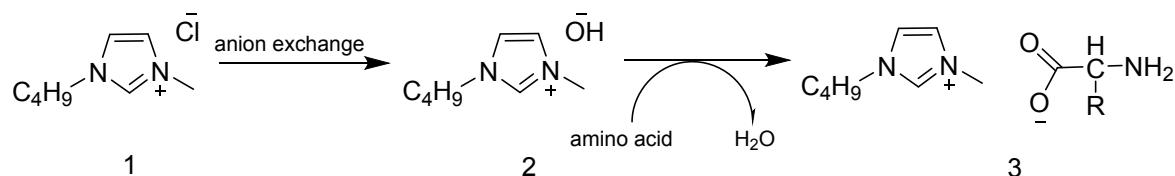


**Figure S32.** UV-vis spectra of compound **7i** (at 356 nm), obtained in the reaction of Paraoxon® in Bmim[Pro].



**Figure S33.** Set of dyes used for derive the Kamlet-Taft parameters; (a) Reichardt's dye (Reichardt's dye #30), (b) 4-nitroaniline (4N), (c) *N,N*-diethyl-4-nitroaniline (NN).

### Experimental method and characterization data



**Scheme S1.** Synthesis of amino acid ionic liquids.

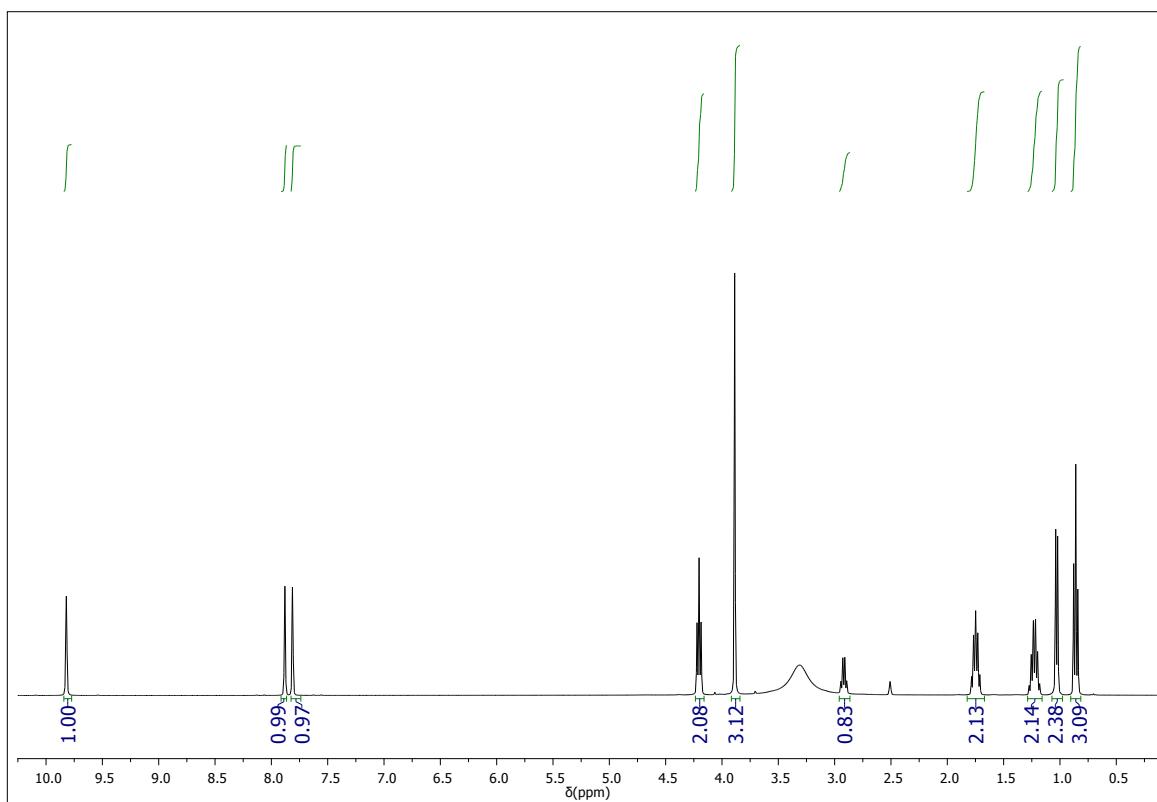
The chemical structures of Bmim[AA] were characterized by NMR and mass spectrometry. The mass spectrum and NMR spectrum of Bmim[Ala], Bmim[His], Bmim[Pro], Bmim[Phe], Bmim[Cys], Bmim[Met], Bmim[Gly], Bmim[Asp], and Bmim[Ser] are shown as following:

### General experimental methods

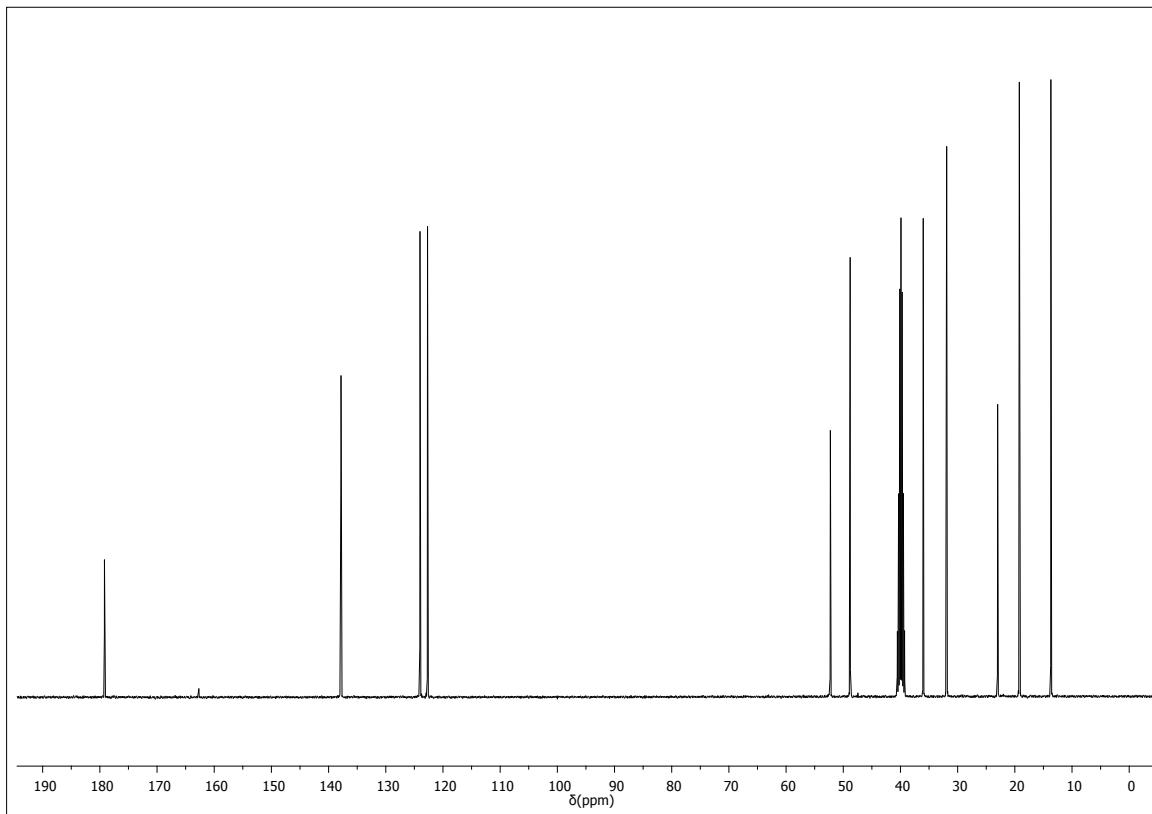
The NMR analysis was performed on a Brucker AVANCE-400 NMR spectrometer operating at 400 MHz for <sup>1</sup>H-NMR and <sup>13</sup>C-NMR. Samples were run in deuterated dimethyl sulfoxide (DMSO) where appropriate. High resolution mass spectrometer Exactive™ Plus Orbitrap, ThermoFisher Scientific (Bremen, Germany). The scan parameters: Resolution: 140000, AGC target: 1e 6, Max. inject time: 200 HESI source: Sheath gas flow: 30, Aux gas flow

rate: 3, Sweep gas flow rate: 0, Capillary temp.: 250°C, S-lens RF level: 0, Heater temp: 50°C.

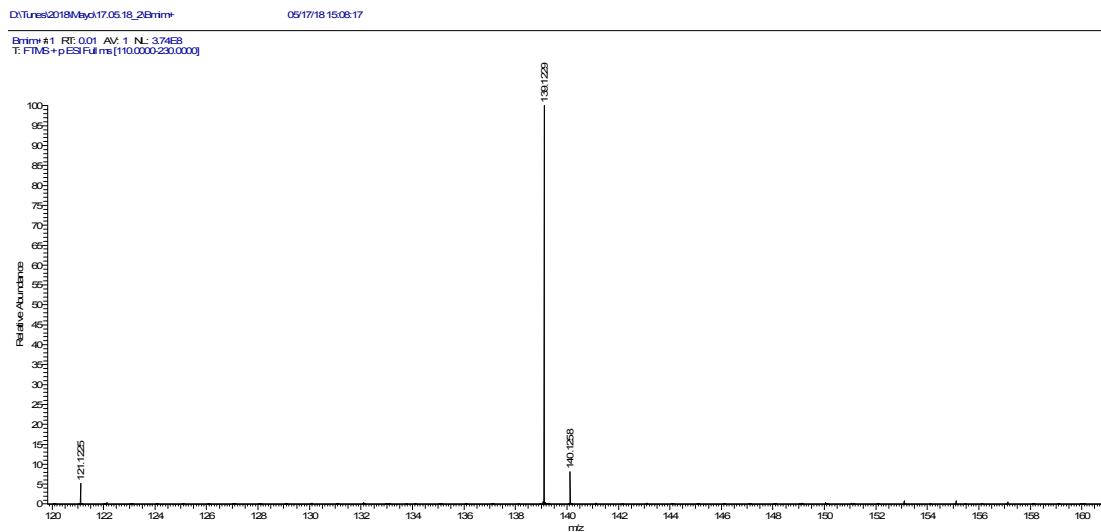
**1-Butyl-3-methylimidazolium alanine** (Bmim[Ala]) Obtained as light-yellow oil in 96% yield.  $^1\text{H}$  NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.82 (s, 1H), 7.88 (s, 1H), 7.81 (s, 1H), 4.20 (t,  $J$ = 7.2 Hz, 2H), 3.89 (s, 3H), 2.92 (q,  $J$ = 6.8 Hz, 1H), 1.82 – 1.67 (m, 2H), 1.29 – 1.16 (m, 2H), 1.04 (d,  $J$ = 6.9 Hz, 3H), 0.86 (t,  $J$ = 7.4 Hz, 3H); NH<sub>2</sub> may appear as very broad signal around 1.5 ppm.  $^{13}\text{C}$  NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$ , ppm: 13.7; 19.2; 23.0; 31.9; 36.0; 48.8; 52.0; 122.7; 124.0; 137.8; 179.2. HRMS-ESI (+ mode): found m/z 139.1229; calculated for cation C<sub>8</sub>H<sub>15</sub>N<sub>2</sub> m/z 139.1230 ( $\Delta$ = 0.7 ppm)



**Figure S34 (a).**  $^1\text{H}$  NMR spectrum of Bmim[Ala].



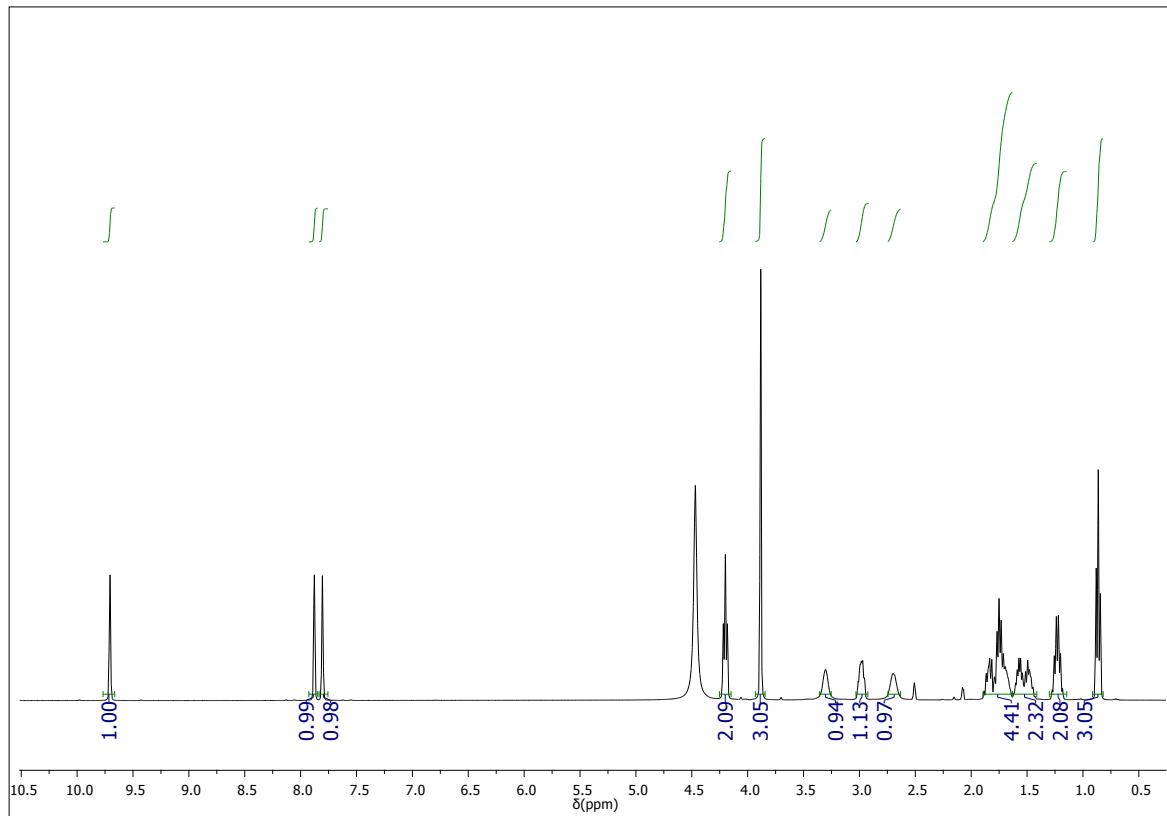
**Figure S34 (b).**  $^{13}\text{C}$  NMR spectrum of Bmim[Ala].



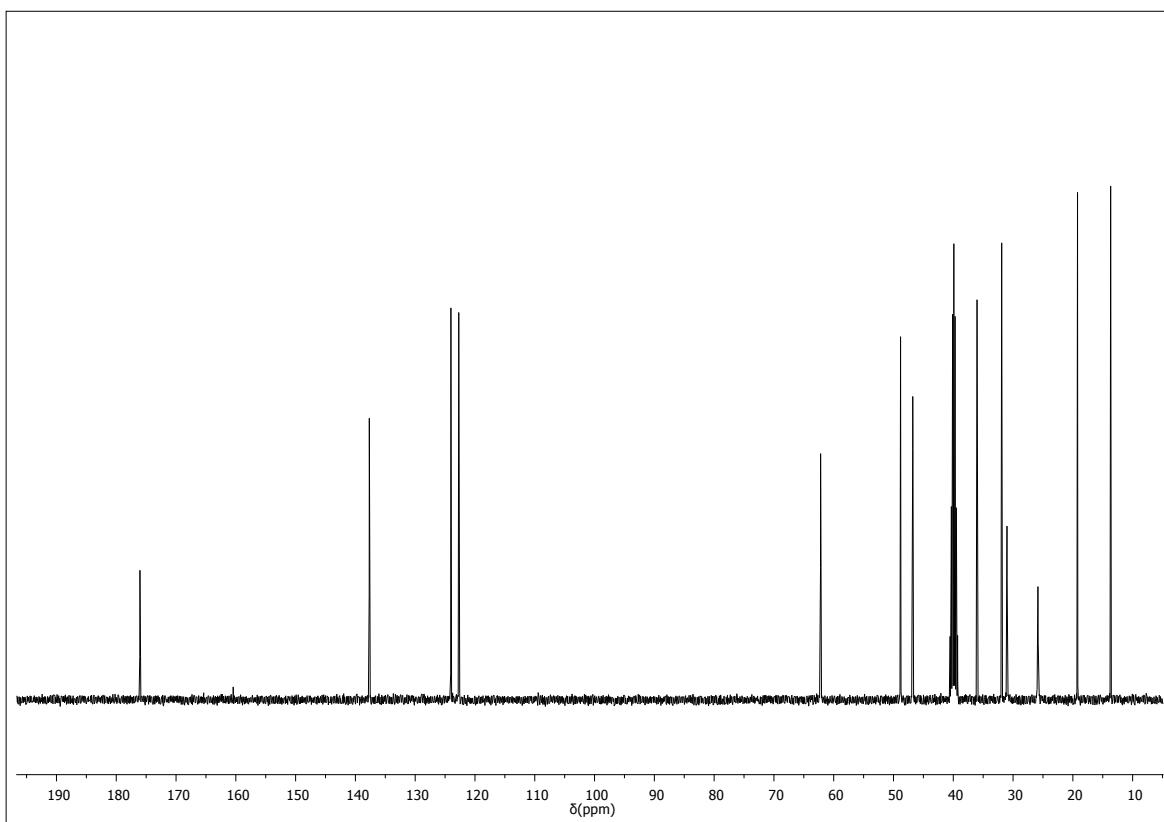
**Figure S34 (c).** HRMS-ESI(+) spectrum of Bmim[Ala].

**1-Butyl-3-methylimidazolium proline (Bmim[Pro])** Obtained as light-yellow oil in 94% yield.  $^1\text{H}$ -RMN (400 MHz, DMSO-d<sub>6</sub>)  $\delta$ , ppm: 9,71 (s, 1H), 7,88 (s, 1H), 7,80 (s, 1H), 4,20 (t,  $J$  = 7,1 Hz, 2H), 3,88 (s, 3H), 3,03 – 2,92 (m, 1H), 2,70 (s, 1H), 1,84 (dd,  $J$  = 11,5, 8,2 Hz,

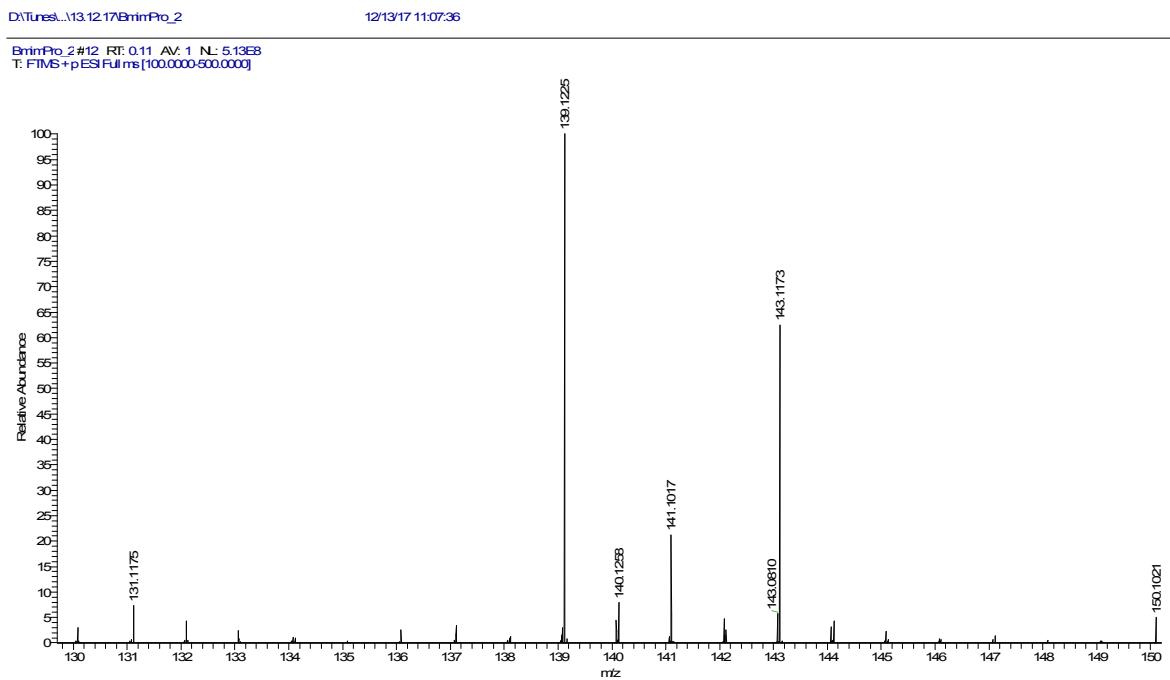
1H), 1,78 – 1,64 (m, 4H), 1,63 – 1,41 (m, 2H), 1,30 – 1,14 (m, 2H), 0,86 (t,  $J = 7,3$  Hz, 3H).  $^{13}\text{C}$ -RMN (400 MHz, DMSO-d<sub>6</sub>)  $\delta$ , ppm: 176,0, 137,7, 124,0, 122,7, 62,1, 48,9, 46,8, 36,0, 31,9, 31,0, 25,8, 19,2, 13,7. HRMS-ESI (+ mode): found m/z 139.1225; calculated for cation C<sub>8</sub>H<sub>15</sub>N<sub>2</sub> m/z 139.1230 ( $\Delta = 3.6$  ppm)



**Figure S35 (a).**  $^1\text{H}$  NMR spectrum of Bmim[Pro].

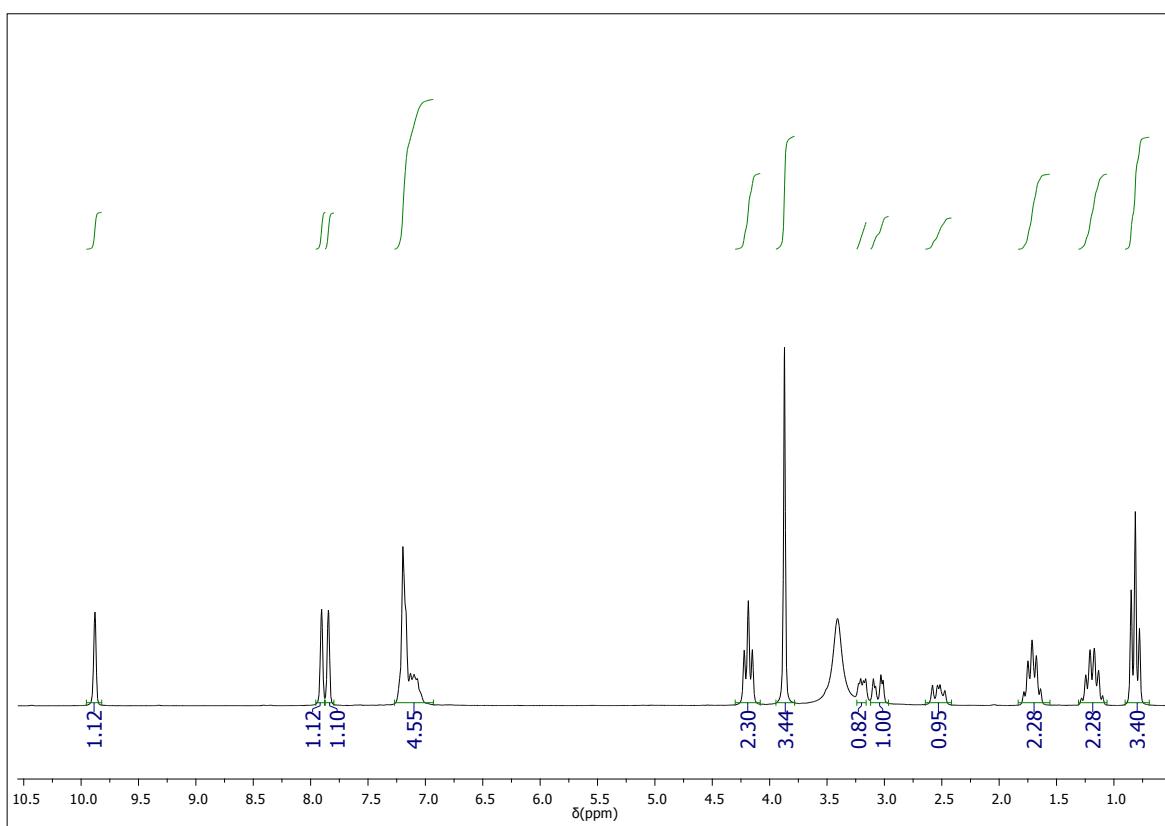


**Figure S35 (b).** <sup>13</sup>C NMR spectrum of Bmim[Pro].

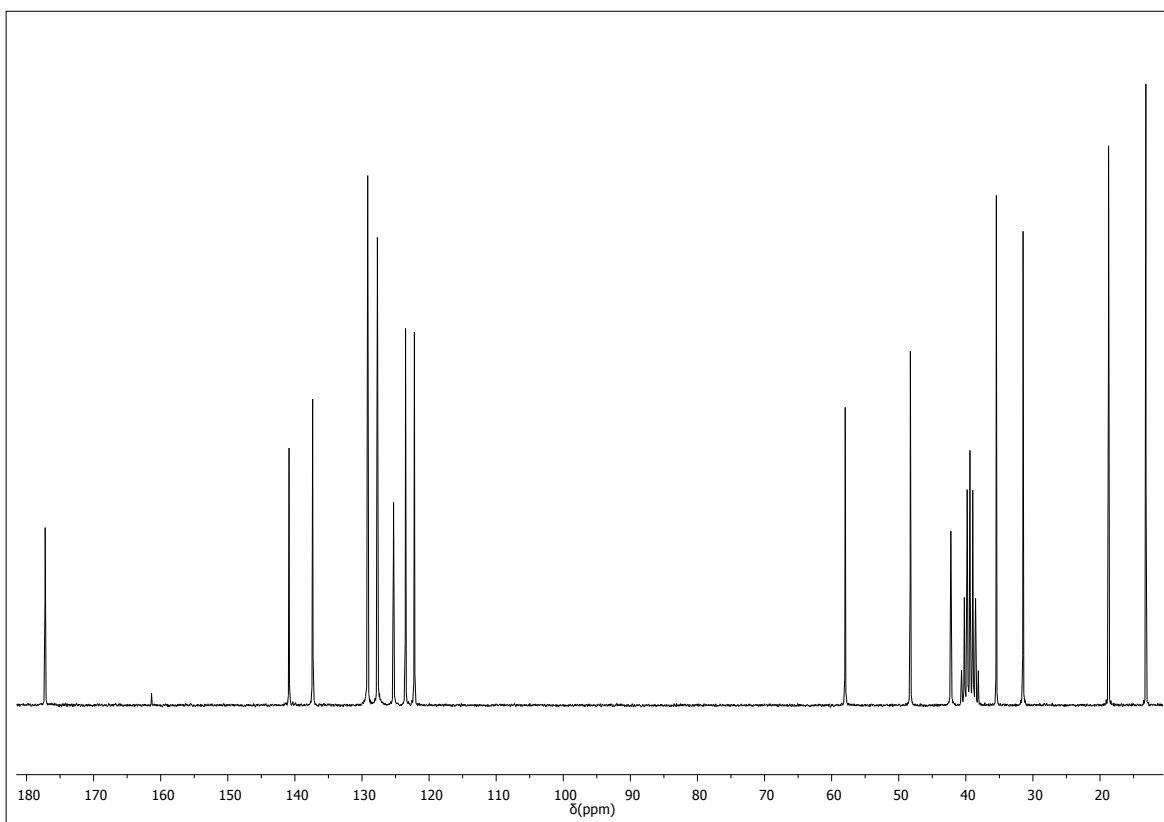


**Figure S35 (c).** HRMS-ESI(+) spectrum of Bmim[Pro].

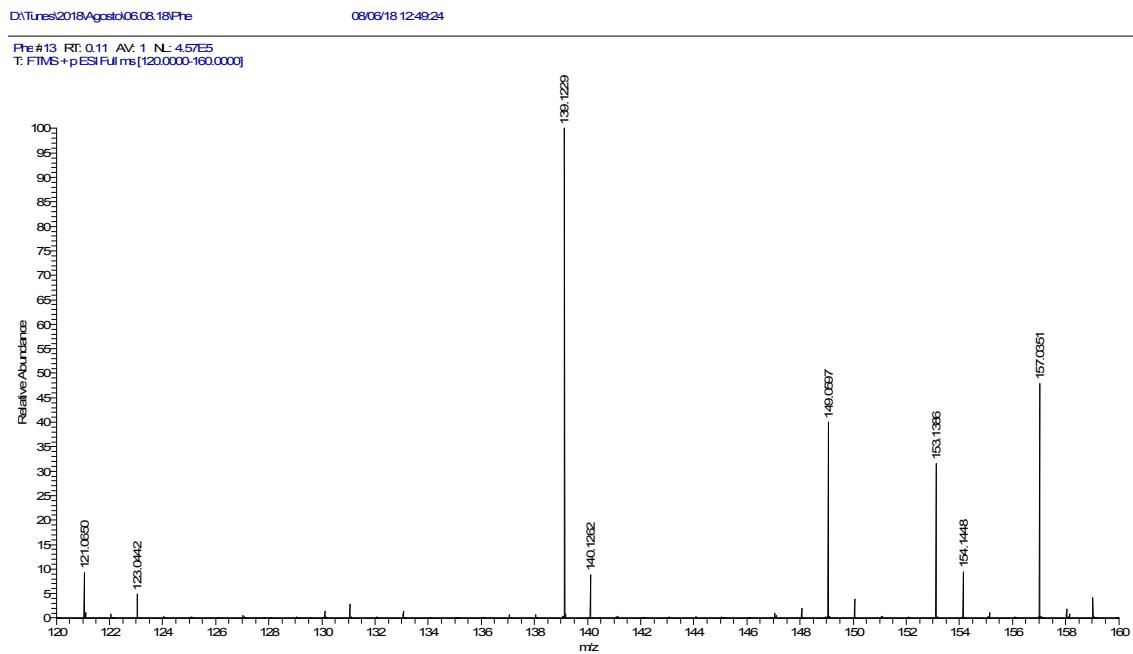
**1-Butyl-3-methylimidazolium phenylalanine (Bmim[Phe])** Obtained as light-yellow oil, 95% yield.  $^1\text{H}$  NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.88 (s, 1H), 7.90 (s, 1H), 7.85 (s, 1H), 7.27 – 6.93 (m, 5H), 4.19 (t,  $J$  = 7.1 Hz, 2H), 3.87 (s, 3H), 3.19 (dd,  $J$  = 8.4, 3.6 Hz, 1H), 3.05 (dd,  $J$  = 13.2, 3.8 Hz, 1H), 2.53 (dd,  $J$  = 13.0, 8.7 Hz, 1H), 1.83 – 1.56 (m, 2H), 1.31 – 1.06 (m, 2H), 0.81 (t,  $J$  = 7.3 Hz, 3H); NH<sub>2</sub> may appear as very broad signal around 1.5 ppm.  $^{13}\text{C}$  NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$ , ppm: 13.2; 18.7; 31.5; 35.5; 42.2; 48.3; 58.0; 122.2; 123.5; 125.3; 127.7; 129.2; 137.2; 140.9; 177.2. HRMS-ESI (+ mode): found m/z 139.1229; calculated for cation C<sub>8</sub>H<sub>15</sub>N<sub>2</sub> m/z 139.1230 ( $\Delta$  = 0.7 ppm)



**Figure S36 (a).**  $^1\text{H}$  NMR spectrum of Bmim[Phe].

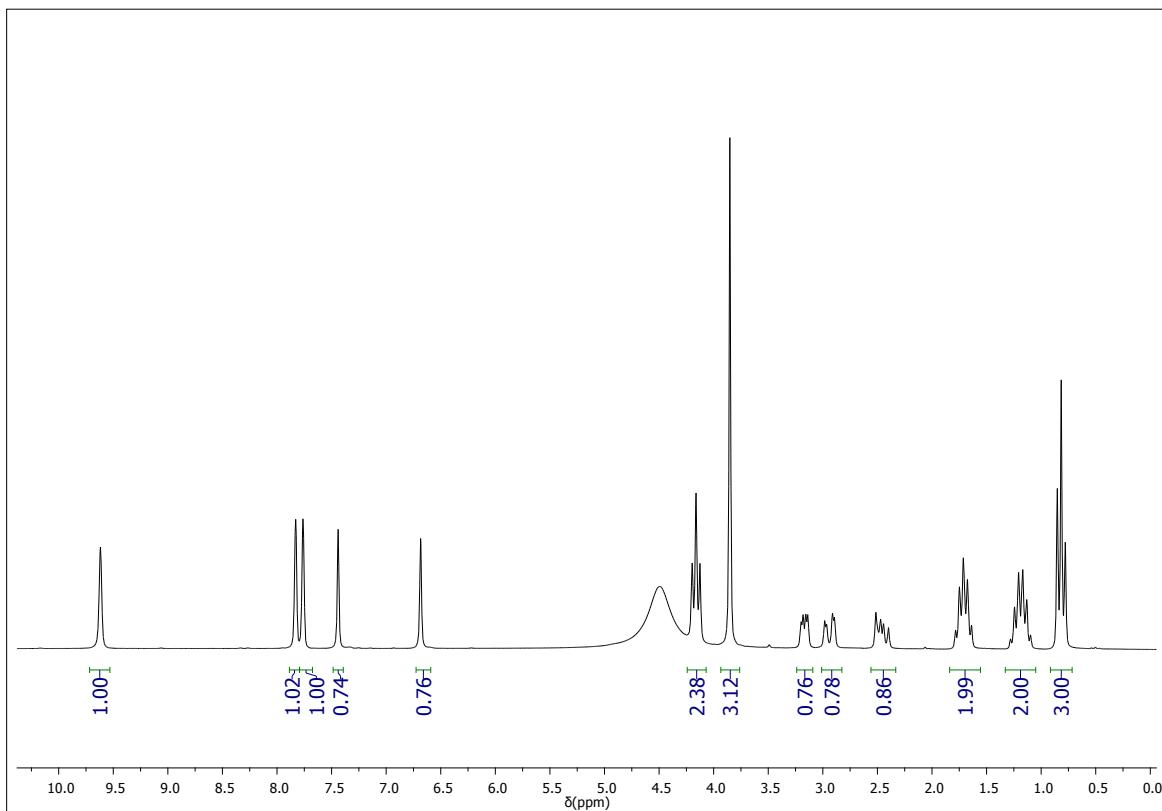


**Figure S36 (b).**  $^{13}\text{C}$  NMR spectrum of Bmim[Phe].

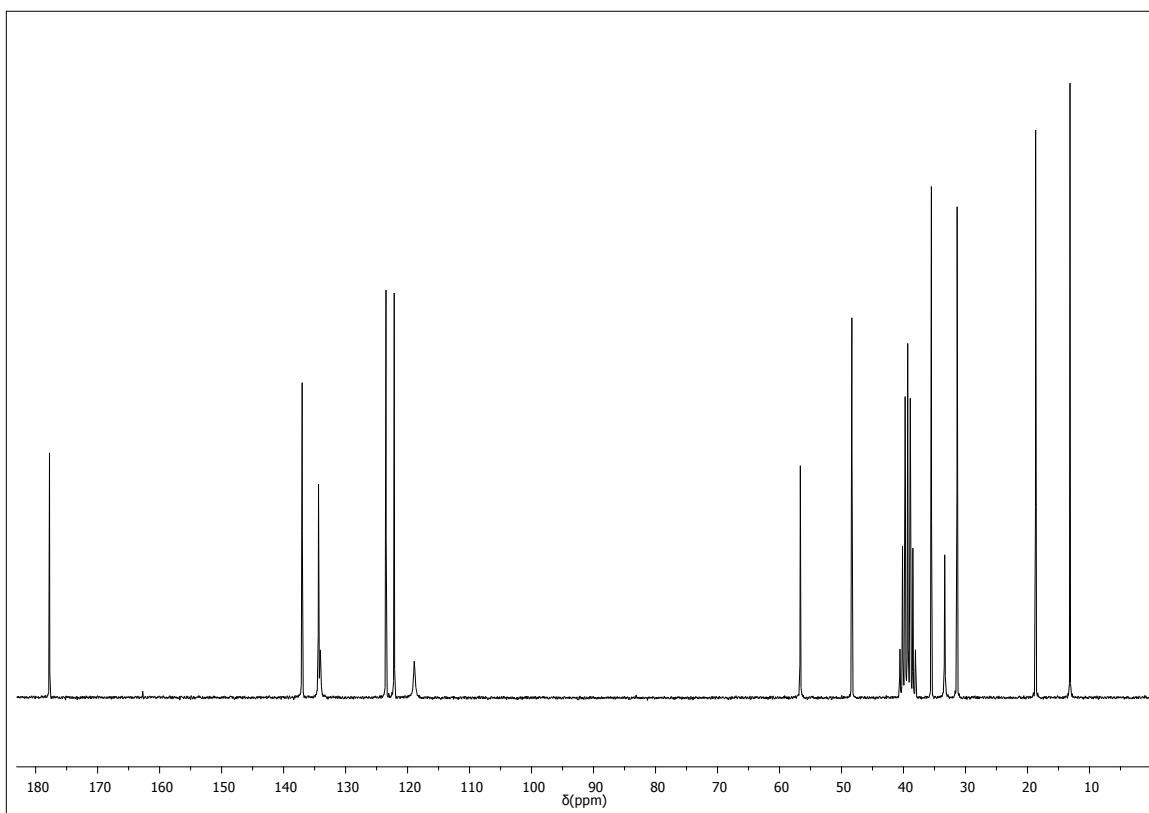


**Figure S36 (c).** HRMS-ESI(+) spectrum of Bmim[Phe].

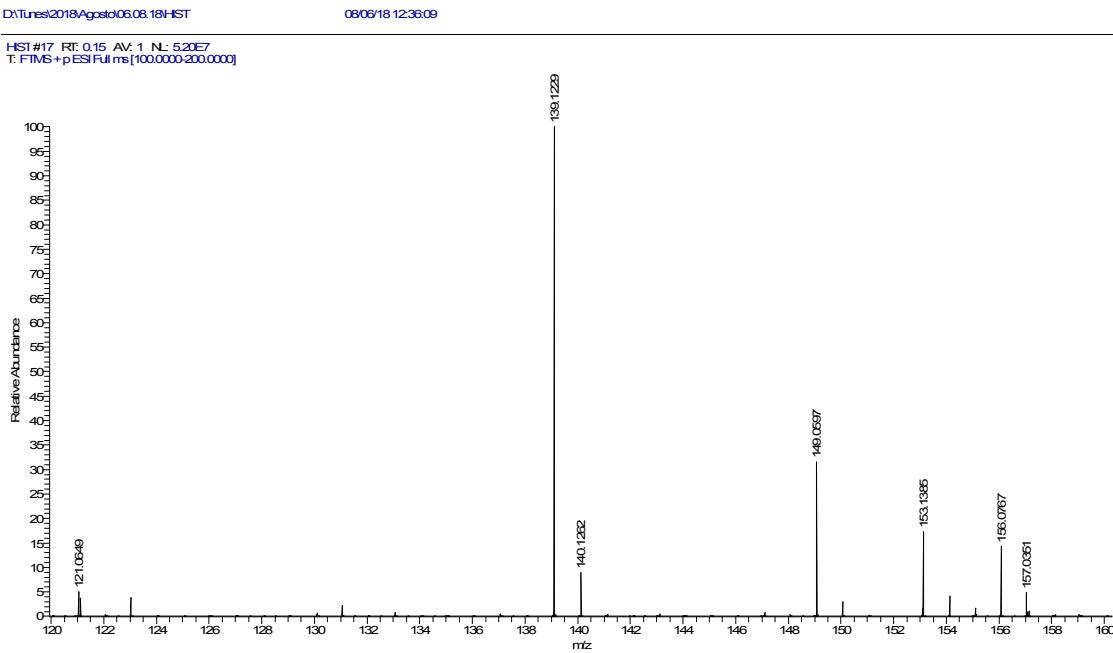
**1-Butyl-3-methylimidazolium Histidine (Bmim[His])** Obtained as light-yellow in 97% yield.  $^1\text{H}$ -RMN (400 MHz, DMSO-d<sub>6</sub>)  $\delta$ , ppm: 9,62 (s, 1H), 7,83 (s, 1H), 7,76 (s, 1H), 7,44 (s, 1H), 6,68 (s, 1H), 4,16 (t,  $J$  = 7,1 Hz, 2H), 3,85 (s, 3H), 3,17 (dd,  $J$  = 8,7, 3,6 Hz, 1H), 2,94 (dd,  $J$  = 14,3, 3,5 Hz, 1H), 2,46 (dd,  $J$  = 14,2, 8,8 Hz, 1H), 1,84 – 1,56 (m, 2H), 1,33 – 1,05 (m, 2H), 0,82 (t,  $J$  = 7,3 Hz, 3H); NH<sub>2</sub> may appear as very broad signal around 1.5 ppm.  $^{13}\text{C}$ -RMN (400 MHz, DMSO-d<sub>6</sub>)  $\delta$ , ppm: 177,8, 137,0, 134,4, 123,5, 122,2, 56,6, 48,3, 35,5, 33,4, 31,4, 18,7, 13,1. HRMS-ESI (+ mode): found m/z 139.1229; calculated for cation C<sub>8</sub>H<sub>15</sub>N<sub>2</sub> m/z 139.1230 ( $\Delta$ = 0.7 ppm)



**Figure S37 (a).**  $^1\text{H}$  NMR spectrum of Bmim[His].

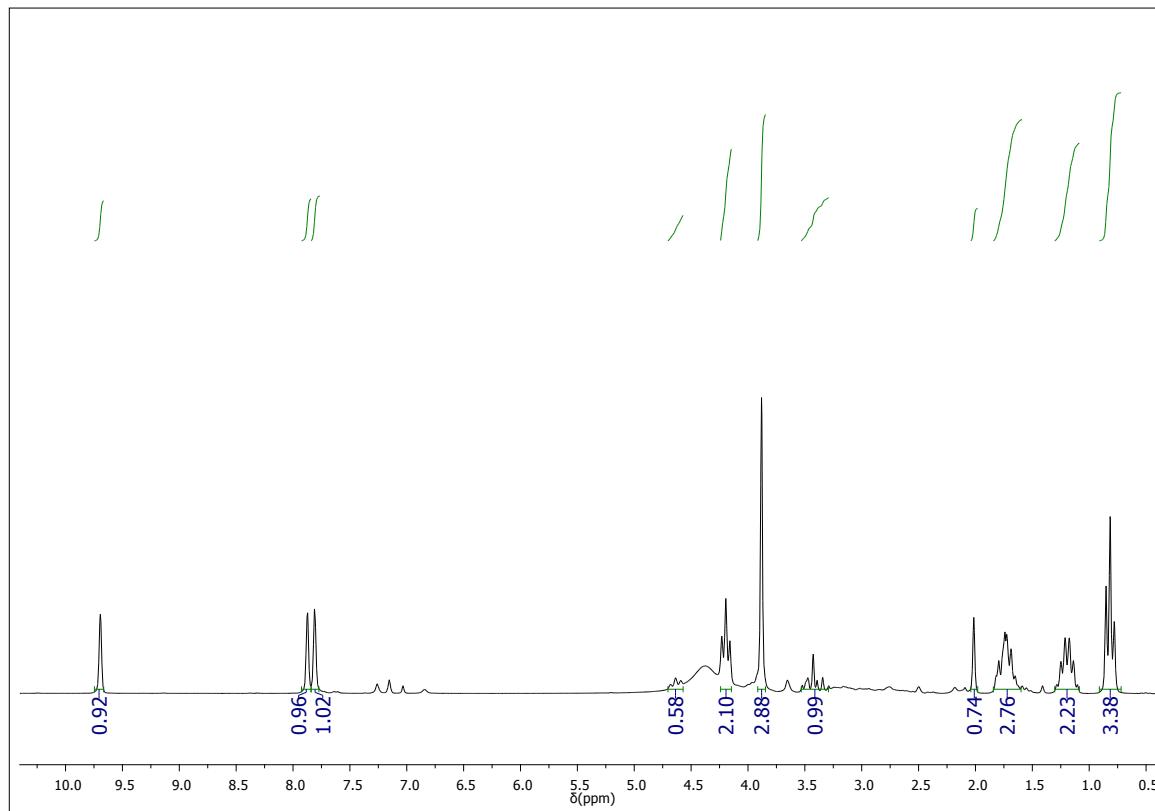


**Figure S37 (b).**  $^{13}\text{C}$  NMR spectrum of Bmim[His].

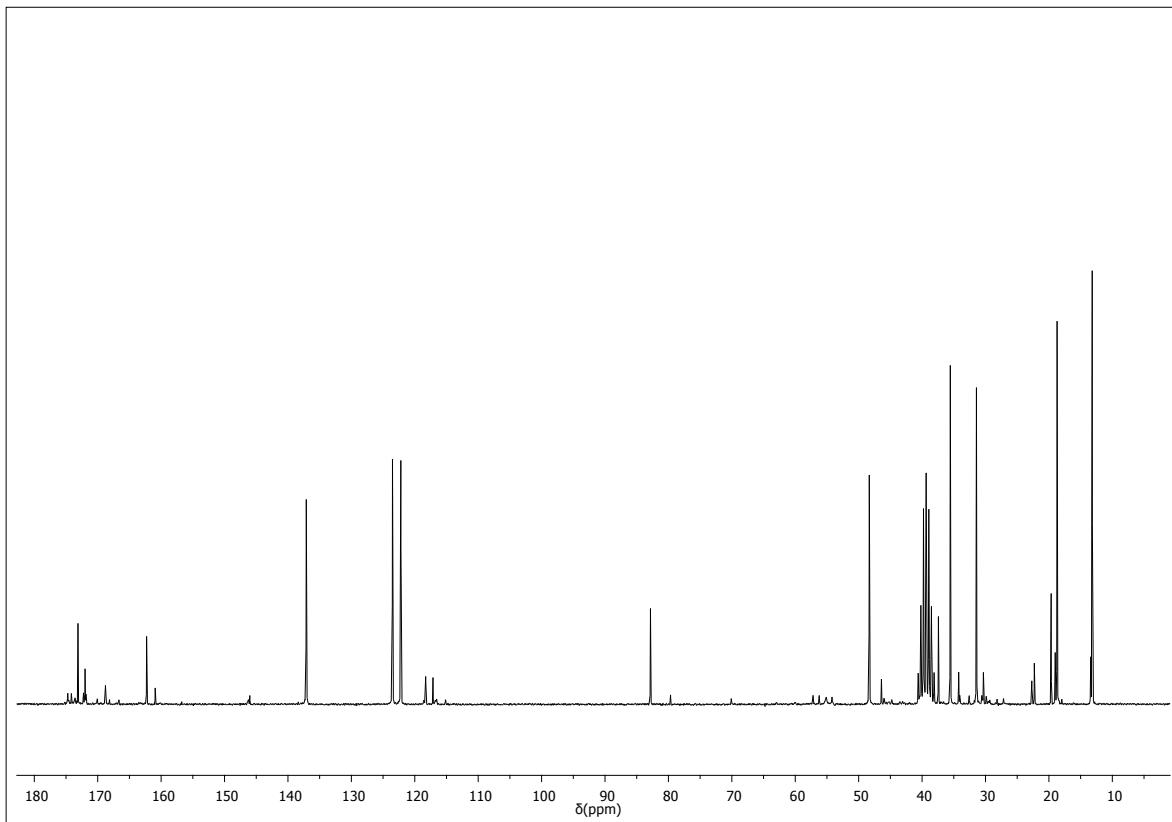


**Figure S37 (c).** HRMS-ESI(+) spectrum of Bmim[His].

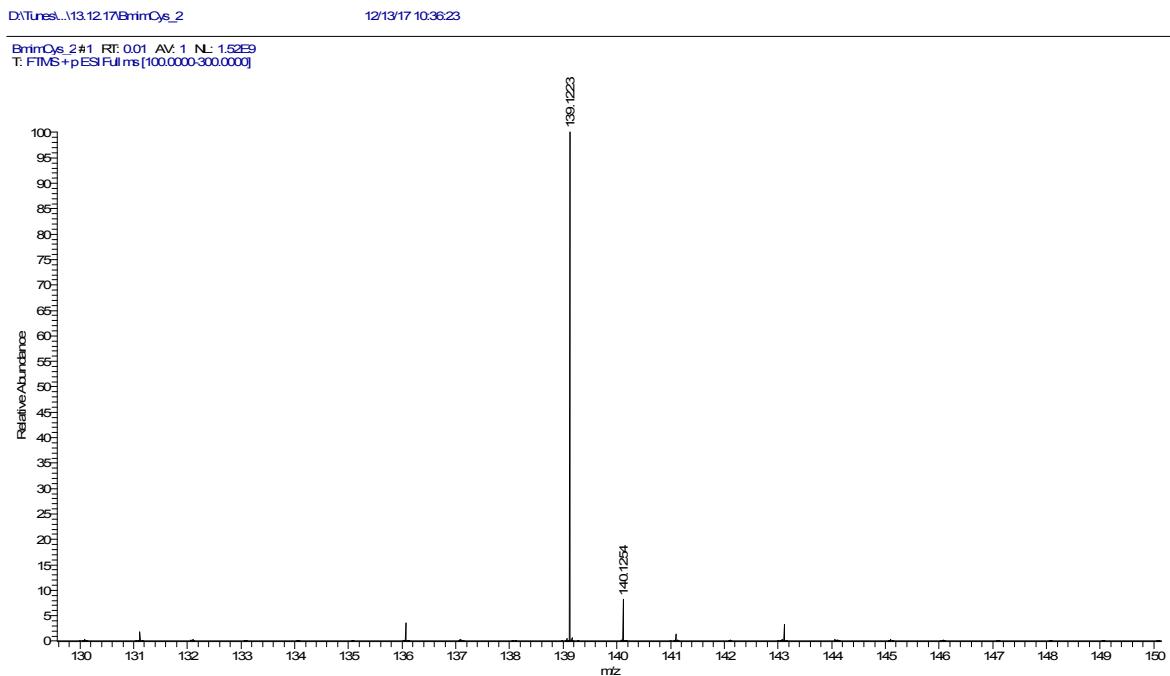
**1-Butyl-3-methylimidazolium cysteine (Bmim[Cys])** Obtained as light-yellow oil in 93% yield.  $^1\text{H}$  NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.69 (s, 1H), 7.87 (s, 1H), 7.81 (s, 1H), 4.70 – 4.57 (m, 1H), 4.19 (t,  $J$  = 7.1 Hz, 2H), 3.88 (s, 3H), 3.41 (t,  $J$  = 13.2 Hz, 1H), 2.01 (s, 1H), 1.74 (td,  $J$  = 15.1, 5.8 Hz, 3H), 1.30 – 1.09 (m, 2H), 0.82 (t,  $J$  = 7.3 Hz, 3H); NH<sub>2</sub> may appear as very broad signal around 1.5 ppm.  $^{13}\text{C}$  NMR (400 MHz, dmso-d<sub>6</sub>)  $\delta$ , ppm: 13.2; 18.7; 31.5; 35.5; 48.3; 58.0; 82.9; 122.2; 123.6; 137.1; 162.2; 173. HRMS-ESI (+ mode): found m/z 139.1223; calculated for cation C<sub>8</sub>H<sub>15</sub>N<sub>2</sub> m/z 139.1230 ( $\Delta$ = 5.0 ppm)



**Figure S38 (a).**  $^1\text{H}$  NMR spectrum of Bmim[Cys].

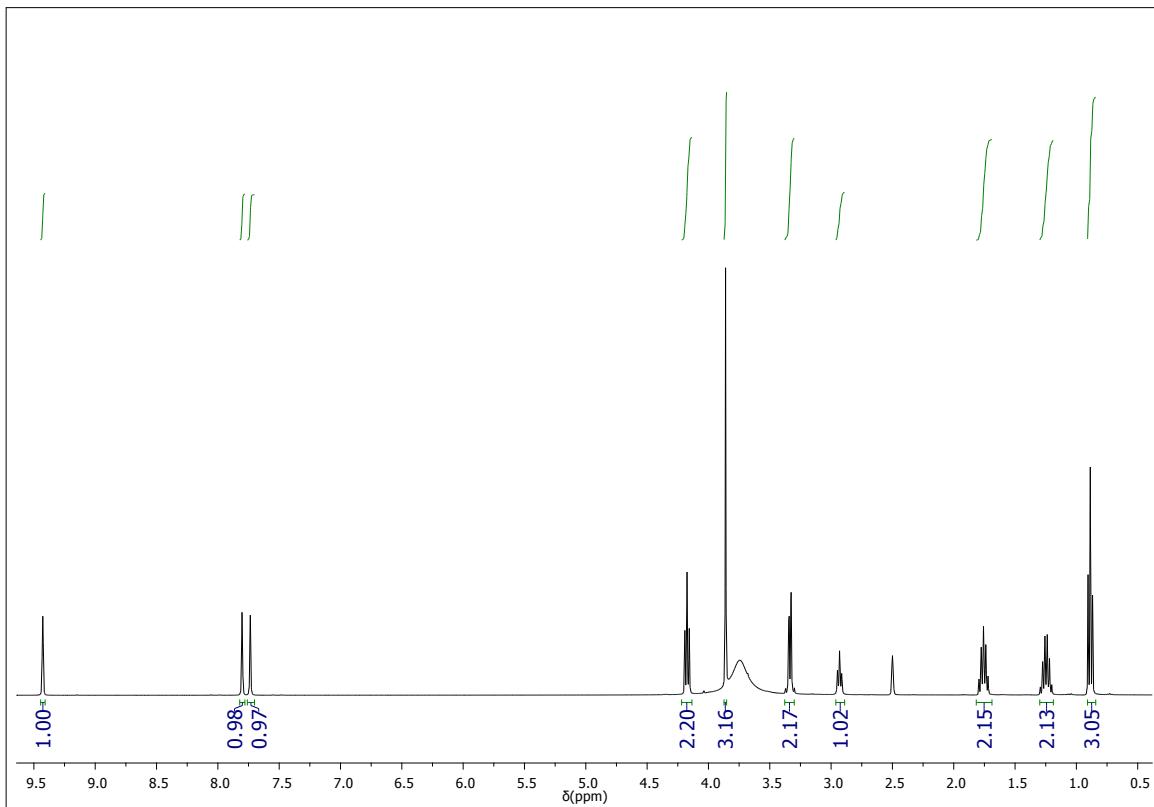


**Figure S38 (b).** <sup>13</sup>C NMR spectrum of Bmim[Cys].

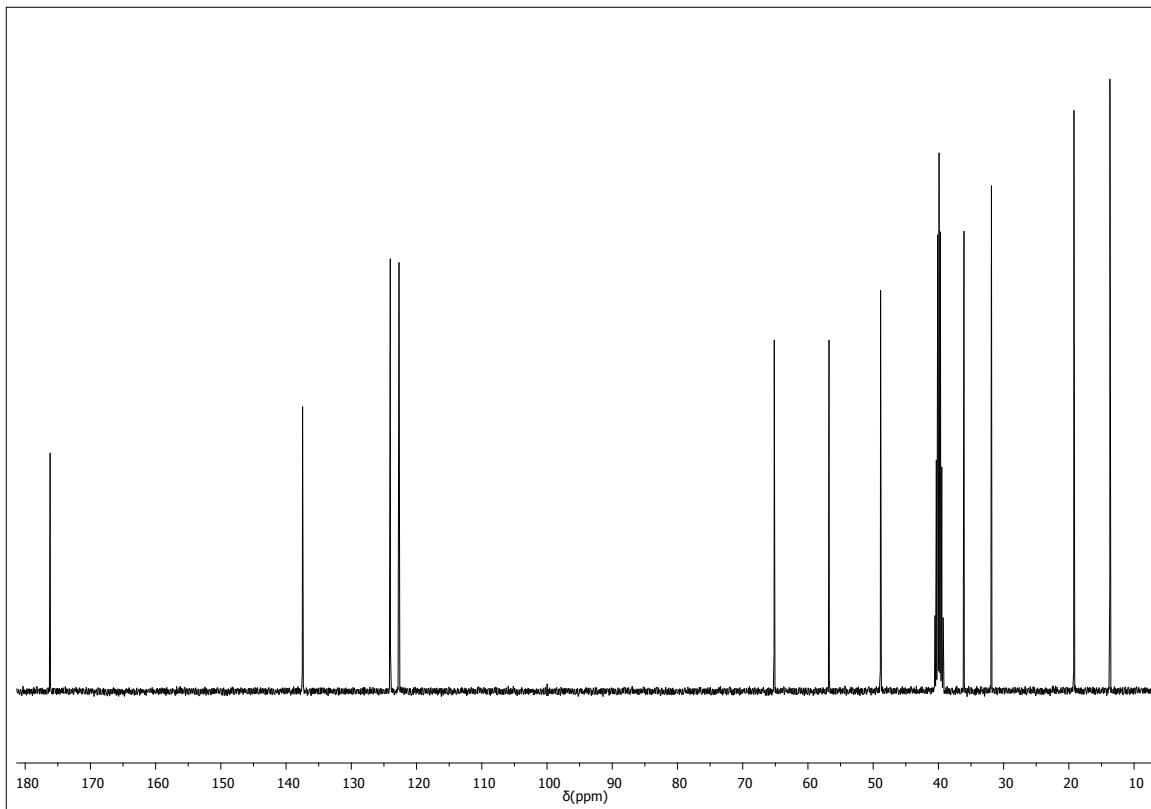


**Figure S38 (c).** HRMS-ESI(+) spectrum of Bmim[Cys].

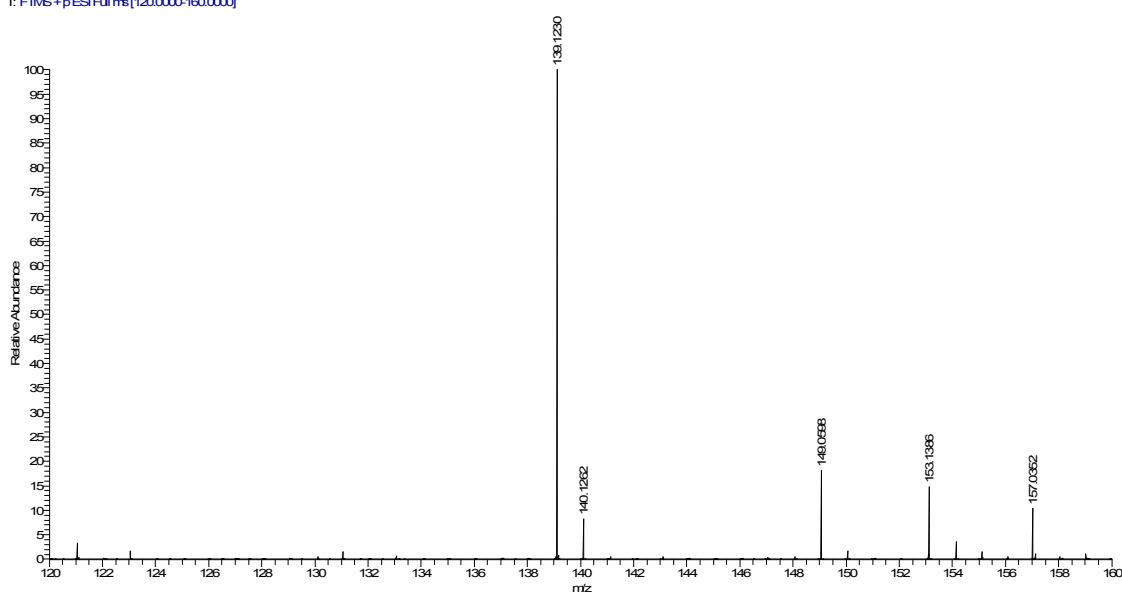
**1-Butyl-3-methylimidazolium serine (Bmim[Ser])** Obtained as light-yellow oil in 95% yield.  $^1\text{H}$  NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$ , ppm: 9.43 (s, 1H), 7.80 (s, 1H), 7.74 (s, 1H), 4.17 (t,  $J$  = 7.2 Hz, 2H), 3.86 (s, 3H), 3.39 – 3.27 (m, 2H), 2.93 (t,  $J$  = 6.8 Hz, 1H), 1.82 – 1.70 (m, 2H), 1.32 – 1.17 (m, 2H), 0.89 (t,  $J$  = 7.4 Hz, 3H). NH<sub>2</sub> may appear as very broad signal around 1.5 ppm and OH may appear as very broad signal around 1.5–4.0 ppm.  $^{13}\text{C}$  NMR (400 MHz, dmsso-d<sub>6</sub>)  $\delta$ , ppm: 13.3, 18.8, 31.5, 35.7, 48.5, 56.4, 64.8, 122.3, 123.6, 137.0, 175.8. HRMS-ESI (+ mode): found m/z 139.1230; calculated for cation C<sub>8</sub>H<sub>15</sub>N<sub>2</sub> m/z 139.1230 ( $\Delta$  = 0 ppm)



**Figure S39 (a).**  $^1\text{H}$  NMR spectrum of Bmim[Ser].

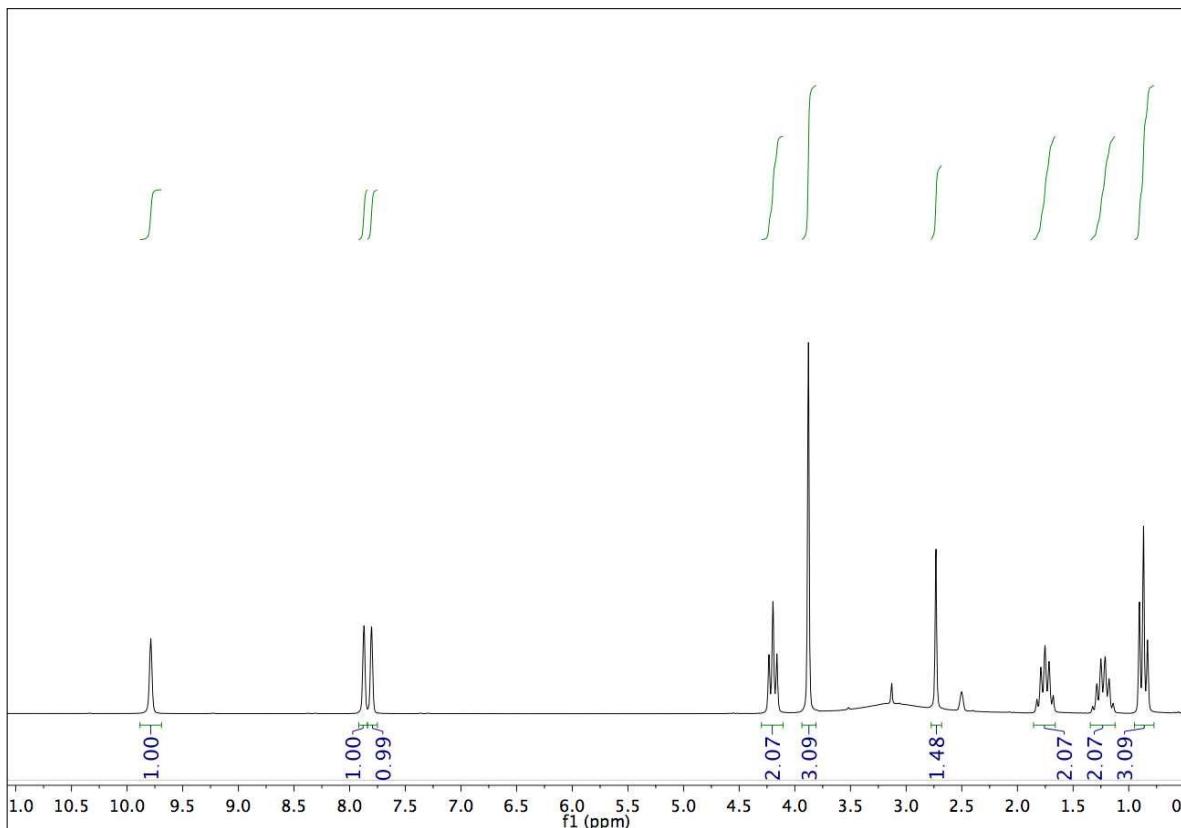


**Figure S39 (b).**  $^{13}\text{C}$  NMR spectrum of Bmim[Ser].

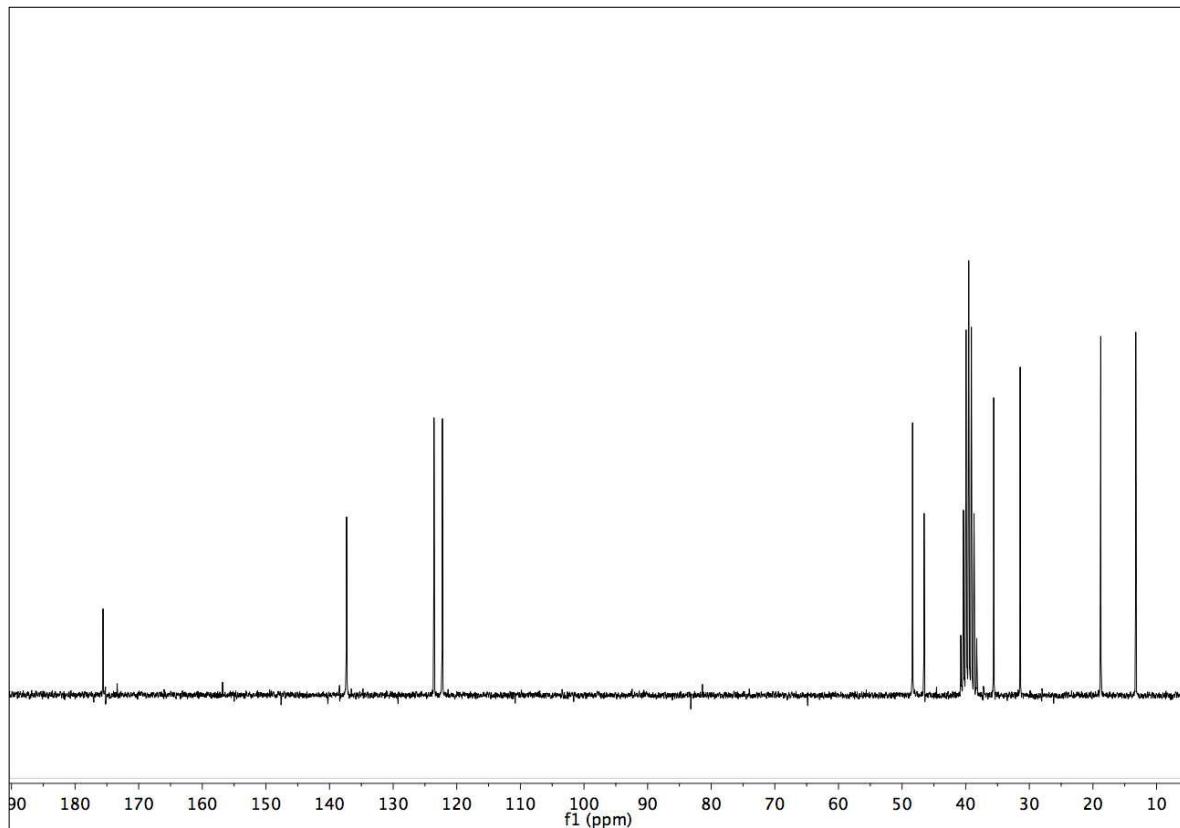


**Figure S39 (c).** HRMS-ESI(+) spectrum of Bmim[Ser].

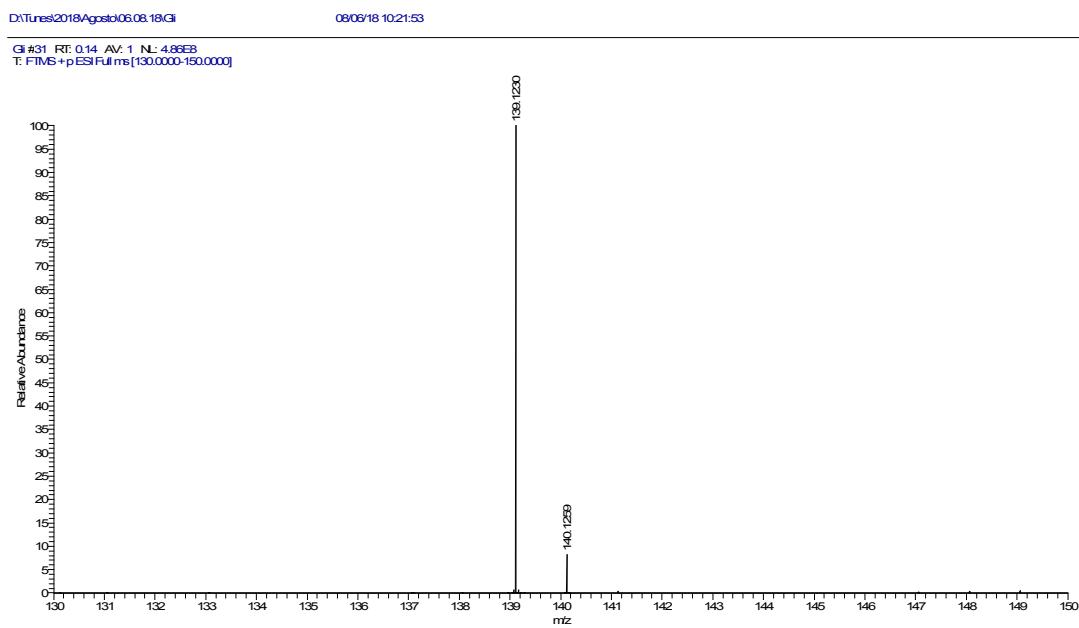
**1-Butyl-3-methylimidazolium glycine** (Bmim[Gly]) Obtained as light-yellow oil in 95% yield.  $^1\text{H}$  NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.79 (s, 1H), 7.87 (s, 1H), 7.80 (s, 1H), 4.20 (t,  $J$ = 7.1 Hz, 2H), 3.88 (s, 3H), 2.73 (s, 1H), 1.75 (p,  $J$ = 7.2 Hz, 2H), 1.21 (dt,  $J$ = 14.4, 7.3 Hz, 2H), 0.87 (t,  $J$ = 7.3 Hz, 3H). NH<sub>2</sub> may appear as very broad signal around 1.5 ppm and OH may appear as very broad signal around 1.5-4.0 ppm.  $^{13}\text{C}$  NMR (400 MHz, dmsso-d<sub>6</sub>)  $\delta$  175.61, 137.32, 123.57, 122.26, 48.35, 46.53, 35.59, 31.44, 18.77, 13.27. HRMS-ESI (+ mode): found m/z 139.1230; calculated for cation C<sub>8</sub>H<sub>15</sub>N<sub>2</sub> m/z 139.1230 ( $\Delta$ = 0 ppm)



**Figure S40 (a).**  $^1\text{H}$  NMR spectrum of Bmim[Gly].

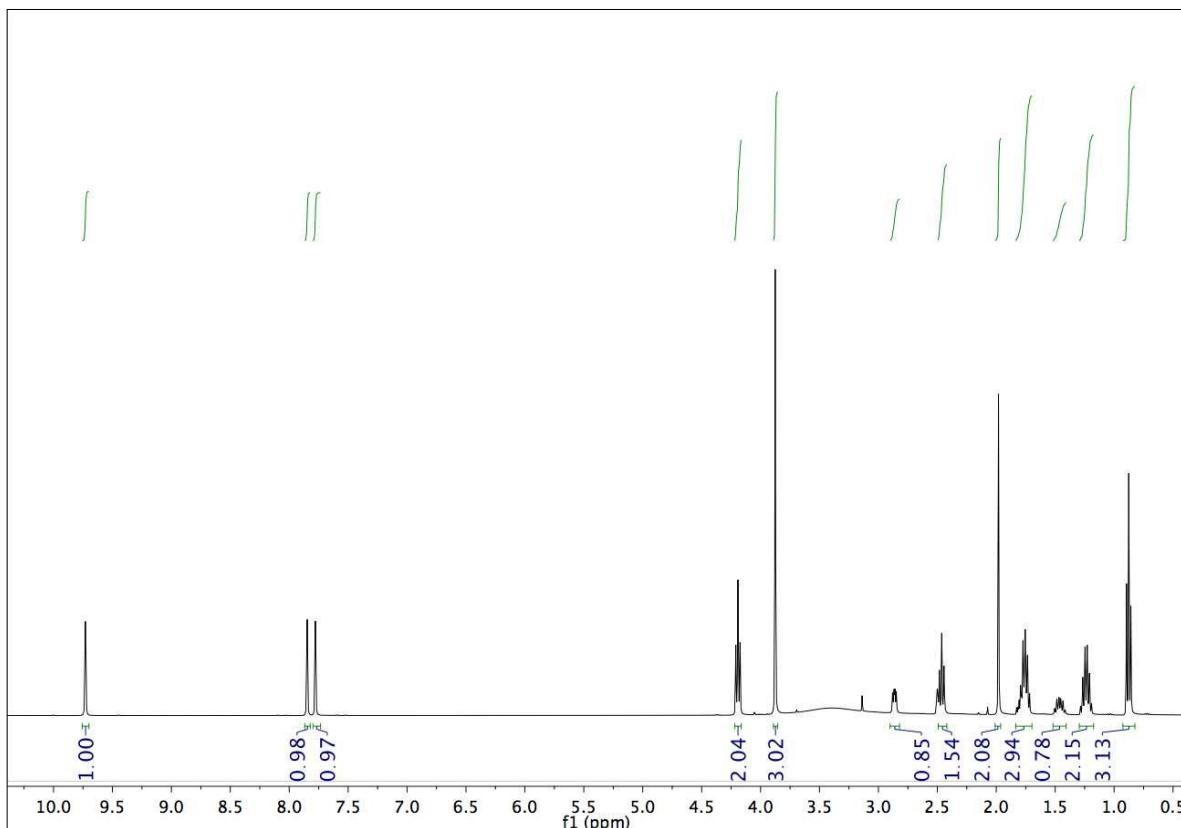


**Figure S40 (b).** <sup>13</sup>C NMR spectrum of Bmim[Gly].

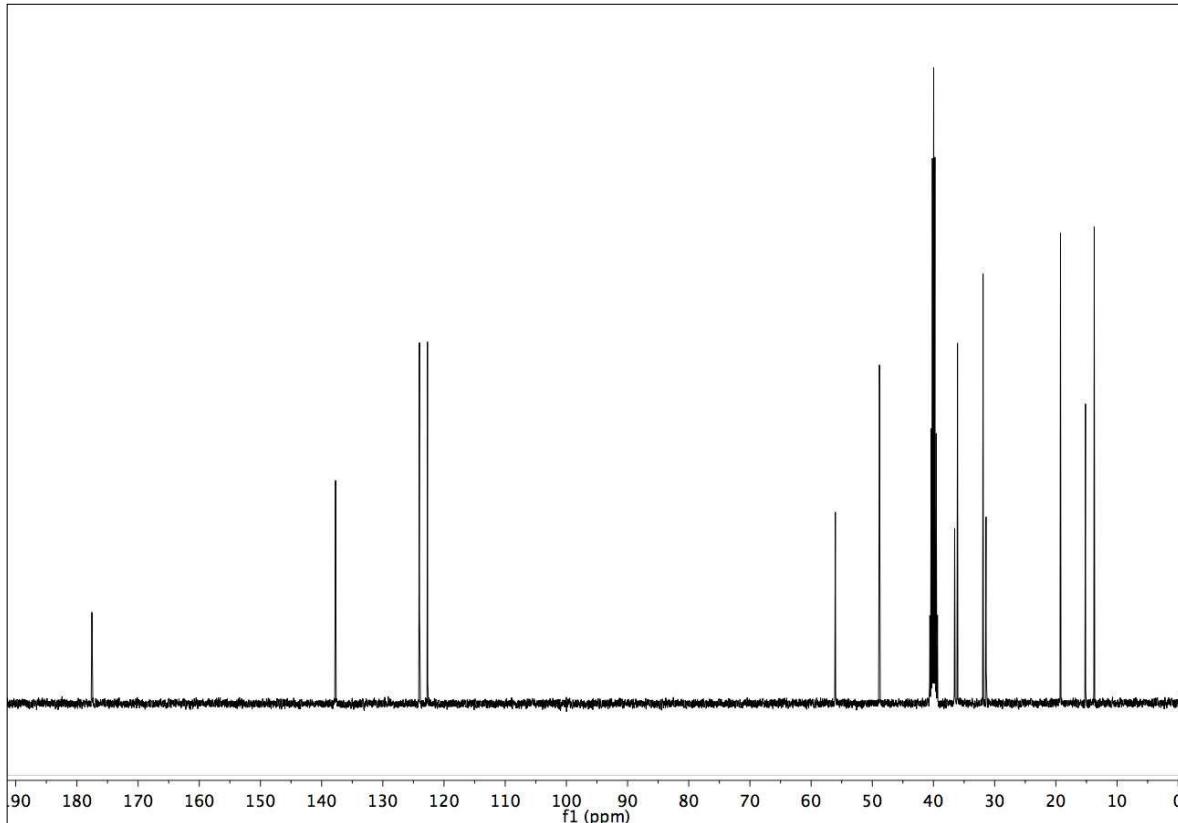


**Figure S40 (c).** HRMS-ESI(+) spectrum of Bmim[Gly].

**1-Butyl-3-methylimidazolium methionine (Bmim[Met])** Obtained as light-yellow oil in 96% yield.  $^1\text{H}$  NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.73 (s, 1H), 7.85 (t,  $J$  = 1.6 Hz, 1H), 7.78 (s, 1H), 4.19 (t,  $J$  = 7.1 Hz, 2H), 3.88 (s, 3H), 2.86 (dd,  $J$  = 7.9, 4.6 Hz, 1H), 2.45 (d,  $J$  = 7.9 Hz, 2H), 1.98 (s, 2H), 1.83 – 1.70 (m, 3H), 1.46 (dq,  $J$  = 15.1, 7.6 Hz, 1H), 1.24 (h,  $J$  = 7.4 Hz, 2H), 0.88 (t,  $J$  = 7.4 Hz, 3H). NH<sub>2</sub> may appear as very broad signal around 1.5 ppm and OH may appear as very broad signal around 1.5-4.0 ppm.  $^{13}\text{C}$  NMR (400 MHz, dmso-d<sub>6</sub>)  $\delta$  177.55, 137.73, 124.02, 122.70, 56.04, 48.83, 36.54, 36.07, 31.90, 31.41, 19.24, 15.15, 13.73. HRMS-ESI (+ mode): found m/z 139.1230; calculated for cation C<sub>8</sub>H<sub>15</sub>N<sub>2</sub> m/z 139.1230 ( $\Delta$  = 0 ppm)



**Figure S41 (a).**  $^1\text{H}$  NMR spectrum of Bmim[Met].

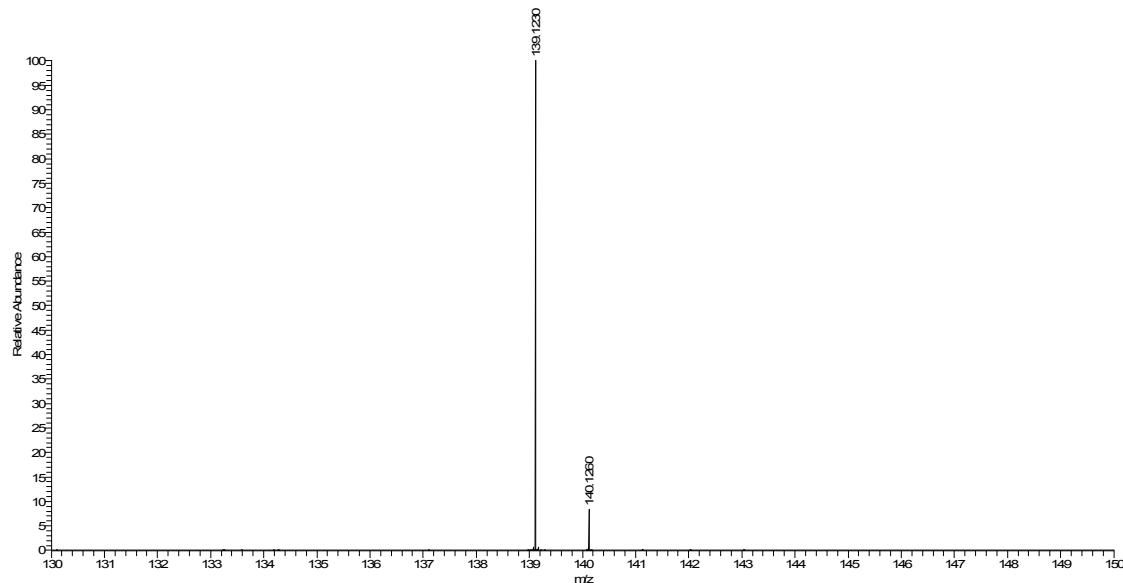


**Figure S41 (b).** <sup>13</sup>C NMR spectrum of Bmim[Met].

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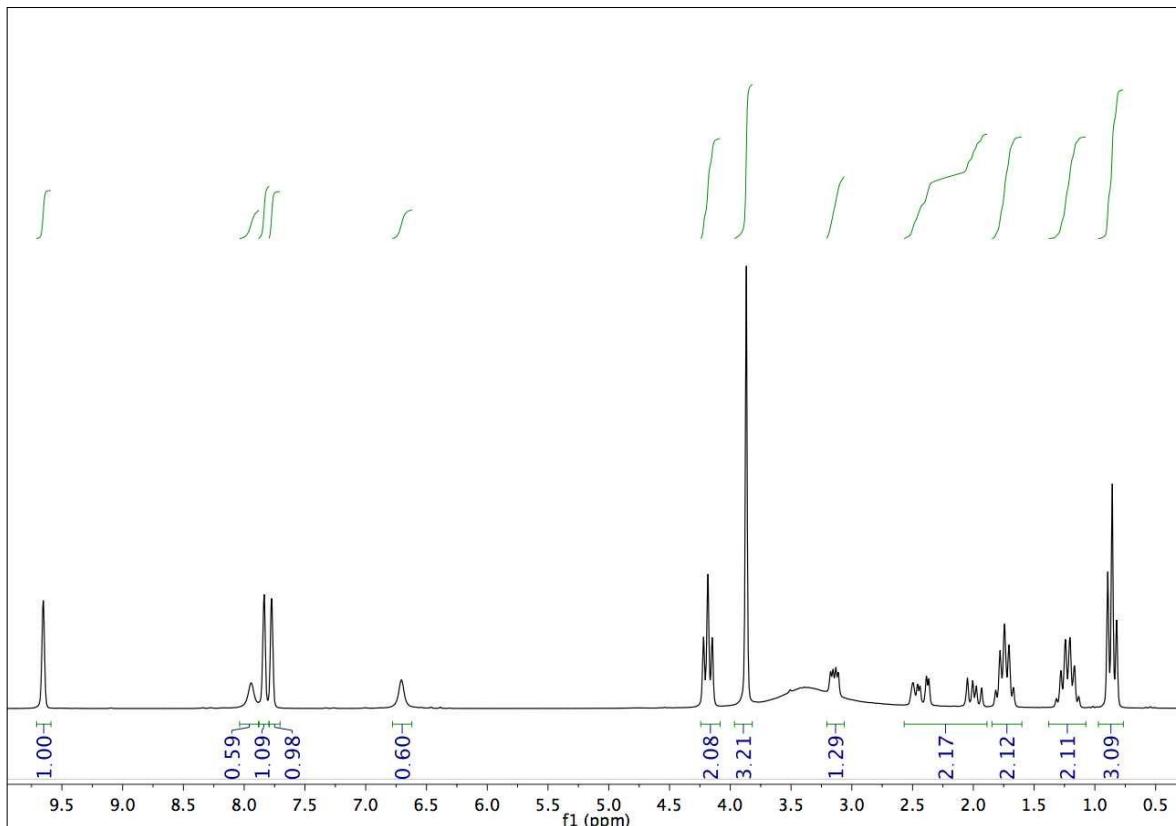
09/08/18 10:15:52

MET#1 RT: 0.01 AV: 1 NL: 361EB  
T: FTMS+PESI Full ms[130.0000-150.0000]

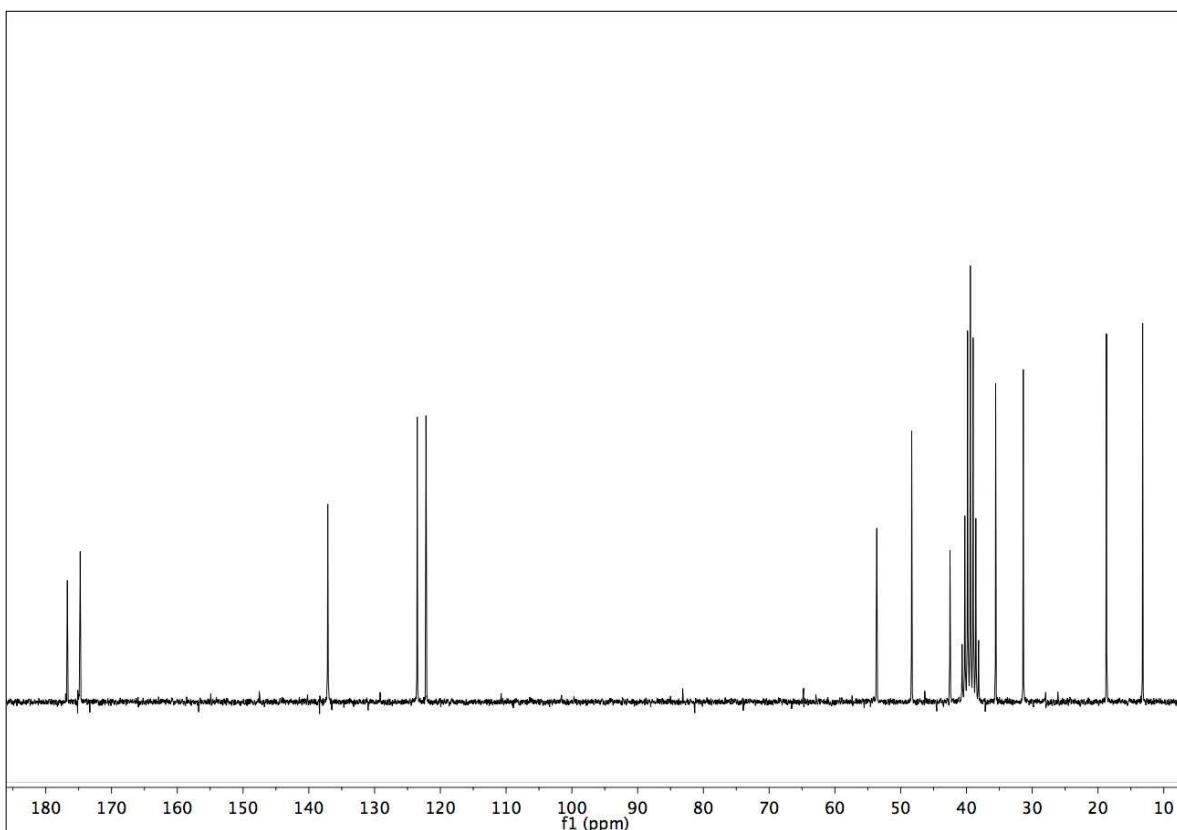


**Figure S41 (c).** HRMS-ESI(+) spectrum of Bmim[Met].

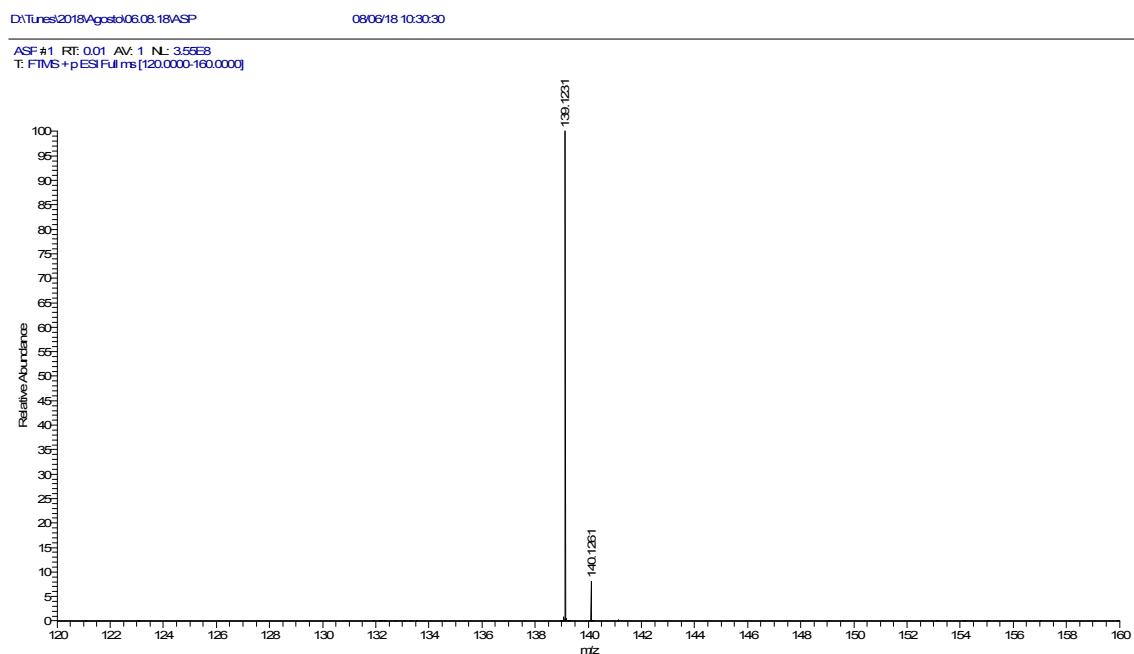
**1-Butyl-3-methylimidazolium asparagine (Bmim[Asp])** Obtained as light-yellow oil in 97% yield.  $^1\text{H}$  NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.65 (s, 1H), 7.94 (s, 1H), 7.84 (d,  $J$  = 1.7 Hz, 1H), 7.77 (d,  $J$  = 1.8 Hz, 1H), 6.71 (s, 1H), 4.18 (t,  $J$  = 7.2 Hz, 2H), 3.14 (dd,  $J$  = 9.0, 4.1 Hz, 1H), 2.57 – 1.89 (m, 2H), 1.74 (p,  $J$  = 7.3 Hz, 2H), 1.22 (h,  $J$  = 7.3 Hz, 2H), 0.97 – 0.77 (m, 3H).  $^{13}\text{C}$  NMR (50 MHz, DMSO-d<sub>6</sub>)  $\delta$  176.72, 174.77, 137.11, 123.51, 122.18, 53.64, 48.32, 42.50, 35.56, 31.36, 18.71, 13.20. HRMS-ESI (+ mode): found m/z 139.1231; calculated for cation C<sub>8</sub>H<sub>15</sub>N<sub>2</sub> m/z 139.1230 ( $\Delta$ = 0.7 ppm)



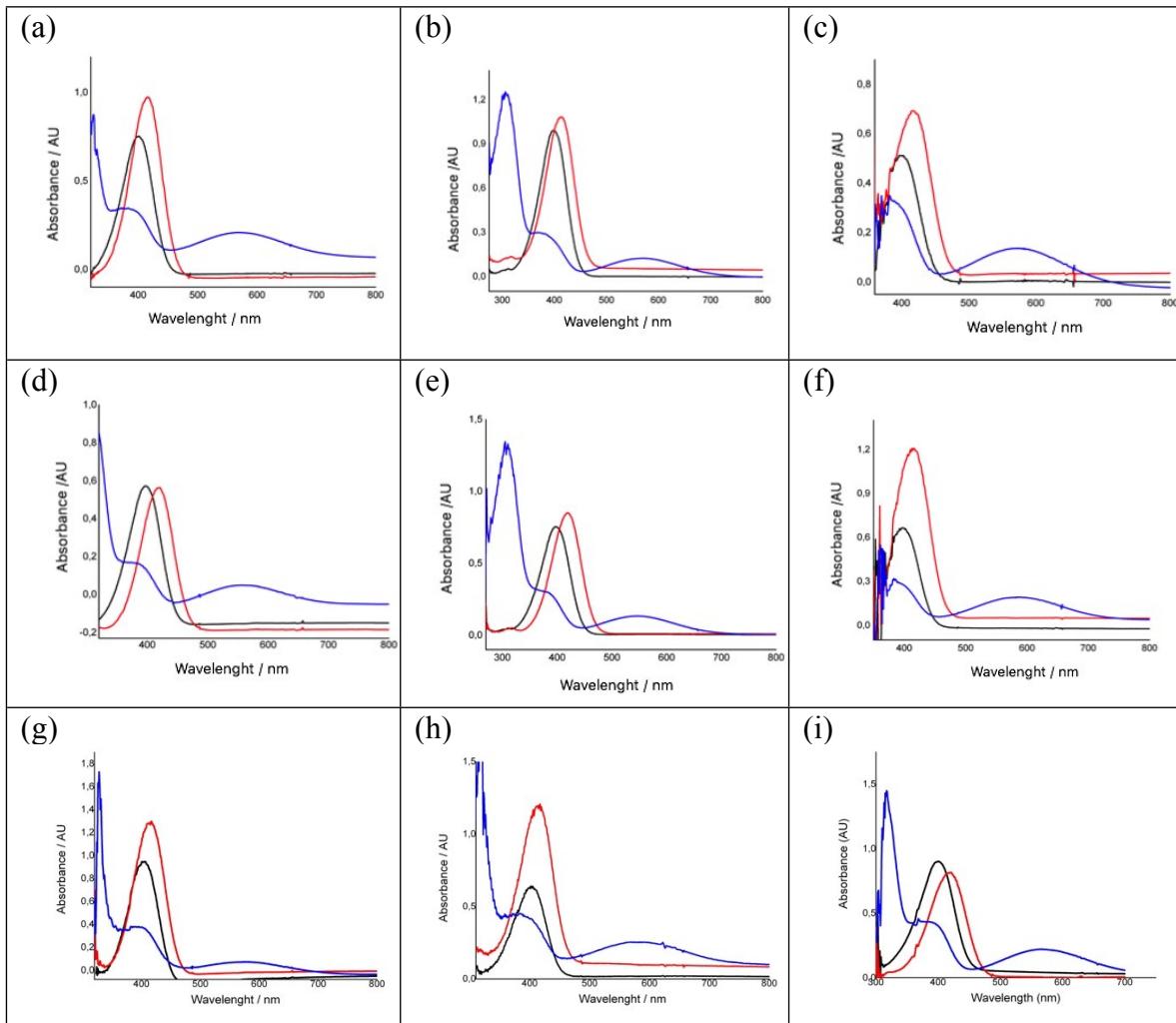
**Figure S42 (a).**  $^1\text{H}$  NMR spectrum of Bmim[Asp].



**Figure S42 (b).** <sup>13</sup>C NMR spectrum of Bmim[Asp].



**Figure S42 (c).** HRMS-ESI(+) spectrum of Bmim[Asp].



**Figure S43.** Solvatochromic shift for each dye used: (—) *N,N*-diethyl-4-nitroaniline, (–) 4-nitroaniline and (—) Reichardt's dye#30 in (a) Bmim[Ala], (b) Bmim[Pro], (c) Bmim[Cys], (d) Bmim[Ser], (e) Bmim[His], (f) Bmim[Phe], (g) Bmim[Gly], (h) Bmim[Met] and (i) Bmim[Asp] at 25°C.

**Table S1.** Relative product distribution (%) for the nucleophilic attack of each Bmim[AA] to Paraoxón.

Bmim[AA]	%S <sub>N</sub> (C)	%S <sub>N</sub> Ar	%S <sub>N</sub> (P)
Bmim[Ala]	8	29	63
Bmim[Cys]	15	85	-
Bmim[Phe]	15	72	13
Bmim[His]	10	90	-
Bmim[Pro]	26	31	43
Bmim[Ser]	20	26	54
Bmim[Asp]	22	42	36
Bmim[Gly]	-	11	89
Bmim[Met]	-	48	52

**Table S2.** Molar amount of the different products at various time for the reaction of Paraoxon with Bmim[Pro] at 25.0 °C. These amount was obtained by integration of the corresponding of <sup>31</sup>P-NMR spectra.

Time	Substrate (10 <sup>3</sup> /moles)	Product 2b (10 <sup>3</sup> /moles)	Product 3 (10 <sup>3</sup> /moles)	Product 4 and 5b (10 <sup>3</sup> /moles)
21 min	7.89	0.81	0.71	0.59
30 min	6.24	1.43	1.22	1.11
42 min	5.30	1.87	1.53	1.30
50 min	4.43	2.58	1.61	1.38
67 min	3.28	2.87	2.15	1.73
75 min	3.17	2.90	2.07	1.87
84 min	2.08	3.13	2.53	2.26
2.35 h	1.28	3.33	2.85	2.54
3.3 h	0.28	4.08	3.07	2.57
4.73 h	-	4.29	3.20	2.51

1.3 days	-	4.21	3.15	2.64
2 days	-	4.29	3.13	2.58
8 days	-	4.29	3.13	2.58

**Table S3.** Pseudo-First-Order Rate Constants ( $k_{\text{obsd}}$ ) for the degradation of Paraoxon in the Bmim[AA].

Bmim[AA]	$10^2 k_{\text{obsd}}/\text{min}^{-1}^*$	$R^2$
Bmim[Ala]	5.06	0,992
Bmim[Pro]	1.95	0,991
Bmim[Cys]	4.95	0,990
Bmim[Phe]	3.08	0,979
Bmim[His]	1.90	0,996
Bmim[Ser]	1.68	0,993
Bmim[Asp]	1,82	0,994
Bmim[Gly]	**	-
Bmim[Met]	**	-

\*Each measurement was made in triplicate.

\*\*It was impossible to obtain an accurate  $k_{\text{obsd}}$  value in both solvents, due to kinetic technique used in this study ( $^{31}\text{P}$ -NMR take almost 3 minutes).

**Table S4.** Half-life ( $t_{1/2}$ ) for the degradation of Paraoxon® in Bmim[Ala] with different water amount added.

Water amount (uL)	$t_{1/2}(\text{min})$
40	28,7
80	79,1
120	136,7