

Supplementary Material (ESI) for Chemical Communications  
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*Supporting information for:*

## **Ionic liquids enable electrospray ionisation mass spectrometry in hexane**

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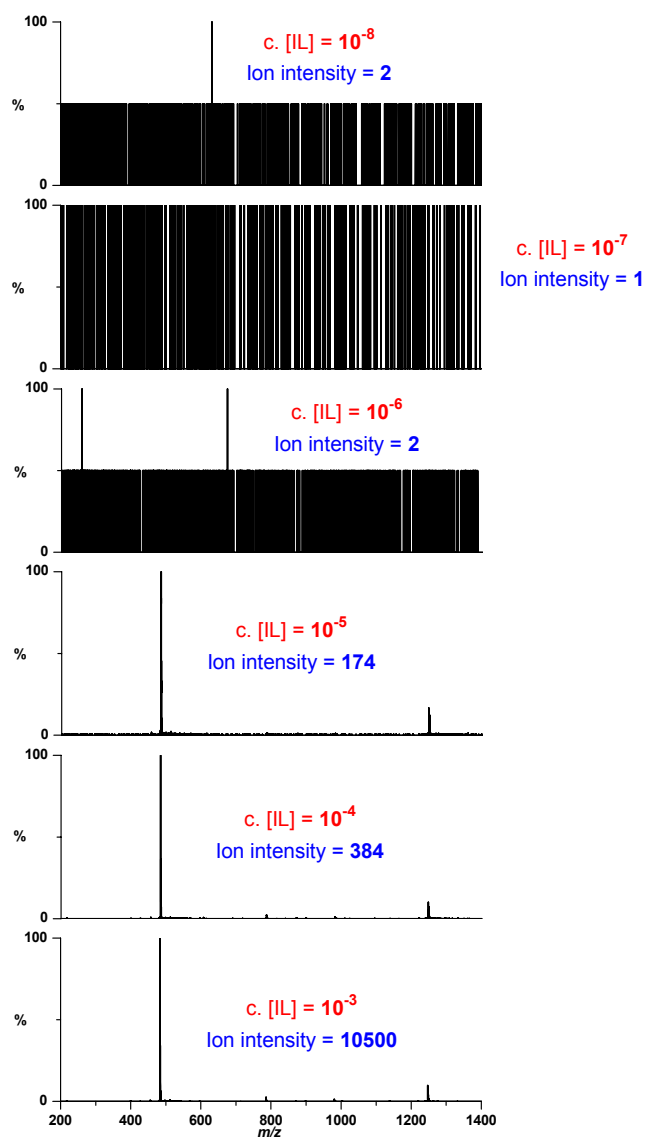
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### *General experimental details*

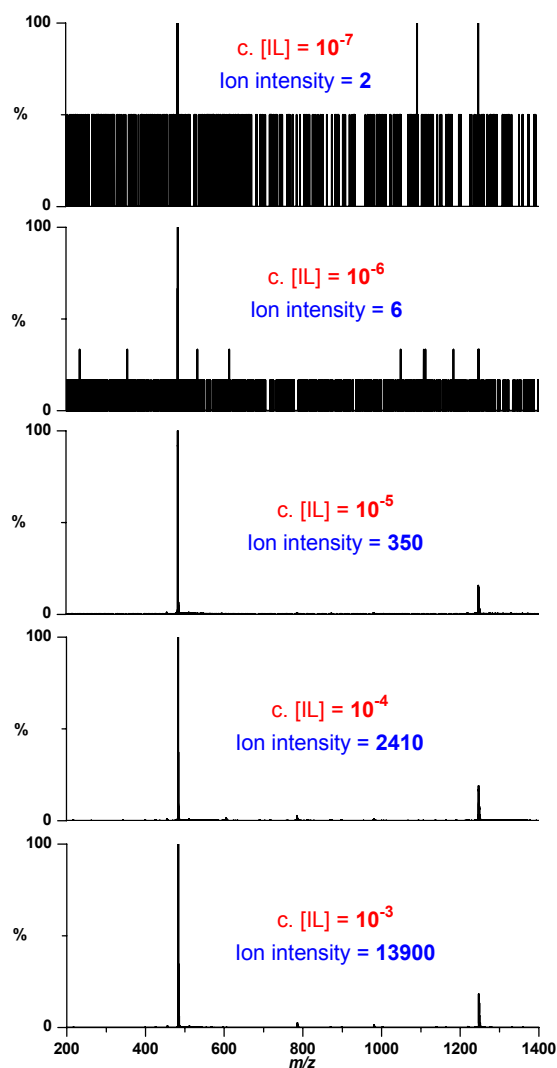
**1** was purchased from Aldrich and used as provided but handled in an inert-atmosphere glovebox. Hexane and toluene were HPLC-grade, and were dried and purged of oxygen using an MBraun solvent-purification system. Pentane, cyclohexane and benzene were HPLC-grade. (C<sub>2</sub>H<sub>4</sub>O)<sub>6</sub> (“18-crown-6”) was purchased from Aldrich.

### *Mass spectra of 1 in various non-polar solvents*

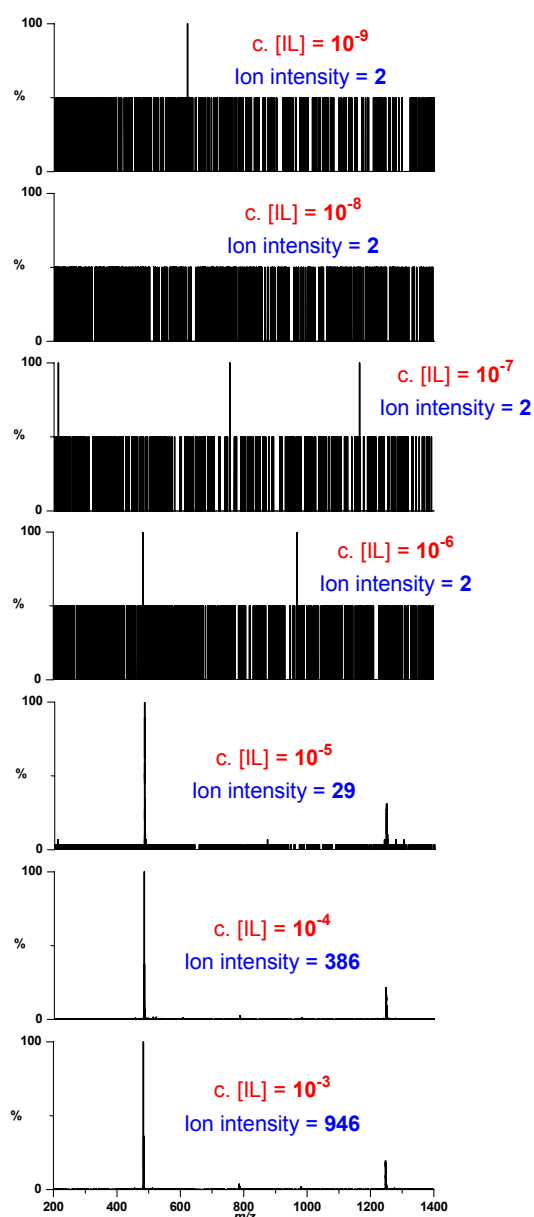
ESI-MS of **1** were collected in positive-ion mode in hexane, pentane, cyclohexane, benzene and toluene. Concentrations of **1** are noted on the spectra. “Ion intensity” refers to the ion current for the base peak. Spectra were collected for 1 minute in all cases, summing 60 individual mass spectra. Relatively high solvent flow rates tend to improve spectra quality; these spectra were collected at 10  $\mu\text{L min}^{-1}$  but flow rates of up to 40  $\mu\text{L min}^{-1}$  often improved the ion current significantly.



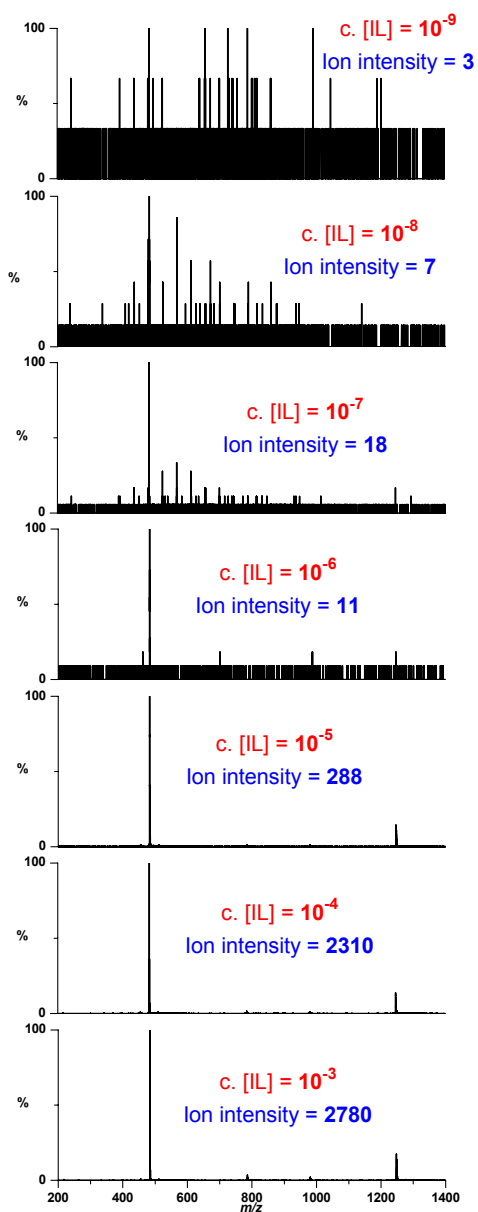
**Figure S11.** Positive-ion ESI mass spectra of **1** at differing concentrations in hexane. Each spectrum was collected over 1 minute (60 summed spectra). A stable spray and good spectra are obtained at a threshold of  $\sim 10^{-5}$  mol L<sup>-1</sup>.



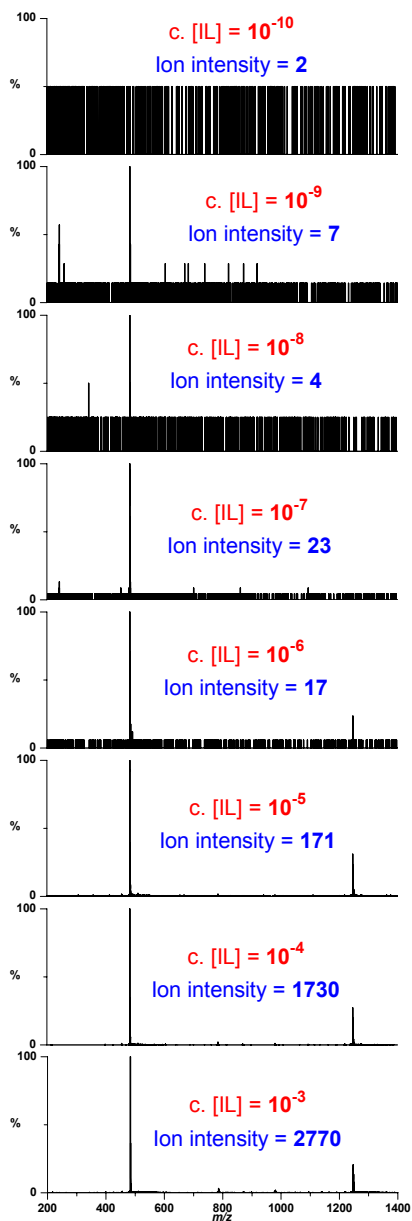
**Figure SI2.** Positive-ion ESI mass spectra of **1** at differing concentrations in pentane. Each spectrum was collected over 1 minute (60 summed spectra). A stable spray and good spectra are obtained at a threshold of  $\sim 10^{-5}$  mol L<sup>-1</sup>.



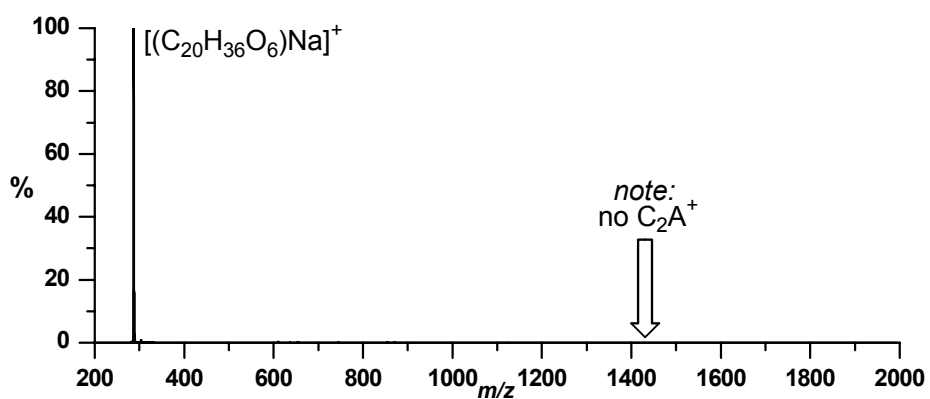
**Figure SI3.** Positive-ion ESI mass spectra of **1** at differing concentrations in cyclohexane. Each spectrum was collected over 1 minute (60 summed spectra). A stable spray and good spectra are obtained at a threshold of  $\sim 10^{-5}$  mol L<sup>-1</sup>.



**Figure S14.** Positive-ion ESI mass spectra of **1** at differing concentrations in benzene. Each spectrum was collected over 1 minute (60 summed spectra). A stable spray and good spectra are obtained at a threshold of  $\sim 10^{-5} \text{ mol L}^{-1}$ , though the IL can be detected at a satisfactory signal-to-noise ratio at  $\sim 10^{-7} \text{ mol L}^{-1}$ .



**Figure S15.** Positive-ion ESI mass spectra of **1** at differing concentrations in toluene. Each spectrum was collected over 1 minute (60 summed spectra). A stable spray and good spectra are obtained at a threshold of  $\sim 10^{-5}$  mol L<sup>-1</sup>, though the IL can be detected at a satisfactory signal-to-noise ratio at  $\sim 10^{-7}$  mol L<sup>-1</sup>.



**Figure SI6.** Positive-ion ESI mass spectrum of **3** in toluene. Similarly, the negative-ion spectrum shows no  $CA_2^-$  ion, only  $A^-$ .