Supporting Information

- **Title:** Nanopore stochastic detection of a liquid explosive component and sensitizers using boromycin and an ionic liquid supporting electrolyte
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Abstract:

This supporting information includes a theoretical explanation for open channel current and dwell time change when ionic liquid was used as the background electrolyte solution. In addition to that, Figures S1 and S2 represents typical single channel current recording traces for the detection of TMA and for the simultaneous detection of TEA and HZ respectively.

Theoretical explanation for open channel current and dwell time change

According to the Nernst-Einstein equation,¹ the molar conductivity of an electrolyte (λ) is related to the diffusion coefficients of its ions (D) as:

$$\lambda = z^2 DF^2 / RT$$

where z is the number of charges on ions, F is the Faraday constant, R is gas constant, and T is absolute temperature.

The diffusion coefficient of an ion is related to the viscosity of the medium (η) through Stokes-Einstein equation:¹

$$D = kT / 6\pi \eta a$$

where k is the Boltzmann constant, and a is the hydrodynamic radius of the ion.

The combination of these two provides the final expression of conductivity:

$$\lambda = z^2 F^2 k / R6 \pi \eta a$$

Therefore, the conductivity of an electrolyte solution is inversely proportional to both the viscosity of the medium and the hydrodynamic radius of the ion. However, the higher viscosity of BMIM-Cl dramatically decreases its conductivity by counteracting the size effect. As a result of these combined effects of size and viscosity, a smaller open channel current is observed in ionic liquid containing solutions than in NaCl solutions.

Since the identical analyte and pore were used in both conditions, specifically, in the experiments with both the NaCl solution and the BMIM-Cl solution as the electrolytes, the dwell time of the boromycin events depends primarily on the migration rate of the analyte as well as the binding

affinity between boromycin and the α HL pore. The former can be primarily governed by the diffusion and charge selectivity of the pore. The effect of diffusion can be attributed using the above Stokes-Einstein equation. According to the equation, the only variable which governs the diffusion is viscosity, because all the other factors can be considered as identical in both systems. When the BMIM-Cl solution was used instead of NaCl, the viscosity of the bulk solution increased by 71% (from 1.438 mm²/s to 2.464 mm²/s). The increased value was much smaller than the percentage of the increase (i.e., 160%) in the experimental event mean dwell times. Since the characteristic time for a molecule to diffuse the 10 nm length pore such as α HL is 50–500 ns,² the relatively small change in the viscosity of the medium could not explain the observed large boromycin residence time. Therefore, it is more likely that the electrolyte change may significantly affect the charge selectivity³ and the binding of boromycin to the pore. It should be noted, our experiments showed that the values for both reversal potentials and streaming potentials of the wild-type α HL protein were different in BMIM-Cl and NaCl solutions (data not shown). However, due to the lack of data for the activity coefficient of BMIM-Cl solution, the actual charge selectivity of the pore could not be obtained. It was reported that the change of the charge selectivity of a protein pore could be reflected from streaming potential and reversal potential.³ Thus, different streaming potential and reversal potential values obtained in NaCl and BMIM-Cl solutions suggests that the charge selectivities of the α HL protein pore are different in these two electrolyte solutions.



Figure S1. Typical single channel current recording trace for the detection of Tetramethylammonium chloride (1.25 mM). The experiments were performed in 1 M BMIM-Cl and with 12.5 μ M boromycin as a host.



Figure S2. Typical single channel current recording traces for the simultaneous detection of TEA and HZ in 1 M BMIM-Cl (aq). a) Boromycin + TEA (2 : 200); b) boromycin + HZ (2 : 200); and c) boromycin + HZ + TEA (2 : 100 : 100).

References

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- (3) Zhao, Q.; Jayawardhana, D. A.; Guan, X. Biophys. J. 2008, 94, 1267-1275.