Supporting Information

Design and Characterization of a 2-(2'-Hydroxyphenyl)benzimidazole -Based Sr^{2+}-Selective Fluorescent Probe in Organic and Micellar Solution Systems

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Measurement of the fluorescence spectrum of M^{n+}-BIC complexes in DMSO

A 10 mM stock solution of **BIC** was prepared by dissolving the appropriate amount of **BIC** in DMSO. Stock solutions (1.0 mM) of metal ions (K^+, Ca^{2+}, Sr^{2+}, and Ba^{2+}) were prepared by dissolving appropriate amounts of sodium chloride, potassium chloride, calcium chloride, strontium chloride, and barium chloride in water. Solutions of M(**BIC**)$^{n+}$ complexes were prepared by adding 1.5 μL of the stock **BIC** solution and appropriate amounts of a stock metal ion solution and DMSO in a quartz cell (the total amount of the M(**BIC**)$^{n+}$ complex solution was 3000 μL). Note that in the case of Na^+-**BIC** solution, the fluorescence spectrum did not change. Therefore, we did not show the data in here.

Upon addition of M^{n+} (M^{n+} = K^+, Ca^{2+}, Sr^{2+}, and Ba^{2+}), the fluorescence intensity of **BIC** is enhanced with a large shift in the wavelength. The peak shift would be due to the formation of M(**BIC**)$^{n+}$ complexes.

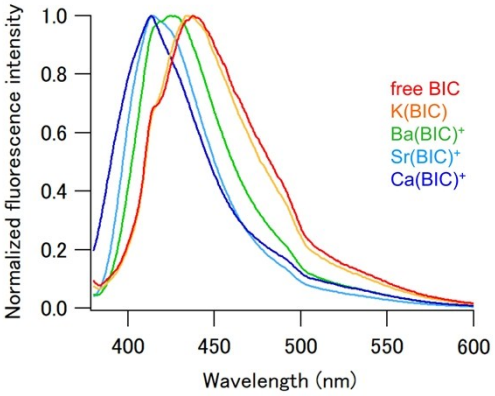

Figure S1 Fluorescence spectra of the M^{n+}-**BIC** (M^{n+} = K^+, Ca^{2+}, Sr^{2+}, and Ba^{2+}) complexes in DMSO.

Table 1. Emission maximum of the M^{n+}-**BIC** complexes in DMSO.

Metal	Free ligand	K^+	Ca^{2+}	Sr^{2+}	Ba^{2+}
Emission maximum wavelength (nm)	437.5	434	413.5	414	424.5

Result of neutron reflectivity (NR) analysis

We carried out NR analysis to reveal the localized structure of Sr(**BIC**)$^+$ complex in LaNa surfactant using a model LaNa sample. The NR measurements were performed on a BL17 SHARAKU reflectometer installed at the Materials and Life Science Experimental Facility (MLF) in J-PARC [1]. The incident beam power of the proton accelerator was 300 kW for all the measurements. The wavelength (λ) range of the incident neutron beam was tuned to be approximately λ = 1.1–8.8 Å using disk choppers. The covered Q_z range was Q_z = 0.01 – 0.24 Å^{-1}, where $Q_z = (4\pi/\lambda)\sin\theta$ (here, θ represents the incident angle). The Motofit program [2] was used to fit the NR profiles using the least-squares approach to minimize deviations in the fit; the thickness, scattering length density (SLD), and Gaussian roughness were evaluated by the program. A LaNa

molecule layer was synthesized by using SAM layer synthesis method (M. Dubey, *et al*, *Langmuir*, **26**, 14747 (2010)) on the surface of Si-substrate with minor changes. The prepared LaNa sample was dipped into a 1 mM Sr(**BIC**)$^+$ complex solution (D_2O/EtOH-d_6 = 1:1 mixture). After 1 hour standing at room temperature, the NR measurement of the model sample was performed on a BL17 SHARAKU reflectometer. The result indicated that adsorption of the Sr(**BIC**)$^+$ complex was occurred in the LaNa model sample. It implied that LaNa molecules are likely present in the outer sphere as counter ions and/or [Sr(**BIC**)]$^+$ complexes are localized in the hydrophobic core of LaNa micelles. A detailed consideration of the [Sr(**BIC**)]$^+$ complex and micelle structure will be performed to understand the detailed mechanism of micelle-mediated fluorescence detection systems.

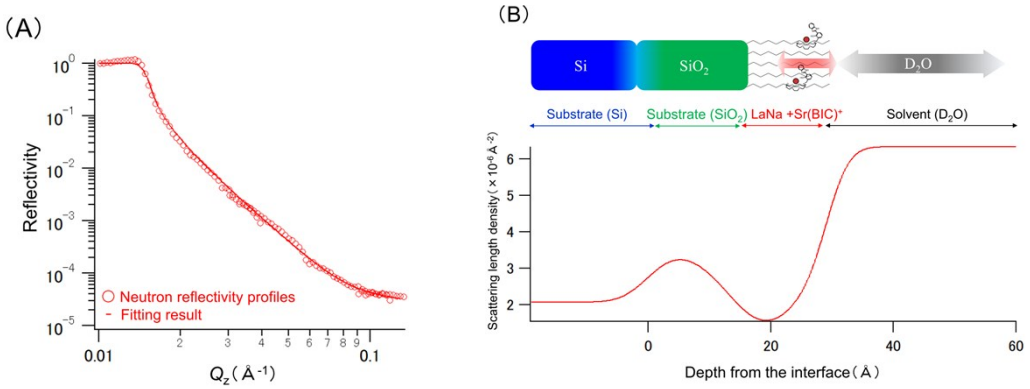

Fig. S2. (A) Neutron reflectivity profiles of the Sr[BIC]$^+$ complex/LaNa molecule sample. (B) Depth profiles of the Sr[BIC]$^+$ complex/LaNa molecule sample calculated by the obtained structural parameters (bottom), and the schematic structure on the surface of LaNa molecules (top).

Acknowledgements

The neutron reflectivity experiments were conducted at the BL17 SHARAKU apparatus in the J-PARC, Tokai, Japan (proposal No. 2016I0017).

References

1 K. Akutsu, T. Niizeki, S. Nagayama, N. Miyata, M. Sahara, A. Shimomura, M. Yoshii and Y. Hasegawa, *J. Ceram. Soc. Japan*, 2016, **124**, 172–176.

2 A. Nelson, *J. Appl. Crystallogr.*, 2006, **39**, 273–276.