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Supportive information

Self-agglomerated crystalline needles harnessing ESIPT and AIEE features for the 'turnon' fluorescence detection of Al³⁺ ions at nanomolar level

> Pranshu Puri, Gulshan Kumar, Kamaldeep Paul and Vijay Luxami* School of Chemistry and Biochemistry, Thapar University, Patiala E-mail: vluxami@thapar.edu

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Figure S1. ¹H-NMR of Probe 2



Figure S2. ¹³C NMR of Probe 2



Figure S3. HR-MS spectrum of Probe 2



Proton Transfer

Figure S4. Optimized structures of probe 2 in ground and excited States



Figure S5. Optimized structure of probe **2** as dimer get insight of aggregation with (a) side and (b) front view.



Figure S6. DLS histogram for hydrodynamic diameter of Probe 2 in (a) THF; (b) 90% H₂O-THF



Figure S7. Plot for determination of binding constant of Probe 2 (Benesi Hildebrand plot)



Figure S8. The linear response of probe **2** for Al^{3+} ions

Table S1. A comparison of literature reported Al ³⁺ selective receptors				
Group	Detection	Emission Response	Mechanism	Ref.
	limit			
Gui <i>et al</i> .	21.6 nM	"Turn-on"	AIE	1
Misra et al.	8.6 nM	"Turn-on"	PET-AIE	2
Tang et al.	21.7 μM	"Turn-on"	ESIPT	3
Lee <i>et al.</i>	24 nM	"Turn-on"	ESIPT	4
Luxami et	0.27 μM	"Turn-on"	AIE+ESIPT	5
al				
Pang <i>et al</i> .	0.5 nM	"Turn-on"	ESIPT	6
Chen <i>et al.</i>	2.2 μM	"Turn-on"	AIE-ESIPT	7
Present	10 nM	"turn-on"	AIE+ESIPT	
Work				

- 1. S. Gui, Y. Huang, F. Hu, Y. Jin, G. Zhang, L. Yan, D. Zhang and R. Zhao, *Anal. Chem.*, 2015, 87, 1470-1474.
- 2. M. Shyamal, P. Mazumdar, S. Maity, G. P. Sahoo, G. Salgado-Morán and A. Misra, *J. Phys. Chem. A*, 2016, 120, 210-220.
- 3. J. Zhao, Y. Zhao, S. Xu, N. Luo and R. Tang, *Inorg. Chim. Acta*, 2015, 438, 105-111.
- 4. J. J. Lee, G. J. Park, Y. S. Kim, S. Y. Lee, H. J. Lee, I. Noh and C. Kim, *Biosens. Bioelectron.*, 2015, 69, 226-229.
- 5. G. Kumar, K. Paul and V. Luxami, *Sens. Actuators, B*, 2018, 263, 585-593.
- 6. J. Wang and Y. Pang, *RSC Adv.*, 2014, 4, 5845-5848.
- 7. Y. Chen, T. Wei, Z. Zhang, T. Chen, J. Li, J. Qiang, J. Lv, F. Wang and X. Chen, *Ind. Eng. Chem. Res.*, 2017, 56, 12267-12275.