Electronic supplementary information (ESI)

Reporting a new siderophore based Ca²⁺ selective chemosensor that works as staining agent in live organism *Artemia*

M. Raju,^a Ratish R. Nair,^a Ishan H. Raval,^b Soumya

Haldar*bc and Pabitra B. Chatterjee*ac

"Analytical Discipline and Centralized Instrument Facility (AD&CIF), CSIR-CSMCRI, Bhavnagar, Gujarat, India.

^bMarine Biotechnology and Ecology Discipline, CSIR-CSMCRI, Bhavnagar, Gujarat, India.

^cAcademy of Scientific and Innovative Research (AcSIR), CSIR-CSMCRI, Bhavnagar, Gujarat, India.

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Table S2. Comparison of optical properties of **HL** with the organic and water-organic mixture soluble Ca^{2+} -selective chemosensors.

Figure S1. ¹³C NMR of HL in the absence and in the presence of calcium salts.



Figure S2. Mass spectrum of HL



Mass spectrum of CaL indicating 1:1 binding of HL with Ca²⁺



Figure S3. Fluorescence intensity of HL (10 μ M) and Ca²⁺ (10 μ M) mixture in the presence of 1 mM Mg²⁺.



Figure S4. Effect of Ca²⁺ (10 μ M) binding to **HL** (10 μ M) in presence of EDTA²⁻ (5-equiv) and L-cysteine (5-equiv), separately.



Figure S5. Effect of Cu²⁺ (10 μ M) binding to **HL** (10 μ M) in presence of EDTA²⁻ (5-equiv) and L-cysteine (5-equiv), separately.



No. of Artemia	Control	Sensor, HL (20 µM)	Sensor, HL (60 µM)
50	50	50	48
50	50	50	48
50	50	50	48

 Table S1. Toxicity results of HL studied with Artemia

Table S2. Comparison of optical properties of **HL** with the organic and water-organic mixture soluble Ca^{2+} -selective chemosensors.

Receptor	Kd	LO	$\Phi_{\rm f}$	$\Phi_{\rm f}$	$\Phi_{\rm f}$	Inter	Solvent	Bio-	Excitation	Ref
	(µM)	D	(free)	(bound)	Enhancement	ference	system	imaging	Region (nm)	
9-AA-2	0.275	NA	0.00030	0.0039	13	NA	CH ₃ CN	NA	362	4 <i>a</i>
9-AA-3	0.176	NA	0.00026	0.0042	16	NA	CH ₃ CN	NA	362	4a
9-AA-4	0.152	NA	0.00033	0.014	42	NA	CH ₃ CN	NA	362	4 <i>a</i>
Squaraine-bichromophoric podands 3a		NA	0.008	NA		NA	CH ₃ CN	NA	570	4 <i>c</i>
Squaraine-bichromophoric podands 3b			0.014			NA	CH ₃ CN	NA	570	4 <i>c</i>
Squaraine-bichromophoric podands 3c			0.023			NA	CH ₃ CN	NA	570	4 <i>c</i>
Squaraine-bichromophoric podands 4a			0.06			NA	CH ₃ CN	NA	570	4 <i>c</i>
Squaraine-Foldamer-1b	0.23	NA	0.032	0.008	0.25	NA	CH ₃ CN	NA	580	4 <i>d</i>
BODIPY-calixarene	0.019	NA	NA	NA		NA	CH ₃ CN	NA	485	4 <i>h</i>
DMDAP	0.1	NA	NA	NA	NA	NA	CH ₃ CN	NA	247	4 <i>e</i>
Chemo sensor 1	0.176	NA	NA	NA	NA	NA	CH ₃ CN	NA	438	4f
Chemo sensor 2	0.161	NA	NA	NA	NA	NA	CH ₃ CN	NA	438	4 <i>f</i>
acridinedione- bichromophoric podand-1b	0.261	NA	0.122	NA	NA	NA	CH ₃ CN	NA	381	4 <i>i</i>
acridinedione- bichromophoric podand-1c	0.207	NA	0.123	NA	NA	NA	CH ₃ CN	NA	381	4 <i>i</i>

Notes and references

4 (a) T. Morozumi, T. Anada and H. Nakamura, J. Phys. Chem. B, 2001, 105, 2923-2931; (c) E. Arunkumar, P. Chithra and A. Ajayaghosh, J. Am. Chem. Soc., 2004, 126, 6590-6598; (d) E. Arunkumar, A. Ajayaghosh and J. Daub, J. Am. Chem. Soc., 2005, 127, 3156-3164; (e) C. -F. Lin, Y. -H. Liu, C. -C. Lai, S. -M. Peng and S. -H. Chiu, Chem. Eur. J., 2006, 12, 4594-4599; (f) J. Kim, T. Morozumi and H. Nakamura, Org. Lett., 2007, 9, 4419-4422; (g) M. Suresh and A. Das, Tetrahedron Lett., 2009, 50, 5808-5812; (h) H. J. Kim and J. S. Kim, Tetrahedron Letters, 2006, 47, 7051-7055; (i) P. Ashokkumar, V. T. Ramakrishnan and P. Ramamurthy, Eur. J. Org. Chem., 2009, 5941-5947.