Supporting Information

Selective Recognition and Reversible "Turn-Off" Fluorescence Sensing of Acetate (CH_3COO^-) Anion at ppb Level Using a Simple Quinizarin Fluorescence Dye

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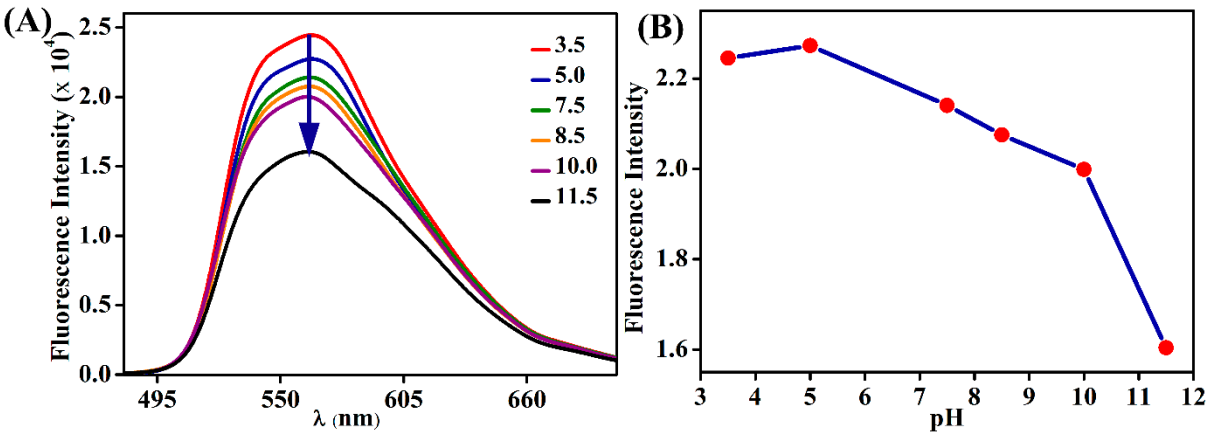
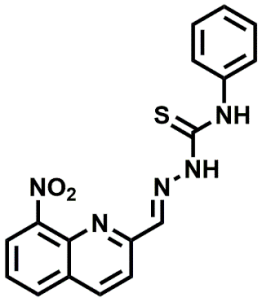
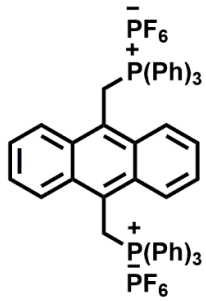
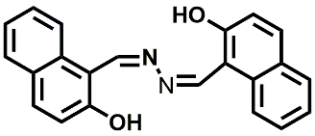
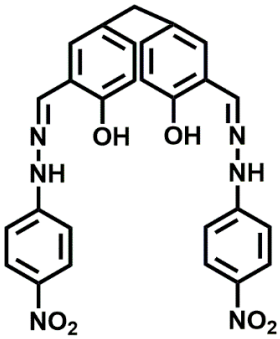
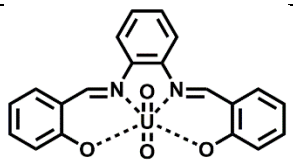
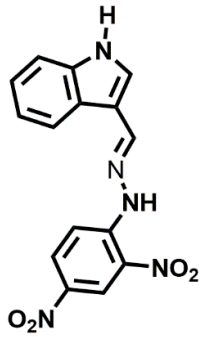
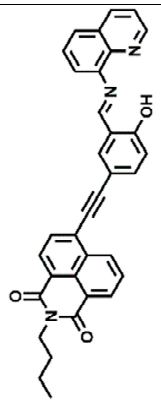
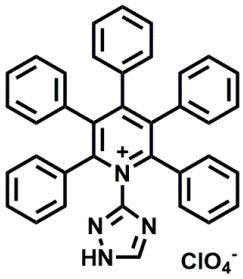
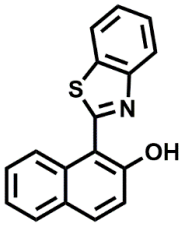
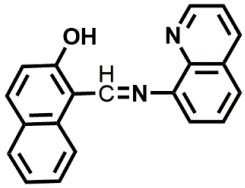
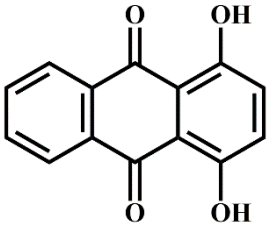


Figure S1. (A) pH-dependent emission titration for **QZ** measured in the DMSO solution; (B) corresponding plot of emission intensity (monitored at λ = 562 nm) *vs* pH showing that the fluorescence intensity is low at basic pH.

Figure S2. Energy-minimized structures of sensor **QZ** before and after binding with CH_3COO^- anion leads to the formation of anion-induced deprotonation of $\mathbf{QZ^{2-}}$.

Table S1. Comparison of sensing properties of various reported small-molecule fluorescence sensors with quinizarin sensor reported in this article.

Sensor	Emission Maxima (λ_{max})	Selectivity for	Binding constant for CH_3COO^-	LoD	[Ref.]
	468 nm	CH_3COO^- F^- $H_2PO_4^-$	K_a = 1.20±0.41 L mol^{-1} (from fluorescence) K_a = 1.95±0.93 L mol^{-1} (from absorbance)	N/A	**[50]**
	429 nm 451 nm	CH_3COO^-	K_a = 15.29±0.31 L mol^{-1} (from fluorescence) K_a = 15.78±0.19 L mol^{-1} (from absorbance)	N/A	**[51]**
	621 nm	CH_3COO^- Al^{3+}	K_{SV} = 5.67 × 10^4 M^{-1}	1.0 × 10^{-7} M	**[52]**
	410 nm 560 nm	CH_3COO^- F^-	K_a = 12,500 L mol^{-1} (from fluorescence) K_a = 5,556 L mol^{-1} (from fluorescence)	N/A	**[53]**
	452 nm	CH_3COO^-	K_a = 6.82±0.11 (from fluorescence)	2.5 × 10^{-8} M	**[54]**

	520 nm	CH_3COO^- F^- $H_2PO_4^-$	$K_a = 1.27 \times 10^5$ M (from absorbance)	N/A	**[55]**
	491 nm	CH_3COO^- F^- OH^-	N/A	1.32×10^{-7} M	**[56]**
	469 nm	CH_3COO^- F^-	$K_a = 177500$ M^{-1} (from fluorescence)	1.09×10^{-5} M	**[57]**
	411 nm	CH_3COO^-	$K_a = 2.6 \times 10^4$ M^{-1} (from absorbance) $K_a = 4.0 \times 10^4$ M^{-1} (from fluorescence)	4.4×10^{-5} M	**[58]**
	500 nm	CH_3COO^-	N/A	4.0×10^{-7} M	**[59]**
	562 nm	CH_3COO^-	$K_a = 7.63 \times 10^3$ M^{-1} (from absorbance) $K_{SV} = 2.3 \times 10^3$ M^{-1} (from fluorescence)	3.8×10^{-8} M	**This work**

References:

50. Shao, J. Quinoline-Based "On-Off" Fluorescent Sensor for Acetate: Effect of Link Mode between Binding Sites and Fluorophore on Fluorescence Changes. *Spectrosc. Lett.* **2012**, *45*, 262–268.
51. Huang, W.; Lin, H.; Lin, H. Fluorescent Acetate-Sensing in Aqueous Solution. *Sens. Actuators, B.* **2011**, *153*, 404–408.
52. Ghosh, A.; Sengupta, A.; Chattopadhyay, A.; Das, D. A Single Probe for Sensing Both Acetate and Aluminum(III): Visible Region Detection, Red Fluorescence, and Human Breast Cancer Cell Imaging. *RSC Adv*. **2015**, *5*, 24194–24199.
53. Liu, G.; Shao, J. Selective Ratiometric Fluorescence Detection of Acetate Based on a Novel Schiff Base Derivative. *J. Fluoresc*. **2012**, *22*, 397–401.
54. Hosseini, M.; Ganjali, M.R.; Veismohammadi, B.; Faridbod, F.; Abkenard, S.D.; Salavati-Niasarie, M. Selective Recognition of Acetate Ion Based on Fluorescence Enhancement Chemosensor. *Luminescence*. **2012**, *27*, 341–345.
55. Li, Y.; Lin, H.; Cai, Z.; Lin, H. Colorimetric Sensing of Biologically Important Acetate Ion Based on Indole Derivation. Mini-Rev. *Org. Chem.* **2011**, *8*, 25–30.
56. Zhao, L.Y.; Wang, G.K.; Chen, J.H.; Zhang, L.M.; Liu, B.; Zhang, J.F.; Zhao, Q.H.; Zhou, Y. 1,8-Naphthalimide-based Visible Colorimetric Sensor for the Selective Sensing of Fluoride, Acetate, and Hydroxyl Anions. *J. Fluorine Chem.* **2014**, *158*, 53–59.
57. Wang, G.; Zheng, T.; Zhang, S.; Ye, J.; Ning, G. Fluorescence Chemosensor for Acetate Ion and Fluorine Ion based on 1,2,4-Triazolyl Substituted Pentaphenylpyridinium. *J. Mol. Struct*. **2021,** *1230,* 129918.
58. Goswami, S.; Das, A.K.; Aich, K.; Manna, A. Competitive Intra- and Inter-Molecular Proton Transfer in Hydroxynaphthyl Benzothiazole: Selective Ratiometric Sensing of Acetate. *Tetrahedron Lett*, **2013**, *54*, 4215–4220.
59. Lin, Q.; Liu, X.; Wei, T.B.; Zhang, Y.M. TICT–ICT State Change Mechanism-based Acetate Fluorescent Sensor Act as an "Off–On–Off" Switch and Logic Gate. Sens. *Actuators, B*. **2014**, *190*, 459–463.