Supporting Information

A new fluorescence and colorimetric sensor for highly selective and sensitive detection of glucose in 100% water

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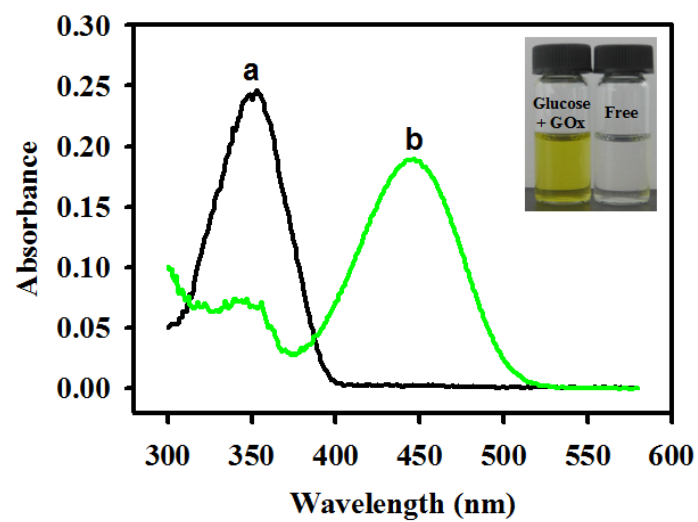
Fig. S1 UV-vis absorption spectra of probe on interaction with 120 μM glucose in the presence (b) and absence (a) of 10 μg/mL GOx in PBS buffered solution (50 mM, pH = 7.0).

Table S1 Determination of glucose in urine samples spiked with glucose (n = 3)

Samples	Test (μM)	Added (μM)	Recovery (%)	RSD (%)
Blank	Not found	0	-	-
1	32.3	30	106.8	2.13
2	61.8	60	105.7	3.63
3	93.2	90	102.2	1.67

Table S2 Calculated absorption wavelengths (λ_{abs}), excitation energies (Ex), oscillator

strengths f, and dominant excitation character of compound **1** and **1**-H_2O_2 reaction

product. Calculations were performed at PCM (H_2O)-TD-B3LYP/6-31+G (d, p) //

B3LYP/6-31+G (d, p) level.

Compound	Transition	λ_{abs}	Ex	f	composition
1	$S_0 \rightarrow S_1$	359.87	3.45 eV	0.363	H→L (98%)
	$S_0 \rightarrow S_2$	326.77	3.79 eV	0.042	H-1→L (89%)
1-H_2O_2	$S_0 \rightarrow S_1$	445.35	2.78 eV	0.219	H→L (97%)
	$S_0 \rightarrow S_3$	307.63	4.03 eV	0.056	H→L+1 (66%)
					H→L+2 (13%)
					H-2→L (12%)

Table S3 Calculated emission wavelengths (λ_{em}), emission energies (Em), oscillator strengths f, and dominant excitation character of compound **1** and **1**-H_2O_2 reaction product. Calculations were performed at PCM (H_2O)-TD-B3LYP/6-31+G (d, p) // TD-B3LYP/6-31+G (d, p) level.

Compound	Transition	λ_{em}	Em	f	Composition
1	$S_1 \rightarrow S_0$	404.86	3.06 eV	0.346	H→L (98%)
	$S_3 \rightarrow S_0$	337.82	3.67 eV	0.026	H-1→L (89%)
1-H_2O_2	$S_1 \rightarrow S_0$	536.93	2.31 eV	0.126	H→L (98%)
	$S_3 \rightarrow S_0$	315.69	3.93 eV	0.037	H→L+1 (71%)
					H-2→L (11%)

178.339

164.347
164.324

135.764
135.262
134.984
131.258
130.912
129.806
127.867
127.095
126.946
124.684

84.615

40.177
33.667
27.723
26.547
24.993
24.387

0.014

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0