SUPPLEMENTARY INFORMATION

An imine-based colorimetric chemodosimeter for the detection of hypochlorite (ClO^-) in aqueous media: its application in test strips and real water samples

DONGJU YUN, JU BYEONG CHAE and CHEAL KIM*

Department of Fine Chem., Seoul National Univ. of Science and Tech., Seoul 139-740, Republic of Korea.

Email: chealkim@snut.ac.kr

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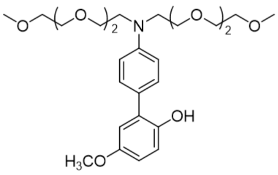
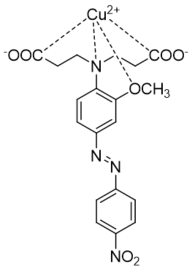
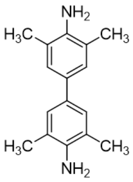
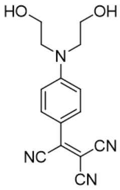
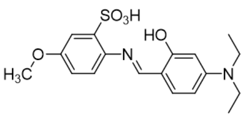
Table S1. Examples of colorimetric chemosensors for detection of ClO^- in a near perfect aqueous media.

No.	Structure	Detection limit (μM)	Reaction media	Method of detection	Test strip	Reference
1		1.74	PBS pH 7.4	colorimetric	No	[1]
2		2	HEPES pH 7.4	colorimetric	No	[2]
3		0.2	Water	colorimetric	No	[3]
4		4	PBS pH 7.4	colorimetric	No	[4]
5		0.95	PBS pH 7.4	colorimetric	Yes	This work

References

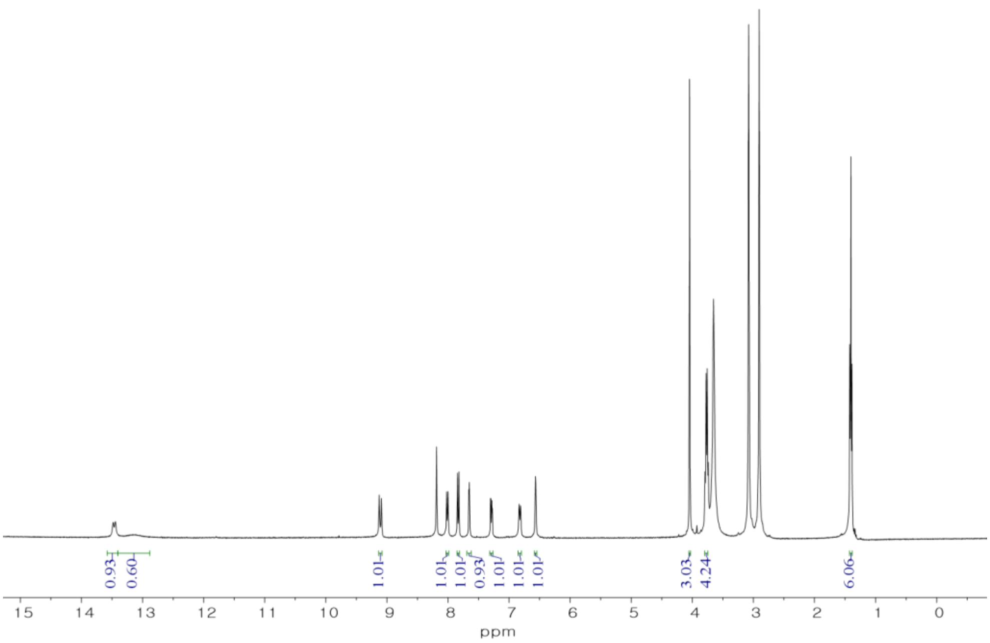
1. Cui K, Zhang D, Zhang G and Zhu D 2010 A highly selective naked-eye probe for hypochlorite with the p-methoxyphenol-substituted aniline compound *Tetrahedron Lett.* **51** 6052

2. Lou X, Zhang Y, Qin J and Li Z 2012 Colorimetric hypochlorite detection using an azobenzene acid in pure aqueous solutions and real application in tap water *Sensors Actuators B Chem.* **161** 229

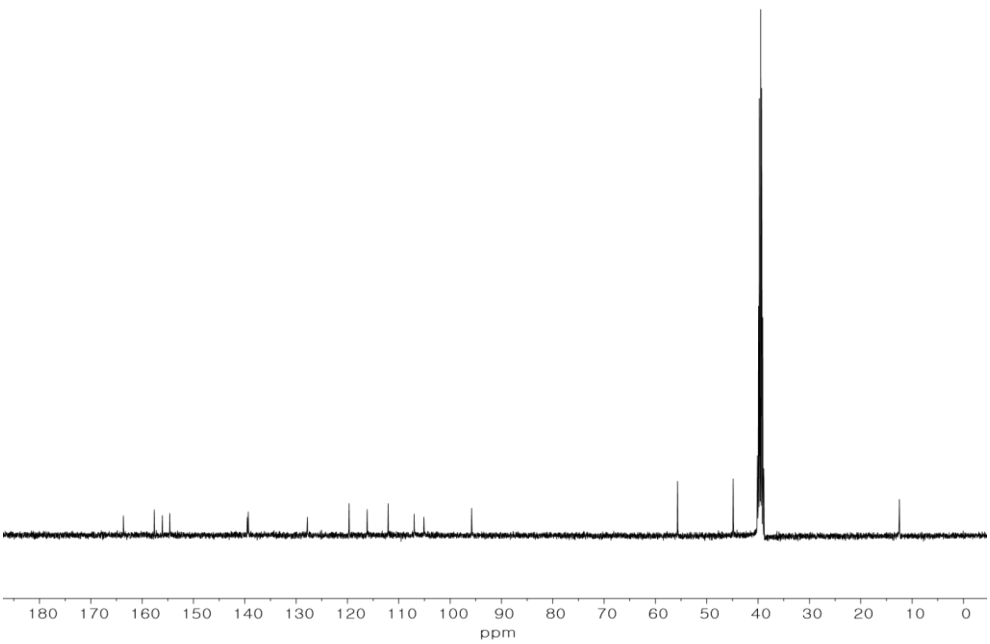
3. Zhang J and Yang X 3013 A simple yet effective chromogenic reagent for the rapid estimation of bromate and hypochlorite in drinking water *Analyst* **138** 434

4. Zhu B, Xu Y, Liu W, Shao C, Wu H, Jiang H, Du B and Zhang X 2014 A highly selective colorimetric probe for fast and sensitive detection of hypochlorite in absolute aqueous solution *Sensors Actuators B Chem.* **191** 473

(a)


0.93
0.60
1.01
1.01
1.01
0.93
1.01
1.01
1.01
3.03
4.24
6.06
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
ppm

(b)


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

(c)

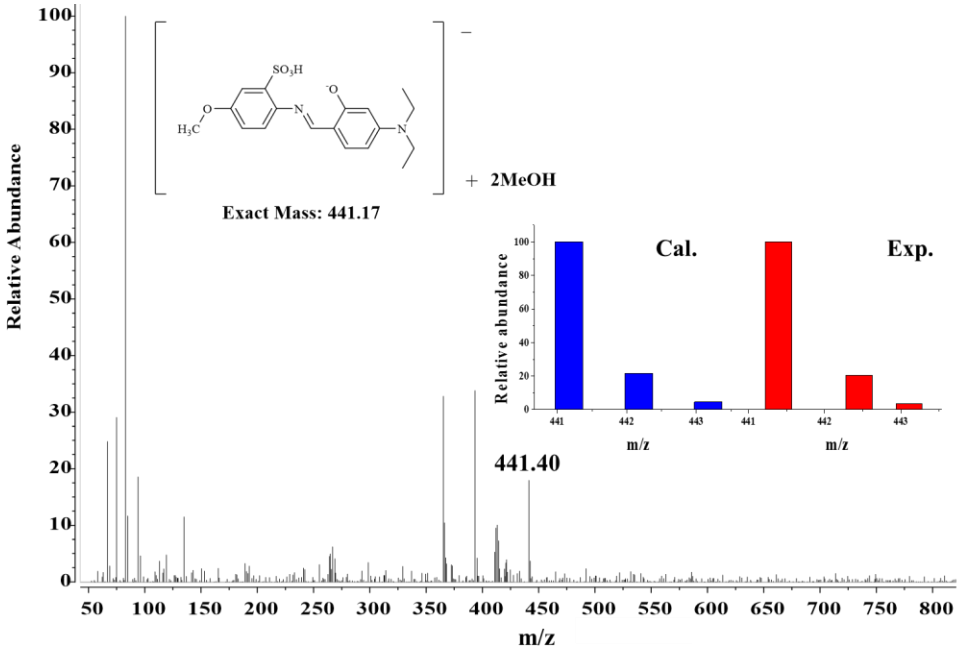


Figure S1. (a) [1]H NMR and (b) [13]C NMR spectra of **ASAD**. (c) Negative-ion electrospray ionization mass spectrum of **ASAD**.

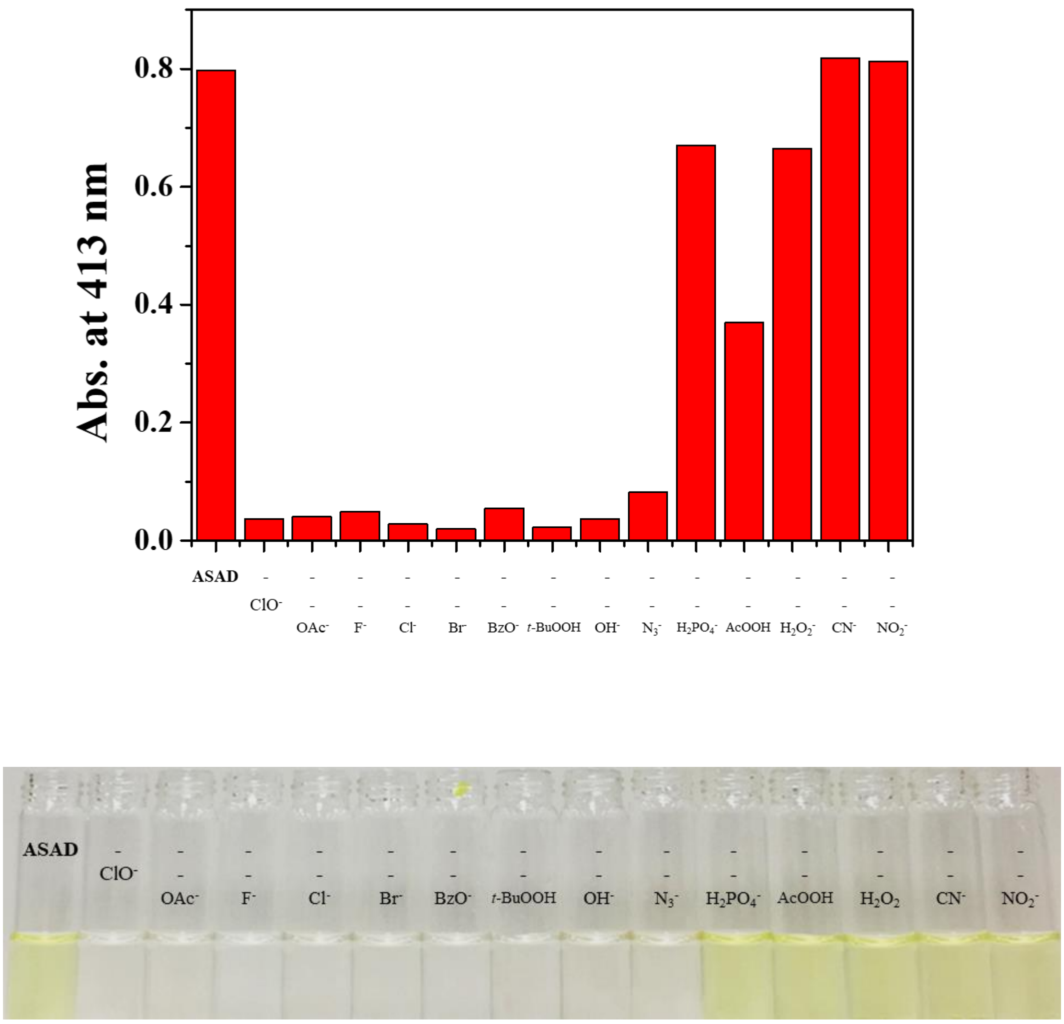


Figure S2. (a) Absorption spectral and (b) color changes of competitive selectivity of **ASAD** (20 μM) toward ClO^- (18 equiv.) in the presence of other guest analytes (18 equiv).

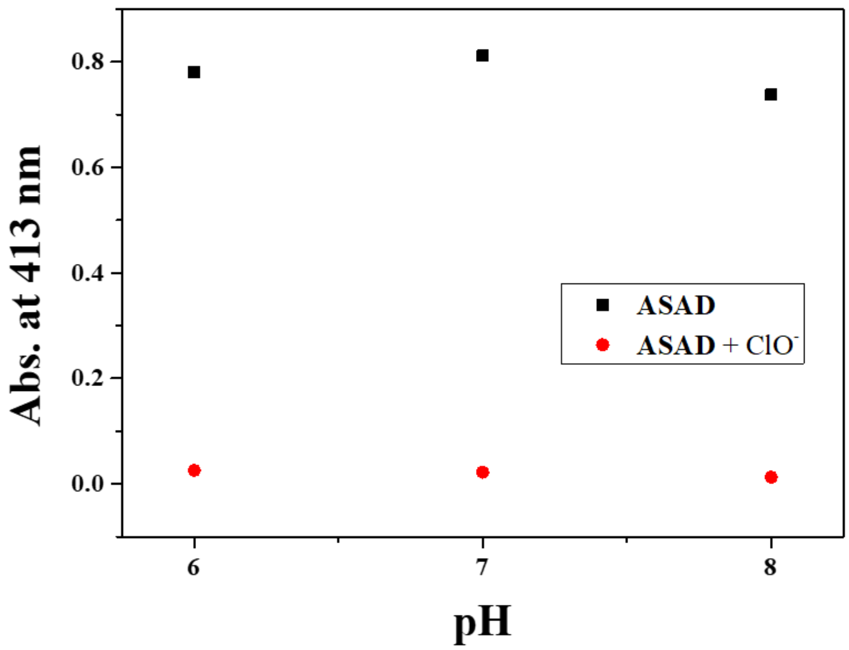
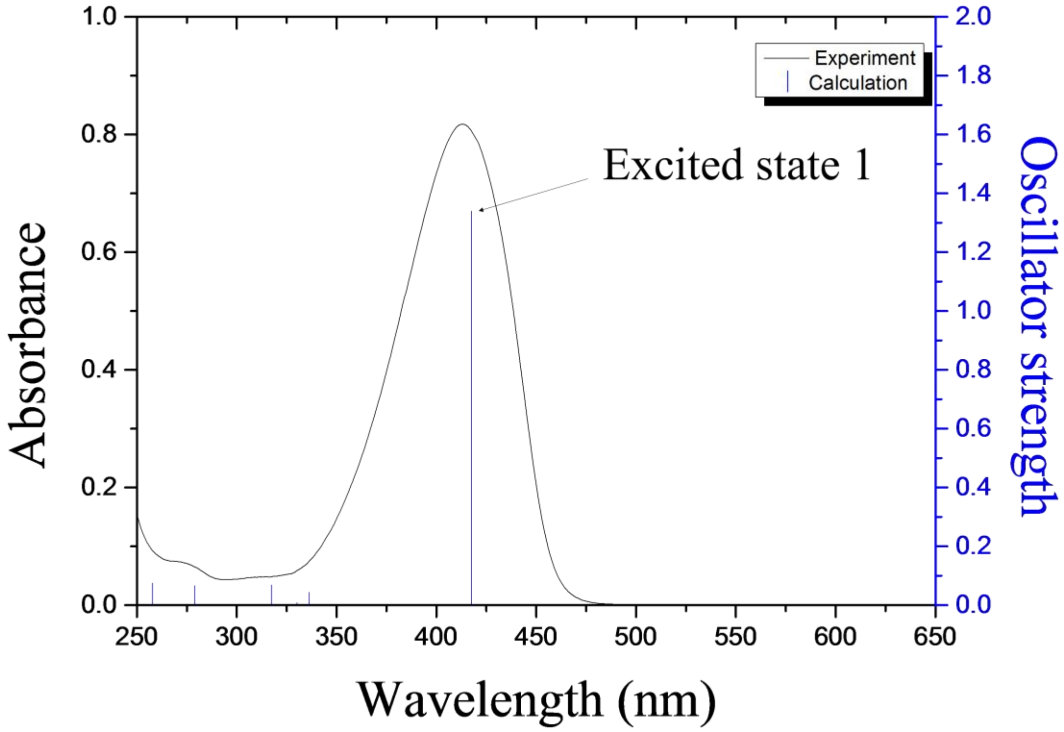


Figure S3. Absorbance (at 413 nm) of **ASAD** and **ASAD** + ClO^- at pH values from 6 to 8.

(a)

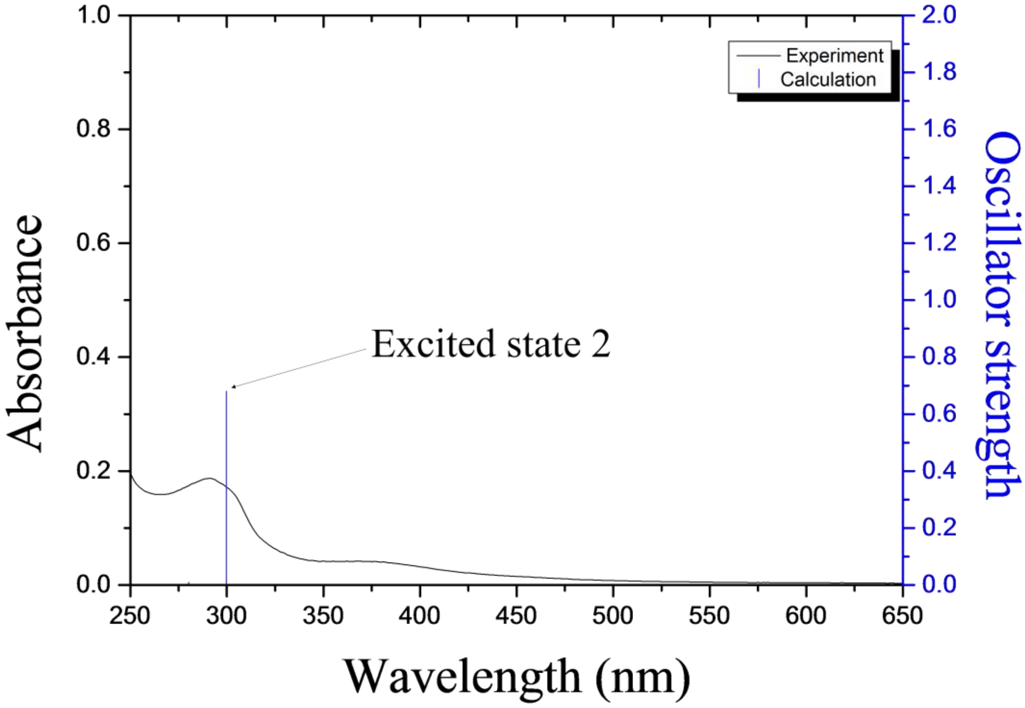


(b)

Excited state 1	Wavelength (nm)	Percent (%)	Main Character	Oscillator strength
H → L	417.41	98	ICT	1.3398

Figure S4. (a) The theoretical excitation energies and the experimental UV-vis spectrum of **ASAD**. (b) The major electronic transition energies and molecular orbital contributions of **ASAD** (H = HOMO and L = LUMO).

(a)



(b)

Excited state 2	Wavelength (nm)	Percent (%)	Main Character	Oscillator strength
H → L	299.75	98	ICT	0.6804

Figure S5. (a) The theoretical excitation energies and the experimental UV-vis spectrum of **DAS**. (b) The major electronic transition energies and molecular orbital contributions of **DAS** (H = HOMO and L = LUMO).

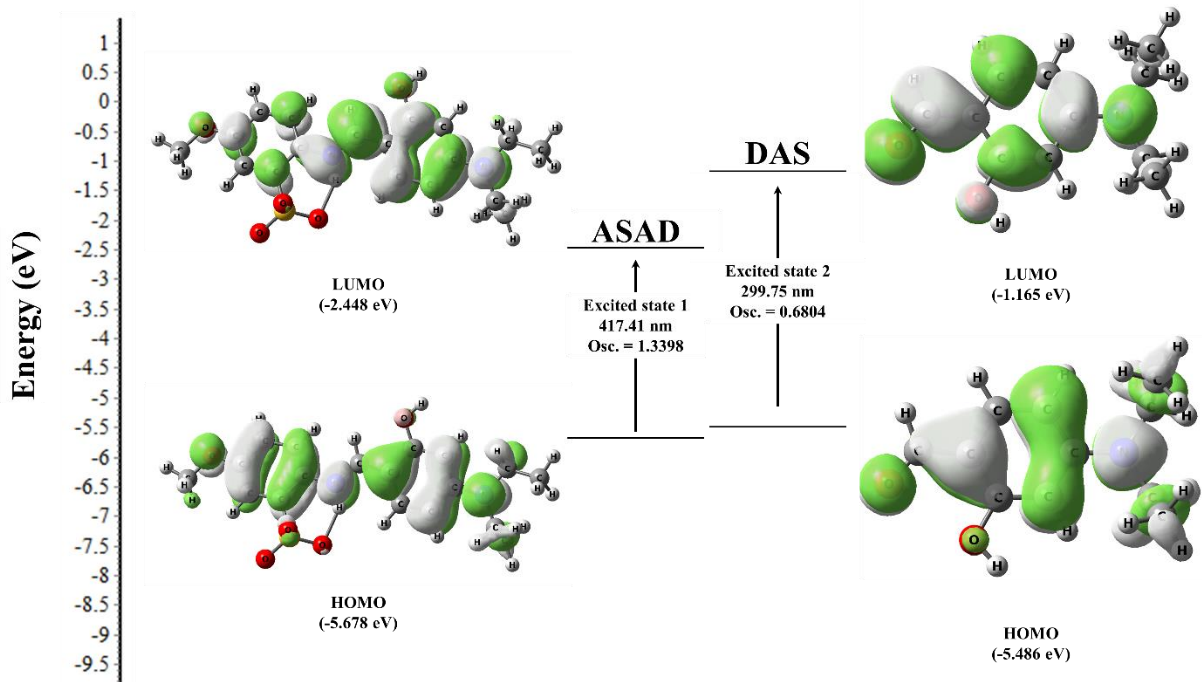


Figure S6. The major molecular orbital transitions and excitation energies of **ASAD** and **DAS**.