Hydroxychalcone Color Indicators for pH and Fluoride Ion

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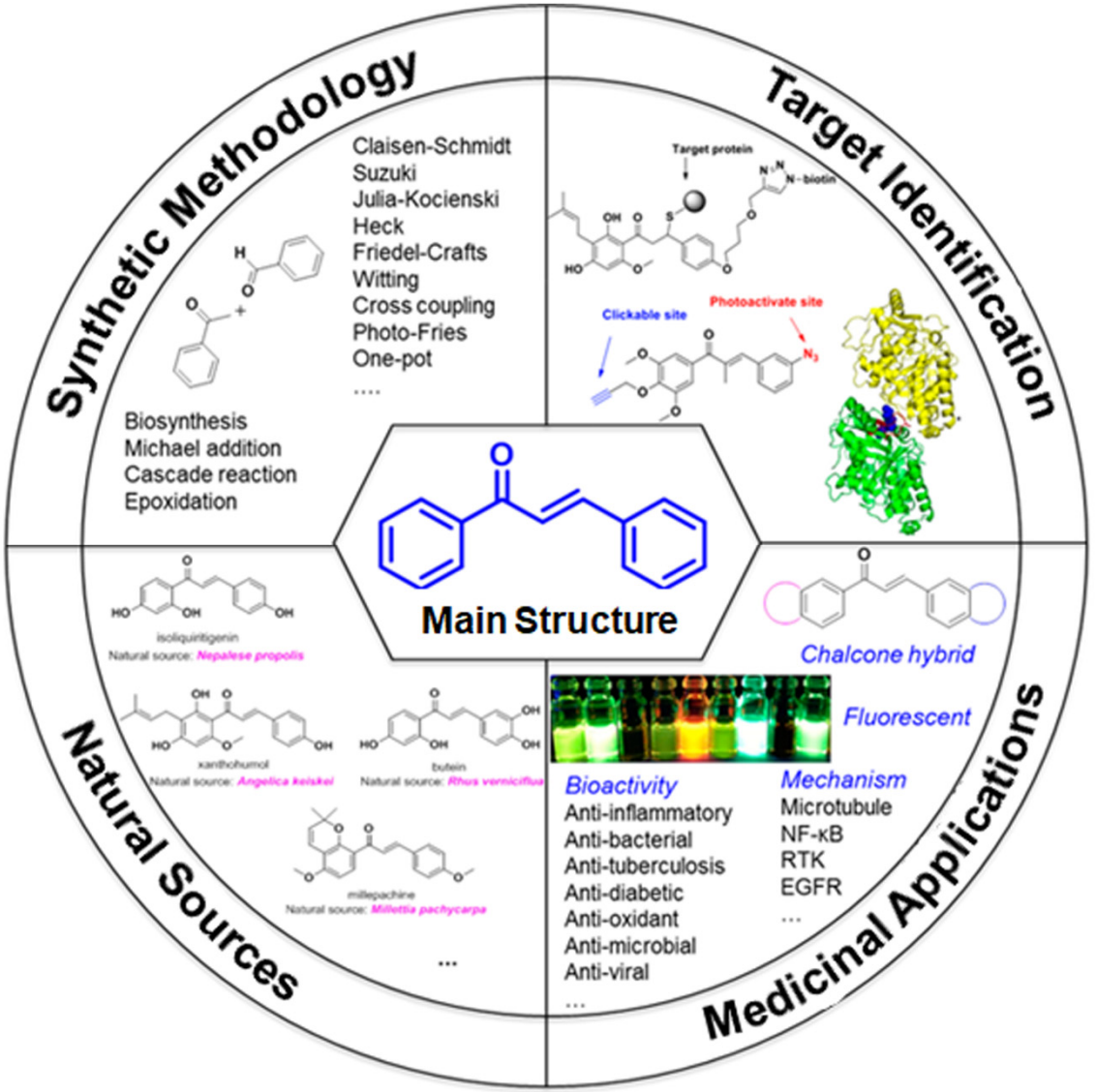
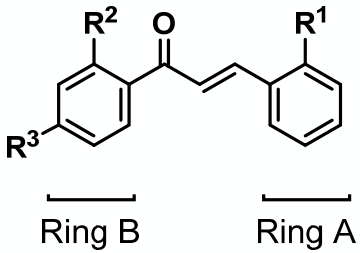
Chalcone

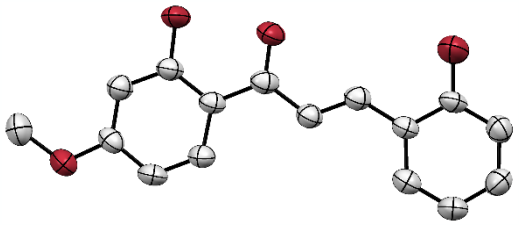


C. Zhuang, W. Zhang, C. Sheng, W. Zhang, C. Xing, Z. Miao, *Chem. Rev*. **2017**, *117*, 7762–7810.

Synthesis of CLN1-6



CLN	R^1	R^2	R^3
1	OH	OH	OCH_3
2	H	H	OCH_3
3	H	OH	OCH_3
4	OH	H	OCH_3
5	OH	OH	H
6	OH	OH	F

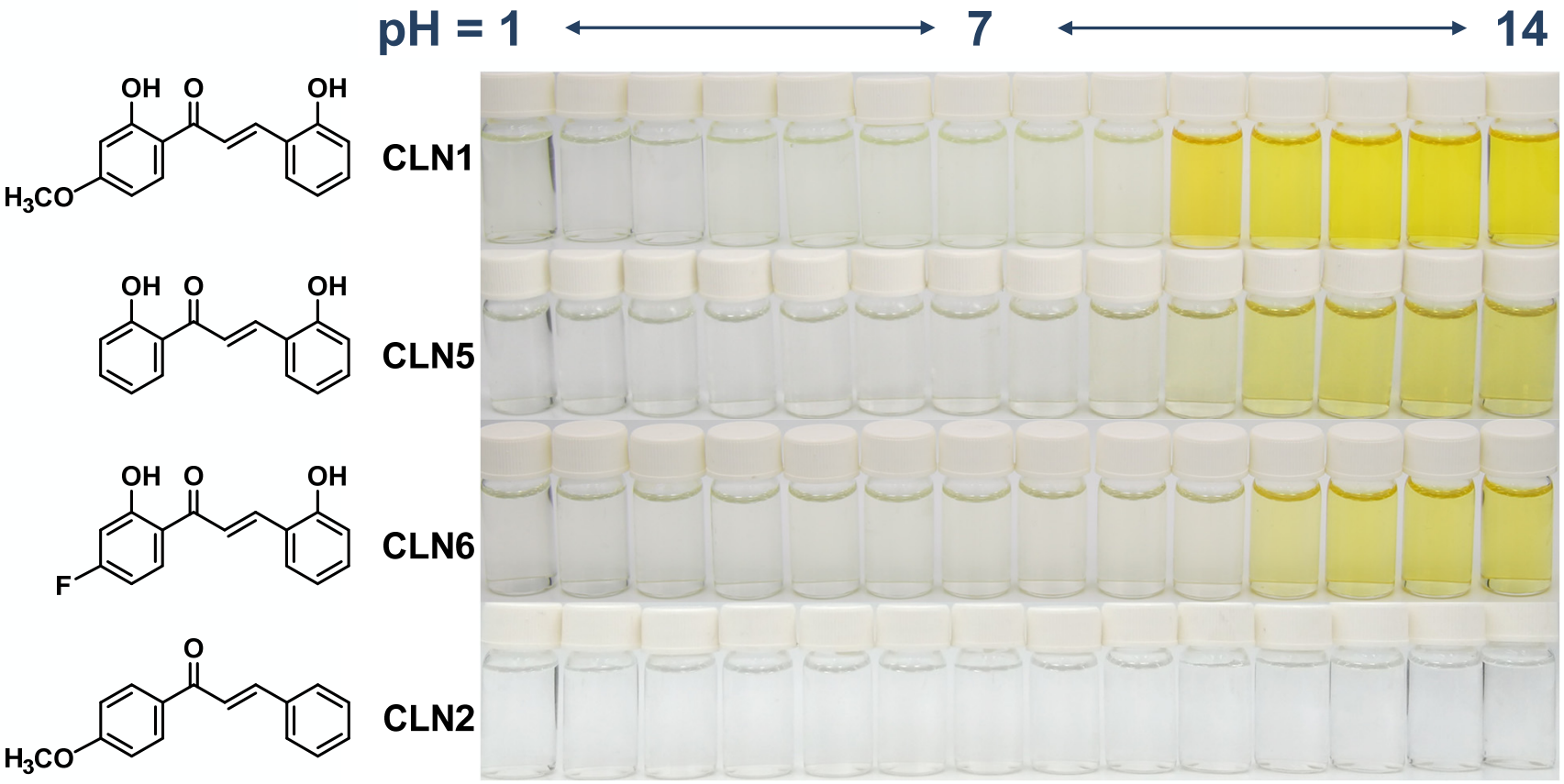


X-ray Crystal Structure of CLN**1**

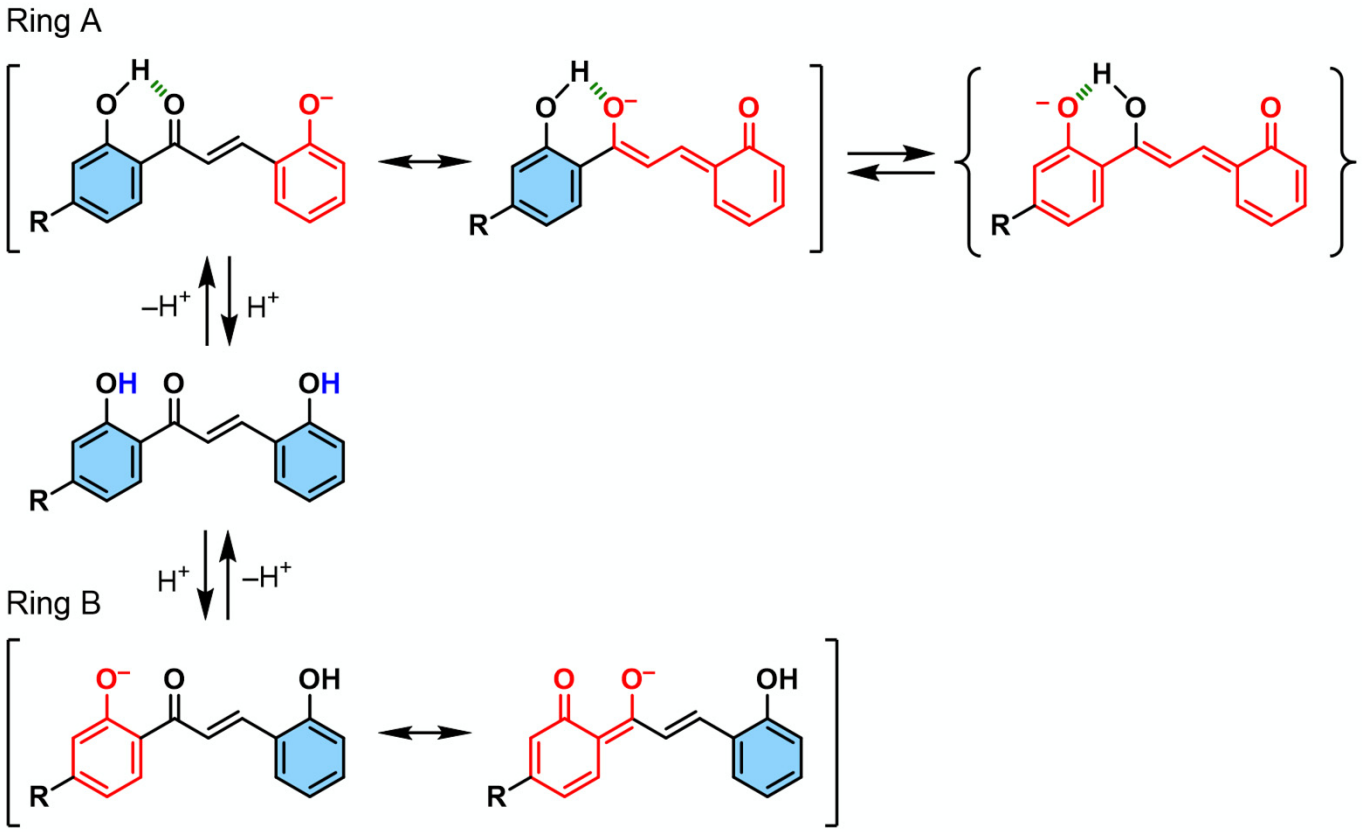
Little attention has been paid to water-soluble chalcones. In this study, we focused on a chalcone diol, in which its two OH groups are directly attached to the phenyl ring A and B. In this work, we report synthesis of CLN**1**-**6** and their applications as chemosensors.

Y. Du, F. Liang, M. Hu, R. Bu, M. Wang, A. Tsuda, C. Eerdun,
RSC Adv. **2020**, *10*, 37463.

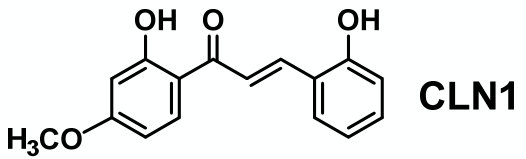
pH Dependent Color Changes of CLN in Water



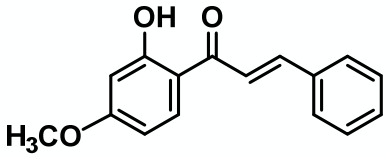
A Schematic Illustration of the Possible Ionization of Chalcone Diol



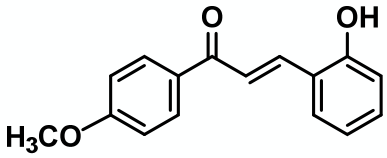
Visible Coloration of CLN1, 3 and 4 upon F^- Sensing in CH_3CN



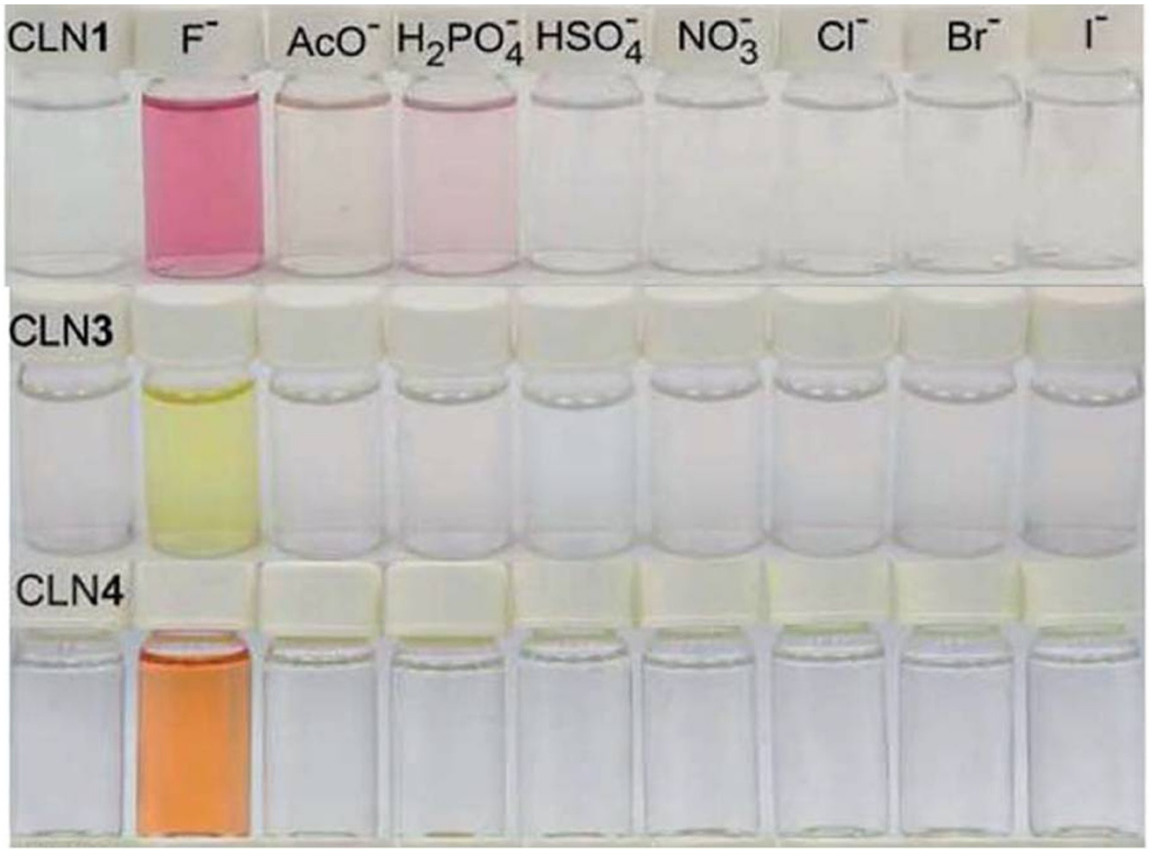
CLN1



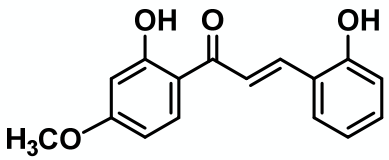
CLN3



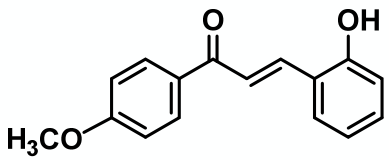
CLN4



Absorption Spectral Changes

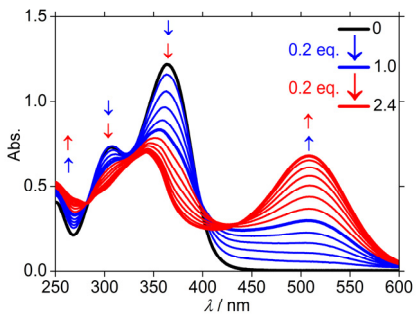


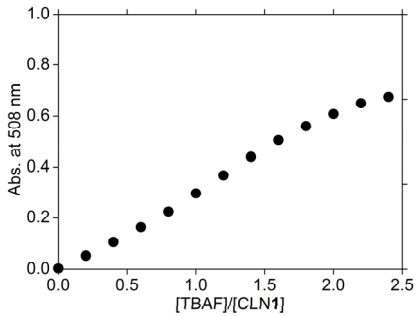
CLN1

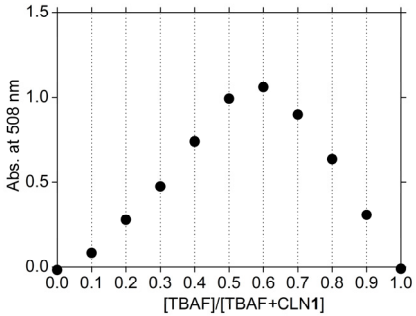


CLN4

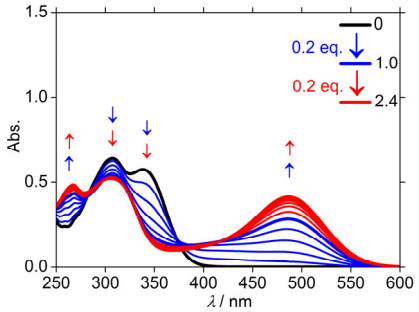
(a)

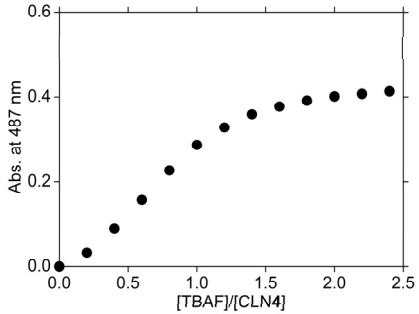


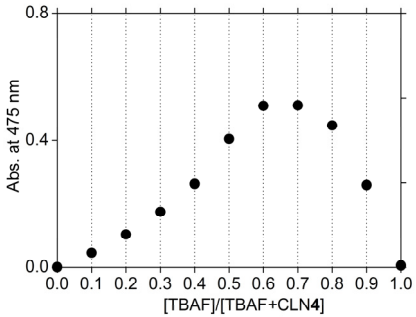




(b)

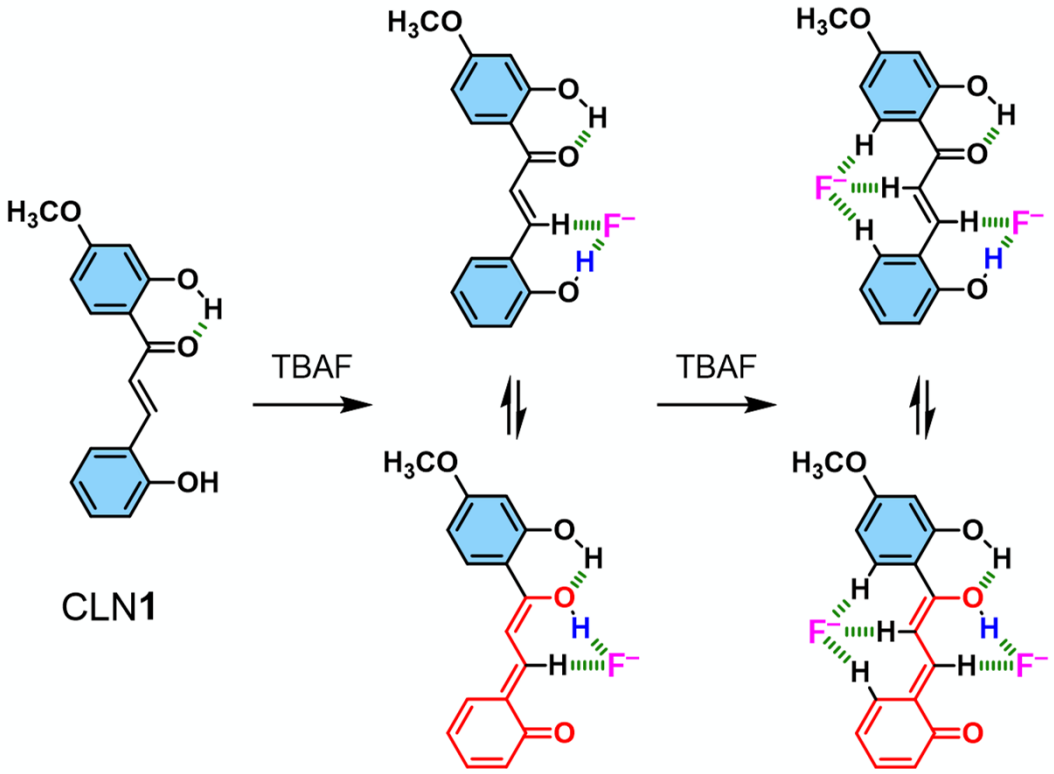




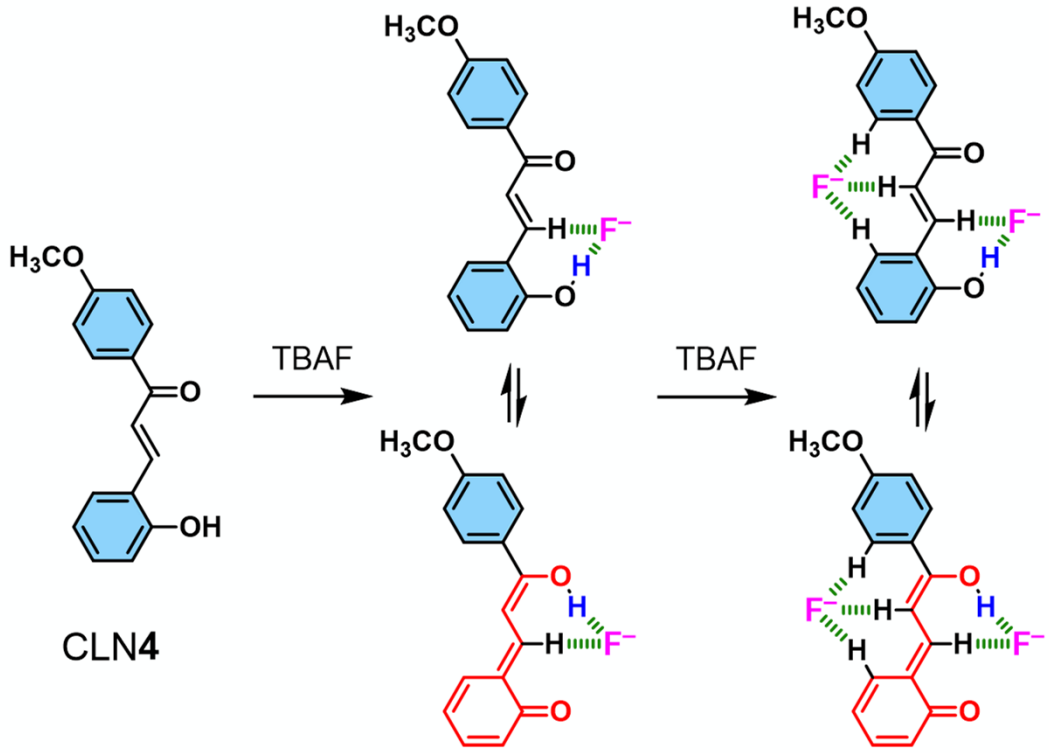


UV-vis absorption spectral titrations of (a) CLN**1**, (b) CLN**4** (4.0×10^{-5} mol·L^{-1}) with TBAF in CH_3CN at 298 K (left), plots of the absorbance change at λ_{max} with respect to [TBAF]/[CLN] (center), and Job plots for the absorbance changes with respect to [TBAF]/[TBAF + CLN] (right).

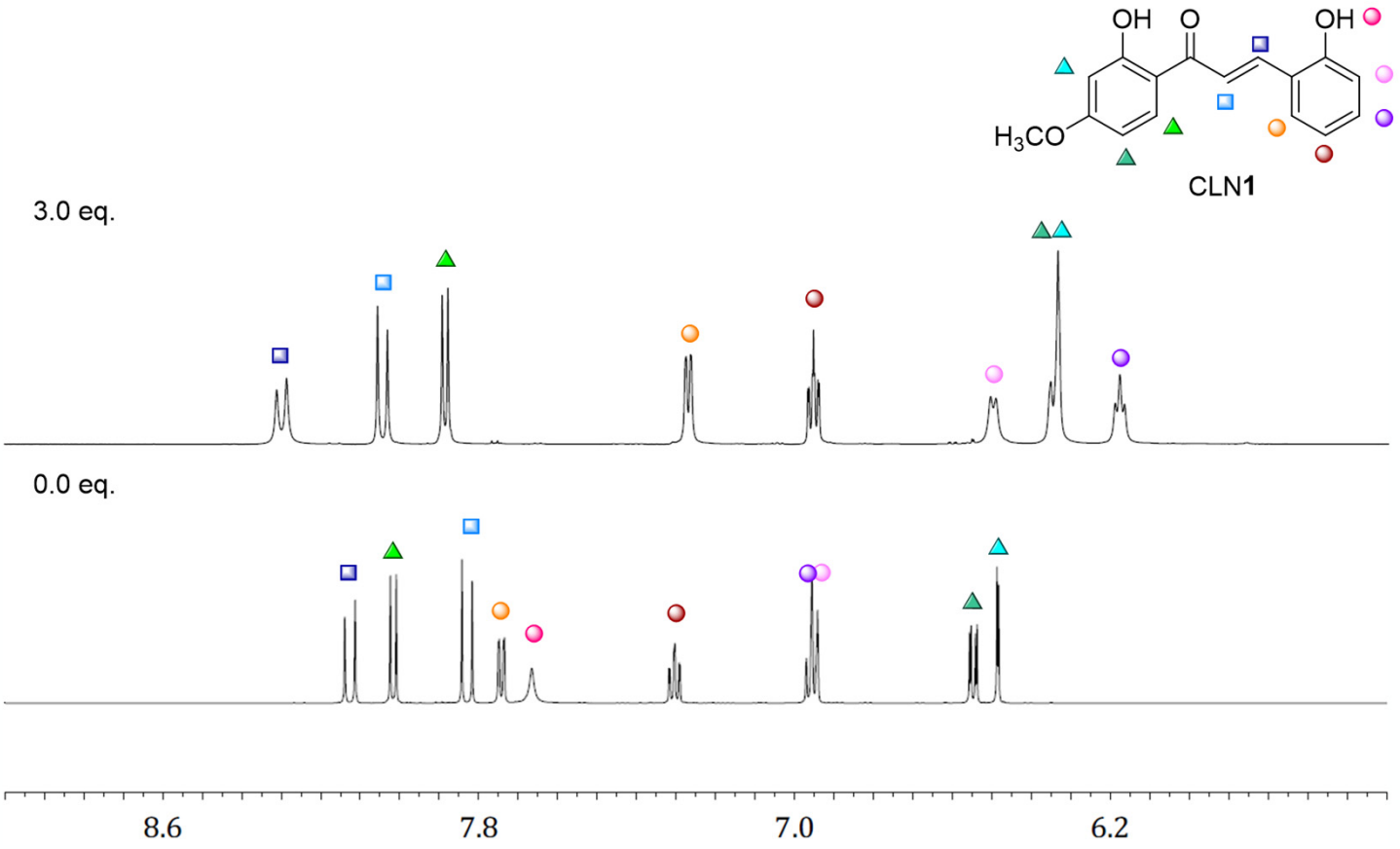
A Possible Mechanism for the Interactions of CLN1 and F^-



A Possible Mechanism for the Interactions of CLN4 and F^-

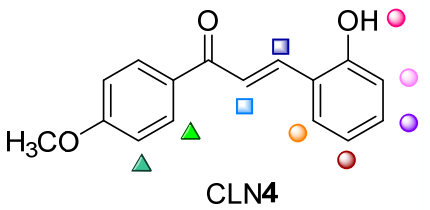


^{1}H NMR Spectrum

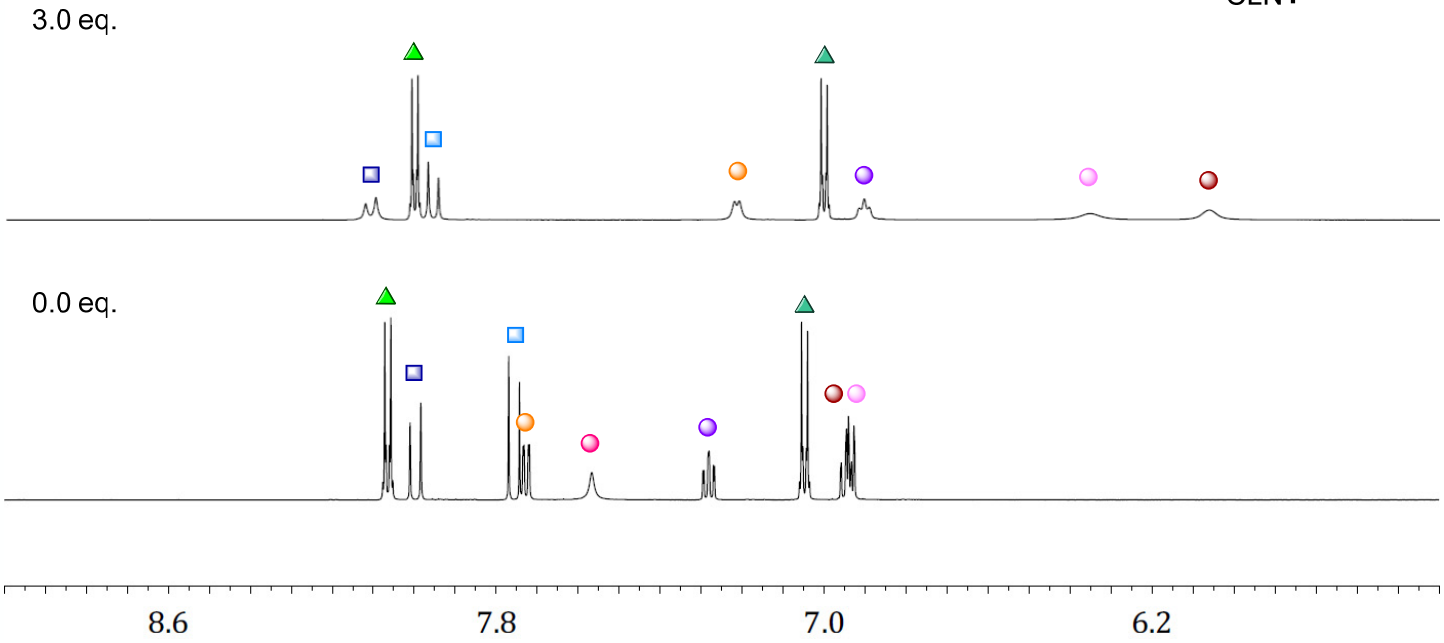


The changes observed in the ^{1}H NMR spectra (600 MHz) of CLN**1** (1.4×10^{-2} mol·L^{-1}) upon titration with TBAF in CD_3CN at 293 K.

^{1}H NMR Spectrum

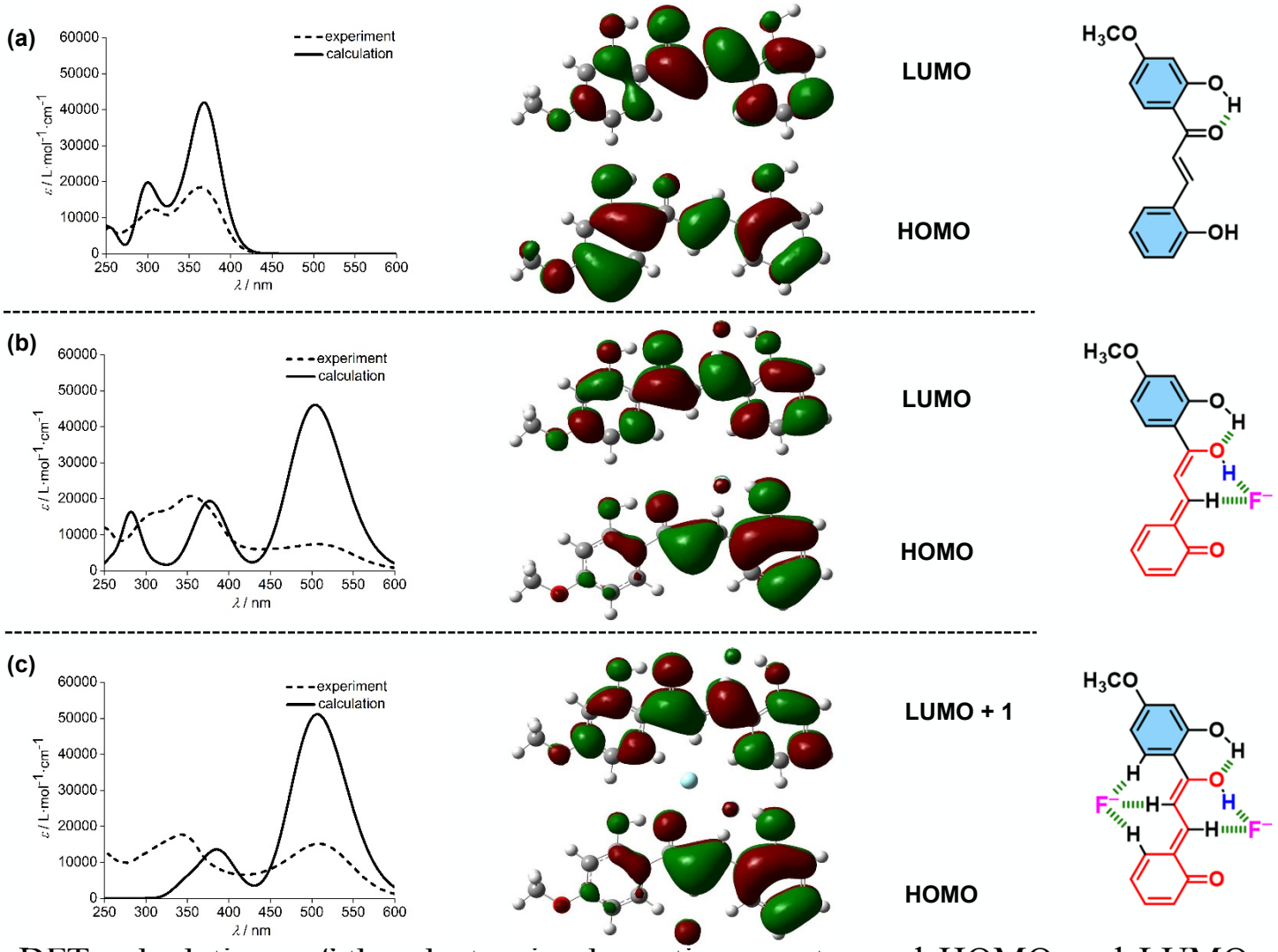


CLN4



The changes observed in the ^{1}H NMR spectra (600 MHz) of CLN**4** (1.4×10^{-2} mol·L^{-1}) upon titration with TBAF in CD_3CN at 293 K.

TD-DFT Calculations



The DFT calculations of the electronic absorption spectra and HOMO and LUMO of (a) CLN**1**, (b) CLN**1**·F^- and (c) CLN**1**·$2F^-$ at the B3LYP/6-311++g(d,p) level. The calculations were demonstrated with X-ray crystallographic data of CLN**1** with OH–F^- distance = 1.34 Å.

Summary

◆CLN**1** shows a vivid color change from colorless to yellow (halochromism) in water at pH ≥ 10.

◆These chalcone diols showed selective vivid colorations from colorless to red upon the addition of TBAF in CH_3CN.

◆This study provides future strategies for the molecular design of chalcone-based chemical sensors and bioactive chemical substances.

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