

Electronic Supplementary Information

for

Theoretical study on the sensing mechanism of chalcone-based fluorescence probe for detecting hydrogen sulfide and biothiols

Yunjian Cao^{a,1}, Lingling Wang^{b,c,1}, Ziqi Liu^a, Chaofan Sun^{a,*}, Yuanzuo Li^{a,*}

^a College of Science, Northeast Forestry University, Harbin 150040, Heilongjiang, China

^b College of Chemistry, Chemical Engineering and Resource Utilization, Northeast Forestry University, Harbin 150040, Heilongjiang, China

^c Key Laboratory of Forest Plant Ecology, Ministry of Education, Northeast Forestry University, Harbin 150040, Heilongjiang, China

¹ These authors contributed equally to this work and should be considered co-first authors.

*Corresponding authors: Chaofan Sun; Yuanzuo Li

E-mail addresses: cfsun@nefu.edu.cn; yzli@nefu.edu.cn

Table S1. The maximum absorption and fluorescence peaks (nm) of Pr1 and Comp2 in DMSO with various functional at 6-311G(d) basis set via the TD-DFT method.

	B3LYP	Cam-B3LYP	B3PW91	mPW1PW91	PBEPBE	Exp. ^a
Pr1- λ_{abs} .	419.79	366.46	420.01	406.26	500.51	420
Comp2- λ_{abs} .	439.98	382.78	440.35	426.40	510.54	426~458
Comp2-k- λ_{flu}	553.17	496.60	551.52	537.28	624.40	580

^a Represents the maximum absorption peak measured in the experiment.