

Supporting Information

Squaramide-based lab-on-a-molecule for the detection of silver ion and nitroaromatic explosives

Bo Shan^a, Rui Shi^a, Shaohua Jin^a, Shusen Chen^a, Yunfei Liu^a, Qinghai Shu^{a*}

^a School of Material Science and Engineering, Beijing Institute of Technology, 100081 Beijing, PR China

Contents

Fig. S1 ¹ H NMR Spectrum of probe SA	P2
Fig. S2 The mass spectrum of SA	P2
Fig. S3 The absorption spectra of SA with different metal ions	P3
Fig.S4 Emission and absorption spectra of SA and TNT	P3
Fig.S5 Emission spectra of SA with different explosives	P4
Fig.S6 Emission spectra of SA upon addition of various equiv. of NT	P4
Fig.S7 Emission spectra of SA upon addition of various equiv. of DNT	P5
Fig.S8 Emission spectra of SA upon addition of various equiv. of TNT	P5
Fig.S9 The UV-vis spectra of SA with different explosives	P6
Fig.S10 UV-Vis spectra of SA, TNT, SA and TNT mix solution	P6
Fig.S11 UV-vis absorption titration of SA upon addition of various equiv. of TNT	P7

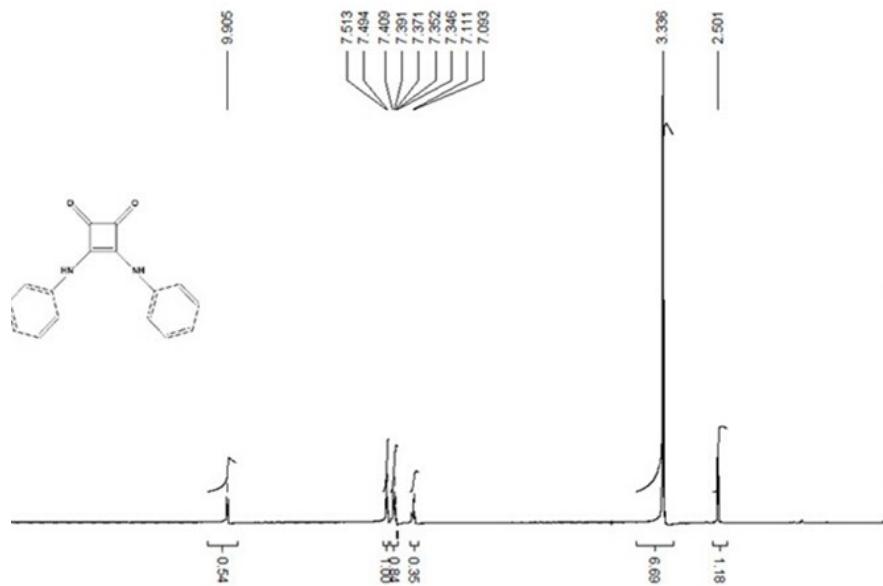


Fig. S1 ^1H NMR spectra of probe SA in DMSO-d_6 .

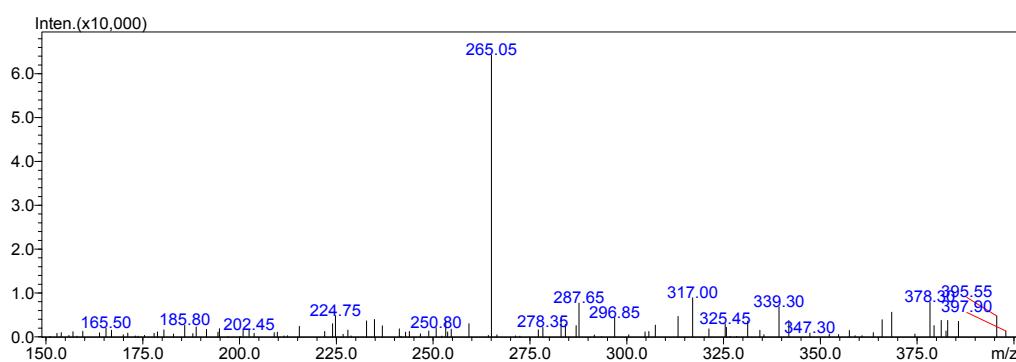


Fig. S2 The mass spectrum of SA.

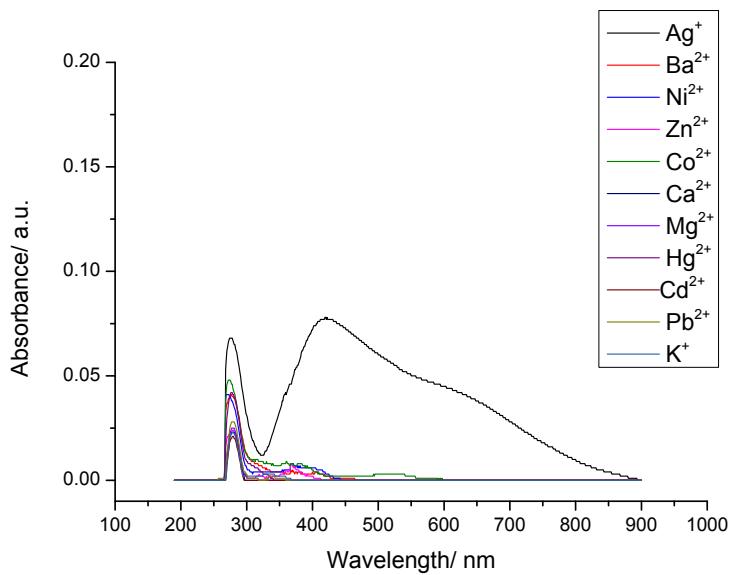


Fig. S3 The UV-vis absorption of **SA** (10 μ M) in the presence of 50 equiv of different metal ions in DMSO buffered solution (pH = 7.24, DMSO: H₂O = 90:10, v/v).

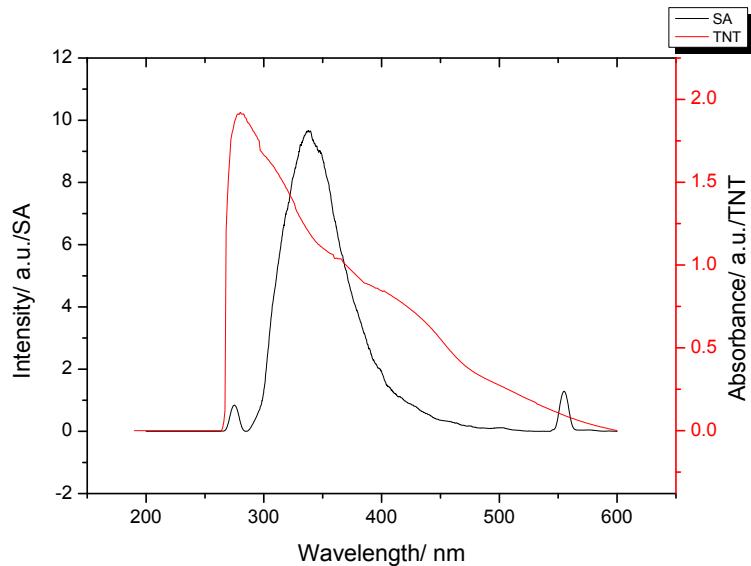


Fig. S4 Emission of **SA** and absorption of **TNT** in DMSO buffered solution (pH = 7.24, DMSO: H₂O = 90:10, v/v).

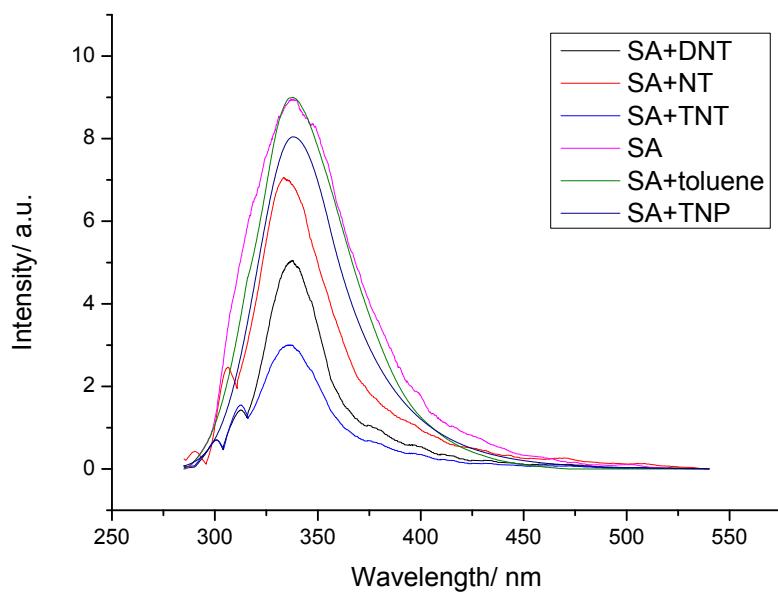


Fig. S5 Emission spectra of **SA** in the presence of 1 equiv of different analytes in DMSO buffered solution (pH = 7.24, DMSO: H₂O = 90:10, v/v).

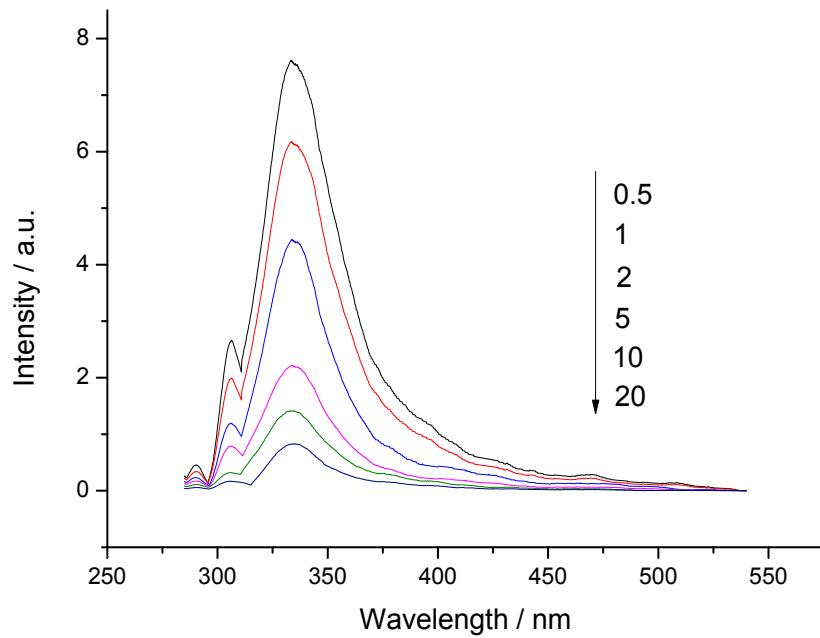


Fig. S6 Emission spectra of **SA** upon addition of 0.5, 1, 2, 5, 10, 20 μM of NT in DMSO buffered solution (pH = 7.24, DMSO: H₂O = 90:10, v/v).

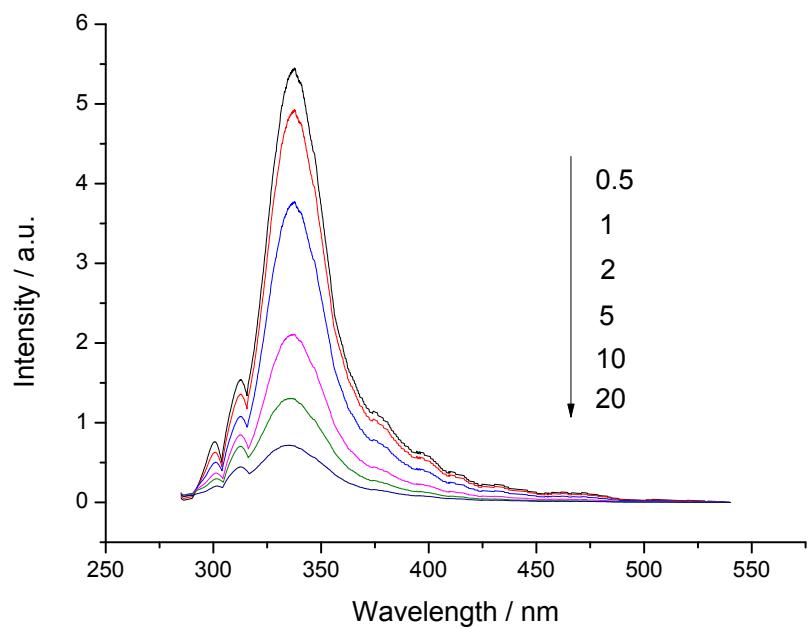


Fig. S7 Emission spectra of **SA** upon addition of 0.5, 1, 2, 5, 10, 20 μM of DNT in DMSO buffered solution (pH = 7.24, DMSO: H_2O = 90:10, v/v).

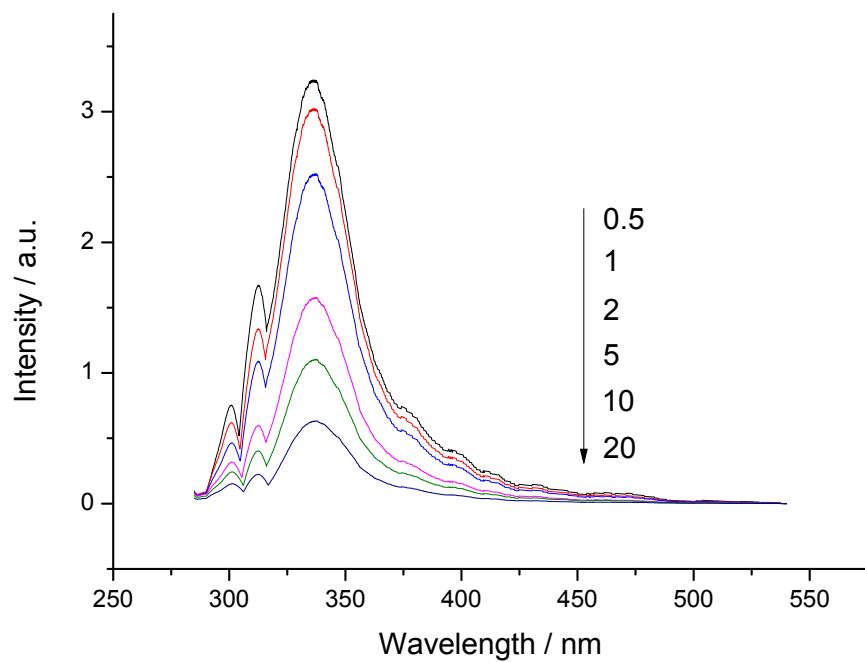


Fig. S8 Emission spectra of **SA** upon addition of 0.5, 1, 2, 5, 10, 20 μM of TNP in DMSO buffered solution (pH = 7.24, DMSO: H_2O = 90:10, v/v).

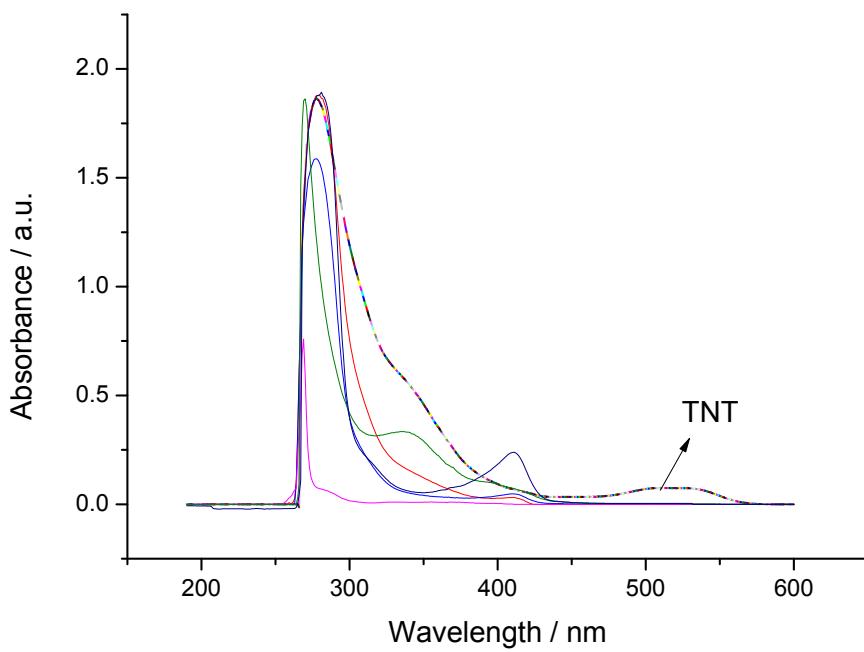


Fig. S9 The UV-vis absorption of SA in the presence of 50 equiv of different explosives in DMSO buffered solution (pH = 7.24, DMSO: H₂O = 90:10, v/v).

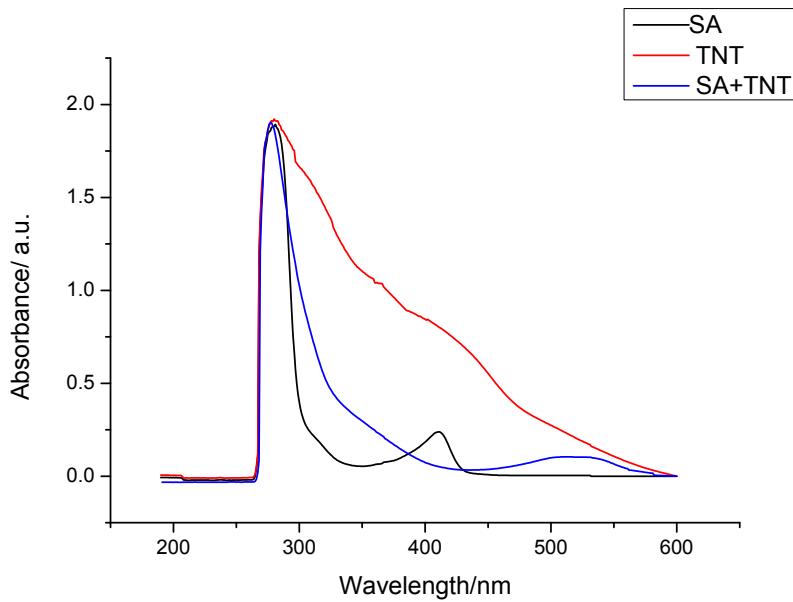


Fig. S10 UV-Vis absorption of SA (black), TNT (red), SA and TNT mixture solution (blue) in DMSO buffered solution (pH = 7.24, DMSO: H₂O = 90:10, v/v).

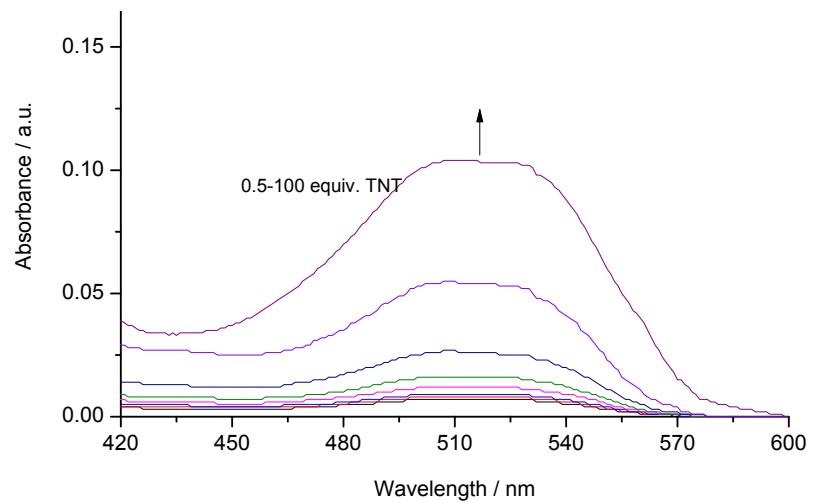


Fig. S11 UV-vis absorption titration of SA ($10 \mu\text{M}$) upon addition of 0.5, 1, 2, 5, 10, 20, 50, 100 μM of TNT in DMSO.