

Supplementary Material

Synthesis and Characterization of Newly Designed and Highly Solvatochromic Double Squaraine Dye for Sensitive and Selective Recognition towards Cu²⁺

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CC1=CC=C2C(=C1)N(C)C(=C2)C
 I^{-}
 C_2H_5

8.38602
 8.32611
 8.31149
 8.25025
 8.16597
 8.14540
 8.03568
 7.82187
 7.81355
 7.80523
 7.80528
 7.80339
 7.78853
 7.72444
 7.71059
 7.70812
 7.70813
 7.69187
 4.85261
 4.72331
 4.70480
 4.67719
 3.31891
 3.31182
 3.30966
 3.30577
 3.29526
 2.95146
 2.95256
 1.84007
 1.83953
 1.64353
 1.62867

-0.00015

Current Data Parameters
 NAME May28-2021TD11
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210528
 Time 22.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 32
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767959 sec
 RG 34.06
 DW 50.000 usec
 DE 6.50 usec
 TE 294.4 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SF01 500.0730881 MHz
 NUC1 1H
 P1 9.60 usec
 PLW1 22.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.0700085 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

1.013
 1.001
 1.004
 1.000
 1.001
 1.001
 1.000
 4.014
 2.058
 0.584
 0.112
 0.098
 6.113
 3.042

MeOD
 MeOH

Chemical structure: CC1=C(C)C(=C2C=CC=CC=C2N1C)C(=O)O

¹H NMR spectrum (MeOD) showing peaks and integration values:

- 139.44955, 138.15678, 135.15678, 132.46135, 131.00409, 129.03465, 128.62631, 124.41184 (aromatic region)
- 113.75797 (aromatic region)
- 57.21075, 49.33833, 49.16884, 48.82733, 48.65464, 45.17490 (aromatic region)
- 22.33758, 14.08660, 14.01462, 13.45585, 13.25734, 13.25766, 13.37557 (methyl and ethyl region)
- 0.04392 (TMS)

Current Data Parameters

NAME	May28-2021TD11
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20210528
Time	23.51
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	MeOD
NS	2048
DS	2
SWH	34090.310 Hz
FIDRES	0.520186 Hz
AQ	0.9611947 sec
RG	188.4
DW	14.667 usec
DE	6.50 usec
TE	295.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TDO	1

CHANNEL f1

SFO1	125.757619 MHz
NUC1	13C
P1	10.30 usec
PLW1	110.00000000 W

CHANNEL f2

SFO2	500.0720003 MHz
NUC2	1H
CPDPRG2	waltz16
PCPD2	80.00 usec
PLW2	22.00000000 W
PLW12	0.31680000 W
PLW13	0.20275000 W

F2 - Processing parameters

SI	32768
SF	125.7425340 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

S1

2. Mass spectral analysis:

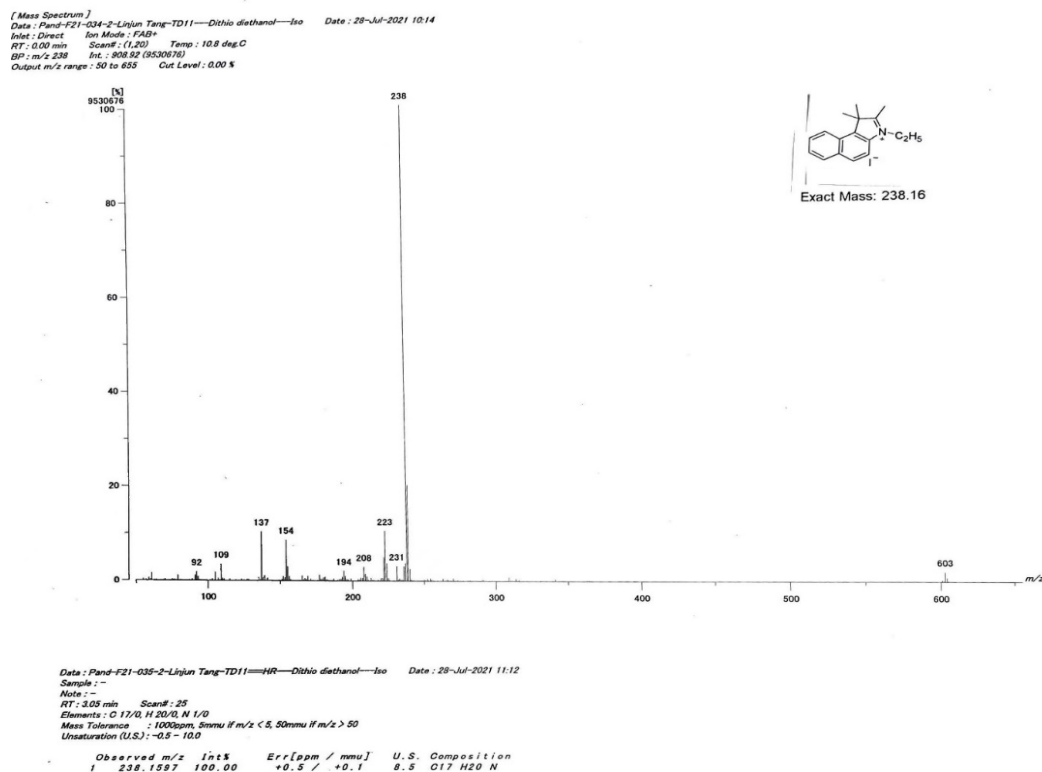


Figure S11. HR-MS spectrum of 3.

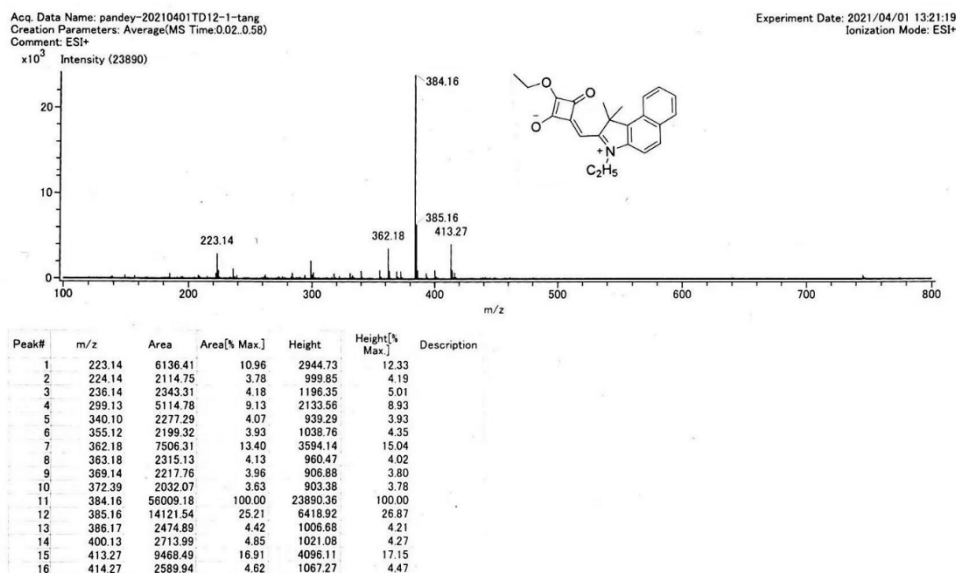


Figure S12. TOF-MS spectrum of 4.

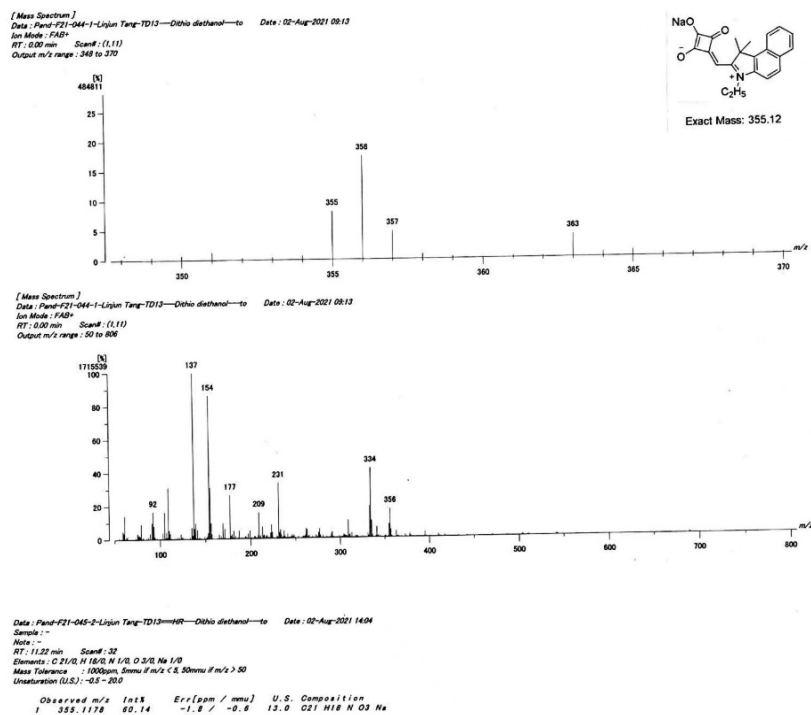


Figure S13. HR-MS spectrum of 5.

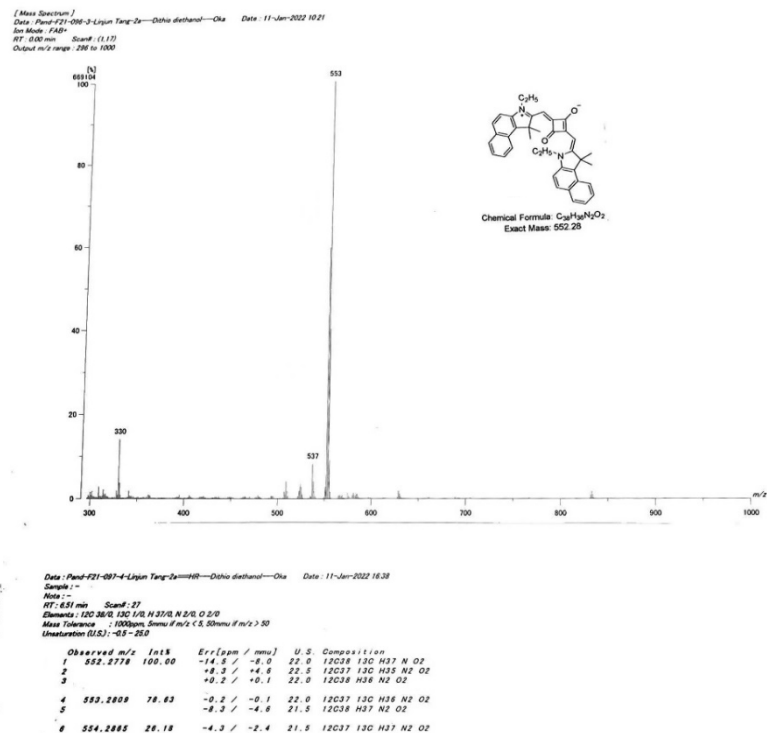
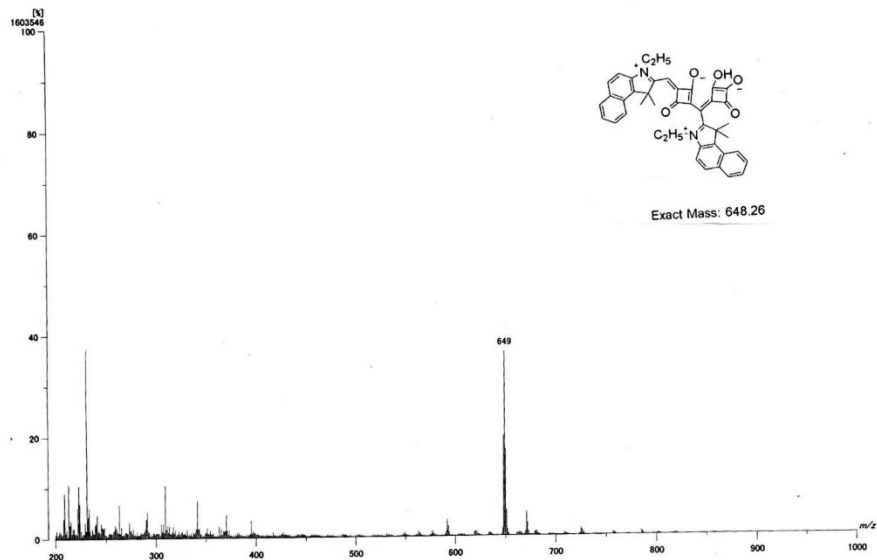


Figure S14. HR-MS spectrum of 6.

[Mass Spectrum]
 Data: Pand-F22-059-3-Jirjun Tang-TM-DithiodE1OH-Oka Date: 04-Jul-2022 10:59
 Ion Mode: FAB+
 RT: 0.00 min Scan#: (1,16)
 Output m/z range: 199 to 1000



Data: Pand-F22-060-2-Jirjun Tang-TM-DithiodE1OH-Oka Date: 04-Jul-2022 11:25
 Sample: -
 Note: -
 RT: 1.72 min Scan#: 8
 Elements: 12C 42/0, 13C 2/0, H 37/0, N 2/2, O 5/5
 Mass Tolerance: 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
 Unsaturation (U.S.): -0.5 - 30.0

Observed m/z	IntS	Err(ppm / mmu)	U.S.	Composition
1 648.2639	64.93	+16.1 / +10.4	25.0	12C40 13C2 H34 N2 O5
2		+9.2 / +5.9	26.5	12C41 13C H35 N2 O5
3		+2.3 / +1.5	26.0	12C42 H36 N2 O5
4 649.2712	100.00	+15.2 / +9.9	26.5	12C40 13C2 H35 N2 O5
5		+8.4 / +5.4	26.0	12C41 13C H36 N2 O5
6		+1.5 / +1.0	25.5	12C42 H37 N2 O5
7 650.2757	44.24	+10.1 / +6.6	26.0	12C40 13C2 H36 N2 O5
8		+3.2 / +2.1	25.5	12C41 13C H37 N2 O5
9 651.2834	12.68	+9.9 / +6.4	25.5	12C40 13C2 H37 N2 O5

Figure S15. HR-MS spectrum of 1.

3. UV-Vis Spectroscopic Studies:

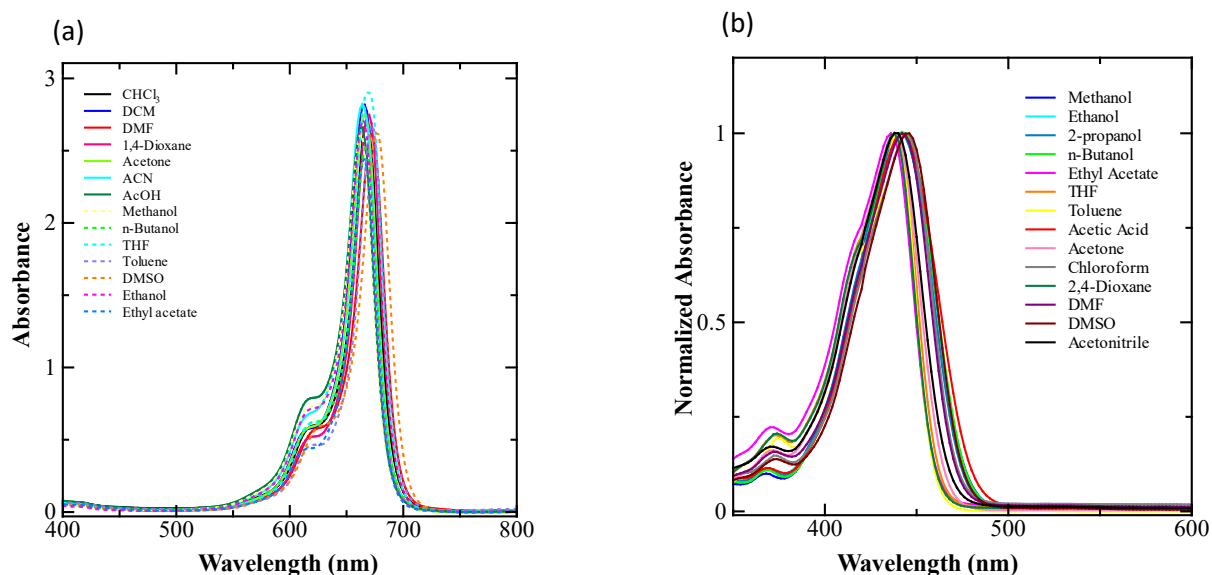


Figure S16. (a) UV-Vis spectra of **6** dissolved in different super dehydrated solvent (25 μM) and (b) UV-Vis spectra of **4** dissolved in different super dehydrated solvents (10 μM).

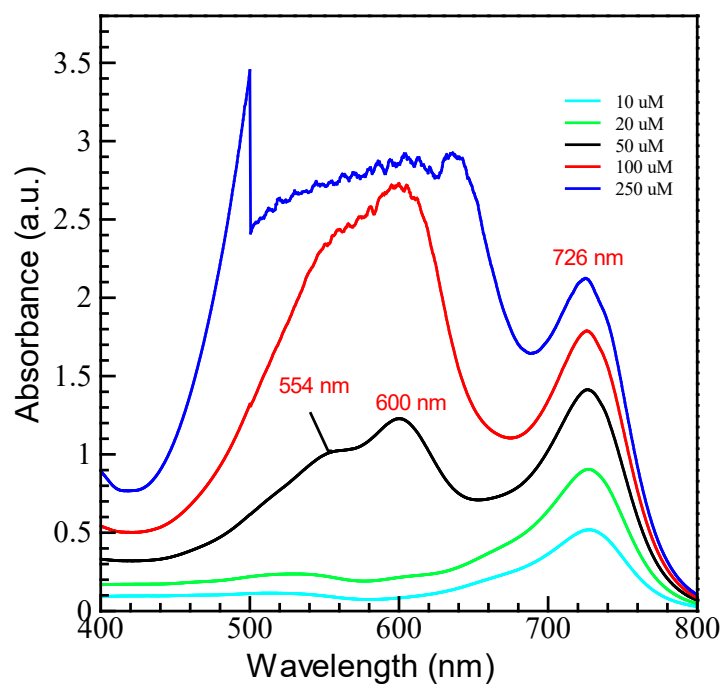


Figure S17. UV-Vis absorption of different concentration of DSQ (**1**) dissolved in DMF

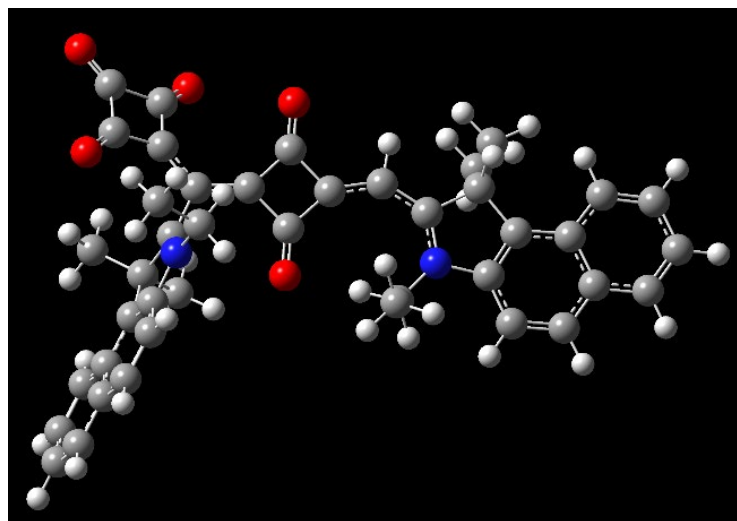


Figure S18. The three-dimensional structure of **1** utilizing Theoretical MO calculation (Gaussian G09 program)

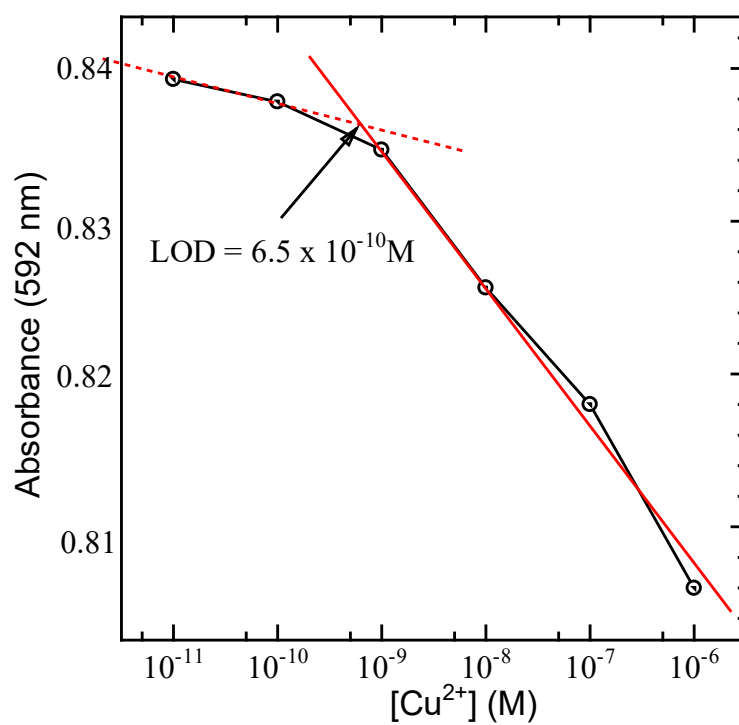


Figure S19. Change in absorbance at 592 nm upon addition of Cu²⁺ ions showing limit of detection

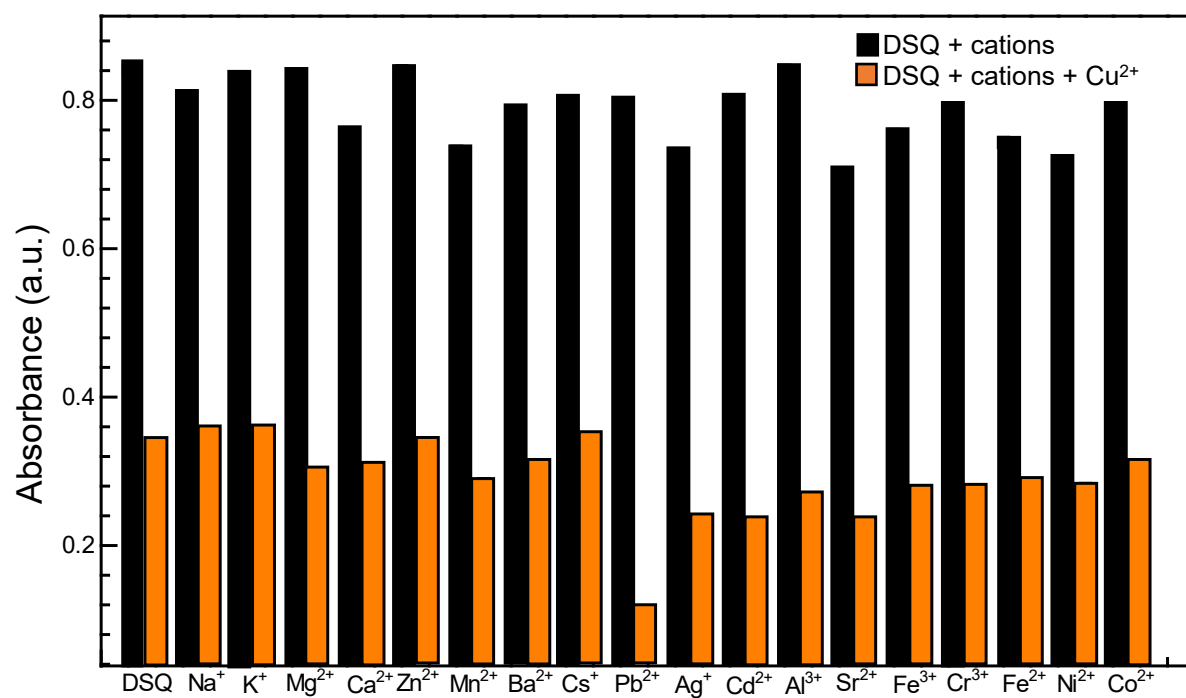


Figure S20. UV-Vis absorption at 592 nm of 10 μM DSQ (**1**) (dissolved in DMF/ACN, 1:99, v/v) in different ion solutions after addition of Cu^{2+}