

Supporting Information for

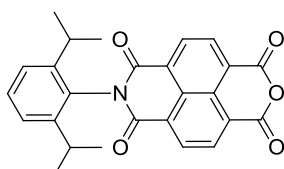
A new N-substituted heteroacene can detect CN⁻ and F⁻ anions via anion- π interaction

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Chemical Formula: C₂₆H₂₁NO₅
Exact Mass: 427.14

2

Shimadzu Biotech Axima ToF² 2.9.3.20110624; Mode Reflectron_HiRes_neg, Power: 110
%Int. 333 mV[sum= 15969 mV] Profiles 1-48: (48 Tagged) Smooth Av 20 -Baseline 20

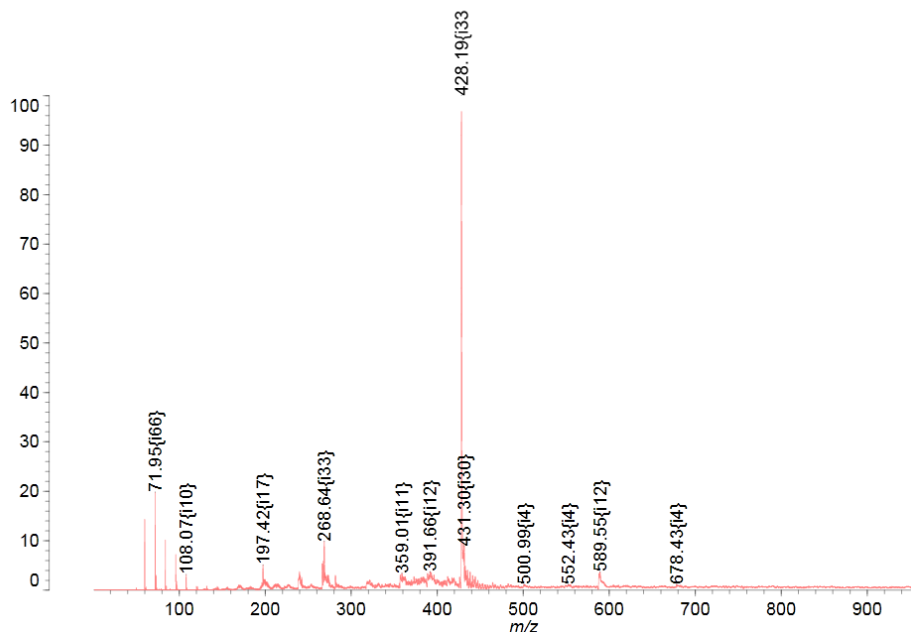
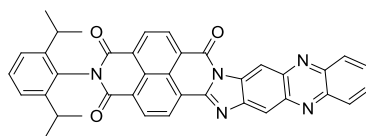


Figure S1 MALDI TOF of 2 without further purification



Chemical Formula: C₃₈H₂₇N₅O₃
Exact Mass: 601.21

1

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

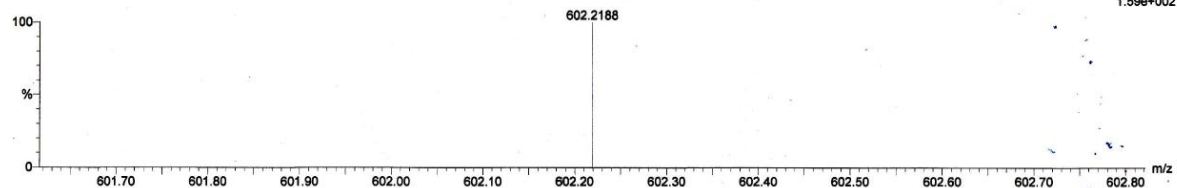
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 38-40 H: 25-29 N: 0-5 O: 0-3

C₃₈H₂₇N₅O₃

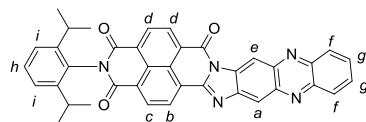
LIULEI3 2 (0.064)



Minimum: -1.5
Maximum: 5.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
602.2188	602.2192	-0.4	-0.7	27.5	20.6	0.0	C ₃₈ H ₂₈ N ₅ O ₃

FigureS2 HiRes MALDI TOF of 1



Chemical Formula: C₃₈H₂₇N₅O₃
Exact Mass: 601.21

1

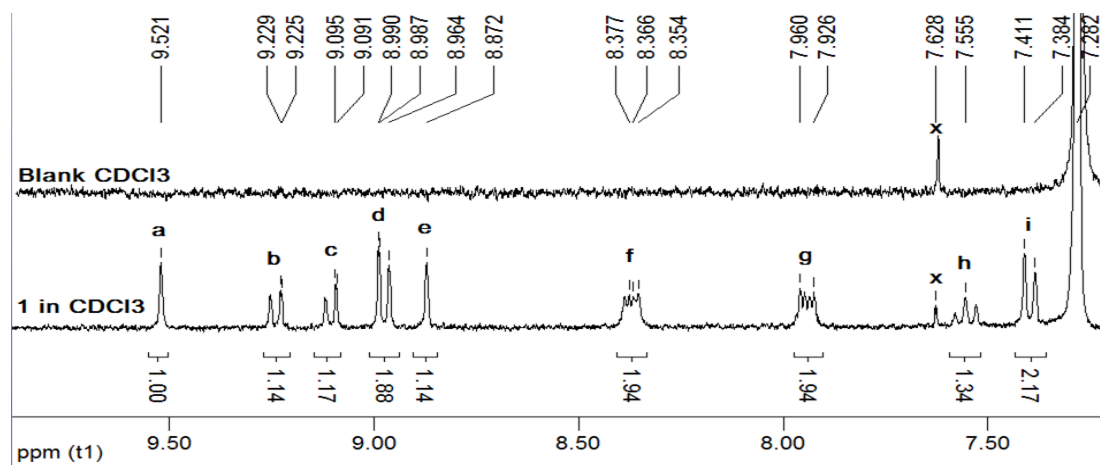


Figure S3. Blank CDCl₃ and aromatic proton peaks distribution of 1 in CDCl₃ via ¹H NMR (400 MHz) as labeled in molecular structure of 1.

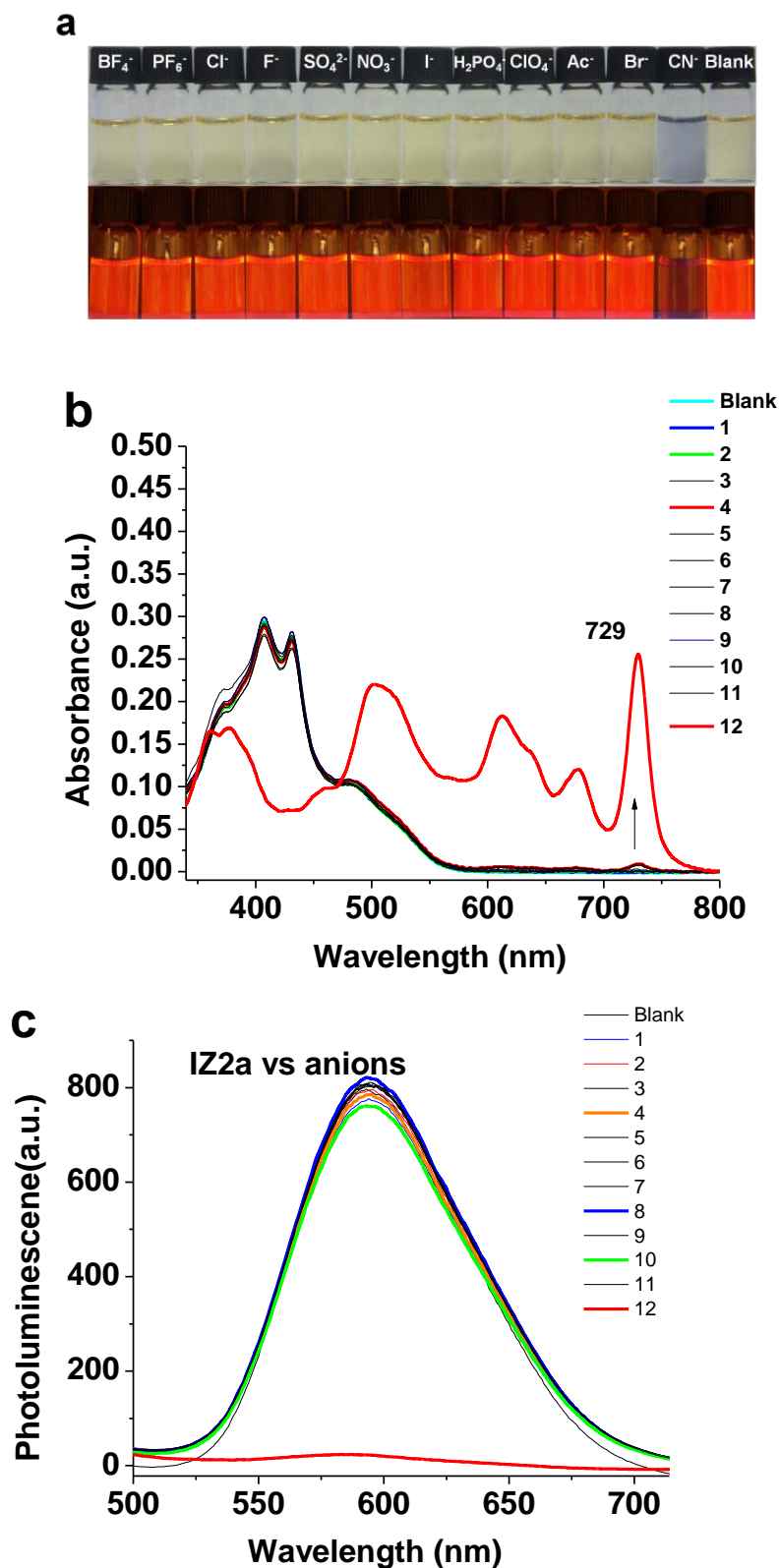


Figure S4. The picture of color change (a), UV-vis (b) and PL (c) spectra of **1** (1 eq., 2 mL, 1.0×10^{-5} M) in THF solution upon addition of anions 1-12 (BF_4^- , PF_6^- , Cl^- , F^- , SO_4^{2-} , NO_3^- , I^- , H_2PO_4^- , ClO_4^- , Ac^- , Br^- , and CN^-) as TBA salts DMF solution (15 eq., 30 μL , 1.0×10^{-2} M).

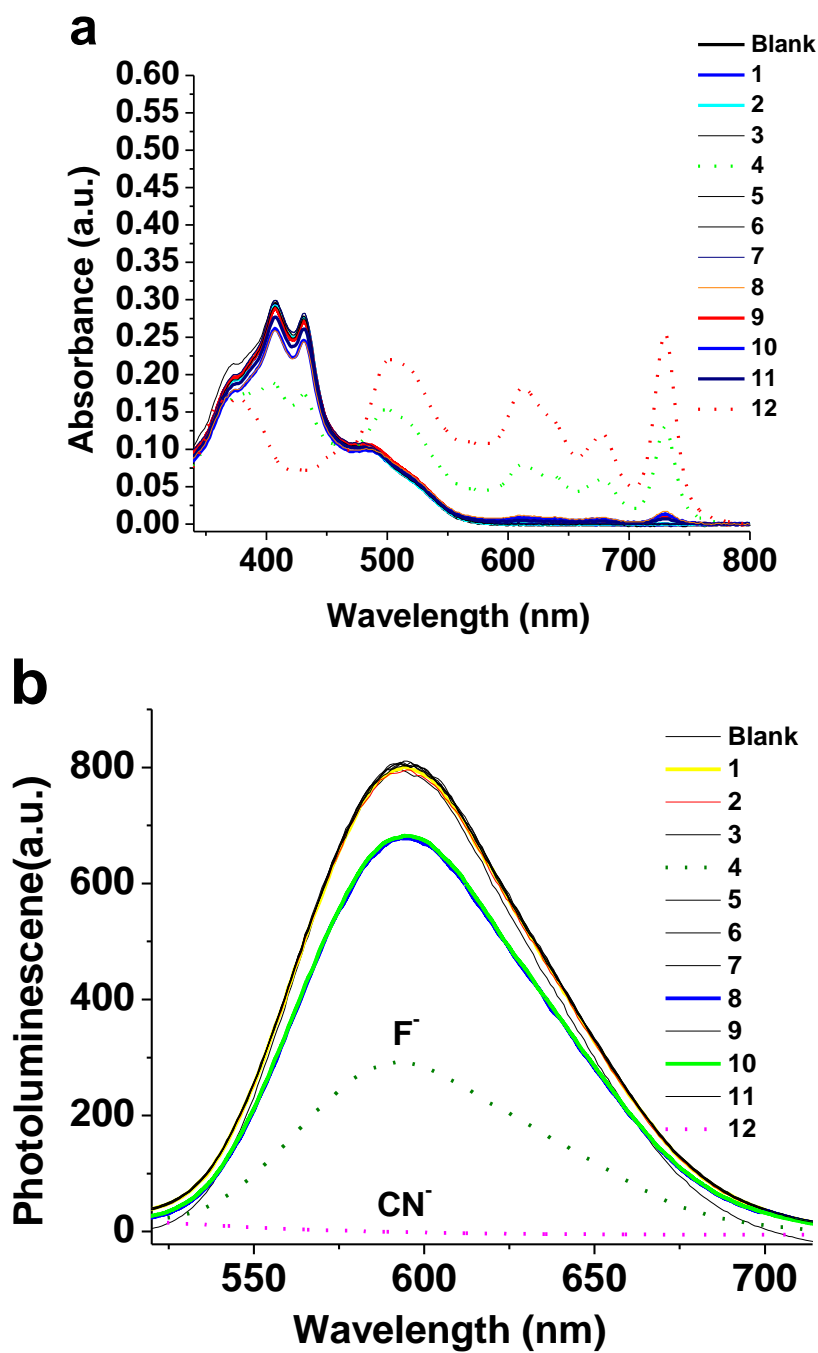


Figure S5. UV-vis (a) and PL (b) spectra of **1** (1 eq., 2 mL, 1.0×10^{-5} mol/L) in THF solution without changes upon the addition of 9 anions 1, 2, 5, 6, 7, 8, 9, 10, and 11 (see Figure S4) as TBA salts in DMF solution (30 eq., 60 μ L, 1.0×10^{-2} mol/L), respectively.

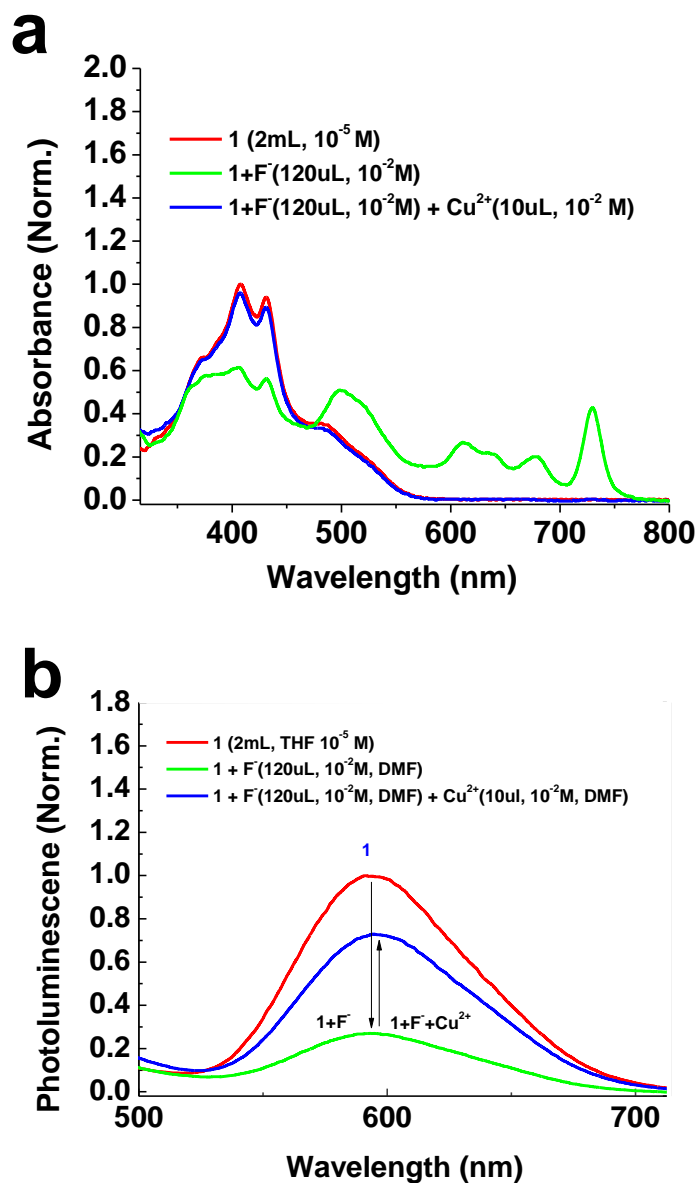


Figure S6. Normalized UV-Vis (a) and PL (b) spectra of **1** (1×10^{-5} M) in THF solution upon addition of **60 eq.** of F⁻ (120 μ L in DMF) and followed by the addition of 5 eq. Cu²⁺ (10 μ L in DMF).

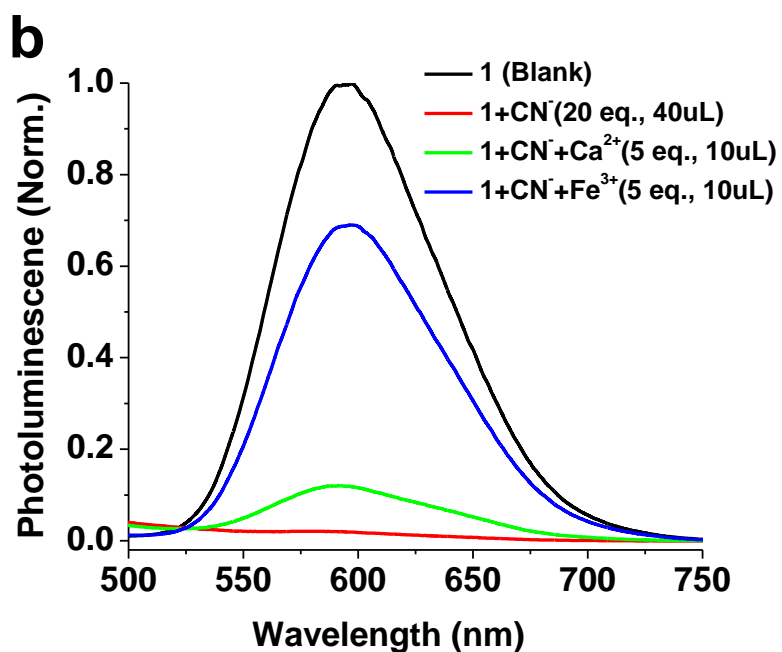
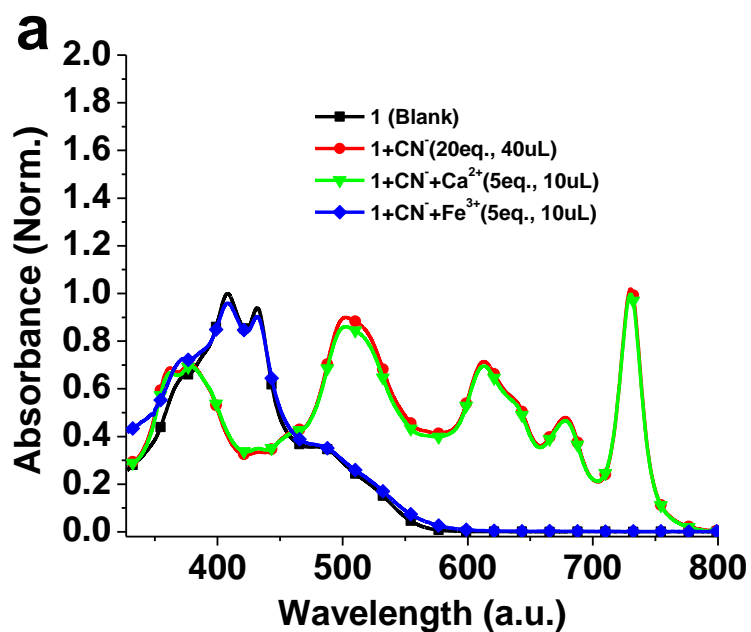


Figure S7. Normalized UV-Vis (a) and PL (b) spectra of **1** (1 eq., 2 mL, 1×10^{-5} M) in THF solution upon addition of 20 eq. of CN⁻ (40 μL in DMF) and followed by the addition of 5 eq. Ca²⁺ and Fe³⁺ (10 μL in DMF) compared to Cu²⁺ (10 μL in DMF).