3-hydroxyflavone derivatives synthesized by a new simple method as chemosensors for cyanide anions

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Supporting Information

1. Crystal data, data collections and structure refinements of compounds 1 and 2

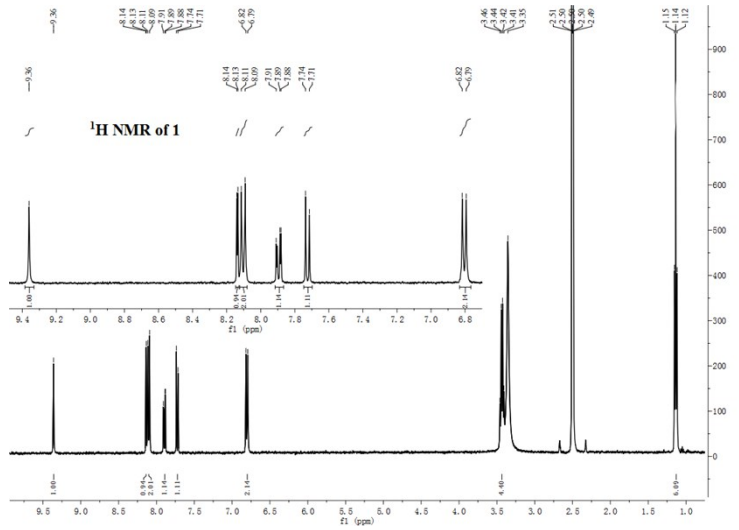
Table S1. Crystal data, date collections and structure refinements of compounds **1** and **2**

Crystal data	**1**	**2**
Empirical formula	$C_{20}H_{18}NO_5$	$C_{19}H_{18}BrNO_3$
Formula mass	352.35	388.25
Crystal system	triclinic	monoclinic
Space group	P-1	$P2_1/c$
a [Å]	7.0399(7)	13.3522(19)
b [Å]	7.3275(7)	13.823(3)
c [Å]	17.4123(17)	9.515(2)
α [º]	89.658(8)	90.00
β [º]	82.561(8)	92.847(18)
γ [º]	76.168(8)	90.00
V [Å^3]	864.53(15)	1753.9(6)
Z	2	4
ρ_{calc} [g cm^{-3}]	1.354	1.470
μ [mm^{-1}]	0.098	2.360
F(000)	370.0	792.0
Crystal size [mm]	0.42×0.18×0.046	0.42 × 0.088 × 0.036
θ_{min}-θ_{max} [º]	52.74-6.74	52.72-5.9
T/K	293.15	293.15
scan mode	ω, φ	ω, φ
Index range	-8 ≤ h ≤ 8	-16 ≤ h ≤ 11
	-9 ≤ k ≤ 9	-16≤ k ≤ 17
	-21 ≤ l ≤ 21	-11 ≤ l ≤ 11
Collected reflections	10358	9853
Unique reflections	3915	3503
Refined parameters	238	220
R1, wR2	0.0532, 0.1454	0.0665, 0.2086

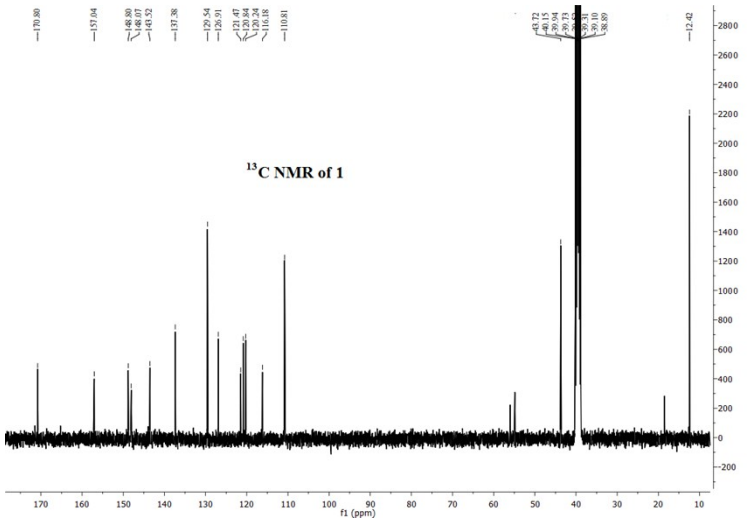
Table S2. Selected geometric parameters (Å,◦) of the crystal structures

	O3-C9 (Å)	O3-C1 (Å)	C8-C9 (Å)	C7-O1 (Å)	C7-C8 (Å)	C6-C7 (Å)	O2-C8 (Å)	Dihedral angle α(º)[a]
1	1.379(2)	1.360(2)	1.371(2)	1.247(2)	1.437(3)	1.456(3)	1.358(2)	11.52
2	1.381(6)	1.366(6)	1.358(7)	1.243(6)	1.441(7)	1.450(7)	1.381(6)	9.74

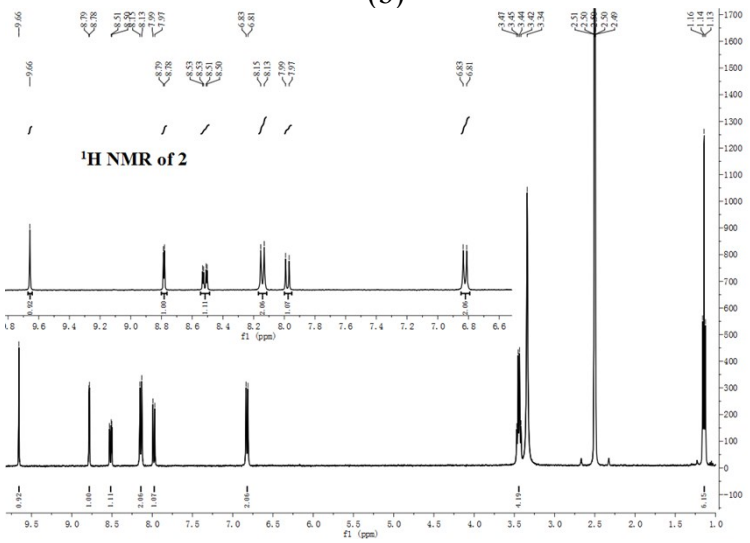
2. N MR spectra of compounds 1 and 2



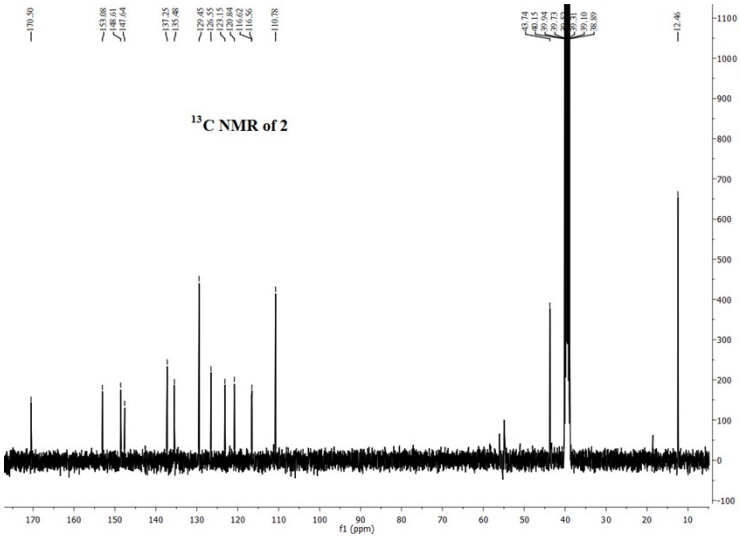
(a)



(b)



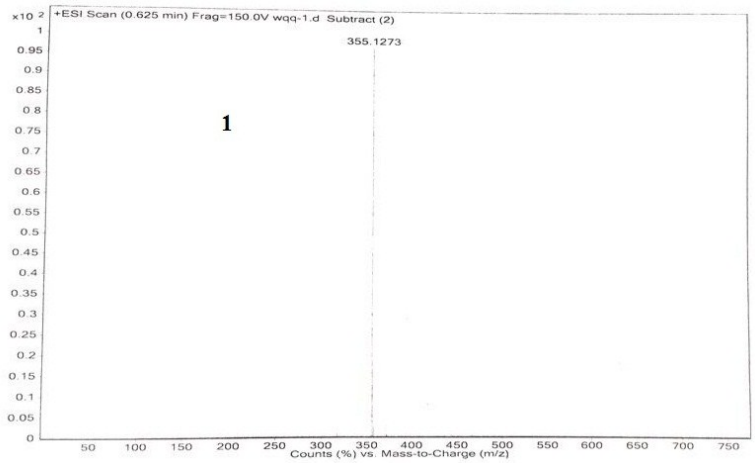
(c)



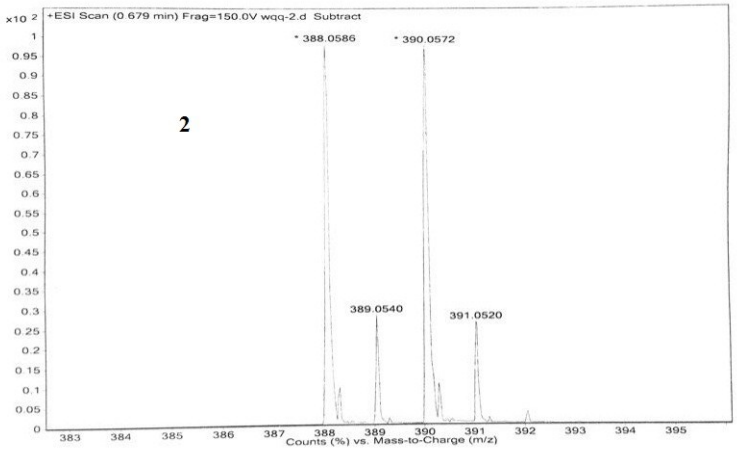
(d)

Figure S1. ^{1}H and ^{13}C NMR spectra of compounds **1** (a, b) and **2** (c, d) in dimethyl sulfoxide.

3. High-resolution mass spectra of compounds 1 and 2



(a)



(b)

Figure S2. High-resolution mass spectra of compounds **1** (a) and **2** (b).

4. Fluorescence spectral change of compound 1 with CN^- in acetonitrile

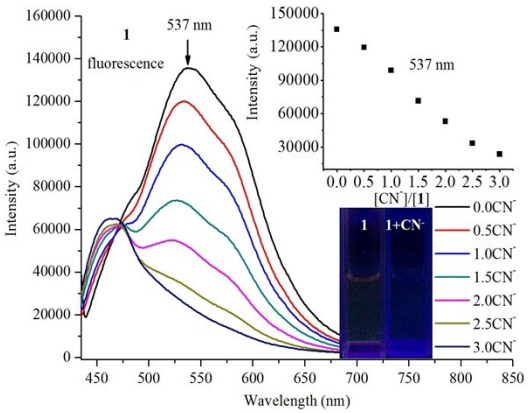


Figure S3. Fluorescence spectral change of compound **1** upon the addition of CN^- in acetonitrile.

5. UV-vis absorption spectral change of compound 3 with CN^- in acetonitrile

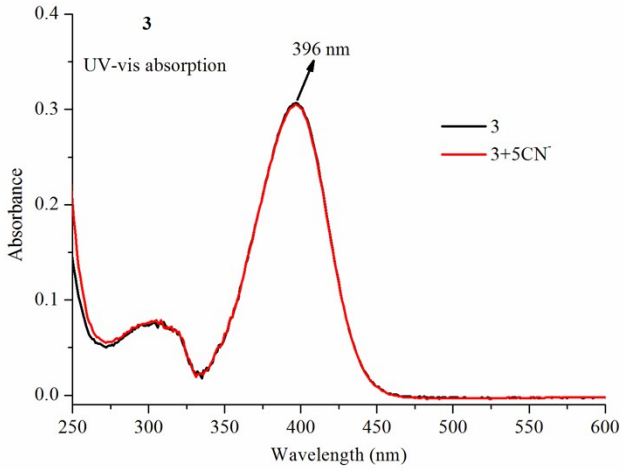


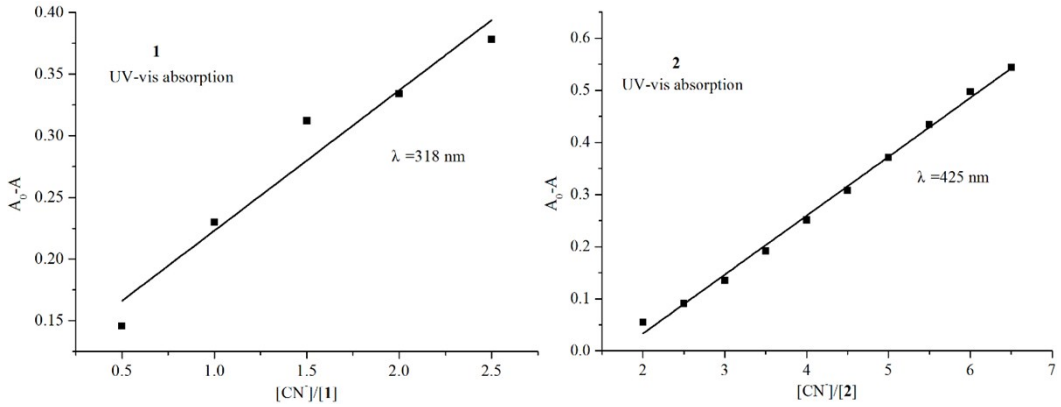
Figure S4. Changes in UV-vis absorption spectra of compound **3** in acetonitrile upon the addition of 5 equivalent of TBACN.

6. Determination of the detection limits

The detection limits DL of the compounds for CN^- were determined from the following equation:

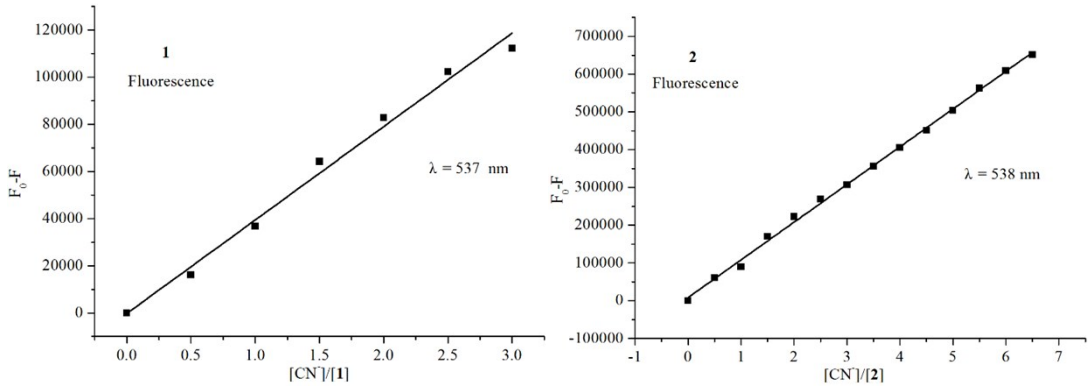
DL = K*Sb1/S

Where K = 2 or 3; Sb1 is the standard deviation of the blank solution; S is the slope of the calibration curve. Here K = 3, Sb1 = 0.002 for absorption; K = 3, Sb1 = 2 for fluorescence.



(a) 0.070 μM (b) 0.053 μM

Figure S5. The absorbance changes of compounds **1** and **2** in acetonitrile with adding CN^- at specific wavelength.



(a) 0.00015μM (b) 0.000060μM

Figure S6. The fluorescence changes of compounds **1** and **2** in acetonitrile with adding CN^- at specific wavelength

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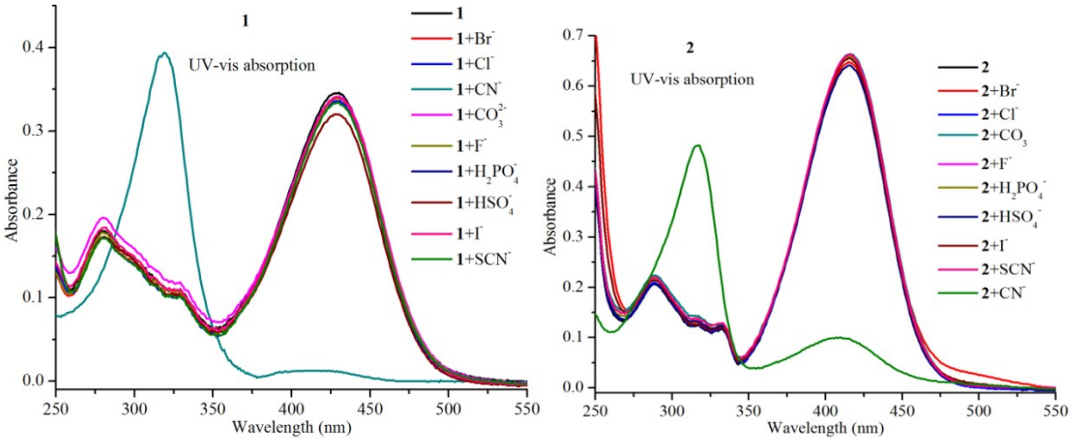
7. UV-vis absorption spectral change of compounds 1 and 2 towards various anions



(a) (b)

Figure S7. UV-vis spectral changes of **1** (a) and **2** (b) with C = 10 μM in acetonitrile observed upon the addition of various anions.

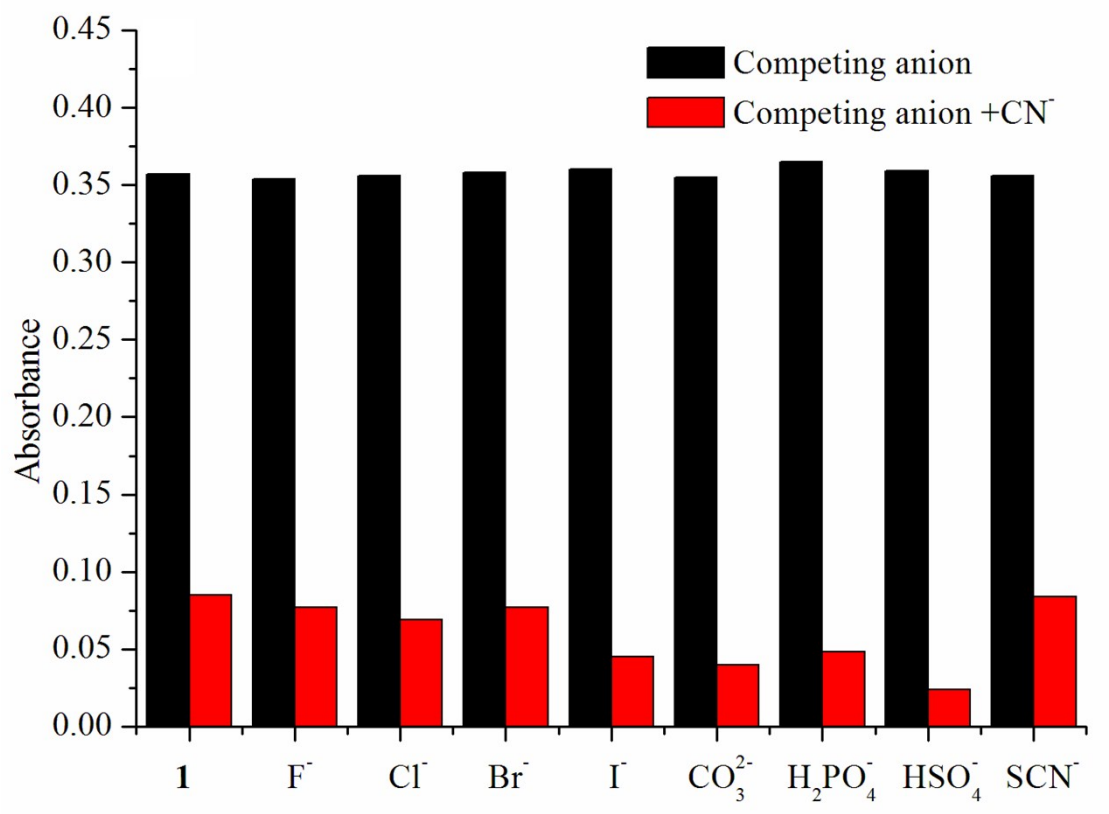


Figure S8. Changes in UV-vis absorption of compound **1** at 426 nm in the presence of various anions (3 equiv.) in acetonitrile in response to CN^- (3 equiv.).