Supplementary Information (SI)

For

A new ratiometric, colorimetric and ‘‘turn-on’’ fluorescent chemosensor for detection of cyanide ion based on phenol–bisthiazolopyridine hybrid

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Table of contents

Page

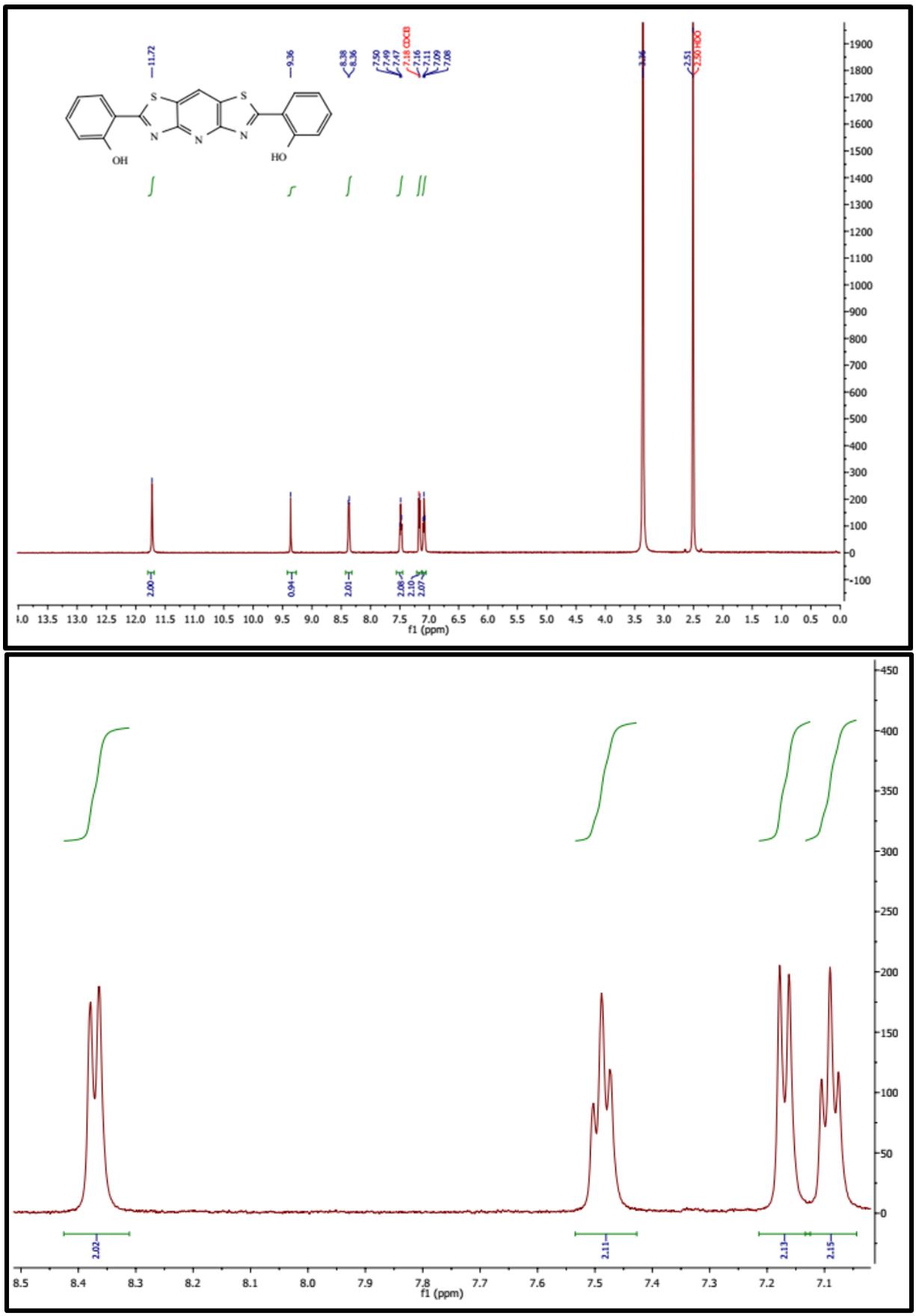


Figure S1. ^{1}H NMR of compound **1** and its expantion spectrum (DMSO-d_6, 500 MHz).

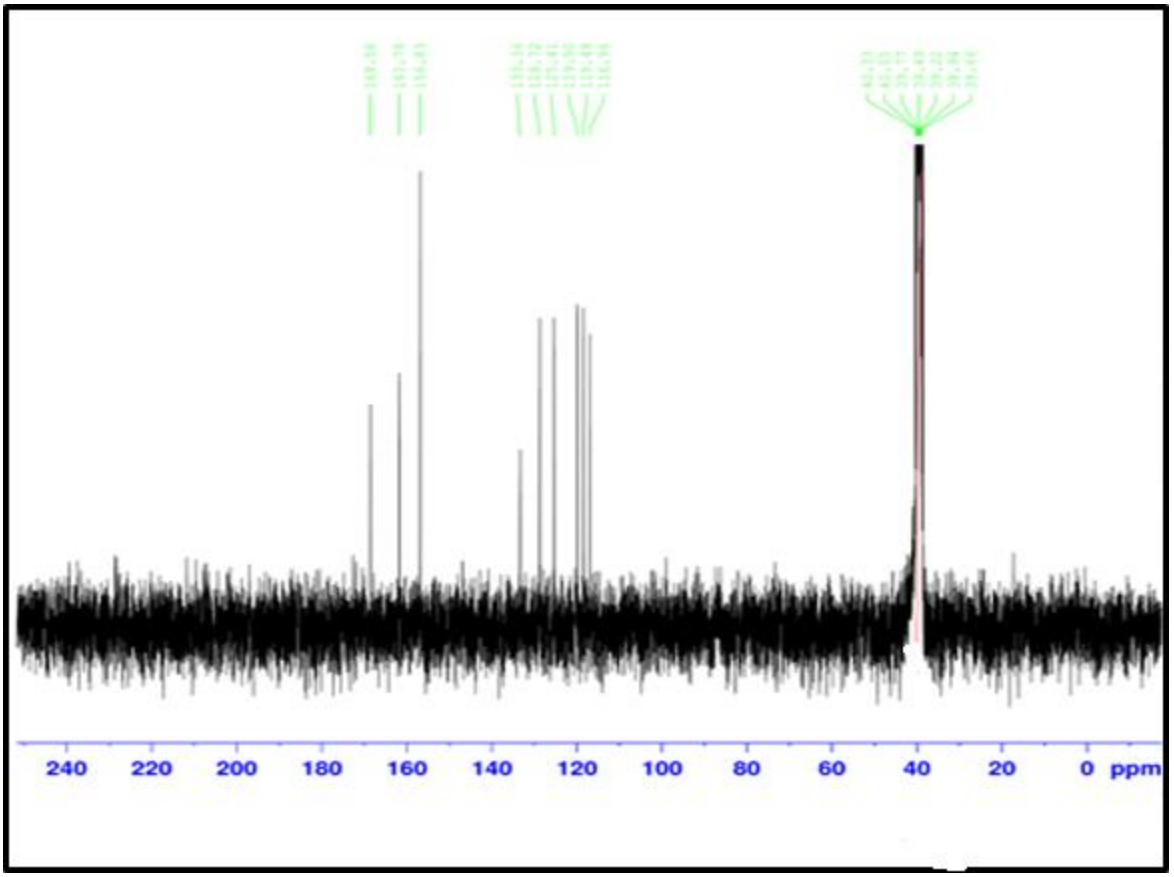
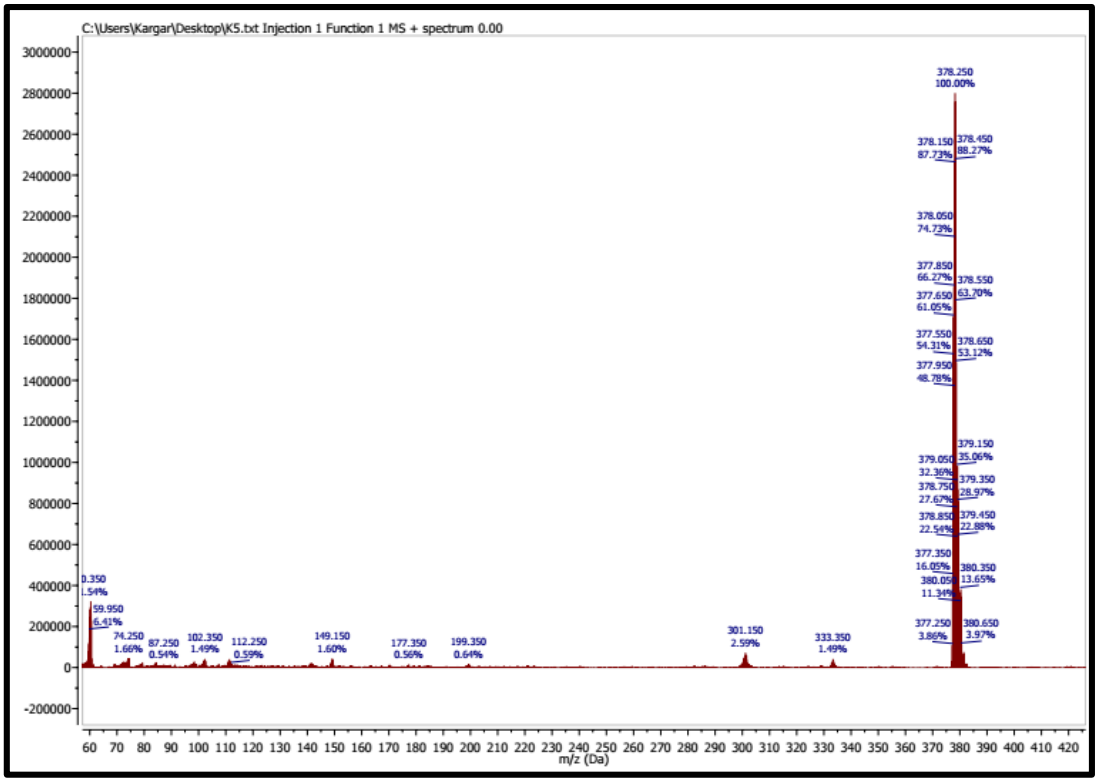


Figure S2. ^{13}C NMR spectrum of compound **1** (DMSO-d_6, 100 MHz).



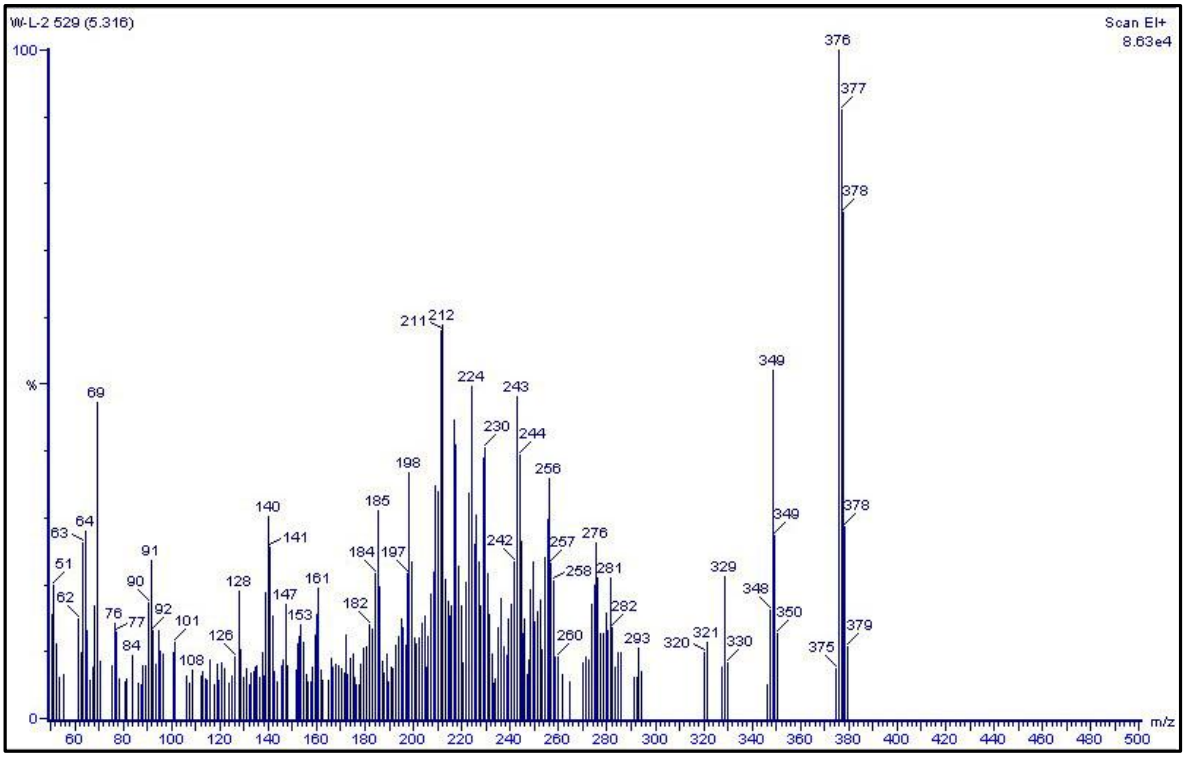


Figure S3. TOF MS ES+ mass and Mass spectrum of compound **1**.

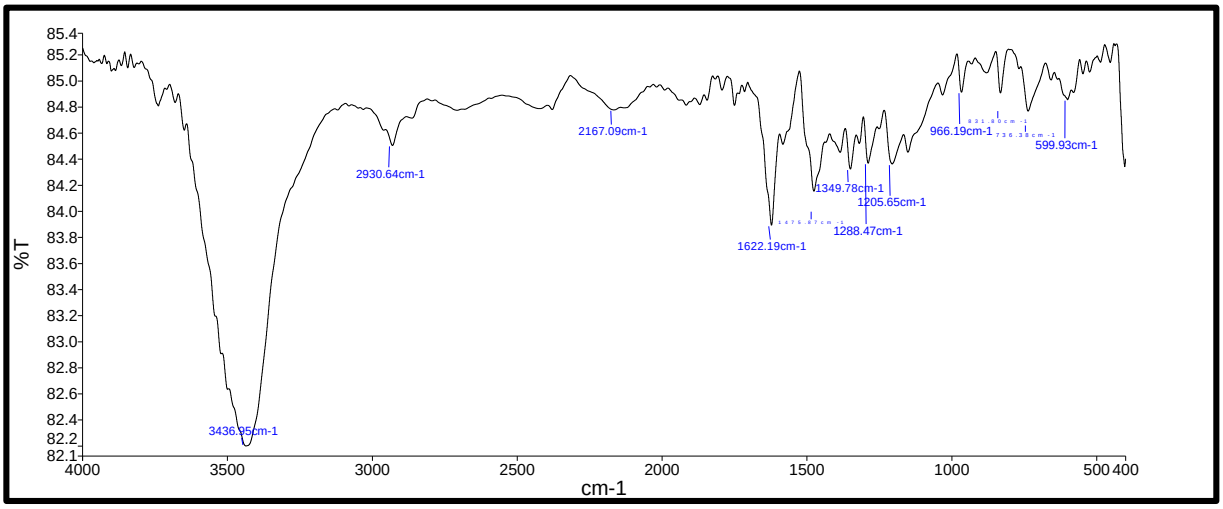


Figure S4. IR spectra of compound **1.**

Table S1. Absorbance titration of **1** with various concentration of CN^-.

V_0	V_t	C_0	C_t	eq	A_{438}	A_{394}	A_{438}/A_{394}
1000	0	0.00005	0	0	0.023864	2.372758	0.010057
1000	20	4.9E-05	1.96E-05	0.4	0.017145	2.310209	0.007421
1000	40	4.81E-05	3.85E-05	0.8	0.072063	2.245557	0.032091
1000	60	4.72E-05	5.66E-05	1.2	0.151919	2.142961	0.070892
1000	80	4.63E-05	7.41E-05	1.6	0.228	2.03182	0.112215
1000	100	4.55E-05	9.09E-05	2	0.291531	1.933491	0.15078
1000	120	4.46E-05	0.000107	2.4	0.358893	1.830863	0.196024
1000	140	4.39E-05	0.000123	2.8	0.412911	1.75173	0.235716
1000	160	4.31E-05	0.000138	3.2	0.458978	1.65529	0.277279
1000	180	4.24E-05	0.000153	3.6	0.503754	1.577458	0.319345
1000	200	4.17E-05	0.000167	4	0.540374	1.502205	0.359721
1000	240	4.03E-05	0.000194	4.8	0.570311	1.431914	0.398285
1000	260	3.97E-05	0.000206	5.2	0.590196	1.382478	0.426911
1000	280	3.91E-05	0.000219	5.6	0.616201	1.313823	0.469014
1000	300	3.85E-05	0.000231	6	0.640322	1.258056	0.508977
1000	320	3.79E-05	0.000242	6.4	0.663762	1.211843	0.547729
1000	340	3.73E-05	0.000254	6.8	0.678571	1.170157	0.579897
1000	360	3.68E-05	0.000265	7.2	0.687393	1.127566	0.609626
1000	380	3.62E-05	0.000275	7.6	0.696812	1.091545	0.638372
1000	400	3.57E-05	0.000286	8	0.705998	1.057835	0.667399
1000	420	3.52E-05	0.000296	8.4	0.702582	1.034633	0.679064
1000	440	3.47E-05	0.000306	8.8	0.696156	1.016213	0.685049

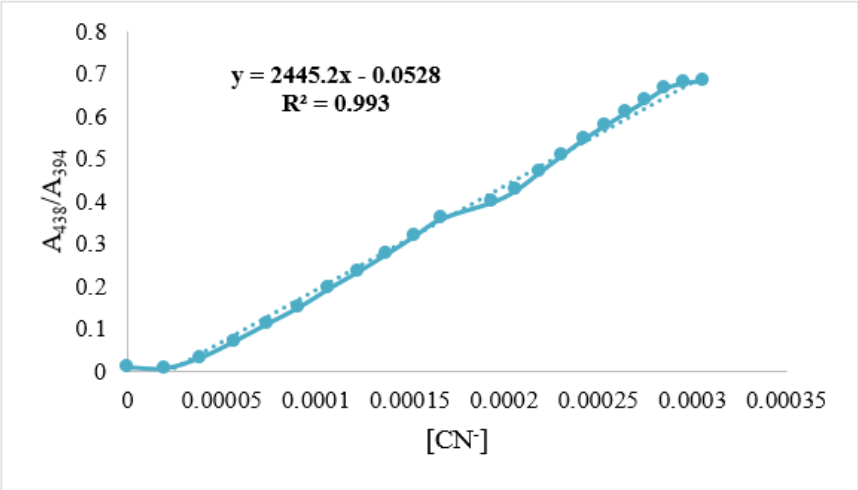


Figure S5. Absorbance ratio changes (A_{438}/A_{394}) of **1** upon gradual addition of CN^-.

Table S2. Fluoresence titration of **1** with various concentration of CN^-.

V_0	V_t	C_0	C_t	eq	I_{420}	I_{515}	A_{420}/A_{515}
1000	0	0.000032	0	0	237.956	34.7844	6.840883
1000	10	3.17E-05	3.17E-05	1	164.435	28.4547	5.778834
1000	15	3.15E-05	4.73E-05	1.5	130.919	27.2438	4.80546
1000	20	3.14E-05	6.27E-05	2	108.254	27.333	3.96056
1000	25	3.12E-05	7.8E-05	2.5	90.2188	26.3415	3.424968
1000	35	3.09E-05	0.000108	3.5	60.4495	27.8854	2.167783
1000	45	3.06E-05	0.000138	4.5	45.7349	28.7886	1.588646
1000	55	3.03E-05	0.000167	5.5	33.5363	30.7737	1.089771
1000	65	3E-05	0.000195	6.5	28.2686	32.3842	0.872913
1000	75	2.98E-05	0.000223	7.5	25.535	34.0518	0.749887
1000	90	2.94E-05	0.000264	9	22.1667	37.7039	0.587915
1000	105	2.9E-05	0.000304	10.5	20.9209	40.8709	0.511878
1000	120	2.86E-05	0.000343	12	18.4569	43.9998	0.419477
1000	135	2.82E-05	0.000381	13.5	17.8581	46.3784	0.385052
1000	155	2.77E-05	0.000429	15.5	17.3951	49.4042	0.352098
1000	175	2.72E-05	0.000477	17.5	16.264	53.3104	0.305081
1000	195	2.68E-05	0.000522	19.5	16.095	55.6268	0.289339
1000	220	2.62E-05	0.000577	22	15.5511	59.5531	0.26113
1000	245	2.57E-05	0.00063	24.5	15.165	59.2113	0.256117
1000	275	2.51E-05	0.00069	27.5	14.9024	62.7435	0.237513
1000	350	2.37E-05	0.00083	35	14.608	65.3445	0.223554

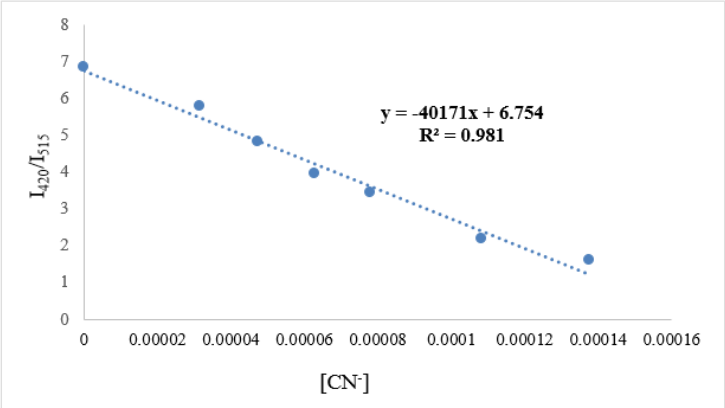


Figure S6. Emission ratio changes (I_{420}/I_{515}) of **1** upon gradual addition of CN^-.

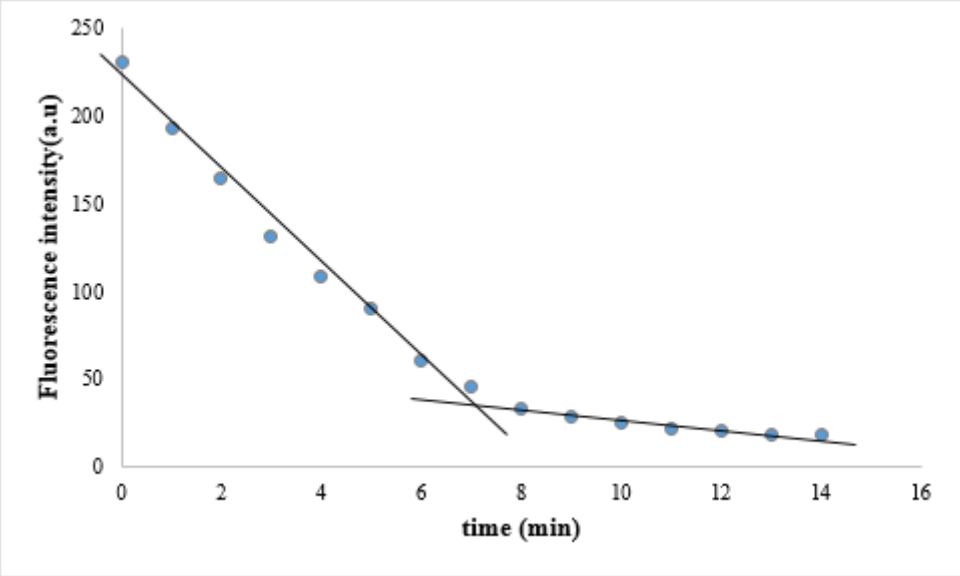


Fig. S7. Time dependent fluorescence study of **1** at 420 nm.

Table S3. Comparison of **1** with other probes for detection of cyanide ions *via* hydrogen bonding.

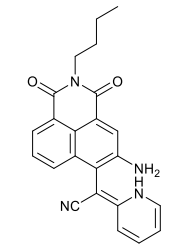
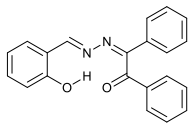
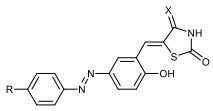
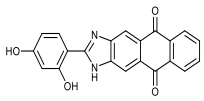
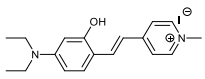
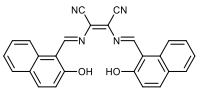
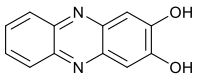
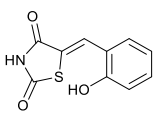
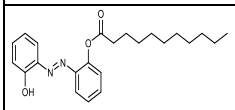
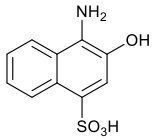
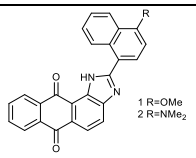
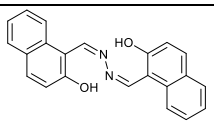
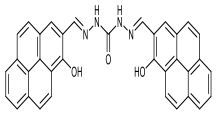
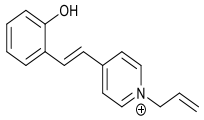
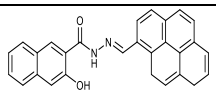
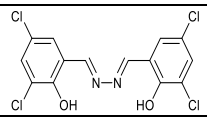
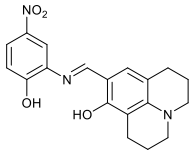
Chemical Structure	Method	Sensing ions	Solvent medium	Mechanism	LOD	Applications	Reference Nomber
	Colorimetric & Fluorescent	CN^-	water	Hydrogen bonding	0.18 µmol	test strips	6
	Colorimetric & Fluorescent	CN^-	DMSO/H_2O (v/v = 3:2)	Hydrogen bonding	0.61 nm	Test kit	7
	Colorimetric	CN^-	CH_3CN/H_2O	Hydrogen bonding	0.74 µM	Test kit	8
	Colorimetric & Fluorescent	CN^-	DMSO/H_2O / THF	Hydrogen bonding	0.11 µM	water & cow urine	9
	Colorimetric & Fluorescent	CN^-	CH_3CN	Hydrogen bonding	0.38 µM	Test kit	10
	Colorimetric & Fluorescent	CN^-	DMSO/H_2O	Hydrogen bonding	-	Cell imaging	11
	Fluorescent	CN^-	H_2O	Hydrogen bonding	56 µM	Bitter seed, Potato, Test kit	12
	Fluorescent	CN^-	CH_3CN/H_2O	Hydrogen bonding	15 µM	Test kit	13

Table S4. Comparison of **1** with other probes for detection of cyanide ions *via* deprotonation.

Chemical Structure	Method	Sensing ions	Solvent medium	Mechanism	LOD	Applications	Reference Nomber
	colorimetric & fluorescent	CN^-, $HCO3^-$, $CO3^{2-}$ the weak selectivity and weak sensitivity	H_2O–MeOH (v/v,2/5)	deprotonation	-	-	14
	colorimetric & fluorescent (on to off)	Cyanide	H_2O	deprotonation	0.32 µmol		15
	colorimetric	Fluoride & Cyanide	CH_3CN–H_2O (9:1)	deprotonation	17.7 µmol		16
	colorimetric & fluorescent (ON)	CN Job (2:1)	DMSO/H_2O (9:1)	deprotonation	0.4 µmol		17
	colorimetric & fluorescent	cyanide	CH_3CN-DMSO-H_2O (94:1:5)	deprotonation	0.25 µmol	Cell imaging	18
	colorimetric	cyanide	CH_3CN–H_2O (95 : 5)	deprotonation	8 µmol	test paper	19
	colorimetric	cyanide	CH_3CN - buffer (1:1)	deprotonation	1.2 µmol		20
	colorimetric	cyanide Job (1:1)	CH_3CN/bis-tris buffer solution (3:7).	deprotonation	210 µM		21
	colorimetric	cyanide Job (1:1) Intereferes in organic media		deprotonation	105 mM	test kit	22