

**Colorimetric, Turn-on fluorescent detection of fluoride ions using simple indole
based receptor in live cells.**

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Synthesis of FI-1:

1.09 mmol of Fluorescein hydrazide and 1.09 mmol of 3- formyl indole mixed with ethanol and the suspension was refluxed overnight in the presence of catalytic amount of acetic acid. The upon cooling the reaction mixture to room temperature, had thrown out colorless solid. FI-1: ¹H NMR (300 MHz, DMSO) δ 11.55 (s, 1H), 9.88 (s, 2H), 9.45 (s, 2H), 8.93 (s, 1H), 8.37 (d, *J* = 7.6 Hz, 1H), 8.02 – 7.91 (m, 1H), 7.75 (s, 1H), 7.65 (dd, *J* = 7.8, Hz, 1H), 7.50 (d, *J* = 7.9 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.18 (dd, *J* = 6.3 Hz, 2H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 1.6 Hz, 1H), 6.59 – 6.44 (m, 2H). ¹³C NMR (75 MHz, DMSO) δ 162.25, 157.88, 152.13, 148.59, 136.48, 132.73, 130.68, 130.26, 128.49, 127.78, 123.46, 122.02, 121.60, 119.84, 111.59, 111.18, 110.29, 101.75, 65.03. Mass (ESI): 474.3233(M+1), 473.1211(calculated)

Synthesis of FI-2:

The procedure used for synthesise FI-1 is followed here instead of 3- formyl indole, here we used N-methyl 3- formyl indole. FI-2: ¹H NMR (300 MHz, DMSO) δ 9.88 (s, 2H), 9.45 (s, 2H), 8.93 (s, 1H), 8.37 (d, *J* = 7.6 Hz, 1H), 8.01 – 7.91 (m, 1H), 7.74 (s, 1H), 7.65 (dd, *J* = 7.8, Hz,

1H), 7.50 (d, $J = 7.9$ Hz, 1H), 7.37 (d, $J = 8.0$ Hz, 1H), 7.18 (dd, $J = 6.3$ Hz, 2H), 6.98(t, $J = 7.5$ Hz, 1H), 6.69 (d, $J = 1.6$ Hz, 1H), 6.59 – 6.42 (m, 2H). 3.6(s,3H). Mass (ESI): 459.1611(M+1), 458.1520 (calculated)

Synthesis of FB-1:

The procedure used for synthesizing FI-1 is followed here instead of 3- formyl indole, here we used N-methyl 3- formyl indole. FB-1: $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 9.11 (s, 9H), 8.63 (s, 4H), 7.41 – 7.33 (m, 9H), 7.32 (dd, $J = 9.0, 5.1$ Hz, 11H), 7.26 (s, 3H), 7.15 – 7.08 (m, 10H), 6.94 (dd, $J = 5.7, 2.1$ Hz, 4H), 6.56 (d, $J = 2.2$ Hz, 7H), 6.38 (s, 2H), 6.36 (s, 4H), 6.30 (d, $J = 2.3$ Hz, 5H), 6.28 (d, $J = 2.3$ Hz, 3H). Mass (ESI): 409.7421(M+1), 407.3011 (calculated)

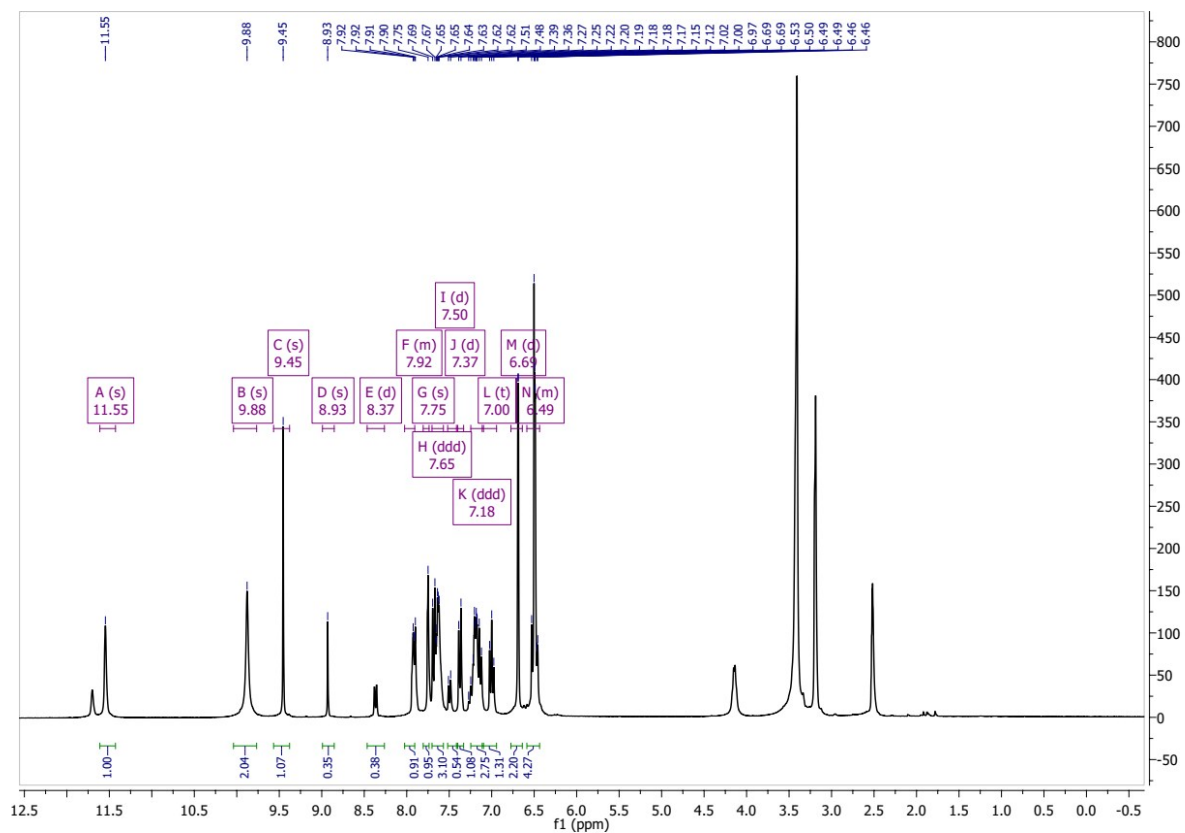


Fig-S1: ¹H-NMR of probe FI-1 in DMSO-d₆.

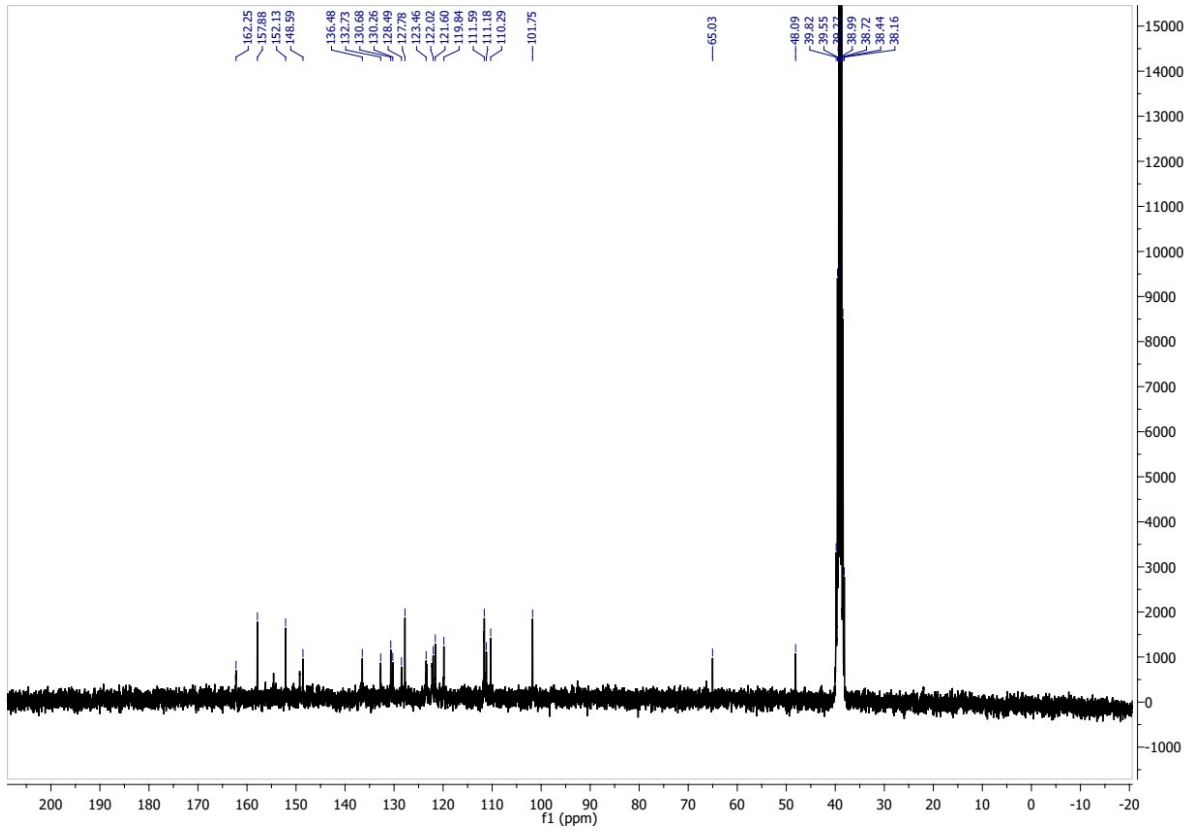


Fig-S2: ¹³C-NMR of probe FI-1 in DMSO-d₆.

S4 #117 RT: 1.78 AV: 1 NL: 1.21E3
T: ITMS + c ESI Full ms [50.00-1500.00]

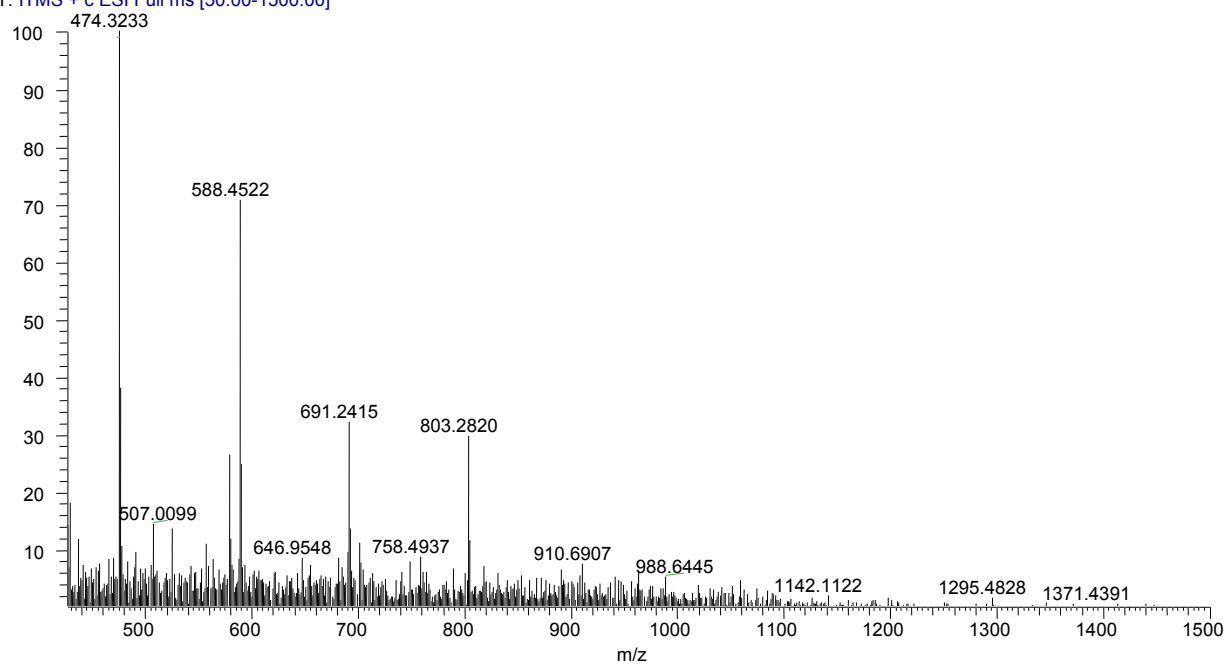


Fig-S3: ESI-MS spectrum of FI-1

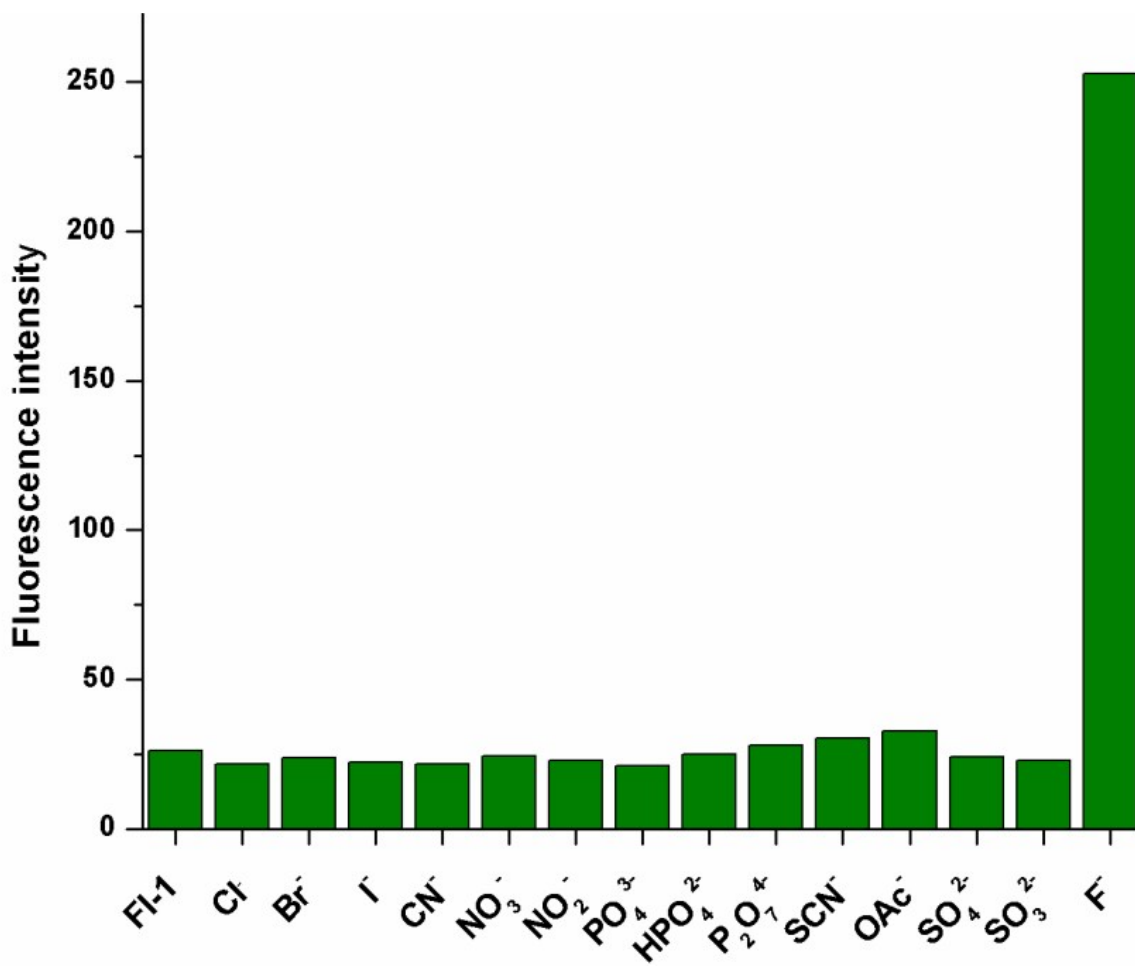


Fig S4: Fluorescence selectivity response of FI-1 with different anions.

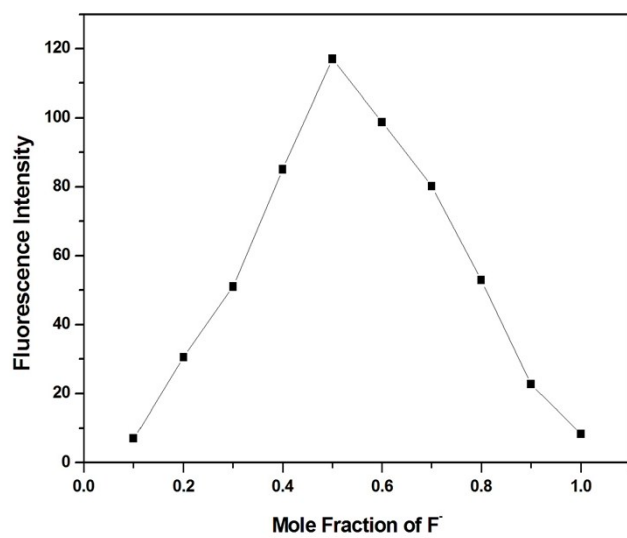


Figure S5: Jobs plot of fluoride ions Vs FI-1.

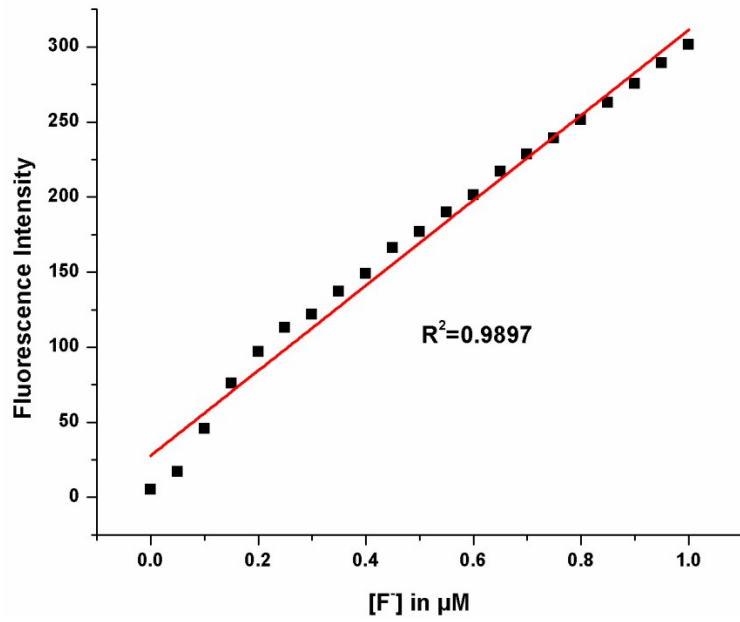


Figure-S6 Plot of fluorescence intensity Vs concentration of fluoride ions added.

Fig-S7: ¹⁹F-NMR of FI-1 with fluoride ions:

Table S1. Determination of F⁻ ion in real samples.

Probe	Sample	F ⁻ spiked (μM)	Found F ⁻	Recovery
			mean ^[a] ± SD ^[b] (μM)	(%)
L -120.84	Tap water 1	10	7.6 ± 0.01	76
	Tap water 2	15	13.3 ± 0.15	86
	Tap water 3	20	18 ± 0.10	90
	Urine- 1	10	8.8 ± 0.01	88
	Urine-2	15	14.0 ± 0.02	90
	Urine-3	20	19.8 ± 0.11	99

^amean of three determination

^bSD, standard deviation

Table-S2: Comparison Chart of the fluoride detection methods with the existing methods.

Sl No	Sensor	Fluorescence switching	LoD	Reference
1.	N-imidazolyl- 1,8-naphthalimide	off	5×10^{-7} M	1
2.	Imidazophenazine	Ratiometric	86 μ M	2
3.	Coumarin tetrazole	On	207 nM	3
4.	Silylated fluorescein	On	1 μ M	4
5.	Fluorine triazolium ion	On	1 μ M	5
6	Rhodamine-imidazole	On	8.52 nM	6

7	Fluorescein Indole	On	31.8 nM	Present work
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References:

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Fig-S8: Photograph of the probe FI-1 in aqueous solution without and with fluoride ions

FI-1 Alone



FI-1 with F⁻ ions

