Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Ratiometric fluorophore for quantification of iodide under physiological conditions : Applications in urine analysis and live cell imaging

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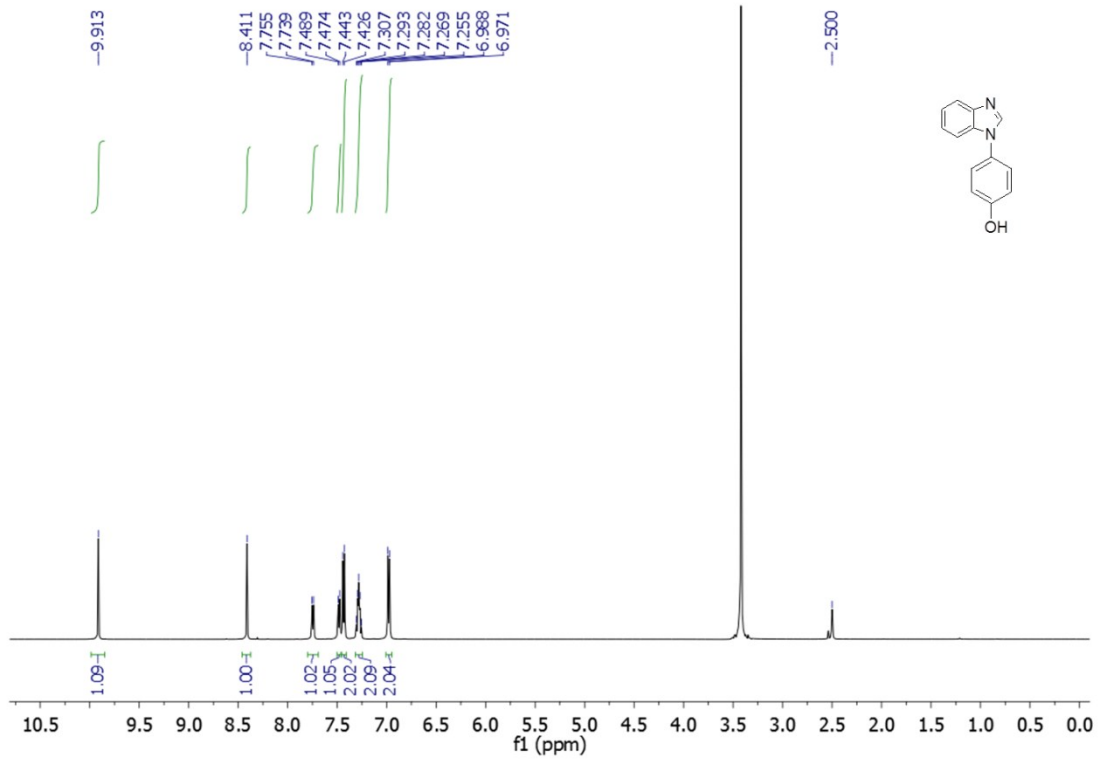
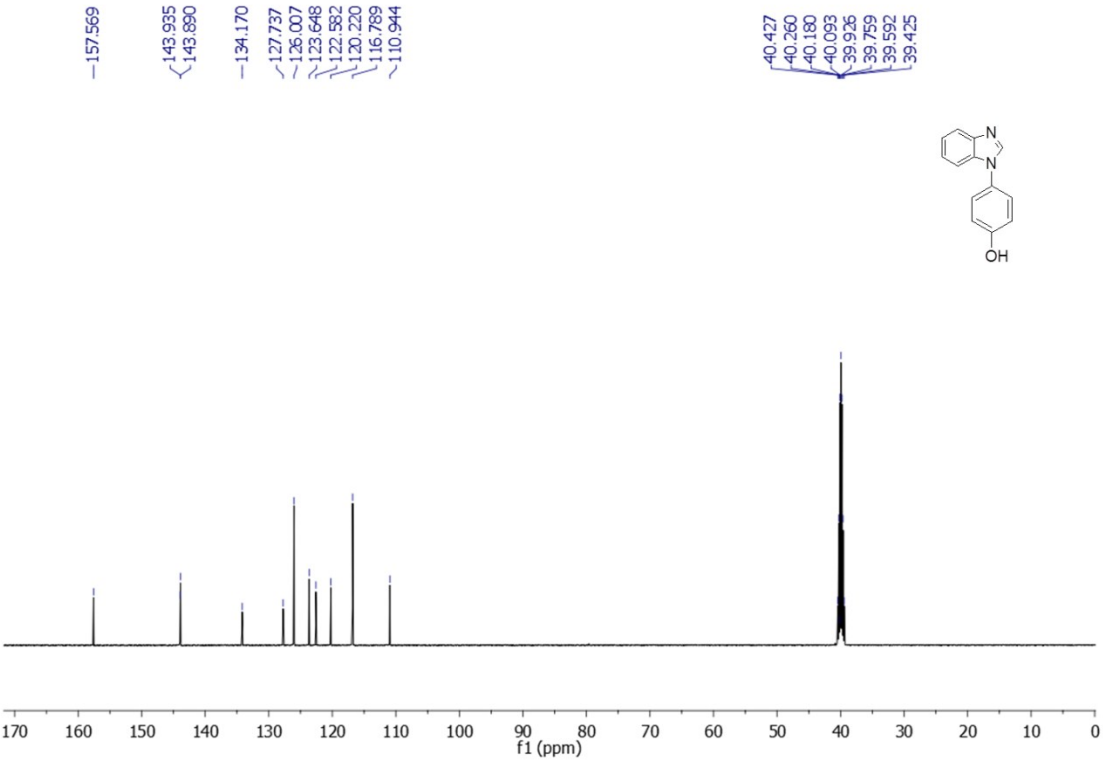
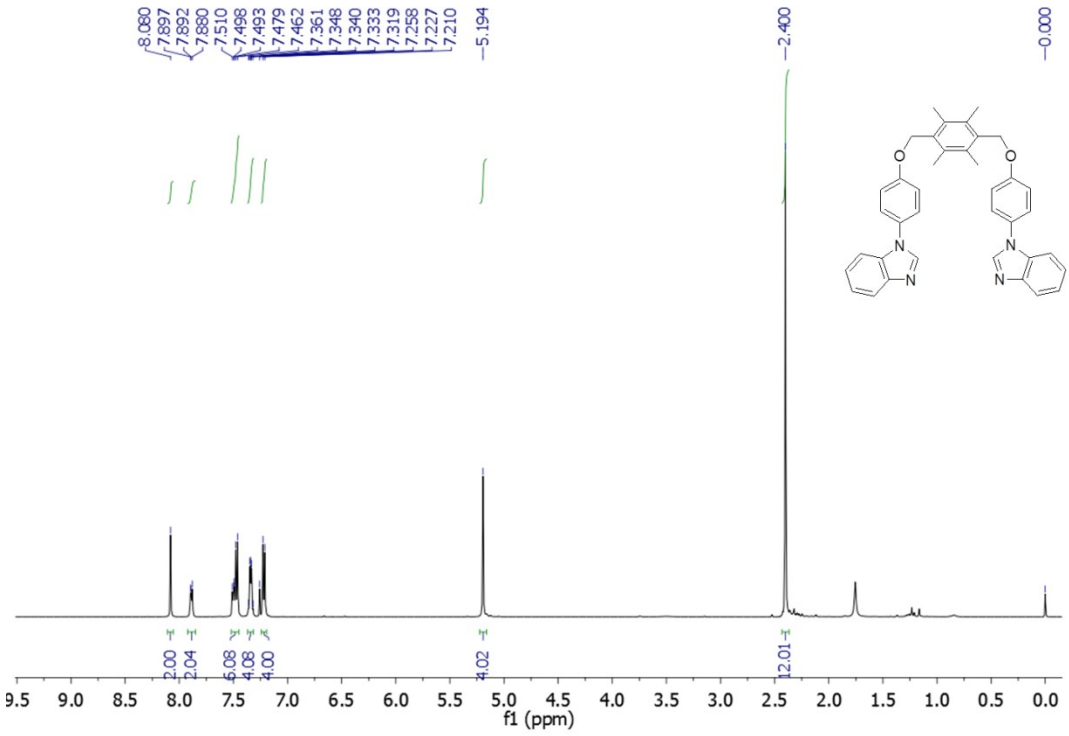
1. Experimental Details

General Remarks: All chemicals were obtained from common suppliers (Aldrich, Across, SDFCL, Spectrochem etc.) and used without further purification. ^{1}H and ^{13}C NMR spectra were recorded on BRUKER Bio spin AVANCE-III FT NMR HD-500 spectrophotometer using $CDCl_3$ or DMSO-d_6 as solvent and tetramethylsilane (TMS) as internal standard. Data are reported as follows: chemical shifts in ppm, coupling constants J in Hz; multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet). High resolution mass spectra were recorded on BRUKER DALTONIK micrOTOF-Q11 spectrometer. The fluorescence titrations were performed on Varian Carey Eclipse fluorescence spectrophotometer and BH-CHRONOS spectrophotometer. The life-time studies were performed on BH-CHRONOS spectrophotometer and absorption spectra were recorded on Shimadzu-2450 spectrophotometer. The spectral data were analyzed through curve fitting procedures by using non-linear regression analysis SPECFIT 3.0.36 to determine the stability constants and the distribution of various species.

2. ^{1}H and ^{13}C NMR spectra of compound 4, 6 and dipod 1



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7.319
7.258
7.227
7.210
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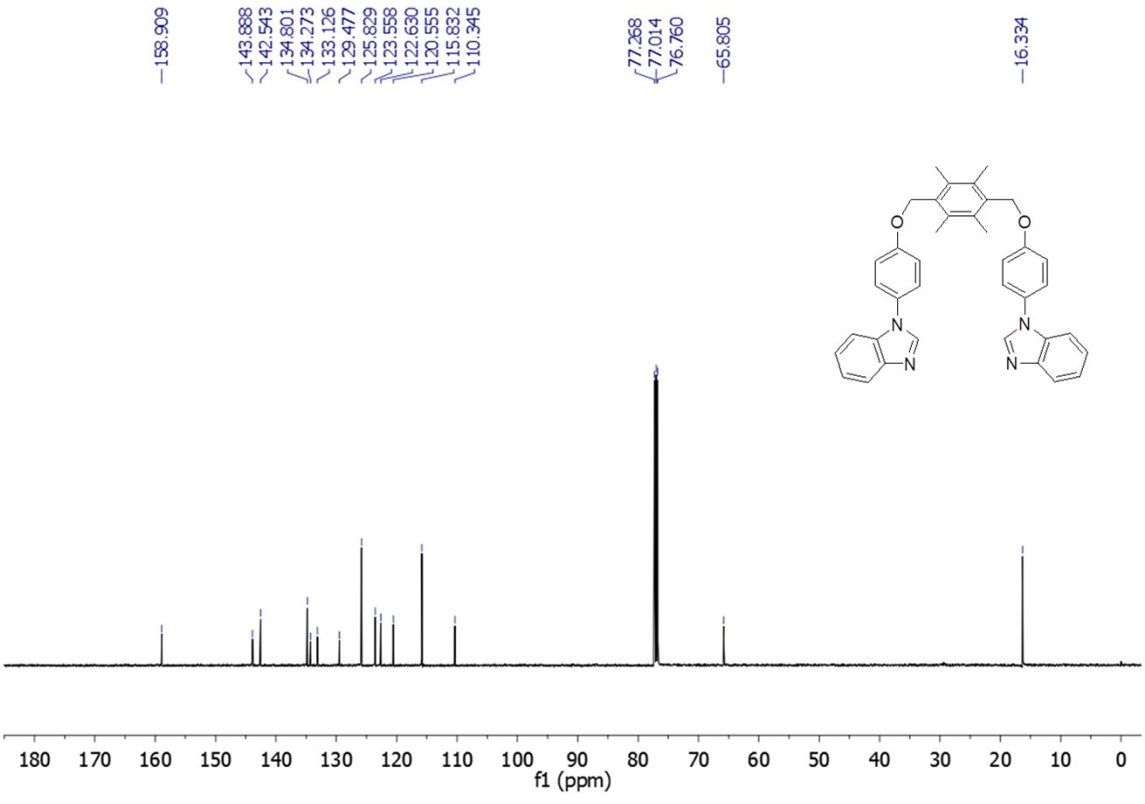
0.000
2.00
2.04
6.08
4.08
4.00
4.02
12.01
f1 (ppm)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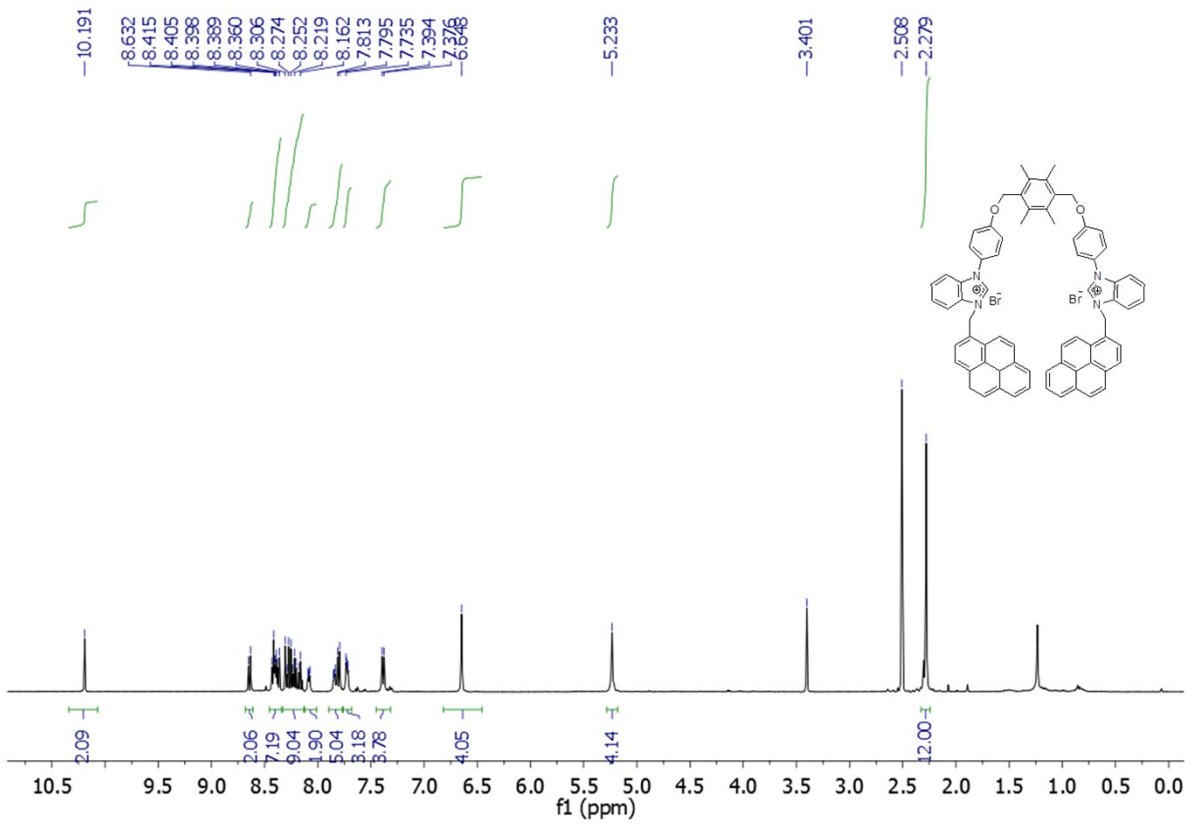
16.334
f1 (ppm)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8.162
7.813
7.795
7.735
7.394
7.376
6.648
5.233
3.401
2.508
2.279
Br⁻
Br⁻
2.09
2.06
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9.04
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4.05
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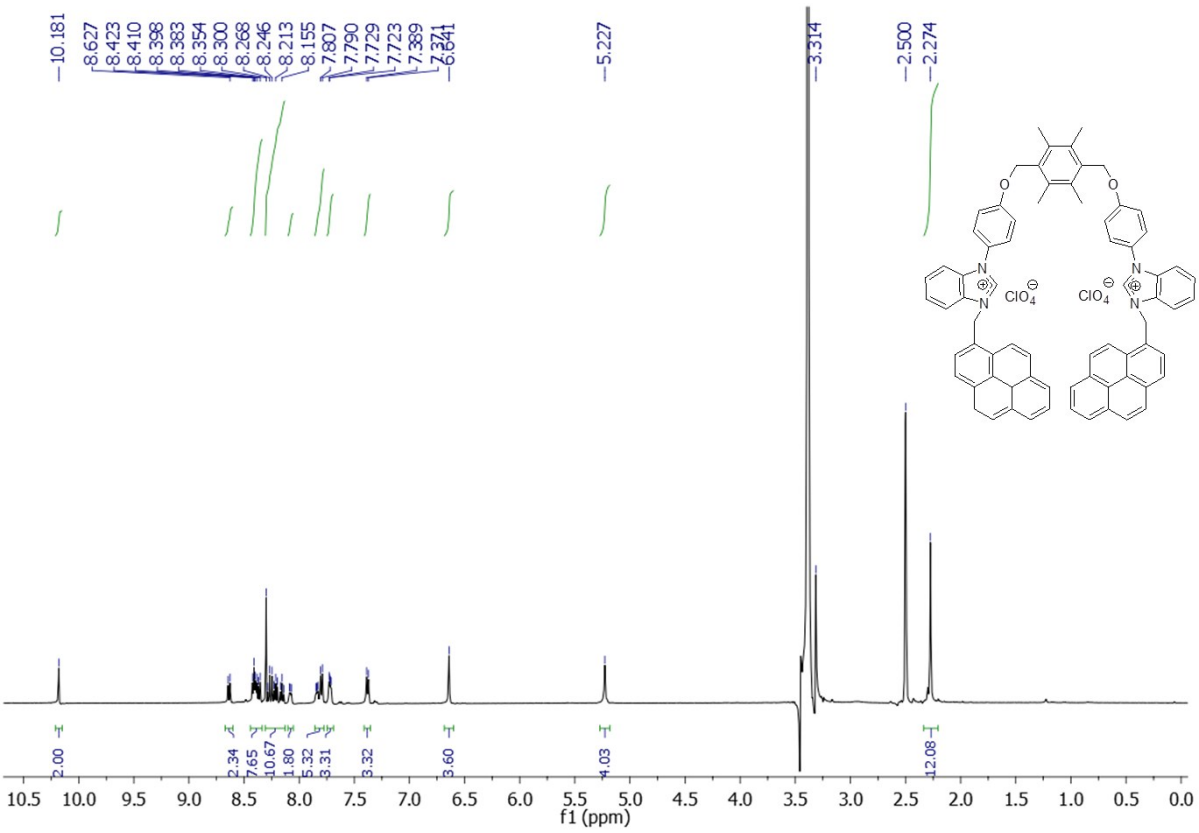
f1 (ppm)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7.729
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7.389
7.371
6.641
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2.274
ClO4⁻
ClO4⁻
2.00
2.34
7.65
10.67
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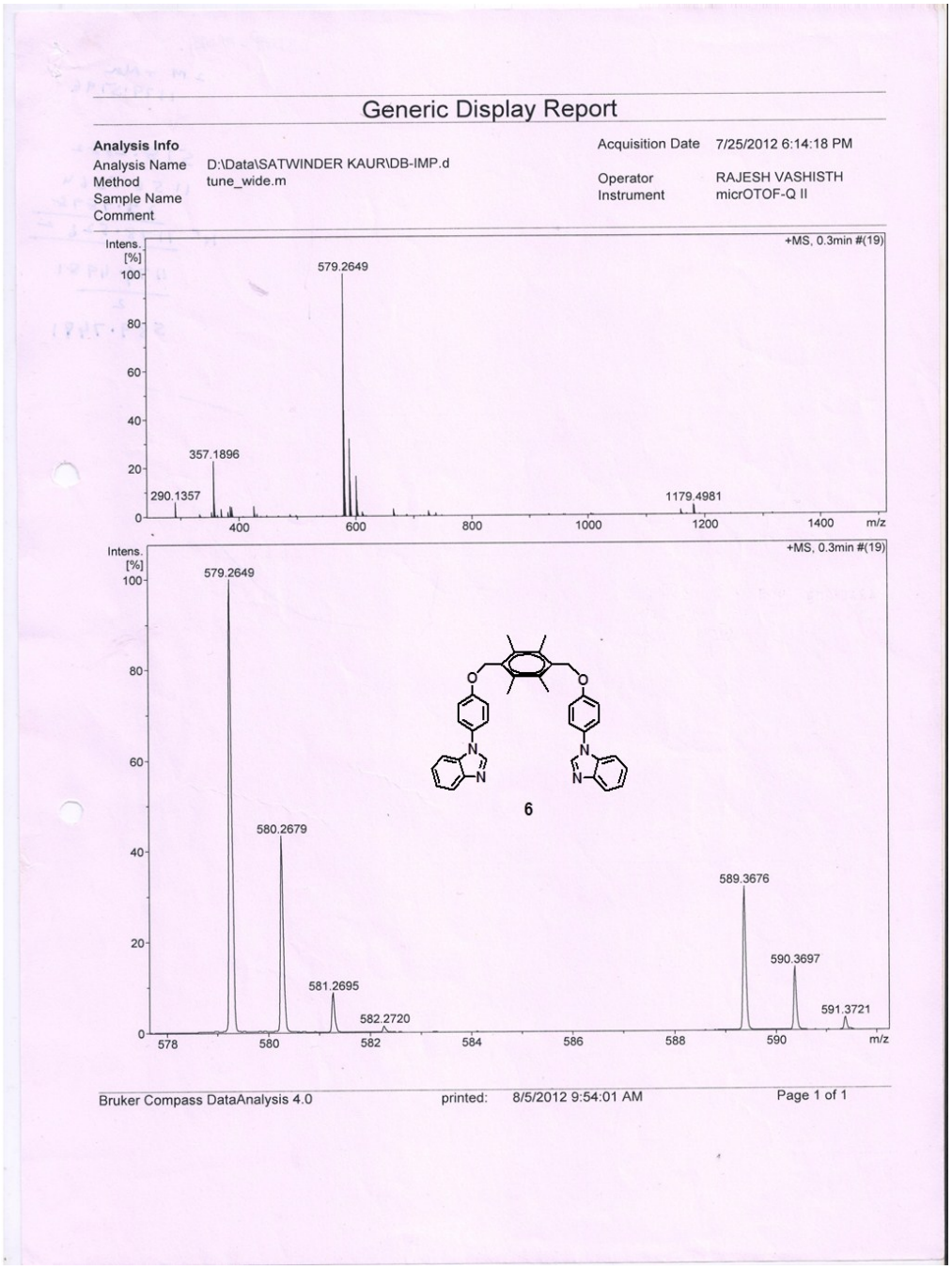
3.31
3.32
3.60
4.03
12.08
f1 (ppm)

3. HRMS spectra of compound 6 and dipod 1, 2



Guru Nanak Dev University-Amritsar

Analysis Info

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Sample Name	sh-35	Instrument	micrOTOF-Q II 10356
Comment			

Acquisition Parameter

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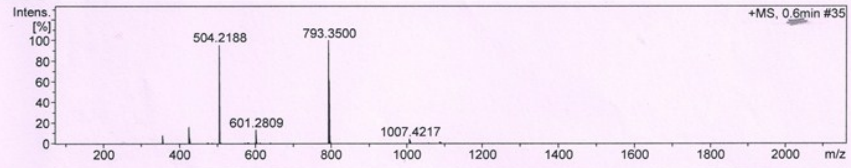
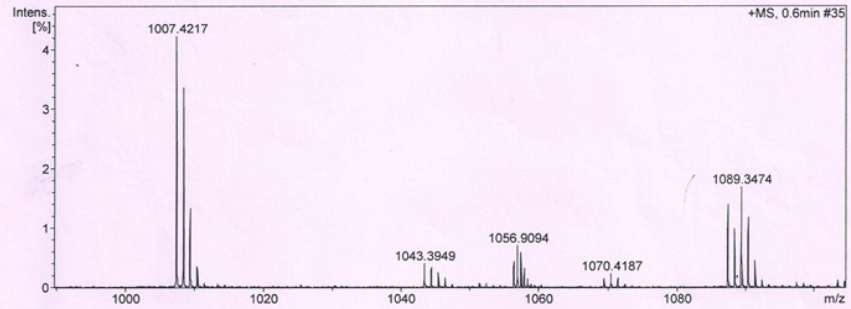
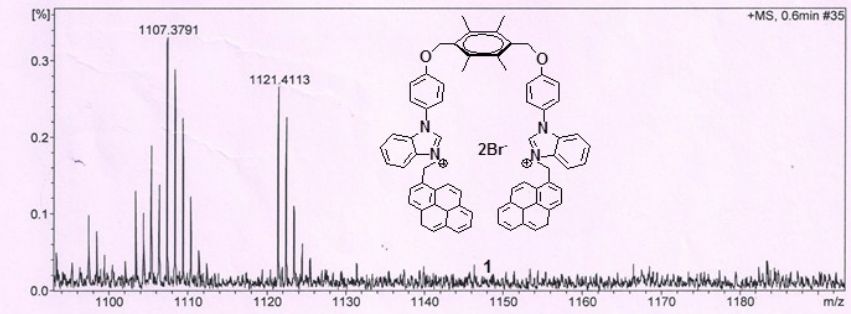
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste







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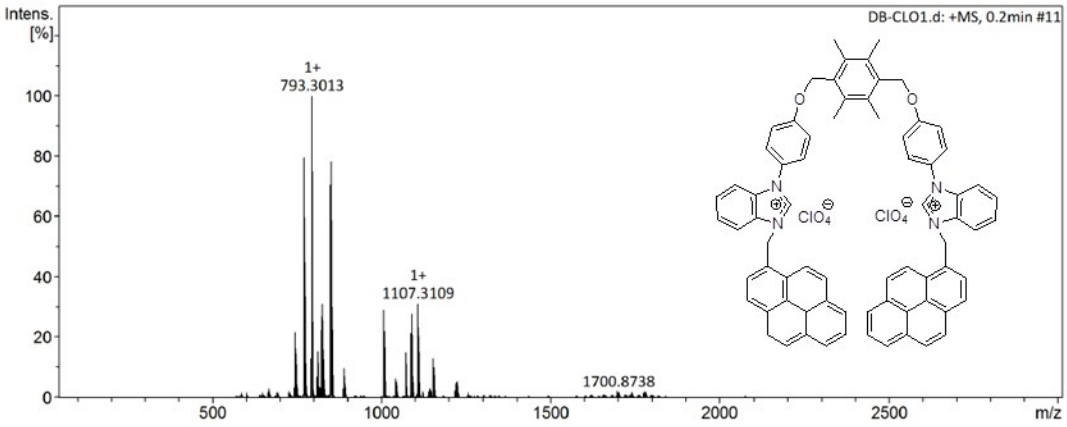

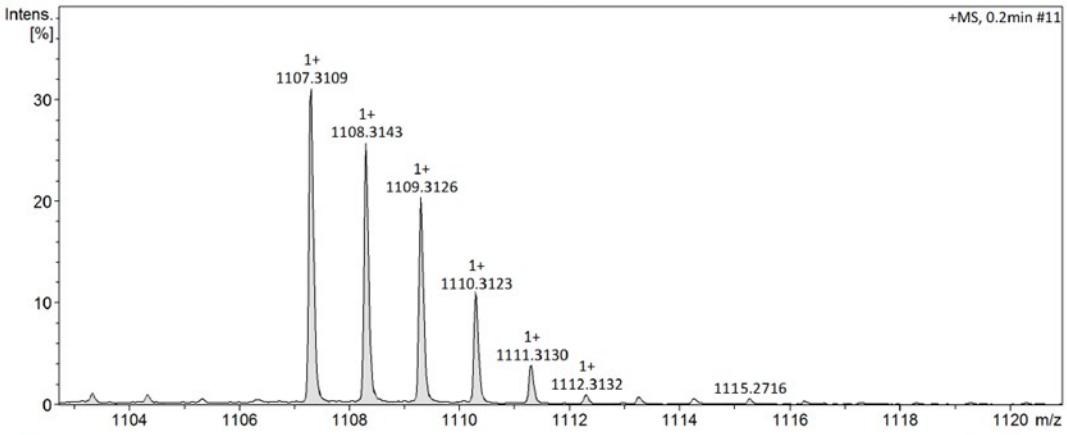

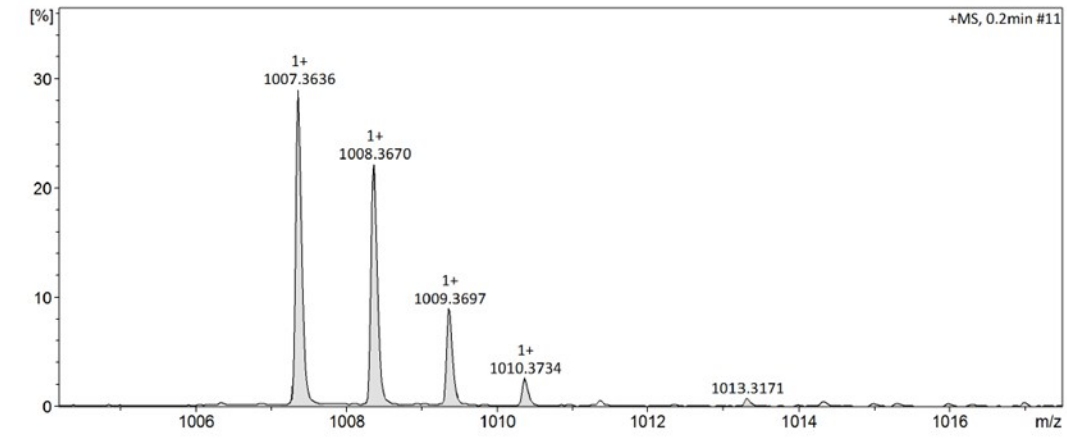

4. UV and Fluorescence Studies of dipod 1 with anions

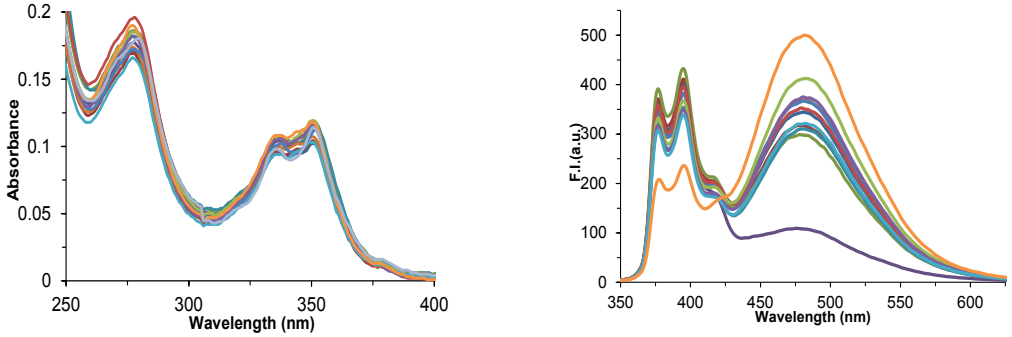

Figure SI-1: UV-Visible and emission spectra (λ_{ex} = 330 nm) of dipod **1** (5μM) with various anions (F^-, Cl^-, Br^-, I^-, CN^-, SCN^-, SO_4^{2-}, $H_2PO_4^{2-}$, NO_3^-, AcO^-, OH^-, ClO_4^-, 25 μM) in 95 % aqueous Hepes buffer (5 % DMSO), pH = 7.4

5. Interference studies of dipod 1

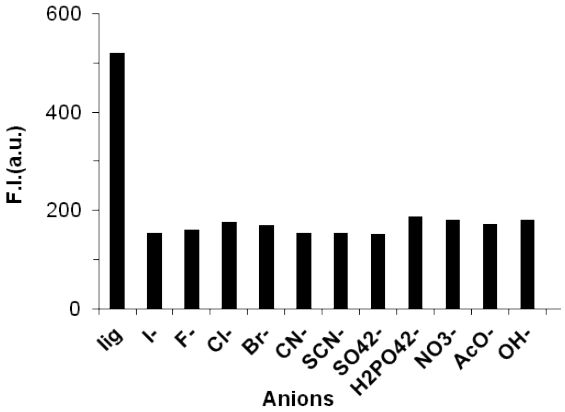

Figure SI-2: Variation of fluorescence intensity at 480 nm for complex between dipod **1** (5 μM) and iodide (5 μM) in the presence of different anions (50 μM) in pH 7.4 HEPES buffer - 5% DMSO (λ_{ex} = 330 nm)

6. ^{1}H NMR titration of dipod 1 with iodide

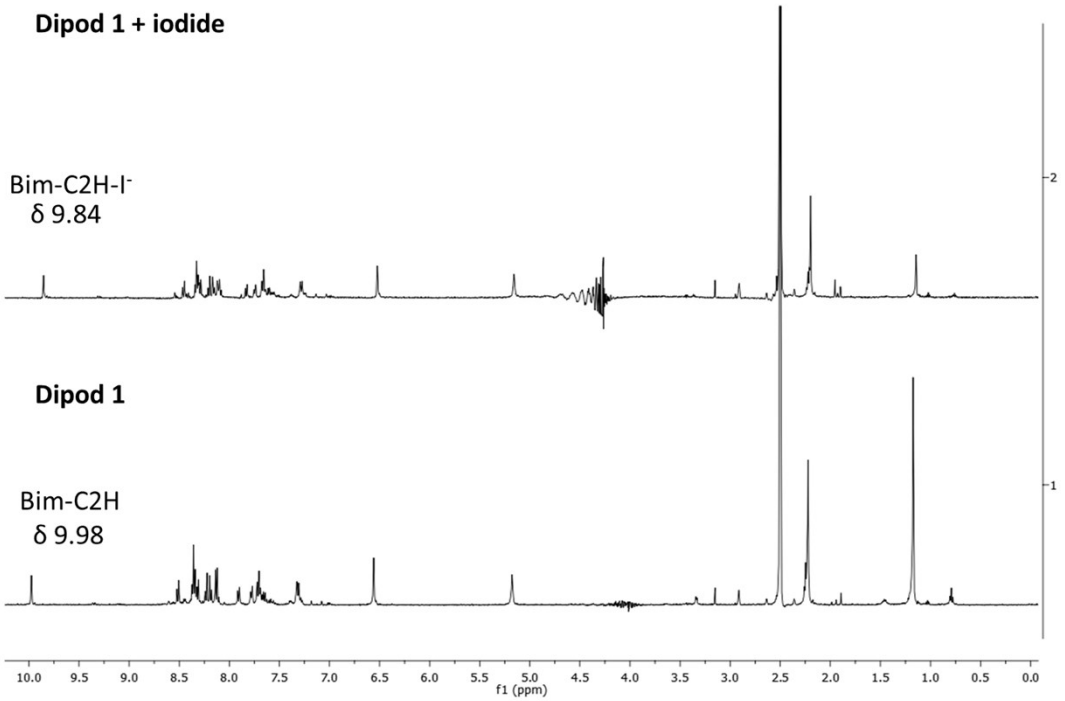

Figure SI-3: ^{1}H NMR titration of dipod **1** with iodide ions in dmso-d_6-H_2O mixture at 500 MHz

7. Analysis of urine sample

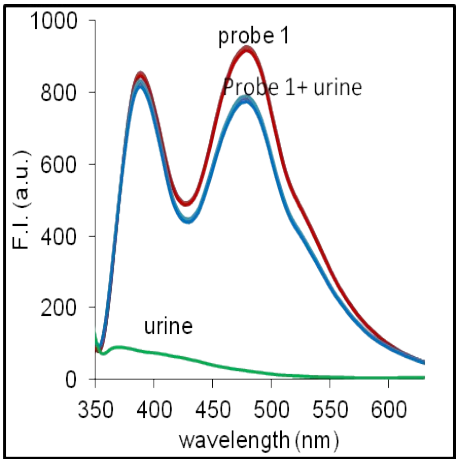

Figure SI-4: Fluorescence spectra of probe **1**, probe **1**+ urine and urine sample

8. Table SI-1: Application of dipod 1 in determination of iodide ions in tap water, in the presence of NaCl and in blood serum samples

S. No.	Conc. ClO_4^- (nM)	Conc. determined ± SD[a] (nM)	Relative error (%)
Tap water ***Maximum relative standard deviation ≤ 1.70 and PRSD = 1.46*** ***Maximum relative error ≤ 1.30 and PRE = 1.08***			
1	0.5	0.51 ± 0.007	1.04
2	5	5.21 ± 0.09	1.30
3	50	50.15 ± 0.63	0.9
4	500	501.5 ± 8.02	1.20
5	5000	5005 ± 66.4	1.01
In presence of NaCl ***Maximum relative standard deviation ≤ 1.82 and PRSD = 1.38*** ***Maximum relative error ≤ 1.41 and PRE = 1.02***			
1	0.5	0.52 ± 0.006	1.04
2	5	5.10 ± 0.12	1.41
3	50	50.12 ± 0.69	1.02
4	500	502.0 ± 5.7	0.80
5	5000	5001.0 ± 60.5	0.84

9. MTT assay for bioimaging of iodide ions in live C6 glioma cells

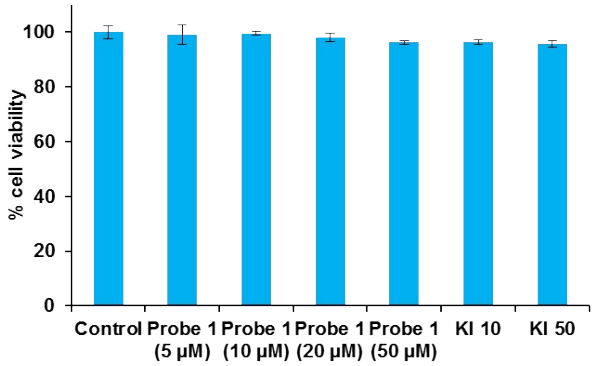

Figure SI-5: MTT assay of dipod **1** and KI