

A Highly Selective Economical Sensor for 4-Nitrophenol

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Supporting Information

Table S1. Concentration and volume of NaFI and nitroaromatics solution in the reaction vials

No.	NaFI molarity (μM)	Volume of NaFI needed from stock solution of 1mM (μL)	Nitroaromatics molarity (μM)	Volume of nitroaromatic needed from stock solution of 3 mM (μL)	Volume of DI water (μL) or MeCN (μL)
1	50	250	100	166.7	4583.3
2	50	250	90	150	4600
3	50	250	80	133.3	4616.7
4	50	250	70	116.7	4633.3
5	50	250	60	100	4650
6	50	250	50	83.3	4666.7
7	50	250	40	66.7	4683.3
8	50	250	30	50	4700
9	50	250	20	33.3	4716.7
10	50	250	10	16.7	4733.3
11	50	250	0	0	4750

Table S2: Kamlet- Taft Parameters which measures separately the acidity or proticity or Hydrogen bond donating ability (α), basicity or hydrogen bond accepting ability (β) and dipolarity/polarizability (π^*) properties of solvents [1].

Solvent	π^*	α	β
Water	1.09	1.17	0.18
MeCN	0.75	0.19	0.31
DMF	0.88	0.00	0.69
THF	0.58	0.00	0.55
Chloroform	0.58	0.00	0.44

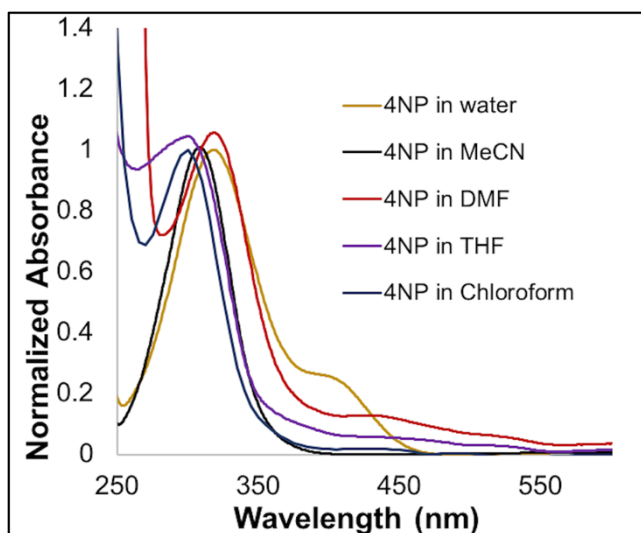


Figure S1. Normalized absorption spectra of 4NP in different solvents

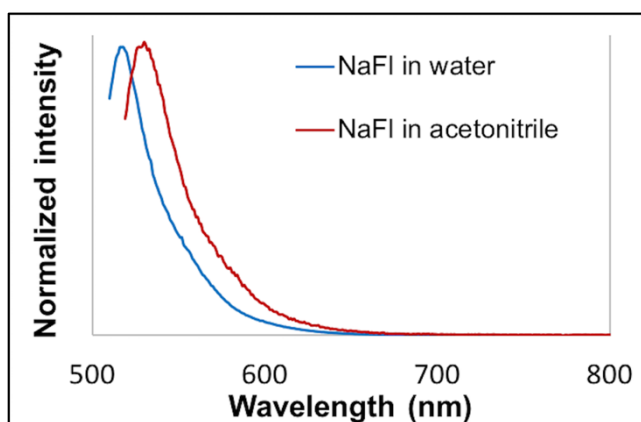


Figure S2. Normalized fluorescence emission spectra of NaFl in two different solvents. The fluorescence emission of NaFl was recorded in water and MeCN at an excitation wavelength of 490 nm and 510 nm, respectively.

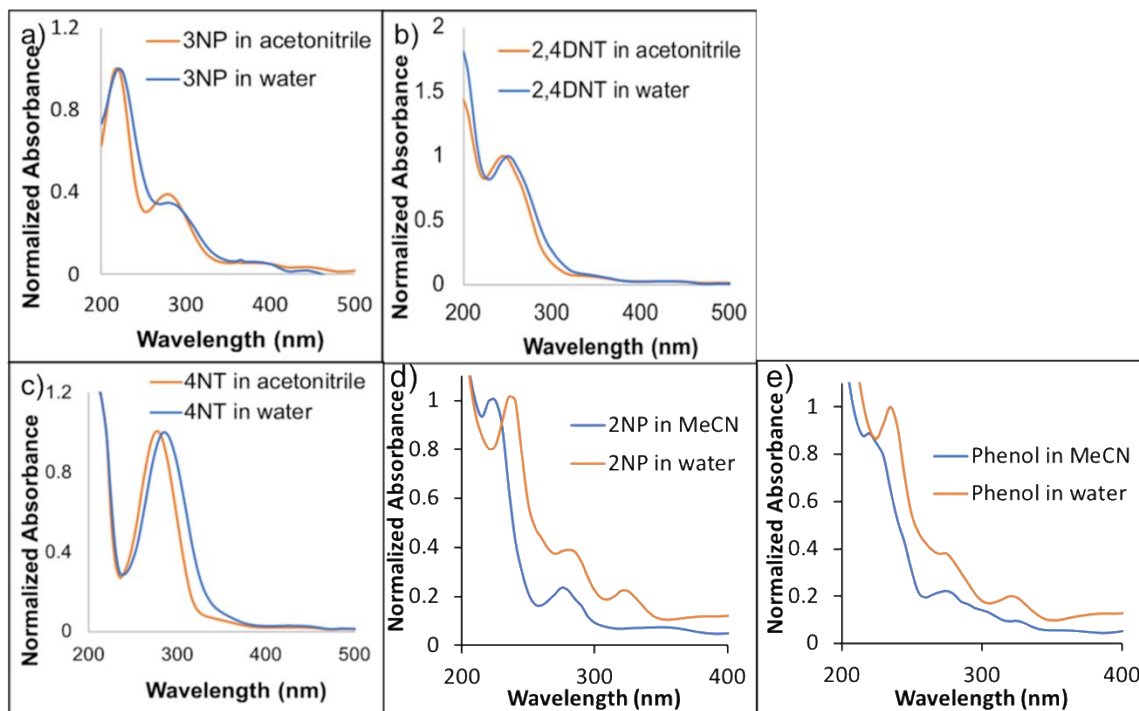


Figure S3. Normalized absorption spectra of a) 3NP, b) 2,4DNT, c) 4NT, d) 2NP, and e) phenol in acetonitrile and in water.

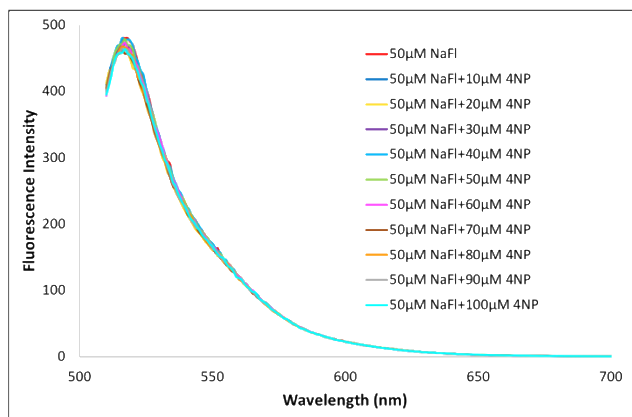


Figure S4. Fluorescence emission spectra of NaFl at the excitation wavelength of 490 nm in the presence of 4NP in water.

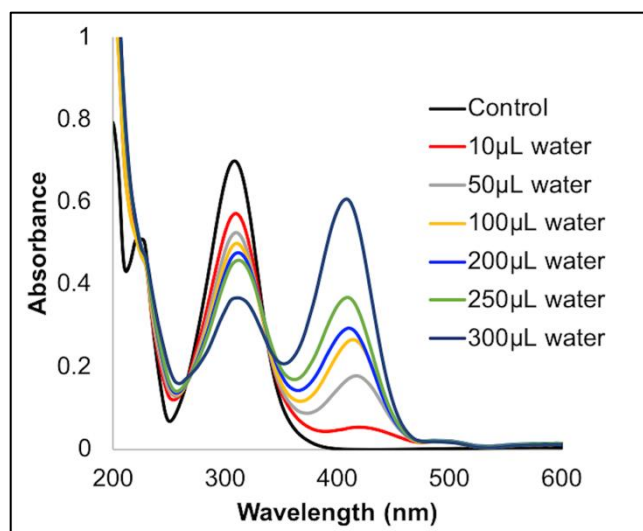


Figure S5. Absorption spectra of 4NP in MeCN and upon addition of different volume (μL) of water.

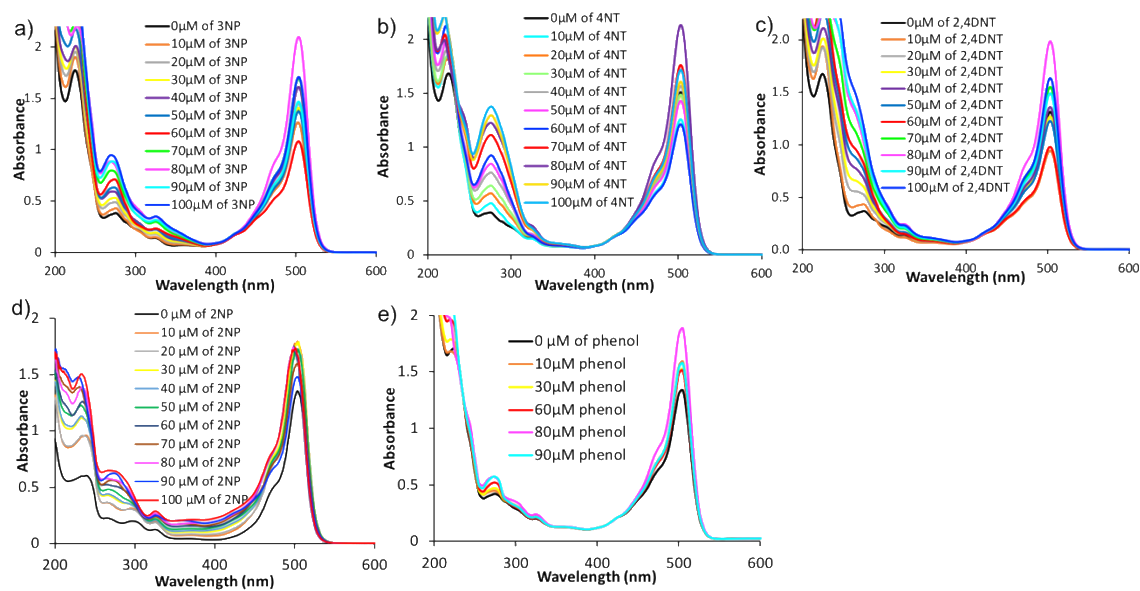


Figure S6. Absorption spectra of 50 μM of NaFl in the presence of different concentrations of a) 3NP, b) 4NT, c) 2,4DNT d) 2NP, and e) phenol in MeCN.

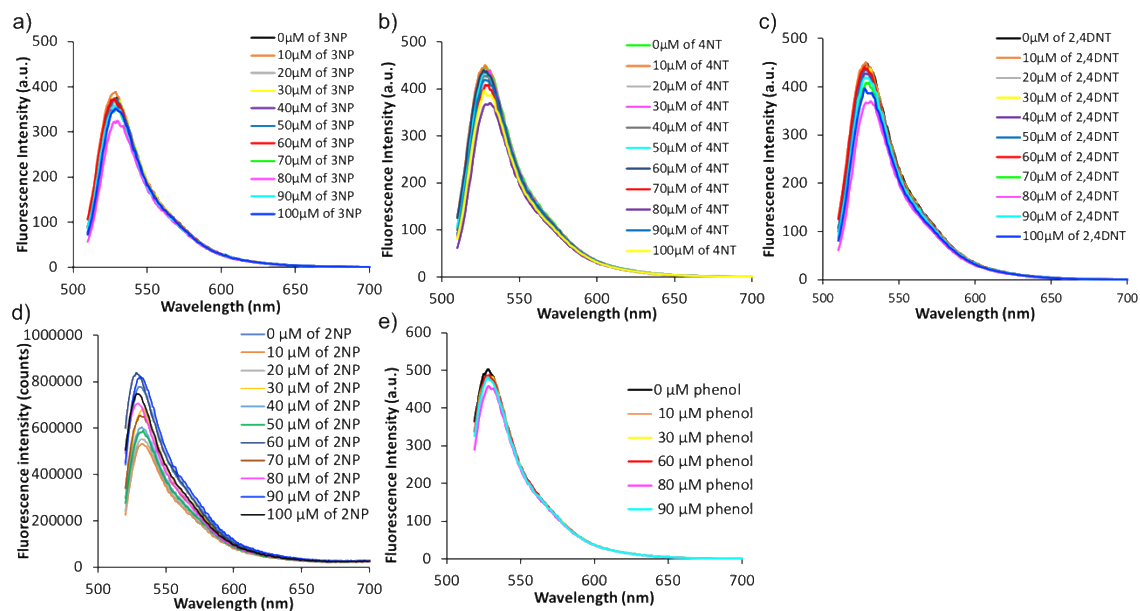


Figure S7. Fluorescence emission spectra of 50 μM of NaFI at the excitation wavelength of 510 nm in the presence of different concentrations of a) 3NP, b) 4NT, c) 2,4DNT, d) 2NP, and e) phenol in MeCN.

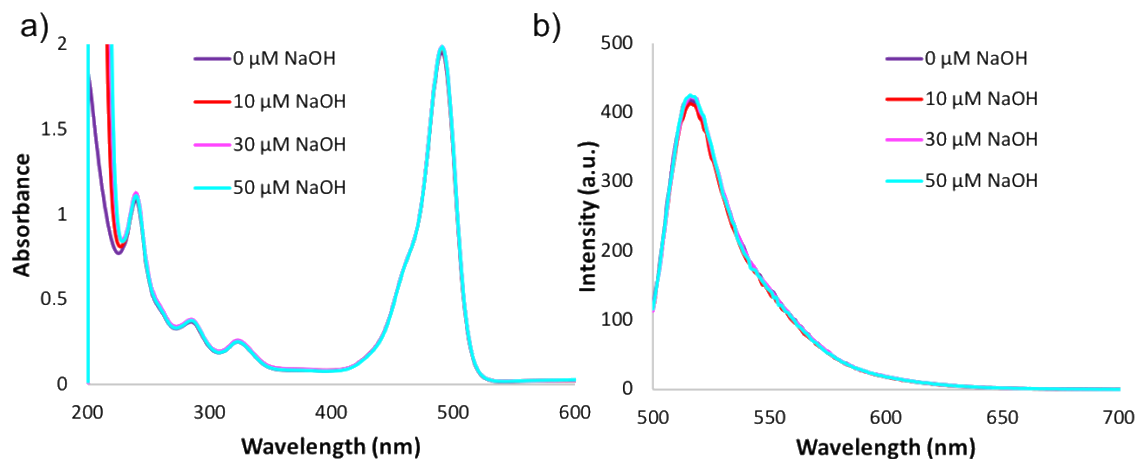


Figure S8. a) Absorption and b) fluorescence emission spectra (at excitation wavelength of 490 nm) of 30 μM of NaFI in alkaline media.

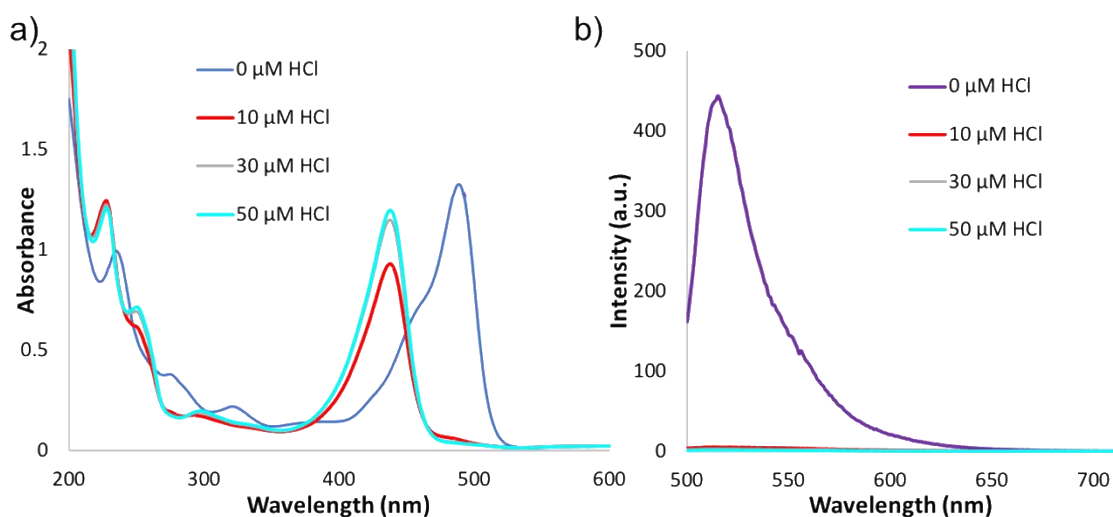


Figure S9. a) Absorption and b) fluorescence emission spectra (at an excitation wavelength of 490 nm) of 30 μM of NaFl in acidic media.

Table S3. 4NP toxic concentration reported by EPA [2].

	Lethal dose, 50% (LD50)
Oral	230 ppm (for rat)
Dermal	> 5000 mg/Kg (for rabbit) > 920 mg/Kg (for mammal)
Inhalation	> 4.7 ppm (for rat in 4 hours)

Animals and organisms	Toxicity
Freshwater algae	EC50= 2.3-7.71 ppm for 96 hours
Freshwater fish	LC50= 6.6 ppm for 96 hours
Water flea	EC50= 3.1-7.1 ppm for 48 hours

Table S4. Detection limit and quenching efficiency of fluorescent sensors to nitroaromatic compounds from previous works as compared to our work.

Sensors	Nitroaromatic compounds	Detection of Limit (mol/L)	Quenching efficiency (%)	References
Pyrimidine-based fluorophores	4NP	1.95×10^{-5}	< 10	[3]
Pyrimidine-based containing carbazole	4NP	1.65×10^{-4}	< 15	[4]
1,4-diazine-based dyes	4NP	3.26×10^{-6}	~ 0.3	[5]
Gold nanoparticle @sulfur-doped graphene quantum dots (Au NP@S-GQD)	4NP	3.5×10^{-9}	---	[6]
Bovine serum albumin functionalized fluorescent gold nanoclusters (BSA Au-NCs)	4NP	1.0×10^{-9}	~ 85	[7]
CdTe quantum dots	4NP	4.0×10^{-8}	---	[8]
Molecular imprinted polymers based on carbon dots (MIP C-dots)	4NP	6.0×10^{-8}	---	[9]
Sodium fluorescein in MeCN	4NP	2.07×10^{-6}	~ 98	This work

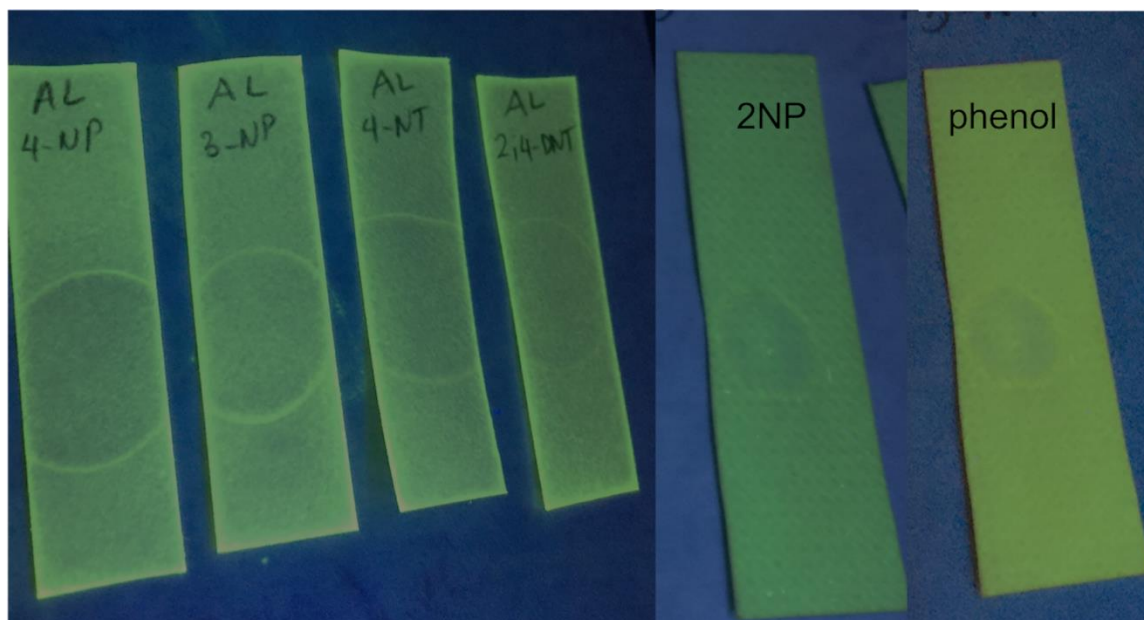


Figure S10. Filter paper based NaFI sensor for nitroaromatic detection.

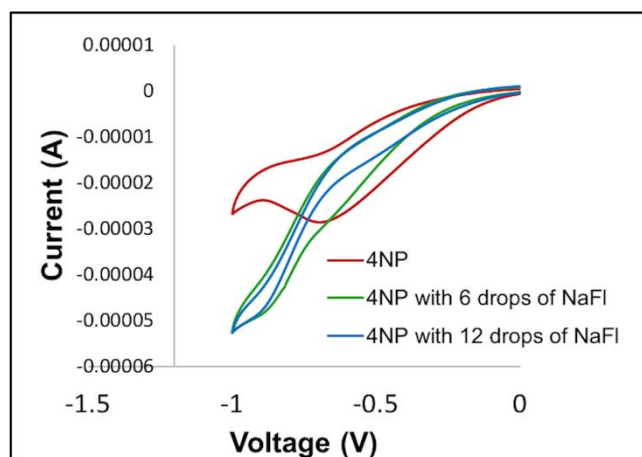


Figure S11. Cyclic voltammogram of 4NP in the presence of NaFI

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