Supporting Information

Simple Devising of N-doped Carbon Dots (N-CDs) as Low-Cost Probe for Selective Detection of Environment Toxin and Security Applications

Kumaresan Annamalai [a], Arun Annamalai [a], Ramya Ravichandran [a], Anandhavalli Jeevarathinam [a], Padmanaban Annamalai [b], Hector Valdes [b] Sundaravadivel Elumalai*

a. Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu – 603 203, India.

b. Facultad de Ingeniería, Universidad Catolica de la Santísima Concepcion, Concepcion, Chile.

*Corresponding author's E-mail: sundaravadivelchem@gmail.com

Stability and Surface Charge Studies of N-CDs.

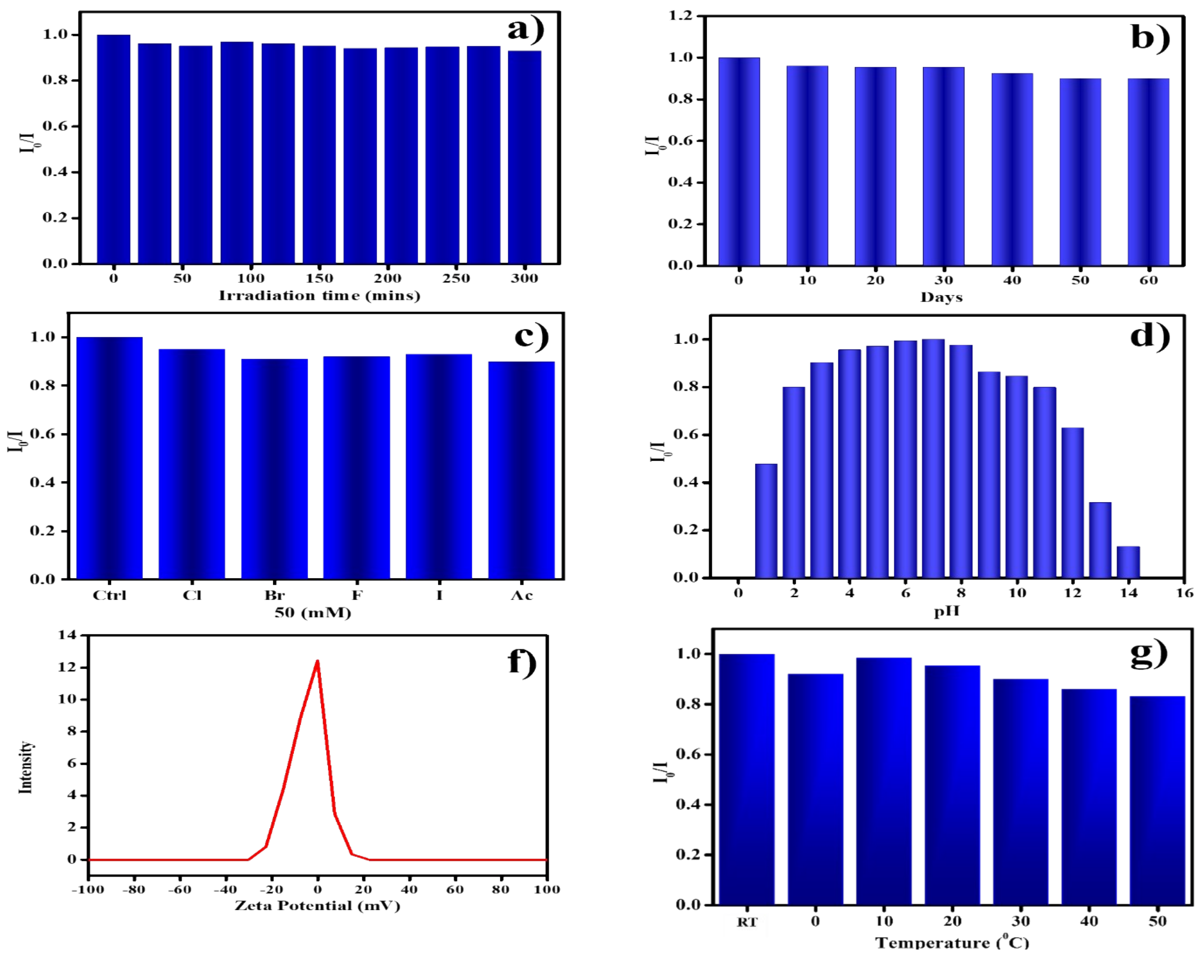

Figure S1. (a) Photostability of N-CDs, (b) PL intensity against 60 days of N-CDs storage time, (c) PL intensity against Photobleaching studies of different ions, (d) pH studies of N-CDs and (f) Zeta potential of N-CDs, (g) temperature dependent studies on N-CDs.

Table S1. Comparison of LOD with Reported PA Sensor Probes.

Detection Probe	Detection Method	Linear Range	Limit of Detection	Reference
CDs	Fluorescence	1-10 µM	0.24 µM	1
N-CDs	Fluorescence	0.3-3.3 µM	0.11 µM	2
N-CDs	Fluorescence	2-45 µM	0.45 µM	3
N-CDs	Fluorescence	1 - 26 µM	82.9 nM (0.08 µM)	Present work

Table S2. Comparison of LOD with Reported Fe^{3+} Sensor Probes.

Detection Probe	Detection Method	Linear Range	Limit of Detection	Reference
Citric acid-Glycine based CDs	Fluorescence	0-3.5 µM	0.21 µM	4
N-doped Cellulose based CDs	Fluorescence	0-100 µM	1.14 µM	5
Functionalized Citric acid-based CDs	Fluorescence	0-300 µM	13.68 µM	6
N-CDs	Fluorescence	1-40 µM	30 nM (0.03 µM)	Present work

Table. S3. Comparison of LOD with Reported Hg^{2+} Sensor Probes

Detection Probe	Detection Method	Linear Range	Limit of Detection	Reference
N, S, P co-doped Cucumber based CDs	Fluorescence	1-70 µM	0.18 µM	7
Hetero atom doped CDs	Fluorescence	0-12 µM	226 nM	8
CDs	Fluorescence	0-50 µM	0.41 µM	9
N-CDs	Fluorescence	6.5 - 50 µM	160 nM (0.016 µM)	Present work

Table S4: Detection of Fe^{3+} & Hg^{2+} and PA in Drinking Water (n=3).

Sample	Spiked (µM)	Detected (µM)	Recovery (%)	RSD (%)
Fe^{3+}	10	8.96	89.6	2.45
	20	19.12	95.6	2.33
	30	29.99	99.9	4.12
Hg^{2+}	10	9.41	94.0	1.76
	20	19.79	98.9	2.56
	30	28.1	93.6	2.56
PA	10	8.43	84.3	2.34
	20	18.87	93.4	2.65
	30	30.96	103.2	3.92

Table S5. Comparison of N-CDs as Probe for Detection of Nitro-explosives and Metal ions.

Nitro-explosives and Metal ions	K_{sv} Value	Linear Range	Limit of Detection	Lifetime (ns)	Mechanism
PA	3.3×10^4 M^{-1}	1 - 26 µM	82.9 nM	10.2	FRET
Fe^{3+}	1.8×10^5 M^{-1}	1-40 µM	30 nM	10.8	IFE
Hg^{2+}	3.6×10^4 M^{-1}	6.5 - 50 µM	160 nM	10.4	PET

Table S6. Comparison of High Quantum Dots with Unique Properties

Starting Material	Synthesis Method	Quantum Yield (%)	Applications	Reference
Citric acid-Glycine based CDs	Hydrothermal	29.8	Fe^{3+} and Fingerprint detection	4
N-doped Cellulose based CDs	Hydrothermal	30.3	Fe^{3+} detection and Bioimaging	5
Ammonium citrate based CDs	Hydrothermal	22.79	Mercury (II) and Glutathione Detection	9
N-CDs	Microwave	33	Fe^{3+}, Hg^{2+} and PA detection, Anti-counterfeiting studies	Present work

REFERENCES

1. Khan, Z. M. S. H. *et al.* A facile one step hydrothermal synthesis of carbon quantum dots for label -free fluorescence sensing approach to detect picric acid in aqueous solution. *J Photochem Photobiol A Chem* **388**, (2020).
2. Kalanidhi, K. & Nagaraaj, P. Facile and Green synthesis of fluorescent N-doped carbon dots from betel leaves for sensitive detection of Picric acid and Iron ion. *J Photochem Photobiol A Chem* **418**, (2021).
3. Abbasi, A. & Shakir, M. Simple One-step Solid-state Synthesis of Highly Crystalline N Doped Carbon Dots As Selective Turn Off-sensor for Picric Acid and Metanil Yellow. *J Fluoresc* **32**, 1239–1246 (2022).
4. Feng, R. Q., Yuan, Z. Y. & Ren, T. Z. A facile hydrothermal method for preparation of fluorescent carbon dots on application of Fe3+ and fingerprint detection. *Methods Appl Fluoresc* **7**, (2019).
5. Liu, Z. *et al.* Oxidized nanocellulose facilitates preparing photoluminescent nitrogen-doped fluorescent carbon dots for Fe3+ ions detection and bioimaging. *Chemical Engineering Journal* **384**, (2020).

6. Xie, Z., Sun, X., Jiao, J. & Xin, X. Ionic liquid-functionalized carbon quantum dots as fluorescent probes for sensitive and selective detection of iron ion and ascorbic acid. *Colloids Surf A Physicochem Eng Asp* **529**, 38–44 (2017).

7. Wang, C., Sun, D., Zhuo, K., Zhang, H. & Wang, J. Simple and green synthesis of nitrogen-, sulfur-, and phosphorus-co-doped carbon dots with tunable luminescence properties and sensing application. *RSC Adv* **4**, 54060–54065 (2014).

8. Shangguan, J. *et al.* Highly Fe3+-Selective Fluorescent Nanoprobe Based on Ultrabright N/P Codoped Carbon Dots and Its Application in Biological Samples. *Anal Chem* **89**, 7477–7484 (2017).

9. Cai, L., Fu, Z. & Cui, F. Synthesis of Carbon Dots and their Application as Turn Off–On Fluorescent Sensor for Mercury (II) and Glutathione. *J Fluoresc* **30**, 11–20 (2020).