Supporting information

Nanoarchitectonics of Congo Red Dye to Biocompatible Fluorescent Carbon Dots for Highly Sensitive Fe^{3+} and Ferritin Detection

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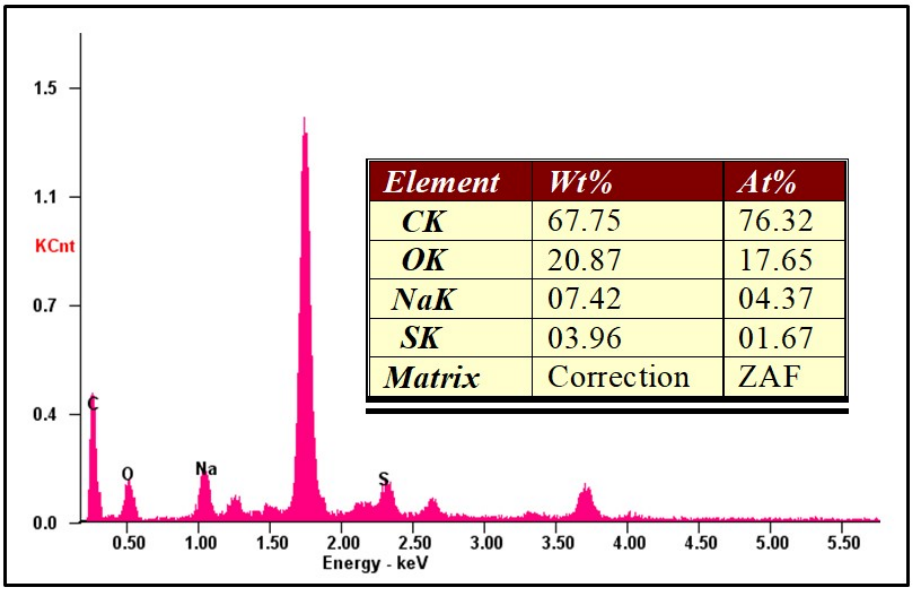

Element	Wt%	At%
CK	67.75	76.32
OK	20.87	17.65
NaK	07.42	04.37
SK	03.96	01.67
Matrix	Correction	ZAF

Figure S1: EDAX spectrum of CDs particles.

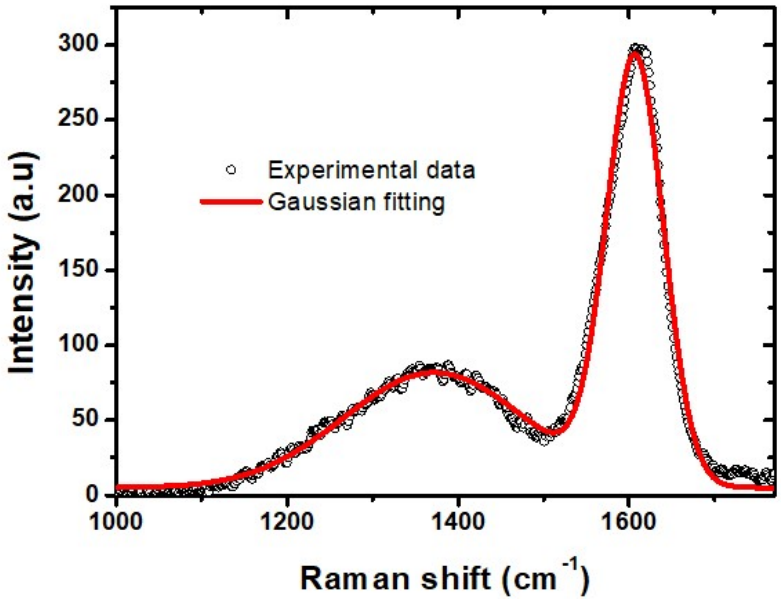

Figure S2: Raman spectrum of as-synthesized CDs.

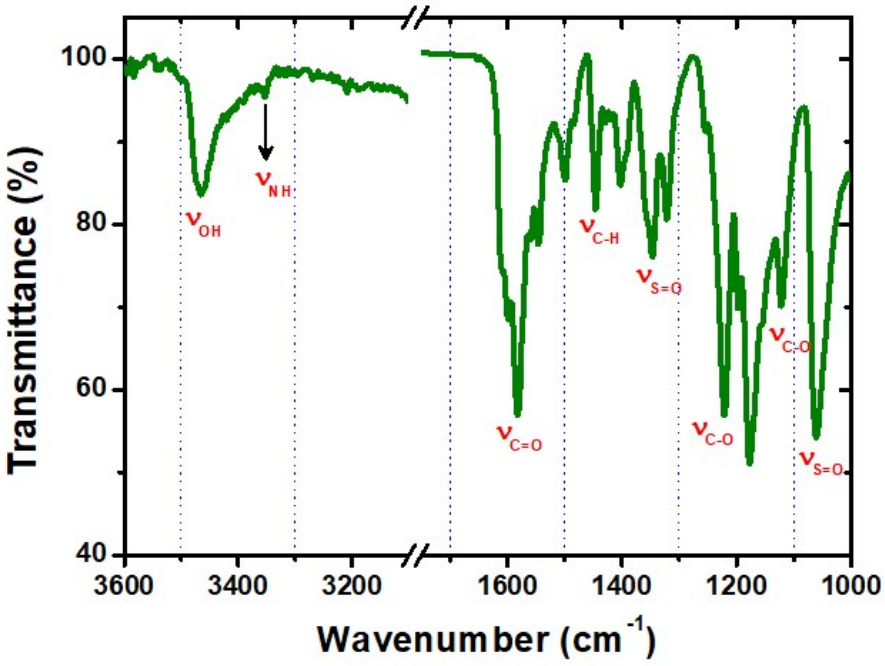

Figure S3: FTIR spectrum of as-synthesized CDs particles.

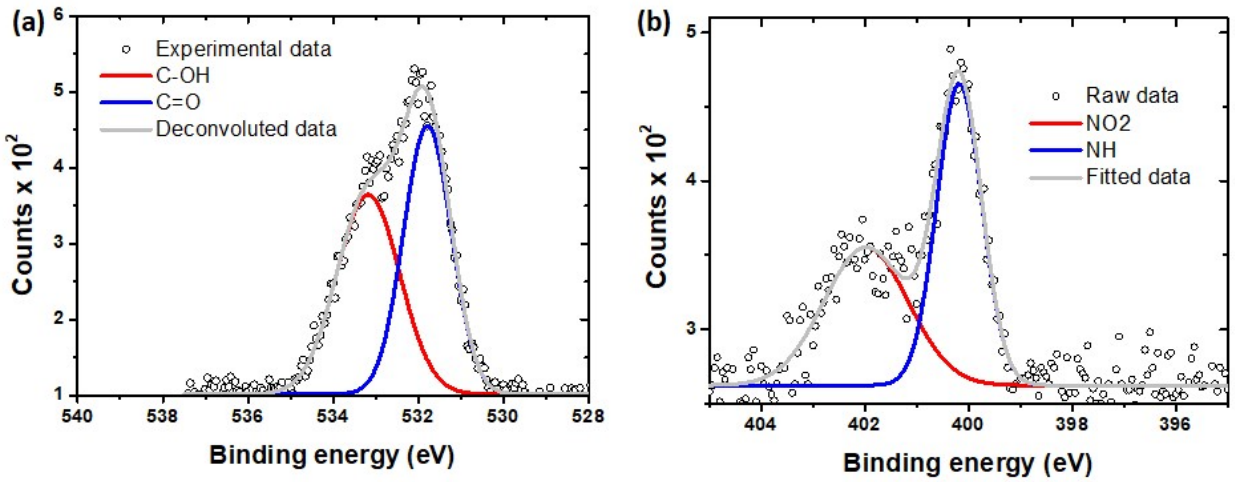

Figure S4: (a) O1s and (b) N1s spectra of CDs.

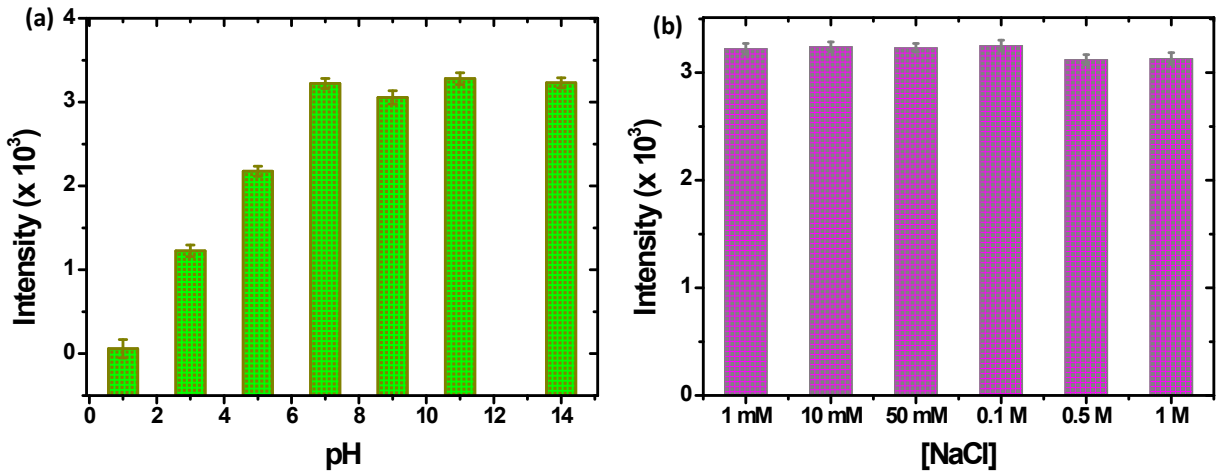

Figure S5: The fluorescence intensity responses of CDs (a) at different pH and (b) as a function of concentration of NaCl.

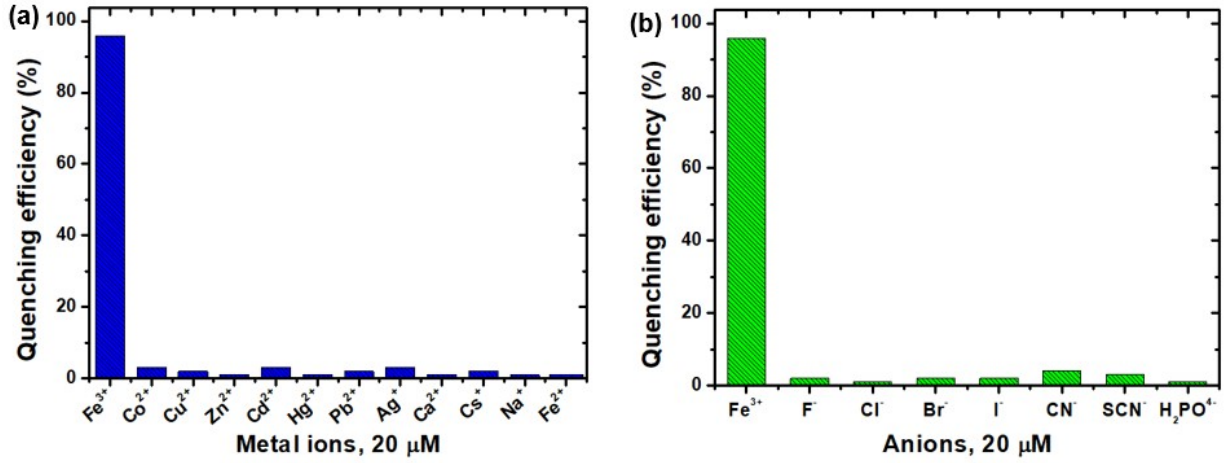

Figure S6: Selectivity of the fluorescence quenching ability of the CDs towards Fe^{3+} over other (a) cations; (b) anions

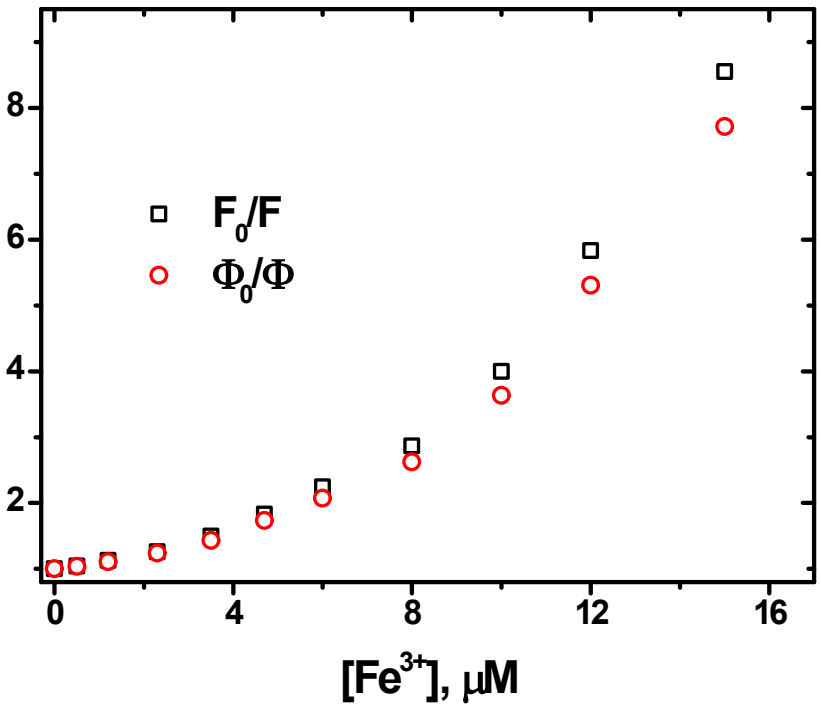

Figure S7: Stern-Volmer plot for the fluorescence quenching of CDs with respect to Fe^{3+} ions.

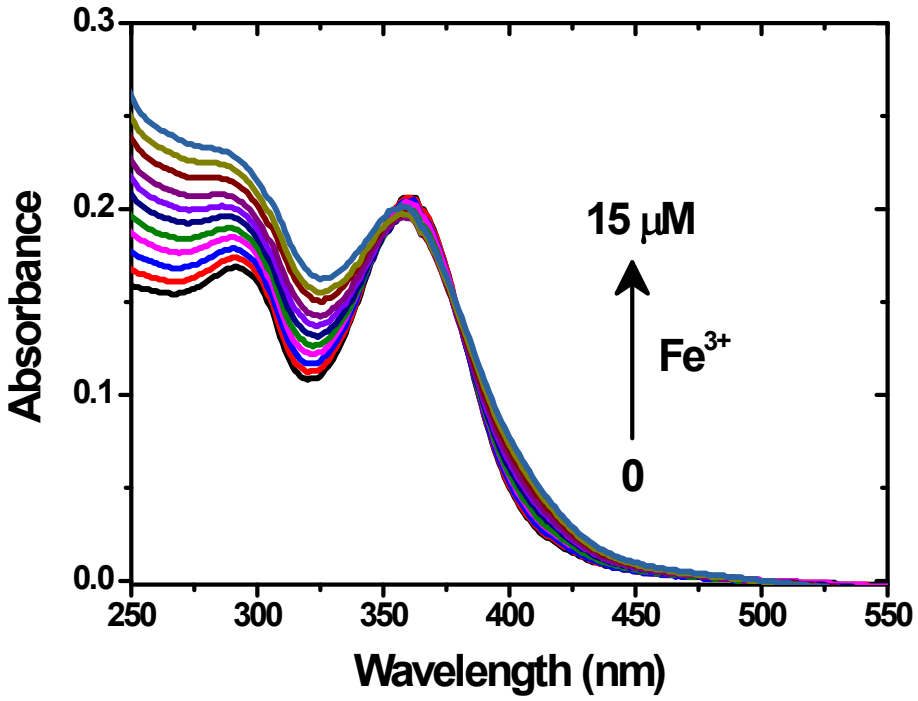

Figure S8: Absorption spectra of CDs with increasing concentration of Fe^{3+} (0 to 15 μM) in water

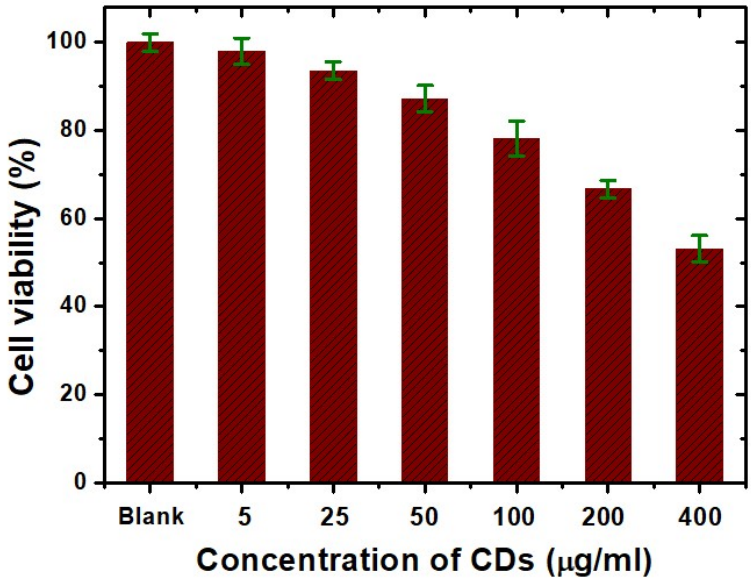

Figure S9: Cell viability of breast cancer cells (MDA-MB-231) incubated with different concentrations (5, 25, 50, 100, 200 and 400 μg/mL) of CDs for 24 h. The percentage of cell viability was calculated with respect to 100% control.

Table S1: Comparison of previously reported CDs probes for Fe^{3+} detection with their respective LOD, with present work.

S.No.	Sources of CDs	LOD	Ref.
1	Yellow banana peel	211 nM	1
2	Straw	200 nM	2
3	Soybean oil	60 nM	3
4	Colistin	56 nM	4
5	Tuberlose	200 nM	5
6	Urea and citric acid	50 nM	6
7	Salicylic acid	52 nM	7
8	Dried astragalus	92 nM	8
9	Betel leaves	50 nM	9
10	N-methyl 2-pyrrolidone	66 nM	10
11	Congo red	12 nM	**This work**

Table S2: Determination of Fe^{3+} concentrations in spiked-water samples.

Sample	Added (μM)	Found (μM)	Recovery (%)	RSD (%, n=3)
Pond water	0.5	0.51	102	1.14
	1	1.00	100	0.35
	3	2.94	98	1.41
	5	5.00	100	0.14
Lake water	0.5	0.51	102	1.07
	1	1.00	101	0.70
	3	2.90	97	0.45
	5	5.01	100	0.21
Tap water	0.5	0.51	102	1.00
	1	0.99	99	1.77
	3	2.95	98	0.75
	5	4.97	99	0.78

References

(1) Vikneswaran, R.; Ramesh, S.; Yahya, R. Green Synthesized Carbon Nanodots as a Fluorescent Probe for Selective and Sensitive Detection of Iron(III) Ions. Mater. Lett.2014, 136, 179–182.

(2) Liu, R.; Gao, M.; Zhang, J.; Li, Z.; Chen, J.; Liu, P.; Wu, D. An Ionic Liquid Promoted Microwave-Hydrothermal Route towards Highly Photoluminescent Carbon Dots for Sensitive and Selective Detection of Iron(III). RSC Adv.2015, 5, 31, 24205–24209.

(3) Chen, T. H.; Tseng, W. L. Self-Assembly of Monodisperse Carbon Dots into High-Brightness Nanoaggregates for Cellular Uptake Imaging and Iron(III) Sensing. Anal. Chem.2017, 89, 21, 11348–11356.

(4) Chandra, S.; Mahto, T. K.; Chowdhuri, A. R.; Das, B.; Sahu, S. kumar. One Step Synthesis of Functionalized Carbon Dots for the Ultrasensitive Detection of Escherichia Coli and Iron (III). Sensors Actuators, B Chem.2017, 245, 835–844.

(5) Rooj, B.; Dutta, A.; Islam, S.; Mandal, U. Green Synthesized Carbon Quantum Dots from Polianthes Tuberose L. Petals for Copper (II) and Iron (II) Detection. J. Fluoresc.2018, 28, 5, 1261–1267.

(6) Omer, K. M.; Tofiq, D. I.; Hassan, A. Q. Solvothermal Synthesis of Phosphorus and Nitrogen Doped Carbon Quantum Dots as a Fluorescent Probe for Iron(III). Microchim. Acta2018, 185, 10, 4–11.

(7) Li, L.; Shi, L.; Jia, J.; Jiao, Y.; Gao, Y.; Liu, Y.; Dong, C.; Shuang, S. “On-off-on” Detection of Fe3+ and F−, Biological Imaging, and Its Logic Gate Operation Based on Excitation-Independent Blue-Fluorescent Carbon Dots. Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.2020, 227, 3, 117716.

(8) Li, L.; Shi, L.; Jia, J.; Chang, D.; Dong, C.; Shuang, S. Fe3+detection, Bioimaging, and Patterning Based on Bright Blue-Fluorescent N-Doped Carbon Dots. Analyst2020, 145, 16, 5450–5457.

(9) Raja, D.; Sundaramurthy, D. Facile Synthesis of Fluorescent Carbon Quantum Dots from Betel Leafs (Piper Betle) for Fe3+sensing. Mater. Today Proc.2018, 34, 488–492.

(10) Zhang, Z.; Chen, X.; Wang, J. Bright Blue Emissions N-Doped Carbon Dots from a Single Precursor and Their Application in the Trace Detection of Fe3+ and F−. InorganicaChim. Acta2021, 515, 120087.