Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2021

Protection of lead-induced cytotoxicity using paramagnetic Nickel-Insulin quantum clusters.

Deepinder Sharda[1], Komal Attri[1,2], Pawandeep Kaur[1], Diptiman Choudhury[1,2,*]

[1]School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, 147004, Punjab, India.

[2]Thapar Institute of Engineering and Technology-Virginia Tech (USA) Center for Excellence and Material Sciences, Thapar Institute of Engineering and Technology, Patiala, Punjab- 147004, India.

Corresponding email: diptiman@thapar.edu, Phone: +91-8196949843.

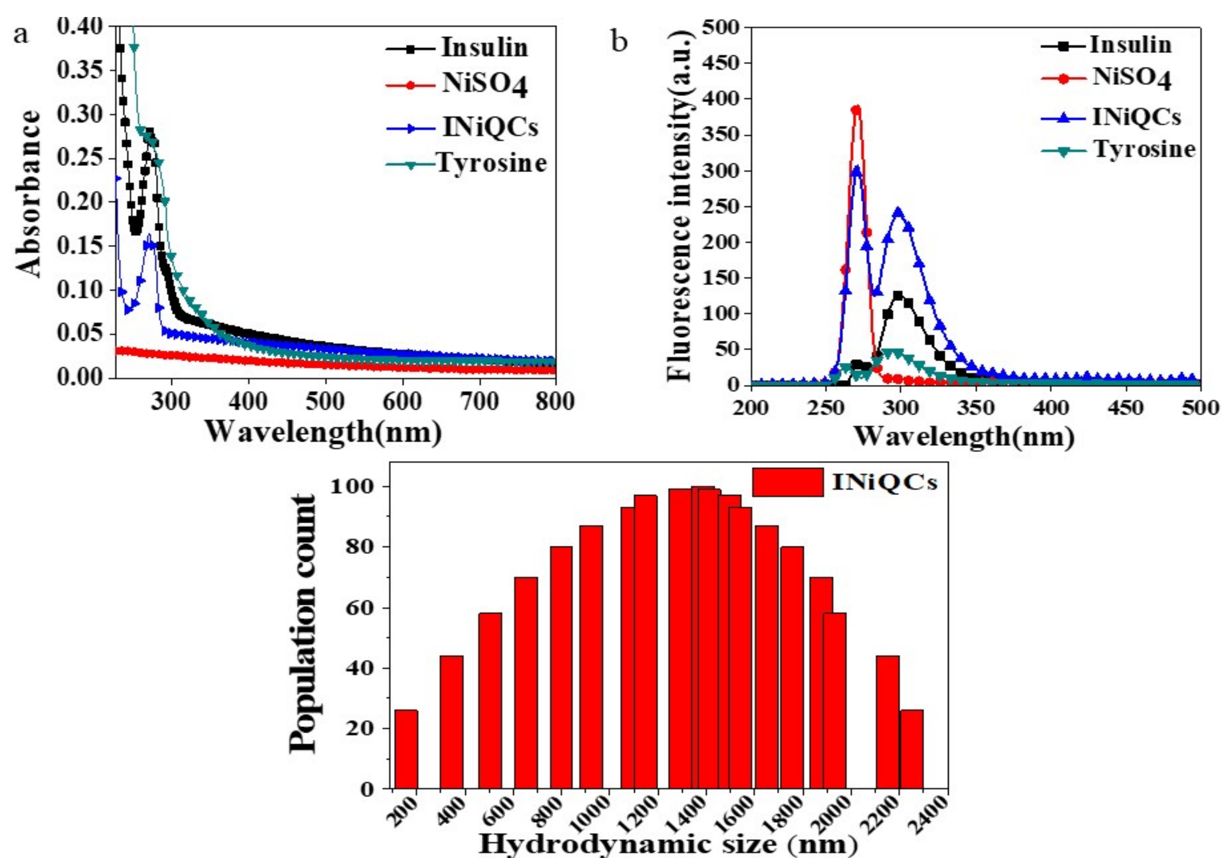

Fig. S1 Spectroscopic characterization of INiQCs (a) It shows a comparison of absorbance value between Insulin, INiQCs, $NiSO_4$, and tyrosine (standard). (b) It shows a comparison of the fluorescence intensity value of Insulin, INiQCs, $NiSO_4$, and tyrosine (standard). (c) The hydrodynamic size of

INiQCs was found to be 1400 ± 150 nm.

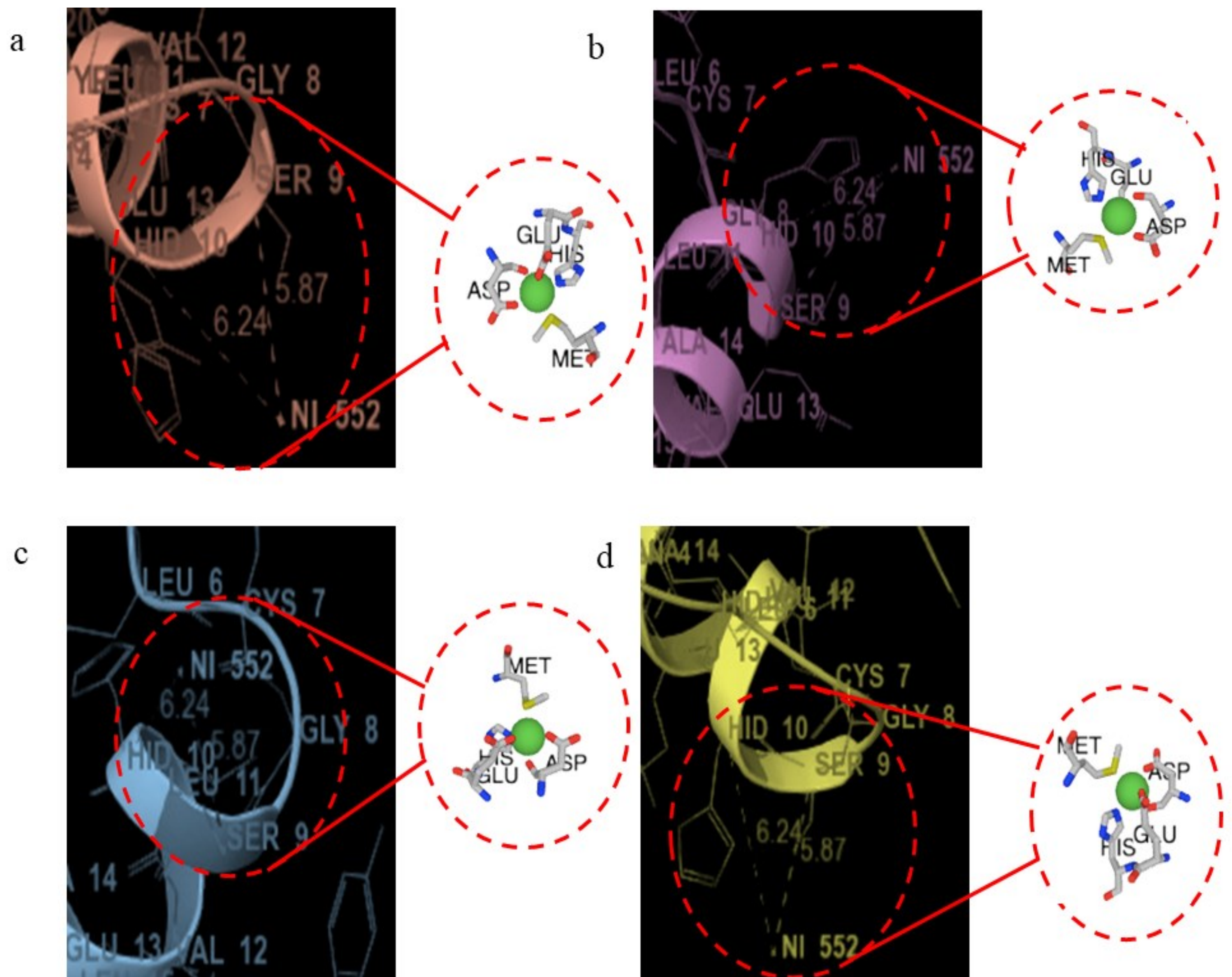

Fig. S2 MIB docking for the **interaction of nickel with insulin protein.** (a, b, c, and d) Metal ion binding residues: Depicts the binding site for Ni with the amino acid residues within 3.55 Ǻ diameter that can participate in binding on chain B of insulin in 4 different orientations. It shows the distance between different functional groups and Ni^{2+} ions.

Table ST1. It shows the binding score for different amino acids present in chain B of insulin with Ni^{2+} ion. Here the binding score is maximum for SER and HIS amino acids.

Residue Number	Amino Acid	Score
1	PHE	-0.899
2	VAL	-0.899
3	ASN	0.617
4	GLN	1.557
5	HIS	1.557
6	LEU	0.821
7	CYS	1.471
8	GLY	0.912
9	SER	2.103
10	HIS	2.103
11	LEU	0.630
12	VAL	-0.899
13	GLU	-0.899
14	ALA	0.726
15	LEU	-0.176
16	TYR	-0.899
17	LEU	-0.899
18	VAL	-0.899
19	CYS	0.416
20	GLY	0.625
21	GLU	0.625
22	ARG	-0.899
23	GLY	-0.264
24	PHE	0.096
25	PHE	-0.899
26	TYR	-0.899
27	THR	-0.899
28	PRO	-0.899
29	LYS	-0.899
30	THR	-0.899

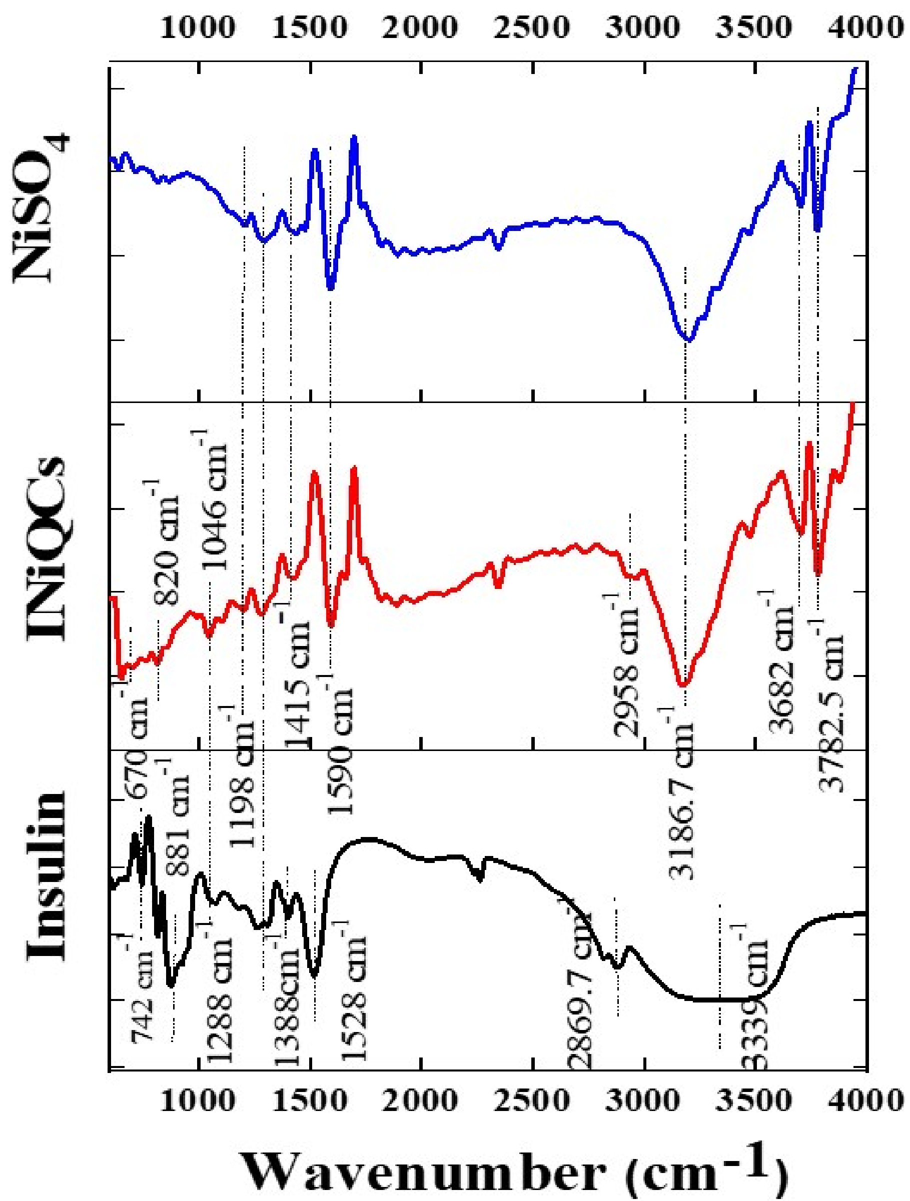

Fig. S3. FTIR spectroscopic studies to find the interaction between insulin protein and nickel-metal ion. The comparison shows the formation of new bonds between Ni-OH and Ni=O, which were otherwise not present.

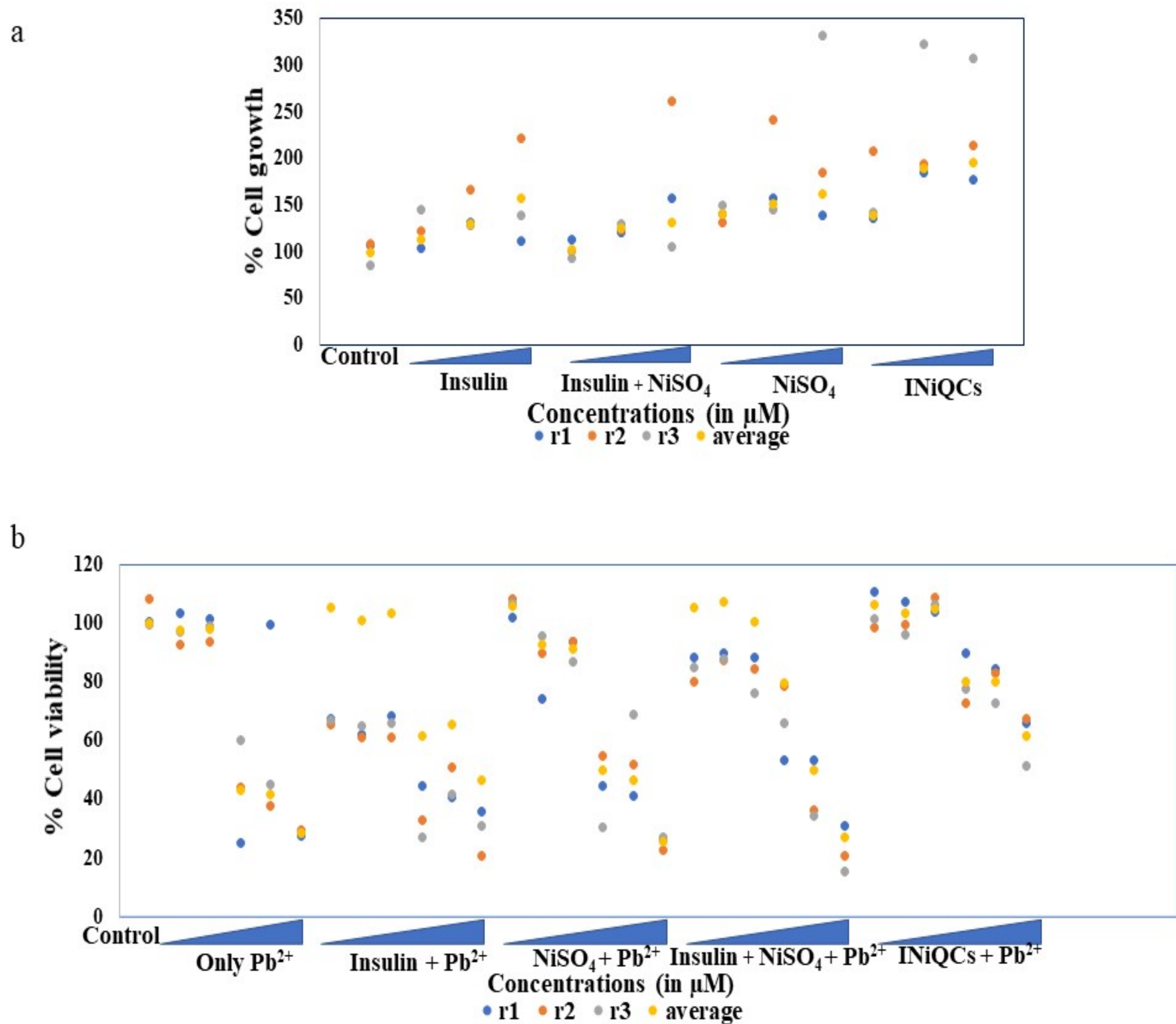

Fig. S4. It represents an MTT assay to determine the metabolism rate of cells. (a) Data shows treatment of HEK-293 cells with control, including insulin, $NiSO_4$, insulin + $NiSO_4$, and INiQCs ranging from 1.5, 7.5, and 30 µM concentrations, respectively, of each sample. (b) Data shows treatment of HEK-293 cells with 0.45 µM of insulin, $NiSO_4$, insulin + $NiSO_4$, and INiQCs. Then the same cells were treated with 0, 1, 10, 100, 500, 1000 (µM) concentration of Pb^{2+} after 3 h, and data were plotted using individual readings rather than non-descriptive error bars. Here r1, r2, and r3 in both the figures represent three individual readings taken for MTT assay after normalizing to control.