

Novel Magnetic Relaxation Nanosensors: An Unparalleled “Spin” on Influenza Diagnosis

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

www.rsc.org/

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Supporting Information

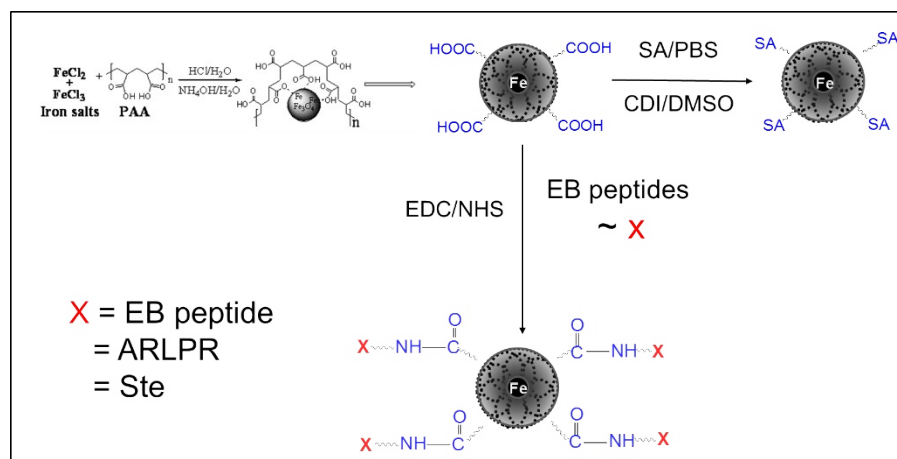
Experimental Section:

Computational Analyses and Modeling. Prior to conducting the binding and competition assays, the ligands and peptides used for functionalization of the MRnS were analyzed via computational modeling. Programs used for this method of analysis included Avogrado, Open Babel, and Autodock 4. Shown below are verified dockings between H1N1/HA1 and 2,6-sialic acid, ARLPR, EB Peptide and Ste (Figures S2-S6). K_d values for 2,6-sialic acid, ARLPR and Ste were 12.92 mM, 27.78 μ M, 4.62 mM, respectively. The interaction between EB Peptide and H1N1/HA1 is shown in Figure S5.

As well, binding between H5N1/HA1 and 2,3-sialic acid, EB Peptide, ARLPR and Ste was analyzed computationally. One of the differences between active residues in H5N1/HA1 vs H1N1/HA1 is the replacement of Glu190 with Leu190. The K_d values for 2,3-sialic acid, ARLPR and Ste binding were reported as 2.82 mM, 52.05 μ M and 12.7 mM, respectively.

In addition, it was noted that the Ste K_d values observed through Autodock 4 were in the millimolar range, in contrast to both literature reports, and our experimental data, which both showed a K_d value in the micromolar range. This discrepancy may be due to the rigidity of the docking files used for this computational experiment.

Synthesis of IONPs and functional MRnS:



Scheme S1: Preparation of iron oxide nanoparticles and subsequent conjugation with targeting ligands via EDC/NHS or CDI chemistry.

Characterization of IONPs and MRnS:

IONPs and conjugated MRnS were characterized using size and charge data collected via zetasizer.

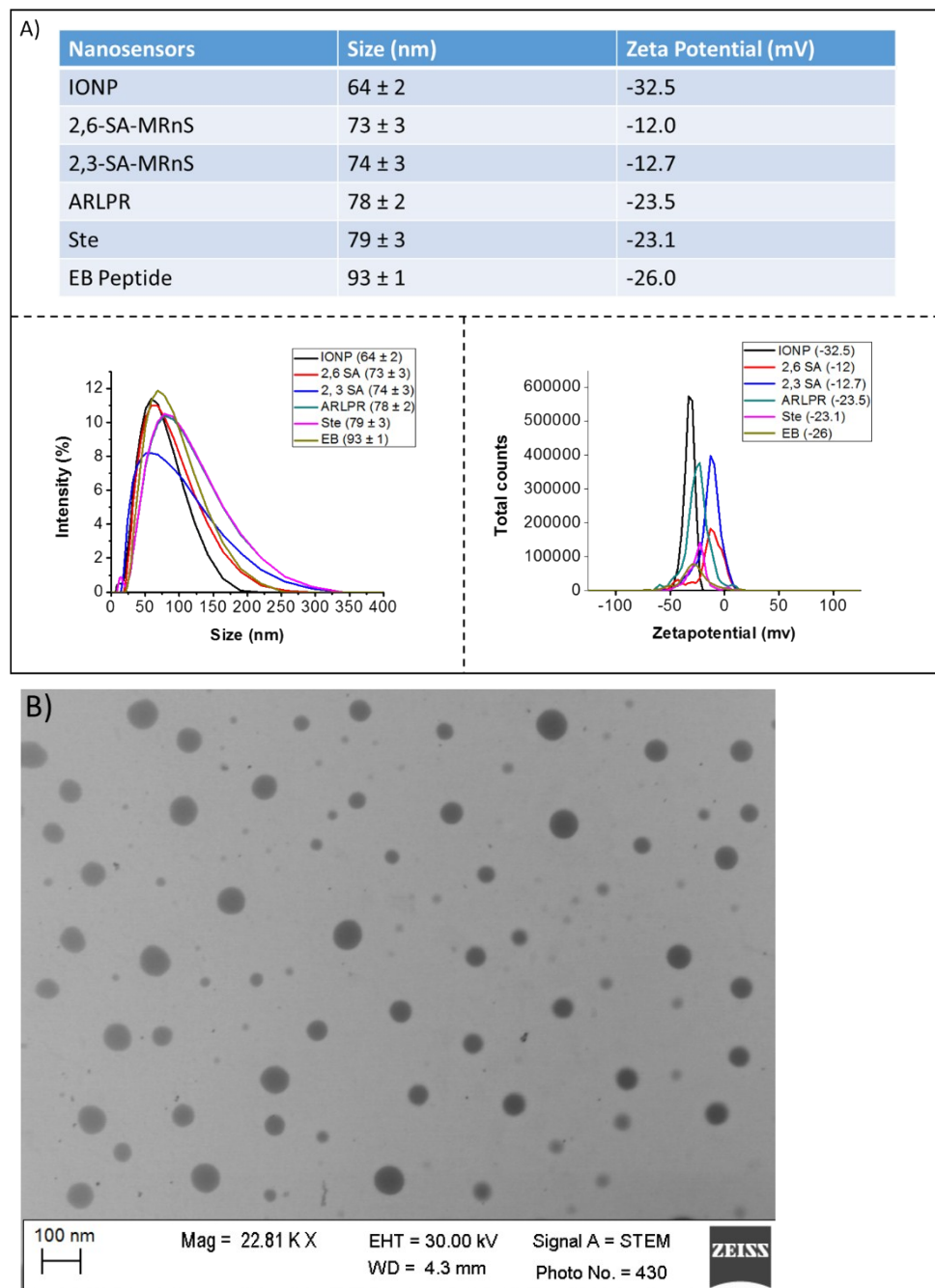
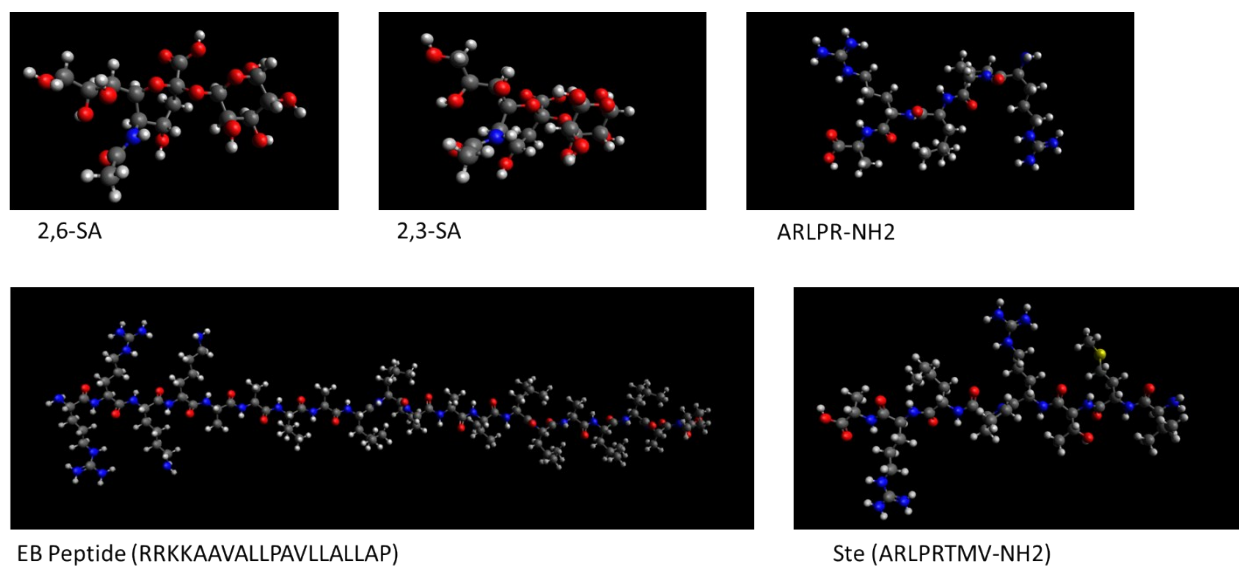
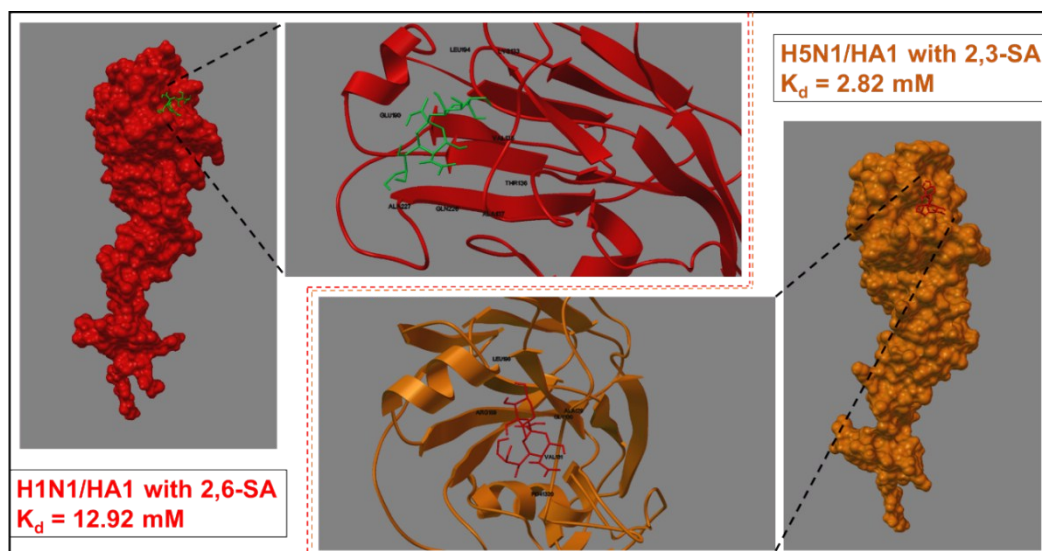


Figure S1: Characterization of iron oxide nanoparticles and conjugated MRnS using A) zeta-sizer and B) STEM image.

Structure of sialic acids and EB peptides:**Figure S2:** 3D modelling of targeting ligands using Avogadro.**Autodock 4 studies between hemagglutinin variants and sialic acids:****Figure S3:** Computational analysis of sialic acid cell receptors (2,6 and 2,3) with hemagglutinin (H1 and H5).

Nanoscale

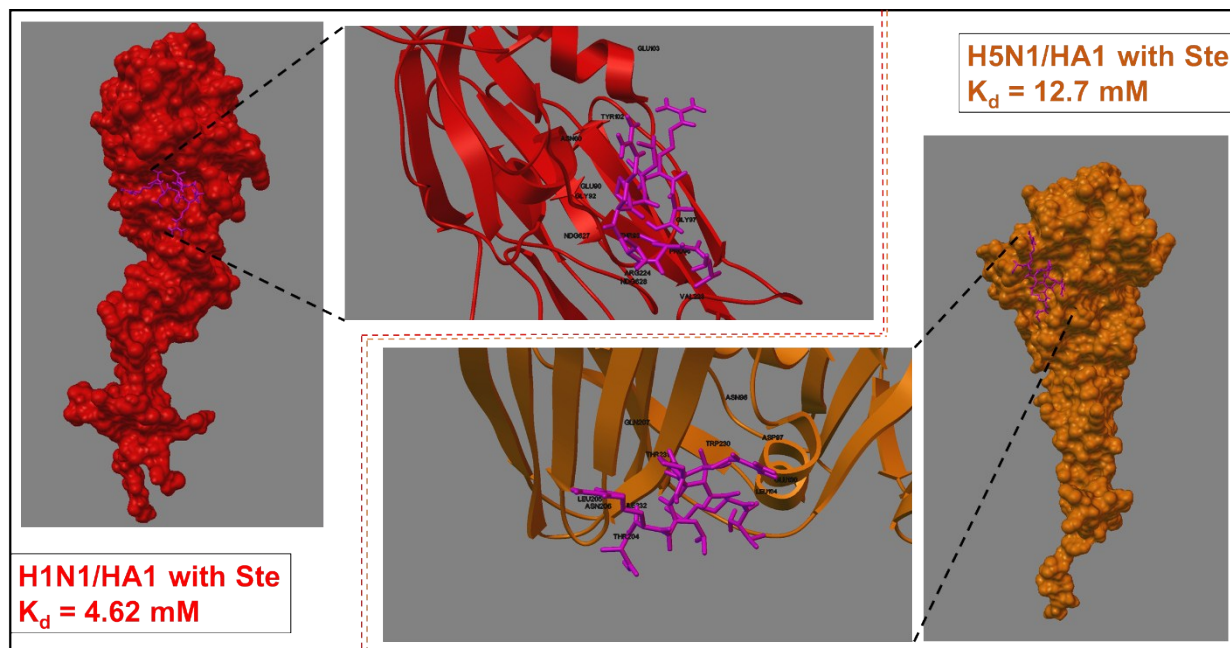


Figure S6: Computational analysis of Ste with hemagglutinin (H1 and H5).

Binding and competition assays using Ste-MRnS

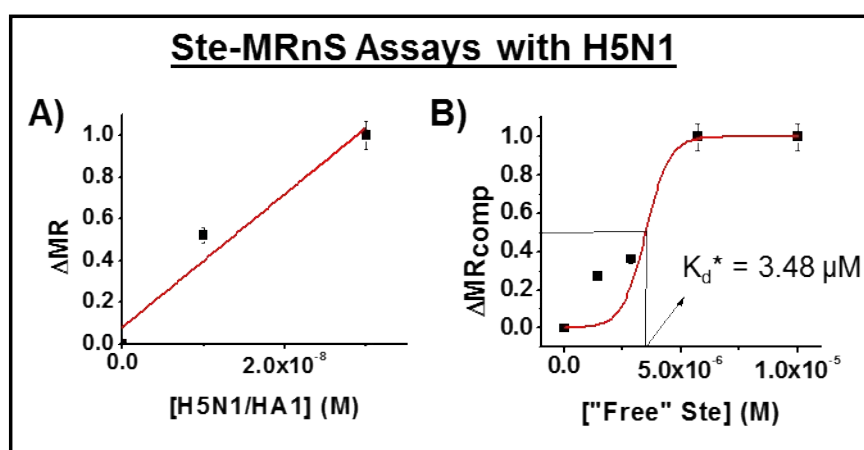


Figure S7: Binding and competition assays with Ste ($7.5 \times 10^{-3} \text{ M}$) and H5N1/HA1 ($0-10 \times 10^{-6} \text{ M}$).

