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Cleavable ester linked magnetic nanoparticles for labeling of solvent exposed primary amine groups of peptides/proteins

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ABSTRACT

Covalent labeling of solvent exposed amino acid residues using chemical reagents/crosslinkers followed by mass spectrometric analysis can be used to determine the solvent accessible amino acids of a protein. A variety of chemical reagents containing cleavable bonds were developed to label abundantly found lysine residues on the surface of protein. To achieve efficient separation of labeled peptides prior to mass spectrometric analysis, magnetic nanoparticles can be decorated with amino acid reactive functional groups and utilized for quick recovery of labeled peptides. [1] In this work, iron oxide magnetic nanoparticles (Fe_3O_4 MNPs) were synthesized by thermal decomposition method and coated with silica (SiO_2@Fe_3O_4 MNPs) by reverse micro emulsion approach. The Fe_3O_4 MNPs and SiO_2@Fe_3O_4 MNPs were characterized by TEM and XRD. The SiO_2@Fe_3O_4 MNPs were further coated with amine groups and conjugated to *N*-hydroxysuccinimidyl (NHS) ester groups via a cleavable ester bond. Fluorescence based qualitative analysis of ester linked NHS ester modified SiO_2@Fe_3O_4 MNPs was performed to confirm the presence of NHS ester group. The active NHS ester sites on the surface of SiO_2@Fe_3O_4 MNPs were determined by depletion approach and found to be 694 active sites per 1 mg of SiO_2@Fe_3O_4 MNPs. Free amine groups of a small peptide, ACTH (4–11) were labeled by ester linked, NHS ester modified SiO_2@Fe_3O_4 MNPs under physiological conditions.

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Superparamagnetic nature of SiO_2@Fe_3O_4 MNPs allowed quick and efficient magnetic separation of labeled peptides from the solution. The ester bond was further cleaved to separate labeled peptides followed by mass spectrometric analysis. The ester linked, NHS ester modified SiO_2@Fe_3O_4 MNPs introduced a mass shift of 115.09 Da on amine groups of ACTH (4–11), which was confirmed by mass spectrometry.

1. Specifications table

Subject area	Biochemistry, Materials chemistry
More specific subject area	Surface Proteomics
Type of data	Text file, figure
How data was acquired	X-ray diffraction, mass spectrometry, and fluorescence spectroscopy
Data format	Analyzed
Experimental factors	The SiO_2@Fe_3O_4 MNPs were modified with NHS ester groups via a cleavable ester bond. Quantitative fluorometric characterization of ester linked NHS ester modified SiO_2@Fe_3O_4 MNPs was performed to determine active NHS ester sites on the surface of SiO_2@Fe_3O_4 MNPs. Solvent exposed free amine residues of peptides were labeled using cleavable ester linked NHS ester linked silica coated iron oxide magnetic nanoparticles. The labeling reaction was performed under physiological conditions to preserve the native structure of proteins. The ester bond was subsequently cleaved followed by magnetic separation of nanoparticles
Experimental features	The label generated on the solvent exposed free amine groups of peptides and proteins were identified by mass spectrometric analysis.
Data source location	New Orleans, Louisiana, USA
Data accessibility	Data is included in this article

2. Value of the data

- The surface exposed amine groups of peptides can be determined by labeling with ester linked NHS ester modified SiO_2@Fe_3O_4 MNPs under physiological conditions.
- Cleavable ester linked NHS ester modified SiO_2@Fe_3O_4 MNPs provide an effective approach to magnetically separate the labeled peptides from the solution without adding extra step of purification.
- The flurometric quantification of active NHS ester sites on the surface of SiO_2@Fe_3O_4 MNPs can allow quantitative control over the labeling reaction.

3. Data, experimental design and methods

The data shown here is divided into four major steps: a) synthesis and characterization of SiO_2@Fe_3O_4 MNPs, b) synthesis of ester linked NHS ester modified SiO_2@Fe_3O_4 MNPs, c) fluorometric quantification of active NHS ester sites on the surface of SiO_2@Fe_3O_4 MNPs and, d) labeling and identification of primary amine groups of ACTH (4–11) using ester linked NHS ester modified SiO_2@Fe_3O_4 MNPs.