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Surface Analysis of Organic- and Bio-conjugated Nanoparticles Using Mass Spectrometric Imaging and FT-IR Spectroscopy

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Recent improvements in synthesis methods and protective coatings or conjugated molecules for water solubility make quantum dots (QDs) promising markers for biomedical imaging research. For the application, we need to understand which molecules are conjugated on QDs during their synthesis. However, methods for direct characterization of organic- or bio-conjugated QDs are still lacking. We have carried out a label-free analysis of CdSe/ZnS QDs and silica nanoparticles conjugated with ligands and biomolecules by using time-of-flight secondary ion mass spectrometry (TOF-SIMS) imaging and FT-IR spectroscopy. TOF-SIMS imaging provides mass spectral images from a sample surface pattern resulting from the nanoparticles aggregates self-assembled on a substrate. In our technique, ligands conjugated onto nanoparticles yield a pattern that overlaps well with the pattern of nanoparticles, whereas other residual chemical species present on the substrate show another pattern void of nanoparticles. Thus, the image contrast with a micron-scale spatial resolution allows for a mass spectral identification of chemical and biological species conjugated onto nanoparticles and the monitoring of ligand exchange processes and impurities remaining in solution. Although this simple and novel technique has great potential in the characterization of organic ligands and biomolecules capped on nanoparticles and self-assembled nanostructures, it does not provide their binding modes or their quantitative information. In this regard, the FT-IR spectroscopy with TOF-SIMS imaging technique can help us to understand the ligand types, the binding modes of ligands, type of chemical linkage along with their quantities.