Hyphenated Mass Spectrometric techniques for smart materials architecture: Theranostic applications

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Rapid early detection is crucial for transboundary/ emerging/ zoonotic disease outbreak prevention. Several international organizations such as WHO, OIE, FAO and EPA called upon the development of rapid, sensitive, low cost, and easy to use early diagnosis of pathogens as "rapid field tests" or "point of care diagnostics". Molecular recognition plays an important role in biological systems and is observed in between receptor-ligand, antigen-antibody, DNA-protein, sugar-lectin, RNA-ribosome, substrate-enzyme, etc. (The lock and the key theory, Pauling, 1940). My investigations show that the characteristics of the functional biomimetic system of "molecular architecture" for certain biological organisms and systems should be designed by computational approach. Molecular imprinted polymers (MIPs) have been applied as artificial antibodies, catalysts, sensors, drug assay tools, and affinity separations. Targets including epitopes or haptens, which are the major antigenic determinants of microorganisms like bacteria or viruses, lead to innovations in disease theragnosis. MALDI-TOF MS bio typing was highly successful in rapid identification of Brucella cultures through dendrodrogram analysis, despite the high phenotypic and genotypic similarity among members of the genus Brucella. From the species perspective, B. suis and B. ovis were more related to B. melitensis than to B. abortus, which had a separate cluster. Strain-specific mass spectral peaks were observed among almost all strains examined Tandem mass spectrometric experiments reveal individual polymer end groups; in contrast, the 1-D MS spectrum provides insight about the sum of chain end substituents present in the oligomer, which may also contain partial or complete monomer unit(s). Additionally, MS can be employed to analyze copolymer sequences and to differentiate polymer architectures. Hyphenated mass spectrometric techniques are machines driving these innovations to successful marketable products based on patents. Computational chemistry tools will aid this developmental approach upon conformational decisions of diagnostic biomarkers/ biomimetic smart polymers.

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