Investigation of the contribution of molecular imprinted hydrogels in the metabolomic analysis of biological systems

Moschovi A.M.[1,2#], Yannopoulos S.N.[3], Dracopoulos V.[2], Klapa M.I [1*]

[1]Metabolic Engineering & Systems Biology Laboratory, Institute of Chemical Engineering Sciences, Foundation for Research and Technology – Hellas (FORTH/ICE-HT), [2] Ionic Liquid and Molten Salts Laboratory, [3] Vibrational Spectroscopy Laboratory, Institute of Chemical Engineering Sciences, Foundation for Research and Technology – Hellas (FORTH/ICE-HT), Patras

Presenting author: Moschovi A.M., email:natassamoschovi@iceht.forth.gr

*** CORRESPONDING AUTHOR: KLAPA M., EMAIL:MKLAPA@ICEHT.FORTH.GR**

Metabolomics refers to the high-throughput analysis of the metabolic state of a biological system based on the quantification of the concentration profile of all measurable free small molecules that act as reactants or products in the metabolic reaction pathways. Metabolomics is an integral part of the systems biology analytical toolbox and its standardization will contribute to the development of accurate methods for the comprehensive analysis of biological systems. Mass spectrometry metabolomics exhibits several advantages such as high sensitivity, which decreases the amount of raw material needed for the analysis, extensive availability in compound databases, experimental protocols and procedures, relatively low cost and user-friendliness. Still, there are issues to be resolved regarding the differentiation and accurate quantification of molecules of similar chemical structure or the presence of certain molecules in such high concentration that affects the accurate quantification of others. In both cases, there is a need for the selective filtration of particular molecules from a complex pool of metabolite extracts.

Hydrogels are insoluble crosslinked polymer network structures composed of hydrophilic co- or homo-polymers which exhibit the ability to absorb significant amount of water. Molecular imprinting (MI) in hydrogels is a technique in which functional groups of the hydrogel are allowed to form a network around a template molecule. After the removal of the template molecule, cavities with specific recognition sites and size are generated for the adsorption of the template.[1] These materials are candidates for molecular recognition, drug delivery, highly specific catalysis, quantitative analysis and separation materials in conjunction with chromatographic techniques. Depending on the application, it is possible to tailor these materials to recognize and bind cells, viruses, proteins or small molecules by covalent and/or non covalent bonding.

Here, we investigate the hypothesis that the resolution of the metabolic profile obtained by mass spectrometry could be improved by the recognition capabilities of MI hydrogels (MIH). For this reason, we use an MIH based on a crosslinked poly(allylamine) PAA·HCl polymer imprinted with and/or without small organic molecules as templates. Results on gelation dynamics, structural characterization and binding tests will be shown and discussed.

REFERENCES

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