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Solid phase extraction of Phorbol Esters (PEs) from pinion cake (*Jatropha curcas* L.) based on computationally-designed polymers in combination with deep eutectic solvents

Maria A Sandoval-Riofrio, Joanna Czulak and Elena Piletska
University of Leicester, UK

Molecular imprinting and computational modeling are technologies which could be used to develop specific absorbents capable of recognizing particular compounds of interest and extract them from complex plant matrices. As a renewable resource is needed for the development of green technologies and sustainable society, it was found that *Jatropha curcas* L. and its waste (pinion cake) have a big amount of biomolecules. But it was also found that there are some toxic compounds such as Phorbol Esters (PEs) present in it, which prevents this waste to be used as fertilizer or balanced feed for animals. The extracted PE could potentially be used as a biopesticide or as building blocks for development of new drugs. Phorbol 12-merystate-13-acetate (PMA) was used as a template for the design of the polymer which is specific for PEs using commercial modeling software Sybyl 7.3 (Tripos, USA) which helped to select the functional monomers possessing the highest affinity towards PMA. In accordance with computational modeling, several polymers have been prepared, tested and screened with PMA's model solution in methanol. In order to extract PEs from the pinion cake, several extraction methods have been tested using the traditional organic solvents and various DES (Deep Eutectic Solvents). PEs has been purified using optimized Solid Phase Extraction (SPE) protocol using the HEM-DVB-based polymer which demonstrated the highest binding capacity towards PMA. Preliminary results show that, DES could be successfully used for the extraction of PE from the pinion cake waste. Spectrophotometer and HPLC-MS will be used for the quantification and identification of the PEs and extracted components from samples.

Biography

Maria A Sandoval-Riofrio is a Research Student at the University of Leicester, UK. She is a Scientist with a research experience in several engineering fields related to clean and renewable energy production, biotechnology focusing on the environmental sustainability and green chemistry oriented towards the development of environmentally friendly processes. Her main research expertise was in designing and scaling up reactors for biofuel elaboration from different sources, collaborative research for environmental management procedures in efficiency energetic, photovoltaic technology and carbon capture using living organisms. She is now working on implementation of new nanotechnology tools that can be scaled-up and applied in developing countries.

masr2@le.ac.uk

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