MS09-P03

A bioconjugate of lipase with polypyrrole–methyl anthranilate functionalized "worm-like" titanium dioxide nanocomposite as promising nanobiocatalyst

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Recently the development of unique nanoscaffolds have gained quite an attention for the preparation of highly stable nanobiocatalysts in order to exploit them for the synthesis of novel compounds and biodiesel. Biodiesel is a key paradigm towards the development of sustainable environment in the future. We show this by the fabrication of novel polypyrrole–methyl anthranilate functionalized titanium dioxide nanomaterial and its conjugation to lipase for the synthesis of flavoured compound and potential in biodiesel synthesis. We demonstrated successful immobilization of lipase from *Rhizopus oryzae* on a Ppy–MA/TiO2 NM by physical adsorption and a glutaraldehyde-activated covalent coupling procedure. The catalytic efficiencies of the free and immobilized preparations were determined for the hydrolysis of p-nitrophenyl palmitate. The covalently immobilized lipase displayed a significantly higher activity yield (effectiveness factor of 0.97) in comparison with the adsorbed counterpart (effectiveness factor of 0.86). The binding of lipase to the Ppy–MA/TiO2 NM was confirmed by transmission electron microscopy, Fourier transform infrared spectroscopy and scanning electron microscopy. TGA and DTA were performed to investigate the thermal stability of the synthesised biocatalysts. The storage stability, solvent tolerance, and reusability of the resulting nanobiocatalyst and the effect of pH and temperature on its catalytic activities were also investigated. The prepared nanobiocatalysts displayed remarkably improved activity in terms of solvent tolerance (activity recovery of 150% and 125% in acetone and isopropanol, respectively) in comparison with its free counterpart. We envisage that the covalent binding method played a profound role in enhancing the properties of the enzyme immobilized on the Ppy–MA/TiO2 NM. The immobilized lipase successfully synthesised flavour ester in solvent free media and n-hexane having 25.5% and 85.5% ester yields respectively and also holds vital potential for enzymatic biodiesel synthesis. Molecular docking results confirmed the successful conjugation of the enzyme-nanocomposite complex.

Keywords: Nanobiocatalyst, Molecular docking, Flavor synthesis

MS09-P04

Crystal structure of inositol 1,3,4,5,6-pentakisphosphate 2-kinase from *Cryptococcus neoformans*

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The fungal pathogen *Cryptococcus neoformans* is a causative agent of meningoencephalitis in humans. For its pathogenicity, the inositol polyphosphate biosynthetic pathway plays critical roles. In particular, an inositol 1,3,4,5,6-pentakisphosphate 2-kinase (Ipk1) catalyzes the phosphorylation of IP_5 to form IP_6, a substrate for subsequent reaction to produce inositol pyrophosphates, such as PP-IP_5/IP_7. In fact, deletion of *IPK1* significantly reduces the virulence of *C. neoformans*, indicating that Ipk1 from *C. neoformans* (CnIpk1) is a major virulence contributor. We initiated structural analysis of CnIpk1 to provide structural information for the possible development of drug design for treatment of cryptococcosis. A crystal structure of the unliganded CnIpk1, the first structure for a fungal Ipk1, will be presented at 2.35 Å resolution. Structure comparisons of CnIpk1 with those from *Arabidopsis thaliana* and *Mus musculus* suggest structural similarities and discrepancies for fungal Ipk1 among members of the Ipk1 family. This work was supported by Next Generation BioGreen 21 program of Rural Development Administration (Plant Molecular Breeding Center) of Republic of KOREA.

References:

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