



**REGIONAL CENTRE FOR BIOTECHNOLOGY**  
**Seminar series**

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**Influence of the Protein Environment on the  
Mechanistic Function of Cytochrome P450 (CYP)  
Enzymes**

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The Hebrew University of Jerusalem, Israel

**Tuesday, 10<sup>th</sup> September, 2013**  
**3:00 PM**  
**Seminar Room**

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### Abstract

Cytochrome P450s (CYPs) are a ubiquitous super-family of enzymes, which play vital roles in many biological process. CYPs generate an iron-oxo intermediate to oxidize relatively inert/hydrophobic substrates and drugs in diverse ways (hydroxylation, epoxidation, O-dealkylation etc). Elucidation of these oxidation reaction mechanisms and identifying how a specific protein affects its function is of immense interest in drug industry and biomedical research. The complex and dynamic nature of this enzyme structure and multistep reactions that undergo in the catalytic cycles often challenges both experimental and theoretical groups to identify the underlying physical principles of the mechanisms and versatile nature of these enzymes.

In view of this, I will first illustrate how our recent theoretical investigations on site-directed mutation of CYP 2B4 enzyme for the catalytic activity and the synthesis of a neurotransmitter serotonin by CYP 2D6 have added insights into the mechanisms at molecular level that complements experiment. These studies illustrate the various factors that the protein environment induces to control the mechanistic function of a P450 enzyme. Fascinated by the mechanisms that enzymes operate to perform complex tasks, I will discuss my vision for the future research areas (a) computational biocatalysts towards developing technologies for greener industrial process and (b) rationalize disease mechanisms for better living of life.