The modeling of new enzymes helps develop therapies for cocaine abuse

July 26 2012

Researchers from the University of Kentucky have designed and discovered a series of highly efficient enzymes that effectively metabolize cocaine. These high-activity cocaine-metabolizing enzymes could potentially prevent cocaine from producing physiological effects, and could aid in the treatment of drug dependency. The results of this study by Chang-Guo Zhan et al are published in the journal *PLOS Computational Biology*.

The effectiveness of the enzymes' work was evaluated through modeling cocaine pharmacokinetics, the study of the body's action on administered external substances, such as cocaine, when the enzyme exists in the body. As there is no FDA-approved anti-cocaine medication, the medical and social consequences of cocaine abuse have made the development of anti-cocaine medication a high priority. Administration of an enzyme to enhance cocaine metabolism has been recognized as a promising treatment strategy for overdose and abuse. A remarkable feature of the enzyme-based therapeutic approach is that one enzyme molecule can degrade many thousands of drug molecules per minute.

This pharmacokinetic modelling is a crucial step of enzyme-based therapy development for cocaine abuse. Furthermore, the general insights of the research should also be valuable for future development of an enzyme therapy for any addictive drug, as the general methodology of the modelling may be used to develop valuable models for evaluating the effectiveness of metabolic enzymes in detoxifying other drugs.

More information: Zheng F, Zhan C-G (2012) Modeling of Pharmacokinetics of Cocaine in Human Reveals the Feasibility for Development of Enzyme Therapies for Drugs of Abuse. *PLoS Comput Biol* 8(7): e1002610. doi:10.1371/journal.pcbi.1002610