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## PERSONALIZED DRUG IN THE ERA OF BIG DATA AND PRECISION MEDICINE

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**T**he cytochrome P450 (CYP450) superfamily plays an important role in the oxidation of almost 90% drugs used currently. As variations of single nucleotide polymorphism (SNPs) in human CYP450 genes will cause different drug effects and even adverse effects, studies on SNPs of human CYP450 genes can be used for indicating the most possible genes associated with human diseases and relevant therapeutic targets, predicting the drug efficacy and adverse drug response, investigating individual gene specific properties and then providing personalized and optimal clinical therapies. We have done extensive bioinformatics studies on CYP450 SNPs and its impact on the drug metabolism in the frame work of personalized medicine, i.e., SNPs prediction, the substrate specificity, comparative molecular field analysis,

molecular dynamics simulation and QM/MM studies of the metabolic mechanism. Based on the structure of membrane protein targets acquired by bioinformatics tools, and database of molecules extracted from traditional Chinese medicines, various cheminformatics procedures, in the context of network pharmacology, were performed to screen for potential active compounds. A molecule named wgx-50 was obtained, which is an effective component from the Sichuan pepper. Extensive experiments strongly suggest that wgx-50 possesses biologic functions against AD. Discoveries were also made in its potential role in anti-aging.

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