

NMR metabolomics and drug discovery

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Drug discovery is a complex and unpredictable endeavor with a high failure rate. Current trends in the pharmaceutical industry have exasperated these challenges and are contributing to the dramatic decline in productivity observed over the last decade. The industrialization of science by forcing the drug discovery process to adhere to assembly-line protocols is imposing unnecessary restrictions, such as short project time-lines. Our disease-centered systems biology approach to drug discovery provides a unique infrastructure to identify novel druggable targets and therapeutic agents to increase the efficiency and success rate of drug discovery. One important component of our approach is the use and development of NMR-based metabolomics techniques to monitor the *in vivo* activity and selectivity of potential drugs. Similarly, NMR metabolomics can be used to monitor disease development, identify *in vivo* mechanisms of action for novel drugs, and evaluate mechanisms of drug resistance. Additionally, NMR metabolomics may be an invaluable approach to easily and rapidly diagnose human disease and assist in personalized medicine by monitoring a patient's response to a particular treatment. Our NMR metabolomics technology, including our development of metabolomic tree diagrams and protocols for metabolite identification will be discussed. Also, our analysis of the mechanism of action and resistance of D-cycloserine (a TB drug), a metabolic signaling pathway for biofilm formation in *S. aureus* and *S. epidermis*, drug resistance in pancreatic cancer, and a potential diagnostic tool for multiple sclerosis will be presented.

Biography

Dr. Robert Powers is an Associate Professor of Chemistry at the University of Nebraska-Lincoln. He received a BA from Rutgers University in 1984, a Ph.D. from Purdue University in 1989, and completed a post-doctoral IRTA fellowship at the National Institutes of Health in 1993. He was an Associate Director at Wyeth before arriving at UNL in 2003. He has 7 patents and over 80 journal articles and book chapters on the application of NMR for drug discovery. He is an associate editor for the Journal of Integrated-omics, Comb. Chem. High Throughput Screening, and founding member of the International Chemical Biology Society.