## AbbVie Workshop Series Driven to Discover<sup>21</sup> in Synthetic Organic & Medicinal Chemistry 4:15 p.m. Friday, Oct. 24, 2014, 331 Smith Hall



Professor

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## Orthogonality Unravels Metabolomic and Residually Complex Chemistry

Research Interests: Secondary metabolites from natural sources across the phylogenetic tree have always played an important role in physiology, biochemistry, pharmacology, drug discovery and pharmaceutical analysis. Their separation, analysis and pharmacological evaluation are core elements of modern pharmacognosy, representing an interdisciplinary field of research. Website: http://tigger.uic.edu/~gfp/

## Abstract

Nature's metabolomic approach to chemistry generates numerous challenges in the biomedical and basic sciences. Recently, it has been becoming increasingly clear that just the small molecules in metabolomes represent highly complex mixtures comprised of 105 species, or even more, regardless of the source organism. This not only generates incredible chemical diversity, but also produces species that are very closely related and can appear to be nearly identical, while having distinct biological functions.

This combination of diversity and subtlety challenges pharmacognosy research at the interface of chemistry, biology and health science. Our approach utilizes analytical orthogonality as a means to unravel the chemistry of complex extracts, characterize their bioactive constituents, develop lead compounds, and investigate the residual complexity of reference materials. Multi-dimensional orthogonality is achieved by the development of liquid-liquid (countercurrent) and liquid-solid chromatography, qualitative and quantitative NMR, as well as hyphenated MS. Furthermore, the joint evaluation of chromatographic and spectroscopic data by statistical and computational methods advances key aspects such as structural dereplication and the targeted characterization of bioactives.

Using examples of newly developed techniques and recent progress, the presentation will highlight the importance of orthogonality for the significance and reproducibility of interdisciplinary study of metabolomic or residually complex materials.



Host: Professor Thomas Hoye