University of Minnesota
Driven to Discover℠

Department of Chemistry
Gassman Lectureship in Chemistry
October 3 through October 7, 2011

Professor

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Research interests: physical and bioorganic chemistry of synthetic and natural receptors and molecular recognition.

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Lecture #1 3:45 p.m. Monday, October 3, 100 Smith Hall (reception following 117/119 Smith Hall)

Supramolecular Analytical Chemistry

The use of synthetic and designed receptors for the analysis of complex analytes in real-life settings will be presented. Analytes in beverages, chiral mixtures, and blood/saliva have been targeted by mimicking the mammalian senses of taste and smell. The receptors derive from a combination of rational chemical design and modeling, with combinatorial synthesis techniques. Optical signaling derives either from indicator-displacement, or indicator-uptake, assays. It will be shown that a union of designed receptors targeted to a class of analytes, with combinatorial methods, gives fingerprints that differentiate between the individual members of the class. The strategy is to use a core-binding element that imparts a bias to each and every member of the library, ensuring affinity of the library members for the class of analytes being targeted. The design of this core derives from standard molecular recognition principles: preorganization, complementary, pair-wise interactions between receptor and analyte, and desolvation. Imparting a bias to the affinity of the library members dramatically reduces the diversity space needed in the library. Combinatorial techniques impart the differential behavior and cross-reactivity desired in an array sensing application. The fingerprints of the solutions are created using artificial neural networks, principle component analysis, and/or discriminate analysis. The technique represents a marriage of supramolecular chemistry and pattern recognition protocols.

Lecture #2: 9:45 a.m. Tuesday, October 4, 331 Smith Hall

Supramolecular Approaches to High-Throughput Screening of Enantiomeric Excess

The need for increasingly user-friendly and rapid assays for ee has arisen recently due the advent of parallel synthesis protocols for asymmetric reaction discovery and optimization. Many studies require hundreds to thousands of assays per day. A primary goal of our group is to design and implement high-throughput screening (HTS) assays for enantiomeric excess (ee) and reaction yield in catalytic asymmetric reaction screening. Our approach to the HTS of ee combines supramolecular chemistry with chemometrics. We create very simple synthetic receptors that are targeted to classes of chiral functional groups, and record absorbance or circular dichroism spectra for diastereomeric or enantiomeric complex formation. LDA, PCA, or ANN interprets the optical data. The analysis is performed in microtiter plates where the ee values, as well as concentration (reaction yield), of 96 crude reaction mixtures can be read within 1 minute to 2 hrs depending upon the particular assay. Assays for diols, amines, carboxylic acids, ketones, and alcohols have been created. Examples of each along with practical applications will be discussed.

Chalk Talk #1: 1-2:30 p.m. Tuesday, October 4, 114 STSS

Solvation, Molecular Recognition

Chalk Talk #2: 1-2:30 p.m. Thursday, October 6, 230 STSS

Chirality and Stereochemical Principles

Chalk Talk #3: 9:30-11 a.m. Friday, October 7, 118 STSS

Bonding: Hybridization versus Qualitative MOT

Regents Professor Paul G. Gassman, internationally known in the chemical community, died in April 1993, at the age of 57. He left behind a legacy of achievement. During his career, he served as mentor and adviser to 85 doctoral and master's candidates as well as dozens of postdoctoral associates and undergraduate students. Numerous awards, honors, and honorary degrees were bestowed in recognition of his contributions to research and his service to the scientific, professional, and university communities. Some of these awards include election to the National Academy of Sciences (1989) and the American Academy of Arts and Sciences (1992), the James Flack Norris Award in Physical Organic Chemistry (1985), Arthur C. Cope Scholar Award (1986), and the National Catalyst Award of the Chemical Manufacturers Association (1990). He served as president of the American Chemical Society in 1990. He was co-chair of the organizing committees of the National Organic Symposium (1991) and the National Conferences on Undergraduate Research meeting (1992), on the University of Minnesota campus. It was his wish that a lectureship be established to bring distinguished organic chemists to the Department of Chemistry. We are proud to present this lecture series in his honor.