

Chemical and Biomolecular Engineering

Fall 2009 Seminar Series

Steven M. Cramer

Professor of Chemical Engineering and William Weightman Walker
Professor of Polymer Engineering, Rensselaer Polytechnic Institute

“Intelligent Design of Chemically Selective Displacers and Multimodal Chromatographic Systems Using Protein Libraries, NMR, SPR and Multi-Scale Simulations”

Abstract

The design of novel multimodal chromatographic and chemically selective displacement systems requires a fundamental understanding of the binding of the ligands involved in these processes to protein surfaces. In this presentation a variety of experimental and theoretical approaches are employed to provide insight into the binding mechanisms involved in these processes and to exploit them for the design of chromatographic systems with unique selectivities. Studies were carried out with various combinations of protein libraries, stationary phase ligands and/or selective displacers. Protein libraries included protein charged ladders as well as homologous libraries of protein variants. Mixed mode ligands included a range of chemically diverse ligands and chemically selective displacers were selected from libraries designed for selective binding to specific protein classes. The tools employed in this work include high throughput screening, NMR, SPR and simulations. Nuclear Magnetic Resonance was conducted on a range of protein/stationary phase ligand or displacer mixtures to verify the binding to targeted proteins and the location of the binding event on both the ligand and protein surfaces. Surface plasmon resonance experiments were carried out to study the inherent kinetics of these processes. Molecular dynamic simulations were conducted to corroborate the NMR results and to provide further insight into the binding and preferred protein-binding orientations on the chromatographic surfaces. Finally, this data is integrated into multi-scale models to aid in the development of novel chromatographic processes with unique selectivities and high performance.

Wednesday, September 16, 2009, 3:00 P.M.

Wu and Chen Auditorium, Levine Hall

