

## **Exploiting Protein Structure Information to Expedite Drug Discovery**

Kristin Koretke

*GlaxoSmithKline, Computational & Structural Chemistry*

Detailed knowledge of a protein family – whether mechanism of action, known active compounds, or three-dimensional structures – can expedite drug discovery. This knowledge is not constrained to the exact protein that is being targeted for a therapeutic effect. In fact, understanding how multiple members of a protein family interact with small molecules can advance lead optimization in multiple ways. It can identify tool compounds early in drug discovery process, aid in selectivity issues and provide information about the flexibility of a protein. Using examples from the protein kinase family, this talk will provide a basic understanding of structure based drug design and demonstrate how using the structure information across a protein family can provide insights that can expedite drug discovery.