

A Statistician's Tour of Duty in the World of Drug Discovery

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As a precursor stage to animal testing, drug discovery is a critical path towards medicinal development. Even though our participation is not mandated by the Food and Drug Administration, statisticians are valuable contributors to drug discovery efforts. Discovery of a new drug involves screening large chemical libraries to identify new and diverse active compounds. In this talk, I will highlight some contributions to design and analysis of high throughput screening studies. One project capitalizes on the fact that screening efficiency can be improved by testing compounds in pools. The other two projects work with screening individuals then using recursive partitioning (RP) models to provide information for future screening efforts. In one case, an RP model is optimized to provide simple interpretations of important chemical configurations. In the other case, an ensemble model is built from individual RP models and is shown to be more effective for prediction of rare actives.