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Intersection of Biophysical Studies and Drug Design. Use of the "Efficiency Coefficient" and "Drug Design Matrix"

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As we all know, the NCE that reach market have been dwindling even though our ability to use technology has increased. This might be due to the fact that all the easy targets are well studied and only the intractable systems are being investigated and/or; this means we must be doing something fundamentally incorrect. In the seminar today, I will present the basis of fragment based drug design and some of the tools that can be used to evaluate what to do next. In addition I will discuss the limitations of some of tools in understanding molecular recognition and perhaps what we can do about this situation. I will also talk about some of our results using NMR spectroscopy, which unfortunately has fallen out of favor recently in the drug discovery process, showing how it can aid the understanding of the molecular recognition process by providing us information not easily attainable by any other method.