

POSTER PRESENTATION

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Free-Wilson in the 21st Century—evolution of a versatile toolkit for SAR analysis

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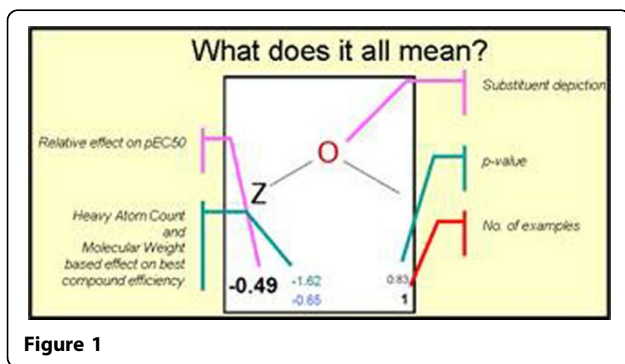
When drug discovery projects are transferred, then rapidly assessing the available SAR in both overview and in numerical detail is a prerequisite for effective computational chemistry input. Following multiple company acquisitions, regular requirements for the approach has led to an effective and fast platform for Free-Wilson [1] based SAR review: in fact the utility is sufficient that it can for a useful reporting or project browsing tool for the busy modeller. Figure 1

In this talk it is shown how a carefully crafted PDF report can be combined with “on the fly” Matched Molecular Pair [2] and other drill downs to provide a versatile platform for SAR exploration and presentation that is appealing and to medicinal chemists.

2. Leach AG, Jones HD, Cosgrove DA, Kenny PW, Ruston L, MacFaul P, Wood JM, Colclough N, Law B: Matched molecular pairs as a guide in the optimization of pharmaceutical properties; a study of aqueous solubility, plasma protein binding and oral exposure. *J Med Chem* 2006, **49**:6672-6682.

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1. Free SM Jr, Wilson JW: A Mathematical Contribution to Structure-Activity Studies. *J Med Chem* 1964, **7**:395-399.

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