The current paradigm of drug discovery utilising chemical library synthesis coupled with high throughput screening technologies often gives rise to a situation whereby drug discovery programmes are compound rich although poor in ADME properties. As such, the ADME properties of compounds require optimisation, through the phases of lead optimisation, prior to progression for clinical development increasing the cost and duration of the process. A prime driver of drug discovery is therefore the early identification of compounds from diverse chemical spaces with optimal ADME properties.

This poster was displayed at the ISSX international meeting in Japan, 2007.

ADMEnsa Interactive is an *in silico* suite of software which enables an estimation of a compounds likelihood of success based upon a balance of the ADME properties required to meet a product profile within a diverse range of therapeutic areas. Prior to initiation of chemical synthesis the key ADME and physicochemical parameters may be predicted from a virtual screening strategy. With the initiation of chemical synthesis, any potential ADME limitations flagged by the in silico predictions can be given priority testing in the ADME/PK laboratory. Using such information SAR relationships may be established leading to the rapid, cost effective, identification of high-quality potential new chemical entities (NCEs) suitable for pre-clinical evaluation. Examples will be presented demonstrating the use of AI and experimental generated ADME data in the identification of NCEs suitable for progression to pre-clinical evaluation.

This poster is available as a PDF file.