

SkelGen: academic use

- **UPGRADED SOFTWARE**
 - Powerful, validated *de novo* design algorithm
 - Applicable to structure- and ligand-based design
 - Graphical user interface enables routine use by medicinal chemists and computational scientists
- **NO REQUIREMENT FOR EXPENSIVE COMPUTING INFRASTRUCTURE**
 - Can be run on a laptop or desktop computer
- **BUILT-IN HELP**
 - Extensive help files
 - Tutorials
 - Detailed reference manual
- **USER CONTROL OF MULTIPLE PARAMETERS**
 - eg molecular size, polarity
 - Default values provided for all parameters
- **ENABLES END-USER KNOWLEDGE TO BE INCORPORATED IN DESIGN STRATEGIES**
 - Interactive 'site-file builder' allows specification of required interactions between the novel ligand and the protein
 - eg particular hydrogen-bonding interactions can be specified
- **ANY NUMBER OF LIGANDS CAN BE GENERATED BY MULTIPLE USERS**
 - Fair-use policy
 - Not less than 20,000 decryptions during the licence term
 - 5 users per academic institution
 - Short term access by larger numbers can be arranged for undergraduate teaching
- **PRICING**
 - Annual fee: £2000
- **INTELLECTUAL PROPERTY**
 - Discoveries using SkelGen are owned by the academic institution