

SkelGen: Pay-Per-View

UPGRADED SOFTWARE

- Powerful, validated de novo design algorithm
- Applicable to structure-and ligand-based design
 - De Novo can provide a service to generate pharmacophore models for ligand-based design
- Graphical user interface enables routine use by medicinal chemists and computational scientists

PAY-PER-VIEW MODEL

- Avoid high up-front access fees
- Pay only for structures that you want to see

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 – ONLY PAY FOR THOSE YOU WANT TO SEE

- Scores are visible before commitment to pay
- Results are clustered to allow low-cost assessment (a small number of cluster members can be viewed to make a decision on the value of that cluster)

ADDITIONAL SUPPORT

- Online 'frequently asked questions'
- Online user forum
 - Get help from other SkelGen users (and/or give help!)
- Training Days/Webinars
 - Get expert help on the application of SkelGen to a variety of problems
- 'Ticket' support system
 - Installation support free-of-charge
 - Additional support queries quoted at hourly rate

PRICING

- Activation fee: £2000
- Low per-structure cost: £0.50