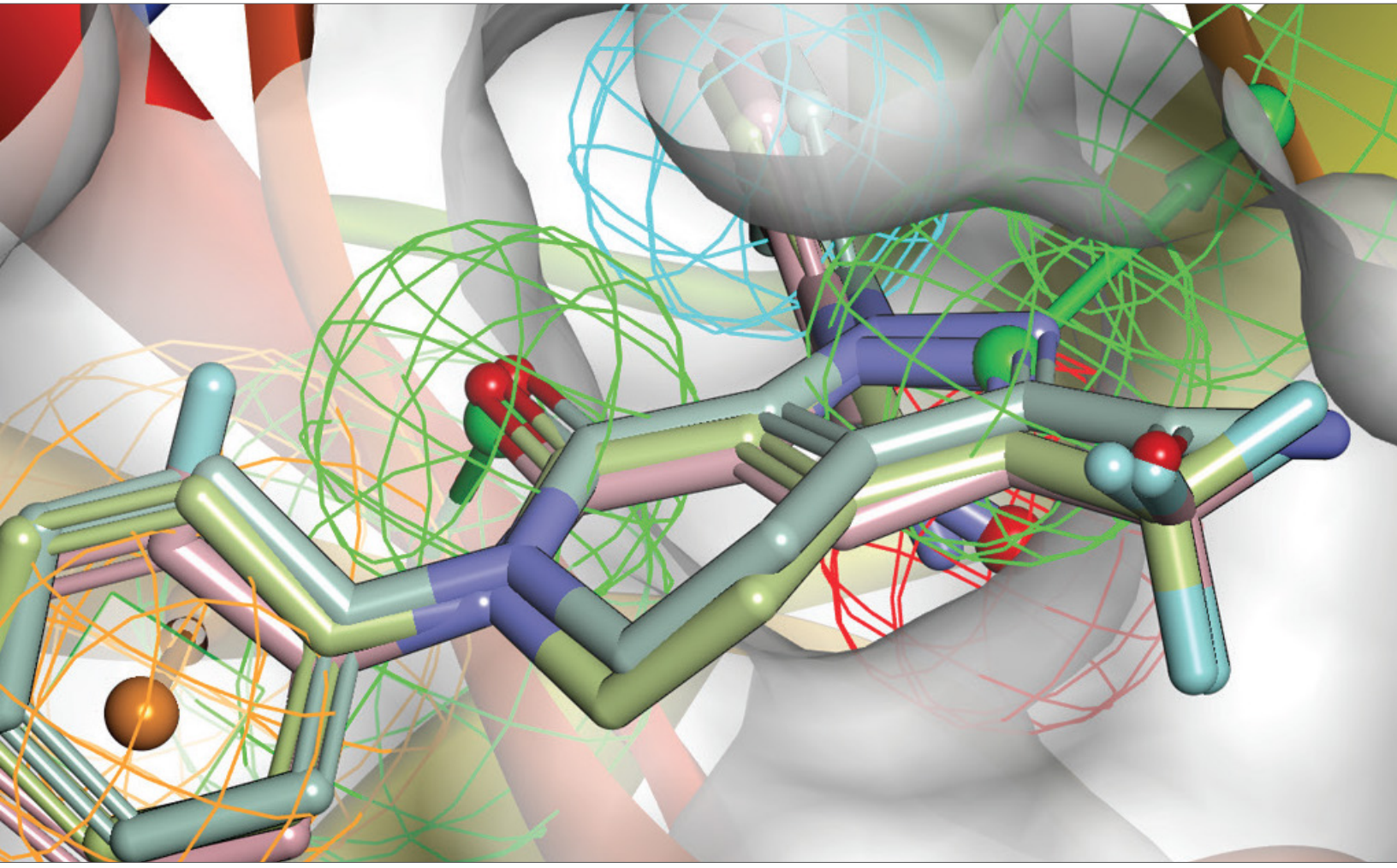
DASSAULT SYSTEMES

BIOVIA

PHARMACOPHORE AND LIGAND-BASED DESIGN WITH BIOVIA DISCOVERY STUDIO®

DATASHEET



ENHANCING RATIONAL LIGAND DESIGN

Ligand-based design, including pharmacophore model generation and virtual screening, are now well established strategies in the rational development of small molecule drugs. BIOVIA Discovery Studio® allows users to visualize, profile and analyze diverse sources of chemical libraries to design and optimize compound selection. Additional comprehensive and scalable tools for hit and lead identification, lead optimization and virtual screening are also available in BIOVIA Discovery Studio. The foundation of many of these is Catalyst®, the most cited and successful collection of pharmacophore modeling tools, offering solutions in de novo design, multi-target drug design as well as activity profiling to offer a full suite of tools to aid the drug design and discovery process.

LIGAND AND LIBRARY DESIGN

- Enumerate reaction- or core-based libraries
- Enumerate ionization states, tautomers and isomers
- Calculate numerous physicochemical and fingerprint properties
- Filter poor candidates with undesirable functional groups and Lipinski and Veber rules
- Multiple rapid and exhaustive conformation generation and analysis methods
- Build multi-conformational indexed databases for rapid searching

SELECTION AND ANALYSIS TOOLS

- 3D visualization of libraries using PCA analysis
- Diverse, focused and similar subset selections
- Clustering tools
- Selection and sorting with Pareto multiple objective optimization
- Compare and augment libraries

FEATURE PERCEPTION

- Robust default **Catalyst**® pharmacophore feature definitions, including shape and excluded volume

Create and edit customized pharmacophore features to tailor to your chemistry

CATALYST PHARMACOPHORE GENERATION

- Generate qualitative common feature pharmacophores **(HipHop)**
- Generate quantitative SAR pharmacophores correlating binding activity with pharmacophore features **(HypoGen)**
- Refine ligand-based pharmacophores using inactive compounds **(HipHopRefine/HypoGenRefine)**
- Generate pharmacophores from protein-ligand complexes and protein active sites
- Generate fragment-based pharmacophores
- Automatically validate generated hypotheses

CATALYST VIRTUAL SCREENING

- Rapidly screen millions of ligands to identify potential lead candidates
- Sophisticated pharmacophore matching (minimum, maximum, partial mapping, required features, group features, negative features)
- Fast, complementary alternative to classical docking
- Characterize protein active sites and identify key residues and features

LEAD IDENTIFICATION AND OPTIMIZATION

- Explore alternative scaffolds
- Predict activities with quantitative pharmacophores
- Modify functional groups of ligands to better match to pharmacophores
- Study multiple mappings and alignments to understand SAR
- Screen fragments to optimize a scaffold

LIGAND PROFILING

- Explore off-target activity and drug repurposing using **PharmaDB**, a database of structure-based pharmacophores derived from over 7000 protein-ligand x-ray complexes*
- Create your own database of annotated pharmacophores
- Analyze profiling results with interactive heatmaps and the ligand alignments

POST-PROCESSING AND ANALYSIS

- Rank identified ligands with FitValue or predicted activities
- Filter virtual screening poses for specific features
- Cluster, merge and compare pharmacophores
- Manage and compare search hitlists
- Generate ROC curves, hit-rate plots and heatmaps

*** Built in collaboration with Dr Didier Rognan of the University of Strasbourg using the scPDB database (bioinfo-pharma.u-strasbg.fr/scPDB/)**

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