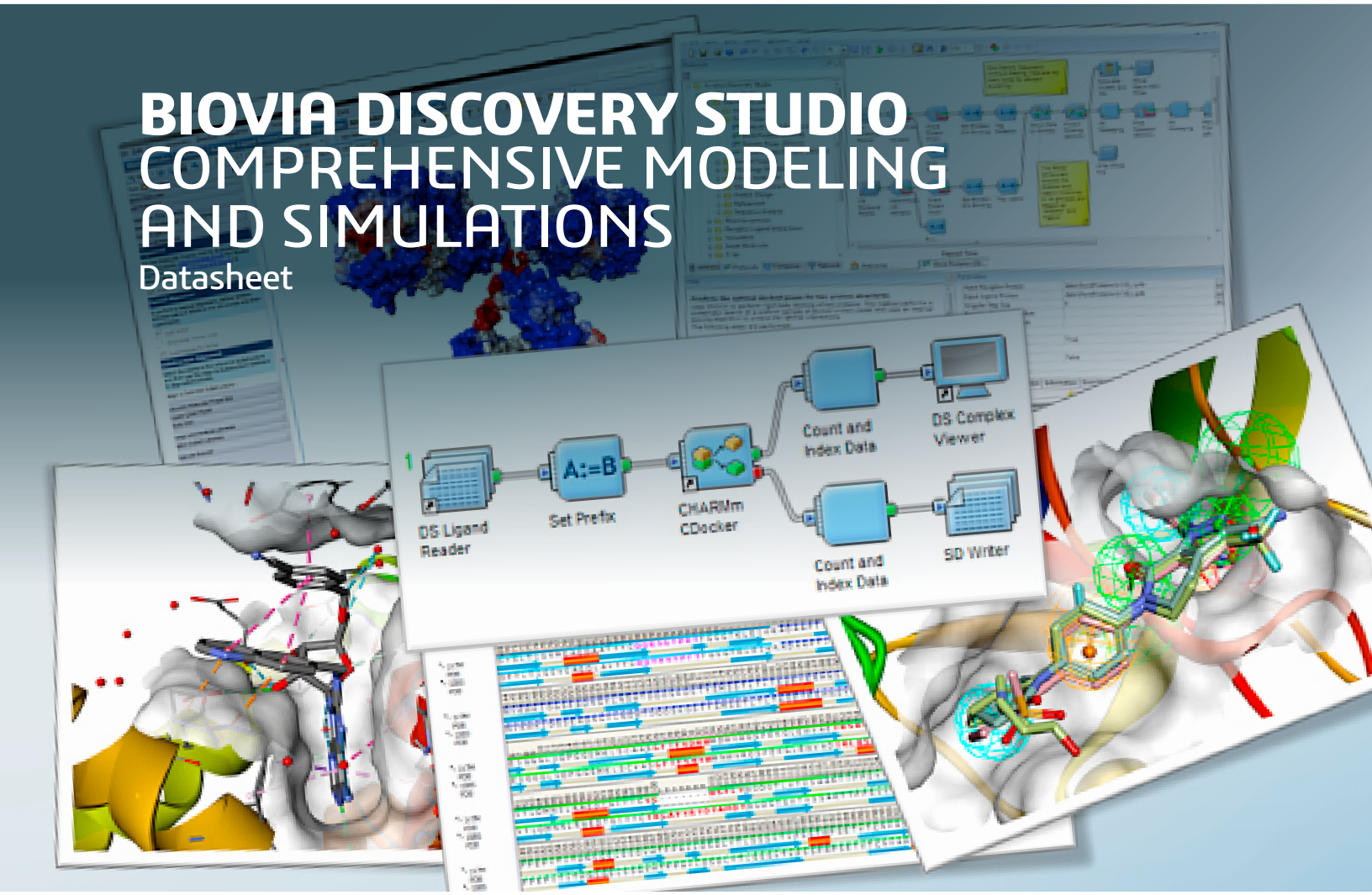
BIOVIA

3DEXPERIENCE®

BIOVIA DISCOVERY STUDIO
COMPREHENSIVE MODELING AND SIMULATIONS
Datasheet



A SUITE OF VALIDATED SCIENCE TECHNOLOGIES

Drug discovery is a multi-objective optimization. Scientists have to optimize both biochemical potency and at the same time, optimize other characteristics such as ADME and toxicity. Built on BIOVIA Pipeline Pilot and utilizing gold-standard applications backed by years of peer-reviewed research (e.g., **CHARMm, MODELER, ZDock, Delphi, Catalyst, DMol³, Vamp, TopKat, AggMap** and **Developability Index**), BIOVIA Discovery Studio® software is the most comprehensive, scalable, collaborative research environment for Life Sciences discovery research.

DASSAULT SYSTEMES

BIOVIA DISCOVERY STUDIO

BIOVIA Discovery Studio is a comprehensive suite of validated science applications built on **BIOVIA Pipeline Pilot**. The software delivers a unique blend of open, scalable, collaborative research tools designed for today's Life Sciences discovery research needs.

Comprehensive science portfolio

- Science solutions address research needs from early stage discovery through to preclinical and biotherapeutic formulations development

Mature science

- The core science underpinning Discovery Studio is backed by up to 30 years of peer-reviewed research

Collaborative research

- With DS Visualizer, Discovery Studio offers a genuinely free visualization and collaboration framework

Discovery Studio: A native Pipeline Pilot-based application

- Every Discovery Studio task is a Pipeline Pilot protocol ensuring a truly open modeling and simulation environment
  - Customizable, extensible science
  - Scalable architecture
  - Deployable workflows
  - Enables scientific innovation
- Out of the box integration with third party applications, including CCDC **GOLD*** and University of Illinois at Urbana-Champaign **NAMD†**
- Discovery Studio sub-licenses the following Pipeline Pilot component collections: Core, Integration, Reporting, Chemistry, Sequence Analysis, ADMET

COMPREHENSIVE PREDICTIVE SCIENCE SUITE

Simulations:

- Best-in-class simulations based on **BIOVIA CHARMm® forcefield engine**, including single point, minimization, Molecular Dynamics simulations and Free energy calculations
- Full ab initio DFT-based Quantum Mechanics with **DMol³**, semi empirical (**VAMP**) and hybrid QM/MM (**DMol³/CHARMm**)

Macromolecule Design and Analysis:

- Market leading **MODELER** homology modeling algorithm
- Best-in-class pH-based protein ionization tools
- Unique pH-based protein stability and binding affinity mutation analysis
- Reliable protein-protein binding prediction with **ZDOCK**

Antibody Development

- The first and most complete set of structure prediction and simulation tools specifically for antibody research
- Proven automated structure prediction workflows designed to deliver best in class antibody homology models
- Unique patented **AggMap** protein aggregation and **Developability Index**
- Rapidly identify sequence motifs associated with post-translational modification (PTM) sites in biotherapeutics

Structure-based design (SBD)

- Novel physics-based (**CHARMm CDOCKER**) docking engine
- Unique set of non-bond analysis monitors that include favourable, unfavourable and unsatisfied interaction types
- Novel MMP-based Activity Cliffs

Fragment-based design (FBD)

- Use classical Medicinal Chemistry reactions to enumerate ***in situ***, using ***ca***. 10k pre-filtered reagents from **BIOVIA ACD**
- Scaffold hop ***in situ*** using ***ca.*** 1.5M commercially available compounds from **BIOVIA SCD**
- Novel Karplus **MCSS** (Multiple Copy Simultaneous Search) fragment docking engine

Pharmacophore and Ligand-based design:

- Market leading **CATALYST** pharmacophore engine
- Includes unique receptor-ligand pharmacophore creation
- The largest validated ligand profiling database, **PharmaDB**

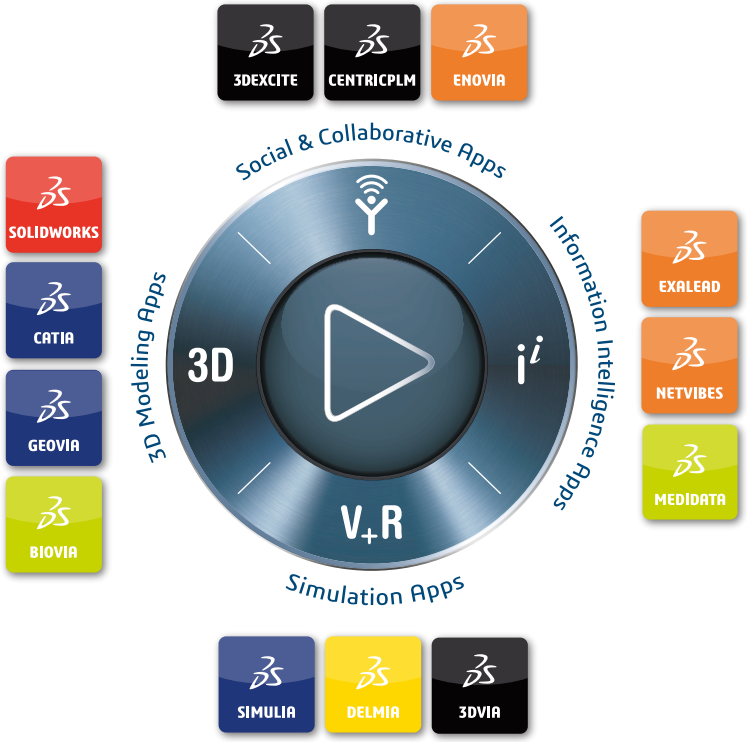
QSAR, ADMET and TOPKAT Predictive Toxicology

- QSAR: Calculate physicochemical, topological fingerprint properties and create PLS, GFA, MLR and more
- Most extensive set of ADMET and predictive toxicology models, including BBB penetration, Hepatotoxicity, CYP2D6, AMES, Rat Oral LD50 and many more

X-ray

- Using **CNX**, generate electron density maps, perform full refinements and use **HT-X PIPE** to run automated structure determination of protein-ligand complexes

To learn more about BIOVIA Discovery Studio, go to:
3ds.com/biovia



Our **3D**EXPERIENCE® platform powers our brand applications, serving 11 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the **3D**EXPERIENCE® Company, provides business and people with virtual universes to imagine sustainable innovations. Its world-leading solutions transform the way products are designed, produced, and supported. Dassault Systèmes' collaborative solutions foster social innovation, expanding possibilities for the virtual world to improve the real world. The group brings value to over 250,000 customers of all sizes in all industries in more than 140 countries. For more information, visit **www.3ds.com**.

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