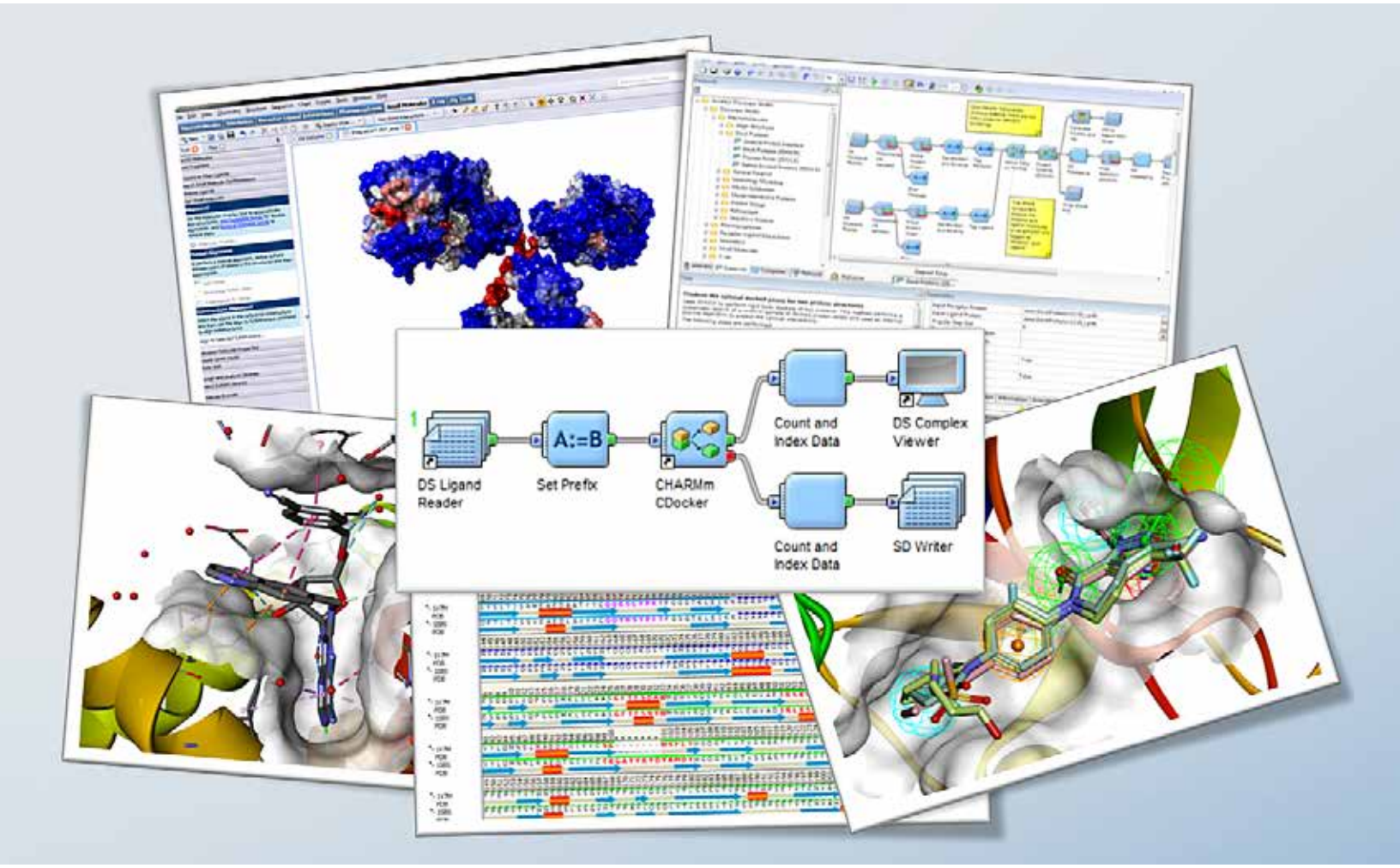
DASSAULT SYSTEMES

BIOVIA

BIOVIA DISCOVERY STUDIO

COMPREHENSIVE MODELING AND SIMULATIONS FOR LIFE SCIENCES

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.

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 accelrys.com/products/collaborative-science/biovia-discovery-studio

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*** GOLD** is available from the Cambridge Crystallographic Data Centre: http://www.ccdc.cam.ac.uk/products/life_sciences/gold
† NAMD is distributed with Discovery Studio in agreement with the University of Illinois at Urbana-Champaign. *http://www.ks.uiuc.edu/Research/namd/*

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