3DEXPERIENCE®

Introducing Discovery Studio

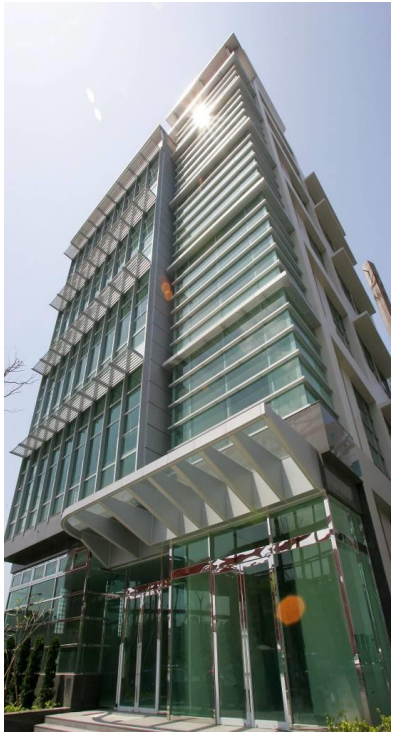
What's New in DS2022

創源生技 分子數位中心

Copyright and Disclaimer

- Copyright © 2022 GGA corp. All rights reserved.
  - This presentation and/or any related documents contains statements regarding our plans or expectations for future features, enhancements or functionalities of current or future products (collectively "Enhancements"). Our plans or expectations are subject to change at any time at our discretion. Accordingly, GGA Corp. is making no representation, undertaking no commitment or legal obligation to create, develop or license any product or Enhancements.
  - The presentation, documents or any related statements are not intended to, nor shall, create any legal obligation upon GGA Corp., and shall not be relied upon in purchasing any product. Any such obligation shall only result from a written agreement executed by both parties.
  - In addition, information disclosed in this presentation and related documents, whether oral or written, is confidential or proprietary information of GGA Corp.. It shall be used only for the purpose of furthering our business relationship, and shall not be disclosed to third parties.

GGA is part of the BIONET Group (訊聯生物科技)



CEO: Christopher Tsai, Ph.D. 蔡政憲 博士

Established: Nov. 2008

Main Product & Service Areas:

1. Genetic Testing
2. Molecular Diagnosis
3. **Scientific Informatics & Bio IT**

IPO Date: September 17, 2012

Stock Ticker: 4160 (Taiwan OTC)

版本差異

版本別	Biology	Chemistry
DS2020	• Solubility and Viscosity prediction for biologics • Explicit membrane-based MD simulations. • Prepare Proteins: Can now take multiple protein molecules as input and runs in parallel • Predict Humanizing Mutations: V and J genes can be specified for both the H and L chains	• Multi-Site Lambda Dynamics via CHARMm-DOMDEC for both GPU and CPU, for exploring large congeneric chemistry space in early lead optimization. • Ensemble Pharmacophore Generation: A new protocol to generate ensemble pharmacophores from large sets of active and inactive ligands. • The 2D binding sites diagram can now also be used with nucleic acid-ligand complexes.
DS2021	• Accelerate calculations by GPU - Dock Proteins (ZDOCK), Solvate with Explicit Membrane • Calculate Protein Formulation Properties: Viscosity and Aggregation prediction	• Accelerate calculations by GPU - Dynamics (NAMD) & MSLD Bias Optimization and Production 、CHARMm Relative FEP Calculations • MSLD Bias Optimization and Production: combine three steps in one protocol. • CHARMm Relative FEP Calculations: run FEP calculations of multiple systems.
DS2022	• Added a new protocol, Predict Excipient Interactions, that predicts the preferential interaction of common excipients with antibody surface residues for antibody formulation • Enhanced the Calculate Protein Formulation Properties protocol to create aggregation sites and surfaces that can be analyzed using the View Aggregation Sites tools.	• Enhanced the Interaction Pharmacophore Generation protocol • Added an option to the Ligand Profiler protocol to maximize the number of features or maximize the pharmacophore fit • Added a new parameter to the Screen Library protocol, Screen Best Only

版本差異

版本別	Core/Platform
DS2020	• PharmaDB: Updated to the latest version based on scPDB release 2017. It now contains over 250,000 pharmacophore models with 16,034 entries. • Dock Ligands (GOLD): Now supports covalent ligand docking. • CHARMm: Incorporates the latest release of the academic CHARMM, version c43b23. • NAMD: Distributed with the CPU edition, version 2.12 • MODELER: Incorporates the latest release of the academic MODELLER, version 9.224. • BLAST+: The BLAST+ version in Discovery Studio has been updated to version 2.9 • GOLD: Supports GOLD 2019 (version 5.7)
DS2021	• CHARMm: Incorporates the latest release of the academic CHARMm code, version c44b2 • NAMD: Distributed with the CPU and GPU edition, version 2.13. • MODELER: Incorporates the latest release of the academic MODELLER, version 9.24 . • BLAST+: The BLAST+ version in Discovery Studio has been updated to version 2.10.1. • GOLD: Supports GOLD 2020 DATABASES • Antibody database、PDB、PDB_nr95、Uniprot、Swiss-Prot: Updated using the July 2020 release.
DS2022	• You can now access the AlphaFold Protein Structure Database from the Open URL dialog. • Added a new visualization script, Color by AlphaFold Model Confidence, to color protein loaded from AlphaFold Protein Structure Database based on the per-residue confidence score. • Updated the Dock Ligands (GOLD) protocol to be compatible with GOLD 2021 • Enhanced the Assign Forcefield protocol to work with RNA and DNA templates from custom RTF files.

NEW AND ENHANCED SCIENCE

- New!
  - Excipient Interactions Prediction - predict molecular interactions for 6 formulation excipients – sorbitol, sucrose, trehalose, proline, arginine·HCl and NaCl.
  - Feature Generation Component - Calculate Protein Features and Calculate Sequence Descriptors components calculate structure- and sequence-based descriptors for machine learning.
- Enhanced!
  - Calculate Protein Formulation Properties protocol now automatically creates aggregation sites and surfaces for analysis with the View Aggregation Sites tools
  - Assign Forcefield protocol now works with RNA and DNA templates from custom RTF files.
  - Nucleic acids supported in the Interaction Pharmacophore Generation protocol.
  - Reduced the memory usage of large solvated systems when running simulations.
  - Access the AlphaFold Protein Structure Database from the Open URL dialog
  - Color proteins from the AlphaFold Protein Structure Database based on the per-residue confidence score.

COMPATIBILITY

- PARTNER SCIENCE
  - CHARMm: Incorporates the academic release CHARMM, version c44b22.
  - NAMD: Distributed with both CPU and GPU editions, version 2.13.
  - MODELER: Incorporates the latest release of the academic MODELLER, version 9.243.
  - BLAST+: The BLAST+ version 2.10.1.
  - GOLD: Supports GOLD 2021.
  - COMPATIBILITY Discovery Studio 2022 is built on BIOVIA Pipeline Pilot 2022

Performance test by GGA corp. - 2022

- HPZ4G4 RTX A6000 GPU
- Motherboard: hp z4 g4 workstation
- CPU: Intel® Xeon® W-2225 4.10 GHz 4core , 8 threads
- RAM: 64GB
- SSD: 512GB
- HDD: 1TB
- GPU: Nvidia RTX A6000
- Power: 750 W
- OS: CentOS Linux release 8.5.2111 (Linux HPZ4G4A6000 4.18.0-348.el8.x86_64 #1 SMP Tue Oct 19 15:14:17 UTC 2021 x86_64 x86_64 x86_64 GNU/Linux)
- V Development Tools
- V RPM Development Tools
- GPU Driver: NVIDIA-Linux-x86_64-460.91.run

Ampere GPU

10,752 NVIDIA® CUDA® 核心
336 NVIDIA® Tensor 核心
84 NVIDIA® RT 核心
48GB GDDR6 記憶體
高達 768GB/s 記憶體頻寬
最大功耗:300W
繪圖匯流排 PCI-E 4.0 x16
主動式散熱
支援 Quadro vDWS虛擬工作站
顯示介面:DP 1.4 (4)
NVLink:2槽位/3槽位低結構橋接器

Performance test by GGA corp.

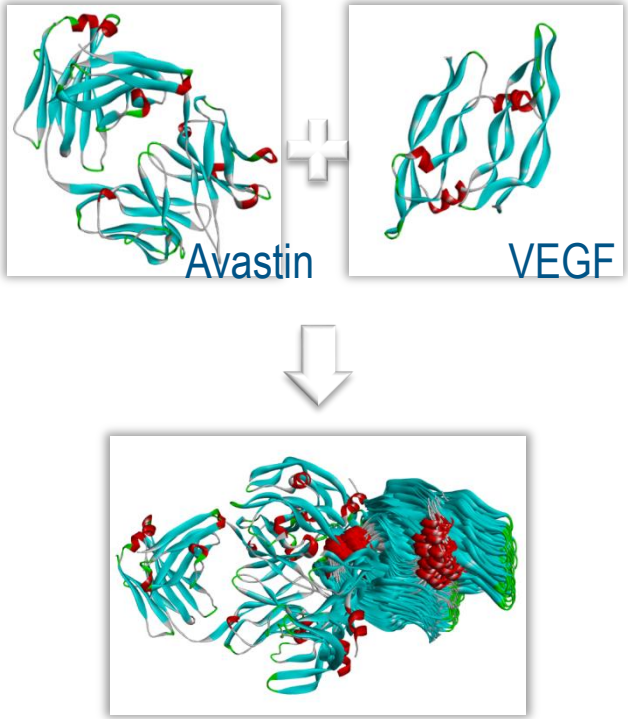
- Test Machine A: (ASUSTek TUF GAMING X570-PLU)
  - CPU: AMD Ryzen 9 3950X 16-Core Processor
  - RAM: 64GB
  - GPU: Nvidia RTX 3070 Super
  - OS: CentOS Linux release 8.3.2011 (4.18.0-240.10.1.el8_3.x86_64)
  - GPU Driver: NVIDIA-Linux-x86_64-460.67 .run
- Discovery Studio Version: 21.1.0.20298

Performance test by GGA corp. - ZDOCK

Sample: Avastin and VEGF

Test Machine A (SuperWorkstation SYS-7039A-i (Black) 工作站):
CPU：SKL-SP Silver 4116 12C/24T 2.1G 16.5M 9.6GT
RAM：96GB (8GBx12) DDR4-2666 1Rx8 ECC REG DIMM
SSD：Intel D3-S4510 240GB, SATA 6Gb/s, 3D, TLC 2.5", 7.0mm, up to 2DWPD
GPU： NVIDIA RTX2080TI 11GB

Platform (RTX2080)	Angular Step Size	Elapse time
CPU: 8 processors	6	1:03:00
GPU	6	0:29:46
CPU: 8 processors	15	0:06:40
GPU	15	0:03:51

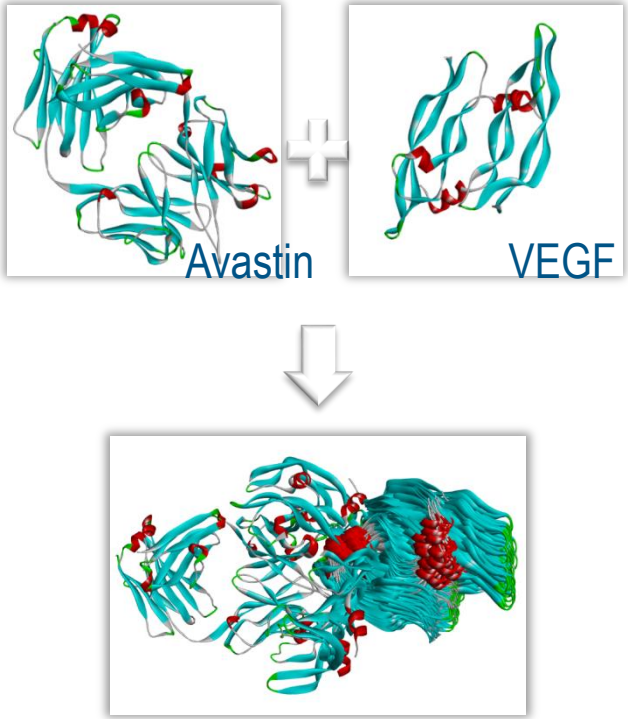


Performance test by GGA corp. - ZDOCK

Sample: Avastin and VEGF

Test Machine B: (ASUSTek TUF GAMING X570-PLU)
CPU: AMD Ryzen 9 3950X 16-Core Processor
RAM: 64GB
GPU: Nvidia RTX 3070 Super
OS: CentOS Linux release 8.3.2011 (4.18.0-240.10.1.el8_3.x86_64)
GPU Driver: NVIDIA-Linux-x86_64-460.67.run

Platform (RTX3070)	Angular Step Size	Elapse time
CPU: 8 processors	6	0:36:05
GPU	6	0:22:52
CPU: 8 processors	15	0:04:22
GPU	15	0:02:09



Performance test by GGA corp. - ZDOCK

Sample: Avastin and VEGF

Test Machine A (SYS-7039A-i (Black) 工作站):
CPU：SKL-SP Silver 4116 12C/24T 2.1G 16.5M 9.6GT
RAM：96GB (8GBx12) DDR4-2666 1Rx8 ECC REG DIMM
SSD：Intel D3-S4510 240GB, SATA 6Gb/s, 3D, TLC 2.5", 7.0mm, up to 2DWPD
GPU： NVIDIA RTX2080TI 11GB

Test Machine B: (ASUSTek TUF GAMING X570-PLU)
CPU: AMD Ryzen 9 3950X 16-Core Processor
RAM: 64GB
GPU: Nvidia RTX 3070 Super
OS: CentOS Linux release 8.3.2011 (4.18.0-240.10.1.el8_3.x86_64)
GPU Driver: NVIDIA-Linux-x86_64-460.67.run

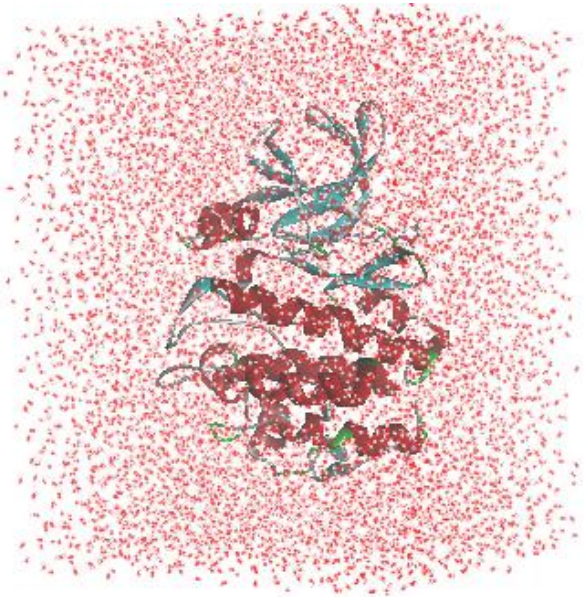
Test Machine C: (hp z4 g4 workstation)
CPU: Intel® Xeon® W-2225 4.1GHz 4core , 8 threads
RAM: 64GB
GPU: Nvidia RTX A6000
OS: CentOS Linux release 8.3.2011 (4.18.0-240.10.1.el8_3.x86_64)
GPU Driver: NVIDIA-Linux-x86_64-450.66.run

Platform	Angular Step Size	Elapse time RTX 2080	Elapse time RTX 3070	Elapse time RTX A6000
CPU: 8 processors	6	1:03:00	0:36:05	0:30:00
GPU	6	0:29:46	0:22:52	0:19:24
CPU: 8 processors	15	0:06:40	0:04:22	0:03:18
GPU	15	0:03:51	0:02:09	0:02:22

Performance test by GGA corp. – Dynamic (Production)

Sample: TBK1 region in explicit solvent model, 28,940 atoms

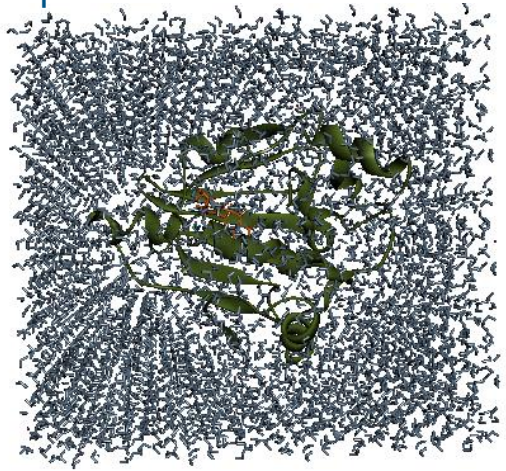
Platform (A)	Simulation time	Elapse time (RTX3070)	Elapse time (RTX A6000)
CPU: 8 processors	500ps	4:22:02(~260min)	-
GPU	500ps	0:06:24(~6min)	0:04:53(~5min)
GPU	1ns	0:13:22(~13min)	0:09:14(~9min)
GPU	10ns	1:50:43 (~110min)	1:29:13(~90min)



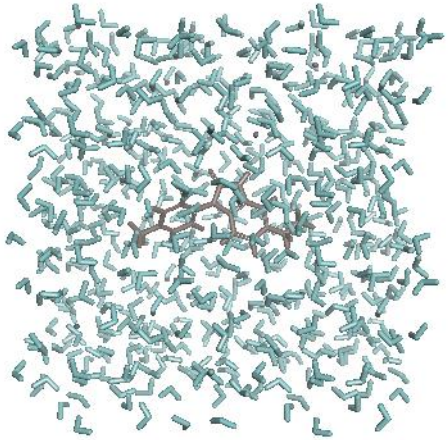
Multi-Site Lambda Dynamics

▶ MSLD Bias Optimization and Production

Complex



Ligand



Platform	Simulation time	Elapse time
GPU (A)	20ns	62:04:25
GPU (B)	20ns	112:32:29
A6000	10ns	40:23:52

MSLD Bias Optimization and Production

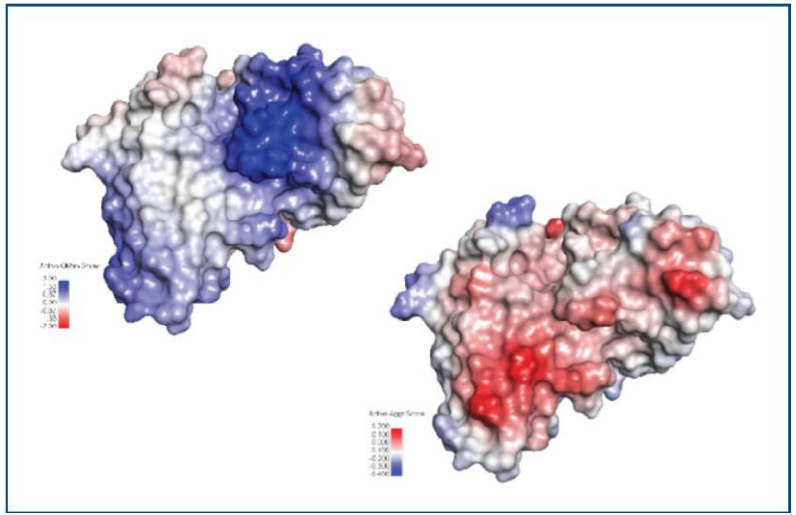
Parameter Name	Parameter Value
Input MSLD Systems	Binding
Solvated Complex	MSLD_systems:Complex
Solvated Ligand	MSLD_systems:Ligand
Vacuum Ligand	
Platform	DOMDEC GPU
GPU Device	
Number of Cores per Simulation	1
Bias Optimization	Start
Production	True
Number of Simulations	3
Simulation Time (ps)	20000
Equilibration Time (ps)	200
Save Results Interval (ps)	100
Number of Simulations to ...	1
Advanced	
Parallel Processing	False

NEW AND ENHANCED SCIENCE

- New!
  - MSLD Bias Optimization and Production: combine three steps in one protocol.
  - CHARMm Relative FEP Calculations: run FEP calculations of multiple systems.
- New! Accelerate calculations by GPU
  - Solvate with Explicit Membrane 、Dynamics (NAMD) & Dock Proteins (ZDOCK)
  - MSLD Bias Optimization and Production 、CHARMm Relative FEP Calculations
- Enhanced!
  - Calculate Protein Formulation Properties: Viscosity and Aggregation prediction
  - Additional non-bond Pharmacophores features
  - Protein modeling and database update

Calculate Protein Formulation Properties

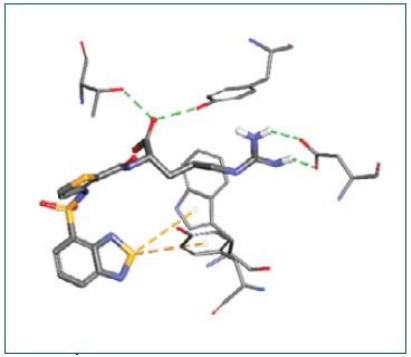
- Viscosity and Aggregation prediction for biologics.
- Calculate Protein Formulation Properties protocol automatically generates Charge Map3 and Aggregation Scores3 surfaces.

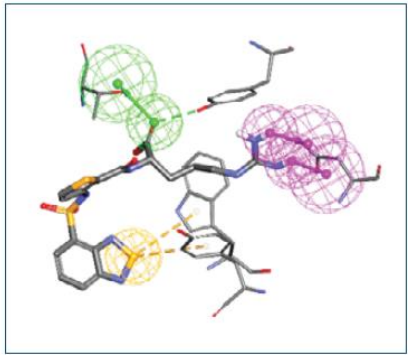


Charge QMap (left) and Aggregation Scores (right) surfaces on an antibody structure.

Additional Non-bond pharmacophore features

- Non-bond pharmacophore features
  - Ligand-based pharmacophore protocols
  - Edit and Cluster Features tool panel
- PharmaDB scPDB receptor-ligand targets updated with nonbond pharmacophore features. (Ligand Profiler)





Interactions pharmacophores harmonize with non-bond feature perception.

NEW AND ENHANCED SCIENCE

- New! CHARMm GPU support via OpenMM interface for running molecular dynamics simulations
- Enhanced! Grid support for simulation protocols
- Enhanced! Various protein modeling enhancements
- New! New protocol, Analyze Crystal Contacts, to generate and analyze crystal contacts

Update!

- **PARTNER SCIENCE**
  - **CHARMm**: Incorporates the latest release of the academic CHARMm code, version c44b2
  - **NAMD**: Distributed with the CPU and GPU edition, version 2.13.
  - **MODELER**: Incorporates the latest release of the academic MODELLER, version 9.24 .
  - **BLAST+**: The BLAST+ version in Discovery Studio has been updated to version 2.10.1.
  - **GOLD:** Supports GOLD 2020
- **DATABASES**
  - Antibody database、PDB、PDB_nr95、Uniprot、Swiss-Prot: Updated using the July 2020 release.