

# Product Licenses and Token Usage for Schrödinger Release 2024-1

## Small Molecule Drug Design

Product Dependencies	Tokens
Maestro	**
(Deep)AutoQSAR#	2
Canvas	1
ConfGen	1
Core Hopping	5
Shape Screening	
Epik	1
Field-based QSAR	5
Glide	5
Glide, SMILES input (optional, recommended)	5
Glide XP Visualizer	6
Epik (required)	
Glide (required)	
Glide, SMILES input (optional, recommended)	6
Jaguar	2
NBO 7 (optional, recommended)	
Jaguar pKa	3
Jaguar (required)	
MacroModel (optional, recommended)	
KNIME	**
LigPrep	1
MacroModel	2
Membrane Permeability	8
Epik (required)	
LigPrep (required)	
Prime (required)	
QikProp (required)	
OPLS	**
P450 Site-of-Metabolism (SOM)	8
Prime (required)	
Glide (required)	
Phenix/OPLS	8
Prime (required)	
Phenix (third party)	

Product Dependencies	Tokens
Phase	5
Epik (required)	
LigPrep (required)	
MacroModel (optional, recommended)	
Prime	8
Prime MM-GBSA	8
Prime (required)	
PrimeX	8
Epik (optional, recommended)	
QikProp	2
QSite	4
Jaguar (required)	
Shape Screening	
CPU	1
GPU	8
SiteMap	1

**Product Dependencies:** A selection of products utilize the functionalities of separate products for full featured job execution.

**Tokens:** The number of tokens simultaneously used during the course of execution on one processor/core. Select job types may utilize fewer tokens.

**Workflows:** The number of tokens simultaneously used during the course of execution on one processor/core. Select job types may utilize fewer tokens.

\*\* Access license

# Also available as an access license

# Small Molecule Drug Design

Workflows	Tokens
Covalent Docking	8
ConfGen ( <b>required</b> )	
Glide ( <b>required</b> )	
MacroModel ( <b>required</b> )	
Prime ( <b>required</b> )	
e-Pharmacophores	5
Phase ( <b>required</b> )	
Glide EM	8
Glide ( <b>required</b> )	
Jaguar (optional, recommended)	
Prime (optional, recommended)	
PrimeX ( <b>required</b> )	
Induced Fit Docking	8
Glide ( <b>required</b> )	
Prime ( <b>required</b> )	
Ligand Designer~	5/10
Glide ( <b>required</b> )	
Phase ( <b>required</b> )	
Prime (optional, recommended)	
FPSim-GPU (optional, recommended)	
LigPrep (optional, recommended)	
Macrocycle Docking	8
Glide ( <b>required</b> )	
LigPrep ( <b>required</b> )	
OPLS ( <b>required</b> )	
Prime ( <b>required</b> )	
Macrocycle Permeability	8
Membrane Permeability ( <b>required</b> )	
Prime ( <b>required</b> )	
Macrocycle Sampling	8
Prime ( <b>required</b> )	
Macrocycle Stability	8
Prime ( <b>required</b> )	
PathFinder^	
Protein Preparation Wizard	1
Epik (optional, recommended)	
Glide (optional, recommended)	
QM-Polarized Ligand Docking (QPLD)	5

Workflows	Tokens
Glide ( <b>required</b> )	
QSite ( <b>required</b> )	
Virtual Screening (VSW)	5
Glide	
LigPrep	
Epik (optional, recommended)	
MacroModel (optional, recommended)	
Prime (optional, recommended)	
QikProp (optional, recommended)	

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~ Standard mode requires 5 tokens and fast mode requires 10 tokens.

^ Also included with Maestro access license

## Materials Science

### Product Dependencies Tokens

MS Maestro*	
(Deep)AutoQSAR	2
Canvas	1
Epik	1
GA Optoelectronics	10
Jaguar	2
Jaguar pKa	3
LigPrep	1
MacroModel	2
MS CG	1
MS Maestro (required)	
Desmond GPU (required)	
MS Dielectric	1
MS Maestro (required)	
Desmond GPU (required)	
Jaguar (required)	
MS Informatics	1
MS Maestro (required)	
Canvas (required)	
(Deep)AutoQSAR (optional, recommended)	
MS Microkinetics	1
MS Maestro (required)	
MS Morph	1
MS Maestro (required)	
Desmond GPU (required)	
MS Penetrant	1
MS Maestro (required)	
Desmond GPU (required)	
MS Transport	1
MS Maestro (required)	
Desmond GPU (required)	
QikProp	2
Quantum Espresso Interface	1
MS Maestro (required)	

### Workflows Tokens

MS Reactivity	2
Canvas (required)	1
FF Builder (required)	**
Jaguar (required)	2
MacroModel (required)	2
MS Maestro (required)	1
MS Reactivity (required)	1
OPLS (required)	1

## Biologics

### Product Dependencies Tokens

Maestro	**
BioLuminate*	
Canvas	1
Epik	1
Jaguar	2
MacroModel	2
PIPER*	
Prime	8
QSite	4
SiteMap (optional)	1

### Workflows Tokens

Antibody Structure Prediction	8
BioLuminate (required)	**
Prime (required)	8
Antibody Humanization	8
BioLuminate (required)	**
Prime (required)	8
Protein Preparation Wizard	1
Epik (optional, recommended)	
Glide (optional, recommended)	
Protein-Protein Docking+	
BioLuminate (required)	**
PIPER+	
Residue Scanning	8
BioLuminate (required)	**
Prime (required)	8

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+ BioLuminate, PIPER, and MS Maestro licenses are provided outside of the token library.

\*\* Access license

## Advanced Technologies Requires Additional License

Active Learning Glide\*

Active Learning Access\*\* (required)

(Deep)AutoQSAR (required)

Epik (required)

Glide (required)

AutoTS

Jaguar (required)

MacroModel (required)

Desmond GPU\*

Constant pH in Desmond GPU requires a FEP+ license to run

FEP+\*

Force Field Builder

FPSim-GPU

IFD-MD\*

Desmond GPU (required)

WaterMap (required)

Macro pKa

Mopac

WaterMap\*

## Token Usage per GPU For Desmond GPU, FEP+ and WaterMap

GPU Card	Tokens per GPU
A100	22
H100	46
L4	24
T4	8
Quadro RTX 5000	10
Quadro RTX A5000	26
Quadro RTX A4000	19
V100	16

Schrödinger GPU-based products (Desmond, WaterMap, and FEP+) scale license usage based on the number of GPU cores on which a user is running.

\* Requires a GPU

\*\* Access license

For additional information, please contact your **Account Manager** or email [help@schrodinger.com](mailto:help@schrodinger.com).

