



MolDesk Basic ver.1.1

Software package for in silico drug design www.moldesk.com

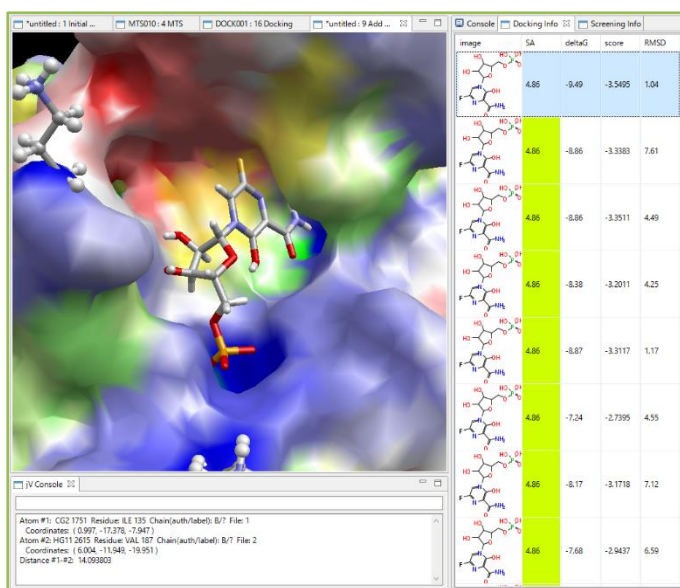
Anything MD, Anywhere Docking

Fully automated, most PDB structure optimization, MD calculations, and docking calculations for most PDBs.

myPresto(*) is used as the calculation engine.

GROMACS can also be used as an MD calculation program.

Protein-compound docking simulation



MolDesk shows results of docking simulation in order of docking scores and allows users to visually confirm the docking poses.

MolDesk provides a list with docking scores as well as corresponding ΔG values estimated with a simple regression model and the RMSD value against the initial coordinates of each compound's molecules.

By clicking the score or the arrow keys, the user can view each docking pose. The user can also superimpose multiple docking poses.

Boost docking by Solution NMR data

Solution NMR data (DIRECTION epitope-mapping method) of non-label solution NMR data can improve your protein-compound docking poses.

Y. Mizukoshi, et al., An accurate pharmacophore mapping method by NMR spectroscopy. *Angew. Chem. Int. Ed. Engl.*, **2012**, *51*(6), 1362-1365.

Figure 1. Docking simulation result.

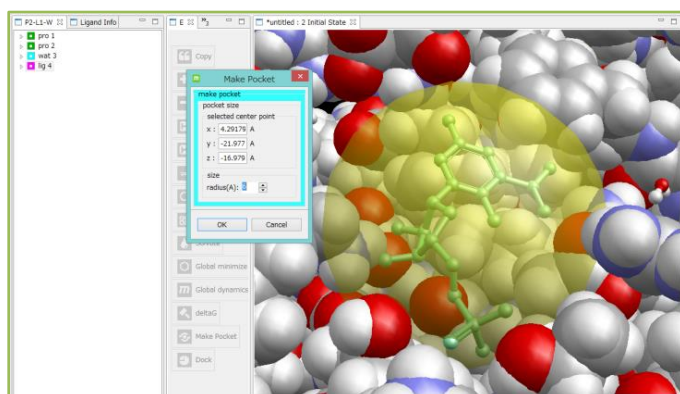


Figure 2. Ligand-binding pocket addressing.

Users can indicate the center of the binding site by either directly entering the coordinates or selecting multiple atoms of the target protein.

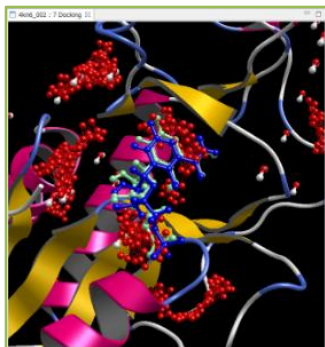
MolDesk shows the synthetic accessibility (SA) of all compounds in the list based on their 2D chemical structures. SA value is updated in real time in molecular editing process.

image	name	SA
	lig 4	7.84
	lig 5	2.76
	lig 6	5.71
	lig 7	3.94

Figure 3. Synthetic accessibility.

※1 myPresto is the software of Japan Biological Informatics Consortium developed by the National Institute of Advanced Industrial Science and Technology, JBIC, Osaka University Institute of Protein Research, etc. supported by AMED, Ministry of Economy, Trade and Industry, and NEDO.

Pocket search (with parallel processing)

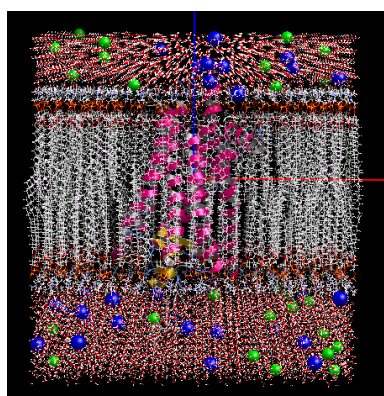


MolDesk can search ligand-binding pockets of a given protein structure with Molecular-docking binding-Site finding (MolSite). This method uses a probe compound library consisting of sets of arbitrarily selected compounds. MolSite performs round-robin docking simulation of the compounds from the compound library against the protein's whole surface, and suggests the protein site that shows the strongest affinity as ligand-binding sites (ligand-binding pocket.)

Figure 4 shows the structure of reconstructed model in a self-docking example (PDBID: 4kn6) with an accuracy of RMSD=1.08Å (Blue: experimental data, Green: predicted ligand structure, Red dots: suggested ligand-binding pockets.) Pocket search does not always provide predictions with such high accuracy, but produces much better results compared to existing geometrical approaches. Pocket search runs with thread-parallel processing similarly to virtual screening.

Figure 4. A docking pose in a ligand-binding pocket found by MolSite (PDBID 4kn6.)

Creation of lipid bilayer system



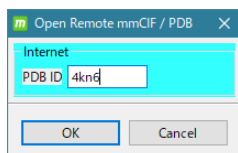
In addition to the creation of general MD calculation systems, lipid bilayer systems can be created automatically by simply selecting a protein or other material.

Lipid bilayers can be created with six different lipid molecule composition ratios. MD calculations can be performed by creating cubic water-soluble systems containing neutralizing ions.

- * Fast MD calculation and trajectory analysis with GROMACS. (Windows has GROMACS already implemented and does not require user installation.) (Linux and MAC require user installation of GROMACS.)
- * MD calculations with myPresto are serviced by MolDesk Screening for high-speed parallel calculations using MPI/GPU, and by MolDesk Basic for sequential calculations only.

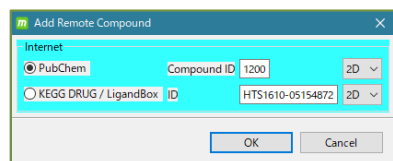
Figure 5. Lipid bilayer system

Molecular Input and Display of electrostatic potential surface



Users can remotely download mmCIF and PDB files by entering PDB IDs (4-character codes) in MolDesk and immediately start calculation / simulation.

Figure 6. Protein downloader window.



Users can remotely download molecular structure files by entering the compound's LigandBox/PubChem ID in MolDesk.

Figure 7. Compound downloader window.

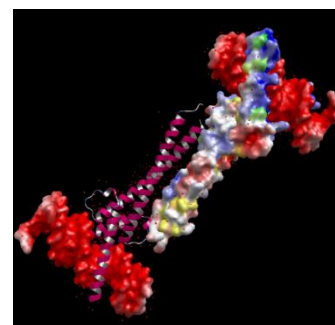
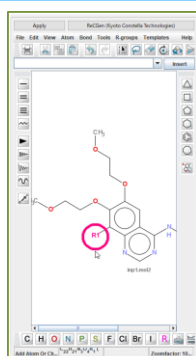


Figure 8. Electrostatic potential surface.

MolDesk can display precise electrostatic potential surface of the protein provided by eF-site and the surface of the protein's cavity.

JChemPaint (2D compound editing)



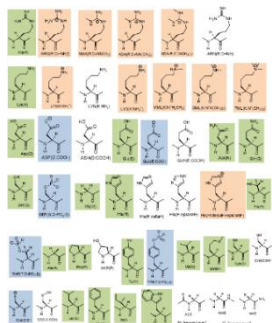
As shown in Figure 8, a user can prepare a molecular structure using JChemPaint, and MolDesk converts its 2D molecular structure to 3D molecular structure to be used in user's own drug design calculation.

Figure 9. Editing 2D compounds.

Compound 2D → 3D batch conversion

Create 3D mol2 files with multiple sdf / mol / mol2 / SMILES files as input, adding H atoms and charges to all molecules and taking into account conformers and optical isomers in the AMBER GAFF2 force field. Some characteristic values such as molecular weight, charge, HOMO/LUMO, etc. are also described.

Chemical modification of amino-acid residue



Users can replace any kind of amino-acid residues of a protein with 40 kinds of chemically modified residues registered in the program.

For example, when you convert the ARN (arginine in AMBER force field), MolDesk produces a table of candidates for conversion as shown on the right. Users can easily process replacement by selecting respective amino acid residues.

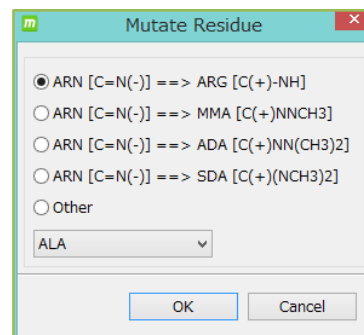


Figure 6. 40 kinds of chemically modified residues.

Figure 7. ARN converter window.

MolDesk Basic Function List

Contents	Functions
Operating System	Windows 11 / 10 (64bit), Linux (64bit) macOS ver. 10.11 or higher (Does not work with Ventura 13.0 or later)
input file	mmCIF pdb mol2 sdf mol SMILES (multi is also possible for mol2 / SMILES) mmCIF(pdb) and compound files can be input via the Internet
output file	mmCIF, pdb, mol2, topology file, MD / Docking calculation setup file, MD / Docking calculation result files, etc. (above, myPresto specification) 3D screen png image file (pixel size can be changed)
External molecular input	Load any mmCIF pdb mol2 sdf mol SMILES (mol2 / SMILES can be multi) into an existing system by mouse click point or file coordinates
Compound (ligand) editing	2D editor (JChemPaint), 2D chemical structure and ease of synthesis list view, H-atom deletion/addition, atom(s) deletion/substitution/addition, structure substitution H atom deletion/addition, atom(s) deletion/substitution/addition, structure substitution, bond deletion/order substitution/rotation, structure optimization (Clean Geometry) Bond deletion, order substitution, rotation, structure optimization (Clean Geometry) Charge calculation (Gasteiger or MOPAC7 AM1 / PM3 / AM1-BCC)
Solvent and ion addition	The TIP3P group of rectangles and spheres (Cap) are generated at the margin from the molecule. Or, add arbitrary size to the center of the mouse click point. Ion (Na ⁺ ,K ⁺ ,Cl ⁻) neutralized concentration, added by concentration/number specification etc.
Automatic generation of lipid bilayer systems	Automatic arrangement of proteins and other substances in lipid bilayer systems with arbitrary composition ratios of six lipid molecules
Compound 2D -> 3D batch conversion	Create 3D mol2 files using AMBER GAFF2 force field, taking into account conformer and optical isomers
structural optimization (Clean Geometry)	Amber ff99SB force field, GAFF2 force field, positional constraints on mouse-selected atoms, and Positional constraint of protein main chain, fast structural optimization of ligand and periphery only
MD Calculation	Amber ff99SB force field, GAFF2 force field, mouse-selected atoms can be position-constrained. Positional constraints on the protein main chain, NVT, NPT, NVE ensemble, and Coulomb force: FMM (solvent water is a sphere) / PME (solvent water is a rectangle). Restart function, automatic loading of boundary conditions when recalculating. GROMACS can be used as MD calculation program.

MolDesk Basic Function List

Contents	Functions
MD Calculation result analysis	Trajectory movies (GROMACS, AMBER, etc. are acceptable), Various energies, Temperature, Atomic distance between any two points, Arbitrary two-sided angle, Time-varying graphs linked to movies Graphical display of almost all GROMACS trajectory analysis results in conjunction with the animation.
Manual docking calculation	Structural optimization of docking poses by placing ligands near protein pockets, Listing of binding free energy ΔG
Search for ligand binding pockets in proteins	Search by fast and simple method of prediction based on protein structure alone. Highly accurate Molsite method with docking calculations is available at MolDesk Screening
Synthetic Accessibility of compounds	Calculate and list the Synthetic Accessibility of a compound.
Docking calculations	List display of docking poses and various property values obtained from docking calculations. Switching between docking poses in the list view by using the up \uparrow and down \downarrow keys on the 3D diagram of the docking poses. Pocket side can be user-specified protein, nucleic acid, ion, metal, or water molecule complexes. Mouse selection of pocket center atoms, deletion of pocket probe points, specification of number of candidate structures, and structural clustering of multiple candidate structures, Fast calculations when docking many ligands (Grid Potential Reuse).
Docking calculations using solution NMR experimental signals.	Prediction of docking structure by solution NMR experimental signal
Project Management	Create new project, open existing project, copy, export, import
UNDO REDO	Unlimited number of times. All processes can be saved and restored. User-created 3D views of each process can be saved in full, atom-by-atom
Molecular display	Wireframe, Stick, Ball stick, Space fill, Protein backbone view, Tube view, Ribbon view, Cartoon view, Surface view (Polygon view), Cavity view, SNFG, Label view, and Slab display (z-clipping plane function), three types of center resets, and Hydrogen bonding display, Electrostatic potential surface display, Stereo display with anaglyphs, and switch between perspective (perspective projection) and parallel (parallel projection) projection modes.
color coordination	Monochrome display, CPK display, Shapely display, Group display, Chain display, Temperature display, Structure display, Charge display, Residue display, Polygon transparency specification
molecular manipulation	Zoom in/out with mouse wheel, rotate, move, delete with mouse

License

Product name	Price (excluding tax)
MolDesk Basic	[Please contact us.] perpetual licence + 1 year maintenance 1 node
	A separate contract is required for maintenance after the second year. Maintenance includes version upgrades and bug support.

Operating OS : Windows 11/10(64bit), Linux(64bit), macOS 10.11 or later.



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