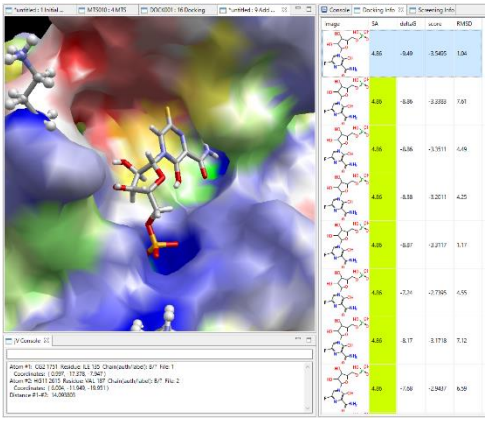
MolDesk Basic ver.1.1

In silico drug discovery drug design package software **www.moldesk.com**

Anything MD, Anywhere Docking

Fully automated, structural optimization, MD and docking calculations for most PDBs.
The following is an example. We use myPresto(*) and GROMACS as the calculation engine.



A list of docking poses from the docking calculation is shown below. The list is sorted by score. The bond free energy ΔG and RMSD (for the input structure) are also displayed.

Clicking the ↑↓ key with the mouse on the list will display the Displays the docking poses in order.

Docking structure correction by solution NMR experimental signals

Predict the structure of a protein-compound complex by entering experimental data of the compound's signal (spin relaxation time of hydrogen atoms) in solution NMR.

MolDesk Basic Function List

contents	Function
Operating System	Windows 11 / 10 / 8.1 / 8 / 7 / Vista (64bit) Linux (64bit) macOS ver. 10.11 or higher
input file	mmCIF pdb mol2 sdf mol SMILES (multi is also possible for mol2 / SMILES) mmCIF (pdb) and compound files can be entered on the Internet
output file	mmCIF pdb mol2 tpl file MD calculation setting file Docking calculation setting file MD calculation and docking calculation result file, etc. (These are myPresto specifications.) 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 / Cl) neutralized saline concentration, added by concentration/number specification
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
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

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The software is provided by Japan Biological Informatics Consortium.

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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.
MD Calculation result analysis	Video of trajectory (GROMACS, AMBER, etc. are also possible), various energies, temperature, atomic distance between any two points, video of any two plane angles and time linked time change graph Graphical display of almost all GROMACS trajectory analysis results in conjunction with video
Manual docking calculation	Structural optimization of the docking pose by simply placing the ligand near the (presumed) pocket of the protein. List the bond free energy ΔG
Search for ligand binding pockets in proteins	A fast and simple method for predicting protein structure alone. (For a highly accurate Molsite method using docking calculations, see MolDesk Screening) (Serviced by)
Ease of synthesis of compounds	Calculate and list the Synthetic Accessibility of a compound.
Docking calculations	List docking poses and various characteristic values obtained from docking calculations In the list view, use the ↑ and ↓ keys to switch the 3D view of the docking pose. The pocket side can be a complex of user-specified proteins, ions, metals, and water molecules. Mouse selection of the pocket center atom, deletion of the pocket probe point, and Specify the number of candidate structures, structure clustering of multiple candidate structures, and Fast computation when docking many ligands (grid potential reuse)
Docking calculations using solution NMR experimental signals.	Docking structure prediction by solution NMR experimental signals
Project Management	Create new project, open existing project, copy, export, import
UNDO REDO	No limit on the number of times, all processes can be saved and restored. User-created 3D views of each process can be fully saved atom by atom.
Molecular display	Wireframe, stick, ball stick, space fill, and Protein backbone view, tube view, ribbon view, and Cartoon view, surface view (polygon view), cavity view, 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, and 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. Permanent + 1 year maintenance 1 node
	A separate contract is required for maintenance after the second year. Maintenance includes version upgrades and bug fixes.

For more information, please visit the MolDesk website at www.moldesk.com

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