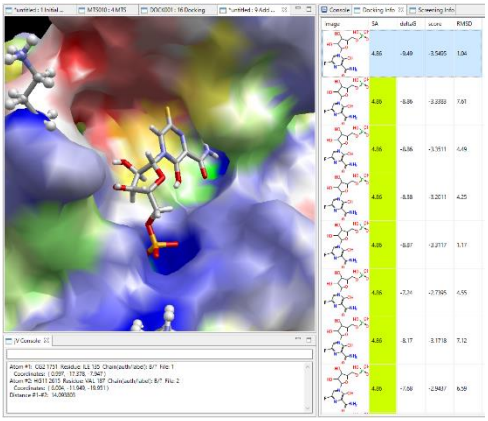
MolDesk Basic ver.1.1

Drug Design Package Software by In Silico Drug Discovery **www.moldesk.com**

Anything MD, Anywhere Docking

Fully automated, most PDB structure optimization, MD calculations, and docking calculations docking calculations for most PDBs.
myPresto(*) is used as the calculation engine.
GROMACS can also be used as an MD calculation program.



Lists docking poses from docking calculations in order of score.
The bond free energy ΔG and RMSD (for the input structure) are also displayed.
Clicking the ↑↓ keys on the list with the mouse displays the docking poses in order.

Docking Structure Correction by Solution NMR Experimental Signals
Predicts protein-compound complex structures by inputting experimental data from solution NMR compound signals (spin relaxation times of hydrogen atoms).

MolDesk Basic Function List

Contents	Functions
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 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
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

myPresto was developed by the National Institute of Advanced Industrial Science and Technology, JBIC, and the Institute for Protein Research, Osaka University, with support from AMED, METI, and NEDO.
The software is provided by Japan Biological Informatics Consortium.

MolDesk Basic Function List

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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	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 ↑ and down ↓ 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 fixes.

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

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