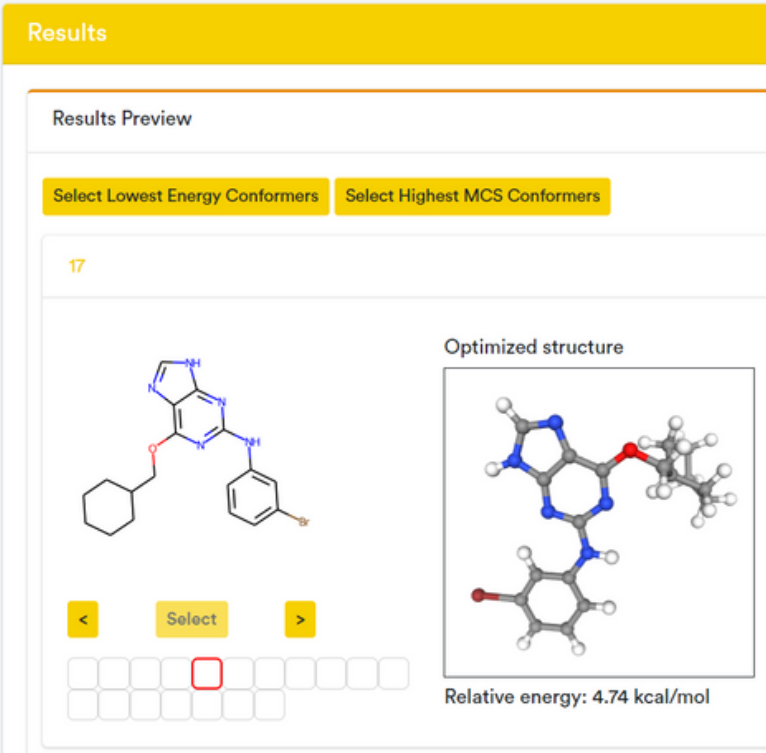
QSIMULATE

LigClean: Fast and Consistent Ligand Preparation



Benefits include:

- **Ligands are positioned in the same binding site**
- **Numerous conformers to select from with complete visualization in the platform**
- **Ligands are prepared in just minutes**

Accelerate your ligand prep!

LigClean speeds up the process of preparing 3D ligand structures required as input for QUELO and other QSP modules through automated conformer generation and alignment to a reference ligand with a receptor bound structure.

Rapid Ligand Alignment

Take a reference ligand in its receptor-bound state and a series of unbound ligands to generate good starting structures for QSP modules like QUELO and QuValent in minutes.

Review All Unique Conformations

When extra care is required to select a conformer, you know your system best. Visualize and review every distinct conformer in three dimensions and its alignment with the reference ligand.

Automatic Conformer Selection

Expedite selection of aligned ligand structures consistent by choosing the lowest energy conformer or the conformer with the largest structural overlap with the reference ligand in a single click.

Why Choose Us

- Our team is built on quantum mechanics excellence.
- Seamless integration with QSP Life, accelerating your R&D.
- Best in class support for all of your scientific and technical questions.