QC SCORE

GPU-ACCELERATED, QUANTUM CHEMISTRY (DFT) SCORING TOOL FOR ADVANCING DRUG DISCOVERY

TRANSFORM YOUR DRUG DISCOVERY PROCESS

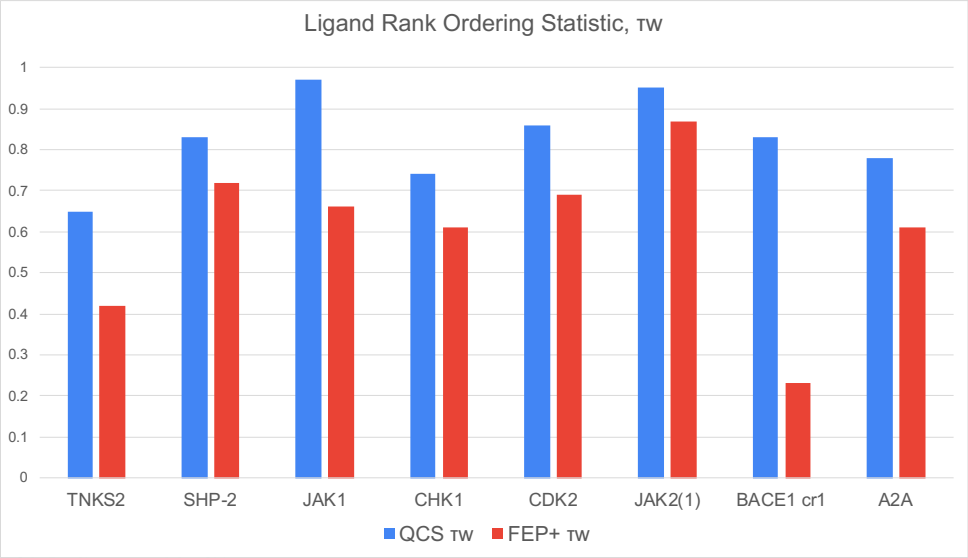
Part of the industry-leading Promethium GPU-powered molecular discovery platform, QC Score delivers unprecedented speed and accuracy in protein-ligand interaction analysis, enabling high-throughput quantum chemical scoring earlier in your optimization funnel. System size: Promethium can handle systems that were formerly intractable with quantum methods.

BREAKTHROUGH PERFORMANCE

- **5-15 minutes** per drug-like ligand
- **Up to 1000s** of ligands in parallel
- <1 hour for 1000 ligands
- 100% parameter-free

PROVEN SUPERIOR PERFORMANCE

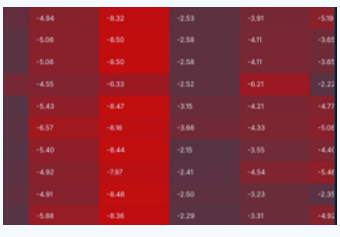
The QC Score tool delivers competitive accuracy with dramatically faster computation times. Easily correlate QC Score with experimental benchmark data to optimize for your target system.



QC Score is a fully first-principles tool and has been benchmarked against industry-standard methods and datasets[1].

SUPERCHARGE YOUR PROTEIN-LIGAND DATA ANALYTICS

- QC Score provides rich quantitative data on individual ligand-residue interaction energies that allow drug hunters to diver deeper into what makes the most potent candidates work.
- Download the complete data set in CSV or JSON formats for further data analytics to identify the most critical ligand-residue interactions to be optimized



[1]Ross, G.A., Lu, C., Scarabelli, G. et al. The maximal and current accuracy of rigorous protein-ligand binding free energy calculations. Commun Chem 6, 222 (2023). https://doi.org/10.1038/s42004-023-01019-9

ULTRA-FAST GPU PROCESSING

Powered by Promethium's GPU quantum chemistry engine, process thousands of ligands in parallel. Typical calculations complete in **5-15 minutes** per system, with 1000 ligands finishing in under an hour.

QUANTUM-LEVEL ACCURACY

Fully *ab initio* calculations with no empirical parameters required. Advanced solvation modeling via PCM ensures accurate ranking of congeneric ligand series across diverse protein targets.

FULLY AUTOMATED WORKFLOW

Intuitive interface requires minimal setup with automated clash removal and geometry optimization. Results obtained in minutes with cloud-native scalability and parallel processing.

EARLY-STAGE OPTIMIZATION

Apply high-accuracy quantum methods earlier in your lead optimization funnel, avoiding premature screening of ligands that would ultimately meet your experimental profile.

WHY CHOOSE QC SCORE?

TRADITIONAL METHODS	QC SCORE
Complex setup and configuration	Minimal setup, intuitive interface
Requires extensive parameterization	No experimental data required
Days for high-throughput screening	Hours for 1000s of ligands
Limited accuracy for charged species	Fully *ab initio* and parameter-free
Poor scalability for large studies	Excellent for charged ligands
	Ligand strain calculation

KEY PLATFORM FEATURES

- Proprietary fragmentation-based quantum chemistry
- Advanced PCM solvation modeling
- Automated binding site cutout definition (3-10 Å)
- One-click export to InteractionMap with F-SAPT for functional-group analysis
- Cloud-native scalability for high-throughput

READY TO ACCELERATE YOUR DISCOVERY?

Join leading pharmaceutical companies already using QC Score to revolutionize their drug discovery pipelines.

READY TO LEARN MORE?