



# QUANTUM

pharmaceuticals

## Quantum LogP calculation module

### Key Capabilities

QUANTUM software predicts octanol-water partition coefficient, LogP, for any small organic molecule (both charged and non-charged molecular structures), calculates LogD for dissociative systems at a given pH, and drug-likeness. The accuracy of calculations for most structures is normally about 0.7 logP units. The results of calculations are represented in logarithmic (LogP) units.

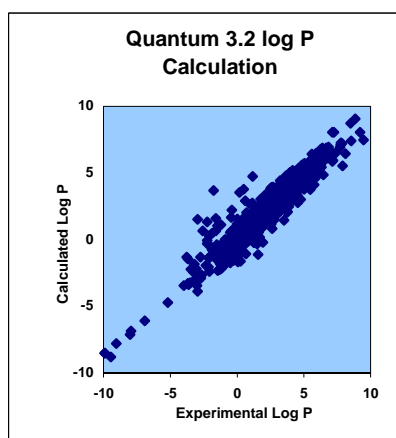
### Technological advantage

The main advantage of QUANTUM is the quality of underlying physical models. Most of competing approaches use different kinds of fragment based descriptors to calculate the molecular properties from known properties of similar compounds (QSAR). Such models rely heavily on additivity of molecular properties, are often overparametrized and lack direct physical justification. As a result, the prediction power of the models may be very good for structures similar to those used in the training set and may not be sufficient for absolutely novel compounds. QUANTUM derives molecular properties from first principles based models directly using advanced quantum mechanical analysis of molecular interactions and thermodynamics.

### Quantum LogP calculations (QlogP)

The octanol-water partition coefficient is a measure of differential solubility of a compound in two solvents - water and octanol. It is a measure of relative hydrophobicity and hydrophilicity of a substance. In the context of

drug-like substances, together with the molecular size, number of rotatable bonds and ability to form hydrogen bonds, the LogP value is related to absorption, bioavailability, hydrophobic drug-receptor interactions, metabolism and toxicity.



The Figure demonstrates the correlation between the experimental and calculated LogP values for over 900 organic molecules (actually drugs from [The Drug Bank database](#)). Root mean squared error is 0.7 LogP units, correlation coefficient  $r = 0.97$ . **No calculated points were removed.**

### Software Description

The software runs both under Windows XP and Linux OSes (see technical requirements below).

Users can either import structures in any popular third-party formats or design a molecule using an array of build in tools. QUANTUM software includes user friendly chemical drawing utility.

QUANTUM software does not require molecules provided in a three dimensional format or optimized to minimum energy geometry. The necessary conformation is obtained in the course of the LogP calculation.

The key features of the software are summarized in the following table:

Import from .mol file	✓
Import from .hin file	✓
Import from .pdb file	✓
Import from .sdf file	✓
Import from SMILES text file	✓
Calculation of octanol-water partition coefficient for compounds in neutral state	✓
Calculation of the effective partition coefficient for dissociative systems (the octanol-water distribution coefficient, logD) at a given pH	✓

Calculation and report of the "Rule of 5" properties	✓
Report of the molecular weight, the number of freely rotatable bonds (FRB), the number of H-bond donors and the number of H-bond acceptors	✓
Automatic calculation of $\log P(D)$ values for an unlimited number of compounds at once	✓

QlogP software lets users search and select compounds within desired ranges of calculated properties and export such molecular libraries in any of the listed file formats (multi-molecular files or folders).

### TRY IT FREE ONLINE

You can easily see how our QlogP works. Upload a small molecule with known the logP value and calculate QlogP instantly on our web-site (<http://q-lead.com>)

### Web-Based Services

In case a customer prefers ordering services rather than

acquiring software QUANTUM offers

opportunity to submit customer's library of compounds through the web interface in SMILES, .sdf, .mol2, .hin or .pdb formats and get the result of the calculations shortly. Full confidentiality and customer's IP protection are guaranteed.

The online version of the QlogP software has most of the functionality of the stand-alone version.

### Software/Hardware Requirements

#### Linux:

Linux-32/64-bit Intel compatible CPU, glibc >2.3 Glibc 2.3 Python 2.4 wxPython 2.6;

#### Windows:

Windows 2000, Windows XP

#### Hardware:

Processor: Intel P4 or higher, AMD Athlon 64 (with SSE support) or higher Memory: at least 1 GB RAM Disk Space: 1 GB

#### References:

1) P. Fedichev, L. Men'shikov, *Long-Range Interactions of Macroscopic Objects in Polar Liquids*, [ArXiv:cond-mat/0601129.pdf](http://arxiv.org/abs/cond-mat/0601129) submitted for publication.

2) P. Fedichev, L. Men'shikov, A. Vinnik, *Novel ab initio molecular modeling tools for drug discovery*, submitted for publication.

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