

# ClogP/CMR

INCLUDE MOLAR REFRACTIVITY AND LOGP IN QSAR AND ADME MODELS



Octanol/water partition coefficients (logP) are often a critical piece of information in the compound discovery process. As a measure of the hydrophobicity of a compound, logP is often correlated with activity and is a common descriptor in QSAR. Molar refractivity (MR) serves as a convenient estimate of molecular polarizability which is also a useful descriptor in establishing QSAR relationships. Measuring either property directly requires synthesis of a relatively large amount of any given compound.

The ClogP/CMR application provides highly accurate calculated logP and MR values. These methods were originally developed during the Pomona College Medicinal Chemistry Project, as part of over two decades of research by Dr. Corwin Hansch and Dr. Albert Leo (now of BioByte Corporation).

These highly accurate, industry standard algorithms are available as a component of Tripos' SYBYL expert molecular modeling environment.

#### Hardware and Software Requirements

ClogP/CMR requires a separate license and runs on workstations operating under IRIX<sup>®</sup> (SGI<sup>®</sup>) or Linux<sup>®</sup> (x86).

#### Complementary Software

- **Advanced CoMFA<sup>®</sup>** for refining and enhancing 3D QSAR models.
- **Almond<sup>™</sup>** for calculating and utilizing alignment independent molecular descriptors.
- **Distill<sup>™</sup>** for determining and visualizing SARs.
- **DiverseSolutions<sup>®</sup>** for designing, comparing, or selecting compound libraries.
- **HQSAR<sup>™</sup>** for performing automated QSAR analyses.
- **Legion<sup>™</sup>/CombiLibMaker<sup>™</sup>** for generating virtual compound libraries.
- **OptDesign<sup>®</sup>** for designing and editing combinatorial libraries.
- **QSAR with CoMFA<sup>®</sup>** for building predictive structure-activity and structure-property models.
- **Selector<sup>™</sup>** for characterizing and sampling compound libraries.
- **VolSurf<sup>™</sup>** for predicting ADME properties.

#### Acknowledgements

Software Partner: BioByte Corporation, Claremont, CA

Scientific Partners: Dr. Albert Leo, Dr. Corwin Hansch, Mr. David Hoekman



WWW.TRIPOS.COM				CONTACT_US@TRIPOS.COM		
AUSTRALIA +61 (7) 5439 9775	CANADA +1 450 4334500	FRANCE +33 1 69 59 29 49	GERMANY +49 89 45 10 300	JAPAN +81 3 5166 1721	UNITED KINGDOM +44 1 908 650000	UNITED STATES 800 323 2960 +1 314 647 1099
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