

**COMPU DRUG INC. SIGNS AGREEMENT WITH MOLCODE LTD.**

**SEDONA, US. – August 1, 2005-** CompuDrug, Inc., a niche software corporation that has been specializing in developing and generating ADME and drug discovery software for the past two decades, today announced that MolCode Ltd. has signed a software distribution agreement for the distribution of CodessaPRO (*Comprehensive Descriptors for Structural and Statistical Analysis*).

**About the CodessaPRO**

CODESSA PRO™ (Comprehensive Descriptors for Structural and Statistical Analysis) is a comprehensive program for developing quantitative structure-activity/property relationships (QSAR/QSPR) that integrates all necessary mathematical and computational tools to:

- calculate a large variety of molecular descriptors on the basis of the 2D/3D geometrical structure and/or quantum-chemical wave function of chemical compounds;
- develop (multi)linear and non-linear QSPR models on the chemical and physical properties or biological activity of chemical compounds;
- carry out cluster analysis of the experimental data and molecular descriptors;
- interpret the developed models;
- predict property values for any chemical compound with known molecular structure

CODESSA PRO has been developed at the Center of Heterocyclic Compounds of the University of Florida under the guidance of Professors A. R. Katritzky and M. Karelson.

**About CompuDrug Inc.**

CompuDrug International, Inc. ([www.compu drug.com](http://www.compu drug.com)) has been developing expert systems and knowledge bases for ADME/Tox and drug discovery since its inception in 1983. Their products combine advanced graphics and modeling techniques with scientific simulation and computation to help researchers understand key structure activity relationships.

**About MolCode Ltd.**

MolCode, Ltd. delivers highly expert consultations and research on the computational modeling of chemical reactivity and molecular properties, and on the molecular design of new chemical compounds, drugs and materials. The expertise is based on the long-time leading scientific research and software development in quantum chemistry, especially in the quantum chemistry of molecular systems in condensed disordered media (liquids, solutions, polymers) and in quantitative structure activity/property relationships (QSAR/QSPR).

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