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ACD and Crystal Impact Partnership: Crystal Impact distributes ACD/ChemSketch molecular drawing software along with Endeavour

Bonn, Germany -- February 28, 2001 - Advanced Chemistry Development Inc. (ACD), a leader in the field of physical property prediction, desktop chromatography and spectroscopy management, systematic naming, and Web-based access to chemistry prediction, and Crystal Impact GbR, a leader in PC-based crystal structure solution and visualization software, today announce the distribution of the ACD molecular drawing software "ChemSketch" (freeware version) along with Crystal Impact's innovative software "Endeavour" for crystal structure solution from powder diffraction data.

Knowledge of the crystal structure, i.e. the way in which atoms and molecules are arranged in solid materials, is an extremely important issue both in the pharmaceutical as well as the pigment industry and also in academic and industrial research. Most compounds nowadays cannot be synthesized as single crystals (for which this would be a routine task) but only as microcrystalline powders. Hence, there is a rapidly growing demand for software able to determine the crystal structure even from these macroscopically disordered materials.

Programs which perform this task such as Crystal Impact's "Endeavour" have become available only recently due to their tremendous demand for computational power. Their application is generally most successful if the connectivity and 3-dimensional structure of the molecule are known prior to the actual crystal structure solution calculation. Typically, the user will first draw a flat molecule and then transform this 2-dimensional sketch into a 3-dimensional structure. Hence, it is extremely valuable to have well thought-out and user-friendly tools like ACD's "ChemSketch" at hand which allow a rapid and safe realization of this task.

The "ChemSketch" software has been developed and distributed by ACD since 1994; today it is a leading program for drawing and optimization of molecular structures. The combination of this matured software tool with Crystal Impact's innovative program "Endeavour" allows easy application of the most recent software technology, even for non-specialist users. Both programs cooperate without any modifications: "ChemSketch" Mol-files can directly be read and used by "Endeavour". We hope that this relationship, though originally established around inclusion of a freeware package, will be extended in the near future to take advantage of other ACD tools.

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