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University of Cambridge Applies ACD/Labs Property-based Design Tools to Natural Product Research

Toronto, Canada, February 17, 2005 - Advanced Chemistry Development, Inc., (ACD/Labs) is pleased to announce that the Ley Research Group at the University of Cambridge has chosen ACD/Labs' sophisticated property-based design studio, ACD/MedChem Advisor, to aid them in the development of complex natural products.

Through ACD/MedChem Advisor, the Group will have access to prediction algorithms that will enable them to evaluate the physicochemical properties for their synthesized compounds, namely logD, pKa, logP, and aqueous solubility. The knowledge of their compounds' structure-property relationships will provide a working hypothesis towards chemically-relevant structural modifications that aid in compound optimization.

ACD/MedChem Advisor will also provide the Group with a compilation of databases to help them identify substituents or heterocycles that can favorably shift the physical properties of their compounds. Containing compilations of popular heterocycles, as well as neutral, acidic, and basic organic substituents, the databases can be queried on a number of search parameters to identify similar topology, synthetic feasibility, and molecular stability.

Professor Steven Ley, Head of Organic Chemistry at the University of Cambridge, states, "We are pleased to have the opportunity to evaluate ACD/MedChem Advisor in a number of our synthesis programmes and look forward to working closer with ACD/Labs and AGB Scientific Solutions on this initiative."

The Ley Research Group purchased ACD/MedChem Advisor through AGB Scientific Solutions, Inc., the official ACD/Labs Distributor for the UK and Ireland. Mike Partington, Managing Director for AGB Scientific Solutions, comments on the purchase, "We are enjoying increasing success within academia and we are delighted to be working with Cambridge University. MedChem Advisor will help the group gain a critical insight into the relationship between a compound's structure and its physical properties, enabling the focus of synthetic effort into a direction more likely to improve drug-like properties. We are looking forward to working with Cambridge and other Universities to help chemists in this vital area."

Antony Williams, VP and Chief Science Officer for ACD/Labs, adds "ACD/Labs has long been the accepted provider of physicochemical property prediction. Our tools are utilized by thousands of medicinal chemists in the majority of drug discovery organizations. By delivering ACD/MedChem Advisor we have extended the potential impact of ACD/PhysChem software since scientists now have the ability to design molecules with optimized properties, without sacrificing their potency. We look forward to developing a relationship with Cambridge University as they navigate a new territory for computer-based molecular design."

Further information about ACD/MedChem Advisor can be found at www.acdlabs.com/sds.

