ACD/Labs becomes an associate partner of Open PHACTS project

The Open PHACTS consortium is pleased to announce an Associate Partner relationship with Advanced Chemistry Development, Inc. (ACD/Labs) who will be supplying a number of predicted physicochemical properties for inclusion within the project data. ACD/Labs is one of the primary suppliers of prediction algorithms to the life sciences industry and their contribution of data provides enhanced querying options for the users. Daria Thorp, President of ACD/Labs, comments "The Open PHACTS project represents a promising approach that leverages existing pharmacological knowledge to make new discoveries. ACD/Labs, with our 18 years of *in silico* physicochemical and ADME-Tox modeling experience, is excited to provide our industry leading molecular property predictions notably log*D* at physiologically relevant pH, "rule of 5", and log*P* values to this project." The ACD/Labs data will be offered via RSC ChemSpider which provides the chemical compound data in a format consumable by the Open PHACTS platform.

The Open PHACTS consortium is building a semantic data integration platform for pharmacological data, to reduce the barriers to drug discovery, creating an Open Pharmacological Space. Open PHACTS will deliver a single view across available data resources, and will be freely available to users.

Scientific text, difficult to analyse by computer, will have factual assertions extracted as semantic triples, allowing for the first time the prospect of querying textual and database data together to give answers needed to identify new drug targets and pharmacological interactions. While the semantic approach has been delivered in small-scale and targeted approaches so far, its promise for multiscale data integration has remained largely unfulfilled - Open PHACTS is a major project including many of the top semantic web experts, committed to deliver on this promise.

About Advanced Chemistry Development (ACD/Labs)
Advanced Chemistry Development, Inc., (ACD/Labs) is a chemistry software company that develops and commercializes enterprise and desktop solutions to support R&D efforts, and preserve and re-use legacy knowledge. ACD/Labs' areas of expertise include a unique knowledge management solution; spectroscopic data processing and interpretation for NMR, MS, LC/MS, IR, UV, other optical, and hyphenated instrumental techniques; chemical structure confirmation, verification, and elucidation; impurity, metabolism, and degradation research; ADME-Tox and physicochemical property prediction, and property-based lead optimization; chromatographic method development and optimization; and chemical nomenclature. We provide integration with existing Informatics systems

and undertake custom projects including enterprise-level automation. A private company founded in 1994, ACD/Labs has worldwide sales and support presence, with offices in N. America, Europe, and Asia. (www.acdlabs.com)

About Open PHACTS

Open PHACTS is a 3-year knowledge management project of the Innovative Medicines Initiative, running from March 2011, and will deliver a sustainable service to continue after the project funding ends. The project consortium consists of leading academics in semantics, pharmacology and informatics, driven by solid industry business requirements: 27 partners, including 9 pharmaceutical companies and 3 biotechs.

The project is on track, with new partners joining the project in February 2012 and an internal prototype to be delivered to the consortium members in March 2012. A public prototype release is scheduled for September 2012.

www.openphacts.org