

Digital Science transfers SureChem patent chemistry data to EMBL-EBI

December 11 2013



Digital Science, a Macmillan company, and EMBL-EBI are transferring SureChem data on patented chemical structures into the public domain. It is the first time a world patent chemistry structure collection of this size has been made publicly and freely available, making it a significant advance in Open Data for use in drug discovery. This donation from Digital Science will give researchers access to a new source of highly relevant compounds related to the curing of human disease.

SureChem, developed by Digital Science, extracts chemical structure data from the full text and images of patents. This makes it easier to check whether a newly developed drug or other product is actually novel. Previously these data were held within commercial systems and inaccessible to most researchers; now, they are freely available from

EMBL-EBI as SureChEMBL.

Nicko Goncharoff, Digital Science: "Our mission is to give researchers better tools and services and from the start Digital Science has preferred solutions that support Open Science and Open Data communities whenever possible. By placing this collection into the trusted hands of EMBL-EBI, we're opening up an entire new class of life science data to the public that has previously been locked behind paywalls, and inaccessible for data mining. We couldn't think of a better home for SureChem, anywhere."

John Overington, Head of Chemical Biology at EMBL-EBI: "Patents are the foundation of high-tech enterprise and innovation and form the basis of the knowledge economy. We hope that making chemical patents more discoverable in the [public domain](#) will considerably speed up the identification of promising molecules. This new source of data will be a major boost to translational research and the discovery of novel bioactive molecules. By putting all this data together in a structured way with other EBI resources, we can help increase competitive innovation."

Academic researchers particularly stand to benefit from SureChEMBL, notes chemistry luminary Christopher Lipinski, Scientific Advisor at Melior Discovery: "Having the SureChem patented [chemical structures](#) freely available to researchers would by itself be an excellent idea. Having the interface through EMBL-EBI is an even better idea, since the new SureChEMBL system takes advantage of EMBL-EBI's nearly 20 years' expertise in technical and professional aspects of interfacing data sets, internal analysis and customer service to the broad genomic, chemo-bioinformatic, chemical biology and drug-discovery communities."

SureChEMBL joins a wide array of connected life-science informatics resources at EMBL-EBI (www.ebi.ac.uk/services), which offers a comprehensive source of freely available molecular data. Today's

transfer opens the door to integrating disease and drug-target data in more meaningful ways, enhancing links between chemical structures and other biological data and their discoverability through the scientific literature.

More information: Researchers working in the public and private domain are invited to explore these data at www.surechembl.org.

Provided by European Molecular Biology Laboratory

Citation: Digital Science transfers SureChem patent chemistry data to EMBL-EBI (2013, December 11) retrieved 3 May 2024 from <https://phys.org/news/2013-12-digital-science-surechem-patent-chemistry.html>

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