

10 doctoral (PhD) positions in Big Data Analysis in Chemistry, Marie Skłodowska-Curie ITN BIGCHEM (<http://bigchem.eu>)



BIGCHEM (BIG data in CHEMistry) is a Marie Skłodowska-Curie Innovative Training Network (ITN) for Early Stage Researchers (ESR) funded by the European Commission under the H2020 Programme. The BIGCHEM ITN will provide a comprehensive and cross-disciplinary structured curriculum for doctoral students in large chemical data analysis using machine-learning, computational chemistry and chemoinformatics methods. The innovative research program will be implemented with the target users, large pharma companies and SMEs, which generate and analyse large chemical data.

BIGCHEM is a collaborative action of 9 groups in 5 countries from academia and pharmaceutical industry. The complementary expertise of partners in different aspect of large chemical data, including data production, data security, analysis, and development of theoretical methods is the basis of the research topics and allocation of individual tasks and resources.

The project will train ten Early Stage Researchers (ESR). Each ESR will spend at least 50% of time with industrial partners and will be employed for 36 months in total (18 months with academic partner and 18 months with industrial partner or vice versa). The ESRs will be enrolled in the respective Universities and will study towards their PhD degrees.

ESR1: Machine learning methodologies for mining very large compound data sets. (Boehringer Ingelheim GmbH & Co KG and University of Bonn, Germany)

ESR2: Computational compound screening and profiling by large-scale mining of pharmaceutical data. (University of Bonn, Germany and Boehringer Ingelheim GmbH & Co KG, Germany)

ESR3: Big data visualization and modeling using Generative Topographic Mapping (GTM). (University of Strasbourg and Boehringer Ingelheim GmbH & Co KG, Germany)

ESR4: Development of frequent hitters filters for HTS screening. (Helmholtz Zentrum München & Lead Discovery Center GmbH, Germany)

ESR5: Analysis of Compound Promiscuity Based on Bioassay Ontology. (University of Bonn & AstraZeneca, Germany & Sweden)

ESR6: Developing virtual screening methods to exploit large virtual chemical space. (University of Bern & AstraZeneca, Sweden & Switzerland)

ESR7: Exploration of uncharted regions of the chemical space by reaction-driven de novo design. (Boehringer Ingelheim GmbH & Co KG and ETH Zürich, Germany and Switzerland)

ESR8: Accessing new chemical space for lead optimization based on QSAR models. (AstraZeneca & Helmholtz Zentrum München, Germany & Sweden)

ESR9: Integrated ligand- and structure-based approaches for predicting compound polypharmacology based on big data. (University of Modena and Reggio Emilia & AstraZeneca, Italy & Sweden)

ESR10: Secure sharing of information using ensemble of machine learning methods and surrogate data. (Helmholtz Zentrum München & AstraZeneca, Germany & Sweden)

Further information about the recruitment process as well as the eligibility criteria are indicated on the BIGCHEM site <http://bigchem.eu> (or from info AT bigchem.eu). Applications should be submitted on-line through the project website <http://bigchem.eu>.

Deadline for applications is **20.03.2016**.