Research outputs:

**Nomenclature for alleles of the human carboxylesterase 1 gene**
Research output: Research - peer-review › Journal article – Annual report year: 2017

**Synthesis and biological evaluation of dihydropyrano-[2,3-c]pyrazoles as a new class of PPARγ partial agonists**
Research output: Research - peer-review › Journal article – Annual report year: 2017

**ChemProt-3.0: a global chemical biology diseases mapping**
Research output: Research - peer-review › Journal article – Annual report year: 2016

**Investigating the impact of missense mutations in hCES1 by in silico structure-based approaches**
Research output: Research - peer-review › Journal article – Annual report year: 2016

**Synthesis and biological evaluations of cytotoxic and antiangiogenic triterpenoids-jacaranone conjugates**
Research output: Research - peer-review › Journal article – Annual report year: 2016

**Evidence of interactions between aroma compounds and the CB1 receptor opens new routes for regulation of food intake**
Research output: Research - peer-review › Conference abstract in journal – Annual report year: 2015

**Evolution of substrate recognition sites (SRSs) in cytochromes P450 from Apiaceae exemplified by the CYP71AJ subfamily**
Research output: Research - peer-review › Journal article – Annual report year: 2015

**Individualization of treatments with drugs metabolized by CES1: combining genetics and metabolomics**
Research output: Research - peer-review › Journal article – Annual report year: 2015

**Identification of Odorant-Receptor Interactions by Global Mapping of the Human Odorome**
Research output: Research - peer-review › Journal article – Annual report year: 2014

**Pharmacology profiling of chemicals and proteins**
Research output: Research › Ph.D. thesis – Annual report year: 2015

**Solid-Phase Synthesis and Biological Evaluation of N-Dipeptido L-Homoserine Lactones as Quorum Sensing Activators**
Research output: Research - peer-review › Journal article – Annual report year: 2014

**ChemProt-2.0: visual navigation in a disease chemical biology database**
Research output: Research - peer-review › Journal article – Annual report year: 2013

**ChemProt: A disease chemical biology database**
Research output: Research - peer-review › Book chapter – Annual report year: 2013

**Discovery of a novel selective PPARγ ligand with partial agonist binding properties by integrated in silico / in vitro work flow**
Research output: Research - peer-review › Journal article – Annual report year: 2013

**HExpoChem: a systems biology resource to explore human exposure to chemicals**
Research output: Research - peer-review › Journal article – Annual report year: 2013
Identification of LasR Ligands through a Virtual Screening Approach
Research output: Research - peer-review | Journal article – Annual report year: 2013

Pharmacological profiling of drugs by linking chemoinformatics and bioinformatics data
Research output: Research - peer-review | Conference abstract in journal – Annual report year: 2013

Scientific competency questions as the basis for semantically enriched open pharmacological space development
Research output: Research - peer-review | Journal article – Annual report year: 2013

Temporal variability in urinary phthalate metabolite excretion based on spot, morning, and 24-h urine samples: Considerations for epidemiological studies
Research output: Research - peer-review | Journal article – Annual report year: 2013

The effect of network biology on drug toxicology.
Research output: Research - peer-review | Journal article – Annual report year: 2013

Association between chemical pattern in breast milk and congenital cryptorchidism: modelling of complex human exposures
Research output: Research - peer-review | Journal article – Annual report year: 2012

A Steered Molecular Dynamics Study of Binding and Translocation Processes in the GABA Transporter
Research output: Research - peer-review | Journal article – Annual report year: 2012

Enantioselective determination of methylphenidate and ritalinic acid in whole blood from forensic cases using automated solid-phase extraction and liquid chromatography-tandem mass spectrometry.
Research output: Research - peer-review | Journal article – Annual report year: 2012

Established and Emerging Trends in Computational Drug Discovery in the Structural Genomics Era
Research output: Research - peer-review | Journal article – Annual report year: 2012

Of possible cheminformatics futures
Research output: Research - peer-review | Journal article – Annual report year: 2012

System chemical biology studies of endocrine disruptors
Research output: Research - peer-review | Conference abstract for conference – Annual report year: 2012

The impact of network biology in pharmacology and toxicology
Research output: Research - peer-review | Journal article – Annual report year: 2012

Toxicogenomics Investigation Under the eTOX Project
Research output: Research - peer-review | Journal article – Annual report year: 2012

Associating Drugs, Targets and Clinical Outcomes into an Integrated Network Affords a New Platform for Computer-Aided Drug Repurposing
Research output: Research - peer-review | Conference article – Annual report year: 2011

ChemProt: a disease chemical biology database
Research output: Research - peer-review | Journal article – Annual report year: 2010

In Silico Predictions of hERG Channel Blockers in Drug Discovery: From Ligand-Based and Target-Based Approaches to Systems Chemical Biology
Country-specific chemical signatures of persistent environmental compounds in breast milk

Deciphering Diseases and Biological Targets for Environmental Chemicals using Toxicogenomics Networks

Homology Modelling of the GABA Transporter and Analysis of Tiagabine Binding

Mutational Mapping and Modeling of the Binding Site for (S)-Citalopram in the Human Serotonin Transporter

Classification of Cytochrome P450 1A2 Inhibitors and Non-Inhibitors by Machine Learning Techniques

Location of the Antidepressant Binding Site in the Serotonin Transporter IMPORTANCE OF SER-438 IN RECOGNITION OF CITALOPRAM AND TRICYCLIC ANTIDEPRESSANTS

Virtual Screening and Prediction of Site of Metabolism for Cytochrome P450 1A2 Ligands

hERG classification model based on a combination of support vector machine method and GRIND descriptors

Projects:

Mapping of Secondary Metabolism in Biotechnologically Important aspergillus Species

Kemisk Biologi af Mikrobielle Anticancer Naturstoffer

Prediction of protein structural features by use of artificial neural networks

Deciphering the clinical effect of drugs trough large-scale data integration

Pharmacogenomics and personalized medicine in the treatment of ADHD