Svava Osk Jonsdottir - DTU Orbit (06/08/2016)

Jonsdottir, Svava Osk
sojo@food.dtu.dk

National Food Institute - Associate Professor, Former

Publications:

Physiologically Based Toxicokinetic Models of Tebuconazole and Application in Human Risk Assessment
Jonsdottir, S. O., Reffstrup, T. K., Petersen, A. & Nielsen, E. 2016 In : Chemical Research in Toxicology. 29, 5, p. 715-734
Publication: Research - peer-review › Journal article – Annual report year: 2016

QSAR screening of 70,983 REACH substances for genotoxic carcinogenicity, mutagenicity and developmental toxicity in the ChemScreen project
Wedebeye, E. B., Dybdahl, M., Nikolov, N. G., Jonsdottir, S. O. & Niemelä, J. R. 2015 In : Reproductive Toxicology. 55, p. 64-72
Publication: Research - peer-review › Journal article – Annual report year: 2015

hERG blocking potential of acids and zwitterions characterized by three thresholds for acidity, size and reactivity
Publication: Research - peer-review › Journal article – Annual report year: 2014

Identification of cytochrome P450 2D6, 2C9 and 3A4 substrates and inhibitors by QSAR models based on human clinical data
Publication: Research - peer-review › Journal article – Annual report year: 2014

Optimization of the cumulative risk assessment of pesticides and biocides using computational techniques: Pilot project
Publication: Research - peer-review › Report – Annual report year: 2014

QSAR pre-screen of 70,983 substances for genotoxic carcinogenicity, mutagenicity and developmental toxicity in the EU FP7 project ChemScreen
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2014

Simple estimate of the influence of competitive inhibition on PBTK based risk assessment
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2014

Discovery of a novel selective PPARγ ligand with partial agonist binding properties by integrated in silico / in vitro workflow
Publication: Research - peer-review › Journal article – Annual report year: 2013
Structural insight into the UNC-45–myosin complex
Fratev, F., Jonsdottir, S. O. & Pajeva, I. 2013 In : Proteins. 81, 7, p. 1212-1221
Publication: Research - peer-review › Journal article – Annual report year: 2013

Identification of cytochrome P450 2D6 and 2C9 substrates and inhibitors by QSAR analysis
Publication: Research - peer-review › Journal article – Annual report year: 2012

Prediction of drug efficacy for cancer treatment based on comparative analysis of chemosensitivity and gene expression data
Publication: Research - peer-review › Journal article – Annual report year: 2012

QSAR model for human pregnane X receptor (PXR) binding: Screening of environmental chemicals and correlations with genotoxicity, endocrine disruption and teratogenicity
Publication: Research - peer-review › Journal article – Annual report year: 2012

The phosphorylation specificity of B-RAF(WT), B-RAF(D594V), B-RAF(V600E) and B-RAF(K601E) kinases: An in silico study
Publication: Research - peer-review › Journal article – Annual report year: 2010

An in silico study of the molecular basis of B-RAF activation and conformational stability
Publication: Research - peer-review › Journal article – Annual report year: 2009

Molecular Basis of Inactive B-RAF(WT) and B-RAF(V600E) Ligand Inhibition, Selectivity and Conformational Stability: An in Silico Study
Fratev, F. F., Jonsdottir, S. O., Mihaylova, E. & Pajeva, I. 2009 In : Molecular Pharmaceutics. 6, 1, p. 144-157
Publication: Research - peer-review › Journal article – Annual report year: 2009

Identification of biomarkers for genotyping Aspergilli using non-linear methods for clustering and classification
Kouskoumvekaki, I., Yang, Z., Jonsdottir, S. O., Olsson, L. & Panagiotou, G. 2008 In : BMC Bioinformatics. 9, p. 59
Publication: Research - peer-review › Journal article – Annual report year: 2008

Prediction of pH-dependent aqueous solubility of Histone Deacetylase (HDAC) inhibitors
Publication: Research - peer-review › Journal article – Annual report year: 2008

Monitoring novel metabolic pathways using metabolomics and machine learning; induction of the phosphoketolase pathway in A. nidulans cultivations
Panagiotou, G., Kouskoumvekaki, I., Jonsdottir, S. O. & Olsson, L. 2007 In : Metabolomics. 3, p. 503-516
Publication: Research - peer-review › Journal article – Annual report year: 2007

Monitoring the Induction of the Phosphoketolase Pathway in Aspergillus nidulans Cultivations using Metabolomics and Machine Learning
Publication: Research - peer-review › Journal article – Annual report year: 2007

Prediction of pH-dependent aqueous solubility of druglike molecules
Publication: Research - peer-review › Journal article – Annual report year: 2006

Vapor-liquid (VLE) and liquid-liquid (LLE) phase equilibria calculations for polystyrene plus methylecyclohexane and polystyrene plus cyclohexane solutions
Publication: Research - peer-review › Journal article – Annual report year: 2006

Wilczura-Wachnik, H. & Jonsdottir, S. O. 2005 In : Journal of Molecular Modeling. 11, 1, p. 87-87
Publication: Research - peer-review › Journal article – Annual report year: 2005

Prediction methods and databases within chemoinformatics: emphasis on drugs and drug candidates
Publication: Research - peer-review › Journal article – Annual report year: 2005

QSRR models based on molecular mechanics and quantum chemical calculations. 2. Thermodynamic properties of alkanes, alcohols, polyols, and ethers
Dyekjær, J. D. & Jonsdottir, S. O. 2003 In : Industrial & engineering chemistry research. 42, 18, p. 4241-4259
Publication: Research - peer-review › Journal article – Annual report year: 2003

A thermodynamic study of glucose and related oligomers in aqueous solution: Vapor pressures and enthalpies of mixing
Publication: Research - peer-review › Journal article – Annual report year: 2002

Modeling and measurements of solid-liquid and vapor-liquid equilibria of polyols and carbohydrates in aqueous solution
Publication: Research - peer-review › Journal article – Annual report year: 2002

Phase equilibria of carbohydrates: the study of a series of glucose oligomers from glucose to maltopentaose in aqueous solution - Experimental versus predicted data using various UNIQUAC/UNIFAC models
Publication: Research - peer-review › Journal article – Annual report year: 2002

QSRR models based on molecular mechanics and quantum chemical calculations. 1. Construction of Boltzmann averaged descriptors for alkanes, alcohols, diols, ethers and cyclic compounds.
Dyekjær, J. D., Rasmussen, K. & Jonsdottir, S. O. 2002 In : Journal of molecular modeling. 8, 9, p. 277-289
Publication: Research - peer-review › Journal article – Annual report year: 2002

The vapour pressure of water as a function of solute concentration above aqueous solutions of fructose, sucrose, raffinose, erythritol, xylitol, and sorbitol
Publication: Research - peer-review › Journal article – Annual report year: 2002

Phase equilibria of carbohydrates: The study of a series of glucose oligomers from glucose to maltopentaose in aqueous solution
Jonsdottir, S. O. 2001
Publication: Research › Poster – Annual report year: 2001
Modelling of the phase equilibria of polyisobutylene in diisobutylketone with Molecular Mechanics
Jonsdottir, S. O. & Welsh, W. J. 2000 In : Computational and Theoretical Polymer Science. 10, p. 125-131
Publication: Research - peer-review › Journal article – Annual report year: 2000

The Consistent Force Field. Part 6: An optimized set of potential energy functions for primary amines
Publication: Research - peer-review › Journal article – Annual report year: 2000

Phase equilibria of carbohydrates in polar solvents.
Publication: Research - peer-review › Journal article – Annual report year: 1999

The critical role of force-fields in property prediction
Publication: Research - peer-review › Journal article – Annual report year: 1999

Phase Equilibria of Polymer Solutions Determined by Molecular Mechanics
Jonsdottir, S. O., Welsh, W. J., Rasmussen, P. & Rasmussen, K. 1998 In : Computational and Theoretical Polymer Science. 8, p. 75-81
Publication: Research - peer-review › Journal article – Annual report year: 1998

Vapor-liquid equilibria of polymer solutions determined by molecular mechanics
Jonsdottir, S. O., Rasmussen, K., Rasmussen, P. & Welsh, W. J. 1998 In : Computational and Theoretical Polymer Science. 8, p. 75-81
Publication: Research - peer-review › Journal article – Annual report year: 1998

Aspects of conformational mobility in charged oligosaccharides
Publication: Research - peer-review › Journal article – Annual report year: 1997

UNIQUAC interaction parameters for molecules with -OH groups on adjacent carbon atoms in aqueous solution determined by molecular mechanics - glycols, glycerol and glucose
Publication: Research - peer-review › Journal article – Annual report year: 1997

UNIQUAC interaction parameters for alkane/amine systems determined by Molecular Mechanics
Publication: Research - peer-review › Journal article – Annual report year: 1996

Projects:

Kemoinformatiske Modeller til Forudsigelse af Toksicitet
Larsen, J. E. P., Brunak, S., Jonsdottir, S. O. & Jørgensen, F. S.
15/04/2005 → 04/05/2011
Project: PhD

Phase Equilibria and Thermodynamic Properties of Biological Polymers.
Jonsdottir, S. O., Dyekjær, J. D., Macedo, E. A. & Westh, P.
01/01/1999 → ...
Project

Phase Equilibria by Molecular Mechanics
Jonsdottir, S. O., Rasmussen, K., Rasmussen, P. & Klein, R. A.
01/03/1997 → 31/12/2000
Teoretisk bestemmelse af UNIFAC-parametre
Jonsdottir, S. O. & Rasmussen, K.
01/04/1992 → 18/04/1995
Project: PhD