

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

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### Publications:

#### **Physicologically 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**

Wedebye, 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**

Nikolov, N. G., Dybdahl, M., Jonsdottir, S. O. & Wedebye, E. B. 2014 In : *Bioorganic & Medicinal Chemistry*. 22, 21, p. 6004-6013 10 p.

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**

Jonsdottir, S. O., Ringsted, T., Nikolov, N. G., Dybdahl, M., Wedebye, E. B. & Niemelä, J. R. 2014 In : *Basic & Clinical Pharmacology & Toxicology*. 115, 1, p. 156-156 1 p.

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**

Jonsdottir, S. O., Reffstrup, T. K., Petersen, A., Nielsen, E. & Larsen, J. C. 2014 Copenhagen: Danish Ministry of the Environment. 183 p.

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**

Wedebye, E. B., Dybdahl, M., Nikolov, N. G., Jonsdottir, S. O. & Niemelä, J. R. 2014 *Abstract Book - DTU Sustain Conference 2014*. Kgs. Lyngby: Technical University of Denmark, 1 p.

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**

Reffstrup, T. K., Petersen, A., Nielsen, E. & Jonsdottir, S. O. 2014 In : *Toxicology Letters*. 229, Supplement, p. S1215-S216

Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2014

#### **Simple estimate of the influence of competitive inhibition on PBTK based risk assessment**

Reffstrup, T. K., Petersen, A., Nielsen, E. & Jonsdottir, S. O. 2014

Publication: Research - peer-review › Poster – Annual report year: 2014

#### **Discovery of a novel selective PPAR $\gamma$ ligand with partial agonist binding properties by integrated in silico / in vitro work flow**

Kouskoumvekaki, I., Petersen, R. K., Fratev, F. F., Taboureau, O., Nielsen, T. E., Oprea, T., Sonne, S. B., Flindt, E. N., Jonsdottir, S. O. & Kristiansen, K. 2013 In : *Journal of Chemical Information and Modeling*. 53, 4, p. 923-937

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**

Jónsdóttir, S. Ó., Ringsted, T., Nikolov, N. G., Dybdahl, M., Wedebye, E. B. & Niemelä, J. R. 2012 In : *Bioorganic & Medicinal Chemistry*. 20, 6, p. 2042-2053  
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**

Wan, P., Li, Q., Larsen, J. E. P., Eklund, A. C., Parlesak, A., Rigina, O., Nielsen, S. J., Björkling, F. & Jonsdottir, S. O. 2012 In : *Bioorganic & Medicinal Chemistry*. 20, 1, p. 167-176  
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**

Dybdahl, M., Nikolov, N. G., Wedebye, E. B., Jónsdóttir, S. Ó. & Niemelä, J. R. 2012 In : *Toxicology and Applied Pharmacology*. 262, 3, p. 301-309  
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**

Fratev, F. F. & Jonsdottir, S. O. 2010 In : *Journal of Molecular Graphics and Modelling*. 28, 7, p. 598-603  
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**

Fratev, F. F. & Jonsdottir, S. O. 2009 In : *BMC Structural Biology*. 9, 47, 17 p.  
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**

Kouskoumvekaki, I., Hansen, N. T., Björkling, F., Vadlamudi, S. M. & Jonsdottir, S. O. 2008 In : *SAR and QSAR in Environmental Research*. 19, 1-2, p. 167-177  
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**

Panagiotou, G., Kouskoumvekaki, I., Jonsdottir, S. O. & Olason, L. 2007 In : *Metabolomics*. 3, p. 503-516  
Publication: Research - peer-review › Journal article – Annual report year: 2007

#### **Prediction of pH-dependent aqueous solubility of druglike molecules**

Kouskoumvekaki, I., Brunak, S. & Jonsdottir, S. O. 2006 In : *Journal of Chemical Information and Modeling*. 46, p. 2601-2609

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**

Wilczura-Wachnik, H. & Jonsdottir, S. O. 2006 In : Polish Journal of Chemistry. 80, 1, p. 65-79

Publication: Research - peer-review › Journal article – Annual report year: 2006

**Modeling of the phase equilibria of polystyrene in methylcyclohexane with semi-empirical quantum mechanical methods I (vol 9, pg 108, 2003)**

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**

Jonsdottir, S. O., Jorgensen, F. S. & Brunak, S. 2005 In : BIOINFORMATICS. 21, 10, p. 2145-2160

Publication: Research - peer-review › Journal article – Annual report year: 2005

**Modeling of the phase equilibria of polystyrene in methylcyclohexane with semi-empirical quantum mechanical methods I**

Wilczura-Wachnik, H. & Jonsdottir, S. O. 2003 In : Journal of molecular modeling. 9, 2, p. 108-113

Publication: Research - peer-review › Journal article – Annual report year: 2003

**QSPR models based on molecular mechanics and quantum chemical calculations. 2. Thermodynamic properties of alkanes, alcohols, polyols, and ethers**

Dyckjær, 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**

Cooke, S. A., Jonsdottir, S. O. & Westh, P. 2002 In : JOURNAL OF CHEMICAL AND ENGINEERING DATA. 47, 5, p. 1185-1192

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**

Jonsdottir, S. O., Cooke, S. A. & Macedo, E. A. 2002 In : CARBOHYDRATE RESEARCH. 337, 17, p. 1563-1571

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**

Cooke, S. A., Jonsdottir, S. O. & Westh, P. 2002 In : FLUID PHASE EQUILIBRIA 194: 947-956 Sp. Iss. SI, MAR 30 2002. 194, p. 947-956

Publication: Research - peer-review › Journal article – Annual report year: 2002

**QSPR models based on molecular mechanics and quantum chemical calculations. 1. Construction of Boltzmann averaged descriptors for alkanes, alcohols, diols, ethers and cyclic compounds.**

Dyckjær, 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**

Cooke, S. A., Jonsdottir, S. O. & Westh, P. 2002 In : JOURNAL OF CHEMICAL THERMODYNAMICS. 34, 10, p. 1545-1555

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**

Jonsdottir, S. O. & Rasmussen, K. 2000 In : New J. Chem.. 24, p. 243-247

Publication: Research - peer-review › Journal article – Annual report year: 2000

**Phase equilibria of carbohydrates in polar solvents.**

Jonsdottir, S. O. & Rasmussen, P. 1999 In : Fluid Phase Equilibria. 158-160, p. 411-418

Publication: Research - peer-review › Journal article – Annual report year: 1999

**The critical role of force-fields in property prediction**

Jonsdottir, S. O., Welsh, W. J., Rasmussen, K. & Klein, R. A. 1999 In : New Journal of Chemistry. 23, 2, p. 153-163

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**

Klein, R. A., Jonsdottir, S. O. & Egge, H. 1997 In : J. Molec. Struct. (Theochem). 395-396, p. 313-332

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**

Jonsdottir, S. O. & Klein, R. A. 1997 In : Fluid Phase Equilibria. 132, p. 117-137

Publication: Research - peer-review › Journal article – Annual report year: 1997

**UNIQUAC interaction parameters for alkane/amine systems determined by Molecular Mechanics**

Jonsdottir, S. O., Klein, R. A. & Rasmussen, K. 1996 In : Fluid Phase Equilibria. 115, 1-2, p. 59-72

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

Project

**Teoretisk bestemmelse af UNIFAC-parametre**

Jonsdottir, S. O. & Rasmussen, K.

01/04/1992 → 18/04/1995

Project: PhD