Curriculum Vitae
for Catrin Hasselgren

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Pepparedsleden 1
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Private Address:
Bergsfoten 6
436 40 Askim
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Born
12th December 1970

Educational degrees
1998 – 2002 PhD Chemistry, Chalmers University of Technology, Sweden
1994 – 1997 Bachelor of Science, Uppsala Univ., Sweden (including 1 year exchange studies at the Univ. of New South Wales, Sydney, Australia and Bachelor Thesis work at the Univ. of South Florida, Tampa, USA)

Current Position
2012 – Present Associate Director, Computational ADME and Safety (currently on parental leave)

Previous Positions
2010 - 2012 Principal Scientist, Computational Toxicology, Global Safety Assessment, AstraZeneca R&D Mölndal, Sweden.
2006 - 2010 Associate Principal Scientist, Computational Toxicology, Global Safety Assessment, AstraZeneca R&D Mölndal, Sweden.
2003 - 2010 Senior Scientist, Computational Toxicology, Global Safety Assessment, AstraZeneca R&D Mölndal, Sweden.
2002- 2003 Post Doc at Enabling Science and Technology, Chemical Computing, AstraZeneca R&D Mölndal, Sweden

Internal Network Membership (current and past)
Global Chemistry Network
PSSG Mölndal
Predictive Chemistry Network
Discovery Informatics Strategy Group

External Oral Presentations
Department of Internal Medicine - Grand Rounds, 14th November 2013, University of New Mexico, School of Medicine.

"Computational Toxicology in drug Discovery"

Invited lecture at the BrazMedChem 2014 – Title not yet submitted.

Workshop on Drug Safety and Computational Methods at the University of New Mexico. October 2011.

American College of Toxicology, 6-9 November 2011, Phoenix, USA.
"An Industrial Perspective on Mutagenicity Modeling"

BrazMedChem, November 2008, Puerto de Galinhas, Brazil.
"Modeling and Informatics Support for Safety and Metabolism Studies in Early Drug Discovery Projects"

EuroQSAR, September 21-26 2008, Uppsala, Sweden.
"Using All the Data in Comprehensive Risk Assessment of the Mutagenic Potential of Drugs"

ICCS, June 5-9, 2005, Noordwijkerhout, The Netherlands.
"SPORCalc – Fingerprint Based Probabilistic Scoring of Metabolic Sites"

A number of poster presentations (including three at the SoT 2012)

Publications

Toplak, M.; Močnik, R.; Polajnar, M.; Bosnic, Z.; Carlsson, L.; **Hasselgren, C.**; Demsar, J.; Boyer, S.; Zupan, B.; Stålring, J.; Assessment of machine learning reliability methods for quantifying the applicability domain of QSAR regression models. *Accepted in J. Chem. Inf. Mod.*

Stålring, J., Almeida, P. R., Carlsson, L., Ahlberg, E., **Hasselgren, C.**, Boyer, S., Localized Heuristic Inverse Quantitative Structure Activity Relationship with Bulk Descriptors Using Numerical Gradients. *J. Chem. Inf. Mod.* 2013 *53* (8), 2001-2017.

Muthas, D., Boyer, S., **Hasselgren, C.**, A critical assessment of modeling Safety-related drug attrition. MedChemComm (2013), 4(7), 1058-1065.

Hasselgren, C.,Muthas, D., Ahlberg, E., Andersson, S., Carlsson, L., Noeske, T., Stålring, J., Boyer, S., Chemoinformatics and Beyond – moving from simple models to complex relationships in pharmaceutical computational toxicology. Bookchapter in "Chemoinformatics For Drug Discovery" Published by Wiley, 2013.

Dobo, K. L., Greene, N., Fred, C., Glowienke, S., Harvey, J. S., **Hasselgren**, **C.**, Jolly, R., Kenyon, M. O., Munzner, J. B., Muster, W., Neft, R., Reddy, M. V., White, A. T., Weiner. A., In silico methods combined with expert knowledge rule out mutagenic potential of pharmaceutical impurities: An industry survey. *Reg. Toxic. And Pharm.*, 2012, 62, 449-455.

Shamovsky, I., Ripa, L., Börjesson, L., Mee, C., Nordén, B., Hansen, P., **Hasselgren, C.**, O'Donovan, M., Sjö, P., Explanation for Main Features of Structure–Genotoxicity Relationships of Aromatic Amines by Theoretical Studies of Their Activation Pathways in CYP1A2. *J. Am. Chem. Soc.,* 2011, 133, 16168-16185.

Glowienke, S., **Hasselgren, C.**, Use of structure activity relationship (SAR) evaluation as a critical tool in the evaluation of the genotoxic potential of impurities. Chapter in "Genotoxic impurities – Strategies for Identification and Control" 2010 Edited by Andrew Teasdale, John Wiley & Sons Inc.

Yang, C., **Hasselgren, C.**, Boyer, S., Arvidson, K., Aveston, S., Dierkes, P., Benigni, R., Benz, R. D., Contrera, J., Kruhlak, N. L., Matthews, E. J., Han, X., Jaworska, J., Kemper, R. A., Rathman, J. F., Richard, A. M. Understanding Genetic Toxicity Through Data Mining: The Process of Building Knowledge by Integrating Multiple Genetic Toxicity Databases. *Toxicol. Mech. Methods* (2008), 18(2-3), 277-295.

Gleeson, M. P., Davis, A. M., Chohan, K. K., Paine, S. W., Boyer, S., Gavaghan, C. L., **Hasselgren Arnby, C.**, Kankkonen, C., Albertson, N. Generation of in-silico cytochrome P450 1A2, 2C9, 2C19, 2D6, and 3A4 inhibition QSAR models. *J. Comput. Aided Mol. Des.* (2007), 21(10-11), 559-573.

Gavaghan, C. L., **Hasselgren Arnby, C.**, Blomberg, N., Strandlund, G., Boyer, S. Development, interpretation and temporal evaluation of a global QSAR of hERG electrophysiology screening data. *J. Comput. Aided Mol. Des.* (2007), 21(4), 189-206.

Afzelius, L., **Hasselgren Arnby, C.**, Broo, A., Carlsson, L., Isaksson, C., Jurva, U., Kjellander, B., Kolmodin, K., Nilsson, K., Raubacher, F., Weidolf, L. State-of-the-art tools for computational site of metabolism predictions: comparative analysis, mechanistical insights, and future applications. *Drug Metab. Rev.* (2007), 39(1), 61-86.

Boyer, S., **Hasselgren Arnby, C.**, Carlsson, L., Smith, J., Stein, V., Glen, R. C. Reaction Site Mapping of Xenobiotic Biotransformations. *J. Chem. Inf. Model.* (2007), 47(2), 583-590.

Glen, R. C., Bender, A., **Hasselgren Arnby, C.**, Carlsson, L., Boyer, S., Smith, J. Circular fingerprints: flexible molecular descriptors with applications from physical chemistry to ADME. *IDrugs* (2006), 9(3), 199-204.

Hasselgren Arnby, C., Jagner, S., Dance, I. Questions for crystal engineering of halocuprate complexes. Concepts for a difficult system. *CrystEngComm* (2004), 6 257-275.

Hasselgren, C., Jagner, S. Halocuprates(I) crystallising with the $Ph_3PNPPh_3^+$ cation: preparation and structural characterisation of $(Ph_3PNPPh_3)_2[Cu_4Br_6]$ and $(Ph_3PNPPh_3)[CuBrCl]$. *Inorg. Chim. Acta,* (2002), **336** 137-141.

Hasselgren, C., Jagner, S., Dance, I. Three-coordinate $[Cu^{II}X_3]$- (X = Cl, Br), trapped in a molecular crystal. *Chem. Eur. J.,* (2002), **8**(6), 1269-1278.

Hasselgren, C., Park, H. I., Ming, L-J. Metal ion binding and activation of Streptomyces griseus dinuclear aminopeptidase: cadmium(II) binding as a model. *JBIC,* (2001), **6**(2), 120-127.

Hasselgren, C., Fisher, K., Jagner, S., Dance, I. Supramolecular assemblies of quaternary ammonium cations and halide anions in the gas phase: ESMS-FTICR data and computer modelling. *Chem. Eur. J.,* (2000), **6**(20), 3671-3678.

Hasselgren, C., Jagner, S., *Acta Cryst.* Dirubidium catena-poly[dichloroargentate(I)-□ -chloro]. (1999), C55(8), 1208-1210.

Hasselgren, C., Stenhagen, G., Öhrstrom, L., Jagner, S. On tuning the copper(I) coordination number in halocuprate(I) anions: new insights into cation control. *Inorg. Chim. Acta,* (1999), 292(2), 266-271.

Hasselgren, C., Dean, P. A. W., Scudder, M. L., Craig, D. C., Dance, I. Dominant cation-cation supramolecular motifs in crystals. Hexagonal arrays of sextuple phenyl embraces in halometalate salts of $MePh_3P^+$. *J. Chem. Soc. Dalton Trans.,* (1997), (12), 2019-2027.