

## Personal Data

Full name Age Klaas Smilde  
Date of birth February 14, 1957  
Place of birth Leeuwarden

## Work address

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## Education

1984-1990 **PhD** *University of Groningen* Analytical Chemistry (Cum Laude)  
Thesis title: Multivariate Calibration of Reversed-Phase Chromatographic Systems  
1975-1984 **MSc** *University of Groningen* Econometrics  
Thesis title: Errors in variables models

## Experience

### Primary employments

2004– **Professor of Biosystems Data Analysis** *University of Amsterdam*  
1993-2004 **Professor of Process Analysis and Chemometrics** *University of Amsterdam*  
1984-1993 **Assistant Professor of Chemometrics** *University of Groningen*

### Secondary employments

2013– **Professor of Computational Systems Biology** *Faculty of Sciences, University of Copenhagen*  
2014–2017 **Principal Investigator** *Academic Medical Centre, University of Amsterdam*  
2014–2016 **Professor of Computational Systems Biology** *Faculty of Health and Medical Sciences, University of Copenhagen*  
2012–2017 **Professor of Biosystems Data Analysis** *Academic Medical Centre*  
2003–2008 **Program Manager Biostatistics** *TNO, Zeist (NL)*  
1992 **Visiting Scientist (NWO scholarship)** *CPAC, Seattle (USA)*

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## Awards and Achievements

- 2017 **Kowalski Award for Best Applied Paper 2015-2016** *Journal of Chemometrics* Wiley, USA
- 2015 **Best 2014 Paper Award** *Metabolomics Society* San Francisco, USA
- 2013 **Highest 2013 Download Award** *Metabolomics Society* Glasgow, United Kingdom
- 2013 **Best Pre-2013 Paper Award** *Metabolomics Society* Glasgow, United Kingdom
- 2012 **I.M. Kolthoff Award for thesis Nutrikinetics (Van Velzen)** *Royal Netherlands Chemical Society* Netherlands
- 2006 **Achievements in Chemometrics Award** *Eastern Analytical Symposium* New Jersey, USA
- 2003- **Invited Secondary Employments** *TNO, AMC, Copenhagen*
- 1996 **Chair Elect** *Gordon Research Conference Statistics in Chemistry and Chemical Engineering* Oxford, United Kingdom

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## Management Activities

- 2015- **Board member of the Netherlands Metabolomics Centre (NMC)**
- 2012-2014 **Board member of the Netherlands Institute for Systems Biology**
- 2007-2013 **Co-founder and member of the Executive Committee of the NMC**

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## Outreach Activities

### Organizing committees

- 2018- **SSC16** *Member of the International Scientific Committee*
- 2016- **Metabolomics Society** *Member of the International Organizing Committee*
- 2000- **Chemometrics in Analytical Chemistry (CAC)** *Member of the International Scientific Committee*
- 1994- **International Chemometrics Research Meetings (ICRM)** *Member of the International Scientific Committee*
- 1993- **Three-way Analysis in Chemistry and Psychology (TRICAP)** *Co-founder and member of the International Scientific Committee*

### Scientific Advisory Boards

- 2014- **Member of the Scientific Advisory Board of the ASK Consortium** *Sogndal, Norway*
- 2014- **Member of the Scientific Advisory Board of the BIOPROD II Consortium** *Copenhagen, Denmark*
- 2013-2017 **Member of the Scientific Advisory Board of the Consortium MIMOmics** *European Union, Brussels*

### Invited Lectures (selection)

- 2017 **Numerical Representations of Metabolic Systems** *MOVISS, Vorau, Austria*
- 2017 **Fusing data of different measurement scales** *SSC15, Naantali, Finland*
- 2015 **Challenges in analyzing metabolomics data** *International Symposium on Profiling (ISPROF), Lisbon, Portugal*

## External assessments

- 1993- **External reviewer for foreign Research Councils** *Canada, USA, Sweden, Norway, Belgium, Switzerland, UK, Cyprus*
- 1993- **External assessor for tenure track positions** *USA, UK, Netherlands, Belgium, Sweden, Italy, Norway*

## Earning capacity (2010-2018)

Source	Period	Amount (Euro)
BioAssist (NGI)	May 2010 - Dec 2013	220,000
NMC-Valorisation	July 2011 - Dec 2012	100,000
NMC-Admit	Jan 2013 - Dec 2013	100,000
Stategra (EU)	Oct 2012 - Sept 2015	600,000
COPSAC (DK)	Oct 2014 - Sept 2016	160,000
AAA-Fonds (VU/UvA)	Jan 2015 - Dec 2018	160,000
Counterstrike (KU/UvA)	April 2015 - Aug 2019	250,000
Chemosense (UvA/LU/WUR/Unilever/DSM)	June 2018 - May 2021	300,000
<b>Total</b>		<b>1,890,000</b>

## Contributions to publications

### Editorial Boards

- 2018- **Editor-in-Chief of the Journal of Chemometrics**
- 2017- **Member of the Editorial Advisory Board of Metabolites**
- 2003-2018 **Member of the Editorial Advisory Board of the Journal of Chemometrics**
- 1994-2002 **Editor-Europe of the Journal of Chemometrics**
- 1990-1994 **Member of the Editorial Advisory Board of Chemometrics and Intelligent Laboratory Systems**

### Reviewing activities

- 1986- **Reviewer** *Analytical Chemistry, Analytica Chimica Acta, The Analyst, Bioinformatics, BMC Bioinformatics, British Journal of Mathematical and Statistical Psychology, Chemometrics and Intelligent Laboratory Systems, Computational Statistics and Data Analysis, Journal of Chemometrics, Linear Algebra and its Applications, Metabolomics, Nature, PLoS Computational Biology, PLoS One, Psychometrika, Technometrics.*

### Publications

- 1986- **Peer reviewed publications: 250**
- 1986- **Books: 3**
- 1986- **Book chapters: 7**
- 1986- **Proceedings contributions: 3**
- H-index: 51 (WoS), 62 (GS)**

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## Supervision and Teaching

- 1993- **Supervision of 36 PhD students**
- 1993- **Supervision of many BSc and MSc students**
- 2014-2015 **Systems Biology BSc Course** Amsterdam University College
- 2014- **ASCA PhD Course** Copenhagen School of Chemometrics, Copenhagen
- 2013-2015 **Data Fusion PhD Course** EMBO, Hinxton, United Kingdom
- 2010- **Matrix Algebra PhD Course** Faculty of Sciences
- 2004- **Biosystems Data Analysis MSc course** Faculty of Sciences
- 1993-2004 **Process Analysis MSc course** Faculty of Chemistry
- 1993-2004 **Numerical Techniques MSc course** Faculty of Chemistry

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## List of PhD theses

### Systems Biology, Proteomics and Metabolomics

- 2017 **Use of prior knowledge in biological systems modelling** *P. Reshetova* University of Amsterdam
- 2016 **Computational interaction proteomics: from proteome to complexome** *J. Kutzera* University of Amsterdam
- 2015 **Validation of systems biology models** *D. Hasdemir* University of Amsterdam
- 2013 **Network inference from time-resolved metabolomics data** *D.M. Hendrickx* University of Amsterdam
- 2012 **Fusing prior knowledge with microbial metabolomics** *M.P.H. Verouden* University of Amsterdam
- 2010 **Nutrikinetics** *E.J.J. van Velzen* University of Amsterdam
- 2010 **Real-life metabolomics data analysis: how to deal with complex data?** *C.M. Rubingh* University of Amsterdam
- 2010 **Endocrine Dynamics: Quantifying Events and Rhythms** *D.J. Vis* University of Amsterdam
- 2009 **Statistical data processing in clinical proteomics** *S. Smit* University of Amsterdam
- 2008 **Crossing borders between biology and data analysis** *R.A. van den Berg* University of Amsterdam
- 2005 **ASCA** *J.J. Jansen* University of Amsterdam

### Process Analysis and Chemometrics

- 2008 **Optimal sensor placement and timing: where and when to measure?** *O. Stanimirovic* University of Amsterdam
- 2005 **PAT and Beyond** *E.T.S. Skibsted* University of Amsterdam
- 2005 **Chromametrics** *V. van Mispelaar* University of Amsterdam
- 2005 **Methods to improve quantitative and qualitative analysis of spectroscopic measurements** *H.F.M. Boelens* University of Amsterdam
- 2004 **Temperature-robust multivariate calibration** *F. Wulfert* University of Amsterdam
- 2004 **Statistical batch process monitoring** *H.J. Ramaker* University of Amsterdam

- 2004 **Statistical batch process monitoring** *E.N.M. van Sprang* University of Amsterdam
- 2001 **Optimal process analyzer selection and positioning for plant-wide monitoring** *F.W.J. van den Berg* University of Amsterdam
- 2000 **Quantifying sources of variation in process analytical measurements** *R.H. Jellema* University of Amsterdam
- 2000 **Estimating rate constants of chemical reactions using spectroscopy** *S. Bijlsma* University of Amsterdam
- 1998 **Multi-way Analysis in the Food Industry. Models, Algorithms, and Applications** *R. Bro* University of Amsterdam
- Co-supervised**
- 2017 **Mastering data pre-processing for accurate quantitative molecular profiling with liquid chromatography coupled to mass spectrometry** *V. Mitra* University of Groningen
- 2012 **Optimized data processing algorithms for biomarker discovery by LC-MS** *C. Christin* University of Groningen
- 2006 **Practical and Computational Aspects in Chemometric Data Analysis** *G. Tomasi* Royal Veterinary and Agricultural University Copenhagen
- 2005 **Biomarker discovery in life sciences** *R.A.N. Lamers* Leiden University
- 2003 **In-line monitoring of controlled radical copolymerisation reactions with near infrared spectroscopy** *C. Beyers* Technical University Eindhoven
- 2002 **Pattern recognition techniques applied to NMR spectra in life sciences** *J.T.W.E. Vogels* Leiden University
- 1998 **Multiway calibration in 3D QSAR. Applications to dopamine receptor ligands** *J. Nilsson* University of Groningen
- 1996 **Chemometric analysis of aged RP-HPLC stationary phases** *A. Bolck* University of Groningen
- 1993 **Construction and analysis of mixture-process variables designs as applied to table formulations** *C.A.A. Duineveld* University of Groningen
- 1992 **Chemometrical aspects of quality in pharmaceutical technology** *J.H. de Boer* University of Groningen

## Languages

Dutch	<b>Native</b>
English	<b>Fluent</b>
German	<b>Advanced</b>
French	<b>Moderate</b>
Spanish	<b>Moderate</b>
Frisian	<b>Moderate</b>

## Personal Interests

- Making music
- Philosophy of Science
- Traveling (see [www.awayfrom63.com](http://www.awayfrom63.com))

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## Peer-reviewed Papers

- [a250] V. Mitra, A. K. Smilde, R. Bischoff, and P. Horvatovich. “Tutorial: Correction of shifts in single-stage LC-MS(/MS) data”. In: *Analytica Chimica Acta* 999 (2018), pp. 37–53.
- [a249] V. Aru, C. Lam, B. Khakimov, H. C. J. Hoefsloot, G. Zwanenburg, M. V. Lind, H. Schafer, J. van Duynhoven, D. M. Jacobs, A. K. Smilde, and S. B. Engelsen. “Quantification of lipoprotein profiles by nuclear magnetic resonance spectroscopy and multivariate data analysis”. In: *Trends in Analytical Chemistry* 94 (2017), pp. 210–219.
- [a248] S. M. Centelles, H. C. J. Hoefsloot, B. Khakimov, P. Ebrahimi, M. V. Lind, M. Kristensen, N. de Roo, D. M. Jacobs, J. van Duynhoven, C. Gannet, F. Fang, E. Humpfer, H. Schafer, M. Spraul, S. B. Engelsen, and A. K. Smilde. “Toward Reliable Lipoprotein Particle Predictions from NMR Spectra of Human Blood: An Interlaboratory Ring Test”. In: *Analytical Chemistry* 89.15 (2017), pp. 8004–8012.
- [a247] M. Coccia et al. “Cellular and molecular synergy in AS01-adjuvanted vaccines results in an early IFN gamma response promoting vaccine immunogenicity”. In: *NPJ Vaccines* 2 (Sept. 2017), p. 25.
- [a246] K. Liland, A.K. Smilde, F. Marini, and T. Naes. “Confidence ellipsoids for ASCA models based on multivariate regression Theory”. In: *Journals of Chemometrics* Accepted (2017).
- [a245] A. K. Smilde, I. Mage, T. Naes, T. Hankemeier, M. A. Lips, H. A. L. Kiers, E. Acar, and R. Bro. “Common and distinct components in data fusion”. In: *Journal of Chemometrics* 31.7 (July 2017), e2900.
- [a244] Y. Song, J A. Westerhuis, N. Aben, M. Michaut, L.F.A. Wessels, and Smilde A.K. “Principal component analysis of binary genomics data”. In: *Briefings in Bioinformatics* Accepted (2017).
- [a243] R. I. Versteeg, D. J. Stenvers, D. Visintainer, A. Linnenbank, M. W. Tanck, G. Zwanenburg, A. K. Smilde, E. Fliers, A. Kalsbeek, M. J. Serlie, S. E. la Fleur, and P. H. Bisschop. “Acute effects of morning light on plasma glucose and triglycerides in healthy men and men with Type 2 Diabetes”. In: *Journal of Biological Rhythms* 32.2 (2017), pp. 130–142.
- [a242] R. Vitale, J A. Westerhuis, T. Naes, A.K. Smilde, O.E. de Noord, and A. Ferrer. “Selecting the number of factors in Principal Component Analysis by permutation testing - Theoretical and practical aspects”. In: *Journal of Chemometrics* Accepted (2017).
- [a241] P. Fazelzadeh, R. Hangelbroek, M. Tieland, L. de Groot, L. Verdijk, L. van Loon, A.K. Smilde, R. Alves, J. Vervoort, M. Mueller, J. van Duynhoven, and M. Boekschoten. “The muscle metabolome differs between healthy and frail subjects of older age”. In: *Journal of Proteomics Research* 15.2 (2016), pp. 499–509.
- [a240] A. Gardlo, A.K. Smilde, K. Hron, M. Hrda, R. Karlikova, D. Friedecky, and T. Adam. “Normalization techniques for PARAFAC modeling of urine metabolomics”. In: *Metabolomics* 12.7 (2016), e117.
- [a239] F.M. Van der Kloet, P. Sebastian-Leon, A. Conesa, Smilde A.K., and J A. Westerhuis. “Separating common from distinctive variation”. In: *BMC Bioinformatics* 17.5 (2016), e271.
- [a238] V. Mitra, N. Govorukhina, G. Zwanenburg, H. Hoefsloot, I. Westra, A.K. Smilde, T. Reijmers, A. van der Zee, F. Suits, R. Bischoff, and P. Horvatovich. “Identification of analytical factors affecting complex proteomics profiles acquired in a factorial design study with ANOVA - simultaneous component analysis”. In: *Analytical Chemistry* 88.8 (2016), pp. 4229–4238.
- [a237] J. H. M. Stroeve, E. Saccenti, J. Bouwman, A. Dane, K. Strassburg, J. Vervoort, T. Hankemeier, A. Astrup, A. K. Smilde, B. van Ommen, and W. H. M. Saris. “Weight loss predictability by plasma metabolic signatures in adults with obesity and morbid obesity of the DiOGenes study”. In: *Obesity* 24.2 (2016), pp. 379–388.

- [a236] D. Hasdemir, H.C.J. Hoefsloot, and A.K. Smilde. “Validation and selection of ODE based systems biology models: how to arrive at more reliable decisions”. In: *BMC Systems Biology* 9 (2015), e32.
- [a235] J. Kutzera, A.K. Smilde, T.F. Wilderjans, and H.C.J.; Hoefsloot. “Towards a hierarchical strategy for finding protein complexes in multi scale IP/MS data”. In: *PLoS One* 10.10 (2015), e0139704.
- [a234] P. Reshetova, A.K. Smilde, J.A. Westerhuis, and A.H.C. van Kampen. “Using Petri nets for experimental design in a multi-organ elimination pathway.” In: *Computers in biology and medicine* 63 (2015), pp. 19–27.
- [a233] E. Saccenti, J.H.M. van Duynhoven, D.M. Jacobs, A.K. Smilde, and H.C.J. Hoefsloot. “Strategies for individual phenotyping of linoleic and arachidonic Acid metabolism using an oral glucose tolerance test.” In: *PloS One* 10.3 (2015), e0119856.
- [a232] A.K. Smilde, M.E. Timmerman, E. Saccenti, J.J. Jansen, and H.C.J. Hoefsloot. “Covariances Simultaneous Component Analysis: a new method within a framework for modeling covariances”. In: *Journal of Chemometrics* 29.5 (2015), pp. 277–288.
- [a231] M.E. Timmerman, H.C.J. Hoefsloot, A.K. Smilde, and E. Ceulemans. “Scaling in ASCA”. In: *Metabolomics* 11.5 (2015), pp. 1265–1276.
- [a230] K. Van Deun, L. Thorrez, R.A. van den Berg, A.K. Smilde, and I. Van Mechelen. “Not just a sum? Identifying different types of interplay between constituents in combined interventions”. In: *Plos One* 10.5 (2015), e0125334.
- [a229] D.J. Vis, J.A. Westerhuis, D.M. Jacobs, J.P.M. van Duynhoven, S. Wopereis, B. van Ommen, M.M.W.B. Hendriks, and A.K. Smilde. “Analyzing metabolomics-based challenge tests”. In: *Metabolomics* 11.1 (2015), pp. 50–63.
- [a228] A.M. Willemsen, D.M. Hendrickx, H.C.J. Hoefsloot, M.M.W.B. Hendriks, S.A. Wahl, B. Teusink, A.K. Smilde, and A.H.C. van Kampen. “MetDFBA: incorporating time-resolved metabolomics measurements into dynamic flux balance analysis”. In: *Molecular Biosystems* 11.1 (2015), pp. 137–145.
- [a227] R. Bro and A.K. Smilde. “Principal component analysis”. In: *Analytical Methods* 6.9 (2014), pp. 2812–2831.
- [a226] M. Coccia, C. Herve, C. Collignon, K. Van Deun, R.A. van den Berg, I. Van Mechelen, A.K. Smilde, S. Morel, N. Garcon, R. van der Most, M. Van Mechelen, and A.M. Didierlaurent. “Early NK cell activation as a result of MPL and QS-21 combination controls the adjuvant effect induced by the human Adjuvant System AS01”. In: *Immunology* 143 (2014), p. 61.
- [a225] D. Hasdemir, H.C.J. Hoefsloot, J.A. Westerhuis, and A.K. Smilde. “How informative is your kinetic model?: Using resampling methods for model invalidation”. In: *BMC Systems Biology* 8 (2014), e61.
- [a224] M. Kaduk, H.C.J. Hoefsloot, D.J. Vis, T. Reijmers, J. van der Greef, A.K. Smilde, and M.M.W.B. Hendriks. “Correlated measurement error hampers association network inference”. In: *Journal of Chromatography B-analytical Technologies In the Biomedical and Life Sciences* 966 (2014), pp. 93–99.
- [a223] O.M. Kvalheim, R. Arneberg, O. Bleie, T. Rajalahti, A.K. Smilde, and J.A. Westerhuis. “Variable importance in latent variable regression models”. In: *Journal of Chemometrics* 28.8 (2014), pp. 615–622.

- [a222] V.V. Mihaleva, D.B. van Schalkwijk, A.A. de Graaf, J.P.M. Van Duynhoven, F.A. Van Dorsten, J. Vervoort, A.K. Smilde, J.A. Westerhuis, and D.M. Jacobs. “A systematic approach to obtain validated partial least square models for predicting lipoprotein subclasses from serum NMR spectra”. In: *Analytical Chemistry* 86.1 (2014), pp. 543–550.
- [a221] V. Mitra, A.K. Smilde, H.C.J. Hoefsloot, F. Suits, R. Bischoff, and P. Horvatovich. “Inversion of peak elution order prevents uniform time alignment of complex liquid-chromatography coupled to mass spectrometry datasets”. In: *Journal of Chromatography A* 1373 (2014), pp. 61–72.
- [a220] P. Reshetova, A.K. Smilde, A.H.C. van Kampen, and J.A. Westerhuis. “Use of prior knowledge for the analysis of high-throughput transcriptomics and metabolomics data”. In: *BMC Systems Biology* 8 (2014), S2.
- [a219] E. Saccenti, H.C.J. Hoefsloot, A.K. Smilde, J.A. Westerhuis, and M.M.W.B. Hendriks. “Reflections on univariate and multivariate analysis of metabolomics data”. In: *Metabolomics* 10.3 (2014), pp. 361–374.
- [a218] E. Saccenti, L. Tenori, P. Verbruggen, M.E. Timmerman, J. Bouwman, J. van der Greef, C. Luchinat, and A.K. Smilde. “Of Monkeys and Men: A Metabolomic Analysis of Static and Dynamic Urinary Metabolic Phenotypes in Two Species”. In: *Plos One* 9.9 (2014), e106077.
- [a217] S. Smit, E. Szymanska, I. Kunz, V.G. Roldan, M.W.E.M. van Tilborg, P. Weber, K. Prudence, F.M. van der Kloet, J.P.M. van Duynhoven, A.K. Smilde, R.C.H. de Vos, and I. Bendik. “Nutrikinetic modeling reveals order of genistein phase II metabolites appearance in human plasma”. In: *Molecular Nutrition & Food Research* 58.11 (2014), pp. 2111–2121.
- [a216] E.J.J. van Velzen, J.A. Westerhuis, C.H. Grun, D.M. Jacobs, P.H.C. Eilers, T.P. Mulder, M. Foltz, U. Garczarek, R. Kemperman, E.E. Vaughan, J.P.M. van Duynhoven, and A.K. Smilde. “Population-based nutrikinetic modeling of polyphenol exposure”. In: *Metabolomics* 10.6 (2014), pp. 1059–1073.
- [a215] D.J. Vis, M.M.W.B. Hendriks, M. Sailer, A.K. Smilde, H. Daniel, and J.A. Westerhuis. “A technical note on challenge tests in human volunteers for multidimensional phenotyping”. In: *Chemometrics and Intelligent Laboratory Systems* 136 (2014), pp. 81–84.
- [a214] D.J. Vis, J.A. Westerhuis, H.C.J. Hoefsloot, F. Roelfsema, J. Van der Greef, M.M.W.B. Hendriks, and A.K. Smilde. “Network Identification of Hormonal Regulation”. In: *Plos One* 9.5 (2014), e96284.
- [a213] Y. Zha, J.A. Westerhuis, B. Muilwijk, K.M. Overkamp, B.M. Nijmeijer, L. Coulier, A.K. Smilde, and P.J. Punt. “Identifying inhibitory compounds in lignocellulosic biomass hydrolysates using an exometabolomics approach”. In: *BMC Biotechnology* 14 (2014), p. 22.
- [a212] C. Christin, H.C.J. Hoefsloot, A.K. Smilde, B. Hoekman, F. Suits, R. Bischoff, and P. Horvatovich. “A critical assessment of feature selection methods for biomarker discovery in clinical proteomics”. In: *Molecular and Cellular Proteomics* 12.1 (2013), pp. 263–276.
- [a211] J. Kutzera, H.C.J. Hoefsloot, A. Malovannaya, A.B. Smit, I. Van Mechelen, and A.K. Smilde. “Inferring protein-protein interaction complexes from immunoprecipitation data.” In: *BMC Research Notes* 6 (2013), pp. 468–468.
- [a210] C.M. Rubingh, H. Martens, H. van der Voet, and A.K. Smilde. “The costs of complex model optimization”. In: *Chemometrics and Intelligent Laboratory Systems* 125 (2013), pp. 139–146.
- [a209] K. Van Deun, A.K. Smilde, L. Thorrez, H.A.L. Kiers, and I. Van Mechelen. “Identifying common and distinctive processes underlying multiset data”. In: *Chemometrics and Intelligent Laboratory Systems* 129 (2013), pp. 40–51.

- [a208] S. Ellero-Simatos, E. Szymanska, T. Rullmann, W.H.A. Dokter, R. Ramaker, R. Berger, T.M.P. van Iersel, A.K. Smilde, T. Hankemeier, and W. Alkema. “Assessing the metabolic effects of prednisolone in healthy volunteers using urine metabolic profiling”. In: *Genome Medicine* 4 (2012), p. 94.
- [a207] D. Hasdemir, G.J. Smits, J.A. Westerhuis, and A.K. Smilde. “Topology of transcriptional regulatory networks: testing and improving”. In: *Plos One* 7.7 (2012), e40082.
- [a206] D.M. Hendrickx, H.C.J. Hoefsloot, M.M.W.B. Hendriks, A.B. Canelas, and A.K. Smilde. “Global test for metabolic pathway differences between conditions”. In: *Analytica Chimica Acta* 719 (2012), pp. 8–15.
- [a205] D.M. Hendrickx, H.C.J. Hoefsloot, M.M.W.B. Hendriks, D.J. Vis, A.B. Canelas, B. Teusink, and A.K. Smilde. “Inferring differences in the distribution of reaction rates across conditions”. In: *Molecular Biosystems* 8.9 (2012), pp. 2415–2423.
- [a204] J.J. Jansen, E. Szymanska, H.C.J. Hoefsloot, D.M. Jacobs, K. Strassburg, and A.K. Smilde. “Between metabolite relationships: an essential aspect of metabolic change”. In: *Metabolomics* 8.3 (2012), pp. 422–432.
- [a203] J.J. Jansen, E. Szymanska, H.C.J. Hoefsloot, and A.K. Smilde. “Individual differences in metabolomics: individualised responses and between-metabolite relationships”. In: *Metabolomics* 8.1 (2012), S94–S104.
- [a202] A.K. Smilde, M.E. Timmerman, M.M.W.B. Hendriks, J.J. Jansen, and H.C.J. Hoefsloot. “Generic framework for high-dimensional fixed-effects ANOVA”. In: *Briefings In Bioinformatics* 13.5 (2012), pp. 524–535.
- [a201] E. Szymanska, J. Bouwman, K. Strassburg, J. Vervoort, A.J. Kangas, P. Soinen, M. Ala-Korpela, J.A. Westerhuis, J.P.M. van Duynhoven, D.J. Mela, I.A. Macdonald, R.J. Vreeken, A.K. Smilde, and D.M. Jacobs. “Gender-dependent associations of metabolite profiles and body fat distribution in a healthy population with central obesity: towards metabolomics diagnostics”. In: *Omics-a Journal of Integrative Biology* 16.12 (2012), pp. 652–667.
- [a200] E. Szymanska, F. A. van Dorsten, J. Troost, I. Paliukhovich, E.J.J. van Velzen, M.M.W.B. Hendriks, E.A. Trautwein, J.P.M. van Duynhoven, R.J. Vreeken, and A.K. Smilde. “A lipidomic analysis approach to evaluate the response to cholesterol-lowering food intake”. In: *Metabolomics* 8.5 (2012), pp. 894–906.
- [a199] E. Szymanska, E. Saccenti, A.K. Smilde, and J.A. Westerhuis. “Double-check: validation of diagnostic statistics for PLS-DA models in metabolomics studies”. In: *Metabolomics* 8.1 (2012), S3–S16.
- [a198] K. Van Deun, I. Van Mechelen, L. Thorrez, M. Schouteden, B. De Moor, M.J. van der Werf, L. De Lathauwer, A.K. Smilde, and H.A.L. Kiers. “DISCO-SCA and properly applied GSVD as swinging methods to find common and distinctive processes”. In: *Plos One* 7.5 (2012), e37840.
- [a197] J.P.M. Van Duynhoven, E.J.J. van Velzen, J A. Westerhuis, M. Foltz, D.M. Jacobs, and A.K. Smilde. “Nutrikinetics: Concept, technologies, applications, perspectives”. In: *Trends In Food Science & Technology* 26.1 (2012), pp. 4–13.
- [a196] D.J. Vis, J.A. Westerhuis, H.C.J. Hoefsloot, F. Roelfsema, M.M.W.B. Hendriks, and A.K. Smilde. “Detecting regulatory mechanisms in endocrine time series measurements”. In: *Plos One* 7.3 (2012), e32985.

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