

Personal Data

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

Work address

Group Biosystems Data Analysis, University of Amsterdam
Address Science Park 904, 1098 XH, Amsterdam
Phone +31 20 525 5062
Email a.k.smilde@uva.nl
Website www.bdagroup.nl

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

2020– **Research Professor of Machine Learning methods for Life Science Data**
Simula, Oslo, Norway
2013– **Professor of Computational Systems Biology** *Faculty of Sciences, University of Copenhagen*
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)*

Awards and Achievements

- 2020 **Highest download award 2019-2020** *Journal of Chemometrics* Wiley, USA
- 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
- 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, Oslo*
- 1996 **Chair Elect** *Gordon Research Conference Statistics in Chemistry and Chemical Engineering* Oxford, United Kingdom

Management Activities

- 2019- **Program Leader Research Priority Area Host-Microbiome Interaction**
- 2019- **Member of the Management Team of SILS**
- 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**

Outreach Activities

Organizing committees

- 2019 **Metabolomics Society** *Co-chair of the MX2019 (> 1000 participants)*
- 2018- **SSC16** *Member of the International Scientific 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*

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 (2012-2020)

Source	Period	Amount (Euro)
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 (DK)	April 2015 - Aug 2019	250,000
Chemosense (NWO)	June 2018 - May 2021	300,000
RPA-Systems Biology (UvA)	April 2019 - April 2024	350,000
MiCROP (NWO)	Dec 2020 - Dec 2023	250,000
Moonlight (NWO)	Oct 2020 - Oct 2022	300,000
RPA-Personal Microbial Health (UvA)	Jan 2021 - Dec 2025	300,000
Total		2,670,000

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: 295**
- 1986- **Books: 3**
- 1986- **Book chapters: 9**
- 1986- **Proceedings contributions: 3**
- H-index: 57 (WoS), 69 (GS)**

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
- 2014-2018 **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

List of PhD theses

Systems Biology, Proteomics and Metabolomics

- 2019 **Fusing heterogeneous data sets** *Y. Song* University of Amsterdam
- 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. Wülfert* 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
- 2021 **From micro to macro level characterization of early childhood health** *S.K. Nørgaard* University of Copenhagen
- 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 tablet 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	Native
English	Fluent
German	Advanced
French	Moderate
Spanish	Moderate

Personal Interests

- Making music
- Philosophy of Science
- Traveling (see www.awayfrom63.com)

Peer-reviewed Papers

- [a280] M. Alinaghi, H.C. Bertram, A. Brunse, A.K. Smilde, and J.A. Westerhuis. “Common and distinct variation in data fusion of designed experimental data”. In: *Metabolomics* 16.1 (2020), p. 2.
- [a281] J. Camacho, A.K. Smilde, E. Saccenti, J.A. Westerhuis, and R. Bro. “All sparse PCA models are wrong, but some are useful. Part II: Limitations and problems of deflation”. In: *Chemometrics and Intelligent Laboratory Systems* (2020), p. 104212.
- [a281] L. De Mot, V. Bechtold, V. Bol, A. Callegaro, M. Coccia, A. Essaghir, D. Hasdemir, F. Ulloa-Montoya, E. Siena, A. K. Smilde, et al. “Transcriptional profiles of adjuvanted hepatitis B vaccines display variable interindividual homogeneity but a shared core signature”. In: *Science Translational Medicine* 12.569 (2020).
- [a279] D. Hasdemir, R.A. van den Berg, A. van Kampen, and A.K. Smilde. “Modeling adaptive response profiles in a vaccine clinical trial”. In: *BMC Medical Research Methodology* 20.1 (2020), pp. 1–13.
- [a281] F.M. van der Kloet, J. Buurmans, M.J. Jonker, A.K. Smilde, and J.A. Westerhuis. “Increased comparability between RNA-Seq and microarray data by utilization of gene sets”. In: *PLoS computational biology* 16.9 (2020), e1008295.
- [a278] R.F. Kranenburg, D. Peroni, S. Affourtit, J.A. Westerhuis, A.K. Smilde, and A.C. van Asten. “Revealing hidden information in GC–MS spectra from isomeric drugs: Chemometrics based identification from 15 eV and 70 eV EI mass spectra”. In: *Forensic Chemistry* 18 (2020), p. 100225.
- [a277] T. Næs, R. Romano, O. Tomic, I. Måge, A.K. Smilde, and K.H. Liland. “Sequential and orthogonalized PLS (SO-PLS) regression for path analysis: Order of blocks and relations between effects”. In: *Journal of Chemometrics* e3243 (2020).
- [a281] S.K. Nørgaard, K. Linder-Steinlein, A.U. Eliassen, J. Stokholm, B.L. Chawes, K. Bønnelykke, H. Bisgaard, A.K. Smilde, and M.A. Rasmussen. “On using kernel integration by graphical LASSO to study partial correlations between heterogeneous data sets”. In: *Journal of Chemometrics* (2020), e3324.
- [a275] S.J. Roeters, M. Sawall, C.E. Eskildsen, M. Panman, G. Tordai, M. Koeman, K. Neymeyr, J. Jansen, A.K. Smilde, and S. Woutersen. “Unraveling VEALYL amyloid formation using advanced vibrational spectroscopy and microscopy”. In: *Biophysical Journal* (2020).
- [a274] E. Saccenti, M.M.W.B. Hendriks, and A.K. Smilde. “Corruption of the Pearson correlation coefficient by measurement error and its estimation, bias, and correction under different error models”. In: *Scientific Reports* 10.1 (2020), pp. 1–19.
- [a273] E. Saccenti, M.M.W.B. Hendriks, and A.K. Smilde. “Corruption of the Pearson correlation coefficient by measurement error and its estimation, bias, and correction under different error models”. In: *Scientific Reports* 20.1 (2020), pp. 1–19.
- [a272] A.K. Smilde and T. Hankemeier. “Numerical Representations of Metabolic Systems”. In: *Analytical chemistry* 92.20 (2020), pp. 13614–13621.
- [a271] A.K. Smilde, Y. Song, J.A. Westerhuis, H.A.L. Kiers, N. Aben, and L.F.A. Wessels. “Heterofusion: Fusing genomics data of different measurement scales”. In: *Journal of Chemometrics* (2020), e3200.

- [a270] Y. Song, J.A. Westerhuis, and A.K. Smilde. “Logistic principal component analysis via non-convex singular value thresholding”. In: *Chemometrics and Intelligent Laboratory Systems* 204 (2020), p. 104089.
- [a269] Y. Song, J.A. Westerhuis, and A.K. Smilde. “Separating common (global and local) and distinct variation in multiple mixed types data sets”. In: *Journal of Chemometrics* 34.1 (2020), e3197.
- [a268] H.W. Uh, L. Klarić, I. Ugrina, G. Lauc, A.K. Smilde, and J.J. Houwing-Duistermaat. “Choosing proper normalization is essential for discovery of sparse glycan biomarkers”. In: *Molecular Omics* (2020).
- [a267] R. Vitale, O.E. de Noord, J.A. Westerhuis, A.K. Smilde, and A. Ferrer. “Divide et impera: How disentangling common and distinctive variability in multiset data analysis can aid industrial process troubleshooting and understanding”. In: *Journal of Chemometrics* (2020), e3266.
- [a266] J Camacho, A.K. Smilde, E. Saccenti, and J.A. Westerhuis. “All sparse PCA models are wrong, but some are useful. Part I: Computation of scores, residuals and explained variance”. In: *Chemometrics and Intelligent Laboratory Systems* (2019), p. 103907.
- [a264] I. Måge, F.M. van der Kloet, and A.K. Smilde. “Performance of methods that separate common and distinct variation in multiple data blocks”. In: *Journal of Chemometrics* 33.1 (2019), e3085.
- [a263] S. Monsonis-Centelles, H.C.J. Hoefsloot, S.B. Engelsen, A.K. Smilde, and M.V. Lind. “Repeatability and reproducibility of lipoprotein particle profile measurements in plasma samples by ultracentrifugation”. In: *Clinical Chemistry and Laboratory Medicine (CCLM)* 58.1 (2019), pp. 103–115.
- [a262] R. Romano, O. Tomic, K. Liland, Smilde A.K., and T. Naes. “A comparison of two PLS based approaches to Structural Equation Modeling”. In: *Journal of Chemometrics* 33 (2019), e3105.
- [a261] K. Van Deun, L. Thorrez, M. Coccia, D. Hasdemir, J.A. Westerhuis, A.K. Smilde, and I. Van Mechelen. “Weighted sparse principal component analysis”. In: *Chemometrics and Intelligent Laboratory Systems* 195 (2019), p. 103875.
- [a260] N. Aben, J. A. Westerhuis, Y. P. Song, H. A. L. Kiers, M. Michaut, A. K. Smilde, and L. F. A. Wessels. “iTOP: inferring the topology of omics data”. In: *Bioinformatics* 34.17 (Sept. 2018), pp. 988–996.
- [a259] A. Folch-Fortuny, B. Teusink, H. C. J. Hoefsloot, A. K. Smilde, and A. Ferrer. “Dynamic elementary mode modelling of non-steady state flux data”. In: *BMC Systems Biology* 12 (2018), p. 71.
- [a258] 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.
- [a257] J.J. de Rooi, S.K. Pedersen, M.A. Rasmussen, K. Bonnelykke, and H. Bisgaard. “Data representations and -analyses of binary diary data in pursuit of stratifying children based on common childhood illnesses”. In: *PLoS One* accepted (2018).

- [a256] E. Saccenti, A. K. Smilde, and J. Camacho. “Group-wise ANOVA simultaneous component analysis for designed omics experiments”. In: *Metabolomics* 14.6 (2018), p. 73.
- [a255] Y. Song, J.A. Westerhuis, N. Aben, L.F.A Wessels, P.F.J. Groenen, and A.K. Smilde. “Generalized Simultaneous Component Analysis of Binary and Quantitative data”. In: *arXiv:1807.04982* (2018).
- [a254] V. Aru, C. Lam, B. Khakimov, H.C.J. Hoefsloot, G. Zwanenburg, M.V. Lind, H. Schäfer, 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: *TrAC Trends in Analytical Chemistry* 94 (2017), pp. 210–219.
- [a253] G.U. Balcke, S. Bennewitz, N. Bergau, B. Athmer, A. Henning, P. Majovsky, J.M. Jiménez-Gómez, W. Hoehenwarter, and A. Tissier. “Multi-omics of tomato glandular trichomes reveals distinct features of central carbon metabolism supporting high productivity of specialized metabolites”. In: *The Plant Cell* 29.5 (2017), pp. 960–983.
- [a252] 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.
- [a251] 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.
- [a250] 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).
- [a249] S. Monsonis-Centelles, H.C.J. Hoefsloot, B. Khakimov, P. Ebrahimi, M.V. Lind, M. Kristensen, N. De Roo, D.M. Jacobs, J. Van Duynhoven, C. Cannel, 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.
- [a248] 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.
- [a247] Y. Song, J A. Westerhuis, N. Aben, M. Michaut, L.F.A. Wessels, and A.K. Smilde. “Principal component analysis of binary genomics data”. In: *Briefings in Bioinformatics* Accepted (2017).
- [a246] 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.

- [a245] 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* 31.12 (2017), e2937.
- [a244] 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.
- [a243] 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.
- [a242] 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.
- [a241] 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.
- [a240] 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.
- [a239] 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.
- [a238] 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.
- [a237] 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.
- [a236] 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.
- [a235] 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.
- [a234] M.E. Timmerman, H.C.J. Hoefsloot, A.K. Smilde, and E. Ceulemans. “Scaling in ASCA”. In: *Metabolomics* 11.5 (2015), pp. 1265–1276.
- [a233] 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.

- [a232] 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.
- [a231] 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.
- [a230] R. Bro and A.K. Smilde. “Principal component analysis”. In: *Analytical Methods* 6.9 (2014), pp. 2812–2831.
- [a229] 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.
- [a228] 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.
- [a227] 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.
- [a226] 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.
- [a225] 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.
- [a224] 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.
- [a223] 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.
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