Age K. Smilde

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

2004-2023	**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

2020-2023	**Research Professor of Machine Learning methods for Life Science Data** *Simula Metropolitan Center for Digital Engineering, Oslo, Norway*
2013-2025	**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

2021	**Herman Wold Gold Medal** *Swedish Chemical Society,* Sweden
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 Yersey, 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

2026-	**Member of Supervisory Board of the Holomicrobiome**
2019-2023	**Program Leader Research Priority Area Host-Microbiome Interaction**
2019-2022	**Member of the Management Team of SILS**
2015-2020	**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)*
2018-2023	**SSC16** *Member of the International Scientific Committee*
2000-2023	**Chemometrics in Analytical Chemistry (CAC)** *Member of the International Scientific Committee*
1994-2023	**International Chemometrics Research Meetings (ICRM)** *Member of the International Scientific Committee*
1993-2023	**Three-way Analysis in Chemistry and Psychology (TRICAP)** *Co-founder and member of the International Scientific Committee*

Scientific Advisory Boards

2014-2020	**Member of the Scientific Advisory Board of the ASK Consortium** *Sogndal,* Norway
2014-2022	**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

1993-2023   **External reviewer for foreign Research Councils** *Canada, USA, Sweden, Norway, Belgium, Switzerland, UK, Cyprus*

1993-2023   **External assessor for tenure track positions** *USA, UK, Netherlands, Belgium, Sweden, Italy, Norway*

Contributions to publications

Editorial Boards

2023-   **Member of the Editorial Advisory Board of the Journal of Chemometrics**

2021-2023   **Member of the Editorial Advisory Board of BioMedInformatics**

2018-2023   **Editor-in-Chief of the Journal of Chemometrics**

2017-2023   **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: 327**

1986-   **Books: 5**

1986-   **Book chapters: 9**

1986-   **Proceedings contributions: 4**

   H-index: 65 (WoS), 79 (GS)

Supervision and Teaching

1993-2023	**Supervision of 38 PhD students**
1993-2023	**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
2010-2023	**Matrix Algebra** *PhD Course* Faculty of Sciences
2004-2023	**Biosystems Data Analysis** *MSc course* Faculty of Sciences

List of PhD theses

Systems Biology, Proteomics and Metabolomics

2026	**Microbiome Data Analysis using Multi-way Methods** *G.R. van der Ploeg* University of Amsterdam
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 dopmanine 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

Personal Interests

- Making music
- Philosophy of Science
- Traveling (see www.awayfrom147.com)

Peer-reviewed Papers

[a309] G.R. van der Ploeg, F.T.G. White, R.R. Jakobsen, J.A. Westerhuis, A. Heintz-Buschart, and A.K. Smilde. "ACMTF-R: Supervised multi-omics data integration uncovering shared and distinct outcome-associated variation". In: *PLoS One* 21.1 (2026), e0339650.

[a308] F. Abegaz, D. Abedini, L. Dong, J.A. Westerhuis, F. Van Eeuwijk, H. Bouwmeester, and A.K. Smilde. "Analysis of microbiome high-dimensional experimental design data using generalized linear models and ANOVA simultaneous component analysis". In: *Frontiers in Microbiomes* 4 (2025), p. 1584516.

[a307] H. Bouwmeester, L. Dong, K. Wippel, T. Hofland, and A.K. Smilde. "The chemical interaction between plants and the rhizosphere microbiome". In: *Trends in Plant Science* 30.9 (2025), pp. 1002–1019.

[a306] J. Camacho, A.K. Smilde, E. Saccenti, J.A. Westerhuis, and R. Bro. "All Sparse PCA Models are Wrong, But Some are Useful. Part III: Model Interpretation". In: *Chemometrics and Intelligent Laboratory Systems* 266.105498 (2025).

[a305] P.E. Cornejo Ulloa, G.R. van der Ploeg, A. Heintz-Buschart, J.A. Westerhuis, A.K. Smilde, E. Zaura, B.W.. Brandt, M.J. Buijs, N. Bostanci, A. Silbereisen, et al. "Shifting hormones, shaping health: Gender-affirming therapy & oral care". In: *International Journal of Transgender Health* (2025), pp. 1–17.

[a304] A.C. Georgiou, G.R. van der Ploeg, J.A. Westerhuis, S.V. van der Waal, A. Heintz-Buschart, A.K. Smilde, and B.W. Brandt. "Modelling of the Systemic Inflammatory Host Response in Relation to the Microbiome of the Endodontic Infection". In: *International Endodontic Journal* 58.12 (2025), pp. 1926–1939.

[a303] S. Leygeber, C. Diez-Simon, J.L. Großmann, A.C. Dubbelman, A.C. Harms, J.A. Westerhuis, D.M. Jacobs, P.W. Lindenburg, M.M.W.B. Hendriks, B.C.H. Ammerlaan, et al. "A Data-Driven Approach to Link GC-MS and LC-MS with Sensory Attributes of Chicken Bouillon with Added Yeast-Derived Flavor Products in a Combined Prediction Model". In: *Metabolites* 15.5 (2025), p. 317.

[a302] T.S. Madssen, A.K. Smilde, J. Camacho, A.H. Jarmund, J.A. Westerhuis, and G.F. Giskeødegård. "Statistical Validation of Multivariate Treatment Effects in Longitudinal Study Designs". In: *Journal of Chemometrics* 39.8 (2025), e70044.

[a301] G.R. van der Ploeg, J.A. Westerhuis, A. Heintz-Buschart, and A.K. Smilde. "parafac4microbiome: Exploratory analysis of longitudinal microbiome data using Parallel Factor Analysis". In: *MSystems* 10.6 (2025), e00472–25.

[a300] F.T.G. White, A. Heintz-Buschart, L. Dong, H.J. Bouwmeester, J.A. Westerhuis, and A.K. Smilde. "MASCARA: coexpression analysis in data from designed experiments". In: *Computational and Structural Biotechnology Reports* (2025), p. 100052.

[a299] J. Zweigle, S. Tisler, M. Bevilacqua, G. Tomasi, N. Nielsen, N. Gawlitta, J.S. Lübeck, A.K. Smilde, and J. Christensen. "HPLC 2025 Preview: Prioritization Strategies in Non-Target Screening of Environmental Samples by Chromatography with High-Resolution Mass Spectrometry". In: *MJH Life Sciences* (2025).

[a298] F. Abegaz, D. Abedini, F. White, A. Guerrieri, A. Zancarini, L. Dong, J. A. Westerhuis, F. van Eeuwijk, H. Bouwmeester, and A. K. Smilde. "A strategy for differential abundance analysis of sparse microbiome data with group-wise structured zeros". In: *Scientific Reports* 14.1 (2024), p. 12433.

[a297] L. Li, H. Hoefsloot, B.M. Bakker, D. Horner, M.A. Rasmussen, A.K. Smilde, and E. Acar. "Longitudinal metabolomics data analysis informed by mechanistic models". In: *Metabolites* 15.1 (2024), p. 2.

[a296] L. Li, S. Yan, B. M. Bakker, H. Hoefsloot, B. Chawes, D. Horner, M. A. Rasmussen, A. K. Smilde, and E. Acar. "Analyzing postprandial metabolomics data using multiway models: A simulation study". In: *BMC bioinformatics* 25.1 (2024), p. 94.

[a295] L. Li, S. Yan, D. Horner, M. A. Rasmussen, A. K. Smilde, and E. Acar. "Revealing static and dynamic biomarkers from postprandial metabolomics data through coupled matrix and tensor factorizations". In: *Metabolomics* 20.4 (2024), p. 86.

[a294] G.R. van der Ploeg, B.W. Brandt, B.J.F. Keijser, M.H. van der Veen, C.M.C. Volgenant, E. Zaura, A.K. Smilde, J.A. Westerhuis, and A Heintz-Buschart. "Multi-way modelling of oral microbial dynamics and host-microbiome interactions during induced gingivitis". In: *npj Biofilms and Microbiomes* 10.1 (2024), p. 89.

[a293] S. Yan, L. Li, D. Horner, P. Ebrahimi, B. Chawes, L. O. Dragsted, M. A. Rasmussen, A. K. Smilde, and E. Acar. "Characterizing human postprandial metabolic response using multiway data analysis". In: *Metabolomics* 20.3 (2024), p. 50.

[a292] F. Becker, A. K. Smilde, and E. Acar. "Unsupervised EHR-based phenotyping via matrix and tensor decompositions". In: *Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery* 13.4 (2023), e1494.

[a291] B. Erdős, J. A. Westerhuis, M. E. Adriaens, S. D. O'Donovan, R. Xie, C. M. Singh-Povel, A. K. Smilde, and I. C. W. Arts. "Analysis of high-dimensional metabolomics data with complex temporal dynamics using RM-ASCA+". In: *PLoS Computational Biology* 19.6 (2023), e1011221.

[a290] J. L. Großmann, J. A. Westerhuis, T. Næs, and A. K. Smilde. "Critical evaluation of assessor difference correction approaches in sensory analysis". In: *Food Quality and Preference* 106 (2023), p. 104792.

[a289] S. K. Nørgaard, N. Følsgaard, N. H. Vissing, J. N. Kyvsgaard, B. Chawes, J. Stokholm, A. K. Smilde, K. Bønnelykke, H. Bisgaard, and M. A. Rasmussen. "Novel Connections of Common Childhood Illnesses Based on More Than 5 Million Diary Registrations From Birth Until Age 3 Years". In: *The Journal of Allergy and Clinical Immunology: In Practice* 11.7 (2023), pp. 2162–2171.

[a288] J. Skogholt, K. H. Liland, T. Næs, A. K. Smilde, and U. G. Indahl. "Selection of principal variables through a modified Gram–Schmidt process with and without supervision". In: *Journal of Chemometrics* 37.10 (2023), e3510.

[a287] J.L. Castro-Mejía, B. Khakimov, V. Aru, M.V. Lind, E. Garne, P. Paulová, E. Tavakkoli, L.H. Hansen, A.K. Smilde, L. Holm, et al. "Gut Microbiome and Its Cofactors Are Linked to Lipoprotein Distribution Profiles". In: *Microorganisms* 10.11 (2022), p. 2156.

[a286] B. Kim, J.A. Westerhuis, A.K. Smilde, K. Floková, A.K.A. Suleiman, E.E. Kuramae, H.J. Bouwmeester, and A. Zancarini. "Effect of strigolactones on recruitment of the rice root-associated microbiome". In: *FEMS microbiology ecology* 98.2 (2022), fiac010.

[a285] S. Leygeber, J.L. Grossmann, C. Diez-Simon, N. Karu, A.C. Dubbelman, A.C. Harms, J.A. Westerhuis, D.M. Jacobs, P.W. Lindenburg, M.M.W.B. Hendriks, et al. "Flavor Profiling Using Comprehensive Mass Spectrometry Analysis of Metabolites in Tomato Soups". In: *Metabolites* 12.12 (2022), p. 1194.

[a284] L. Li, H. C. J. Hoefsloot, A. A. de Graaf, E. Acar, and A. K. Smilde. "Exploring dynamic metabolomics data with multiway data analysis: a simulation study". In: *BMC Bioinformatics* 23.1 (2022), pp. 1–22.

[a283] N. Davarzani, C. Diez-Simon, J.L. Großmann, D.M. Jacobs, R. van Doorn, M.A. van den Berg, A.K. Smilde, R. Mumm, R.D. Hall, and J.A. Westerhuis. "Systematic selection of competing metabolomics methods in a metabolite-sensory relationship study". In: *Metabolomics* 17.9 (2021), pp. 1–12.

[a282] B. Khakimov, H. C. J. Hoefsloot, N. Mobaraki, V. Aru, M. Kristensen, M. V. Lind, L. Holm, J. L. Castro-Mejía, D. S. Nielsen, D. M. Jacobs, et al. "Human Blood Lipoprotein Predictions from 1H NMR Spectra: Protocol, Model Performances, and Cage of Covariance". In: *Analytical Chemistry* 94.2 (2021), pp. 628–636.

[a281] T. S. Madssen, G. F. Giskeødegård, A. K. Smilde, and J. A. Westerhuis. "Repeated measures ASCA+ for analysis of longitudinal intervention studies with multivariate outcome data". In: *PLoS Computational Biology* 17.11 (2021), e1009585.

[a280] P. B. Skou, E. Hosseini, J. B. Ghasemi, A. K. Smilde, and C. E. Eskildsen. "Orthogonality constrained inverse regression to improve model selectivity and analyte predictions from vibrational spectroscopic measurements". In: *Analytica Chimica Acta* 1185 (2021), p. 339073.

[a279] Y. Song, J.A. Westerhuis, N. Aben, L.F.A. Wessels, P.J.F. Groenen, and A.K. Smilde. "Generalized simultaneous component analysis of binary and quantitative data". In: *Journal of Chemometrics* 35.3 (2021), e3312.

[a278] A. Zancarini, J.A. Westerhuis, A.K. Smilde, and H.J. Bouwmeester. "Integration of omics data to unravel root microbiome recruitment". In: *Current Opinion in Biotechnology* 70 (2021), pp. 255–261.

[a277] 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.

[a276] 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.

[a275] 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).

[a274] 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.

[a273] 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.

[a272] 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.

[a271] 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).

[a270] S.K. Nørgaard, K. Linder-Steinlein, A.U. Eliasen, 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.

[a269] 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).

[a268] 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.

[a267] A.K. Smilde and T. Hankemeier. "Numerical Representations of Metabolic Systems". In: *Analytical chemistry* 92.20 (2020), pp. 13614–13621.

[a266] 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.

[a265] 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.

[a264] 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.

[a263] 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).

[a262] 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.

[a261] 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.

[a260] 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.

[a259] 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.

[a258] 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.

[a257] 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.

[a256] 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.

[a255] 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.

[a254] 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.

[a253] 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* e020717.13(11) (2018).

[a252] 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.

[a251] 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.

[a250] 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.

[a249] 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.

[a248] 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.

[a247]   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).

[a246]   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. Cannet, 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.

[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 A.K. Smilde. "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* 31.12 (2017), e2937.

[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]   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.

[a238]   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.

[a237]   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.

[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. Soininen, 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.

[a195] S. Wopereis, M. Radonjic, C.M. Rubingh, M. J. van Erk, A.K. Smilde, W. van Duyvenvoorde, N. Cnubben, T. Kooistra, B. van Ommen, and R. Kleemann. "Identification of prognostic and diagnostic biomarkers of glucose intolerance in ApoE3Leiden mice". In: *Physiological Genomics* 44.5 (2012), pp. 293–304.

[a194] T.G. Doeswijk, A.K. Smilde, J.A. Hageman, J.A. Westerhuis, and F.A. van Eeuwijk. "On the increase of predictive performance with high-level data fusion". In: *Analytica Chimica Acta* 705.1-2 (2011), pp. 41–47.

[a193] D.M. Hendrickx, M.M.W.B. Hendriks, P.H.C. Eilers, A.K. Smilde, and H.C.J. Hoefsloot. "Reverse engineering of metabolic networks, a critical assessment". In: *Molecular Biosystems* 7.2 (2011), pp. 511–520.

[a192] M.M.W.B. Hendriks, F.A. van Eeuwijk, R.H. Jellema, J.A. Westerhuis, T.H. Reijmers, H.C.J. Hoefsloot, and A.K. Smilde. "Data-processing strategies for metabolomics studies". In: *TRAC-Trends in Analytical Chemistry* 30.10 (2011), pp. 1685–1698.

[a191] C.M. Rubingh, M.J. van Erk, S. Wopereis, T. van Vliet, E.R. Verheij, N.H.P. Cnubben, B. van Ommen, J. van der Greef, H.F.J. Hendriks, and A.K. Smilde. "Discovery of subtle effects in a human intervention trial through multilevel modeling". In: *Chemometrics and Intelligent Laboratory Systems* 106.1 (2011), pp. 108–114.

[a190] E. Saccenti, A.K. Smilde, and W.H.M. Saris. "Beethoven's deafness and his three styles". In: *British Medical Journal* 343 (2011), p. d7589.

[a189] E. Saccenti, A.K. Smilde, J.A. Westerhuis, and M.M.W.B. Hendriks. "Tracy-Widom statistic for the largest eigenvalue of autoscaled real matrices". In: *Journal of Chemometrics* 25.12 (2011), pp. 644–652.

[a188] E. Saccenti, J.A. Westerhuis, A.K. Smilde, M.J. van der Werf, J.A. Hageman, and M.M.W.B. Hendriks. "Simplivariate models: uncovering the underlying biology in functional genomics data". In: *Plos One* 6.6 (2011), e20747.

[a187] M.F. Van Batenburg, L. Coulier, F.A. van Eeuwijk, A.K. Smilde, and J.A. Westerhuis. "New figures of merit for comprehensive functional genomics data: the metabolomics case". In: *Analytical Chemistry* 83.9 (2011), pp. 3267–3274.

[a186] J.P.M. Van Duynhoven, E.E. Vaughan, D.M. Jacobs, R.A. Kemperman, E.J.J. van Velzen, G. Gross, L.C. Roger, S. Possemiers, A.K.. Smilde, J. Dore, J.A. Westerhuis, and T. Van de Wiele. "Metabolic fate of polyphenols in the human superorganism". In: *Proceedings of the National Academy of Sciences of the United States of America* 108 (2011), pp. 4531–4538.

[a185] I. Van Mechelen and A.K. Smilde. "Comparability problems in the analysis of multiway data". In: *Chemometrics and Intelligent Laboratory Systems* 106.1 (2011), pp. 2–11.

[a184] C. Xu, H.C.J. Hoefsloot, and A.K. Smilde. "To aggregate or not to aggregate high-dimensional classifiers". In: *BMC Bioinformatics* 12 (2011), p. 153.

[a183] G. Zwanenburg, H.C.J. Hoefsloot, J.A. Westerhuis, J.J. Jansen, and A.K. Smilde. "ANOVA-principal component analysis and ANOVA-simultaneous component analysis: a comparison". In: *Journal of Chemometrics* 25.10 (2011), pp. 561–567.

[a182] C. Christin, H.C.J. Hoefsloot, A.K. Smilde, F. Suits, R. Bischoff, and P.L. Horvatovich. "Time alignment algorithms based on selected mass traces for complex LC-MS data". In: *Journal of Proteome Research* 9.3 (2010), pp. 1483–1495.

[a181] J.J. Jansen, S. Smit, H.C.J. Hoefsloot, and A.K. Smilde. "The Photographer and the Greenhouse: How to Analyse Plant Metabolomics Data". In: *Phytochemical Analysis* 21.1 (2010), pp. 48–60.

[a180] A.K. Smilde, J.A. Westerhuis, H.C.J. Hoefsloot, S. Bijlsma, C.M. Rubingh, D.J. Vis, R.H. Jellema, H. Pijl, F. Roelfsema, and J. van der Greef. "Dynamic metabolomic data analysis: a tutorial review". In: *Metabolomics* 6.1 (2010), pp. 3–17.

[a179] O. Stanimirovic, H.C.J. Hoefsloot, and A.K. Smilde. "Optimal measurement design for monitoring batch processes". In: *AICHE Journal* 56.3 (2010), pp. 837–840.

[a178] M.J. Van Erk, S. Wopereis, C.M. Rubingh, T. van Vliet, E.R. Verheij, N.H.P. Cnubben, T.L. Pedersen, J.W. Newman, A.K. Smilde, J. van der Greef, H.F.J. Hendriks, and B. van Ommen. "Insight in modulation of inflammation in response to diclofenac intervention: a human intervention study". In: *BMC Medical Genomics* 3 (2010), p. 5.

[a177] I. Van Mechelen and A.K. Smilde. "A generic linked-mode decomposition model for data fusion". In: *Chemometrics and Intelligent Laboratory Systems* 104.1 (2010), pp. 83–94.

[a176] D.J. Vis, J.A. Westerhuis, H.C.J. Hoefsloot, H. Pijl, F. Roelfsema, J. van der Greef, and A.K. Smilde. "Endocrine pulse identification using penalized methods and a minimum set of assumptions". In: *American Journal of Physiology-Endocrinology and Metabolism* 298.4 (2010), E894–E894.

[a175] J.A. Westerhuis, E.J.J. van Velzen, H.C.J. Hoefsloot, and A.K. Smilde. "Multivariate paired data analysis: multilevel PLSDA versus OPLSDA". In: *Metabolomics* 6.1 (2010), pp. 119–128.

[a174] C. Xu, H.C.J. Hoefsloot, M. Dijkstra, K. Havenga, H. Roelofsen, R.J. Vonk, and A.K. Smilde. "Computational modeling of the human serum proteome response to colon resection surgery". In: *Analytica Chimica Acta* 661.1 (2010), pp. 20–27.

[a173] R.G. Boot, M.J. van Breemen, W. Wegdam, R.R. Sprenger, S. de Jong, D. Speijer, C.E.M. Hollak, L. van Dussen, H.C.J. Hoefsloot, A.K. Smilde, C.G. de Koster, J.P.C. Vissers, and J.M.F.G. Aerts. "Gaucher disease: a model disorder for biomarker discovery". In: *Expert Review of Proteomics* 6.4 (2009), pp. 411–419.

[a172] M. Braaksma, A.K. Smilde, M.J. van der Werf, and P.J. Punt. "The effect of environmental conditions on extracellular protease activity in controlled fermentations of Aspergillus niger". In: *Microbiology* 155 (2009), pp. 3430–3439.

[a171] T. Cakir, M.M.W.B. Hendriks, J.A. Westerhuis, and A.K. Smilde. "Metabolic network discovery through reverse engineering of metabolome data". In: *Metabolomics* 5.3 (2009), pp. 318–329.

[a170] J.J. Jansen, N.M. van Dam, H.C.J. Hoefsloot, and A.K. Smilde. "Crossfit analysis: a novel method to characterize the dynamics of induced plant responses". In: *BMC Bioinformatics* 10 (2009), p. 425.

[a169] C.M. Rubingh, S. Bijlsma, R.H. Jellema, K.M. Overkamp, M.J. van der Werf, and A.K. Smilde. "Analyzing longitudinal microbial metabolomics data". In: *Journal of Proteome Research* 8.9 (2009), pp. 4319–4327.

[a168] A.K. Smilde, H.A.L. Kiers, S. Bijlsma, C.M. Rubingh, and M.J. van Erk. "Matrix correlations for high-dimensional data: the modified RV-coefficient". In: *Bioinformatics* 25.3 (2009), pp. 401–405.

[a167] A.K. Smilde, M.J. van der Werf, J.P. Schaller, and C. Kistemaker. "Characterizing the precision of mass-spectrometry-based metabolic profiling platforms". In: *Analyst* 134.11 (2009), pp. 2281–2285.

[a166] U. Thissen, S. Wopereis, S.A.A. van den Berg, I. Bobeldijk, R. Kleemann, T. Kooistra, K. W. van Dijk, B. van Ommen, and A.K. Smilde. "Improving the analysis of designed studies by combining statistical modelling with study design information". In: *Bmc Bioinformatics* 10 (2009), p. 52.

[a165] M.E. Timmerman, H.A.L. Kiers, A.K. Smilde, E. Ceulemans, and J. Stouten. "Bootstrap confidence intervals in multi-level simultaneous component analysis". In: *British Journal of Mathematical & Statistical Psychology* 62 (2009), pp. 299–318.

[a164] R.A. Van den Berg, C.M. Rubingh, J.A. Westerhuis, M.J. van der Werf, and A.K. Smilde. "Metabolomics data exploration guided by prior knowledge". In: *Analytica Chimica Acta* 651.2 (2009), pp. 173–181.

[a163] R.A. Van den Berg, I. Van Mechelen, T.F. Wilderjans, K. Van Deun, H.A.L. Kiers, and A.K. Smilde. "Integrating functional genomics data using maximum likelihood based simultaneous component analysis". In: *BMC Bioinformatics* 10 (2009), p. 340.

[a162] K. Van Deun, A.K. Smilde, M.J. van der Werf, H.A.L. Kiers, and I. Van Mechelen. "A structured overview of simultaneous component based data integration". In: *BMC Bioinformatics* 10 (2009), p. 246.

[a161] E.J.J. Van Velzen, J A. Westerhuis, H.C.J. Hoefsloot, and A.K. Smilde. "Data analysis strategies in nutritional metabolomics". In: *GIT Laboratory Journal* 13.1-2 (2009), pp. 17–19.

[a160] E.J.J. van Velzen, J.A. Westerhuis, J.P.M. van Duynhoven, F.A. van Dorsten, C.H. Grun, D.M. Jacobs, G.S.M.J.E. Duchateau, D.J. Vis, and A.K. Smilde. "Phenotyping tea consumers by nutrikinetic analysis of polyphenolic end-metabolites". In: *Journal of Proteome Research* 8.7 (2009), pp. 3317–3330.

[a159] M.P.H. Verouden, R.A. Notebaart, J.A. Westerhuis, M.J. van der Werf, B. Teusink, and A.K. Smilde. "Multi-way analysis of flux distributions across multiple conditions". In: *Journal of Chemometrics* 23.7-8 (2009), pp. 406–420.

[a158] M.P.H. Verouden, J.A. Westerhuis, M.J. van der Werf, and A.K. Smilde. "Exploring the analysis of structured metabolomics data". In: *Chemometrics and Intelligent Laboratory Systems* 98.1 (2009), pp. 88–96.

[a157] S. Wopereis, C.M. Rubingh, M.J. van Erk, E.R. Verheij, T. van Vliet, N.H.P. Cnubben, A.K. Smilde, J. van der Greef, B. van Ommen, and H.F.J. Hendriks. "Metabolic profiling of the response to an oral glucose tolerance test detects subtle metabolic changes". In: *Plos One* 4.2 (2009), e4525.

[a156] J.M. Aerts, M.J. van Breemen, A.P. Bussink, K. Ghauharali, R. Sprenger, R.G. Boot, J.E. Groener, C.E. Hollak, M. Maas, S. Smit, H.C.J. Hoefsloot, A.K. Smilde, J.P.C. Vissers, S. de Jong, D. Speijer, and C.G. de Koster. "Biomarkers for lysosomal storage disorders: identification and application as exemplified by chitotriosidase in Gaucher disease". In: *Acta Paediatrica* 97 (2008), pp. 7–14.

[a155] R. Bro, K. Kjeldahl, A.K. Smilde, and H.A.L. Kiers. "Cross-validation of component models: A critical look at current methods". In: *Analytical and Bioanalytical Chemistry* 390.5 (2008), pp. 1241–1251.

[a154] C. Christin, A.K. Smilde, H.C.J. Hoefsloot, F. Suits, R. Bischoff, and P.L. Horvatovich. "Optimized time alignment algorithm for LC-MS data: Correlation optimized warping using component detection algorithm-selected mass chromatograms". In: *Analytical Chemistry* 80.18 (2008), pp. 7012–7021.

[a153] S.C. Cruz, G. Rothenberg, J.A. Westerhuis, and A.K. Smilde. "Estimating kinetic parameters of complex catalytic reactions using a curve resolution based method". In: *Chemometrics and Intelligent Laboratory Systems* 91.2 (2008), pp. 101–109.

[a152] J.A. Hageman, R.A. van den Berg, J.A. Westerhuis, M.J. van der Werf, and A.K. Smilde. "Genetic algorithm based two-mode clustering of metabolomics data". In: *Metabolomics* 4.2 (2008), pp. 141–149.

[a151] J.A. Hageman, M.M.W.B. Hendriks, J.A. Westerhuis, M.J. van der Werf, R. Berger, and A.K. Smilde. "Simplivariate models: Ideas and first examples". In: *Plos One* 3.9 (2008), e3259.

[a150] H.C.J. Hoefsloot, S. Smit, and A.K. Smilde. "A classification model for the Leiden proteomics competition." In: *Statistical applications in genetics and molecular biology* 7.2 (2008), p. 8.

[a149] J.J. Jansen, R. Bro, H.C.J. Hoefsloot, F.W.J. van den Berg, J.A. Westerhuis, and A.K. Smilde. "PARAFASCA: ASCA combined with PARAFAC for the analysis of metabolic fingerprinting data". In: *Journal of Chemometrics* 22.1-2 (2008), pp. 114–121.

[a148] A.K. Smilde, H.C.J. Hoefsloot, and J.A. Westerhuis. "The geometry of ASCA". In: *Journal of Chemometrics* 22.7-8 (2008), pp. 464–471.

[a147] S. Smit, H.C.J. Hoefsloot, and A.K. Smilde. "Statistical data processing in clinical proteomics". In: *Journal of Chromatography B-analytical Technologies In the Biomedical and Life Sciences* 866.1-2 (2008), pp. 77–88.

[a146] O. Stanimirovic, H.C.J. Hoefsloot, P.K. De Bokx, and A.K. Smilde. "Variable selection methods as a tool to find sensor locations for distributed parameter systems". In: *Industrial & Engineering Chemistry Research* 47.4 (2008), pp. 1184–1191.

[a145] E.J.J. van Velzen, J.A. Westerhuis, J.P.M. van Duynhoven, F.A. van Dorsten, H.C.J. Hoefsloot, D.M. Jacobs, S. Smit, R. Draijer, C.I. Kroner, and A.K. Smilde. "Multilevel data analysis of a crossover designed human nutritional intervention study". In: *Journal of Proteome Research* 7.10 (2008), pp. 4483–4491.

[a144] J.A. Westerhuis, H.C.J. Hoefsloot, S. Smit, D.J. Vis, A.K. Smilde, E.J.J. van Velzen, J.P.M. van Duijnhoven, and F.A. van Dorsten. "Assessment of PLSDA cross validation". In: *Metabolomics* 4.1 (2008), pp. 81–89.

[a143] J.A. Westerhuis, E.J.J. van Velzen, H.C.J. Hoefsloot, and A.K. Smilde. "Discriminant Q(2) (DQ(2)) for improved discrimination in PLSDA models". In: *Metabolomics* 4.4 (2008), pp. 293–296.

[a142] D. Damian, M. Oresic, E. R. Verheij, J. Meulman, J. Friedman, A. Adourian, N. Morel, A.K. Smilde, and J. van der Greef. "Applications of a new subspace clustering algorithm (COSA) in medical systems biology". In: *Metabolomics* 3.1 (2007), pp. 69–77.

[a141] R. Goodacre, D. Broadhurst, A.K. Smilde, B.S. Kristal, J.D. Baker, R. Beger, C. Bessant, S. Connor, G. Calmani, A. Craig, T. Ebbels, D.B. Kell, C. Manetti, J. Newton, G. Paternostro, R. Somorjai, M. Sjostrom, J. Trygg, and F. Wulfert. "Proposed minimum reporting standards for data analysis in metabolomics". In: *Metabolomics* 3.3 (2007), pp. 231–241.

[a140] M.M.W.B. Hendriks, S. Smit, W.L.M.W. Akkermans, T.H. Reijmers, P.H.C. Eilers, H.C.J. Hoefsloot, C.M. Rubingh, C.G.. de Koster, J.M. Aerts, and A.K. Smilde. "How to distinguish healthy from diseased? Classification strategy for mass specitrometry-based clinical proteomics". In: *Proteomics* 7.20 (2007), pp. 3672–3680.

[a139] H.A.L. Kiers and A.K. Smilde. "A comparison of various methods for multivariate regression with highly collinear variables". In: *Statistical Methods and Applications* 16.2 (2007), pp. 193–228.

[a138] R. Kleemann, L. Verschuren, M.J. Van Erk, Y. Nikolsky, N.H.P. Cnubben, E.R.. Verheij, A.K. Smilde, H.F.J. Hendriks, S. Zadelaar, G.J. Smith, V. Kaznacheev, T. Nikolskaya, A. Melnikov, E. Hurt-Camejo, J. van der Greef, B. van Ommen, and T. Kooistra. "Atherosclerosis and liver inflammation induced by increased dietary cholesterol intake: a combined transcriptomics and metabolomics analysis". In: *Genome Biology* 8.9 (2007), R200.

[a137] M.J. Nueda, A. Conesa, J.A. Westerhuis, H.C.J. Hoefsloot, A.K. Smilde, M. Talon, and A. Ferrer. "Discovering gene expression patterns in time course microarray experiments by ANOVA-SCA". In: *Bioinformatics* 23.14 (2007), pp. 1792–1800.

[a136] E.T.S. Skibsted, J.A. Westerhuis, A.K. Smilde, and D.T. Witte. "Examples of NIR based real time release in tablet manufacturing". In: *Journal of Pharmaceutical and Biomedical Analysis* 43.4 (2007), pp. 1297–1305.

[a135] S. Smit, M.J. van Breemen, H.C.J. Hoefsloot, A.K. Smilde, J.M.F.G. Aerts, and C.G. de Koster. "Assessing the statistical validity of proteomics based biomarkers". In: *Analytica Chimica Acta* 592.2 (2007), pp. 210–217.

[a134] M.E. Timmerman, H.A.L. Kiers, and A.K. Smilde. "Estimating confidence intervals for principal component loadings: A comparison between the bootstrap and asymptotic results". In: *British Journal of Mathematical & Statistical Psychology* 60 (2007), pp. 295–314.

[a133] E.N.M. Van Sprang, M. Streefland, L.A. Van der Pol, E.C. Buevery, H.J. Ramaker, and A.K. Smilde. "Manufacturing vaccines: an illustration of using PAT tools for controlling the cultivation of Bordetella pertussis". In: *Quality Engineering* 19.4 (2007), pp. 373–384.

[a132] D.J. Vis, J.A. Westerhuis, A.K. Smilde, and J. van der Greef. "Statistical validation of megavariate effects in ASCA". In: *BMC Bioinformatics* 8 (2007), p. 322.

[a131] J.A. Westerhuis, E.P.P.A. Derks, H.C.J. Hoefsloot, and A.K. Smilde. "Grey component analysis". In: *Journal of Chemometrics* 21.10-11 (2007), pp. 474–485.

[a130] S. Bijlsma, L. Bobeldijk, E.R. Verheij, R. Ramaker, S. Kochhar, I.A. Macdonald, B. van Ommen, and A.K. Smilde. "Large-scale human metabolomics studies: A strategy for data (pre-) processing and validation". In: *Analytical Chemistry* 78.2 (2006), pp. 567–574.

[a129] J.A. Hageman, R.A. van den Berg, J.A. Westerhuis, H.C.J. Hoefsloot, and A.K. Smilde. "Bagged K-means clustering of metabolome data". In: *Critical Reviews In Analytical Chemistry* 36.3-4 (2006), pp. 211–220.

[a128] H.C.J.. Hoefsloot, M.P.H. Verouden, J.A. Westerhuis, and A.K. Smilde. "Maximum likelihood scaling (MALS)". In: *Journal of Chemometrics* 20.3-4 (2006), pp. 120–127.

[a127] H.J. Ramaker, E.N.M. van Sprang, J.A. Westerhuis, S.P. Gurden, A.K. Smilde, and F.H. van der Meulen. "Performance assessment and improvement of control charts for statistical batch process monitoring". In: *Statistica Neerlandica* 60.3 (2006), pp. 339–360.

[a126] H.J. Ramaker, E.N.M. van Sprang, J.A. Westerhuis, and A.K. Smilde. "Single channel event (SCE) for managing sensor failures in MSPC". In: *Computers & Chemical Engineering* 30.6-7 (2006), pp. 961–969.

[a125] C.M. Rubingh, S. Bijlsma, E.P.P.A. Derks, I. Bobeldijk, E.R. Verheij, S. Kochhar, and A.K. Smilde. "Assessing the performance of statistical validation tools for megavariate metabolomics data". In: *Metabolomics* 2.2 (2006), pp. 53–61.

[a124] E.T.S. Skibsted, H.F.M. Boelens, J.A. Westerhuis, D.T. Witte, and A.K. Smilde. "Simple assessment of homogeneity in pharmaceutical mixing processes using a near-infrared reflectance probe and control charts". In: *Journal of Pharmaceutical and Biomedical Analysis* 41.1 (2006), pp. 26–35.

[a123] O. Stanimirovic, H.C.J.. Hoefsloot, P.K. de Bokx, and A.K. Smilde. "Linking PCA and time derivatives of dynamic systems". In: *Journal of Chemometrics* 20.1-2 (2006), pp. 43–53.

[a122] R.A. Van den Berg, H.C.J. Hoefsloot, J.A. Westerhuis, A.K. Smilde, and M.J. van der Werf. "Centering, scaling, and transformations: improving the biological information content of metabolomics data". In: *BMC Genomics* 7 (2006), p. 142.

[a121] S. Cruz, G. Rothenberg, J.A. Westerhuis, and A.K. Smilde. "Tackling calibration problems of spectroscopic analysis in high-throughput experimentation". In: *Analytical Chemistry* 77.7 (2005), pp. 2227–2234.

[a120] J.A. Hageman, J.A. Westerhuis, and A.K. Smilde. "Temperature robust multivariate calibration: an overview of methods for dealing with temperature influences on near infrared spectra". In: *Journal of Near Infrared Spectroscopy* 13.2 (2005), pp. 53–62.

[a119] J.J. Jansen, H.C.J. Hoefsloot, J. van der Greef, M.E. Timmerman, and A.K. Smilde. "Multilevel component analysis of time-resolved metabolic fingerprinting data". In: *Analytica Chimica Acta* 530.2 (2005), pp. 173–183.

[a118] J.J. Jansen, H.C.J. Hoefsloot, J. van der Greef, M.E. Timmerman, J.A. Westerhuis, and A.K. Smilde. "ASCA: analysis of multivariate data obtained from an experimental design". In: *Journal of Chemometrics* 19.9 (2005), pp. 469–481.

[a117] R.H. Jellema, A.M. Janssen, M.E.J. Terpstra, R.A. de Wijk, and A.K. Smilde. "Relating the sensory sensation 'creamy mouthfeel' in custards to rheological measurements". In: *Journal of Chemometrics* 19.3 (2005), pp. 191–200.

[a116] V.G. van Mispelaar, A.K. Smilde, O.E. de Noord, J. Blomberg, and P.J. Schoenmakers. "Classification of highly similar crude oils using data sets from comprehensive two-dimensional gas chromatography and multivariate techniques". In: *Journal of Chromatography A* 1096.1-2 (2005), pp. 156–164.

[a115] H.J. Ramaker, E.N.M. van Sprang, J.A. Westerhuis, and A.K. Smilde. "Fault detection properties of global, local and time evolving models for batch process monitoring". In: *Journal of Process Control* 15.7 (2005), pp. 799–805.

[a114] E.T.S. Skibsted, H.F.M. Boelens, J.A. Westerhuis, A.K. Smilde, N.W. Broad, D.R. Rees, and D.T. Witte. "Net analyte signal based statistical quality control". In: *Analytical Chemistry* 77.22 (2005), pp. 7103–7114.

[a113] A.K. Smilde, J.J. Jansen, H.C.J. Hoefsloot, R.J.A.N. Lamers, J. van der Greef, and M.E. Timmerman. "ANOVA-simultaneous component analysis (ASCA): a new tool for analyzing designed metabolomics data". In: *Bioinformatics* 21.13 (2005), pp. 3043–3048.

[a112] A.K. Smilde, M.J. van der Werf, S. Bijlsma, B.J.C. van der Werff-van-der Vat, and R.H. Jellema. "Fusion of mass spectrometry-based metabolomics data". In: *Analytical Chemistry* 77.20 (2005), pp. 6729–6736.

[a111] O. Stanimirovic, H.F.M. Boelens, A.J.G. Mank, H.C.J. Hoefsloot, and A.K. Smilde. "Profiling of liquid crystal displays with Raman spectroscopy: Preprocessing of spectra". In: *Applied Spectroscopy* 59.3 (2005), pp. 267–274.

[a110] J. Van der Greef and A. K. Smilde. "Symbiosis of chemometrics and metabolomics: past, present, and future". In: *Journal of Chemometrics* 19.5-7 (2005), pp. 376–386.

[a109] E.N.M. Van Sprang, H.J. Ramaker, J.A. Westerhuis, and A.K. Smilde. "Statistical batch process monitoring using gray models". In: *Aiche Journal* 51.3 (2005), pp. 931–945.

[a108] H.F.M. Boelens, W.T. Kok, O.E. de Noord, and A.K. Smilde. "Performance optimization of spectroscopic process analyzers". In: *Analytical Chemistry* 76.9 (2004), pp. 2656–2663.

[a107] J.J. Jansen, H.C.J. Hoefsloot, H.F.M. Boelens, J. van der Greef, and A.K. Smilde. "Analysis of longitudinal metabolomics data". In: *Bioinformatics* 20.15 (2004), pp. 2438–2446.

[a106] H.J. Ramaker, E.N.M. van Sprang, J.A. Westerhuis, H.F.M. Boelens, and A.K. Smilde. "Dynamic time warping of spectroscopic BATCH data (vol 498, pg 133, 2003)". In: *Analytica Chimica Acta* 526.1 (2004), pp. 111–111.

[a105] H.J. Ramaker, E.N.M. van Sprang, J.A. Westerhuis, and A.K. Smilde. "The effect of the size of the training set and number of principal components on the false alarm rate in statistical process monitoring". In: *Chemometrics and Intelligent Laboratory Systems* 73.2 (2004), pp. 181–187.

[a104] E.T.S. Skibsted, H.F.M. Boelens, J.A. Westerhuis, D.T. Witte, and A.K. Smilde. "New indicator for optimal preprocessing and wavelength selection of near-infrared spectra". In: *Applied Spectroscopy* 58.3 (2004), pp. 264–271.

[a103] R. Bro and A.K. Smilde. "Centering and scaling in component analysis". In: *Journal of Chemometrics* 17.1 (2003), pp. 16–33.

[a102] S.C. Cruz, P.J. Aarnoutse, G. Rothenberg, J.A. Westerhuis, A.K. Smilde, and A. Bliek. "Kinetic and mechanistic studies on the Heck reaction using real-time near infrared spectroscopy". In: *Physical Chemistry Chemical Physics* 5.20 (2003), pp. 4455–4460.

[a101] E.P.P.A. Derks, J.A. Westerhuis, A.K. Smilde, and B.M. King. "An introduction to Multi-block Component Analysis by means of a flavor language case study". In: *Food Quality and Preference* 14.5-6 (2003), pp. 497–506.

[a100] R.H. Jellema, D.J. Louwerse, Smilde A.K., M.J.P. Gerritsen, D. Guldemond, H. Van der Voet, and P.F.G. Vereijken. "A systematic quantification of the sources of variation of process analytical measurements in the steel industry". In: *Quality Engineering* 15 (2003), pp. 391–402.

[a99] V.G. van Mispelaar, A.C. Tas, A.K. Smilde, P.J. Schoenmakers, and A.C. van Asten. "Quantitative analysis of target components by comprehensive two-dimensional gas chromatography". In: *Journal of Chromatography A* 1019.1-2 (2003), pp. 15–29.

[a98] H.J. Ramaker, E.N.M. van Sprang, J.A. Westerhuis, and A.K. Smilde. "Dynamic time warping of spectroscopic batch data". In: *Analytica Chimica Acta* 498.1-2 (2003), pp. 133–153.

[a97]   A.K. Smilde, J.A. Westerhuis, and S. de Jong. "A framework for sequential multiblock component methods". In: *Journal of Chemometrics* 17.6 (2003), pp. 323–337.

[a96]   E.N.M. Van Sprang, H.J. Ramaker, J.A. Westerhuis, A.K. Smilde, S.P. Gurden, and D. Wienke. "Near-infrared spectroscopic monitoring of a series of industrial batch processes using a bilinear grey model". In: *Applied Spectroscopy* 57.8 (2003), pp. 1007–1019.

[a95]   S. Bijlsma, H.F.M. Boelens, H.C.J. Hoefsloot, and A.K. Smilde. "Constrained least squares methods for estimating reaction rate constants from spectroscopic data". In: *Journal of Chemometrics* 16.1 (2002), pp. 28–40.

[a94]   R. Bro, N.D. Sidiropoulos, and A.K. Smilde. "Maximum likelihood fitting using ordinary least squares algorithms". In: *Journal of Chemometrics* 16.8-10 (2002), pp. 387–400.

[a93]   S.P. Gurden, J.A. Westerhuis, and A.K. Smilde. "Monitoring of batch processes using spectroscopy". In: *AICHE Journal* 48.10 (2002), pp. 2283–2297.

[a92]   J.A. Lopes, J.C. Menezes, J.A. Westerhuis, and A.K. Smilde. "Multiblock PLS analysis of an industrial pharmaceutical process". In: *Biotechnology and Bioengineering* 80.4 (2002), pp. 419–427.

[a91]   H.A. Lousberg, H.C.J. Hoefsloot, H.F.M. Boelens, P. Schoenmakers, and A.K. Smilde. "Development and validation of a fast size exclusion chromatographic method for at-line determination of the conversion of a polymerization reaction". In: *International Journal of Polymer Analysis and Characterization* 7.1-2 (2002), pp. 76–92.

[a90]   H.H.A. Lousberg, H.F.M. Boelens, E.P. Le Comte, H.C.J. Hoefsloot, and A.K. Smilde. "On-line determination of the conversion in a styrene bulk polymerization batch reactor using near-infrared spectroscopy". In: *Journal of Applied Polymer Science* 84.1 (2002), pp. 90–98. DOI: 10.1002/app.10241.

[a89]   H.J. Ramaker, E.N.M. van Sprang, S.P. Gurden, J.A. Westerhuis, and A.K. Smilde. "Improved monitoring of batch processes by incorporating external information". In: *Journal of Process Control* 12.4 (2002), pp. 569–576.

[a88]   A.K. Smilde, F.W.J. van den Berg, and H.C.J. Hoefsloot. "How to choose the right process analyzer". In: *Analytical Chemistry* 74.13 (2002), 368A–373A.

[a87]   E.N.M. van Sprang, H.J. Ramaker, J.A. Westerhuis, S.P. Gurden, and A.K. Smilde. "Critical evaluation of approaches for on-line batch process monitoring". In: *Chemical Engineering Science* 57.18 (2002).

[a86]   J.M.F. Ten Berge and A.K. Smilde. "Non-triviality and identification of a constrained Tucker3 analysis". In: *Journal of Chemometrics* 16.12 (2002), pp. 609–612.

[a85]   F.W.J. Van den Berg, H.C.J. Hoefsloot, and A.K. Smilde. "Selection of optimal process analyzers for plant-wide monitoring". In: *Analytical Chemistry* 74.13 (2002), pp. 3105–3111.

[a84]   C.G. Zampronio, S.P. Gurden, L.A.B. Moraes, M.N. Eberlin, A.K. Smilde, and R.J. Poppi. "Direct sampling tandem mass spectrometry (MS/MS) and multiway calibration for isomer quantitation". In: *Analyst* 127.8 (2002), pp. 1054–1060.

[a83] H.K. Barring, H.F.M. Boelens, O.E. de Noord, and A.K. Smilde. "Optimizing meta-parameters in continuous piecewise direct standardization". In: *Applied Spectroscopy* 55.4 (2001), pp. 458–466.

[a82] S. Bijlsma, H.F.M. Boelens, and A.K. Smilde. "Determination of rate constants in second-order kinetics using UV-visible spectroscopy". In: *Applied Spectroscopy* 55.1 (2001), pp. 77–83.

[a81] R. Bro, A.K. Smilde, and S. de Jong. "On the difference between low-rank and subspace approximation: improved model for multi-linear PLS regression". In: *Chemometrics and Intelligent Laboratory Systems* 58.1 (2001), pp. 3–13.

[a80] S.P. Gurden, J.A. Westerhuis, S. Bijlsma, and A.K. Smilde. "Modelling of spectroscopic batch process data using grey models to incorporate external information". In: *Journal of Chemometrics* 15.2 (2001), pp. 101–121.

[a79] S.P. Gurden, J.A. Westerhuis, R. Bro, and A.K. Smilde. "A comparison of multiway regression and scaling methods". In: *Chemometrics and Intelligent Laboratory Systems* 59.1-2 (2001), pp. 121–136.

[a78] A.K. Smilde. "Comments on three-way analyses used for batch process data". In: *Journal of Chemometrics* 15.1 (2001), pp. 19–27.

[a77] A.K. Smilde. "Reply to 'Comment on a recently proposed resampling method'". In: *Journal of Chemometrics* 15.3 (2001), pp. 189–192.

[a76] A.K. Smilde, H.C.J. Hoefsloot, H.A.L. Kiers, S. Bijlsma, and H.F.M. Boelens. "Sufficient conditions for unique solutions within a certain class of curve resolution models". In: *Journal of Chemometrics* 15.4 (2001), pp. 405–411.

[a75] A.K. Smilde and H.A.L. Kiers. "Meerweganalyse als cement tussen de psychologie en de chemie". In: *STAtOR* 2.2 (2001), pp. 5–9.

[a74] A.K. Smilde, A.A. Tates, H.F.M. Boelens, P. Oerlemans, and G. Ruitenberg. "Systematic investigation of process and product variations in a spindraw-winding process". In: *Chemical Engineering Science* 56.17 (2001), pp. 4993–5002.

[a73] F.W.J. Van den Berg, H.F.M. Boelens, A.K. Smilde, and H.C.J. Hoefsloot. "Process analyzer location and performance assessment for optimal process monitoring". In: *AICHE Journal* 47.11 (2001), pp. 2503–2514.

[a72] J.A. Westerhuis, S. de Jong, and A.K. Smilde. "Direct orthogonal signal correction". In: *Chemometrics and Intelligent Laboratory Systems* 56.1 (2001), pp. 13–25.

[a71] J.A. Westerhuis and A.K. Smilde. "Deflation in multiblock PLS". In: *Journal of Chemometrics* 15.5 (2001), pp. 485–493.

[a70] S. Bijlsma, H.F.M. Boelens, H.C.J. Hoefsloot, and A.K. Smilde. "Estimating reaction rate constants: comparison between traditional curve fitting and curve resolution". In: *Analytica Chimica Acta* 419.2 (2000), pp. 197–207.

[a69] S. Bijlsma and A.K. Smilde. "Estimating reaction rate constants from a two-step reaction: a comparison between two-way and three-way methods". In: *Journal of Chemometrics* 14.5-6 (2000), pp. 541–560.

[a68]   H.F.M. Boelens, W.T. Kok, O.E. de Noord, and A.K. Smilde. "Fast on-line analysis of process alkane gas mixtures by NIR spectroscopy". In: *Applied Spectroscopy* 54.3 (2000), pp. 406–412.

[a67]   R.H. Jellema, D.J. Louwerse, A.K. Smilde, M.J.P. Gerritsen, and D. Guldemond. "Identification and quantification of sources of variation in the analysis of steel". In: *Fresenius Journal of Analytical Chemistry* 368.4 (2000), pp. 397–406.

[a66]   D.J. Louwerse and A.K. Smilde. "Multivariate statistical process control of batch processes based on three-way models". In: *Chemical Engineering Science* 55.7 (2000), pp. 1225–1235.

[a65]   M.M. Reis, S.P. Gurden, A.K. Smilde, and M.M.C. Ferreira. "Calibration and detailed analysis of second-order flow injection analysis data with rank overlap". In: *Analytica Chimica Acta* 422.1 (2000), pp. 21–36.

[a64]   A.K. Smilde, J.A. Westerhuis, and R. Boque. "Multiway multiblock component and covariates regression models". In: *Journal of Chemometrics* 14.3 (2000), pp. 301–331.

[a63]   H. Swierenga, F. Wulfert, O.E. de Noord, A.P. de Weijer, A.K. Smilde, and L.M.C. Buydens. "Development of robust calibration models in near infra-red spectrometric applications". In: *Analytica Chimica Acta* 411.1-2 (2000), pp. 121–135.

[a62]   F.W.J. Van den Berg, H.C.J. Hoefsloot, H.F.M. Boelens, and A.K. Smilde. "Selection of optimal sensor position in a tubular reactor using robust degree of observability criteria". In: *Chemical Engineering Science* 55.4 (2000), pp. 827–837.

[a61]   J.A. Westerhuis, S.P. Gurden, and A.K. Smilde. "Generalized contribution plots in multivariate statistical process monitoring". In: *Chemometrics and Intelligent Laboratory Systems* 51.1 (2000), pp. 95–114.

[a60]   J.A. Westerhuis, S.P. Gurden, and A.K. Smilde. "Spectroscopic monitoring of batch reactions for on-line fault detection and diagnosis". In: *Analytical Chemistry* 72.21 (2000), pp. 5322–5330.

[a59]   J.A. Westerhuis, S.P. Gurden, and A.K. Smilde. "Standardized Q-statistic for improved sensitivity in the monitoring of residuals in MSPC". In: *Journal of Chemometrics* 14.4 (2000), pp. 335–349.

[a58]   F. Wulfert, W.T. Kok, O.E. de Noord, and A.K. Smilde. "Correction of temperature-induced spectral variation by continuous piecewise direct standardization". In: *Analytical Chemistry* 72.7 (2000), pp. 1639–1644.

[a57]   F. Wulfert, W.T. Kok, O.E. de Noord, and A.K. Smilde. "Linear techniques to correct for temperature-induced spectral variation in multivariate calibration". In: *Chemometrics and Intelligent Laboratory Systems* 51.2 (2000), pp. 189–200.

[a56]   S. Bijlsma, D.L. Louwerse, and A.K. Smilde. "Estimating rate constants and pure UV-vis spectra of a two-step reaction using trilinear models". In: *Journal of Chemometrics* 13.3-4 (1999), pp. 311–329.

[a55]   S. Bijlsma and A.K. Smilde. "Application of curve resolution based methods to kinetic data". In: *Analytica Chimica Acta* 396.2-3 (1999), pp. 231–240.

[a54] A. Bolck, A.K. Smilde, and C.H.P. Bruins. "Monitoring aged reversed-phase high performance liquid chromatography columns". In: *Chemometrics and Intelligent Laboratory Systems* 46.1 (1999), pp. 1–12.

[a53] R. Boque and A.K. Smilde. "Monitoring and diagnosing batch processes with multiway covariates regression models". In: *AICHE Journal* 45.7 (1999), pp. 1504–1520.

[a52] D.J. Louwerse, A.K. Smilde, and H.A.L. Kiers. "Cross-validation of multiway component models". In: *Journal of Chemometrics* 13.5 (1999), pp. 491–510.

[a51] D.J. Louwerse, A.A. Tates, A.K. Smilde, G.L.M. Koot, and H. Berndt. "PLS discriminant analysis with contribution plots to determine differences between parallel batch reactors in the process industry". In: *Chemometrics and Intelligent Laboratory Systems* 46.2 (1999), pp. 197–206.

[a50] A.K. Smilde and H.A.L. Kiers. "Multiway covariates regression models". In: *Journal of Chemometrics* 13.1 (1999), pp. 31–48.

[a49] A.K. Smilde, R. Tauler, J. Saurina, and R. Bro. "Calibration methods for complex second-order data". In: *Analytica Chimica Acta* 398.2-3 (1999), pp. 237–251.

[a48] A.A. Tates, D.J. Louwerse, A.K. Smilde, G.L.M. Koot, and H. Berndt. "Monitoring a PVC batch process with multivariate statistical process control charts". In: *Industrial and Engineering Chemistry Research* 38.12 (1999), pp. 4769–4776.

[a47] W. Windig, B. Antalek, L. J. Sorriero, S. Bijlsma, D. J. Louwerse, and A. K. Smilde. "Applications and new developments of the direct exponential curve resolution algorithm (DECRA). Examples of spectra and magnetic resonance images". In: *Journal of Chemometrics* 13.2 (1999), pp. 95–110.

[a46] S. Bijlsma, D.J. Louwerse, and A.K. Smilde. "Rapid estimation of rate constants of batch processes using on-line SW-NIR". In: *Aiche Journal* 44.12 (1998), pp. 2713–2723.

[a45] S. Bijlsma, D.J. Louwerse, W. Windig, and A.K. Smilde. "Rapid estimation of rate constants using on-line SW-NIR and trilinear models". In: *Analytica Chimica Acta* 376.3 (1998), pp. 339–355.

[a44] H.A.L. Kiers and A.K. Smilde. "Constrained three-mode factor analysis as a tool for parameter estimation with second-order instrumental data". In: *Journal of Chemometrics* 12.2 (1998), pp. 125–147.

[a43] J. Nilsson, E.J. Homan, A.K. Smilde, C.J. Grol, and H. Wikstrom. "A multiway 3D QSAR analysis of a series of (S)-N-[(1-ethyl-2-pyrrolidinyl)methyl]-6-methoxybenzamides". In: *Journal of Computer-aided Molecular Design* 12.1 (1998), pp. 81–93.

[a42] F. Wulfert, W.T. Kok, and A.K. Smilde. "Influence of temperature on vibrational spectra and consequences for the predictive ability of multivariate models". In: *Analytical Chemistry* 70.9 (1998), pp. 1761–1767.

[a41] J. Nilsson, S. De Jong, and A.K. Smilde. "Multiway calibration in 3D QSAR". In: *Journal of Chemometrics* 11.6 (1997), pp. 511–524.

[a40] J. Nilsson, H. Wikstrom, A.K. Smilde, S. Glase, T. Pugsley, G. Cruciani, M. Pastor, and S. Clementi. "GRID/GOLPE 3D quantitative structure-activity relationship study on a set of benzamides and naphthamides, with affinity for the dopamine D-3 receptor subtype". In: *Journal of Medicinal Chemistry* 40.6 (1997), pp. 833–840.

[a39] A.K. Smilde. "Comments on multilinear PLS". In: *Journal of Chemometrics* 11.5 (1997), pp. 367–377.

[a38] F.W.J. Van den Berg, W.A. van Osenbruggen, and A.K. Smilde. "Process analytical chemistry in the distillation industry using near-infrared spectroscopy". In: *Process Control and Quality* 9.1-3 (1997), pp. 51–57.

[a37] A. Bolck, A.K. Smilde, C.A.A. Duineveld, and P.M.J. Coenegracht. "Multivariate quality assessment of aged RP-HPLC columns". In: *Journal of Chemometrics* 10.5-6 (1996), pp. 351–370.

[a36] O.M. Steijger, H.C.M. den Nieuwenboer, H. Lingeman, U.A.T. Brinkman, J.J.M. Holthuis, and A.K. Smilde. "Enhancement of peroxyoxalate chemiluminescence by copper(II) in flow injection analysis; Optimization by factorial design analysis". In: *Analytica Chimica Acta* 320.1 (1996), pp. 99–105.

[a35] P. Geladi and A.K. Smilde. "The Future of Chemometrics". In: *Journal of Chemometrics* 9.1 (1995), pp. 1–2.

[a34] H.A.L. Kiers and A.K. Smilde. "Some theoretical results on 2nd-order calibration methods for data with and without rank overlap". In: *Journal of Chemometrics* 9.3 (1995), pp. 179–195.

[a33] M.M.A. Ruyken, J.A. Visser, and A.K. Smilde. "Online detection and identification of interferences in multivariate predictions of organic gases using FT-IR spectroscopy". In: *Analytical Chemistry* 67.13 (1995), pp. 2170–2179.

[a32] R. Tauler, A.K. Smilde, and B.R. Kowalski. "Selectivity, local rank, three-way data-analysis and ambiguity In multivariate curve resolution". In: *Journal of Chemometrics* 9.1 (1995), pp. 31–58.

[a31] C.A.A. Duineveld, C.H.P. Bruins, A.K. Smilde, G.K. Bolhuis, K. Zuurman, and D.A. Doornbos. "Multicriteria Steepest Ascent". In: *Chemometrics and Intelligent Laboratory Systems* 25.2 (1994), pp. 183–201.

[a30] A.K. Smilde, R. Tauler, J.M. Henshaw, L.W. Burgess, and B.R. Kowalski. "Multicomponent determination of chlorinated hydrocarbons using a reaction-based chemical sensor .3. Medium-rank 2nd-order calibration with restricted tucker models". In: *Analytical Chemistry* 66.20 (1994), pp. 3345–3351.

[a29] A.K. Smilde, Y.D. Wang, and B.R. Kowalski. "Theory of medium-rank 2nd-order calibration with restricted-tucker models". In: *Journal of Chemometrics* 8.1 (1994), pp. 21–36.

[a28] R. Tauler, A.K. Smilde, J.M. Henshaw, L.W. Burgess, and B.R. Kowalski. "Multicomponent determination of chlorinated hydrocarbons using a reaction-based chemical sensor .2. Chemical speciation using multivariate curve resolution". In: *Analytical Chemistry* 66.20 (1994), pp. 3337–3344.

[a27] C.A.A. Duineveld, A.K. Smilde, and D.A. Doornbos. "Comparison of Experimental-designs Combining Process and Mixture Variables .1. Design Construction and Theoretical Evaluation". In: *Chemometrics and Intelligent Laboratory Systems* 19.3 (1993), pp. 295–308.

[a26] C.A.A. Duineveld, A.K. Smilde, and D.A. Doornbos. "Comparison of Experimental-designs Combining Process and Mixture Variables .2. Design Evaluation On Measured Data". In: *Chemometrics and Intelligent Laboratory Systems* 19.3 (1993), pp. 309–318.

[a25] C.A.A. Duineveld, A.K. Smilde, and D.A. Doornbos. "Designs For Mixture and Process Variables Applied In Tablet Formulations". In: *Analytica Chimica Acta* 277.2 (1993), pp. 455–465.

[a24] O.M. Steijger, H. Lingeman, U.A.T. Brinkman, J.J.M. Holthuis, A.K. Smilde, and D.A. Doornbos. "Liquid-chromatographic Analysis of Carboxylic-acids Using N-(4-aminobutyl)-n-ethylisoluminol As Chemiluminescent Label - Determination of Ibuprofen In Saliva". In: *Journal of Chromatography-biomedical Applications* 615.1 (1993), pp. 97–110.

[a23] J.H. De Boer, A.K. Smilde, and D.A. Doornbos. "Introduction of A Robustness Coefficient In Optimization Procedures - Implementation In Mixture Design-problems .3. Validation and Comparison With Competing Criteria". In: *Chemometrics and Intelligent Laboratory Systems* 15.1 (1992), pp. 13–28.

[a22] R. Ferwerda, L.T.W. De Jong-van den Berg, P.B. van den Berg, and A.K. Smilde. "Drug utilization patterns in pregnancy". In: *Journal of Pharmacoepidemiology* 2.4 (1992), pp. 35–45.

[a21] M.M.W.B. Hendriks, J.H. De Boer, A.K. Smilde, and D.A. Doornbos. "Multicriteria Decision-making". In: *Chemometrics and Intelligent Laboratory Systems* 16.3 (1992), pp. 175–191.

[a20] A.K. Smilde. "Three-way Analyses - Problems and Prospects". In: *Chemometrics and Intelligent Laboratory Systems* 15.2-3 (1992), pp. 143–157.

[a19] A.K. Smilde and D.A. Doornbos. "Simple Validatory Tools For Judging the Predictive Performance of Parafac and 3-way Pls". In: *Journal of Chemometrics* 6.1 (1992), pp. 11–28.

[a18] C.E. Bos, G.K. Bolhuis, C.F. Lerk, J.H. De Boer, C.A.A. Duineveld, A.K. Smilde, and D. A. Doornbos. "The use of a factorial design to evaluate the physical stability of tablets prepared by direct compression .2. Selection of excipients suitable for use under tropical storage-conditions". In: *European Journal of Pharmaceutics and Biopharmaceutics* 37.4 (1991), pp. 210–215.

[a17] C.E. Bos, G.K. Bolhuis, C.F. Lerk, J.H. De Boer, C.A.A. Duineveld, A.K. Smilde, and D.A. Doornbos. "Optimization of direct compression tablet formulations for use In tropical countries". In: *Drug Development and Industrial Pharmacy* 17.18 (1991), pp. 2477–2496.

[a16] C.E. Bos, G.K. Bolhuis, C.F. Lerk, J.H. De Boer, C.A.A. Duinveld, A.K. Smilde, and D.A. Doornbos. "The use of a factorial design to evaluate the physical stability of tablets prepared by direct compression .1. A new approach based on the relative change In tablet parameters". In: *European Journal of Pharmaceutics and Biopharmaceutics* 37.4 (1991), pp. 204–209.

[a15] P.M.J. Coenegrracht, A.K. Smilde, H. Benak, C.H.P. Bruins, H.J. Metting, H. De Vries, and D.A. Dornbos. "Multivariate Characterization of Solvent Strength and Solvent Selectivity In Reversed-phase High-performance Liquid-chromatography". In: *Journal of Chromatography* 550.1-2 (1991), pp. 397–410.

[a14] J.H. De Boer, A.K. Smilde, and D.A. Doornbos. "Introduction of A Robustness Coefficient In Optimization Procedures - Implementation In Mixture Design-problems .2. Some Practical Considerations". In: *Chemometrics and Intelligent Laboratory Systems* 10.3 (1991), pp. 325–336.

[a13] A.K. Smilde and D.A. Doornbos. "Three-way Methods For the Calibration of Chromatographic Systems - Comparing Parafac and 3-way Pls". In: *Journal of Chemometrics* 5.4 (1991), pp. 345–360.

[a12] C. Caramella, F. Ferrari, M. Ronchi, and A.K. Smilde. "An Integrated Computer-aided Approach For Modeling Disintegration-related Phenomena". In: *Acta Pharmaceutica Technologica-International Journal of Drug Formulation and Biopharmaceutics* 36.4 (1990), pp. 249–253.

[a11] J.H. De Boer, A.K. Smilde, and D.A. Doornbos. "Introduction of A Robustness Coefficient In Optimization Procedures - Implementation In Mixture Design-problems .1. Theory". In: *Chemometrics and Intelligent Laboratory Systems* 7.3 (1990), pp. 223–236.

[a10] A.K. Smilde, P.H. Van der Graaf, D.A. Doornbos, T. Steerneman, and A. Sleurink. "Multivariate Calibration of Reversed-phase Chromatographic Systems - Some Designs Based On 3-way Data-analysis". In: *Analytica Chimica Acta* 235.1 (1990), pp. 41–51.

[a9] P.M.J. Coenegracht, A.K. Smilde, and A. Knevelman. "Performance Characterization of Multi-solvent Mobile Phase Systems In Rp-hplc By Multi-criteria Decision-making Illustrated By the Comparison of Ternary and Quaternary Solvent Systems". In: *Journal of Liquid Chromatography* 12.1-2 (1989), pp. 77–94.

[a8] P.M.J. Coenegracht, A.K. Smilde, H.J. Metting, and D.A. Doornbos. "Comparison of Optimization Methods In Reversed-phase High-performance Liquid-chromatography Using Mixture Designs and Multicriteria Decision-making". In: *Journal of Chromatography* 485 (1989), pp. 195–217.

[a7] P.M.J. Coenegracjht, H.J. Metting, A.K. Smilde, and P.J.M. Coenegracht-Lamers. "A Chemometric Investigation of the Selectivity of Multisolvent Mobile Phase Systems In Rp-hplc". In: *Chromatographia* 27.3-4 (1989), pp. 135–141.

[a6] A.K. Smilde, P.M.J. Coenegracht, C.H.P. Bruins, and D.A. Doornbos. "Multivariate Calibration Strategy For Reversed-phase Chromatographic Systems Based On the Characterization of Stationary Mobile Phase Combinations With Markers". In: *Journal of Chromatography* 485 (1989), pp. 169–181.

[a5] J.H. De Boer, A.K. Smilde, and D.A. Doornbos. "Introduction of multi-criteria decision-making In optimization procedures for pharmaceutical formulations". In: *Acta Pharmaceutica Technologica-international Journal of Drug Forumlation and Biopharmaceutics* 34.3 (1988), pp. 140–143.

[a4] A.K. Smilde, C.H.P. Bruins, P.M.J. Coenegracht, and D.A. Doornbos. "Characterization of stationary mobile phase combinations by using markers .1. Preliminary-results for the prediction of reversed-phase retention on various stationary phases". In: *Analytica Chimica Acta* 212.1-2 (1988), pp. 95–104.

[a3] A.K. Smilde, C.H.P. Bruins, D.A. Doornbos, and J. Vink. "Optimization of the reversed-phase high-performance liquid-chromatographic separation of synthetic estrogenic and progestogenic steroids using the multicriteria decision-making method". In: *Journal of Chromatography* 410.1 (1987), pp. 1–12.

[a2] A.K. Smilde and A. Knevelman. "The use of multicriteria decision-making In the optimization of an RP-HPLC separation of sulfonamides". In: *Pharmaceutisch Weekblad-scientific Edition* 9.2 (1987), pp. 147–147.

[a1] A.K. Smilde, A. Knevelman, and P.M.J. Coenegracht. "Introduction of Multicriteria Decision-making In Optimization Procedures For High-performance Liquid-chromatographic Separations". In: *Journal of Chromatography* 369.1 (1986), pp. 1–10.

Books

[b5] A.K. Smilde, F. Marini, J.A. Westerhuis, and K.H. Liland. *Analysis of Variance for High-Dimensional Data: Applications in Life, Food, and Chemical Sciences.* John Wiley & Sons, 2025.

[b4] A.K. Smilde, T. Næs, and K. H. Liland. *Multiblock Data Fusion in Statistics and Machine Learning: Applications in the Natural and Life Sciences.* John Wiley & Sons, 2022.

[b3] A.K. Smilde, R. Bro, and P. Geladi. *Multi-way Analysis. Applications in the Chemical Sciences.* John Wiley and Sons, 2004.

[b2] M.M.W.B. Hendriks, J.H. de Boer, and A.K. Smilde. *Robustness of Analytical Chemical Methods and Pharmaceutical Technological Products.* Elsevier, 1996.

[b1] A.K. Smilde. *Multivariate calibration of reversed-phase chromatographic systems.* Doctoral Thesis. Groningen: University of Groningen, 1990.

Chapters

[c9] A.K. Smilde and I. van Mechelen. "A framework for low-level data fusion". In: *Data Fusion Methodology and Applications.* Ed. by M. Cocchi. Elsevier, 2019, pp. 27–47.

[c8] J.A. Westerhuis, F. van der Kloet, and A.K. Smilde. "Data Fusion in Metabolomics". In: *Metabolomics: Practical Guide to Design and Analysis.* Ed. by R. Wehrens and R. Salek. CRC Press, 2019, pp. 157–.

[c7] J.A. Westerhuis, E.J.J. van Velzen, J.J. Jansen, H.C.J. Hoefsloot, and A.K. Smilde. "Analysis of high-dimensional data from designed metabolomics studies". In: *Metabolic profiling: disease and xenobiotics.* Ed. by M. Grootveld. Issues in Toxicology (21). Cambridge: Royal Society of Chemistry, 2015, pp. 117–136.

[c6] A.K. Smilde, M.M.W.B. Hendriks, J.A. Westerhuis, and H.C.J. Hoefsloot. "Data processing in metabolomics". In: *Metabolomics in Practice: Successful Strategies to Generate and Analyze Metabolic Data.* Ed. by M. Lämmerhofer and W. Weckwerth. Wiley-VCH Verlag, 2013, pp. 261–284.

[c5] J.P.M. van Duynhoven, E.J.J. van Velzen, G. Gross, F.A. van Dorsten, D.M. Jacobs, M. Bingham, R. Draijer, T. Mulder, T. Koning, E.E. Vaughan, T. van der Wiele, J.A. Westerhuis, and A.K. Smilde. "NMR-based metabonomics approaches for the assessment of the metabolic impact of dietary polyphenols on humans". In: *Magnetic resonance in food science: challenges in a changing world.* Cambridge: Royal Society of Chemistry, 2009, pp. 20–28.

[c4] C.E. Bos. "The use of a factorial design to evaluate the physical stability of tablets after storage under tropical conditions". In: *Robustness of Analytical Chemical Methods and Pharmaceutical Technological Products.* Ed. by M.M.W.B. Hendriks, J.H. De Boer, and A.K. Smilde. Elsevier, 1996, pp. 309–341.

[c3] A.K. Smilde. "General introduction of robustness". In: *Robustness of Analytical Chemical Methods and Pharmaceutical Technological Products.* Ed. by M.M.W.B. Hendriks, J.H. De Boer, and A.K. Smilde. Amsterdam: Elsevier, 1996, pp. 1–10.

[c2] A. Bolck and A.K. Smilde. "Multivariate characterization of RP-HPLC stationary phases". In: *Retention Indices in Chromatography.* Ed. by R. Smith. Elsevier, 1994.

[c1] D.A. Doornbos, Smilde A.K., J.H. De Boer, and C.A.A. Duineveld. "Experimental design, response surface methodology and multicriteria decision making". In: *Scientific Computation and Automation.* Ed. by E.J. Karjalainen. Amsterdam: Elsevier, 1990.

Proceedings

[p4] F. Becker, M. Nygård, J. Nygård, A. K. Smilde, and E. Acar. "Phenotyping of cervical cancer risk groups via generalized low-rank models using medical questionnaires". In: *Nordic Artificial Intelligence Research and Development: 4th Symposium of the Norwegian AI Society, NAIS 2022, Oslo, Norway, May 31–June 1, 2022, Revised Selected Papers.* Springer International Publishing Cham. 2023, pp. 94–110.

[p3] E. Acar, R. Bro, and A.K. Smilde. "Data Fusion in Metabolomics using Coupled Matrix and Tensor Factorizations". In: *Proceedings of the IEEE.* Vol. 103. 9. 2015, pp. 1602–1620.

[p2] J.A Westerhuis, E.N.M. van Sprang, H.J. Ramaker, A.K. Smilde, and D. Wienke. "Monitoring of industrial batch process using grey models and NIR spectroscopy". In: *Proceedings PLS2003 conference.* Lisbon, Portugal, 2003, pp. 155–165.

[p1] A.K. Smilde, J.A. Westerhuis, S.P. Gurden, E.N.M. van Sprang, and H.J. Ramaker. "Monitoring batch processes using external information". In: *ADCHEM 2000, International Symposium on Advanced Control of Chemical Processes.* Pisa, Italy, 2000, pp. 33–37.