

Personal Data

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Work address

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Education

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

Experience

Primary employments

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

Secondary employments

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

Awards and Achievements

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

Management Activities

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

Outreach Activities

Organizing committees

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

Scientific Advisory Boards

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

Invited Lectures (selection)

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

External assessments

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

Earning capacity (2010-2018)

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

Contributions to publications

Editorial Boards

- 2017- **Member of the Editorial Advisory Board of Metabolites**
- 2003- **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, PLoS Computational Biology, PLoS One, Psychometrika, Technometrics.*

Publications

- 1986- **Peer reviewed publications: 249**
- 1986- **Books: 3**
- 1986- **Book chapters: 7**
- 1986- **Proceedings contributions: 3**
- H-index: 51 (WoS), 62 (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- **ASCA PhD Course** Copenhagen School of Chemometrics, Copenhagen
- 2013-2015 **Data Fusion PhD Course** EMBO, Hinxton, United Kingdom
- 2010- **Matrix Algebra PhD Course** Faculty of Sciences
- 2004- **Biosystems Data Analysis MSc course** Faculty of Sciences
- 1993-2004 **Process Analysis MSc course** Faculty of Chemistry
- 1993-2004 **Numerical Techniques MSc course** Faculty of Chemistry

List of PhD theses

Systems Biology, Proteomics and Metabolomics

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

Process Analysis and Chemometrics

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

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

Languages

Dutch	Native
English	Fluent
German	Advanced
French	Moderate
Spanish	Moderate
Frisian	Moderate

Personal Interests

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

Peer-reviewed Papers

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

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

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

- [a208] S. Ellero-Simatos, E. Szymanska, T. Rullmann, W.H.A. Dokter, R. Ramaker, R. Berger, T.M.P. van Iersel, A.K. Smilde, T. Hankemeier, and W. Alkema. “Assessing the metabolic effects of prednisolone in healthy volunteers using urine metabolic profiling”. In: *Genome Medicine* 4 (2012), p. 94.
- [a207] D. Hasdemir, G.J. Smits, J.A. Westerhuis, and A.K. Smilde. “Topology of transcriptional regulatory networks: testing and improving”. In: *Plos One* 7.7 (2012), e40082.
- [a206] D.M. Hendrickx, H.C.J. Hoefsloot, M.M.W.B. Hendriks, A.B. Canelas, and A.K. Smilde. “Global test for metabolic pathway differences between conditions”. In: *Analytica Chimica Acta* 719 (2012), pp. 8–15.
- [a205] D.M. Hendrickx, H.C.J. Hoefsloot, M.M.W.B. Hendriks, D.J. Vis, A.B. Canelas, B. Teusink, and A.K. Smilde. “Inferring differences in the distribution of reaction rates across conditions”. In: *Molecular Biosystems* 8.9 (2012), pp. 2415–2423.
- [a204] J.J. Jansen, E. Szymanska, H.C.J. Hoefsloot, D.M. Jacobs, K. Strassburg, and A.K. Smilde. “Between metabolite relationships: an essential aspect of metabolic change”. In: *Metabolomics* 8.3 (2012), pp. 422–432.
- [a203] J.J. Jansen, E. Szymanska, H.C.J. Hoefsloot, and A.K. Smilde. “Individual differences in metabolomics: individualised responses and between-metabolite relationships”. In: *Metabolomics* 8.1 (2012), S94–S104.
- [a202] A.K. Smilde, M.E. Timmerman, M.M.W.B. Hendriks, J.J. Jansen, and H.C.J. Hoefsloot. “Generic framework for high-dimensional fixed-effects ANOVA”. In: *Briefings In Bioinformatics* 13.5 (2012), pp. 524–535.
- [a201] E. Szymanska, J. Bouwman, K. Strassburg, J. Vervoort, A.J. Kangas, P. Soinenen, 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.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.
- [a172] 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.
- [a171] 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.
- [a170] 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.
- [a169] 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.
- [a168] 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.
- [a167] 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.
- [a166] 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.

- [a165] 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.
- [a164] 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.
- [a163] 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.
- [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 Duynhoven, 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 spectrometry-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] 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.
- [a129] 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.
- [a128] 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.
- [a127] 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.
- [a126] 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.
- [a125] 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.
- [a124] 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.

- [a123] 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.
- [a122] 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.
- [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. 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.
- [a119] 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.
- [a118] 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.
- [a117] 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.
- [a116] 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.
- [a115] 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.
- [a114] 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.
- [a113] 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.
- [a112] 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.
- [a111] 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.
- [a110] 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.
- [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. Blik. "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. Guldmond, 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] 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.
- [a94] 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.
- [a93] 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.
- [a92] 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.

- [a91] 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.
- [a90] 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.
- [a89] 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.
- [a88] 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.
- [a87] 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.
- [a86] 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).
- [a85] 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.
- [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] 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.
- [a81] 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.
- [a80] 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.
- [a79] 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.
- [a78] 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.
- [a77] A.K. Smilde. “Comments on three-way analyses used for batch process data”. In: *Journal of Chemometrics* 15.1 (2001), pp. 19–27.
- [a76] A.K. Smilde. “Reply to ‘Comment on a recently proposed resampling method’”. In: *Journal of Chemometrics* 15.3 (2001), pp. 189–192.

- [a75] 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.
- [a74] 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.
- [a73] A.K. Smilde, A.A. Tates, H.F.M. Boelens, P. Oerlemans, and G. Ruitenbergh. "Systematic investigation of process and product variations in a spindraw-winding process". In: *Chemical Engineering Science* 56.17 (2001), pp. 4993–5002.
- [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] 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.
- [a69] 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.
- [a68] 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.
- [a67] 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.
- [a66] 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.
- [a65] 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.
- [a64] 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.
- [a63] 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.
- [a62] 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.
- [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-methoxybenzamide". 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] 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.
- [a40] J. Nilsson, S. De Jong, and A.K. Smilde. "Multiway calibration in 3D QSAR". In: *Journal of Chemometrics* 11.6 (1997), pp. 511–524.
- [a39] 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.
- [a38] A.K. Smilde. "Comments on multilinear PLS". In: *Journal of Chemometrics* 11.5 (1997), pp. 367–377.
- [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 Smilde A.K. "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. 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 .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. Coenegracht, A.K. Smilde, H. Benak, C.H.P. Bruins, H.J. Metting, H. De Vries, and D.A. Doornbos. "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. Coenegracht, 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 Formulation 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

- [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

- [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 metabolomics 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. Bolek 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

- [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.