Appendix

List of Publications

Poster Presentations and Conference Contributions

Oral Presentations

Curriculum Vitae

List of Publications

2003

[37] The First Successful Crystallographic Characterization of a Cyclodextrin Dimer: Efficient Synthesis and Molecular Geometry of a Doubly Sulfur-bridged β-Cyclodextrin.
D.-Q. Yuan, **S. Immel**, K. Koga, M. Yamaguchi, and K. Fujita, *Chem. Eur. J.* **2003**, *9*, 3501-3506.

2002

[36] Metabolism of Sucrose and Its Five α-D-Glucosyl-D-fructose Isomers by *Fusobacterium mortiferum*.
A. Pikis, **S. Immel**, S. A. Robrish, and J. Thompson, *Microbiology* **2002**, *148*, 843-852.

2001

[35] Two Stereoisomeric $3^{I},2^{II}$-Anhydro-α-cyclodextrins: A Molecular Dynamics and Crystallographic Study.
S. Immel, K. Fujita, M. Fukudome, and M. Bolte, *Carbohydr. Res.* **2001**, *336*, 297-308.

[34] Hydroxymethyl-substituted Crown Acetals with 35-C-14 and 40-C-16 Skeletal Backbones: Synthesis and Molecular Geometries.
S. Immel, F. W. Lichtenthaler, H. J. Lindner, and T. Nakagawa, *Tetrahedron: Asymmetry* **2001**, *12*, 2767-2774.

[33] Metabolism of Sucrose and Its Five Linkage-isomeric α-D-Glucosyl-D-fructoses by *Klebsiella pneumoniae*.
J. Thompson, S. A. Robrish, **S. Immel**, F. W. Lichtenthaler, B. G. Hall, and A. Pikis, *J. Biol. Chem.* **2001**, *276*, 37415-37425.

2000

[32] Atropdiastereoisomers of Ellagitannin Model Compounds: Configuration, Conformation, and Relative Stability of D-Glucose Diphenoyl Derivatives.
S. Immel, K. Khanbabaee, Tetrahedron: Asymmetry **2000**, *11*, 2495-2507.

[31] Synthesis and Molecular Geometry of an Achiral 30-Crown-12 Polyacetal from α-Cyclodextrin.
S. Immel, T. Nakagawa, H. J. Lindner, and F. W. Lichtenthaler, *Chem. Eur. J.* **2000**, *6*, 3366-3371.

[30] The 2,3-Anhydro-α-cyclomannin - 1-Propanol Hexahydrate: Topography, Lipophilicity Pattern, and Solid-State Architecture.
S. Immel, F. W. Lichtenthaler, H. J. Lindner, K. Fujita, M. Fukudome, and Y. Nogami, *Tetrahedron: Asymmetry* **2000**, *11*, 27-36.

[29] Structure and Lipophilicity Profile of 2,3-Anhydro-α-cyclomannin and its Ethanol Inclusion Complex.
S. Immel, K. Fujita, H. J. Lindner, Y. Nogami, and F. W. Lichtenthaler, *Chem. Eur. J.* **2000**, *6*, 2327-2333.

[28] The Hydrophobic Topographies of Amylose and its Blue Iodine Complex.
S. Immel and F. W. Lichtenthaler, *Starch/Stärke* **2000**, *52*, 1-8.

[27] Topography of the 1:1 α-Cyclodextrin - Nitromethane Inclusion Complex.
T. Nakagawa, **S. Immel**, H. J. Lindner, and F. W. Lichtenthaler, *Carbohydr. Res.* **2000**, *324*, 141-146.

[26] Flexible Non-glucose Cyclooligosaccharides.
S. Immel, *Proc. 10th Int. Symp. Cyclodextrins* (Ed.: J. Szejtli), Mia Digital Publ., Ann Arbor, Michigan, **2000**, pp. 24-31.

[25] Large-ring Crown Acetals from Cyclodextrins.
T. Nakagawa, **S. Immel**, H. J. Lindner, and F. W. Lichtenthaler, *Proc. 10th Int. Symp. Cyclodextrins* (Ed.: J. Szejtli), Mia Digital Publ., Ann Arbor, Michigan, **2000**, pp. 18-23.

1999

[24] Conformations and Lipophilicity Profiles of some Cyclic β(1→3)- and β(1→6)-linked Oligogalactofuranosides.
H. Gohlke, **S. Immel**, and F. W. Lichtenthaler, *Carbohydr. Res.* **1999**, *321*, 96-104.

[23] Solution Geometries and Lipophilicity Patterns of α-Cycloaltrin.
S. Immel, K. Fujita, and F. W. Lichtenthaler, *Chem. Eur. J.* **1999**, *5*, 3185-3192.

[22] Guest-induced Conformational Change in a Flexible Host: Mono-*altro*-β-Cyclodextrin.
K. Fujita, W.-H. Chen, D.-Q. Yuan, Y. Nogami, T. Koga, T. Fujioka, K. Mihashi, **S. Immel**, and F. W. Lichtenthaler, *Tetrahedron: Asymmetry* **1999**, *10*, 1689-1696.

[21] α-Cycloaltrin: Conformation and Properties in the Solid-State and Aqueous Solution.
S. Immel, G. E. Schmitt, and F. W. Lichtenthaler, *Proceedings of the 9th Internat. Symp. on Cyclodextrins* (Eds.: J. J. Torres-Labandeira and J. L. Vila Jato), Kluwer Acad. Publ., Dordrecht, NL, **1999**, 41-48.

[20] Molecular Geometries of Furanoid β(1→3)- and β(1→6)-linked Cyclogalactins.
H. Gohlke, **S. Immel**, F. W. Lichtenthaler, and G. E. Schmitt, *Proceedings of the 9th Internat. Symp. on Cyclodextrins* (Eds.: J. J. Torres-Labandeira and J. L. Vila Jato), Kluwer Acad. Publ., Dordrecht, NL, **1999**, 63-68.

[19] The Molecular Geometries of Cyclofructins.
S. Immel, G. E. Schmitt, and F. W. Lichtenthaler, *Proceedings of the 9th Internat. Symp. on Cyclodextrins* (Eds.: J. J. Torres-Labandeira and J. L. Vila Jato), Kluwer Acad. Publ., Dordrecht, NL, **1999**, 57-62.

1998

[18] Cyclofructins with Six to Ten β(1→2)-linked Fructofuranose Units: Geometries, Electrostatic Profiles, Lipophilicity Patterns, and Potential for Inclusion Complexation.
S. Immel, G. E. Schmitt, and F. W. Lichtenthaler, *Carbohydr. Res.* **1998**, *313*, 91-105.

1997

[17] Synthesis, Structure, and Conformational Features of α-Cycloaltrin: a Cyclooligosaccharide with alternating $^4C_1$ and $^1C_4$ Pyranose Chairs.
Y. Nogami, K. Nasu, T. Koga, K. Ohta, K. Fujita, **S. Immel**, H. J. Lindner, G. E. Schmitt, and F. W. Lichtenthaler, *Angew. Chem.* **1997**, *109*, 1987-1991; *Angew. Chem. Int. Ed. Engl.* **1997**,*35*, 1899-1902.

1996

[16] The Lipophilicity Patterns of Cyclodextrins and of Non-glucose Cyclooligosaccharides.
F. W. Lichtenthaler and **S. Immel**, *J. Inclusion Phenom. Mol. Recognit. Chem.* **1996**, *25*, 3-16.
F. W. Lichtenthaler and **S. Immel**, *Proceedings of the 8th Internat. Symp. on Cyclodextrins* (Eds.: J. Szejtli and L. Szente), Kluwer Acad. Publ., Dordrecht, NL, **1996**, pp. 3-16.

[15] Permethylated α- and β-CD: Cyclodextrins with Inverse Hydrophobicity.
S. Immel and F. W. Lichtenthaler, *Starch/Stärke* **1996**, *48*, 225-232.

[14] Sucrose as a Renewable Organic Raw Material: New Selective Entry Reactions via Computer Simulation of its Solution Conformations and its Hydroxyl Group Reactivities.
F. W. Lichtenthaler, P. Pokinskyj, and **S. Immel**, *Zuckerindustrie (Berlin)* **1996**, *12*, 170-190.

[13] Towards Understanding the Formation and Stability of Cyclodextrin Inclusion Complexes: The Lipophilicity Patterns of some Typical Examples.
F. W. Lichtenthaler and **S. Immel**, *Starch/Stärke* **1996**, *48*, 145-154.

[12] Molecular Electrostatic and Lipophilic Potential Profiles of α-Cyclofructin: Computation, Visualization, and Conclusions.
S. Immel and F. W. Lichtenthaler, *Liebigs Ann. Chem.* **1996**, 39-44.

[11] On the Hydrophobic Characteristics of Cyclodextrins: Computer-Aided Visualization of Molecular Lipophilicity Patterns.
F. W. Lichtenthaler and **S. Immel**, *Liebigs Ann. Chem.* **1996**, 27-37.

1995

[10] Selective 2-*O*-Benzylation of Sucrose: A Facile Entry to its 2-Deoxy- and 2-Keto-Derivatives and to Sucrosamine.
F. W. Lichtenthaler, **S. Immel**, and P. Pokinskyj, *Liebigs Ann. Chem.* **1995**, 1938-1947.

[9] The Conformation of Sucrose in Water: a Molecular Dynamics Approach.
S. Immel and F. W. Lichtenthaler, *Liebigs Ann. Chem.* **1995**, 1925-1937.

[8] Small Ring Cyclodextrins: their Geometries and Hydrophobic Topographies.
S. Immel, J. Brickmann, and F. W. Lichtenthaler, *Liebigs Ann. Chem.* **1995**, 929-942.

[7] Computer Simulation of Chemical and Biological Properties of Sucrose, the Cyclodextrins, and Amylose.
F. W. Lichtenthaler and **S. Immel**, *Int. Sugar J.* **1995**, *97*, 12-22.

1994

[6] Cyclodextrins, Cyclomannins, and Cyclogalactins with five and six (1→4)-linked Sugar Units: a Comparative Assessment of their Conformations and Hydrophobicity Potential Profiles.
F. W. Lichtenthaler and **S. Immel**, *Tetrahedron: Asymmetry* **1994**, *5*, 2045-2060.

[5] A Practical Synthesis of β-D-Xyl-(1→2)-β-D-Man-(1→4)-β-D-Glc-OMe, a Trisaccharide Component of the Glycosphingolipid of *Hyriopsis schlegelii*.
F. W. Lichtenthaler, T. Schneider-Adams, and **S. Immel**, *J. Org. Chem.* **1994**, *59*, 6735-6738.

1993

[4] Solid-State Conformations of 2,6-cis- and 2,6-trans-substituted Dihydropyran-3-ones.
F. W. Lichtenthaler, S. Rönninger, H. J. Lindner, **S. Immel**, and E. Cuny, *Carbohydr. Res.* **1993**, *249*, 305-326.

[3] Sucrose, Sucralose, and Fructose: Correlations Between Hydrophobicity Potential Profiles and AH-B-X Assignments.
F. W. Lichtenthaler and **S. Immel**, in: *Sweet Taste Chemoreception* (Eds.: M. Mathlouthi, J. A. Kanters, and G. G. Birch), Elsevier Appl. Science, London/New York, **1993**, pp. 21-53.

1992

[2] Some Disaccharide-derived Building Blocks of Potential Industrial Utility.
F. W. Lichtenthaler, **S. Immel**, D. Martin, and V. Müller, *Starch/Stärke* **1992**, *44*, 445-456.

1991

[1] Evolution of the Structural Representation of Sucrose.
F. W. Lichtenthaler, **S. Immel**, and U. Kreis, in: *Carbohydrates as Organic Raw Materials* (F. W. Lichtenthaler, Ed.), VCH, Weinheim/New York, **1991**, pp. 1-32.
Übersetzung ins Japanische: *Shokuhin Kogyo ("The Food Industry")* **1992**, 35, 65-85.

Poster Presentations and Conference Contributions

1999

[13] Large Ring Crown Acetals from Cyclodextrins.

T. Nakagawa, **S. Immel**, H. J. Lindner, and F. W. Lichtenthaler, *XVIIth Japanese Cyclodextrin Symposium*, Osaka, Japan, October 13-14, **1999**.

1998

[12] α-Cyclodextrin: Hydration Properties and Hydrogen Bonding.

S. Immel and G. E. Schmitt, *XIXth International Carbohydrate Symposium*, San Diego, California, August 9-14, **1998**, Abstract AO008.

[11] α-Cycloaltrin: Molecular Shape and Hydration Properties.

S. Immel, G. E. Schmitt, and F. W. Lichtenthaler, *XIXth International Carbohydrate Symposium*, San Diego, California, August 9-14, **1998**, Abstract AP124.

[10] β(1→3)- and β(1→6)-Linked Cyclogalactofuranosides: Conformations and Molecular Shapes.

H. Gohlke, **S. Immel**, F. W. Lichtenthaler, and G. E. Schmitt, *9thInternational Symposium on Cyclodextrins*, Santiago de Compostela, Spain, May 31 - June 3, **1998**, Abstract 2-P-4.

[9] Cyclofructins: Conformations, Molecular Electrostatic and Lipophilicity Patterns, and Inclusion Complexes.

S. Immel, G. E. Schmitt, and F. W. Lichtenthaler, *9thInternational Symposium on Cyclodextrins*, Santiago de Compostela, Spain, May 31 - June 3, **1998**, Abstract 2-P-3.

[8] α-Cycloaltrin: Conformation and Properties in Aqueous Solution.

S. Immel, G. E. Schmitt, and F. W. Lichtenthaler, *9th International Symposium on Cyclodextrins*, Santiago de Compostela, Spain, May 31 - June 3, **1998**, Abstract 2-O-5.

1997

[7] Structure and Conformational Features of α-Cycloaltrin: a Cyclooligosaccharide with alternating $^4C_1$ and $^1C_4$ Pyranose Chairs.

S. Immel, G. E. Schmitt, and F. W. Lichtenthaler, *9th European Carbohydrate Symposium (EUROCARB IX)*, Utrecht, Netherlands, July 6-11, **1997**, Abstract C5.

1996

[6] Cyclofructins: Geometries, Electrostatic and Lipophilicity Patterns, and Inclusion Complexes.

S. Immel, G. E. Schmitt, and F. W. Lichtenthaler, *10th Molecular Modeling Workshop*, Darmstadt, May 14-15, **1996**.
S. Immel, G. E. Schmitt, and F. W. Lichtenthaler, *IVth Intl. Satellite Meeting on Conformational Studies of Carbohydrates*, La Thuile (Aosta), Italy, July 17-20, **1996**.
S. Immel, G. E. Schmitt, and F. W. Lichtenthaler, *XVIIIth International Carbohydrate Symposium*, Milano, Italy, July 21-26, **1996**, Abstract AO027.

1995

[5] A New Look at the Hydrophobic Characteristics of Cyclodextrins, Cyclomannins, Cyclogalactins, Cyclofructins, and of Starch.

S. Immel and F. W. Lichtenthaler, *8th European Carbohydrate Symposium (EUROCARB VIII)*, Seville, Spain, July 2-7, **1995**, Abstract B38.

1992

[4] Sucrose, Fructose, and some Non-Carbohydrate Sweeteners: Correlations Between Hydrophobicity Potential Profiles and AH-B-X Assignments.

S. Immel and F. W. Lichtenthaler, *Symposium on Conformational Studies of Oligosaccharides, Polysaccharides and Glycoconjugates*, Le Croisic, June 29 - July 2, **1992**, Abstract VI-2.
S. Immel and F. W. Lichtenthaler, *XVIth International Carbohydrate Symposium*, Paris, July 5-10, **1992**, Abstract C163.

1991

[3] Structural Representation of Sucrose: From Tollens' 1883 Formula to Graphic Displays of its Hydrophobicity Potential Profile.

U. Kreis, **S. Immel**, and F. W. Lichtenthaler, *6th European Carbohydrate Symposium (EUROCARB VI)*, Edinburgh, September **1991**.

[2] The Electrostatic and Hydrophobicity Potential Profiles of Sucrose and Related Disaccharides.
U. Kreis, **S. Immel**, and F. W. Lichtenthaler, *201st ACS Meeting*, New York, August **1991**, Abstract CARB 3.

[1] Die Hydrophobieverteilung bei Saccharose, und ihre Auswirkung auf derzeitige Struktur-Süßkraft Konzepte.
S. Immel, U. Kreis, and F. W. Lichtenthaler, *5th Molecular Modeling Workshop*, Darmstadt, May **1991**.

Oral Presentations

2003

[16] Flexible und rigide Cyclodextrinderivate: Synthese, Struktur und Eigenschaften.

S. Immel, *Chemiedozententagung*, Technische Universität Chemnitz, Chemnitz, Germany, March 16-19, **2003**, Abstract A20.

2001

[15] Von Cyclodextrinderivaten bis hin zur Stärke: Molecular Modelling der Eigenschaften und Geometrien.

S. Immel, Kolloquium für Anorganische und Organische Chemie, Universität Wuppertal, Prof. Dr. H.-J. Altenbach, Nov. 22, **2001**.

2000

[14] From Rigid Cyclodextrins to Flexible Non-glucose Cyclooligosaccharides.

S. Immel, *10th International Symposium on Cyclodextrins*, Ann Arbor, Michigan USA, May 21-24, **2000**.

[13] The Topographies of Starch and Cyclodextrins: Analogies and Differences.

S. Immel, *51. Stärke Tagung*, Detmold, April 12-14, **2000**.

1999

[12] From Cyclodextrins to Starch: Structures and Hydrophobic Characteristics.

S. Immel, Workshop on the *"Chemistry of Cyclodextrins"* held by Prof. Dr. G. Wenz, Universität Karlsruhe, May 6, **1999**.

1998

[11] - [5] The Hydrophobic Properties of Cyclodextrins and some Non-glucose Cyclooligosaccharides, and Their Properties in Aqueous Solution.

S. Immel, hosted by:

- Prof. Dr. Kahee Fujita, Faculty of Pharmaceutical Sciences, Nagasaki University, Nagasaki, Japan, November 4, **1998**.
- Prof. Dr. Yasuyoshi Nogami, Departement of Pharmaceutical Sciences, Kyushu University, Fukuoka, Japan, November 5, **1998**.
- Prof. Dr. Naoki Kashimura and Prof. Dr. Shinichi Kitamura, *3rd Domestic Meeting on "Bioactive Carbohydrates"*, Department of Biological Resource Chemistry, Kyoto Prefectural University, Kyoto, Japan, November 7, **1998**, Abstract 3-10.
- Prof. Dr. Akihiko Ueno, Department of Chemistry, Faculty of Bioscience and Biotechnology, Tokyo Institute of Technology, Yokohama, Japan, November 10, **1998**.
- Prof. Dr. Ken-ichi Sato, Deptartment of Applied Chemistry, Kanagawa University, Yokohama, Japan, November 11, **1998**.
- Prof. Dr. Seiichiro Ogawa, Department of Applied Chemistry, Faculty of Science and Technology, Keio University, Yokohama, Japan, November 13, **1998**.
- Prof. Dr. Haruhisa Ueda, Department of Physical Chemistry, Faculty of Pharmaceutical Sciences, Hoshi University, Tokyo, Japan, November 14, **1998**.

[4] α-Cyclodextrin: Hydration Properties and Hydrogen Bonding.

S. Immel and G. E. Schmitt, *XIXth International Carbohydrate Symposium*, San Diego, California, August 9-14, **1998**, Abstract AO008.

[3] α-Cycloaltrin: Conformation and Properties in Aqueous Solution.

S. Immel, G. E. Schmitt, and F. W. Lichtenthaler, *9th International Symposium on Cyclodextrins*, Santiago de Compostela, Spain, May 31-June 3, **1998**, Abstract 2-O-5.

1994

[2] Towards Understanding Sweetness: Structure-Activity Relationships on the Basis of Hydrophobicity Potential Profiles.

S. Immel and F. W. Lichtenthaler, *207th ACS Meeting*, San Diego, March 13-18, **1994**, Abstract CARB 11.

1993

[1] Towards Understanding Sweetness: Structure-Activity Relationships on the Basis of Hydrophobicity Potential Profiles.

S. Immel and F. W. Lichtenthaler, *7th European Carbohydrate Symposium (EUROCARB VII)*, Cracow, August 22-27, **1993**, Abstract C026.

Curriculum Vitae

Persönliche Daten

Name:	Dr. Stefan Immel
Privatanschrift:	Bismarckstraße 43d, D-64293 Darmstadt
	Tel.: (+49) 6151 29 36 71
Geburtsdatum:	11. 11. 1965
Geburtsort:	Darmstadt
Staatsangehörigkeit:	Deutsch
Familienstand:	ledig, keine Kinder

Schul- und Universitätsausbildung

08.**1997** - 11.**2003**	Arbeiten an der Technischen Universität Darmstadt mit dem Ziel der Habilitation und dem Schwerpunkt *"Synthese, Struktur und Eigenschaften von Cyclodextrinen und Cyclodextrinderivaten".*
11. - 12.**1998**	Forschungsaufenthalt bei Prof. Dr. K. Fujita, Nagasaki Universität, Japan.
06.**1996** - 07.**1997**	Postdoktorand bei K. B. Sharpless, The Scripps Research Institute, San Diego, Kalifornien, über: *"Computersimulations on the Mechanism of Osmium-Catalyzed Reactions".*
01.**1995** - 05.**1996**	Forschungsarbeiten mit F. W. Lichtenthaler: *"Molecular Dynamics Simulations of Saccharides".*
01.**1995**	Promotion an der Technischen Universität Darmstadt zum Dr.-Ing. *"mit Auszeichnung".*
08.**1990** - 12.**1994**	Dissertation unter Anleitung von F. W. Lichtenthaler über: *"Computersimulations of Chemical and Biological Properties of Saccharides: Sucrose, Fructose, Cyclodextrins, and Starch".*
06. - 08.**1991**	Gastaufenthalt an der ETH Zürich bei W. F. van Gunsteren; Arbeiten über: *“Molecular Dynamics of Sucrose in Aqueous Solution".*
07.**1990**	Hauptdiplom Chemie, Technische Universität Darmstadt (*"mit Auszeichnung"*) Diplom Arbeit unter Anleitung von F. W. Lichtenthaler über die "*Stereoselektivität von Dialdehyd-Nitromethan-Cyclisierungen*".
06.**1987**	Vordiplom Chemie, Technische Universität Darmstadt (*"mit Auszeichnung"*).
10.**1984**	Beginn des Studiums der Chemie an der Technischen Universität Darmstadt.
06.**1984**	Abitur am Lichtenberg Gymnasium in Darmstadt.

Mitgliedschaften in wissenschaftlichen Gesellschaften

Seit **1996**	American Chemical Society
Seit **1990**	Gesellschaft Deutscher Chemiker

Mitgliedschaften in Editorial Boards

Seit **2000**	Editorial Board von *Carbohydrate Research*

Wissenschaftliche Auszeichnungen und Stipendien

1996 - **1997** Postdoktoranden-Stipendium der Deutschen Forschungsgemeinschaft (DFG).

1991 - **1992** Doktoranden-Stipendium des Fonds der Chemischen Industrie.

02.**1988** Preisträger der Dr. Anton-Keller-Stiftung der Technischen Universität Darmstadt, Auszeichnung für herausragende Leistungen im Vordiplom.

Forschungsschwerpunkte

- Synthese, Struktur, und Eigenschaften flexibler und rigider Cyclooligosaccharide: Molekulare Erkennung nach dem "*Induced-Fit*" und "*Schlüssel-Schloss*" Prinzip.
- Von Cyclodextrinen abgeleitete Kronen-Acetale: Neue Kationen-Fänger?
- Molekülmodellierung chemischer und biologischer Eigenschaften von Kohlenhydraten.
- Konformation von Kohlenhydraten im Kristall und in Lösung.
- Anwendung von Kraftfeld-gestützten Rechenverfahren zur Charakterisierung von Kohlenhydraten, insbesondere hydrophober Oberflächenregionen.
- Wechselwirkung von Kohlenhydraten mit Lösungsmitteln (Wasser) und deren Hydratationseigenschaften.
- Struktur-Süßkraft Beziehungen von Zuckern und künstlichen Süßstoffen.

Lehrtätigkeiten und Vorlesungen

- Vorlesung „Metallorganische Chemie“ für Chemiker im Hauptstudium.
- Vorlesung „Grundlagen und Reaktionsmechanismen in der Organischen Chemie“ für Chemiker und Biologen im Grundstudium.
- Begleitende Seminare und Übungen zur Vorlesung „Organische Experimentalvorlesung“ für Chemiker im Grundstudium.
- Blockseminar „Physikalische Methoden in der Organischen Chemie“ (IR, UV, NMR Spektroskopie und MS Spektrometrie) für Chemiker im Fortgeschrittenen Praktikum.
- Vortragsübungen für Chemiker und Biologen im Rahmen der Fortgeschrittenen Praktika.