6 Anhang

6.1 Literatur

Ahlers, M.; W. Müller; A. Reichert; H. Ringsdorf; J. Venzmer (1990)
Spezifische Wechselwirkung von Proteinen mit funktionellen Lipidmonoschichten - Wege zur Simulation von Biomembranprozessen
Angew. Chemie **102**, 1310-1327.

Allen, M.P.; D.J. Tildesley (1987)
Computer simulation of liquids
Oxford University Press, Oxford.

Alper, H.E.; D. Bassolino; T.R. Stouch (1993a)
Computer simulation of a phospholipid monolayer-water system: The influence of long range forces on water structure and dynamics
J. Chem. Phys. **98**, 9798-9807.

Alper, H.E.; D. Bassolino; T.R. Stouch (1993b)
The limiting behavior of water hydrating a phopholipid monolayer: A computer simulation study
J. Chem. Phys. **99**, 5547-5559.

Alving, C.R.; E.C. Richardson (1984)
Mitogenic activities of lipid A and liposome-associated lipid A: Effects of epitope density
Rev. Infect. Dis. **6**, 493-496.

Amano, K.-I.; K. Fukushi; J.C. Williams (1985)
Short communication: Electron microscopic studies of lipopolysaccharides from phase I and phase II *Coxiella burnettii*
J. Gen. Microbiol. **131**, 3127-3129.

Appelmelk, B.J.; J.J. Maaskant; A.M.J.J. Verweij-van Vught; N.M. van der Meer; B.G. Thijs, D.M. MacLaren (1993)
Antigenic and immunogenic differences in lipopolysaccharides of *Escherichia coli* J5 vaccine strains of different origin
J. Gen. Microbiol. **139**, 2641-2647.

Atassi, Z.; C.-L. Lee (1978)
The precise and entire antigenic structure of native lysozyme
Biochem. J. **171**, 429-434.

Bahrami, S.; G. Schlag; Y.-M. Yao; H. Redl (1995)
Significance of translocation/endotoxin in the development of systemic sepsis following trauma and/or haemorrhage
In: Bacterial endotoxins: Lipopolysaccharides from genes to therapy (Hrsg.: Levin, J.; C.R. Alving; R.S. Munford; H. Redl)
Wiley-Liss, New York, 197-208.

Bailat, S.; D. Heumann; D. Le Roy; J.D. Baumgartner; E.Th. Rietschel; M.P. Glauser; F. Di Padova (1997)
Similarities and disparities between core-specific and O-side-chain-specific antilipopolysaccharide monoclonal antibodies in models of endotoxemia and bacteremia in mice
Infect. Immun. **65**, 811-814.

Bates, D.W.; T.H. Lee (1994)
Projected impact of monoclonal anti-endotoxin antibody therapy
Arch. Intern. Med. **154**, 1241-1249.

Baumann, M., L. Brade; E. Fasske; H. Brade (1992)
Staining of surface antigens of *Chlamydia trachomatis* L2 in tissue culture
Infect. Immun. **60**, 4433-4438.

Baumgartner, J.D.; D. Heumann; T. Calandra; M.P. Glauser (1991)
Antibodies to lipopolysaccharides after immunization of humans with the rough mutant *Escherichia coli* J5
J. Infect. Dis. **163**, 769-772.

Beamer, L.J.; S.F. Carroll; D. Eisenberg (1997)
Crystal structure of human BPI and two bound phospholipids at 2.4 Ångstrom resolution
Science **276**, 1861-1864.

Beveridge, T.J. (1983)
In: The Target of Penicillin (Hrsg.: Hakenbeck; R.; J.-V. Höltje, H. Labischinski)
W. de Gruyter, Berlin, 39.

Bhattacharjee, A.K.; S.M. Opal; R. Taylor; R. Naso; M. Semenuk; W.D. Zollinger (1996)
A noncovalent complex vaccine prepared with detoxified *Escherichia coli* J5 (Rc chemotype) lipopolysaccharide and *Neisseria meningitidis* group B outer membrane protein produces protective antibodies against Gram-negative bacteremia
J. Infect. Dis. **173**, 1157-63.

Bhattacharjya, S.; S.A. David; V.I. Mathan; P. Balaram (1997)
Polymyxin B nonapeptide: conformations in water and in the lipopolysaccharide-bound state determined by two-dimensional NMR and molecular dynamics
Biopolymers **41**, 251-265.

Billeter, M. (1992)
Comparison of protein structures determined by NMR in solution and by X-ray diffraction in single crystals
Q. Rev. Biophys. **25**, 325-377.

Birkelund, S.; A.G. Lundemose; G. Christiansen (1989)
Immunoelectron microscopy of lipopolysaccharide in *Chlamydia trachomatis*
Infect. Immun. **57**, 3250-3253.

Blattner, F.R.; G. Plunkett 3rd; C.A. Bloch; N.T. Perna; V. Burland; M. Riley; J. Collado-Vides; J.D. Glasner; C.K. Rode; G.F. Mayhew; J. Gregor; N.W. Davis; H.A. Kirkpatrick; M.A. Goeden; D.J. Rose; B. Mau; Y. Shao (1997)
The complete genome sequence of *Escherichia coli* K-12
Science **277**, 1453-1474.

Bock, K.; J.U. Thomsen; P. Kosma; P. Christian; O. Holst; H. Brade (1992)
A nuclear magnetic resonance spectroscopic investigation of KDO-containing oligosaccharides related to the genus-specific epitope of *Chlamydia* lipopolysaccharides
Carbohydr. Res. **229**, 213-224.

Bock, K.; E.V. Vinogradov; O. Holst; H. Brade (1994)
Isolation and structural analysis of oligosaccharide phosphates containing the complete carbohydrate chain of the lipopolysaccharide from *Vibrio cholerae* strain H11 (non-O1)
Eur. J. Biochem. **225**, 1029-1039.

Böcker, J.; M. Schlenkrich; P. Bopp; J. Brickmann (1992)
Molecular dynamics simulation of a n-hexadecyltrimethylammonium chloride monolayer
J. Phys. Chem. **96**, 9915-9922.

Bogard, W.C., S.A. Siegel; A.O. Leone; E. Damiano; D.J. Shealy; T.M. Ely; B. Frederick; M.A. Mascelli; R.C. Siegel; B. Machielse; D. Naveh; P.M. Kaplan; P.E. Daddona (1993)
Human monoclonal antibody HA-1A binds to endotoxin via an epitope an the lipid A domain of lipopolysaccharide
J. Immunol. **150**, 4438-4449.

Böhm, H.J.; G. Klebe (1996)
Was läßt sich aus der molekularen Erkennung in Protein-Ligand-Komplexen für das Design neuer Wirkstoffe lernen ?
Angew. Chemie **108**, 2750-2778.

Brade, L.; M. Nurminen; H. Mäkelä; H. Brade (1985)
Antigenic properties of *Chlamydia trachomatis* lipopolysaccharide
Infect. Immun. **48**, 569-572.

Brade, L.; K. Brandenburg; H.-M. Kuhn; S. Kusumoto; I. Macher; E.Th. Rietschel; H. Brade (1987a)
The immunogenicity and antigenicity of lipid A are influenced by its physicochemical state and environment
Infect. Immun. **55**, 2636-2644.

Brade, H.; L. Brade; F.E. Nano (1987b)
Chemical and serological investigations on the genus-specific lipopolysaccharide epitope of *Chlamydia*
Proc. Natl. Acad. Sci. **84**, 2508-2512.

Brade, H.; L. Brade; E.Th. Rietschel (1988)
Structure activity relationships of bacterial lipopolysaccharides (endotoxins)
Zbl. Bakt. Hyg. **A 268**, 151-179.

Brade; L.; H. Brunnemann; M. Ernst; Y. Fu; O. Holst; P. Kosma; H. Näher; K. Persson; H. Brade (1994)
Occurence of antibodies against chlamydial lipopolysaccharide in human sera as measured by ELISA using an artificial glycoconjugate antigen
FEMS Immunol. Med. Microbiol. **8**, 27-42.

Brade, H.; W. Brabetz; L. Brade; O. Holst; S. Löbau; M. Lukacova; U. Mamat; A. Rozalski; K. Zych; P. Kosma (1995)
Chlamydial lipopolysaccharide: Chemical and antigenic structure, biosynthesis and biomedical application
Pure Appl. Chem. **67**, 1617-1626.

Brade, L.; H.D. Grimmecke; O. Holst; W. Brabetz; A. Zamojski; H. Brade (1996)
Specificity of monoclonal antibodies against *Escherichia coli* K-12 lipopolysaccharide
J. Endotoxin Res. **3**, 39-47.

Brandenburg, K.; U. Seydel (1984)
Physical aspects of structure and function of membranes made from lipopolysaccharides and lipid A
Biochim. Biophys. Acta **775**, 225-38.

Brandenburg, K.; U. Seydel (1990a)
Investigation into the fluidity of lipopolysaccharide and free lipid A membrane systems by Fourier-transform infrared spectroscopy and differential scanning calorimetry
Eur. J. Biochem. **191**, 229-236.

Brandenburg, K.; M.H.J. Koch; U. Seydel (1990b)
Phase diagram of lipid A from *salmonella minnesota* and *Escherichia coli* rough mutant lipopolysaccharide
J. Struct. Biol. **105**, 11-21.

Brandenburg, K.; U. Seydel (1991)
A comment on the preparation of liposomes from and on the b « a acyl chain melting behaviour of rough mutant lipopolysaccharide
Biochim. Biophys. Acta **1069**, 1-4.

Brandis, H. (1988)
Die Prokaryonten
In: Lehrbuch der Medizinischen Mikrobiologie (Hrsg: Brandis, H.; G. Pulverer)
G. Fischer, Stuttgart, 6. Aufl., 13-26.

Brandis, H.; K.P. Schaal (1988)
Taxonomie der Bakterien
In: Lehrbuch der Medizinischen Mikrobiologie (Hrsg: Brandis, H.; G. Pulverer)
G. Fischer, Stuttgart, 6. Aufl., 38-46.

Brandtzaeg, P.; R. Øvstebø; P. Kierulf (1995)
Bacteremia and compartimentalization of LPS in menigococcal disease
In: Bacterial endotoxins: Lipopolysaccharides from genes to therapy (Hrsg.: Levin, J.; C.R. Alving; R.S. Munford; H. Redl)
Wiley-Liss, New York, 219-233.

Brooks, B.R.; R.E. Bruccoleri; B.D. Olafson; D.J. States; S. Swaminathan; M.J. Karplus (1983)
CHARMM: A program for macromolecular energy, minimization, and dynamics calculations
J. Comput. Chem. **4**,187-217.

Brooks, C.L.; M. Karplus (1989)
Solvent effects on protein motion and protein effects on solvent motion
J. Mol. Biol. **208**, 159-181.

Bufler, P.; G. Stiegler; M. Schuchmann; S. Hess; C. Krüger; F. Stelter; C. Eckerskorn; C. Schütt; H. Engelmann (1995)
Soluble lipopolysaccharide receptor (CD14) is released via two different mechanisms from human monocytes and CD14 transfectants
Eur. J. Immunol. **25**, 604-610.

Bundle, D.R.; E. Eichler; M.A.J. Gidney; M. Meldal; A. Ragauskas; B.W. Sigurskjold; B. Sinnott; D.C. Watson; M. Yaguchi; N.M. Young (1994a)
Molecular recognition of a *Salmonella* trisaccharide epitope by monoclonal antibody Se 155-4
Biochemistry **33**, 5172-5182.

Bundle, D.R.; H. Baumann; J.-R. Brisson; S. Gagné; A. Zdanov; M. Cygler (1994b)
Solution structure of a trisaccharide-antibody complex: Comparison of NMR measurements with a crystal structure
Biochemistry **33**, 5183-5192.

Buttenschoen, K.; D. Berger; N. Hiki; W. Strecker; M. Seidelmann; H.G. Beger (1996)
Plasma concentrations of endotoxin and antiendotoxin antibodies in patients with multiple injuries: A prospective clinical study
Eur. J. Surg. **162**, 853-860.

Caldwell, H.D.; P.J. Hitchcock (1984)
Monoclonal antibody against a genus-specific antigen of *Chlamydia* species
Infect. Immun. **44**, 306-314.

Capodici, C.; S. Chen; Z. Sidorczyk; P. Elsbach; J. Weiss (1994)
Effect of lipopolysaccharide (LPS) chain length on interactions of bactericidal/permeability-increasing protein and its bioactive 23-kilodalton NH_2-terminal fragment with isolated LPS and intact *Proteus mirabilis* and *Escherichia coli*
Infect. Immun. **62**, 259-265.

CDC Centers for Disease Control (1990)
Increase in national hospital discharge survey rates for septicemia - United States 1979-87
MMWR Morb. Mortal. Wkly. Rep. **39**, 31-34.

Cevc, G. (1990)
Membrane electrostatics
Biochim. Biophys. Acta. **1031-3**, 311-382.

Chapman, D. (1993a)
Lipid phase transitions
In: Biomembranes (Hrsg.: Shinitzky, M.)
VCH, Weinheim, 29-62.

Chapman, D. (1993b)
Biomembranes and new hemocompatible materials
Langmuir **9**, 39-45.

Chedid, L.; M. Parent; F. Parent; F. Boyer (1968)
A proposed mechanism for natural immunity to enterobacterial pathogens
J. Immunol. **100**, 292-301.

Chen, C.; R. Brock; F. Luh; P.-J. Chou; J.W. Larrick; R.F. Huang; T.-H. Huang (1995)
The solution structure of the active domain of CAP18 - a lipopolysaccharide binding protein from rabbit leukocytes
FEBS Letters **370**, 46-52.

Chiu, S.-W.; M. Clark; S. Subramaniam; H.L. Scott; E. Jakobsson (1995)
Incorporation of surface tension into molecular dynamics simulation of an interface: A fluid phase bilayer membrane
Biophys. J. **69**, 1230-1245.

Christ, W.J.; O. Asano; A.L.C. Robidoux; M. Perez; Y. Wang; G.R. Dubuc; W.E. Gavin; L.D. Hawkins; P.D. McGuiness; M.A. Mullarkey; M.D. Lewis; Y. Kishi; T. Kawata; J.R. Bristol; J.R. Rose; D.P. Rossignol; S. Kobayashi; I. Hishinuma; A. Kimura; N. Asakawa; K. Katayama; I. Yamatsu (1995)
E5531, a pure endotoxin antagonist of high potency
Science **268**, 80-83.

Clementi, E. (1972)
zit. nach K. Merz
Modelling 97, Erlangen, 1997

Cohen, M.L. (1994)
Epidemiology of drug resistance: Implications for a post-antimicrobial era
Science **264**, 1050-1055.

Connolly, M.J. (1983)
Solvent-accessible surface of proteins and nucleic acids
Science **221**, 709-13.

Coughlin, R.T.; A. Haug; E.J. McGroarty (1983a)
Physical properties of defined lipopolysaccharide salts
Biochemistry **22**, 2007-2013.

Coughlin, R.T.; S. Tonsager; E.J. McGroarty (1983b)
Quantitation of metal cations bound to membranes and extracted lipopolysaccharide of *Escherichia coli*
Biochemistry **22**, 2002-2007.

Coughlin, R.T.; A.A. Peterson; A. Haug; H.J. Pownall; E.J. McGroarty (1985)
A pH-tritration study on the ionic bridging within lipopolysaccharide aggregates
Biochim. Biophys. Acta **821**, 404-412.

Cygler, M.; D.R. Rose; D.R. Bundle (1991)
Recognition of a cell-surface oligosaccharide of pathogenic *Salmonella* by an antibody Fab fragment
Science **253,** 442-445.

Damodaran, K.V.; K.M. Merz Jr. (1994a)
A comparison of DMPC- and DLPE lipid bilayers
Biophys. J. **66**, 1076-1087.

Damodaran, K.V.; K.M. Merz Jr. (1994b)
Computer simulation of lipid systems
Rev. Comput. Chem. **5**, 269-298.

David, S.A.; V.I. Mathan; P. Balaram (1995)
Interactions of linear dicationic molecules with lipid A: structural requisites for optimal binding affinity
J. Endotoxin Res. **2**, 325-336.

Davies, D.R.; E.A. Padlan; S. Sheriff (1990)
Antibody-antigen complexes
Annu. Rev. Biochem. **59**, 439-73.

De Loof, H.; S.C. Harvey; J.P. Segrest; R.W. Pastor (1991)
Mean field stochastic boundary molecular dynamics simulation of a phospholipid membrane
Biochemistry **30**, 2099-2113.

Di Padova, F.E.; H. Brade; G.R. Barclay; I.R. Poxton; E. Liehl; E. Schuetze; H.P. Kocher; G. Ramsay; M.H. Schreier; D.B.L. McClelland; E.Th. Rietschel (1993)
A broadly cross-protective monoclonal antibody binding to *Escherichia coli* and *Salmonella* lipopolysaccharides
Infect. Immun. **61**, 3863-3872.

Di Padova, F.E.; V. Mikol; G.R. Barclay; I.R. Poxton; H. Brade; E.Th. Rietschel (1994)
Anti-lipopolysaccharide core antibodies
In: Bacterial Endotoxins: Basic Science to Anti-Sepsis strategies (Hrsg.: Levin, J.; S.J.H. van Deventer; T. van der Poll; A. Sturke)
Wiley-Liss, New York, 85-94.

Din, Z.Z.; P. Mukerjee; M. Kastowsky; K. Takayama (1993)
Effect of pH on solubility and ionic state of lipopolysaccharide obtained from the deep rough mutant of *Escherichia coli*
Biochemistry **32**, 4579-4586.

Dinarello, C.A. (1996)
Cytokines as mediators in the pathogenesis of septic shock
Curr. Topics Microbiol. Immunol. **216**, 134-165.

Domann, E. (1997)
Infektionskrankheiten heute
Deutsche Apotheker Zeitung **137**, 3478-3482.

Doran, J.E. (1992)
Biological effects of endotoxin
Curr Stud Hematol. Blood Transfus. **59**, 66-99.

Douliez, J.-P.; A. Léonard; E.J. Fufourc (1995)
Restatement of order parameters in biomembranes: Calculation of C-C bond order parameters from C-D quadrupolar splittings
Biophys. J. **68**, 1727-1739.

Edholm, O.; A.M. Nyberg (1992)
Cholesterol in model membranes - A molecular dynamics simulation
Biophys. J. **63**, 1081-1089.

Einstein, A. (1905)
Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen
Ann. Physik **17**, 549-560.

Elbein, A.D.; E.C. Heath (1965)
The biosynthesis of cell wall lipopolysaccharide in *Escherichia coli*
J. Biol. Chem. **240**, 1919-1925.

Elsbach, P.; J. Weiss (1993)
The bactericidal/permeability-increasing protein (BPI), a potent element in host-defense against Gram-negative bacteria and lipopolysaccharide
Immunobiol. **187**, 417-429

Evans, M.E.; M. Pollack; N.L. Koles; N.J. Hardegen; D. Panapoulos (1992)
Lipopolysaccharide heterogeneity in *Escherichia coli* J5 variants: Analysis by flow cytometry
J. Infect. Dis. **166**, 803-811.

Ferris, F.G.; T.J. Beveridge (1986)
Site specificity of metallic ion binding in *Escherichia coli* K-12 lipopolysaccharide
Can. J. Microbiol. **32**, 52-55.

Ferris, F.G. (1989)
Metalic ion interactions with the outer membrane of Gram-negative bacteria
In: Metal ion and bacteria (Hrsg.: Beveridge, T.J.; R.J. Doyle)
J. Wiley & Sons, New York, 295-323.

Fletcher, M.A.; T.M. McKenna, J.L. Quance; N.R. Wainwright; T.J. Williams (1993)
Lipopolysaccharide detoxification by endotoxin neutralizing protein
J. Surg. Res. **55**, 147-154.

Freudenberg, M.A.; T. Neß; Y. Kumazawa; C. Galanos (1993)
Die Bedeutung von Zytokinen beim Endotoxinschock und bei der Endotoxinüberempfindlichkeit
Immun. Infekt. **21**, 40-44.

Fu, Y.; M. Baumann; P. Kosma; L. Brade; H. Brade (1992)
A synthetic glycoconjugate representing the genus-specific epitope of *chlamydial* lipopolysaccharide exhibits the same specificity as its natural counterpart
Infect. Immun. **60**, 1314-1321.

Fujihara, Y.; M.-G. Lei; D.C. Morrison (1993a)
Characterization of specific binding of a human immunoglobin M monoclonal antibody to lipopolysaccharide and its lipid A domain
Infect. Immun. **61**, 910-918.

Fujihara, Y.; W.C. Bogard; M.-G. Lei; P.E. Daddoa; D.C. Morrison (1993b)
Monoclonal anti-lipid A IgM antibodies HA-1A and E-5 recognize distinct epitopes on lipopolysaccharide and lipid A
J. Infect. Dis. **168**, 1429-1435.

Galanos, C.; O. Lüderitz; O. Westphal (1971)
Preparation and propertiesof antisera against the Lipid-A component of bacterial lipopolysaccharides
Eur. J. Biochem. **24**, 116-122.

Galanos, C.; M.A. Freudenberg; F. Jay; D. Nerkar; K. Veleva; H. Brade; W. Strittmatter (1984)
Immunogenic properties of lipid A
Rev. Infect. Dis. **6**, 546-551.

Gazzano-Santoro, H.; J.B. Parent; L. Grinna; A. Horwitz; T. Parsons; G. Theofan; P. Elsbach; J. Weiss; P.J. Conlon (1992)
High-affinity binding of the bactericidal/permeability-increasing protein and a recombinant amino-terminal fragment to the lipid A region of lipopolysaccharide
Infect. Immun. **60**, 4754-4761.

Glaudemans, C.P.J.; L. Lerner; G.D. Daves; P. Kovac; R. Venable; A. Bax (1990)
Significant conformational changes in an antigenic carbohydrate epitope upon binding to a monoclonal antibody
Biochemistry **29**, 10906-10911.

Golenbock, D.T.; R.Y. Hampton; N. Qureshi; K. Takayama; C.R.H. Raetz (1991)
Lipid A-like molecules that antagonize the effects of endotoxins on human monocytes
J. Biol. Chem. **266**, 19490-19498.

Gram, C. (1884)
Ueber die isolirte Färbung der Schizomyceten in Schnitt- und Trockenpräparaten
Fortschr. Med. **2**, 185-189.

Gray, P.W.; G. Flaggs, S.R. Leong; R.J. Gumina (1989)
Cloning of the cDNA of a human neutrophil bactericidal protein
J. Biol. Chem. **264**, 9505-9509.

Gutberlet, T. (1995)
Strukturuntersuchungen von isolierten Lipoteichonsäuren und Lipoteichonsäure-Lipid Mischsystemen
Dissertation, Freie Universität Berlin.

Hailman, E.; J.J. Albers; G. Wolfbauer; A.-Y. Tu; S.D. Wright (1996)
Neutralization and transfer of lipopolysaccharide by phospholipid transfer protein
J. Biol. Chem. 271, 12172-12178.

Halle, B.; L. Piculell (1986)
Water spin relaxation in colloidal systems
J. Chem. Soc., Faraday Trans.1 **82**, 415-429.

Hancock, R.E.W.; A. Bell (1988)
Antibiotic uptake into Gram-negative bacteria
Eur. J. Clin. Microbiol. Infect. Dis. **7**, 713-720.

Hardy, B.J.; R.W. Pastor (1994)
Conformational sampling of hydrocarbon and lipid chains in an orienting potential
J. Comput. Chem. **15**, 208-226.

Hauser, H.; I. Pascher; R.H. Pearson, S. Sundell (1981)
Preferred conformation and molecular packing of phosphatidylethanolamine and phosphatidylcholine
Biochim. Biophys. Acta **650**, 21-51.

Helander, I.M.; B. Lindner; H. Brade; K. Altmann; A.A. Lindberg, E.Th. Rietschel; U. Zähringer (1988)
Chemical structure of the lipopolysaccharide of *Haemophilus influenzae* strain I-69 Rd-/b+: description of a novel deep-rough mutant
Eur. J. Biochem. **177**, 483-492.

Heller, H.; M. Schaefer; K. Schulten (1993)
Molecular dynamics simulation of a bilayer of 200 lipids in the gel and in the liquid-crystal phases
J. Phys. Chem. **97**, 8343-8360.

Hermann, R.B. (1994)
Modelling hydrophobic solvation of nonspherical systems: Comparison of use of molecular surface with accessible surface area
J. Comput. Chem. **18**, 115-25.

Hertz, H.G. (1973)
Nuclear magnetic relaxation spectroscopy
In: Water. A comprehensive treatise, Vol. 3, (Hrsg.: Franks, F.)
Plenum Press, Oxford, 301-399

Heumann, D.; M.P. Glauser (1996)
Anticytokine strategies for the treatment of septic shock: Relevance of animal models
Curr. Topics Microbiol. Immunol. **216**, 299-311.

Hirata, M.; Y. Shimomura; M. Yoshida; J.G. Morgan; I. Palings; D. Wilson; M.H. Yen; S.C. Wright; J.W. Larrick (1994)
Characterization of a rabbit cationic protein (CAP18) with lipopolysaccharide-inhibitory activity
Infect. Immun. **62**, 1421-1426.

Hoess, A.; S. Watson; G.R. Siber; R. Liddington (1993)
Crystal structure of an endotoxin-neutralizing protein from the horseshoe crab, Limulus anti-LPS factor, at 1.5 Å resolution
EMBO J. **12**, 3351-3356.

Holst, O.; L. Brade; P. Kosma; H. Brade (1991)
Structure, serological specifity, and synthesis of artificial glycoconjugates representing the genus-specific lipopolysaccharide epitope of *Chlamydia* spp.
J. Bacteriol. **173**, 1862-1866.

Holst, O.; S. Müller-Loennies; B. Lindner; H. Brade (1993a)
Chemical structure of the lipid A of *Escherichia coli* J-5
Eur. J. Biochem. **214**, 695-701.

Holst, O.; W. Broer; J.E. Thomas-Oates; U. Mamat; H. Brade (1993b)
Structural analysis of two oligosaccharide bisphosphates from the lipopolysaccharide of a recombinant strain of *Escherichia coli* F515 (Re chemotype) expressing the genus-specific epitope of *Chlamydia* lipopolysaccharide
Eur. J. Biochem. **214**, 703-710.

Holst, O. (1995)
Endotoxin-Antagonisten: Potentielle Therapeutica der Gram-negativen Sepsis
Angew. Chemie **107**, 2154-2156.

Holst, O.; A.J. Ulmer; H. Brade; H.-D. Flad; E.Th. Rietschel (1996)
Biochemistry and cell biology of bacterial endodoxins
FEMS Immunol. Med. Microbiol. **16**, 83-104.

Hynninen, M.; M. Valtonen; M. Vaara; H. Markkanen; P. Kuusela; H. Saxen; O. Takkunen (1995)
Plasma endotoxin and cytokine levels in neutropenic and non-neutropenic bacteremic patients
Eur. J. Clin. Microbiol. Infect. Dis. **269**, 1039-1045.

Imoto, M.; S. Kusumoto; T. Shiba; E.Th. Rietschel; C. Galanos; O. Lüderitz (1985a)
Chemical structure of *Escherichia coli* lipid A
Tetrahedron Lett. **26**, 907-908.

Imoto, M.; H. Yoshimura; N. Sakaguchi; S. Kusumoto; T. Shiba (1985b)
Total synthesis of *Escherichia coli* lipid A
Tetrahedron Lett. **26**, 1545-1548.

Israelachvili, J.N.; H. Wennerström (1990)
Hydration or steric forces between amphiphilic surfaces ?
Langmuir **6**, 873-876.

Israelachvili, J.N.; H. Wennerström (1992)
Entropic forces between amphiphilic surfaces in liquids
J. Phys. Chem. **96**, 520-531.

J5 Study group (1992)
Treatment of severe infectious purpura in children with human plasma from donors immunized with *Escherichia coli* J5: A prospective double blind study
J. Infect. Dis. **65**, 695-701.

Jack, R.S.; U. Grunwald; F. Stelter; G. Workalemahu; C. Schütt (1995)
Both membrane-bound and soluble forms of CD14 bind to Gram-negative bacteria
Eur. J. Immunol. **25**, 1436-1441.

Jackson, R.M.; M.J.E. Sternberg (1993)
Protein surface area defined
Nature **366**, 638.

Jansson, P.-E.; R. Wollin; G.W. Bruse; A.-A. Lindberg (1989)
The conformation of core oligosaccharides from *Escherichia coli* and *Salmonella typhimurium* lipopolysaccharides as predicted by semi-empirical calculations
J. Mol. Recog. **2**, 25-36.

Jimenez, R.; G.R. Fleming; P.V. Kumar; M. Maroncelli (1994)
Femtosecond solvation dynamics of water
Nature **369**, 471-473.

Jorgensen, W.L.; J. Chandrasekhar; J.D. Madura (1983)
Comparison of simple potential functions for simulating liquid water
J. Chem. Phys. **79**, 926-935.

Jung, S.; D. Min; R.I. Hollingsworth (1996)
A metropolis Monte Carlo method for analyzing the energetics and dynamics of lipopolysaccharide supramolecluar structure and organization
J. Comput. Chem. **17**, 238-249.

Kabat, A.E. (1954)
Some configurational requirements and dimensions of the combining site on an antibody to a naturally occuring antigen
J. Am. Chem. Soc. **76**, 3709-3713.

Kahle, C.; P.-J. Koch; W. Dürr; M. Kastowsky; H. Bradaczek (1996)
Active penetration of charged peptides into monomolecular films of deep rough mutant lipopolysaccharide
Thin Solid Films **284-285**, 802-804.

Kar L.; S.A. Sherman; M.E. Johnson (1994)
Comparison of protein structures in solution using local conformations derived from NMR data: application to cytochrome c
J. Biomol. Struct. Dyn. **12**, 527-558.

Karaborni, S. (1993)
Molecular dynamics simulations of long-chain amphiphilic molecules in Langmuir monolayers
Langmuir **9**, 1334-1343.

Karimi, S.T.; R.H. Schloemer; C.E. Wilde (1989)
Accumulation of *Chlamydial* Lipopolysaccharide Antigen in the Plasma Membrane of Infected Cells
Infect. Immun. **57**, 1780-1785.

Karplus, M.; G.A. Petsko (1990)
Molecular dynamics simulations in biology
Nature **347**, 631-639.

Kastowsky, M.; A. Sabisch; T. Gutberlet; H. Bradaczek (1991)
Molecular Modelling of bacterial deep rough mutant lipopolysaccharide of *Escherichia coli*
Eur. J. Biochem. **197**, 707-716.

Kastowsky, M.; T. Gutberlet; H. Bradaczek (1992)
Molecular modelling of the three-dimensional structure and conformational flexibility of bacterial lipopolysaccharide
J. Bacteriol. **174**, 4798-4806.

Kastowsky, M. (1993a)
Modelling the three-dimensional structure of lipopolysaccharide
In: Bacterial endotoxin: Recognition and effector mechanisms. (Hrsg.: Levin, J.; C.R. Alving; R.S. Munford; P.L. Stütz)
Elsevier, Amsterdam, 61-70.

Kastowsky, M. (1993b)
Molekülmodellrechnungen und röntgenographische Untersuchungen zur Aufklärung der dreidimensionalen Molekül- und Membranstruktur bakterieller Lipopolysaccharide
Dissertation, Freie Universität Berlin.

Kato, N.; M. Ohta; N. Kido; H. Ito; S. Naito; T. Kuno (1985)
Formation of a hexagonal lattice structure by an R-form lipopolysaccharide of *Klebsiella* sp.
J. Bacteriol. **162**, 1142-1150.

Kato, N.; M. Ohta; N. Kido; H. Ito; S. Naito; T. Hasegawa; T. Watabe; K. Sasaki (1990a)
Crystallization of R-form lipopolysaccharides from *Salmonella minnesota* and *Escherichia coli*
J. Bacteriol. **172**, 1516-1528.

Kato, N.; M. Ohta; N. Kido; H. Ito; Y. Arakawa; S. Naito (1990b)
Electron microscopic observation of crystals of *Escherichia coli* K-12 lipopolysaccharide
Microbiol. Immunol. **34**, 665-674.

Keller, E. (1989)
Some computer drawings of molecular and solid-state structures
J. Appl. Cryst. **22**, 19-22.

Keller, E. (1995)
Grafische Darstellung von Molekül- und Kristallstrukturmodellen
GIT Fachz. Lab. **39**, 232-238.

Kelly, J.L.; C. O' Sullivan; M. O'Riordain; D. O'Riordain; A. Lyons; J. Doherty; J.A. Mannick; M.L. Rodrick (1997)
Is circulating endotoxin the trigger for the systemic inflammatory response syndrom seen after injury ?
Ann. Surg. **225**, 530-543.

Koch, P.-J.; J. Frank; J. Schüler, H. Bradaczek (1997)
Thermodynamic investigations of the binding of Polymyxin B to LPS
Biophys. Chem., eingereicht.

Koch, P.-J. (1998)
Wechselwirkung von polykationischen Substanzen mit bakteriellen Lipopolysacchariden
Dissertation, Freie Universität Berlin, eingereicht.

König, S.; E. Sackmann; D. Richter; R. Zorn; C. Carlile; T.M. Bayerl (1994)
Molecular dynamics of water in oriented DPPC-multilayers studied by quasielastic neutron scattering and deuterium-nuclear magnetic resonance relaxation
J. Chem. Phys. **100**, 3307-3316.

König, S.; T.M. Bayerl; G. Coddens; D. Richter; E. Sackmann (1995)
Hydration dependence of chain dynamics and local diffusion in L-a-Dipalmitoylphosphatidyl-choline multilayers studied by incoherent quasi-elastic neutron scattering
Biophys. J. **68**, 1871-1880.

Krieger, J.I.; R.C. Fletcher; S.A. Siegel; D.T. Fearon; D.S. Neblock; R.H. Boutin; R.P. Taylor; P.E. Daddona (1993)
Human anti-endotoxin antibody HA-1A mediates complement-dependent binding of *Escherichia coli* J5 lipopolysaccharide to complement receptor type 1 of human erythrocytes and neutrophils
J. Infect. Dis. **167**, 865-875.

Kuby, J. (1992)
Immunology
W.H. Freeman & Co., New York, 80-83.

Kuhn, H.-M.; L. Brade; B.J. Appelmelk; S. Kusumoto; E.Th. Rietschel; H. Brade (1992)
Characterization of the epitope specifity of murine monoclonal antibodies directed against lipid A
Infect. Immun. **60**, 2201-2210.

Kuhn, H.-M. (1993)
Cross-reactivity of monoclonal antibodies and sera directed against lipid A and lipopolysaccharides
Infection **21**, 179-186.

Kuhn, H.-M.; L. Brade; B.J. Appelmelk; S. Kusumoto; E.Th. Rietschel; H. Brade (1993)
The antibody reactivity of monoclonal lipid A antibodies is influenced by the acylation pattern of lipid A and the assay system employed
Immunobiol. **189**, 457-471.

Kuntz, I.D. (1992)
Structure-based strategies for drug design and discovery
Science **257**, 1078-82.

Kuzmin, A.; S. Obst; J. Purans (1997)
X-ray absorption spectroscopy and molecular dynamics studies of Zn^{2+} hydration in aqueous solutions
J. Phys.: Condens. Matter **9**, 10069-10078.

Labischinski, H.; G. Barnickel; H. Bradaczek; D. Naumann; E.Th. Rietschel; P. Giesbrecht (1985)
High state of order of isolated bacterial lipopolysaccharide and its possible contribution to the permeation barrier property of the outer membrane
J. Bacteriol. **162**, 9-20.

Labischinski, H.; D. Naumann; C. Schultz; S. Kusumoto, T. Shiba; E.Th. Rietschel; P. Giesbrecht (1989)
Comparative X-ray and Fourier-transform-infrared investigations of conformational properties of bacterial and synthetic lipid A of *Escherichia coli* and *Salmonella minnesota* as well as partial structures and analogues thereof
Eur. J. Biochem. **179**, 659-665.

Landmann, R.; H.-P. Knopf; S. Link; S. Sansano; R. Schumann; W. Zimmerli (1996)
Human monocyte CD14 is upregulated by lipopolysaccharide
Infect. Immun. **64**, 1762-1769.

Larrick, J.W.; M. Hirata; Y. Shimomoura; M. Yoshida; H. Zheng; J. Zhong; S.C. Wright (1994)
Rabbit CAP18 derived peptides inhibit Gram negative and Gram positive bacteria
In: Bacterial Endotoxins: Basic Science to Anti-Sepsis strategies (Hrsg.: Levin, J.; S.J.H. van Deventer; T. van der Poll; A. Sturke)
Wiley-Liss, New York, 125-135.

Laver, W.G.; G.M. Air; R.G. Webster; S.J. Smith-Gill (1990)
Epitopes on protein antigens: Misconceptions and realities
Cell **61**, 553-556.

Lee, B.; F.M. Richards (1971)
The interpretation of protein structures: Estimation of static accessibility
J. Mol. Biol. **55**, 379-400.

Lee, S.H.; P.J. Rossky (1994)
A comparison of the structure and dynamics of liquid water at hydrophobic and hydrophilic surfaces - a molecular dynamics simulation study
J. Chem. Phys. **100**, 3334-3345.

Levitzki, A.; D.E. Koshland Jr. (1972)
Role of an allosteric effector. Guanosine triphosphate activation in cytosine triphosphate synthetase
Biochemistry **11**, 241-246.

Lifson, S.; C.E. Felder; M. Dobler (1987)
Effects of crystal packing and hydration on the conformation of enniatin B
Acta Cryst. **B 43**, 179-187.

López Cascales, J.J.; J.G. de la Torre; S.J. Marrink; H.J.C. Berendsen (1996)
Molecular dynamics simulation of a charged biological membrane
J. Chem. Phys. **104**, 2713-2720.

Lugowski, C.; W. Jachymek; T. Niedziela; S. Rowinski (1996a)
Serological characterization of anti-endotoxin sera directed against conjugates of oligosaccharide core of *Escherichia coli* type R1, R2, R3, J5 and *Salmonella* Ra with tetanus toxoid
FEMS Immunol. Med. Microbiol. **16**, 21-30.

Lugowski, C.; T. Niedziela; W. Jachymek (1996b)
Anti-endotoxin antibodies directed against *Escherichia coli* R1 oligosaccharide core-tetanus toxoid conjugate bind to smooth, live bacteria and smooth lipopolysaccharides and attenuate their tumor necrosis factor stimulating activity
FEMS Immunol. Med. Microbiol. **16**, 31-38.

Lugtenberg, B.; L. van Alphen (1983)
Molecular architecture and functioning of the outer membrane of *Escherichia coli* and other Gram-negative bacteria
Biochim. Biophys. Acta **737**, 51-115.

Lukácová, M.; M. Baumann; L. Brade; U. Mamat; H. Brade (1994)
Lipopolysaccharide smooth-rough phase variation in bacteria of the genus *Chlamydia*
Infect. Immun. **62**, 2270-2276.

MacDonald, R.C.; S.A. Simon (1987)
Lipid monolayer states and their relationship to bilayers
Proc. Natl. Acad. Sci. **84**, 4089-4093.

MacKerell Jr., A.D. (1995)
Molecular dynamics simulation analysis of a sodium dodecyl sulfate micelle in aqueous solution: Decreased fluidity of the micelle hydrocarbon interior
J. Phys. Chem. **99**, 1846-1855.

Mamat, U., M. Baumann; G. Schmidt; H. Brade (1993)
The genus-specific lipopolysaccharide epitope of *Chlamydia* is assembled in *C. psittaci* and *C. trachomatis* by glycosyltransferases of low homology
Mol. Microbiol. **10**, 935-941.

Marra, M.N.; C.G. Wilde; M.S. Collins; J.L. Snabel; M.B. Thornton; R.W, Scott (1992)
The role of bactericidal/permeability-increasing protein as a natural inhibitor of bacterial endotoxin
J. Immunol. **148**, 532-537.

Marsh, D. (1993)
Bilayers, monolayers, multilayers and non-lamellar lipid phases
In: Biomembranes (Hrsg.: Shinitzky, M.)
VCH, Weinheim, 1-28.

Martich, G.D.; A.J. Boujoukos; A.F. Suffredini
Response of man to endotoxin
Immunobiol. **187**, 403-416.

Mattsby-Baltzer, I.; C.R. Alving (1984)
Antibodies to lipid A: Occurence in humans
Rev. Infect. Dis. **6**, 553-557.

Mayeux, P.R (1997)
Pathobiology of lipopolysaccharide
J. Toxicol. Environ. Health **51**, 415-435.

McManus, C. (1997)
Mechanisms of bacterial resistance to antimicrobial agents
Am. J. Health-Syst. Pharm. **57**, 1420-1433.

Mikol, V.; P. Kosma; H. Brade (1994)
Crystal and molecular structure of allyl *O*-(sodium 3-deoxy-α-D-*manno*-2-octulopyranosylate)-(2->8)-*O*-(sodium 3-deoxy-α-D-*manno*-2-octulopyranosidate)-monohydrate
Carbohydr. Res. **263**, 35-42.

Mlot, C. (1996)
Chlamydia linked to atherosclerosis
Science **272**, 1422.

Morrison, D.C. (1989)
The case for specific lipopolysaccharide receptors expressed on mammalian cells
Microb. Pathogen. **7**, 389-398.

Moulder, J. (1984)
Order II. Chlamydiales
In: Bergey´s Manual of Systematic Bacteriology (Hrsg.: Krieg, N.R.; J.G. Holt)
Williams & Wilkins, Baltimore, Band 1, 729-739.

Mouritsen, O.G.; B. Dammann, H.C. Fogedby; J.H. Ipsen; C. Jeppesen; K. Jörgensen; J. Risbo; M.C. Sabra; M.M. Sperotto; M.J. Zuckerman (1995)
The computer as a laboratory for the physical chemistry of membranes
Biophys. Chem. **55**, 55-68.

Müller-Loennies, S.; O. Holst; H. Brade (1994)
Chemical structure of the core region of *Escherichia coli* J-5 lipopolysaccharide
Eur. J. Biochem. **224**, 751-760.

Munford, R.S.; C.L. Hall; P.D. Rick (1980)
Size heterogeneity of *Salmonella typhimurium* lipopolysaccharides in outer membrane and culture supernatant membrane fragments
J. Bacteriol. **144**, 630-640.

Murray, R.G.E. (1984a)
The higher taxa, or, a place for everything ...?
In: Bergey´s Manual of Systematic Bacteriology (Hrsg.: Krieg, N.R.; J.G. Holt)
Williams & Wilkins, Baltimore, Band 1, 31-34.

Murray, R.G.E. (1984b)
Kingdom Procaryotae
In: Bergey´s Manual of Systematic Bacteriology (Hrsg.: Krieg, N.R.; J.G. Holt)
Williams & Wilkins, Baltimore, Band 1, 35-36.

Nano, F.E.; H.D. Caldwell (1985)
Expression of the chlamydial genus-specific lipopolysaccharide epitope in *Escherichia coli*
Science **228**, 742-744.

Neu, H.C. (1992)
The crisis in antibiotic resistance
Science **257**, 1064-1073.

Nicklas, K.; M. Schlenkrich; P. Bopp (1991)
Molecular dynamics studies of the interface between a model membrane and an aqueous solution
Biophys. J. **60**, 261-272.

Nikaido, H; M. Vaara (1985)
Molecular basis of bacterial outer membrane permeability
Microbiol. Rev. **49**, 1-32.

Obst, S.; H. Bradaczek (1996)
Molecular dynamics study of the structure and dynamics of the hydration shell of alkaline and alkaline-earth metal cations
J. Phys. Chem. **100**, 15677-15687.

Obst, S.; H. Bradaczek (1997)
Molecular dynamics simulations of zinc ions in water using CHARMM
J. Mol. Model. **3**, 224-232.

Obst, S.; M. Kastowsky; H. Bradaczek (1997)
Molecular dynamics simulations of six different fully hydrated monomeric conformers of *Escherichia coli* Re-lipopolysaccharide in the presence and absence of Ca^{2+}
Biophys. J. **72**, 1031-1046.

Ørskov, F. (1984)
Genus I. *Escherichia*
In: Bergey´s Manual of Systematic Bacteriology (Hrsg.: Krieg, N.R.; J.G. Holt)
Williams & Wilkins, Baltimore, Band 1, 420-423.

Pastor, R.W.; R.M. Venable (1988)
Brownian dynamics simulation of a lipid chain in a membrane bilayer
J. Chem. Phys. **89**, 1112-1127.

Pastor, R.W.; R.M. Venable; M. Karplus (1991)
Model for the structure of the lipid bilayer
Proc. Natl. Acad. Sci. **88**, 892-896.

Patel, P.; M.A. Menadll; D. Carrington; D.P. Strachan; E. Leatham; N. Molineaux; J. Levy; C. Blakeston; C.A. Seymour; A.J. Camm; T.C. Northfield (1995)
Association of *Helicobacter pylori* and *Chlamydia pneumoniae* infections with coronary heart disease and cardiovascular risk factors
BMJ **311**, 711-714.

Pelletier, C.; P. Bourlioux; J. van Heijenoort (1994)
Effects of sub-minimal inhibitory concentrations of EDTA on growth of *Escherichia coli* and the release of lipopolysaccharide
FEMS Microbiol. Letters **117***,* 203-206.

Peters, G.H.; S. Toxvaerd, A. Svendsen, O.H. Olsen (1994)
Modeling of complex biological systems. I. Molecular dynamics studies of diglyceride monolayers
*J. Chem. Phys.***100**, 5996-6009.

Pfeiffer, R. (1892)
Untersuchungen über das Choleragift
Zf. Hyg. **11**, 393-412.

Poelstra, K.; W.E. Bakker; P.A. Klok; M.J. Hardonk; D.K.F. Meijer (1997)
A physiologic function for alkaline phosphatase: endotoxin detoxifikation
Lab. Invest. **76**, 319-327.

Pollack, M.; C.A. Ohl (1996)
Endotoxin-based molecular strategies for the prevention and treatment of Gram-negative sepsis and septic shock
Curr. Topics Microbiol. Immunol. **216**, 275-297.

Poxton, I.R. (1995)
Antibodies to lipopoysaccharide
J. Immunol. Methods **186**, 1-15.

Raetz, C.R.H. (1990)
Biochemistry of endotoxins
Annu. Rev. Biochem. **59**,129-170.

Raetz, C.R.H.; R.J. Ulevitch; S.D. Wright; C.H. Sibley, A. Ding; C.F. Nathan (1991)
Gram-negative endotoxin: An extraordinary lipid with profound effects on eukaryotic signal transduction
FASEB J. **5**, 2652-2660.

Raghavan, K.; M. Reddy; M.L. Berkowitz (1992)
A molecular dynamics study of the structure and dynamics of water between dilauroylphosphatidylethanolamine bilayers
Langmuir **8**, 233-240.

Ramirez, J.A. and the *C. pneumoniae* study group (1996)
Isolation of *Chlamydia pneumoniae* from the coronary artery of a patient with coronary atherosclerosis
Ann. Int. Med. **125**, 979-982.

Ried, C.; C. Wahl; T. Miethke; G. Wellnhofer; C. Landgraf; J. Schneider-Mergener; A. Hoess (1996)
High affinity endotoxin-binding and neutralizing peptides based on the crystal structure of recombinant *Limulus* anti-lipopolysaccharide factor
J. Biol. Chem. **271**, 28120-28127.

Rietschel, E.Th.; H. Brade (1993)
Bakterielle Endotoxine
Spektrum der Wissenschaft **14**, 34-42.

Rietschel, E.Th.; T. Kirikae; F.U. Schade; A.J. Ulmer; O. Holst; H. Brade; G. Schmidt; U. Mamat; H.-D. Grimmicke; S. Kusumoto; U. Zähringer (1993)
The chemical structure of bacterial endotoxin in relation to bioactivity
Immunobiol. **187**, 169-190.

Rietschel, E.Th.; T. Kirikae; F.U. Schade; U. Mamat; G. Schmidt; H. Loppnow; A.J. Ulmer; U. Zähringer, U. Seydel, F. Di Padova, M. Schreier; H. Brade (1994)
Bacterial endotoxin: molecular relationship of structure to activity and function
FASEB J. **8**, 217-225.

Rietschel, E.Th.; H. Brade, O. Holst; L. Brade, S. Müller-Loennies; U. Mamat; U. Zähringer; F. Beckmann; U. Seydel; K. Brandenburg; A.J. Ulmer; T. Mattern; H. Heine; J. Schletter; H. Loppnow; U. Schönbeck; H.-D. Flad; S. Hauschildt; U.F. Schade; F. Di Padova; S. Kusumoto; R.R. Schumann (1996)
Bacterial endotoxin: chemical constitution, biological recognition, host response, and immunological detoxification
Curr. Topics Microbiol. Immunol. **216**, 40-81.

Roth, R.I.; J.S. Wong; R.L. Hamilton (1996)
Ultrastructural changes in bacterial lipopolysaccharide induced by human hemoglobin
J. Endotoxin Res. **3**, 361-366.

Rottem, S; L. Leive (1977)
Effect of the variations in lipopolysaccharide on the fluidity of the outer membrane of *Escherichia coli*
J. Biol. Chem. **252**, 2077-2081.

Rozalski, A.; L. Brade; H.-M. Kuhn; H. Brade; P. Kosma; B.J. Appelmelk; S. Kusumoto; H. Paulsen (1989)
Determination of the epitope specifity of monoclonal antibodies against the inner core region of bacterial lipopolysaccharides by use of 3-Deoxy-D-manno-octulosonate-containing synthetic antigens
Carbohydr. Res. **193**, 257-270.

Rustici, A.; M. Velucchi; R. Faggioni; M. Sironi; P. Ghezzi; S. Quataert; B. Green; M. Porro (1993)
Molecular mapping and detoxification of the lipid A binding site by synthetic peptides
Science **259**, 361-365.

Sabisch, A. (1988)
Konformationsuntersuchungen am Re-Lipopolysaccharid von *Escherichia coli* mit Hilfe von Potentialenergieberechnungen und computergraphischen Auswertemethoden
Diplomarbeit, Freie Universität Berlin.

Sabisch, A. (1994)
Verbindung von eindimensionalen Röntgendaten an lamellaren Schichten mit *modelling*-Experimenten am Beispiel von bakteriellen Lipopolysacchariden
Dissertation, Freie Universität Berlin.

Saito, M. (1994)
Molecular dynamics simulations of proteins in solution: Artifacts caused by the cutoff approximation
J. Chem. Phys. **101**, 4055-4061.

Salinas, J.; J. Sanchez; A.J. Buendia; A. Souriau; A. Rodolakis; A. Bernabé; F. Cuello (1994)
The LPS localization might explain the lack of protection of LPS-specific antibodies in abortion-causing *Chlamydia psittaci* infections
Res. Microbiol. **145**, 611-620.

Sayle, R.A.; E.J. Milner-White (1995)
RASMOL: Biomolecular graphics for all
Trends Biochem. Sci. **20**, 374-376.

Schachter, J.; H.D. Caldwell (1980)
Chlamydiae
Annu Rev. Microbiol. **34**, 285-309.

Schindler, M.; M.J. Osborn (1979)
Interaction of divalent cations and polymyxin B with lipopolysaccharide
Biochemistry **18**, 4425-4430.

Schlenkrich, M.; K. Nicklas; J. Brickmann; P. Bopp (1990)
A molecular dynamics study of the interface between a membrane and water
Ber. Bunsenges. Phys. Chem. **94**, 133-145.

Schlenkrich, M. (1993)
Entwicklung und Anwendung eines Kraftfeldes zur Simulation von Phospholipidmembransystemen
Dissertation, Technische Hochschule Darmstadt.

Schromm, A.B.; K. Brandenburg; E.Th. Rietschel; H.-D. Flad; S.F. Carroll; U. Seydel (1996)
Lipopolysaccharide-binding protein medicates CD14-independent intercalation of lipopolysaccharide into phospholipid membranes
FEBS Letters **399**, 267-271.

Schultz, C. (1993)
Untersuchungen zur Membran-Organisation lebender Bakterien unter besonderer Berücksichtigung des thermotropen Phasenverhaltens rekonstituierter Lipopolysaccharid-Doppelschichten
Dissertation, Freie Universität Berlin.

Schumann, R.R.; S.R. Leong; G.W. Flaggs; P.W. Gray; S.D. Wright; J.C. Mathison; P.S. Tobias; R.J. Ulevitch (1990)
Structure and function of lipopolysaccharide binding protein
Science **249**, 1429-1431.

Schumann, R.R. (1992)
Function of lipopolysaccharide (LPS)-binding protein (LBP) and CD14, the receptor for LPS/LBP complexes: A short review
Res. Immunol. **143**, 11-15.

Schütt, C.; R. Schumann (1993)
Der Endotoxinrezeptor CD14
Immun. Infekt. **21**, 36-40.

Schwartzer, T.A.; D.V. Alcid; V. Numsuwan; D.J. Gocke (1989)
Immunochemical specifity of human antibodies to lipopolysaccharide from the J5 rough mutant of *Escherichia coli* O111:B4
J. Infect. Dis. **159**, 35-42.

Seelig, J; A. Seelig (1974)
The dynamic structure of fatty acyl chains in a phospholipid bilayer measured by deuterium magnetic resonance
Biochemistry **13**, 4839-4845.

Seifert, M.; G. Schoenherr; D. Roggenbuck; U. Marx; R. von Baehr (1996)
Generation and characterization of a human monoclonal IgM antibody that recognizes a conserved epitope shared by lipopolysaccharides of different Gram-negative bacteria
Hybridoma **15**, 191-198.

Seydel, U.; H. Labischinski; M. Kastowsky; K. Brandenburg (1993)
Phase behaviour, supramolecular structure, and molecular conformation of lipopolysaccharide
Immunobiol. **187**, 191-211.

Shnyra, A.; K. Hultenby; A.A. Lindberg (1993)
Role of the physical state of *Salmonella* lipopolysaccharide in expression of biological and endotoxic properties
Infect. Immun. **61**, 5351-5360

Siegel, S.A.; M.E. Evans; M. Pollack; A.O. Leone ; C.S. Kinney; S.H. Tam; P.E. Daddona (1993)
Antibiotics enhance binding by human lipid A-reactive monoclonal antibody HA-1A to smooth Gram-negative bacteria
Infect. Immun. **61**, 2512-519.

Simmons, D.L.; S. Tan; D.G. Tenen; A. Nicholson-Weller, B. Seed (1989)
Monocyte antigen CD14 is a phospholipid anchored membrane protein
Blood **73**, 284-289.

Singer, S.J.; G.L. Nicolson (1972)
The fluid mosaic model of the structure of cell membranes
Science **175**, 720-731.

Singh, S.P.; Y. U. Williams; W.H. Benjamin; P.E. Klebba; D. Boyd (1996)
Immunoprotection by monoclonal antibodies to the porins and lipopolysaccharide of *Salmonella typhimurium*
Microb. Pathog. **21**, 249-263.

Srimal, S.; N. Surolia; S. Balasubramanian; A. Surolia (1996)
Titration calorimetric studies to elucidate the specificity of the interactions of polymyxin B with lipopolysaccharides and lipid A
Biochem. J. **315**, 679-686.

Staley, J.T.; N.R. Krieg (1984)
Bacterial Classification I. Classification of procaryotic organisms: An overview.
In: Bergey´s Manual of Systematic Bacteriology (Hrsg.: Krieg, N.R.; J.G. Holt)
Williams & Wilkins, Baltimore, Band 1, 1-4.

Stille, W.; G. Just-Nübling (1997)
Argumente für eine Antibiotika-Therapie der Arteriosklerose
Chemotherapie J. **6**, 1-5.

Stone, R. (1994)
Search for sepsis drugs goes on despite past failures
Science **264**, 365-367.

Storm, D.R.; K.S. Rosenthal; P.E. Swanson (1977)
Polymyxin and related peptide antibiotics
Annu. Rev. Biochem. **46**, 723-746.

Stouch, T.R. (1993)
Lipid membrane structure and dynamics studied by all-atom molecular dynamics simulations of hydrated phospholipid bilayers
Mol. Simul. **10**, 335-362.

Strain, S.M.; S.W. Fesik; I.M. Armitage (1983)
Structure and metal-binding properties of lipopolysaccharides from heptoseless mutants of *Escherichia coli* studied by ^{13}C and ^{31}P nuclear magnetic resonance
*J. Biol. Chem.***258**, 13466-13477.

Swart, R.M. (1990)
Monolayers and multilayers of biomolecules
In: Langmuir-Blodgett Films (Hrsg.: Roberts, G.)
Plenum Press New York, 273-316.

Takayama, K.; Z.Z. Din; P. Mukerjee; P.H. Cooke; T.N. Kirkland (1990)
Physicochemical properties of the lipopolysaccharide unit that activates B lymphocytes
J. Biol. Chem. **265,** 14023-14029.

Takayama, K.; D.H. Mitchell; Z.Z. Din; P. Mukerjee; C. Li; D.L. Coleman (1994)
Monomeric Re lipopolysaccharide from *Escherichia coli* is more active than the aggregated form in the *Limulus* amebocyte lysate assay and in inducing Egr-1 mRNA in murine peritoneal macrophages
J. Biol. Chem. **269,** 2241-2244.

Tanaka, S.; T. Nakamura; T. Morita; S. Twanaga (1982)
Limulus anti-LPS factor: An anticoagulant which inhibits the endotoxin mediated activation of *Limulus* coagulation system
Biochem. Biophys. Res. Comm. **105**, 717-723.

Tasaki, K.; S. McDonald; J.W. Brady (1993)
Observations concerning the treatment of long-range interactions in molecular dynamics simulations
J. Comput. Chem. **14**, 278-284.

Taylor, .H.; G.H. Heavner; M. Nedelman; D. Sheeris; E. Brunt; D. Knight; J. Ghrayeb (1995)
Lipopolysaccharide (LPS) neutralizing peptides reveal a lipid A binding site of LPS binding protein
J. Biol. Chem. **270**, 17934-17938.

Tellgmann, R.; E. Keller; V. Krämer (1994)
SCHAKAL 92: 8-bit-graphics of molecular and solid-state structure models on a DOS PC
Z. Kristallogr. Suppl. **8**, 516.

Tesh, V.L.; D.C. Morrison (1988)
The physical-chemical characterization and biologic activity of serum released lipopolysaccharides
*J. Immunol.***141**, 3523-3531.

Tobias, P.S.; K. Soldau; R.J. Ulevitch (1989)
Identification of a lipid A binding site in the acute phase reactant lipopolysaccharide binding protein
J. Biol. Chem. **264**, 10867-10871.

Tobias, P.S.; R.J. Ulevitch (1993)
Lipopolysaccharide binding protein and CD14 in LPS dependent macrophage activation
Immunobiol. **187**, 227-232.

Tobias, P.S.; K. Soldau; J.A. Gegner; D. Mintz; R.J. Ulevitch (1995)
Lipopolysaccharide binding protein-mediated complexation of lipopolysaccharide with soluble CD14
J. Biol. Chem. **270**, 10482-10488.

Tobias, P.S.; K. Soldau; N.M. Iovine; P. Elsbach; J. Weiss (1997)
Lipopolysaccharide (LPS)-binding proteins BPI and LBP form different types of complexes with LPS
J. Biol. Chem. **272**, 18682-18685.

Tocanne, J.-F.; J. Teissié (1990)
Ionization of phospholipids and phospholipid-supproted interfacial lateral diffusion of protons in membrane model systems
Biochim. Biophys. Acta. **1031**, 111-142.

Totrov, M.; R. Abagyan (1996)
The contour-buildup algorithm to calculate the analytical molecular surface
J. Struct. Biol. **116**, 138-143.

Troelstra, A.; P. Antal-Szalmas; L.A.M. de Graaf-Miltenburg; A.J.L Weersink; J. Verhoef; K.P.M. van Kessel; J.A.G. van Strijp (1997)
Saturable CD14-dependent binding of fluorescein-labeled lipopolysaccharide to human monocytes
Infect. Immun. **65**, 2272-2277.

Ulman, A. (1991)
An introduction to ultrathin organic films: From Langmuir-Blodgett to self-assembly
Academic Press, San Diego.

Vaara, M. (1992)
Agents that increase the permeability of the outer membrane
Microbiol. Rev. **56**, 395-411.

van der Meer, B.W. (1993)
Fluidity, dynamics and order
In: Biomembranes (Hrsg. Shinitzky, M.)
VCH Weinheim, 97-158.

van der Ploeg, P.; H.J.C. Berendsen (1982)
Molecular dynamics simulation of a bilayer membrane
J. Chem. Phys. **76**, 3271-3276.

van der Sijs, D.A., Y.K. Levine (1994)
A lattice dynamics model of lipid bilayer systems
J. Chem. Phys. **100**, 6783-6790.

van Gunsteren, W.F.; H.J.C. Berendsen (1977)
Algorithms for macromolecular dynamics and constraint dynamics
Mol. Phys. **34**, 1311-1327.

van Gunsteren, W.F.; M. Karplus (1981)
Effect of constraints, solvent and crystal environment on protein dynamics
Nature **293**, 677-678.

van Gunsteren, W.F.; H.J.C. Berendsen (1990)
Moleküldynamik-Computersimulationen: Methodik, Anwendungen und Perspektiven in der Chemie
Angew. Chemie **102**, 1020-1055.

van Gunsteren, W.F.; A.E. Mark (1992)
On the interpretation of biochemical data by molecular dynamics computer simulation
Eur. J. Biochem **204**, 947-961.

van Saene, J.J.M.; C.P. Stoutenbeek; H.K.F. van Saene; G. Matera; A.E. Martinez-Pellus; G. Ramsay (1996)
Reduction of the intestinal endotoxin pool by three different SDD regimens in human volunteers
J. Endotox. Res. **3**, 337-343.

Vincent, J.L. (1996)
Definition and pathogenesis of septic shock
Curr. Topics Microbiol. Immunol. **216**, 1-13.

Vinogradov, E.V.; R. Stuike-Prill; K. Bock; O. Holst; H. Brade (1993)
The structure of the carbohydrate backbone of the core-lipid-A region of the lipopolysaccharide from *Vibrio cholerae* strain H11 (non-O1)
Eur. J. Biochem. **218**, 543-554.

Vita, N.; S. Lefort; P. Sozzani; R. Reeb; S. Richards; L.K. Borysiewicz; P. Ferrara; M.O. Labéta (1997)
Detection and biochemical characteristics of the receptor for complexes of soluble CD14 and bacterial lipopolysaccharide
J. Immunol. **158**, 3457-3462.

Vretou, A.; E. Psarrou; D. Spiliopoulou (1992)
The role of lipopolysaccharide in the exposure of protective antigenic sites of the major outer membrane protein of *Chlamydia trachomatis*
J. Gen. Microbiol. **138**, 1221-1227.

Wang, Y.; R.I. Hollingsworth (1996)
An NMR spectroscopy and molecular mechanics study of the molecular basis for the supramolecular structure of lipopolysaccharides
Biochemistry **35**, 5647-5654.

Warren, H.S.; M.L. Glennon; N. Wainwright; S.F. Amato; K.M. Black; S.J. Kirsch; G. R. Riveau; R.I. Whyte; W.M. Zapol; T.J. Novitsky (1992)
Binding and neutralization of endotoxin by *Limulus* antilipopolysaccharide factor
Infect. Immun. **60**, 2506-2513.

Weil, M.H. (1994)
Lessons learned from clinical trials on monoclonal anti-endotoxin antibody
Arch. Intern. Med. **154**, 1183.

Wellinghausen, N.; A.B. Schromm; U. Seydel; K. Brandenburg; J. Luhm; H. Kirchner; L. Rink (1996)
Zinc enhances lipopolysaccharide-induced monokine secretion by alteration of fluidity state of lipopolysaccharide
J. Immunol. **157**, 3139-3145.

Westphal, O. (1993)
An old-timer's reflections on endotoxin
In: Bacterial endotoxin: Recognition and effector mechanisms (Hrsg.: Levin, J.; C.R. Alving; R.S. Munford; P.L. Stütz)
Elsevier Science, Amsterdam, 17-36.

Wiese, A.; K. Brandenburg; B. Lindner; A.B. Schromm; S.F. Carroll; E.Th. Rietschel; U. Seydel (1997)
Mechanisms of action of the bactericidal/permeability-increasing protein BPI on endotoxin and phospholipid monolayers and aggregates
Biochemistry **36**, 10301-10310.

Wilde, C.G.; J. Seilhammer; M. McGrogan; N. Ashton; J.L. Snable; J.C. Lane; S.R. Leong; M.B. Thornton; K.L. Miller; R.W. Scott; M.N. Marra (1994)
Bactericidal/permeability-increasing protein and lipopolysaccharide (LPS)-binding protein
J. Biol. Chem. **269**, 17411-17416.

Wilkinson, S.G. (1996)
Bacterial lipopolysaccharides - themes and variations
Prog. Lipid Res. **35**, 283-343.

Wimmer, M.L.J.; R. Sandmann-Strupp; P. Saikku; R.L. Haberl (1996)
Association of chlamydial infection with cerebrovascular disease
Stroke **27**, 2207-2210.

Woods, M.C.; J.M. Haile (1986)
Internal structure of a model micelle via computer simulation. 2. Spherically confined aggregates with mobile head groups
J. Phys. Chem. **90**, 1875-1885.

Wright, S.D.; R.A. Ramos; P.S. Tobias; R.J. Ulevitch; J.C. Mathison (1990)
CD14, a receptor for complexes of lipopolysaccharide (LPS) and LPS binding protein
Science **249**, 1431-1433.

Yu, B.; E. Hailman; S.D. Wright (1996)
Lipopolysaccharide binding protein and soluble CD14 catalyze exchange of phospholipids
J. Clin Invest. **99**, 315-24.

Yu, B.; S.D. Wright (1996)
Catalytic properties of lipopolysaccharide (LPS) binding protein
J. Biol Chem. **271**, 4100-4105.

Zabel, P.; F.U. Schade (1993)
Therapiestrategien gegen Mediatoren beim septischen Schock
Immun. Infekt. **21**, 45-50.

Zähringer, U.; B. Lindner; U. Seydel; E.Th. Rietschel; H. Naoki; F.M. Unger; M. Imoto; S. Kusumoto; T. Shiba (1985)
Structure of De-O-acylated lipopolysaccharide from the *Escherichia coli* Re mutant strain F515
Tetrahedron Lett. **26**, 6321-6324.

Zähringer, U.; B. Lindner; E.Th. Rietschel (1994)
Molecular structure of lipid A, the endotoxic center of bacterial lipopolysaccharides
Adv. Carbohydr. Chem. Biochem. **50**, 211-276.

Zanetti, G.; J.-D. Baumgartner; M.-P. Glauser (1997)
Sepsis and septic shock
Schweiz. Med. Wochenschr. **127**, 489-499.

Ziegler, E.J.; H. Douglas; J.E. Sherman; C.E. Davis; A.I. Braude (1973)
Treatment of *E. coli* and *klebsiella* bacteremia in agranulocytic animals with antiserum to a UDP-gal epimerase-deficient mutant.
J. Immunol. **111**, 433-438.

Ziegler, E.J.; J.A. McCutchan; J. Fierer; M.P. Glauser; J.C. Sadoff; H. Douglas; A.I. Braude (1982)
Treatment of Gram-negative bacteremia and shock with human antiserum to a mutant *Escherichia coli*
N. Engl. J. Med. **307**, 1225-1230.

Ziegler, E.J.; C.J. Fisher; C.L. Sprung; R.C. Straube; J.C. Sadoff; G.E. Foulke; C.H. Wortel; M.P. Fink; R.P. Dellinger; N.N.H. Teng; I.E. Allen; H.J. Berger; G.L. Knatterud; A.F. LoBuglio; C.R. Smith & J5 Study group (1991)
Treatment of Gram-negative bacteremia and septic shock with HA-1A human monoclonal antibody against endotoxin
N. Engl. J. Med. **324**, 429-436.

6.2 Glossar

α	Winkel zwischen Membrannormale und C-D-Vektor (s. S_{CD})
e	Dielektrizitätskonstante
γ	Winkel zwischen den Packungsvektoren a und b
p	Kreiskonstante (3,14159265....)
θ	Tiltwinkel der Fettsäureketten
Å	Ångstrom (Längeneinheit, 1 Å entspricht 10^{-10} m bzw. 0,1 nm)
©	eingetragenes Warenzeichen
a	Packungsvektor
b	Packungsvektor
e	Elementarladung (1 *e* entspricht 1,6 ´ 10^{-19} C)
BPI	bakterizides/permeabilitätserhöhendes Protein (bactericidal / permeability-increasing protein)
BSA	Rinderserum-Albumin (bovine serum albumine)
C	Coulomb (Einheit der elektrischen Ladung)
CAP18	kationisches antibakterielles Protein mit einem Molekulargewicht von 18 kDa (Cationic antibacterial Protein, 18 kDa)
CD14	Cluster of differentiation antigen 14 (bei Monozyten)
Core	Kernzuckerbereich
CSD	Kristallstrukturdatenbank (Cambridge Structural Database System)
Da	Dalton (Masseneinheit, ein Wasserstoffatom hat die Masse 1 Dalton)
DLPE	Dilauroylphosphatidylethanolamin
DMPC	Dimyristoylphosphatidylcholin
DPG	1,2-*sn*-Dipalmitoylglycerol
DPPC	1,2-Dipalmitoyl-3-*sn*-phosphatidylcholin
E. coli	*Escherichia coli*
ENP	Endotoxin-neutralisierendes Protein (s. LALF)
EU	Endotoxin Einheiten (endotoxin units, 1 EU/ml entspricht einer LPS-Konzentration von 100 pg/ml)
Glc	*D*-Glucose
GlcN	*D*-Glucosamin (2-Amino-2-desoxy-*D*-glucose)
GlcNac	N-Acetylglucosamin

GPI	Glykosyl-Phosphatidyl-Inositol
HDL	Lipoproteine mit hoher Dichte (High-density lipoprotein)
Hep	L-Glycero-D-*manno*-heptose
HSEA	hard sphere exo-anomeric
IL	Interleukin
in vitro	im Laborexperiment (außerhalb des Körpers)
in vivo	im lebenden Körper
$InsP_3$	myo-Inositol-1,4,5-trisphosphat
Kdo	2-Keto-3-desoxy-octonsäure (systematisch: 3-Desoxy-*D*-*manno*-2-octulosonsäure, dOclA)
$L_{\beta'}$-Phase	feste oder Gel-Phase von Lipiden mit Tiltwinkel > 0°
L_{β}-Phase	feste oder Gel-Phase von Lipiden ohne Tilt
L_{α}-Phase	fluide Phase von Lipiden (liquid-crystalline)
LALF	*Limulus* Anti-LPS-Faktor (s. ENP)
LBP	Lipopolysaccharid-bindendes Protein
LC-Phase	fest-analoge Phase von Monofilmen (liquid-condensed)
LDL	Lipoproteine mit geringer Dichte (Low-density lipoprotein)
LE-Phase	flüssig-analoge Phase von Monofilmen (liquid-expanded)
LPS	Lipopolysaccharid
MAPK	Mitogen-aktivierte Protein-Kinase
mCD 14	membrangebundenes CD 14
MD	Molekulardynamik (-Simulation)
MOF	multiples Organ-Versagen (multi organ failure)
NFκB	Kernfaktor κ B (nuclear factor κ B)
NMR	Kernspinresonanz (Nuclear magnetic resonance)-Spektroskopie
NO	Stickstoffmonoxid
PAF	Plättchen-aktivierender Faktor (platelet activating factor)
PC	Personal computer
PDB	Protein Datenbank (Brookhaven Protein Database)
PMB	Polymyxin B
PMBN	Polymyxin B Nonapeptid

PMN	Polymorphkernige Zellen (polymorphonuclear cells, neutrophile Granulozyten)
POPC	1-Palmitoyl-2-oleoyl-*sn*-glycero-3-phosphatidylcholin
PTK	Protein-Tyrosin-Kinase
QENS	Quasi-elastische Neutronenstreuung
rBPI	rekombinantes BPI (siehe dort)
RcLPS	LPS einer Rauh-Mutante mit reduziertem Core
ReLPS	LPS einer Rauh-Mutante mit minimalem Core
Residuen	(Zucker)-reste, aus denen ein Molekül aufgebaut ist
R-LPS	Rauhes LPS (ohne O-Antigen, u.U. unvollständiger Core)
RMSD	Mittlere Abweichung (root mean square deviation)
S. minnesota	*Salmonella minnesota*
SAS	Oberfläche, die dem Lösungsmittel zugänglich ist (solvent accessible surface)
sCD 14	lösliches (soluble) CD14
S_{CD}	^{2}H-NMR-Ordnungsparameter
S-LPS	Glattes (Wildtyp-) LPS mit vollständigem Core und O-Antigen
TFE	Trifluorethanol
Tilt	Verkippung der Fettsäureketten relativ zur Membrannormalen
TNF-α	Tumor-Nekrose-Faktor α
V_ϕ	Potential der Bindungswinkel
V_ϖ	Potential der uneigentlichen Torsionswinkel (improper torsions)
V_θ	Potential der Torsionswinkel
V_B	Potential der Bindungslängen
VLDL	Lipoproteine mit sehr geringer Dichte (Very-low-density lipoprotein)

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6.4 Lebenslauf

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6.4.1 Schulbildung

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1979 - 86	Theodor-Heuss-Gymnasium, Wolfsburg
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6.4.2 Studium

Oktober 1988	Beginn des Studiums der Biochemie an der Freien Universität Berlin
Oktober 1991	Vordiplom in Biochemie
1994	Anfertigung der Diplomarbeit *Untersuchungen zur Struktur hydratisierter Lipopolysaccharide* in der Arbeitsgruppe von Prof. Dr. Hans Bradaczek
November 1994	Diplom im Studiengang Biochemie
1995 -97	Anfertigung der vorliegenden Dissertation in der Arbeitsgruppe von Prof. H. Dr. Bradaczek am Institut für Kristallographie, Fachbereich Chemie der Freien Universität Berlin

6.4.3 Erwerbstätigkeiten

1986 - 1988	Softwareentwicklung und Betreuung beim Konstruktionsbüro Eckard-Design, Wolfsburg
1989 und 1990	Werkstudent im Produktionsbereich bei der Volkswagen AG, Werk Wolfsburg
1991 - 1992	Messebau für die Firma Schendel & Pawlaczyk, Berlin und Münster
1993 - 1995	Labortätigkeit und Datenerfassung beim DRK-Blutspendedienst, Berlin
1992 - 1994	Studentische Hilfskraft im DFG-Projekt *Elekronendichte-simulationen* bei Prof. Bradaczek, Freie Universität Berlin
1995 - 1997	Wissenschaftlicher Mitarbeiter im DFG-Projekt *Berechnung dreidimensionaler Modelle von unterschiedlich langen bakteriellen Lipopolysacchariden und Beschreibung daraus abgeleiteter Aggregate* bei Prof. Bradaczek, Freie Universität Berlin
ab 1.1.1998	Procter & Gamble Pharmaceuticals Deutschland

6.5 Eigene Publikationen

6.5.1 Artikel

1. P. Mukerjee; M. Kastowsky; S. Obst; K. Takayama (eingeladene Publikation)
   LPS preparations in aqueous media: Implications for solution versus suspension
   In: Endotoxin in Health and Disease; Chapter III: Chemistry and Physical Chemistry of LPS (Hrsg.: H. Brade, D.C. Morrison, S.M. Opal und S.N. Vogel)
   Marcel Dekker Inc., New York, 1998.

2. M. Popescu, A. Lörinczi, F. Sava, P.-J. Koch, S. Obst, T. Gutberlet, W. Uebach, H. Bradaczek, V. Meriacre, C. Turta, S. Zamfira
   Structure of the evaporated films based on triiron complexes with short carboxylate chains
   Rom. J. Phys., angenommen.

3. A. Kuzmin; S. Obst; J. Purans
   X-ray absorption spectroscopy and molecular dynamics studies of Zn^{2+} hydration in aqueous solutions
   J. Phys.: Condens. Matter, 1997, **9**, 10069-78.

4. S. Obst; Hans Bradaczek
   Molecular dynamics simulations of zinc ions in water using CHARMM
   J. Mol. Model. 1997, **3**, 224-32.

5. S. Obst; M. Kastowsky; H. Bradaczek
   Molecular dynamics simulations of six different fully hydrated monomeric conformers of *Escherichia coli* Re-Lipopolysaccharide in the presence and absence of Ca^{2+}
   Biophys. J. 1997, **72**, 1031-46.

6. S. Obst; H. Bradaczek
   Molecular Dynamics Study of the Structure and dynamics of the Hydration Shell of Alkaline and Alkaline-Earth Metal Cations
   J. Phys. Chem. 1996, **100**, 15677-15687.

7. S. Obst; P.-J. Koch; C. Kahle; H. Bradaczek
   Corrosion Induced by Chromosulfuric Acid Influences Pressure Readings from a Wilhelmy Balance Mounted on a Tombak Spring
   Langmuir 1996, **12**, 3527-3528.

6.5.2 Poster und Vorträge

1. S. Obst, H. Bradaczek (P)
   Molecular dynamics simulations of inorganic cations in water using the CHARMM 22 force field
   11. Darmstädter Molecular Modelling Workshop, Darmstadt, 1997.

2. S. Obst (V)
   Molecular Dynamics of fully hydrated ReLPS
   W.S. Middleton Memorial Veterans Hospital, Madison, WI, 1996.

3. M. Popescu, F. Sava, A. Lörinczi, E. Vateva, D. Nesheva, I.N. Mihailescu, P.-J. Koch, S. Obst, H. Bradaczek (P)
   Amorphous Se/CdSe and SiO_x/CdSe multilayers. Preparation and properties
   5th Confererence in Optics 'ROMOPTO', Bukarest, 1997.

4. M. Popescu, A. Lörinczi, F. Sava, E. Skordeva, E. Vateva, A. Andriesh, M. Iovu, V. Verlan, P.-J. Koch, S. Obst, H. Bradaczek (P)
   Modifications induced by ultraviolet light in amorphous chalcogenide films
   Romanian Conference on Advanced Materials 'ROCAM', Bukarest, 1997

5. S. Obst, M. Kastowsky, H. Bradaczek (P)
   Hydration of monomers of Re-lipopolysaccharides of *E. coli* studied by molecular dynamics simulations
   2nd Symposium on Biological Physics, München, 1995.

6. T. Gutberlet, M. Kastowsky, P.-J. Koch, S. Obst, W. Schwenk, H. Bradaczek (P)
   Strukturuntersuchungen von bakteriellen Lipopolysacchariden mittels Röntgendiffraktometrie und molecular modelling Simulationen
   Jahrestagung der Deutschen Gesellschaft für Biophysik, Berlin, 1994.

7. S. Obst, P.-J. Koch, A. Sabisch, M. Kastowsky, T. Gutberlet, H. Bradaczek (P)
   MD-Simulation eines Lipopolysaccharid-Moleküls in einer Wasser-Box
   8. Darmstädter Molecular Modelling Workshop, Darmstadt, 1994.

8. S. Obst, P.-J. Koch, M. Kastowsky, H. Bradaczek (P)
   Molecular modelling studies on isolated, fully solvated molecules of *E. coli* ReLPS and MD simulation of the influence of polymyxin B on ReLPS monolayers
   3rd Conference of the International Endotoxin Society, Helsinki, 1994.
   J. Endotox. Res. 1994, **1** Suppl. 1, A64