

peer reviewed papers

145. H. Lan; E. T. Abualrous; J. Sticht; L. M. A. Fernandez; T. Werk; C. Weise; M. Ballaschk; P. Schmieder; B. Loll; C. Freund; "Exchange catalysis by tapasin exploits conserved and allele-specific features of MHC-I molecules"; *Nat Commun* **12**, 4236 (2021)
[DOI:10.1038/s41467-021-24401-4](https://doi.org/10.1038/s41467-021-24401-4)
144. T. Urbaniak; K. G. Hoffmann; M. H. Glomm; H. Oschkinat; P. Schmieder; K. Koschek; "How solvent-free crosslinking conditions alter the chemistry and topology of hemiketal based polymer networks"; *Polymer* **229**, 123986 (2021)
[DOI:10.1016/j.polymer.2021.123986](https://doi.org/10.1016/j.polymer.2021.123986)
143. N. Kamdem; Y. Roske; D. Kovalskyy; M. O. Platonov; O. Balinskyi; A. Kreuchwig; J. Saupe; L. Fang; A. Diehl; P. Schmieder; G. Krause; J. Rademann; U. Heinemann; W. Birchmeier; H. Oschkinat; "Small-molecule inhibitors of the PDZ domain of Dishevelled proteins interrupt Wnt signalling"; *Magn. Reson.* **2**, 355-374 (2021)
[DOI:10.5194/mr-2-355-2021](https://doi.org/10.5194/mr-2-355-2021)
142. S. Breinlinger; T. J. Phillips; B. N. Haram; J. Mares; J. A. Martinez Yerena; P. Hrouzek; R. Sobotka; W. M. Henderson; P. Schmieder; S. M. Williams; J. D. Lauderdale; H. D. Wilde; W. Gerrin; A. Kust; J. W. Washington; C. Wagner; B. Geier; M. Liebeke; H. Enke; T. H. J. Niedermeyer; S. B. Wilde; "Hunting the eagle killer: A cyanobacterial neurotoxin causes vacuolar myelinopathy"; *Science* **371**, eaax9050 (2021)
[DOI:10.1126/science.aax9050](https://doi.org/10.1126/science.aax9050)
141. E. Dias D'Andrea; J. Sebastian Retel; A. Diehl; P. Schmieder; H. Oschkinat; J. Ricardo Pires; "NMR structure and dynamics of Q4DY78, a conserved kinetoplast-specific protein from *Trypanosoma cruzi*"; *J. Struct. Biol.* **213**, 107715 (2021)
[DOI:10.1016/j.jsb.2021.107715](https://doi.org/10.1016/j.jsb.2021.107715)
140. A. Hauser; E. Poulou; F. Muller; P. Schmieder; C. P. R. Hackenberger; "Synthesis and Evaluation of Non-Hydrolyzable Phospho-Lysine Peptide Mimics"; *Chemistry* **27**, 2326-2331 (2021)

[DOI:10.1002/chem.202003947](https://doi.org/10.1002/chem.202003947)

139. M. Barone; M. Muller; S. Chiha; J. Ren; D. Albat; A. Soicke; S. Dohmen; M. Klein; J. Bruns; M. van Dinther; R. Opitz; P. Lindemann; M. Beerbaum; K. Motzny; Y. Roske; P. Schmieder; R. Volkmer; M. Nazare; U. Heinemann; H. Oschkinat; P. Ten Dijke; H. G. Schmalz; R. Kuhne; "Designed nanomolar small-molecule inhibitors of Ena/VASP EVH1 interaction impair invasion and extravasation of breast cancer cells". *PNAS* **117**, 29684-29690 (2020)

[DOI:10.1073/pnas.2007213117](https://doi.org/10.1073/pnas.2007213117)

138. T. Chilczuk; R. Monson; P. Schmieder; V. Christov; H. Enke; G. Salmond; T.H.J. Niedermeyer*; "Ambigols from the Cyanobacterium *Fischerella ambigua* Increase Prodigiosin Production in *Serratia* spp"; *ACS Chem. Biol.* **15**, 2929 -2936 (2020)

[DOI:10.1021/acscchembio.0c00663](https://doi.org/10.1021/acscchembio.0c00663)

137. J. Clochard; G. Jerz; P. Schmieder; H. Mitdank; M. Tröger; S. Sama; A. Weng*; "A new acetylated triterpene saponin from *Agrostemma githago* L. modulates gene delivery efficiently and shows a high cellular tolerance"; *Int. J. Pharm.* **589**, 119822 (2020)

[DOI:10.1016/j.ijpharm.2020.119822](https://doi.org/10.1016/j.ijpharm.2020.119822)

136. S. Sreeramulu; C. Richter; T. Kuehn; K. Azzaoui; M.J.J. Blommers; R. Del Conte; M. Fragai; N. Trieloff; P. Schmieder; M. Nazaré; E. Specker; V. Ivanov; H. Oschkinat; L. Banci; H. Schwalbe*; "NMR quality control of fragment libraries for screening"; *J. Biomol. NMR* **74**, 555 - 563 (2020)

[DOI:10.1007/s10858-020-00327-9](https://doi.org/10.1007/s10858-020-00327-9)

135. É. Dias D'Andréa; Y. Roske*; G.A.P. de Oliveira; N. Cremer; A. Diehl; P. Schmieder; U. Heinemann; H. Oschkinat; J. Ricardo Pires*; "Crystal Structure of Q4D6Q6, a Conserved Kinetoplastid-Specific Protein From *Trypanosoma Cruzi*"; *J. Struct. Biol.* **211**, 107536 (2020)

[DOI:10.1016/j.jsb.2020.107536](https://doi.org/10.1016/j.jsb.2020.107536)

134. A.L. Baumann; S. Schwagerus; K. Broi; K. Kemnitz-Hassanin; C.E. Stieger; N. Trieloff; P. Schmieder; C.P.R. Hackenberger*; "Chemically induced vinylphosphonothiolate electrophiles for thiol-thiol bioconjugation"; *J. Am. Chem. Soc.* **142**, 9544 - 9552 (2020)

[DOI:10.1021/jacs.0c03426](https://doi.org/10.1021/jacs.0c03426)

133. T. Wiglenda; N. Groenke; W. Hoffmann; C. Manz; L. Diez; A. Buntru; L. Brusendorf, N. Neuendorf; S. Schnoegl; C. Haenig; P. Schmieder; K. Pagel; E.E.Wanker*; "Sclerotiorin stabilizes the assembly of non-fibrillar Abeta42 oligomers with low toxicity, seeding activity and beta-sheet content"; *J. Mol. Biol.* **432**, 2080 -2098 (2020)
[DOI:10.1016/j.jmb.2020.01.033](https://doi.org/10.1016/j.jmb.2020.01.033)
132. L.M. Gerland; D. Friedrich; L. Hopf; E. Donovan; A. Wallmann; N. Erdmann; A. Diehl; M. Bommer, K. Buzar; M. Ibrahim M; **P. Schmieder**; H. Dobbek; A. Zouni; A.N. Bondar; H. Dau; H. Oschkinat*; "pH-Dependent Protonation of Surface Carboxylates in PsbO Enables Local Buffering and Triggers Structural Changes"; *ChemBioChem* **21**, 1597 - 1604 (2020)
[DOI:10.1002/cbic.201900739](https://doi.org/10.1002/cbic.201900739)
131. X-L. Li; L-P. Chi; A. Navarro-Vázquez; S. Hwang; **P. Schmieder**; X-M. Li; X. Li; S-Q. Yang; X. Lei; B-G. Wang; H. Sun*; "Stereochemical Elucidation of Natural Products from Residual Chemical Shift Anisotropies in a Liquid Crystalline Phase"; *J. Am. Chem. Soc.* **142**, 2301 - 2309 (2020)
[DOI:10.1021/jacs.9b10961](https://doi.org/10.1021/jacs.9b10961)
130. M.A. Kasper; M. Glanz; A. Oder; **P. Schmieder**; J.P. von Kries; C.P.R. Hackenberger*; "Vinylphosphonites for Staudinger-induced chemoselective peptide cyclization and functionalization"; *Chem. Sci.* **10**, 6322 - 6329 (2019)
[DOI:10.1039/c9sc01345h](https://doi.org/10.1039/c9sc01345h)
129. R. Driller, M. Ballaschk, **P. Schmieder**, B. Uchanska-Ziegler, A. Ziegler, B. Loll*; "Metal-triggered conformational reorientation of a self-peptide bound to a disease-associated HLA-B*27 subtype"; *J. Biol. Chem.* **294**, 13269 - 13279 (2019)
[DOI:10.1074/jbc.RA119.008937](https://doi.org/10.1074/jbc.RA119.008937)
128. R.K. Harmel; R. Puschmann; M.N. Trung; A. Saiardi; **P. Schmieder**; D. Fiedler*; "Harnessing ¹³C-labeled myo-inositol to interrogate inositol phosphate messengers by NMR"; *Chem. Sci.* **10**, 5267 - 5274 (2019)
[DOI: 10.1039/C9SC00151D](https://doi.org/10.1039/C9SC00151D)
127. C. Kesten; A. Wallmann; R. Schneider; H.E. McFarlane; A. Diehl; G.A. Khan; B.J. van Rossum; E.R. Lampugnani; W.G. Szymanski; N. Cremer; **P. Schmieder**; K.L. Ford; F. Seiter; J.L. Heazlewood; C. Sanchez-

- Rodriguez; H. Oschkinat*; S. Persson*; "The companion of cellulose synthase 1 confers salt tolerance through a Tau-like mechanism in plants"; *Nat. Commun.* **10**, 875 (2019)
[DOI: 10.1038/s41467-019-08780-3](https://doi.org/10.1038/s41467-019-08780-3)
126. R.G. Brinson*; J.P. Marino; F. Delaglio; L.W. Arbogast; R.M. Evans; A. Kearsley; G. Gingras; H. Ghasriani; Y. Aubin; G.K. Pierens; X. Jia; M. Mobli; H.G. Grant; D.W. Keizer; K. Schweimer; J. Stähle; G. Widmalm; E.R. Zartler; C.W. Lawrence; P.N. Reardon; J.R. Cort; P. Xu; F. Ni; S. Yanaka; K. Kato; S.R. Parnham; D. Tsao; A. Blomgren; T. Rundlöf; N. Trieloff; **P. Schmieder**; A. Ross; K. Skidmore; K. Chen; D. Keire; D.I. Freedberg; T. Suter-Stahel; G. Wider; G. Ilc; J. Plavec; S.A. Bradley; D.M. Baldisseri; M.L. Sforça; A.C.M. M Zeri ; J.Y. Wei; C.M. Szabo; C.A. Amezcua; J.B. Jordan; M. Wikström; "Enabling adoption of 2D-NMR for the higher order structure assessment of monoclonal antibody therapeutics"; *mAbs* **11**, 94 - 105 (2019)
[DOI: 10.1080/19420862.2018.1544454](https://doi.org/10.1080/19420862.2018.1544454)
125. T. Utesch; A. de Miguel Catalina; C. Schattenberg; N Paege; **P. Schmieder**; E. Krause; Y. Miao; J.A. McCammon; V. Meyer; S. Jung; M.A. Mroginski*; "A computational modeling approach predicts interaction of the antifungal protein AFP from *Aspergillus giganteus* with fungal membranes via its γ -core motif"; *mSphere* **5**, e00377-18 (2018)
[DOI: 10.1128/mSphere.00377-18](https://doi.org/10.1128/mSphere.00377-18)
124. S. Sama; G. Jerz; **P. Schmieder**; J.F. Joseph; M.F. Melzig; A. Weng*; "Plant derived triterpenes from *Gypsophila elegans* M.Bieb. enable non-toxic delivery of gene loaded nanoplexes"; *J. Biotechnol.* **284**, 131 -139 (2018)
[DOI: 10.1016/j.jbiotec.2018.07.037](https://doi.org/10.1016/j.jbiotec.2018.07.037)
123. J. Schöne; H. Bel Abed ; **P. Schmieder** ; M. Christmann; M. Nazaré*; "A General One-Pot Synthesis of 2H-Indazoles Using an Organophosphorus-Silane System"; *Chemistry* **24**, 9090 - 9100 (2018)
[DOI: 10.1002/chem.201800763](https://doi.org/10.1002/chem.201800763)
122. A. Diehl; Y. Roske; L Ball; A. Chowdhury; M. Hiller; N. Molière; R. Kramer; D. Stöppler; C.L. Worth; B. Schlegel; M. Leidert; N. Cremer; N. Erdmann;

- D. Lopez; H. Stephanowitz; E. Krause; B. van Rossum; **P. Schmieder**; U. Heinemann; K. Turgay; Ü. Akbey; H. Oschkinat*; "Structural changes of TasA in biofilm formation of *Bacillus subtilis*"; *Proc. Natl. Acad. Sci. USA* **115**, 3237-3242 (2018)
[DOI: 10.1073/pnas.1718102115](https://doi.org/10.1073/pnas.1718102115)
121. S. Sama; G. Jerz; **P. Schmieder**; E. Woith; M.F. Melzig; A. Weng*; "Sapofectosid – Ensuring non-toxic and effective DNA and RNA delivery"; *Int. J. Pharm.* **534**, 195 - 205 (2017)
[DOI: 10.1016/j.ijpharm.2017.10.016](https://doi.org/10.1016/j.ijpharm.2017.10.016)
120. S. Muschiol*; S. Erlendsson; M.S. Aschtgen; V. Oliveira; **P. Schmieder**; C. de Lichtenberg; K. Teilum; T. Boesen; U. Akbey; B. Henriques-Normark*; "Structure of the competence pilus major pilin ComGC in *Streptococcus pneumoniae*"; *J. Biol. Chem.* **292**, 14134 -14149 (2017)
[DOI: 10.1074/jbc.M117.787671](https://doi.org/10.1074/jbc.M117.787671)
119. H. Sun; A. Horatscheck; V. Martos; M. Bartetzko; U. Uhrig; D. Lentz; **P. Schmieder***; M. Nazaré*; "Direct Experimental Evidence for Halogen–Aryl π Interactions in Solution from Molecular Torsion Balances"; *Angew. Chem. Int. Ed. Engl.* **56**, 6454 - 6458 (2017); *Angew. Chem.* **129**, 6554 - 6558 (2017)
[DOI: 10.1002/ange.201700520](https://doi.org/10.1002/ange.201700520)
[DOI: 10.1002/anie.201700520](https://doi.org/10.1002/anie.201700520)
118. J. Bertran-Vicente; M. Penkert; O. Nieto-Garcia; J.M. Jeckelmann; **P. Schmieder**; E. Krause; C.P. Hackenberger*; "Chemoselective synthesis and analysis of naturally occurring phosphorylated cysteine peptides"; *Nat. Commun.* **7**, 12703 (2016)
[DOI: 10.1038/ncomms12703](https://doi.org/10.1038/ncomms12703)
117. J. Hanske; S. Aleksic; M. Ballaschk; M. Jurk; E. Shanina; M. Beerbaum; **P. Schmieder**; B.G. Keller; C. Rademacher*; "An intra-domain allosteric network modulates the calcium affinity of the C-type lectin receptor Langerin"; *J. Am. Chem. Soc.* **138**, 12176-12186 (2016)
[DOI: 10.1021/jacs.6b05458](https://doi.org/10.1021/jacs.6b05458)
116. V. Boschert; C. Frisch; J. W. Back; K. van Pee; S. E. Weidauer; E.-M. Muth; **P. Schmieder**; M. Beerbaum; A. Knappik; P. Timmerman; T. D.

- Mueller*; "The sclerostin-neutralizing antibody AbD09097 recognizes an epitope adjacent to sclerostin's binding site for the Wnt co-receptor LRP6"; *Open Biol.* **6**, 160120 (2016)
[DOI: 10.1098/rsob.160120](https://doi.org/10.1098/rsob.160120)
115. E.D. D'Andréa, A. Diehl, **P. Schmieder**, H. Oschkinat, J.R.M. Pires*; "Chemical shift assignments and secondary structure prediction for Q4DY78, a conserved kinetoplastid-specific protein from *Trypanosoma cruzi*"; *Biomol. NMR Assign.* **10**, 325 - 328 (2016)
[DOI: 10.1007/s12104-016-9693-8](https://doi.org/10.1007/s12104-016-9693-8)
114. M. Preisitsch ; S.E. Heiden; M. Beerbaum; T.H.J. Niedermeyer; M. Schneefeld; J. Herrmann; J. Kumpfmüller; A. Thürmer; I. Neidhardt; C. Wiesner; R. Daniel; R. Müller; F.-C. Bange; **P. Schmieder**; T. Schweder; S. Mundt *; "Effects of Halide Ions on the Carbamidocyclophane Biosynthesis in *Nostoc* sp. CAVN2"; *Mar. Drugs.* **14**, 21 (2016)
[DOI: 10.3390/md14010021](https://doi.org/10.3390/md14010021)
113. M. Lehmann; B. Gottschalk; D. Puchkov; P. Schmieder; S. Schwagerus; C. Hackenberger; V. Haucke; J. Schmoranzner*; "Multicolor 'caged' dSTORM resolves the ultrastructure of synaptic vesicles in the brain"; *Angew. Chem.* **127**, 13428 - 13433 (2015); *Angew. Chem. Int. Ed. Engl.* **54**, 13230 - 13235 (2015)
[DOI: 10.1002/ange.201505138](https://doi.org/10.1002/ange.201505138)
[DOI: 10.1002/anie.201505138](https://doi.org/10.1002/anie.201505138)
112. J. Bertran-Vicente; M. Schuemann; P. Schmieder; E. Krause; C.P.R. Hackenberger*; "Direct access of site-specifically phosphorylated-lysine peptides from solid-support"; *Org. Biomol. Chem* **13**, 6839 - 6843 (2015)
[DOI: 10.1039/C5OB00734H](https://doi.org/10.1039/C5OB00734H)
111. R. Opitz; M. Müller; C. Reuter; M. Barone; A. Soicke; Y. Roske; K. Piotukh; P. Huy; M. Beerbaum; B. Wiesner; M. Beyermann; P. Schmieder; C. Freund; R. Volkmer; H. Oschkinat; H.G. Schmalz; R. Kühne*; "A modular toolkit to inhibit proline-rich motif-mediated protein-protein interactions"; *Proc. Natl. Acad. Sci. USA* **112**, 5011-5016 (2015)
[DOI: 10.1073/pnas.1422054112](https://doi.org/10.1073/pnas.1422054112)

110. K. Diesenberg; M. Beerbaum; U. Fink; P. Schmieder; M. Krauss*; "Septin 9 negatively regulates ubiquitin-dependent downregulation of 2 epidermal growth factor receptor"; *J. Cell Sci.* **128**, 397-407 (2015)
[DOI: 10.1242/jcs.162206](https://doi.org/10.1242/jcs.162206)
109. J. Bertran-Vicente; R. Serwa; M. Schuemann; **P. Schmieder**; E. Krause; C.P.R. Hackenberger*; "Site-specifically phosphorylated lysine peptides"; *J. Am. Chem. Soc.* **136**, 13622-13628 (2014)
[DOI: 10.1021/ja507886s](https://doi.org/10.1021/ja507886s)
108. C. Vargas; G. Radziwill; G. Krause; A. Diehl, S. Keller; N. Kamdem; C. Czekelius; A. Kreuchwig; **P. Schmieder**; D. Doyle; K. Moelling; V. Hagen; M. Schade; H. Oschkinat*; "Small-Molecule Inhibitors of AF6 PDZ-Mediated Protein–Protein Interactions"; *ChemMedChem* **9**, 1458 - 1462 (2014)
[DOI: 10.1002/cmdc.201300553](https://doi.org/10.1002/cmdc.201300553)
107. M. Muehlberg; K.D. Siebertz; B. Schlegel; **P. Schmieder**; C. Hackenberger*; "Controlled Thioamide vs. Amide Formation in the Thioacid–Azide Reaction under Acidic Aqueous Conditions"; *Chem. Commun.* **50**, 4603 - 4606 (2014)
[DOI: 10.1039/C4CC00774C](https://doi.org/10.1039/C4CC00774C)
106. T.H.J. Niedermeyer*; **P. Schmieder**; R. Kurmayer; "Isolation of Microcystins from the Cyanobacterium *Planktothrix rubescens* Strain No80"; *Nat. Prod. Bioprospect.* **4**, 37-45 (2014)
[DOI: 10.1007/s13659-013-0001-3](https://doi.org/10.1007/s13659-013-0001-3)
105. Y. Yang; M. Linke; T. von Haimberger; R. Matute; L. González; **P. Schmieder**; K. Heyne*; "Active and silent chromophore isoforms for phytochrome Pr photoisomerization: An alternative evolutionary strategy to optimize photoreaction quantum yields "; *Struct. Dyn.* **1**, 014701 (2014)
[DOI: 10.1063/1.4865233](https://doi.org/10.1063/1.4865233)
104. M. Dorn; M. Jurk; A. Wartenberg; A. Hahn; **P. Schmieder***; "LOV takes a pick: thermodynamic and structural aspects of the Flavin-LOV-Interaction of the blue-light sensitive Photoreceptor YtvA from *Bacillus subtilis*"; *PLoS ONE* **8**, e81268 (2013)
[DOI: 10.1371/journal.pone.0081268](https://doi.org/10.1371/journal.pone.0081268)

103. J. Fiebig; S. Weidauer; L.-Y. Qiu; M. Bauer; **P. Schmieder**; M. Beerbaum; J.-L. Zhang; H. Oschkinat; W. Sebald; T. Mueller*; "The Clip-Segment of the von Willebrand Domain 1 of the BMP Modulator Protein Crossveinless 2 Is Preformed"; *Molecules* **18**, 11658-11682 (2013)
[DOI: 10.3390/molecules181011658](https://doi.org/10.3390/molecules181011658)
102. G. Schäfer; J. Mili; A. Eldahshan; F. Götz; K. Zühlke; C. Schillinger; A. Kreuchwig; J.M. Elkins; K.R. Abdul Azeez; A. Oder; M.C. Moutty; N. Masada; M. Beerbaum; B. Schlegel; S. Niquet; **P. Schmieder**; G. Krause; J.P. v. Kries; D.M.F. Cooper; S. Knapp; J. Rademann; W. Rosenthal; E. Klusmann*; "Highly Functionalized Terpyridines as Competitive Inhibitors of AKAP-PKA Interactions"; *Angew. Chem.* **125**, 12409-12413 (2013); *Angew. Chem. Int. Ed. Engl.* **52**, 12187-12191 (2013)
[DOI: 10.1002/ange.201304686](https://doi.org/10.1002/ange.201304686)
[DOI: 10.1002/anie.201304686](https://doi.org/10.1002/anie.201304686)
101. V. Hack; C. Reuter; R. Opitz; **P. Schmieder**; M. Beyermann; J.-M. Neudörfl; R. Kühne; H.-G. Schmalz*; "Efficient α -Helix Induction in a Linear Peptide Chain by N-Capping with a Bridged-tricyclic Diproline Analogue"; *Angew. Chem.* **125**, 9718-9722 (2013), *Angew. Chem. Int. Ed.* **52**, 9539-9543 (2013)
[DOI: 10.1002/ange.201302014](https://doi.org/10.1002/ange.201302014)
[DOI: 10.1002/anie.201302014](https://doi.org/10.1002/anie.201302014)
100. M. Beerbaum; M. Ballaschk; N. Erdmann; C. Schnick; A. Diehl; B. Uchanska-Ziegler; A. Ziegler; **P. Schmieder***; "NMR spectroscopy reveals unexpected structural variation at the protein-protein interface in MHC class I molecules"; *J. Biomol. NMR* **57**, 167-178 (2013)
[DOI: 10.1007/s10858-013-9777-z](https://doi.org/10.1007/s10858-013-9777-z)
99. P. Schmieder*; F. Nitschke; M. Steup; K. Mallow; E. Specker; "Determination of glucan phosphorylation using heteronuclear ^1H , ^{13}C double and ^1H , ^{13}C , ^{31}P triple-resonance NMR spectra"; *Magn. Reson. Chem.* **51**, 655-661 (2013)
[DOI: 10.1002/mrc.3996](https://doi.org/10.1002/mrc.3996)
98. F. Nitschke; P. Wang; **P. Schmieder**; G.-M. Girard; D.E. Awrey; T. Wang; J. Israelian; X. Zhao; J. Turnbull; M. Heydenreich; E. Kleinpeter; M. Steup; B.A. Minassian*; "Hyperphosphorylation of glucosyl C6 carbons and

- altered structure of glycogen in the neurodegenerative epilepsy Lafora disease"; *Cell Metab.* **17**, 756-767 (2013)
[DOI: 10.1016/j.cmet.2013.04.006](https://doi.org/10.1016/j.cmet.2013.04.006)
97. B. Uchanska-Ziegler*; A. Ziegler; **P. Schmieder**; "Structural and dynamic features of HLA-B27 subtypes"; *Curr. Opin. Rheumatol.* **25**, 411-418 (2013)
[DOI: 10.1097/BOR.0b013e32836203ab](https://doi.org/10.1097/BOR.0b013e32836203ab)
96. M. Jurk; P. Schramm; **P. Schmieder***; "The blue-light receptor YtvA from *Bacillus subtilis* is permanently incorporated into the stressosome independent of the illumination state"; *Biochem. Biophys. Res. Commun.* **432**, 499-503 (2013)
[DOI: 10.1016/j.bbrc.2013.02.025](https://doi.org/10.1016/j.bbrc.2013.02.025)
95. N. Naue; M. Beerbaum; A. Bogutzki; **P. Schmieder**; U. Curth* ; "The helicase-binding domain of *Escherichia coli* DnaG primase interacts with the highly conserved C-terminal region of single-stranded DNA-binding protein"; *Nucleic Acids Res.* **41**, 4507-4517 (2013)
[DOI: 10.1093/nar/gkt107](https://doi.org/10.1093/nar/gkt107)
94. H. Elgabarty; **P. Schmieder**; D. Sebastiani* ; "Unraveling the existence of dynamic water channels in light-harvesting proteins: alpha-C-phycocyanobilin in vitro"; *Chem. Sci.* **4**, 755-763 (2013)
[DOI: 10.1039/c2sc21145a](https://doi.org/10.1039/c2sc21145a)
93. C.S. Hee; M. Beerbaum; B. Loll; M. Ballaschk; **P. Schmieder**; B. Uchanska-Ziegler; A. Ziegler* ; "Dynamics of free versus complexed $\beta(2)$ -microglobulin and the evolution of interfaces in MHC class I molecules"; *Immunogenetics* **65**, 157-172 (2013)
[DOI: 10.1007/s00251-012-0667-4](https://doi.org/10.1007/s00251-012-0667-4)
92. Y. Yang; M. Linke; T. von Haimberger; J. Hahn; R.A. Matute; L. González; **P. Schmieder**; K. Heyne* ; "Real-time tracking of phytochrome's orientational changes during Pr photoisomerization"; *J. Am. Chem. Soc.* **134**, 1408-1411 (2012)
[DOI: 10.1021/ja209413d](https://doi.org/10.1021/ja209413d)
91. Matthias Dorn; Marcel Jurk; **Peter Schmieder***; "Blue News Update: BODIPY-GTP Binds to the Blue-Light Receptor YtvA While GTP Does Not"; *PLoS ONE* **7**, e29201 (2012)

- [DOI: 10.1371/journal.pone.0029201](https://doi.org/10.1371/journal.pone.0029201)
90. C. Hoppmann*; **P. Schmieder**; N. Heinrich; M. Beyermann; "Photoswitchable Click Amino Acids: Light Control of Conformation and Bioactivity"; *ChemBioChem* **12**, 2555-2559 (2011)
[DOI: 10.1002/cbic.201100578](https://doi.org/10.1002/cbic.201100578)
89. M. Jurk; M. Dorn; **P. Schmieder***; "Blue Flickers of Hope: Secondary Structure, Dynamics and Putative Dimerisation Interface of the Blue-Light Receptor YtvA from *Bacillus subtilis*"; *Biochemistry* **50**, 8163-8171 (2011)
[DOI: 10.1021/bi200782j](https://doi.org/10.1021/bi200782j)
88. M. Röben; **P. Schmieder***; "Assignment of phycocyanobilin in HMPT using triple resonance experiments"; *Magn. Reson. Chem.* **49**, 543-548 (2011)
[DOI: 10.1002/mrc.2776](https://doi.org/10.1002/mrc.2776)
87. C. Hoppmann*; **P. Schmieder**; P. Domaing; G. Vogelreiter; J. Eichhorst; B. Wiesner; I. Morano; K. Rück-Braun; M. Beyermann; "Photocontrol of Contracting Muscle Fibers"; *Angew. Chem.* **123**, 7841-7845 (2011); *Angew. Chem. Int. Ed. Engl.* **50**, 7699-7702 (2011)
[DOI: 10.1002/ange.201101398](https://doi.org/10.1002/ange.201101398)
[DOI: 10.1002/anie.201101398](https://doi.org/10.1002/anie.201101398)
86. Z. Fidan; A. Younis; **P. Schmieder**; R. Volkmer*; "Chemical synthesis of the third WW domain of TCERG1 by native chemical ligation"; *J. Pept. Sci.* **17**, 644-649 (2011)
[DOI: 10.1002/psc.1383](https://doi.org/10.1002/psc.1383)
85. R. Linser; M. Dasari; M. Hiller; V. Higman; U. Fink; J.M. Lopez Del Amo; S. Markovic; L. Handel; B. Kessler; **P. Schmieder**; D. Oesterhelt; H. Oschkinat*; B. Reif*; "Proton-Detected Solid-State NMR Spectroscopy of Fibrillar and Membrane Proteins"; *Angew. Chem.* **123**, 4601-4605 (2011); *Angew. Chem. Int. Ed. Engl.* **50**, 4508-4512 (2011)
[DOI: 10.1002/anie.201008244](https://doi.org/10.1002/anie.201008244)
[DOI: 10.1002/ange.201008244](https://doi.org/10.1002/ange.201008244)
84. T. Schmiederer; S. Rausch; M. Valdebenito; Y. Mantri; E. Mösker; T. Baramov; K. Stelmaszyk; **P. Schmieder**; D. Butz; S.I. Müller; K. Schneider; M.H. Baik; K. Hantke; R.D. Süßmuth*; "The *E. coli* Siderophores Enterobactin and Salmochelin Form Six-Coordinate Silicon

- Complexes at Physiological pH"; *Angew. Chem.* **123**, 4317–4321 (2011);
Angew. Chem. Int. Ed. Engl. **50**, 4230-4233 (2011)
[DOI 10.1002/ange.201005792](https://doi.org/10.1002/ange.201005792)
[DOI 10.1002/anie.201005792](https://doi.org/10.1002/anie.201005792)
83. C. Köhler; J.K. Lighthouse; T. Werther; O.M. Andersen; A. Diehl; **P. Schmieder**; J. Du; B.C. Holdener; H. Oschkinat*; "The Structure of MESD45-184 Brings Light into the Mechanism of LDLR Family Folding"; *Structure* **19**, 337-348 (2011)
[DOI: 10.1016/j.str.2010.12.022](https://doi.org/10.1016/j.str.2010.12.022)
82. F. Christian; M. Szaszak; S. Friedl; S. Drewianka; D. Lorenz; A. Goncalves; J. Furkert; C. Vargas; **P. Schmieder**; F. Goetz; K. Zuehlke; M. Moutty; H. Goettert; M. Joshi; B. Reif; H. Haase; I. Morano; S. Grossmann; A. Klukovits; J. Verli; R. Gaspar; C. Noack; M. Bergmann; R. Kass; K. Hampel; D. Kashin; H.G. Genieser; F.W. Herberg; D. Willoughby; D.M. Cooper; G.S. Baillie; M.D. Houslay; J.P. von Kries; B. Zimmermann; W. Rosenthal; E. Klussmann*; "Small molecule AKAP/PKA interaction disruptors that activate PKA interfere with compartmentalized cAMP signaling in cardiac myocytes"; *J. Biol. Chem.* **286**, 9079-9096 (2011)
[DOI: 10.1074/jbc.M110.160614](https://doi.org/10.1074/jbc.M110.160614)
81. S. Asami; **P. Schmieder**; B. Reif*; "High resolution 1H-detected solid-state NMR spectroscopy of protein aliphatic resonances: access to tertiary structure information "; *J. Am. Chem. Soc.* **132**, 15133-15135 (2010)
[DOI: 10.1021/ja106170h](https://doi.org/10.1021/ja106170h)
80. M. Jurk; M. Dorn; A. Kikhney; D. Svergun; W. Gärtner; **P. Schmieder***; "The switch that does not flip - the blue-light receptor YtvA from *Bacillus subtilis* adopts an elongated dimer conformation independent of the activation state as revealed by a combined AUC and SAXS study"; *J. Mol. Biol.* **403**, 78-87 (2010)
[DOI: 10.1016/j.jmb.2010.08.036](https://doi.org/10.1016/j.jmb.2010.08.036)
79. S. Seedorff; C. Appelt; M. Beyermann; **P. Schmieder***; "Design, synthesis, structure and binding properties of PDZ binding, cyclic β -finger peptides"; *Biochem. Biophys. Res. Commun.* **14**, 535-539 (2010).
[DOI: 10.1016/j.bbrc.2010.04.060](https://doi.org/10.1016/j.bbrc.2010.04.060)

78. M. Röben; J. Hahn; E. Klein; T. Lamparter; G. Psakis; J. Hughes; **P. Schmieder***; "NMR Spectroscopic Investigation of Mobility and Hydrogen Bonding of the Chromophore in the Binding Pocket of Phytochrome Proteins"; *ChemPhysChem*. **11**, 1248-1257 (2010)
[DOI: 10.1002/cphc.200900897](https://doi.org/10.1002/cphc.200900897)
77. A. Weng; K. Jenett-Siems; **P. Schmieder**; D. Bachran; C. Bachran; C. Görick; M. Thakur; H. Fuchs; M.F. Melzig*; "A convenient method for saponin isolation in tumour therapy"; *J. Chromatogr. B. Analyt. Technol. Biomed. Life Sci.* **878**, 713-718 (2010)
[DOI: 10.1016/j.jchromb.2010.01.026](https://doi.org/10.1016/j.jchromb.2010.01.026)
76. C. Hoppmann; S. Seedorff; A. Richter; H. Fabian; **P. Schmieder**; K. Rück-Braun; M. Beyermann*; "Light-directed protein binding of a biologically relevant beta-sheet"; *Angew. Chem.* **121**, 6763-6766 (2009); *Angew. Chem. Int. Ed. Engl.* **48**, 6636-6639 (2009)
[DOI: 10.1002/ange.200901933](https://doi.org/10.1002/ange.200901933)
[DOI: 10.1002/anie.200901933](https://doi.org/10.1002/anie.200901933)
75. A. Rutkowska; M. Beerbaum; N. Rajagopalan; J. Fiaux; **P. Schmieder**; G. Kramer; H. Oschkinat; B. Bukau*; "Large-scale purification of ribosome-nascent chain complexes for biochemical and structural studies"; *FEBS Lett.* **583**, 2407-2413 (2009)
[DOI: 10.1016/j.febslet.2009.06.041](https://doi.org/10.1016/j.febslet.2009.06.041)
74. T. Jacso; M. Grote; **P. Schmieder**; E. Schneider; B. Reif; "NMR assignments of the periplasmic loop P2 of the MalF subunit of the maltose ATP binding cassette transporter" *Biomol. NMR Assign.* **3**, 21-23 (2009)
[DOI: 10.1007/s12104-008-9131-7](https://doi.org/10.1007/s12104-008-9131-7)
73. Ahsanullah; **P. Schmieder**; R. Kühne; J. Rademann*; "Metal-free, regioselective triazole ligations that deliver locked cis peptide mimetics"; *Angew. Chem.* **121**, 5143–5147 (2009); *Angew. Chem. Int. Ed. Engl.* **48**, 5042-5045 (2009)
[DOI: 10.1002/ange.200806390](https://doi.org/10.1002/ange.200806390)
[DOI: 10.1002/anie.200806390](https://doi.org/10.1002/anie.200806390)
72. M. Mroginski*; D. von Stetten; F. Escobar; H. Strauss; S. Kaminski; P. Scheerer; M. Günther; D. Murgida; **P. Schmieder**; C. Bongards; W. Gärtner; J. Mailliet; J. Hughes; L.-O. Essen; Peter Hildebrandt*;

- "Chromophore Structure of Cyanobacterial Phytochrome Cph1 in the Pr State: Reconciling Structural and Spectroscopic Data by QM/MM Calculations "; *Biophysical J.* **96**, 4153-4163 (2009)
[DOI: 10.1016/j.bpj.2009.02.029](https://doi.org/10.1016/j.bpj.2009.02.029)
71. T. Jacso; M. Grote; M. Daus; **P. Schmieder**; S. Keller; E. Schneider; B. Reif*; "The periplasmic loop P2 of the MalF subunit of the maltose ATP binding cassette transporter is sufficient to bind the maltose binding protein MalE"; *Biochemistry* **48**, 2216-2225 (2009)
[DOI: 10.1021/bi801376m](https://doi.org/10.1021/bi801376m)
70. S.E. Weidauer; **P. Schmieder**; M. Beerbaum; W. Schmitz; H. Oschkinat; T.D. Müller*; "NMR structure of the Wnt modulator protein Sclerostin"; *Biochem. Biophys. Res. Commun.* **380**, 160-165 (2009)
[DOI: 10.1016/j.bbrc.2009.01.062](https://doi.org/10.1016/j.bbrc.2009.01.062)
69. V. Agarwal; K. Faelber; **P. Schmieder**; B. Reif*; "High-resolution double-quantum deuterium magic angle spinning solid-state NMR spectroscopy of perdeuterated proteins."; *J. Am. Chem. Soc.* **131**, 2-3 (2009)
[DOI: 10.1021/ja803620r](https://doi.org/10.1021/ja803620r)
68. J. Hahn; H.M. Strauss, **P. Schmieder***; "Heteronuclear NMR Investigation on the Structure and Dynamics of the Chromophore Binding Pocket of the Cyanobacterial Phytochrome Cph1"; *J. Am. Chem. Soc.* **130**, 11170-11178 (2008)
[DOI: 10.1021/ja8031086](https://doi.org/10.1021/ja8031086)
67. I. Coin; M. Beerbaum; **P. Schmieder**; M. Bienert; M. Beyermann*; "Solid-Phase Synthesis of a Cyclodepsipeptide: Cotransin"; *Org. Lett.* **10**, 3857-3860 (2008)
[DOI: 10.1021/ol800855p](https://doi.org/10.1021/ol800855p)
66. C. Appelt; A. Wessolowski; M. Dathe; **P. Schmieder***; "Structures of cyclic, antimicrobial peptides in a membrane-mimicking environment define requirements for activity"; *J. Pept. Sci.* **14**, 524-527 (2008)
[DOI: 10.1002/psc.924](https://doi.org/10.1002/psc.924)
65. I. Coin; **P. Schmieder**; M. Bienert; M. Beyermann*; "The depsipeptide technique applied to peptide segment condensation: Scope and limitations"; *J. Pept. Sci.* **14**, 299-306 (2008)
[DOI: 10.1002/psc.928](https://doi.org/10.1002/psc.928)

64. C. Koehler; S. Bishop; E. F. Dowler; **P. Schmieder**; A. Diehl; H. Oschkinat; L.J. Ball; "Backbone and sidechain ^1H , ^{13}C and ^{15}N resonance assignments of the Bright/ARID domain from the human JARID1C (SMCX) protein" *Biomol. NMR Assign.* **2**, 9-11 (2008)
[DOI: 10.1007/s12104-007-9071-7](https://doi.org/10.1007/s12104-007-9071-7)
63. M. Hupfer*; S. Glöß; **P. Schmieder**; H.-P. Grossart; "Methods for Detection and Quantification of Polyphosphate and Polyphosphate Accumulating Microorganisms in Aquatic Sediments"; *Int. Rev. Hydrobiol.* **93**, 1-30 (2008)
[DOI: 10.1002/iroh.200610935](https://doi.org/10.1002/iroh.200610935)
62. J. Hahn; R. Kühne; **P. Schmieder***; " ^{15}N solution-state NMR study of α -C-phycoerythrin. Implications for the structure of the chromophore binding pocket of the cyanobacterial phytochrome Cph1"; *ChemBioChem* **8**, 524-2249-2255 (2007)
[DOI: 10.1002/cbic.200700256](https://doi.org/10.1002/cbic.200700256)
61. I. Scholz; S. Jehle; **P. Schmieder**; M. Hiller; F. Eisenmenger; H. Oschkinat, B.J. van Rossum*; "J-deconvolution using maximum entropy reconstruction applied to ^{13}C - ^{13}C solid state CP MAS NMR of proteins"; *J. Am. Chem. Soc.* **129**, 6682-6683 (2007)
[DOI: 10.1021/ja070849g](https://doi.org/10.1021/ja070849g)
60. E.F. Dowler; A. Diehl; **P. Schmieder**; C. Brockmann; J. Elkins; M. Soundararajan; H. Oschkinat; L.J. Ball; "Backbone and sidechain ^1H , ^{13}C , ^{15}N resonance assignment of the RGS domain of human RGS14" *Biomol. NMR Assign.* **1**, 95-97 (2007)
[DOI: 10.1007/s12104-007-9029-9](https://doi.org/10.1007/s12104-007-9029-9)
59. C. Appelt; A.K. Schrey; J.A. Söderhäll; **P. Schmieder**; "Design of antimicrobial compounds based on peptide structures"; *Bioorg. Med. Chem. Lett.* **17**, 2334-2337 (2007)
[DOI: 10.1016/j.bmcl.2007.01.075](https://doi.org/10.1016/j.bmcl.2007.01.075)
58. O.Y. Fedorov; V.A. Higman; **P. Schmieder**; M. Leidert; A. Diehl; J. Elkins; M. Soundararajan; H. Oschkinat; L.J. Ball; "Resonance assignment of the RGS domain of human RGS10" *J. Biomolec. NMR* **38**, 191 (2007)
[DOI: 10.1007/s10858-006-9111-0](https://doi.org/10.1007/s10858-006-9111-0)

-
57. C. Köhler C; O.M. Andersen; A. Diehl; G. Krause; **P. Schmieder**; H. Oschkinat*; "The solution structure of the core of mesoderm development (MESD), a chaperone for members of the LDLR-family"; *J. Struct. Funct. Genomics* **7**, 133-138 (2006)
[DOI: 10.1007/s10969-007-9016-5](https://doi.org/10.1007/s10969-007-9016-5)
56. T. Rohmer; H. Strauss; J. Hughes; H. de Groot; W. Gärtner; **P. Schmieder**; J. Matysik*; "15N MAS NMR studies of Cph1 phytochrome: chromophore dynamics and intramolecular signal transduction"; *J. Chem. Phys. B* **110**, 20580-20585 (2006)
[DOI: 10.1021/jp062454+](https://doi.org/10.1021/jp062454+)
55. T.-T. Mac; M. Beyermann; J.R. Pires; **P. Schmieder**; H. Oschkinat*; "High yield expression and purification of isotopically labelled human endothelin-1 for use in NMR studies"; *Protein Expr. Purif.* **48**, 253-260 (2006)
[DOI: 10.1016/j.pep.2006.01.022](https://doi.org/10.1016/j.pep.2006.01.022)
54. T. Neuhof; **P. Schmieder**; M. Seibold; K. Preussel; H. von Döhren*; "Hassallidin B - Second antifungal member of the Hassallidin family"; *Bioorg Med Chem Lett.* **16**, 4220-4222 (2006)
[DOI: 10.1016/j.bmcl.2006.05.094](https://doi.org/10.1016/j.bmcl.2006.05.094)
53. M. Joshi; C. Vargas; P. Boisguerin; A. Diehl; G. Krause; **P. Schmieder**; K. Moelling; V. Hagen; M. Schade; H. Oschkinat*; "Discovery of low-molecular-weight ligands for the AF6 PDZ domain"; *Angew. Chem.* **118**, 3874–3879 (2006), *Angew. Chem. Int. Ed. Engl.* **45**, 3790-3795 (2006)
[DOI: 10.1002/ange.200503965](https://doi.org/10.1002/ange.200503965)
[DOI: 10.1002/anie.200503965](https://doi.org/10.1002/anie.200503965)
52. J. Hahn*; H. Strauss; F. Landgraf; H. Faus Gimenez; G. Lochnit; **P. Schmieder**; J. Hughes; "Probing protein-chromophore interactions in Cph1 phytochrome via mutagenesis"; *FEBS J.* **273**, 1415-1429 (2006)
[DOI: 10.1111/j.1742-4658.2006.05164.x](https://doi.org/10.1111/j.1742-4658.2006.05164.x)
51. C. Appelt; F. Eisenmenger; R. Kühne; **P. Schmieder**; J.A. Söderhäll*; "Interaction of the antimicrobial peptide cyclo(RRWRF) with membranes by molecular dynamics simulations"; *Biophys. J.* **89**, 2296-2306 (2005)
[DOI: 10.1529/biophysj.105.063040](https://doi.org/10.1529/biophysj.105.063040)
-

-
50. C. Appelt; A. Wessolowski; J. A. Söderhäll; M. Dathe; **P. Schmieder***; "Structure of the antimicrobial, cationic hexapeptide cyclo(RRWRF) and its analogs in solution and bound to detergent micelles"; *ChemBioChem* **6**, 1654-1662 (2005)
[DOI: 10.1002/cbic.200500095](https://doi.org/10.1002/cbic.200500095)
49. H.M. Strauss*; **P. Schmieder**; J. Hughes; "Light-dependent dimerisation in the N-terminal sensory module of cyanobacterial phytochrome 1 (Cph1 Δ 2)"; *FEBS Lett.* **579**, 3970-3974 (2005)
[DOI: 10.1016/j.febslet.2005.06.025](https://doi.org/10.1016/j.febslet.2005.06.025)
48. D. Leitner; M. Wahl; D. Labudde; G. Krause; A. Diehl; **P. Schmieder**; J.R. Pires; M. Fossi; U. Wiedemann; M. Leidert; H. Oschkinat*; "The solution structure of an N-terminally truncated version of the yeast CDC24p PB1 domain shows a different beta-sheet topology"; *FEBS Lett.* **579**, 3534-3538 (2005)
[DOI: 10.1016/j.febslet.2005.05.025](https://doi.org/10.1016/j.febslet.2005.05.025)
47. H.M. Strauss; J. Hughes; **P. Schmieder***; "Heteronuclear solution-state NMR studies of the chromophore in cyanobacterial phytochrome Cph1"; *Biochemistry* **44**, 8244-8250 (2005)
[DOI: 10.1021/bi050457r](https://doi.org/10.1021/bi050457r)
46. T. Neuhof; **P. Schmieder**; K. Preussel; R. Dieckmann; H. Pham; F. Bartl; H. von Döhren*; "Hassallidin, a Glycosylated Lipopeptide with Antifungal Activity from the Cyanobacterium *Hassallia* sp."; *J. Nat. Prod.* **68**, 695-700 (2005)
[DOI: 10.1021/np049671r](https://doi.org/10.1021/np049671r)
45. M. Schubert; D. Labudde; D. Leitner; H. Oschkinat; **P. Schmieder***; "A modified strategy for sequence specific assignment of protein NMR spectra based on amino acid type selective experiments"; *J. Biomolec. NMR* **31**, 115-128 (2005)
[DOI: 10.1007/s10858-004-8263-z](https://doi.org/10.1007/s10858-004-8263-z)
44. O.J. Gaiser; L.J. Ball*; **P. Schmieder**; D. Leitner; H. Strauss; M. Wahl; R. Kühne; H. Oschkinat; U. Heinemann; "Solution Structure, Backbone Dynamics, and Association Behavior of the C-Terminal BRCT Domain from the Breast Cancer-Associated Protein BRCA1"; *Biochemistry* **43**, 15983-15995 (2004)
-

[DOI: 10.1021/bi049550g](https://doi.org/10.1021/bi049550g)

43. C. Brockmann; A. Diehl; K. Rehbein; H. Strauss; **P. Schmieder**; B. Korn; R. Kühne; H. Oschkinat*; "The oxidized subunit b8 from human complex I adopts a thioredoxin fold"; *Structure* **12**, 1645-1654 (2004)

[DOI: 10.1016/j.str.2004.06.021](https://doi.org/10.1016/j.str.2004.06.021)

42. J.D. Kahmann; D.A. Wecking; V. Putter; K. Lowenhaupt; Y.G. Kim; **P. Schmieder**; H. Oschkinat; A. Rich; M. Schade*; "The solution structure of the N-terminal domain of E3L shows a tyrosine conformation that may explain its reduced affinity to Z-DNA in vitro"; *Proc. Natl. Acad. Sci. USA* **101**, 2712-2717 (2004)

[DOI: 10.1073/pnas.0308612100](https://doi.org/10.1073/pnas.0308612100)

41. M. Hupfer*; B. Rube, **P. Schmieder**; "Origin and diagenesis of polyphosphate in lake sediments: A ³¹P-NMR study"; *Limnol. Oceanogr.* **49**, 1-10 (2004)

[DOI: 10.4319/lo.2004.49.1.0001](https://doi.org/10.4319/lo.2004.49.1.0001)

40. L. Otte; U. Wiedemann; B. Schlegel; J.R. Pires; M. Beyermann; **P. Schmieder**; G. Krause; R. Volkmer-Engert; J. Schneider-Mergener; H. Oschkinat*; "WW domain sequence activity relationships identified using ligand recognition propensities of 42 WW domains"; *Prot. Sci.* **12**, 491-500 (2003)

[DOI: 10.1110/ps.0233203](https://doi.org/10.1110/ps.0233203)

39. M. Schubert; D. Labudde*; H. Oschkinat; **P. Schmieder***; "A software tool for the prediction of Xaa-Pro peptide bond conformations in proteins based on ¹³C chemical shift statistics"; *J. Biomolec. NMR* **24**, 149-154 (2002)

[DOI: 10.1023/A:1020997118364](https://doi.org/10.1023/A:1020997118364)

38. M. Schubert; M. Kolbe; B. Kessler; D. Oesterhelt; **P. Schmieder***; "Heteronuclear multidimensional NMR-spectroscopy of solubilized membrane proteins: Resonance assignment of native bacteriorhodopsin"; *ChemBioChem* **3**, 1019-1023 (2002)

[DOI: 10.1002/1439-7633\(20021004\)3:10<1019::AID-CBIC1019>3.0.CO;2-C](https://doi.org/10.1002/1439-7633(20021004)3:10<1019::AID-CBIC1019>3.0.CO;2-C)

37. H. Patzelt; B. Simon; A. terLaak; B. Kessler; R. Kühne; **P. Schmieder**; D. Oesterhelt*; H. Oschkinat*; "The structure of the active center in dark-

- adapted Bacteriorhodopsin by solution-state NMR spectroscopy"; *Proc. Natl. Acad. Sci. USA* **99**, 9765-9770 (2002)
[DOI: 10.1073/pnas.132253899](https://doi.org/10.1073/pnas.132253899)
36. M.J.S. Kelly*; L.J. Ball; C. Krieger; Y. Yu; M. Fischer; S. Schiffmann, **P. Schmieder**; R. Kühne; W. Bermel; A. Aacher, G. Richter; H. Oschkinat*; "The NMR Structure of the 47 kDa Dimeric Enzyme 3,4-Dihydroxy-2-Butanone-4-Phosphate Synthase and the Ligand Binding Studies Reveal the location of the active site"; *Proc. Natl. Acad. Sci. USA* **98**, 13025-13030 (2001)
[DOI: 10.1073/pnas.231323598](https://doi.org/10.1073/pnas.231323598)
35. M. Schubert; H. Oschkinat; **P. Schmieder***; "MUSIC and aromatic residues: Amino acid type-selective ^1H - ^{15}N correlations, part III"; *J. Magn. Reson.* **153**, 186-192 (2001)
[DOI: 10.1006/jmre.2001.2447](https://doi.org/10.1006/jmre.2001.2447)
34. M. Schubert; H. Oschkinat; **P. Schmieder***; "Amino acid type-selective ^1H - ^{15}N correlations for Arg and Lys"; *J. Biomolec. NMR* **20**, 379-384 (2001)
[DOI: 10.1023/A:1011206131623](https://doi.org/10.1023/A:1011206131623)
33. M. Schubert; H. Oschkinat; **P. Schmieder***; "MUSIC, selective pulses and tuned delays: Amino acid type-selective ^1H - ^{15}N correlations, part II"; *J. Magn. Reson.* **148**, 61-72 (2001)
[DOI: 10.1006/jmre.2000.2222](https://doi.org/10.1006/jmre.2000.2222)
32. L.J. Ball; R. Kühne; **P. Schmieder**; B. Hoffmann; R. Volkmer-Engert; J. Schneider-Mergener; A. Häfner; M. Hof; M. Wahl; U. Walter; H. Oschkinat*; T. Jarchau; "Dual epitope recognition by the VASP EVH1 domain modulates polyproline ligand specificity and binding affinity"; *EMBO J.* **19**, 4903-4914 (2000)
[DOI: 10.1093/emboj/19.18.4903](https://doi.org/10.1093/emboj/19.18.4903)
31. M. Schubert; L. Ball; H. Oschkinat; **P. Schmieder***; "Bridging the gap: A set of selective ^1H - ^{15}N correlations to link sequential neighbors of proline"; *J. Biomolec. NMR* **17**, 331-335 (2000)
[DOI: 10.1023/A:1008362904205](https://doi.org/10.1023/A:1008362904205)

-
30. E. Krause*; M. Bienert; **P. Schmieder**; H. Wenschuh; "The helix-destabilizing propensity scale of D-amino acids: the influence of side chain steric effects"; *J. Am. Chem. Soc.* **122**, 4865-4870 (2000)
[DOI: 10.1021/ja9940524](https://doi.org/10.1021/ja9940524)
29. M. Schade; C.J. Turner; R. Kühne; **P. Schmieder**; K. Lowenhaupt, A. Herbert; A. Rich*; H. Oschkinat; "The solution structure of the Z α domain of the human RNA editing enzyme ADAR1 reveals a prepositioned binding surface for Z-DNA"; *Proc. Natl. Acad. Sci. USA* **96**, 12465-12470 (1999)
[DOI: 10.1073/pnas.96.22.12465](https://doi.org/10.1073/pnas.96.22.12465)
28. M. Schubert; M. Smalla; **P. Schmieder***; H. Oschkinat; "MUSIC in triple resonance experiments: Amino acid type selective ^1H - ^{15}N correlations"; *J. Magn. Reson.* **141**, 34-43 (1999)
[DOI: 10.1006/jmre.1999.1881](https://doi.org/10.1006/jmre.1999.1881)
27. M. Smalla; **P. Schmieder**; M. Kelly; A. ter Laak; G. Krause; L. Ball; M. Wahl; P. Bork; H. Oschkinat*; "Solution structure of the receptor tyrosine kinase EphB2 SAM domain and identification of two distinct homotypic interaction sites"; *Prot. Sci.* **8**, 1954-1961 (1999)
[DOI: 10.1110/ps.8.10.1954](https://doi.org/10.1110/ps.8.10.1954)
26. M.J.S. Kelly*; C. Krieger; L.J. Ball; Y. Yu; G. Richter; **P. Schmieder**; A. Bacher; H. Oschkinat*; "Application of amino acid type-specific ^1H and ^{14}N -labeling in a ^2H -, ^{15}N -labeled background to a 47 kDa homodimer: potential for NMR structure determination of large proteins"; *J. Biomolec. NMR* **14**, 79-83 (1999)
[DOI: 10.1023/A:1008351606073](https://doi.org/10.1023/A:1008351606073)
25. **P. Schmieder***; M. Leidert; M.J.S. Kelly; H. Oschkinat; "Multiplicity-selective coherence transfer steps for the design of amino-acid selective experiments - a triple resonance experiment selective for Asn and Gln"; *J. Magn. Reson.* **131**, 199-201 (1998)
[DOI: 10.1006/jmre.1997.1348](https://doi.org/10.1006/jmre.1997.1348)
24. J. Schultz; U. Hoffmüller; G. Krause; J. Ashurst; M.J. Macias; **P. Schmieder**; J. Schneider-Mergener; H. Oschkinat*; "Specific interactions
-

- between the syntrophin PDZ domain and voltage-gated sodium channels"; *Nat. Struc. Biol.* **5**, 19-24 (1998)
[DOI: 10.1038/nsb0198-19](https://doi.org/10.1038/nsb0198-19)
23. **P. Schmieder**; A.S. Stern; G. Wagner; J.C. Hoch*; "Quantification of Maximum-Entropy Spectrum Reconstructions"; *J. Magn. Reson.* **125**, 332-339 (1997)
[DOI: 10.1006/jmre.1997.1117](https://doi.org/10.1006/jmre.1997.1117)
22. J-X. Yang, A. Krezel, **P. Schmieder**, G. Wagner, T.F. Havel*; "An evaluation of least-square fits to COSY spectra as a means of estimating proton-proton coupling constants: II. Application to polypeptides"; *J. Biomolec. NMR* **4**, 827-844 (1994)
[DOI: 10.1007/BF00398412](https://doi.org/10.1007/BF00398412)
21. **P. Schmieder**; A.S. Stern; G. Wagner; J.C. Hoch*; "Improved resolution in triple-resonance spectra by non-linear sampling in the constant time domain"; *J. Biomolec. NMR* **4**, 483-490 (1994)
[DOI: 10.1007/BF00156615](https://doi.org/10.1007/BF00156615)
20. **P. Schmieder**; A.S. Stern; G. Wagner; J.C. Hoch*; "Application of non-linear sampling schemes to COSY-type spectra"; *J. Biomolec. NMR* **3**, 569-576 (1993)
[DOI: 10.1007/BF00174610](https://doi.org/10.1007/BF00174610)
19. W. Schüler; U. Christians; **P. Schmieder**; H.-M. Schiebel; I. Holz; K.-F. Sewing; H. Kessler*; "Structural investigation of 13-O-Demethyl-FK506 and its isomers generated by in-vivo metabolism of FK506 Using Human-Liver Microsomes"; *Helv. Chim. Acta* **76**, 2288-2302 (1993)
[DOI: 10.1002/hlca.19930760614](https://doi.org/10.1002/hlca.19930760614)
18. **P. Schmieder**; J.H. Ippel; H. van den Elst; G.A. van der Marel; J.H. van Boom; C. Altona; H. Kessler*; "Heteronuclear NMR of DNA with the heteronucleus in natural abundance: Facilitated assignment and extraction of coupling constants"; *Nucleic Acids Res.* **20**, 4747-4751 (1992)
[DOI: 10.1093/nar/20.18.4747](https://doi.org/10.1093/nar/20.18.4747)

17. **P. Schmieder**; H. Kessler*; "Determination of the ϕ -angle in a peptide-backbone by NMR-spectroscopy with a combination of homonuclear and heteronuclear coupling constants"; *Biopolymers* **32**, 435-440 (1992)
[DOI: 10.1002/bip.360320421](https://doi.org/10.1002/bip.360320421)
16. M. Kurz; **P. Schmieder**; H. Kessler*; "HETLOC, an Efficient Method for Determining Heteronuclear Long-Range Couplings with Heteronuclei in Natural Abundance"; *Angew. Chem.* **103**, 1341-1342 (1991), *Angew. Chem. Int. Ed. Engl.* **30**, 1329-1331 (1991)
[DOI: 10.1002/anie.199113291](https://doi.org/10.1002/anie.199113291)
[DOI: 10.1002/ange.19911031012](https://doi.org/10.1002/ange.19911031012)
15. D. F. Mierke; **P. Schmieder**; P. Karuso; H. Kessler*; "Conformational Analysis of the Cis and Trans Isomers of FK506 from NMR and Molecular Dynamics"; *Helv. Chim. Acta* **74**, 1027-1047 (1991)
[DOI: 10.1002/hlca.19910740513](https://doi.org/10.1002/hlca.19910740513)
14. D. Seebach*; S.Y. Ko; H. Kessler; M. Köck; M. Reggelin; **P. Schmieder**; M.D. Walkinshaw; D. Bevec; "Thiocyclosporins : Preparation, Conformation and Structure-activity Relationship"; *Helv. Chim. Acta* **74**, 1953-1990 (1991)
[DOI: 10.1002/hlca.19910740833](https://doi.org/10.1002/hlca.19910740833)
13. **P. Schmieder**; M. Kurz; H. Kessler*; "Determination of Heteronuclear Long Range Couplings to Heteronuclei in Natural Abundance by Two- and Three-dimensional NMR Spektroskopie"; *J. Biomolec. NMR* **1**, 403-420 (1991)
[DOI 10.1007/BF02192863](https://doi.org/10.1007/BF02192863)
12. **P. Schmieder**; V. Thanabal; L. P. McIntosh; F. W. Dahlquist; G. Wagner*; "Measurement of small H^{α} - H^N Vicinal Coupling Constants in T4 Lysozyme with a new 3D 1H - ^{15}N - ^{13}C Quadruple Resonance NMR Experiment"; *J. Am. Chem. Soc.* **113**, 6323-6324 (1991)
[DOI: 10.1021/ja00016a088](https://doi.org/10.1021/ja00016a088)
11. G. Wagner*; **P. Schmieder**; V. Thanabal; "A new 1H - ^{15}N - ^{13}C Triple Resonance Experiment for Sequential Assignments and Measuring Homonuclear H^{α} - H^N Vicinal Coupling Constants in Polypeptides"; *J. Magn. Reson.* **93**, 436-440 (1991)

- [DOI: 10.1016/0022-2364\(91\)90022-L](https://doi.org/10.1016/0022-2364(91)90022-L)
10. **P. Schmieder**; T. Dohmke; D.G. Norris; M. Kurz; H. Kessler; D. Leibfritz*; "Editing of Multiplicity in Two- and Three-dimensional Heteronuclear NMR Spectroscopy by Fourier Transform of the Pulse Angle Dependency"; *J. Magn. Reson.* **93**, 430-435 (1991)
- [DOI: 10.1016/0022-2364\(91\)90021-K](https://doi.org/10.1016/0022-2364(91)90021-K)
9. **P. Schmieder**; S. Zimmer; H. Kessler*; "Increased Resolution in Proton Detected Heteronuclear NMR Experiments by Folding in the Carbon Dimension"; *Magn. Reson. Chem.* **29**, 375-380 (1991)
- [DOI: 10.1002/mrc.1260290415](https://doi.org/10.1002/mrc.1260290415)
8. H. Kessler*; **P. Schmieder**; "Heteronuclear 2D and 3D NMR Spectroscopy of Carbon-13 in Natural Abundance by Multiplicity Selection and Editing - Application to Peptides"; *Biopolymers* **31**, 621-629 (1991)
- [DOI: 10.1002/bip.360310606](https://doi.org/10.1002/bip.360310606)
7. H. Kessler*; **P. Schmieder**; M. Koeck; M. Reggelin; "Selection of Methyl Resonances in Proton Detected Heteronuclear Shift Correlation, the HMQC"; *J. Magn. Reson.* **91**, 375-379 (1991)
- [DOI: 10.1016/0022-2364\(91\)90199-4](https://doi.org/10.1016/0022-2364(91)90199-4)
6. H. Kessler*; **P. Schmieder**; H. Oschkinat; "3D Heteronuclear NMR Techniques for Carbon-13 in Natural Abundance"; *J. Am. Chem. Soc.* **112**, 8599-8600 (1990)
- [DOI: 10.1021/ja00179a064](https://doi.org/10.1021/ja00179a064)
5. **P. Schmieder**; H. Kessler; H. Oschkinat*; "Fast Heteronuclear 3D NMR Spectroscopy", *Angew. Chem.* **102**, 588-589 (1990), *Angew. Chem. Int. Ed. Engl.* **29**, 546-548 (1990)
- [DOI: 10.1002/anie.199005461](https://doi.org/10.1002/anie.199005461)
- [DOI: 10.1002/ange.19901020534](https://doi.org/10.1002/ange.19901020534)
4. H. Kessler*; **P. Schmieder**; M. Köck; M. Kurz; "Improved Resolution in Proton-Detected Heteronuclear Long-Range Correlation"; *J. Magn. Reson.* **88**, 615-618 (1990)
- [DOI: 10.1016/0022-2364\(90\)90293-I](https://doi.org/10.1016/0022-2364(90)90293-I)
3. H. Kessler*; **P. Schmieder**; W. Bermel; "Complete Assignment of the Non-Carbonylic Carbon-13 Resonances of Tendamistat"; *Biopolymers* **30**, 465-475 (1990)

[DOI: 10.1002/bjp.360300323](https://doi.org/10.1002/bjp.360300323)

2. H. Kessler*; G. Gemmecker; M. Köck; R. Osowski; **P. Schmieder**;
"Improvement of Carbon Detected H,H-TOCSY Experiments by
Employing a DEPT-Transfer"; *Magn. Reson. Chem.* **28**, 62-67 (1990)

[DOI: 10.1002/mrc.1260280112](https://doi.org/10.1002/mrc.1260280112)

1. H. Kessler*; **P. Schmieder**; M. Kurz; "Implementation of the DEPT-
Sequence in Inverse Shift Correlation, the DEPT-HMQC"; *J. Magn.
Reson.* **85**, 400-405 (1989)

[DOI: 10.1016/0022-2364\(89\)90153-4](https://doi.org/10.1016/0022-2364(89)90153-4)

patents

T. Neuhof; R. Dieckmann; H.v. Döhren; K. Preussel; M. Seibold; **P. Schmieder**;
"Lipopeptides having pharmaceutical activity"; Europäisches Patent,
EP05004582, Anm.Tag 02.03.2005

D. Labudde; D. Leitner; H. Oschkinat; **P. Schmieder**; M. Schubert; R. Winter;
"Vorrichtung und Verfahren zur Zuordnung der NMR-Signale von
Polypeptiden"; Dt. Patent, Aktenzeichen 101 44 661.6, Anm.Tag 11.09.2001

other papers

28. A. Ziegler; M. Beerbaum; M. Ballaschk; N. Erdmann; C. Schnick; A. Diehl;
B. Uchanska-Ziegler; **P. Schmieder***; "NMR spectroscopy reveals
unexpected structural variation at the protein-protein interface in MHC
class I molecules" *Hum. Immunol.* **74**, S24 (2013)
 27. M. Hupfer*; C. Herzog; **P. Schmieder**; "Sedimentation and diagenetic
transformation of particulate organic phosphorus in a stratified eutrophic
lake" *Verh. Internat. Verein. Limnol.* **30**, 1389-1392 (2010)
 26. K. Heyne*; Y. Yang; M. Linke; J.; **P. Schmieder**; "Determination of the
Isomerization Dynamics and Transient Ring D Orientation Changes of the
Phytochrome P_{fr} form in Solution by Polarization Resolved Femtosecond
VIS Pump - IR Probe Spectroscopy" *Biophysical J.* **98**, 743a-744a (2010)
 25. C. Hoppmann; S. Seedorff; A. Richter; H. Fabian; **P. Schmieder**; K. Rück-
Braun; M. Beyermann; "Regulation of protein binding by photoswitchable
peptides" *Biopolymers* **92**, 296 (2009)
 24. I. Coin; **P. Schmieder**; M. Bienert; M. Beyermann; "The depsipeptide
technique for the solid phase peptide synthesis: from stepwise assembly
to segment condensation" *Adv. Exp. Med. Biol.* **611**, 127-128 (2009)
 23. I. Coin; **P. Schmieder**; M. Bienert; M. Beyermann; "The depsipeptide
technique for the solid phase peptide synthesis: from stepwise assembly
to segment condensation" *Biopolymers* **88**, 565 (2007)
-

22. **P. Schmieder**; "Multidimensional NMR"; in *Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine*, D. Ganten and K. Ruckpaul (Eds.), Springer, 1204-1208 (2006)
21. T. Neuhof; **P. Schmieder**; M. Seibold; K. Preussel; H. von Döhren*; "Hassallidin B - Second antifungalmember of the Hassallidin family "; *ChemInform* **37**, 51-191 (2006)
20. **P. Schmieder**; "NMR in the structure elucidation of natural products - the Hassalidins"; in *Metalloproteine und Metalloidproteine*, A. Kyriakopoulos, B. Michalke, A. Graebert and D. Behne (Eds.), Herbert Utz Verlag München, 25-31 (2006)
19. C. Appelt; F. Eisenmenger; **P. Schmieder**; R. Kühne; A. Söderhäll; „Antimicrobial Peptide Induces Lethal Membrane Order and Strain: a combined Molecular Dynamics and NMR Investigation“; in *QSAR and Molecular Modelling in Rational Design of Bioactive Molecules*, E. Aki and I. Yalcin (Eds.), Computer Aided Drug Design & Development Society in Turkey, 302-303 (2005)
18. **P. Schmieder**; “Aminosäuretyp-selektive NMR Experimente für die automatische Zuordnung von Protein-NMR-Spektren”; in *Metalloproteine und Metalloidproteine*, A. Kyriakopoulos and D. Behne (Eds.), Wissenschaftliche Verlagsgesellschaft mbH Stuttgart, 15-20 (2004)
17. M. Dathe, H. Nikolenko, A. Wessolowski, **P. Schmieder**, M. Beyermann, and M. Bienert; "The Membrane Activity and Selectivity of Linear and Cyclic Hexapeptides" *J. Liposome Res.* **13**, 58 (2003)
16. D. Labudde; D. Leitner; R. Winter; **P. Schmieder**; M. Schubert; H. Oschkinat; „Automated setup of NMR experiments by PASTE and PAPST“; *International Genomic / Proteomic Technology* (2002)
15. D. Labudde; D. Leitner; R. Winter; **P. Schmieder**; H. Oschkinat; „Automated setup of NMR experiments: New versions of PASTE and PAPST“; *Bruker Spinreport* **150/151**, 8-11 (2002)
14. B. Simon; H. Patzelt; A. ter Laak; G. Krause; **P. Schmieder**; D. Oesterhelt; H. Oschkinat; "The Chromophore Structure of Dark-Adapted Bacteriorhodopsin Solubilized in Detergent Micelles Determined by Solution NMR Spectroscopy"; in *Proceedings of the 29. AMPERE - 13.*

- ISMAR International Conference on Magnetic Resonance and Related Phenomena*, D. Ziessow and W. Lubitz (Eds), Berlin, 109-110 (1998)
13. M. Smalla; **P. Schmieder**; M. Kelly; H. Oschkinat; "Structural studies of the SAM domain "; in *Proceedings of the 29. AMPERE - 13. ISMAR International Conference on Magnetic Resonance and Related Phenomena*, D. Ziessow and W. Lubitz (Eds), Berlin, 452-453 (1998)
 12. **P. Schmieder**; M. Smalla; H. Oschkinat; "New Amino-Acid selective NMR Experiments for the Assignment of Asn and Gln in Proteins"; in *Proceedings of the 29. AMPERE - 13. ISMAR International Conference on Magnetic Resonance and Related Phenomena*, D. Ziessow and W. Lubitz (Eds), Berlin, 134-135 (1998)
 11. D. Winkler; R.-D. Stigler; B. Hoffmann; G. Zahn; W. Hohne; J. Rappsilber; **P. Schmieder**; H. Oschkinat; J. Schneider-Mergener; "Elucidation of the interaction of an anti-TGF α antibody with its peptide epitope using combinatorial cyclic peptide libraries, binding studies, NMR, computer modeling and flexible docking techniques"; in *Pept. 1996, Proc. 24th Eur. Pept. Symp.*, Meeting Date 1996, Ramage, R. and Epton, R. (Eds.), 913-914 (1998)
 10. **P. Schmieder**; "Strukturbestimmung von Proteinen mittels NMR-Spektroskopie"; *BIOforum*, **7-8**, 367-369 (1997)
 9. **P. Schmieder**; A.S. Stern; G. Wagner; J. C. Hoch; "Applications of MaxEnt Reconstructions"; *J. Cell. Biol. Suppl.* 17C, 300 (1993)
 8. H. Kessler; J. Balbach; G. Müller; D.F. Mierke; **P. Schmieder**; S. Seip; "New heteronuclear NMR techniques for the determination of structure and dynamics of peptides and proteins - consequences for drug design"; *J. Cell. Biol. Suppl.* 17C, 246 (1993)
 7. **P. Schmieder**; R. Mamorstein; J.D. Baleja; S.C. Harrison; G. Wagner; "Structural investigation of the GAL4 dimerization domain in solution by NMR-spectroscopy"; *J. Cell. Biol. Suppl.* 17C, 237 (1993)
 6. **P. Schmieder**; "Entwicklung und Anwendung neuer, heteronuklearer NMR-spektroskopischer Methoden mit Protonendetektion"; Dissertation, TU München (1991)

-
5. **P. Schmieder**; "Auf Umwegen zum Ziel"; *Angew. Chem.* **102**, A298 (1990)
 4. **P. Schmieder**; "Die Größe von Weitbereichskopplungen"; *Angew. Chem.* **102**, A122 (1990)
 3. **P. Schmieder**; "Spektrenvereinfachung durch doppelte Halbfilter"; *Angew. Chem.* **102**, A122 (1990)
 2. H. Kessler; **P. Schmieder**; "Proton Detected DEPT Spectroscopy"; *TAMU Letters* 15, 378-379 (1990)
 1. U. Döller; M. Eichhorn; A. Kleemann; W. Knauf; F. Küber; **P. Schmieder**; "Frankfurter Studenten Seminar"; *Chem. Unserer Zeit* **22**, A36 (1988)