

## Publications Daniel Hoffmann

- [1] Karimzadeh H, Kiraithe MM, Kosinska AD, Glaser M, Fiedler M, Oberhardt V, Salimi Alizei E, Hofmann M, Mok JY, Nguyen M, van Esch WJE, Budeus B, Grabowski J, Homs M, Olivero A, Keyvani H, Rodríguez-Frías F, Tabernero D, Buti M, Heinold A, Alavian SM, Bauer T, Schulze Zur Wiesch J, Raziorrouh B, Hoffmann D, Smedile A, Rizzetto M, Wedemeyer H, Timm J, Antes I, Neumann-Haefelin C, Protzer U, Roggendorf M. Amino acid substitutions within HLA-B\*27-restricted T cell epitopes prevent recognition by hepatitis delta virus-specific CD8+ T cells. *Journal of virology*. 2018 April; Available from: <https://doi.org/10.1128/JVI.01891-17>.
- [2] Schürmann S, Steffes G, Manikowski D, Kastl P, Malkus U, Bandari S, Ohlig S, Ortmann C, Rebolledo-Rios R, Otto M, Nüsse H, Hoffmann D, Klämbt C, Galic M, Klingauf J, Grobe K. Proteolytic processing of palmitoylated Hedgehog peptides specifies the 3-4 intervein region of the. *Elife*. 2018 Mar;7.
- [3] Piombo V, Jochmann K, Hoffmann D, Wuelling M, Vortkamp A. Signaling systems affecting the severity of multiple osteochondromas. *Bone*. 2018 Mar;111:71–81. Available from: <https://doi.org/10.1016/j.bone.2018.03.010>.
- [4] Grad JN, Gigante A, Wilms C, Dybowski JN, Ohl L, Ottmann C, Schmuck C, Hoffmann D. Locating Large, Flexible Ligands on Proteins. *Journal of Chemical Information and Modeling*. 2018 Jan;58(2):315–327. Available from: <http://dx.doi.org/10.1021/acs.jcim.7b00413>.
- [5] Ehlers M, Grad JN, Mittal S, Bier D, Mertel M, Ohl L, Bartel M, Briels J, Heimann M, Ottmann C, Sanchez-Garcia E, Hoffmann D, Schmuck C. Rational Design, Binding Studies, and Crystal-Structure Evaluation of the First Ligand Targeting the Dimerization Interface of the 14-3-3 $\zeta$  Adapter Protein. *ChemBioChem*. 2018 Feb; Available from: <http://dx.doi.org/10.1002/cbic.201700588>.
- [6] Tucci FA, Kitanovski S, Johansson P, Klein-Hitpass L, Kahraman A, Dürig J, Hoffmann D, Küppers R. Biased IGH VDJ gene repertoire and clonal expansions in B cells of chronically hepatitis C virus-infected individuals. *Blood*. 2018 Feb;131(5):546–557.
- [7] Jakobs P, Schulz P, Schürmann S, Niland S, Exner S, Rebolledo-Rios R, Manikowski D, Hoffmann D, Seidler DG, Grobe K. Ca(2+) coordination controls sonic hedgehog structure and its Scube2-regulated release. *Journal of cell science*. 2017 Oct;130:3261–3271.
- [8] Drabczyk-Pluta M, Werner T, Hoffmann D, Leng Q, Chen L, Dittmer U, Zelinsky G. Granulocytic myeloid-derived suppressor cells suppress virus-specific CD8(+) T cell responses during acute Friend retrovirus infection. *Retrovirology*. 2017 Aug;14:42.
- [9] Dunkel T, de León Gallegos EL, Bock C, Lange A, Hoffmann D, Boenigk J, Denecke M. Illumina sequencing for the identification of filamentous bulking and foaming bacteria in industrial activated sludge plants. *International Journal of Environmental Science and Technology*. 2017 Aug; Available from: <https://doi.org/10.1007/s13762-017-1484-y>.

- [10] Nemeč M, Hoffmann D. Quantitative Assessment of Molecular Dynamics Sampling for Flexible Systems. *Journal of chemical theory and computation*. 2017 Feb;13:400–414.
- [11] Saeedghalati M, Farahpour F, Budeus B, Lange A, Westendorf AM, Seifert M, Küppers R, Hoffmann D. Quantitative Comparison of Abundance Structures of Generalized Communities: From B-Cell Receptor Repertoires to Microbiomes. *PLoS computational biology*. 2017 Jan;13:e1005362.
- [12] Kletenkov K, Hoffmann D, Böni J, Yerly S, Aubert V, Schöni-Affolter F, Struck D, Verheyen J, Klimkait T, Study SHC. Role of Gag mutations in PI resistance in the Swiss HIV cohort study: bystanders or contributors? *The Journal of antimicrobial chemotherapy*. 2016 Dec;.
- [13] Grossmann L, Jensen M, Heider D, Jost S, Glücksman E, Hartikainen H, Mahamdallie SS, Gardner M, Hoffmann D, Bass D, Boenigk J. Protistan community analysis: key findings of a large-scale molecular sampling. *ISME J*. 2016 Feb; Available from: <http://dx.doi.org/10.1038/ismej.2016.10>.
- [14] Budeus B, Timm J, Hoffmann D. SeqFeatR for the Discovery of Feature-Sequence Associations. *PLoS One*. 2016;11(1):e0146409. Available from: <http://dx.doi.org/10.1371/journal.pone.0146409>.
- [15] Lange A, Jost S, Heider D, Bock C, Budeus B, Schilling E, Strittmatter A, Boenigk J, Hoffmann D. AmpliconDuo: A Split-Sample Filtering Protocol for High-Throughput Amplicon Sequencing of Microbial Communities. *PLoS One*. 2015;10(11):e0141590. Available from: <http://dx.doi.org/10.1371/journal.pone.0141590>.
- [16] Budeus B, Schweigle de Reynoso S, Przekopowicz M, Hoffmann D, Seifert M, Küppers R. Complexity of the human memory B-cell compartment is determined by the versatility of clonal diversification in germinal centers. *Proc Natl Acad Sci U S A*. 2015 Sep;112(38):E5281–E5289. Available from: <http://dx.doi.org/10.1073/pnas.1511270112>.
- [17] Merches K, Khairnar V, Knuschke T, Shaabani N, Honke N, Duhan V, Recher M, Navarini AA, Hardt C, Häussinger D, Tümmler B, Gulbins E, Futerman AH, Hoffmann D, Lang F, Lang PA, Westendorf AM, Lang KS. Virus-Induced Type I Interferon Deteriorates Control of Systemic *Pseudomonas Aeruginosa* Infection. *Cell Physiol Biochem*. 2015;36(6):2379–2392. Available from: <http://dx.doi.org/10.1159/000430200>.
- [18] Sierra S, Dybowski JN, Pironti A, Heider D, Güney L, Thielen A, Reuter S, Esser S, Fätkenheuer G, Lengauer T, Hoffmann D, Pfister H, Jensen B, Kaiser R. Parameters Influencing Baseline HIV-1 Genotypic Tropism Testing Related to Clinical Outcome in Patients on Maraviroc. *PLoS One*. 2015;10(5):e0125502. Available from: <http://dx.doi.org/10.1371/journal.pone.0125502>.
- [19] Klammer M, Dybowski JN, Hoffmann D, Schaab C. Pareto Optimization Identifies Diverse Set of Phosphorylation Signatures Predicting Response to Treatment with Dasatinib. *PLoS One*. 2015;10(6):e0128542. Available from: <http://dx.doi.org/10.1371/journal.pone.0128542>.

- [20] Kefalakes H, Budeus B, Walker A, Jochum C, Hilgard G, Heinold A, Heinemann FM, Gerken G, Hoffmann D, Timm J. Adaptation of the hepatitis B virus core protein to CD8(+) T-cell selection pressure. *Hepatology*. 2015 Jul;62(1):47–56. Available from: <http://dx.doi.org/10.1002/hep.27771>.
- [21] Heider D, Dybowski JN, Wilms C, Hoffmann D. A simple structure-based model for the prediction of HIV-1 co-receptor tropism. *BioData Min*. 2014;7:14. Available from: <http://dx.doi.org/10.1186/1756-0381-7-14>.
- [22] Klammer M, Dybowski JN, Hoffmann D, Schaab C. Identification of significant features by the global mean rank test. *PLoS One*. 2014;9(8):e104504.
- [23] Rebolledo-Rios R, Bandari S, Wilms C, Jakushev S, Vortkamp A, Grobe K, Hoffmann D. Signaling domain of Sonic Hedgehog as cannibalistic calcium-regulated zinc-peptidase. *PLoS computational biology*. 2014 Jul;10:e1003707.
- [24] Dang S, Wang Y, Budeus B, Verheyen J, Yang R, Hoffmann D. Differential selection in HIV-1 gp120 between subtype B and East Asian variant B'. *Virology*. 2014 Feb;29(1):40–7.
- [25] Matena A, Sinnen C, van den Boom J, Wilms C, Dybowski JN, Maltaner R, Mueller JW, Link NM, Hoffmann D, Bayer P. Transient Domain Interactions Enhance the Affinity of the Mitotic Regulator Pin1 toward Phosphorylated Peptide Ligands. *Structure*. 2013 Oct;21(10):1769–77.
- [26] Grum D, Franke S, Kraff O, Heider D, Schramm A, Hoffmann D, Bayer P. Design of a modular protein-based MRI contrast agent for targeted application. *PLoS One*. 2013;8(6):e65346.
- [27] Sowa JP, Heider D, Bechmann LP, Gerken G, Hoffmann D, Canbay A. Novel Algorithm for Non-Invasive Assessment of Fibrosis in NAFLD. *PLoS One*. 2013;8(4):e62439.
- [28] Wang Y, Rawi R, Wilms C, Heider D, Yang R, Hoffmann D. A Small Set of Succinct Signature Patterns Distinguishes Chinese and Non-Chinese HIV-1 Genomes. *PLoS One*. 2013;8(3):e58804.
- [29] Jiang QQ, Bartsch L, Sicking W, Wich PR, Heider D, Hoffmann D, Schmuck C. A new approach to inhibit human  $\beta$ -tryptase by protein surface binding of four-armed peptide ligands with two different sets of arms. *Org Biomol Chem*. 2013 Jan;11(10):1631 – 1639.
- [30] Ohlig S, Pickhinke U, Sirko S, Bandari S, Hoffmann D, Dreier R, Farshi P, Götz M, Grobe K. An emerging role of Sonic hedgehog shedding as a modulator of heparan sulfate interactions. *J Biol Chem*. 2012 Dec;287(52):43708–19.
- [31] Qin B, Budeus B, Cao L, Wu C, Wang Y, Zhang X, Rayner S, Hoffmann D, Lu M, Chen X. The amino acid substitutions rtP177G and rtF249A in the reverse transcriptase domain of hepatitis B virus polymerase reduce the susceptibility to tenofovir. *Antiviral Res*. 2013 Dec;97:93–100.
- [32] Genheden S, Kuhn O, Mikulskis P, Hoffmann D, Ryde U. The Normal-Mode Entropy in the MM/GBSA Method: Effect of System Truncation, Buffer Region, and Dielectric Constant. *J Chem Inf Model*. 2012 Aug;52(8):2079–88.

- [33] Neumann LC, Markaki Y, Mladenov E, Hoffmann D, Buiting K, Horsthemke B. The imprinted NPAP1/C15orf2 gene in the Prader-Willi syndrome region encodes a nuclear pore complex associated protein. *Hum Mol Genet.* 2012 Sep;21(18):4038–48.
- [34] Ruhl M, Chhatwal P, Strathmann H, Kuntzen T, Bankwitz D, Skibbe K, Walker A, Heinemann FM, Horn PA, Allen TM, Hoffmann D, Pietschmann T, Timm J. Escape from a dominant HLA-B\*15-restricted CD8+ T cell response against hepatitis C virus requires compensatory mutations outside the epitope. *J Virol.* 2012 Jan;86(2):991–1000.
- [35] Dybowski JN, Riemenschneider M, Hauke S, Pyka M, Verheyen J, Hoffmann D, Heider D. Improved Bevirimat resistance prediction by combination of structural and sequence-based classifiers. *BioData Min.* 2011 Nov;4(1):26.
- [36] Lederer C, Heider D, van den Boom J, Hoffmann D, Mueller JW, Bayer P. Single-domain parvulins constitute a specific marker for recently proposed deep-branching archaeal subgroups. *Evol Bioinform Online.* 2011;7:135–48.
- [37] Lättig-Tünnemann G, Prinz M, Hoffmann D, Behlke J, Palm-Apergi C, Morano I, Herce HD, Cardoso MC. Backbone rigidity and static presentation of guanidinium groups increases cellular uptake of arginine-rich cell-penetrating peptides. *Nat Commun.* 2011;2:453.
- [38] Ohlig S, Farshi P, Pickhinke U, van den Boom J, Höing S, Jakushev S, Hoffmann D, Dreier R, Schöler HR, Dierker T, Bordych C, Grobe K. Sonic hedgehog shedding results in functional activation of the solubilized protein. *Dev Cell.* 2011 Jun;20(6):764–74.
- [39] Ruhl M, Knuschke T, Schewior K, Glavinic L, Neumann-Haefelin C, Chang DI, Klein M, Heinemann FM, Tenckhoff H, Wiese M, Horn PA, Viazov S, Spengler U, Roggendorf M, Scherbaum N, Nattermann J, Hoffmann D, Timm J, East German HCV Study Group. CD8(+) T-cell response promotes evolution of hepatitis C virus nonstructural proteins. *Gastroenterology.* 2011 Jun;140(7):2064–73.
- [40] Heider D, Verheyen J, Hoffmann D. Machine learning on normalized protein sequences. *BMC Res Notes.* 2011 Mar;4(1):94.
- [41] Horsthemke B, Wawrzik M, Groß S, Lich C, Sauer B, Rost I, Krasemann E, Kosyakova N, Liehr T, Weise A, Dybowski JN, Hoffmann D, Wieczorek D. Parental origin and functional relevance of a de novo UBE3A variant. *Eur J Med Genet.* 2011;54(1):19–24.
- [42] Haferkamp P, Kutschki S, Treichel J, Hemeda H, Sewczyk K, Hoffmann D, Zaparty M, Siebers B. An additional glucose dehydrogenase from *Sulfolobus solfataricus*: fine-tuning of sugar degradation? *Biochem Soc Trans.* 2011 Jan;39(1):77–81.
- [43] Dybowski JN, Heider D, Hoffmann D. Structure of HIV-1 quasi-species as early indicator for switches of co-receptor tropism. *AIDS Res Ther.* 2010 Nov;7(1):41.
- [44] Drogan D, Rauch P, Hoffmann D, Walter H, Metzner KJ. The antiretroviral potency of emtricitabine is approximately 3-fold higher compared to lamivudine in dual human immunodeficiency virus type 1 infection/competition experiments in vitro. *Antiviral Res.* 2010 Jun;86(3):312–5.

- [45] Dybowski JN, Heider D, Hoffmann D. Prediction of co-receptor usage of HIV-1 from genotype. *PLoS Comput Biol*. 2010 Apr;6(4):e1000743.
- [46] Ehrentraut S, Weber JM, Dybowski JN, Hoffmann D, Ehrenhofer-Murray AE. Rpd3-dependent boundary formation at telomeres by removal of Sir2 substrate. *Proc Natl Acad Sci U S A*. 2010 Mar;107(12):5522–7.
- [47] Heider D, Verheyen J, Hoffmann D. Predicting Bevirimat resistance of HIV-1 from genotype. *BMC Bioinformatics*. 2010 Jan;11(1):37.
- [48] Schirling C, Heseding C, Heise F, Kesper D, Klebes A, Klein-Hitpass L, Vortkamp A, Hoffmann D, Saumweber H, Ehrenhofer-Murray AE. Widespread regulation of gene expression in the *Drosophila* genome by the histone acetyltransferase dTip60. *Chromosoma*. 2010 Feb;119(1):99–113.
- [49] Franke S, Herfurth J, Hoffmann D. Estimating affinities of calcium ions to proteins. *Adv Appl Bioinform Chem*. 2010;2:1–6.
- [50] Balduin M, Oette M, Däumer MP, Hoffmann D, Pfister HJ, Kaiser R. Prevalence of minor variants of HIV strains at reverse transcriptase position 103 in therapy-naïve patients and their impact on the virological failure. *J Clin Virol*. 2009 May;45(1):34–8.
- [51] Jakushev S, Hoffmann D. A Novel Algorithm for Macromolecular Epitope Matching. *Algorithms*. 2009;2(1):498–517. Available from: <http://www.mdpi.com/1999-4893/2/1/498>.
- [52] Verheyen J, Knops E, Kupfer B, Hamouda O, Somogyi S, Schuldenzucker U, Hoffmann D, Kaiser R, Pfister H, Kücherer C. Prevalence of C-terminal gag cleavage site mutations in HIV from therapy-naïve patients. *J Infect*. 2009 Jan;58(1):61–7.
- [53] Fischer S, Kohlhase J, Böhm D, Schweiger B, Hoffmann D, Heitmann M, Horsthemke B, Wieczorek D. Biallelic Loss of Function of the Promyelocytic Leukaemia Zinc Finger (PLZF) Gene Causes Severe Skeletal Defects and Genital Hypoplasia. *J Med Genet*. 2008;45:731–737.
- [54] Albert T, Egler C, Jakushev S, Schuldenzucker U, Schmitt A, Brokemper O, Zabe-Kuhn M, Hoffmann D, Oldenburg J, Schwaab R. The B-cell epitope of the monoclonal anti-factor VIII antibody ESH8 characterized by peptide array analysis. *Thromb Haemost*. 2008;99:634–637.
- [55] Gronwald W, Hohm T, Hoffmann D. Evolutionary Pareto-optimization of stably folding peptides. *BMC Bioinformatics*. 2008;9:109.
- [56] Gilsdorf M, Däumer M, Kaiser R, Korn K, Walter H, Hoffmann D. Towards molecular model based prediction of HIV drug resistance. *European Journal of Medical Research*. 2007;12(Suppl. III).
- [57] Egler C, Schuldenzucker U, Hoffmann D. Selection and sequence analysis of TiO<sub>2</sub>-binding peptides. *BIOMaterialien*. 2006;7:142.

- [58] Verheyen J, Litau E, Däumer M, Balduin M, Oette M, Fätgenheuer G, Rockstroh JK, Hoffmann D, Pfister H, Kaiser R. Compensatory mutations at HIV cleavage sites p7/p1 and p1/p6-gag in therapy-naïve and therapy-experienced patients. *Antiviral Therapy*. 2006;11:879–87.
- [59] Roomp K, Beerenwinkel N, Sing T, Schülter E, Büch J, Sierra-Aragon S, Däumer M, Hoffmann D, Kaiser R, Lengauer T, Selbig J. Arevir: A Secure Platform for Designing Personalized Antiretroviral Therapies Against HIV. *Lecture Notes in Computer Science*. 2006;4075:185–94.
- [60] Wefing S, Schnaible V, Hoffmann D. SearchXLinks – A Program for Identifying Crosslinks or Disulfide Bonds in Proteins from Mass Spectra. *Anal Chem*. 2006;78:1235–1241.
- [61] Wendeler M, Werth N, Maier T, Schwarzmann G, Kolter T, Schoeniger M, Hoffmann D, Lemm T, Saenger W, Sandhoff K. The enzyme-binding region of human GM2-activator protein. *FEBS J*. 2006;273:982–91.
- [62] Hohm T, Limbourg P, Hoffmann D. A multiobjective evolutionary method for the design of peptidic mimotopes. *J Comput Biol*. 2006;13:113–125.
- [63] Balduin M, Sierra S, Daumer MP, Rockstroh JK, Oette M, Fätkenheuer G, Kupfer B, Beerenwinkel N, Hoffmann D, Selbig J, Pfister HJ, Kaiser R. Evolution of HIV resistance during treatment interruption in experienced patients and after restarting a new therapy. *J Clin Virol*. 2005;34:277–87.
- [64] Beerenwinkel N, Däumer M, Sing T, Rahnenführer J, Lengauer T, Selbig J, Hoffmann D, Kaiser R. Estimating HIV evolutionary pathways and the genetic barrier to drug resistance. *J Infect Dis*. 2005;191:1953–1960.
- [65] Sing T, Svicher V, Beerenwinkel N, Ceccherini-Silberstein F, Däumer M, Kaiser R, Walter H, Korn K, Hoffmann D, Oette M, Rockstroh JK, Fätkenheuer G, Perno CF, Lengauer T. Characterization of Novel HIV Drug Resistance Mutations Using Clustering, Multidimensional Scaling, and SVM-Based Feature Ranking. In: *Proceedings of ECML/PKDD-2005*. Springer; 2005. p. 285–296.
- [66] Hohm T, Hoffmann D. A multi-objective evolutionary approach to peptide structure redesign and stabilization. In: Beyer HG, editor. *GECCO'05. Proceedings of the Genetic and Evolutionary Computation Conference*. ACM; 2005. p. 423–429.
- [67] Beerenwinkel N, Rahnenführer J, Däumer M, Hoffmann D, Kaiser R, Selbig J, Lengauer T. Learning Multiple Evolutionary Pathways from Cross-sectional Data. *J Comput Biol RECOMB 2004*. 2005;12:584–598.
- [68] Beerenwinkel N, Rahnenführer J, Kaiser R, Hoffmann D, Selbig J, Lengauer T. Mtreemix: a software package for learning and using mixture models of mutagenic trees. *Bioinformatics*. 2005;21:2106–2107.

- [69] Beerenwinkel N, Sing T, Lengauer T, Rahnenführer J, Roomp K, Savenkov I, Fischer R, Hoffmann D, Selbig J, Korn K, Walter H, Berg T, Braun P, Fätkenheuer G, Oette M, Rockstroh J, Kupfer B, Kaiser R, Däumer M. Computational methods for the design of effective therapies against drug resistant HIV strains. *Bioinformatics*. 2005 Sep;21(21):3943–3950. Available from: <http://dx.doi.org/10.1093/bioinformatics/bti654>.
- [70] Wendeler M, Hoernschemeyer J, Hoffmann D, Kolter T, Schwarzmann G, Sandhoff K. Photoaffinity labelling of the human GM2-activator protein. Mechanistic insight into ganglioside GM2 degradation. *Eur J Biochem*. 2004;271:614–627.
- [71] Hoffmann D. Computergestützte molekulare Modellierung für die Suche nach neuen Wirkstoffen gegen HIV/AIDS. In: *Resistenz in der HIV-Therapie – Diagnostik und Management*. Bremen, London, Boston: Uni-Med; 2003. p. 62–65. M. Oette, R. Kaiser, D. Häussinger, eds.
- [72] Wolf K, Walter H, Beerenwinkel N, Kaiser WKR, Hoffmann D, Lengauer T, Selbig J, Vandamme AM, Korn K, Schmidt B. Tenofovir Resistance and Resensitization. *Antimicrob Agents and Chemother*. 2003;47:3478–3484.
- [73] Hoffmann D. Optimierung von Oligomeren; 2003. Deutsches Patentamt, No. 103 436 90.
- [74] Hoffmann D. Detektion von Nanopartikeln; 2003. Deutsches Patentamt, No. 103 44 515.
- [75] Beerenwinkel N, Däumer M, Oette M, Korn K, Hoffmann D, Kaiser R, Lengauer T, Selbig J, Walter H. Geno2pheno: estimating phenotypic drug resistance from HIV-1 genotypes. *Nucl Acids Res*. 2003;31:3850–3855.
- [76] Beerenwinkel N, Lengauer T, Däumer M, Kaiser R, Walter H, Korn K, Hoffmann D, Selbig J. Methods for optimizing antiviral combination therapies. *Bioinformatics*. 2003;19 (suppl. 1):i16–i25.
- [77] Schnaible V, Wefing S, Bücker A, Wolf-Kümmeth S, Hoffmann D. Partial reduction and two step modification of proteins for identification of disulfide bonds. *Analytical Chemistry*. 2002;74:2386–2393.
- [78] Albrecht M, Hoffmann D, Evert BO, Schmitt I, Wüllner U, Lengauer T. Structural Modeling of Ataxin-3 Reveals Distant Homology To Adaptins. *Proteins Struct Funct Genet*. 2003;50:355–370.
- [79] Hoffmann D, Moske M. Elasto-Optischer Biosensor; 2002. Deutsches Patentamt, Nr. 102 21 792.
- [80] Beerenwinkel N, Schmidt B, Walter H, Kaiser R, Lengauer T, Hoffmann D, Korn K, Selbig J. Diversity and complexity of HIV-1 drug resistance: a bioinformatics approach to predicting phenotype from genotype. *Proc Natl Acad Sci U S A*. 2002 Jun;99(12):8271–6.
- [81] Schmid B, Hoffmann D, Famulok M, Quandt E, Schnaible V, Tewes M, Wefing S. Process for detecting biological molecules; 2002. Publication date: April 18, 2002. United States Patent Office, No. 09/973 993.

- [82] Schnaible V, Wefing S, Resemann A, Suckau D, Bücker A, Wolf-Kümmeth S, D H. Screening for Disulfide Bonds in Proteins by MALDI-MS/MS and LIFT-TOF/TOF-MS. *Analytical Chemistry*. 2002;74:4980–4988.
- [83] Hoffmann D. The Protein Information Resource. *Angew Chem Int Ed*. 2002;41:1075.
- [84] Beerenwinkel N, Nolden T, Kupfer B, Selbig J, Däumer M, Hoffmann D, Rockstroh J, Kaiser R. Predicting HIV-1 Cytopathogenicity and Co-Receptor Usage from V3 Envelope Sequences by Machine Learning. In: 1st IAS Conference on HIV Pathogenesis and Treatment. Buenos Aires; 2001. p. Abstr. 268.
- [85] Hoffmann D, Schnaible V, Wefing S, Albrecht M, Hanisch D, Zimmer R. A New Method for the Fast Solution of Protein-3D-Structures, combining Experiments and Bioinformatics. In: Hoffmann KH, editor. *Coupling of biological and electronic systems: proceedings of the 2nd caesarium*, Bonn, November 1-3, 2000. vol. 2. Berlin; New York.: Springer; 2002. p. 59–78. ISBN 3-540-43699-5.
- [86] Beerenwinkel N, Schmidt B, Walter H, Kaiser R, Lengauer T, Hoffmann D, Korn K, Selbig J. Identifying Drug Resistance-Associated Patterns in HIV Genotypes. *Proceedings of the German Conference on Bioinformatics*. 2001;p. 126–130.
- [87] Beerenwinkel N, Däumer M, Hoffmann D, Kaiser R, Korn K, Lengauer T, Schmidt B, Walter H, Selbig J. Neue Wege zur Optimierung von Anti-HIV-Therapien – Erste Analysen mit bioinformatischen Methoden. *BIOforum*. 2001;(12):912–914.
- [88] Beerenwinkel N, Schmidt B, Walter H, Kaiser R, Lengauer T, Hoffmann D, Korn K, Selbig J. Geno2pheno: Interpreting Genotypic HIV Drug Resistance Tests. *IEEE Intelligent Systems*. 2001;16:35–41.
- [89] Schmid B, Hoffmann D, Famulok M, Quandt E, Schnaible V, Tewes M, Wefing S. Verfahren zum Nachweis biologischer Moleküle; 2000. Deutsches Patentamt, Nr. 100 50 632.
- [90] Beerenwinkel N, Selbig J, Kaiser R, Hoffmann D. Arevir: Analysis of HIV Resistance Mutations. *ERCIM news*. 2000;(43):23–24.
- [91] Hoffmann D, Schnaible V, Wefing S. Verfahren zur Bestimmung räumlicher Abstände in Polymeren oder Komplexen von Polymeren mit Hilfe von Gemischen von Cross-Linker Molekülen.; 2000. Deutsches Patentamt, Nr. 100 36 342.
- [92] Jacob J, Gessler K, Hoffmann D, Sanbe H, Koizumi K, Smith SM, Takaha T, Saenger W. Band-flip and kink as novel structural motifs in alpha-(1-> 4)-D-glucose oligosaccharides. Crystal structures of cyclodeca- and cyclotetradecaamylose. *Carbohydrate Research*. 1999;322:228–246.
- [93] Rabenstein B, Hoffmann D, Knapp EW. Simulation of oligopeptide folding or how do residues talk. *AIP Conference Proceedings*. 1999;487(1):54–68. Available from: <http://aip.scitation.org/doi/abs/10.1063/1.59893>.



- [94] Hoffmann D, Zimmer R. Chemical Activation Mediated by the Transfer of Fluorescent Energy for Elucidating the 3D-Structure of Biological Macromolecules; 1999. German Patent Office, PCT WO 99/41607.
- [95] Hoffmann D, Kramer B, Washio T, Steinmetzer T, Rarey M, Lengauer T. Two-Stage Method for Protein-Ligand Docking. *J Med Chem.* 1999;42:4422–4433.
- [96] Saenger W, Jacob J, Gessler K, Steiner T, Hoffmann D, Sanbe H, Koizumi K, Smith SM, Takaha T. Structures of the Common Cyclodextrins and Their Larger Analogues – Beyond the Doughnut. *Chem Rev.* 1998;98:1787–1802.
- [97] Jacob J, Gessler K, Hoffmann D, Sanbe H, Koizumi K, Smith SM, Takaha T, Saenger W. Strain induced flips of glucoses in cyclodecaamylose and higher homologues. *Angew Chem Int Ed.* 1998;37:605–609.
- [98] Hoffmann D, Flörke H. A structural role for glycosylation: lessons from the hp-model. *Folding & Design.* 1998;3:337–343.
- [99] Hoffmann D, Washio T, Gessler K, Jacob J. Tackling Concrete Problems in Molecular Biophysics Using Monte Carlo and Related Methods: Glycosylation, Folding, Solvation. In: Grassberger P, Barkema G, Nadler W, editors. *Monte Carlo approach to Biopolymers and Protein Folding.* Singapore: World Scientific; 1998. p. 153–170. ISBN 981-02-3658-1.
- [100] Hoffmann D, Knapp EW. Folding Pathways of a Helix-Turn-Helix Model Protein. *J Phys Chem B.* 1997;101:6734–6740.
- [101] Hoffmann D, Knapp EW. A Monte Carlo method for simulations of protein folding with detailed protein models. In: *Perspectives on Protein Engineering.* Bingham, UK: Biodigm; 1996. ISBN 0-9529015-0-1.
- [102] Hoffmann D, Knapp EW. Protein Folding Studied by Off-Lattice Monte Carlo Dynamics. *Prog Biophys molec Biol.* 1996;65, Suppl. 1:52.
- [103] Hoffmann D. Monte Carlo Methoden zur Simulation der Langzeitdynamik von Proteinen. vol. 2 of *Bioinformatik.* Berlin: Verlag Köster; 1996. ISBN 3-89574-150-7 (PhD thesis).
- [104] Hoffmann D, Knapp EW. Protein dynamics with off-lattice Monte Carlo moves. *Phys Rev E.* 1996;53:4221–4224.
- [105] Hoffmann D, Knapp EW. Polypeptide folding with off-lattice Monte Carlo dynamics: the method. *Eur Biophysics J.* 1996;24:387–404.
- [106] Hoffmann D, Sartori F, Knapp EW. An off-lattice Monte Carlo Method to simulate the long time dynamics of proteins. *Protein Science.* 1995;4, Suppl. 1:56.