

## Curriculum Vitae – Prof. Dr. Harald Schwalbe 26.03.1966

Lab Institute of Organic Chemistry and Chemical Biology  
Center for Biomolecular Magnetic Resonance (BMRZ)  
Address Johann Wolfgang Goethe-University  
Max-von-Laue -Str. 7  
60438 Frankfurt, Germany  
Phone +49-(0)69-798-29737  
Fax +49-(0)69-798-29515  
e-mail schwalbe@nmr.uni-frankfurt.de  
homepage <http://schwalbe.org.chemie.uni-frankfurt.de/>

### Education

1993-1995 Postdoctoral fellow at the Oxford Centre for Molecular Sciences, Oxford University (Mentor: C.M. Dobson, FRS)  
1990-1993 Chemistry, University of Frankfurt, Germany, Ph.D. (summa cum laude; Mentor: C. Griesinger)  
1985-1990 Chemistry, University of Frankfurt, Germany, Diploma (summa cum laude; Mentor: C. Griesinger)

### Professional Career

2014- EU representative of Goethe University Frankfurt  
2013- Member of the Board of Directors: Cluster of Excellence: Macromolecular Complexes  
2012- Coordinator: DFG-funded Network of German NMR Centres  
2012- Chairman of the Frankfurt section of the Society of German Chemists (GDCh)  
2011- Speaker: DFG-SFB 902: "Molecular principles of RNA-based regulation"  
2011-2016 Chairman of the DFG panel: large equipment ("Apparatausschuß")  
2009-2012 Speaker: DFG-Cluster of Excellence EXC115: "Macromolecular Complexes"  
2009-2010 Member of the DFG panel: large equipment ("Apparatausschuß")  
2007-2009 Speaker: DFG-SFB 579: "RNA-Ligand-Interactions"  
2006-2008 Deputy Director: DFG-Center of Excellence: Macromolecular Complexes  
2005- Member of Senate of Goethe-University Frankfurt  
2003- Coordinator of 5 EU-funded programmes (STREPs, TOKs, Research Infrastructure for NMR (I3))  
2002-2006 Managing Director of the Center for Biomolecular Magnetic Resonance, BMRZ  
2003-2008 Head of the Department (Dekan) "Biochemistry, Chemistry and Pharmacy"  
2002- Full Professor (C4), Institute for Organic Chemistry and Chemical Biology, University of Frankfurt  
2001 Associate Professor for Biological Chemistry, Massachusetts Institute of Technology  
1999-2001 Assistant Professor for Biological Chemistry, Massachusetts Institute of Technology  
1995-1999 Work as Habilitand in Chemistry, University of Frankfurt (Mentor: C. Griesinger)

### Honors and Awards

2015 Best PhD thesis advisor award, University Frankfurt.  
2015 Szent-Györgyi Albert lecturer in Budapest  
2014 "Scientist of the Year" of Kassel Foundation, University Frankfurt.  
2012 Department Prize for Teaching, University Frankfurt  
2006 1822-Prize for Teaching; University Frankfurt  
2002- Vertrauensdozent of the "Studienstiftung des deutschen Volkes"  
2001 Pew Scholar for Biomedical Sciences, Fellow of the Alfred P. Sloan Foundation  
2000 Karl Winnacker Preis of Aventis Foundation  
1999 Gerhard Hess Preis of DFG  
1996 Liebig Stipend of the Fonds der Chemischen Industrie  
1993-1995 Human Capital and Mobility Fellow, EU.  
1993 Studienabschlusspreis of the Fonds der Chemischen Industrie, Promotion

- 1989-1993 Member of the Graduate program: "Chemische und Biologische Synthese von Wirkstoffen", Institut für Organische Chemie, Frankfurt/Main.  
1987-1990 Member of the "Studienstiftung des Deutschen Volkes"

### **Research Interests**

Structural Biology of Proteins and RNA studied by NMR spectroscopy  
Time-Resolved NMR spectroscopy  
RNA Folding and Regulation  
Protein Folding; non-native states of proteins  
NMR-based drug design (kinases, phosphatases, GPCRs)  
Synthesis of isotope labelled RNA, DNA, peptides and photolabile compounds

### **Member of Editorial Boards/Scientific Committees**

ChemBioChem, Board of ISMAR (2002-2010), ICMRBS Council (2006-2016), Kuratorium des Strüngmann-Forums, Kuratorium der Rolf-Sammet-Stiftung, Kuratorium der Oswald- und Boris-Rajewski-Stiftung, Preiskommission der GDCh August-Wilhelm-von-Hofmann-Denk Münze (2009-2015), Preiskommission des Frankfurter Biophysikpreises der Oswald-Stiftung, Member of the „Wissenschaftliche Gesellschaft der Johann Wolfgang Goethe-Universität Frankfurt“, Kuratorium des „Centres for Dialogue“, Kuratorium der Angewandten Chemie.

### **Organization of Large International Conferences**

- 2002 iLab: G-protein coupled receptors (together with G. Wess, Aventis)  
2003 iLab: RNA targeting (together with G. Wess, Aventis, M. Göbel, Uni Frankfurt)  
2004 iLab: Systems Biology challenges Chemistry (together with G. Wess, Aventis)  
2007 ICMRBS Göttingen (co-organizer)  
2009 GDCh Wissenschaftsforum Frankfurt (local organizer)  
2011 EUROMAR Frankfurt (co-organizer), GDCh Wissenschaftsforum Bremen (scientific committee), International symposium of the German Society for Biochemistry and Molecular Biology (scientific committee)  
2013 Elected Co-Chair Gordon Conference: Biopolymers

### **Scientific Advisory Boards**

Center for Magnetic Resonance Florence  
Henry Wellcome Center Birmingham  
Frankfurt Institute for Advanced Studies (2005-2012)

### **Reviewing activity**

DFG Germany, NWO Netherlands, FWO Austria, CNS France, Wellcome-Trust UK, BBSRC UK, National Science Foundation USA, NIH USA, Science Foundation Belgium, Excellence programme Slovenia, German Israel Foundation, Czech Science Foundation, Klaus-Tschira-Preis, DAAD, Czech Science Foundation, EPSRC UK

Accounts in Chemical Research, Angew. Chem. Int. Ed., Biochemistry, Bioorganic and Medicinal Chemistry, Biophysical J., ChemBioChem, ChemComm, Chemistry A European Journal, ChemPhysChem, Febs Lett., J. Am. Chem. Soc., J. Biomol. NMR, J. Chem. Theor. and Computation, J. Magn. Reson., J. Mol. Biol., J. Phys. Chem., Magnetic Resonance in Chemistry, Nature, Nucleic Acids Res., Plos One, Proc. Natl. Acad. Sci. USA, RNA, Science, Structure.

## 10 recent important publications

### Protein Folding

J. Klein-Seetharaman, M. Oikawa, S.B. Grimshaw, J. Wirmer, E. Duchardt, T. Ueda, T. Imoto, L.J. Smith, C.M. Dobson, **H. Schwalbe** (2002) Long-range interactions within a non-native protein *Science* **295**, 1719-1722.

F. Buhr, S. Jha, M. Thommen, J. Mittelstaet, F. Kutz, **H. Schwalbe\***, M. Rodnina\*, A. Komar\* (2016) Synonymous codons direct co-translational folding towards different protein conformations. *Mol. Cell* **61**, 341-351.

### RNA Folding and Regulation

P. Wenter, B. Fürtig, A. Hainard, **H. Schwalbe\***, S. Pitsch\* (2005) Kinetic investigation of photoinduced RNA refolding by realtime NMR spectroscopy. *Angew. Chem.* **117**, 2656-2659.

J. Buck, B. Fürtig, J. Noeske, J. Wöhnert, **H. Schwalbe** (2007) Time-resolved NMR methods resolving ligand-induced RNA folding at atomic resolution. *Proc. Natl. Acad. Sci. USA* **104**, 15699-15704.

A. Reining, S. Nozinovic, K. Schlepckow, F. Buhr, B. Fürtig\*, **H. Schwalbe\*** (2013) Three-state mechanism couples ligand and temperature sensing in riboswitches. *Nature* **499**, 355-359.

H. Steinert, F. Sochor, A. Wacker, J. Buck, C. Helmling, F. Hiller, S. Keyhani, J. Noeske, S. Grimm, M.M. Rudolph, H. Keller, R.A. Mooney, R. Landick, B. Suess, B. Fürtig\*, J. Wöhnert\*, **H. Schwalbe\*** (2017) Pausing guides RNA folding to populate transiently stable RNA structures for riboswitch-based transcription regulation. *eLife*, e21297.

### Membrane Proteins

J. Stehle, R. Silvers, K. Werner, D. Chatterjee, S. Gande, F. Scholz, A. Dutta, J. Wachtveitl, J. Klein-Seetharaman, **H. Schwalbe** (2014) Solution NMR characterization of simultaneous meta II and meta III decay kinetics in rhodopsin. *Angew. Chem. Intl. Ed.* **53**, 2078-2084.

V. Zickermann, C. Wirth, H. Nasiri, K. Siegmund, **H. Schwalbe**, C. Hunte, U. Brandt (2015) Mechanistic insight from the crystal structure of mitochondrial complex I. *Science* **347**, 44-49.

### NMR-based Drug Design

M. Vogtherr, K. Saxena, S. Hoelder, S. Grimme, M. Betz, U. Schieborr, B. Pescatore, M. Robin, T. Langer, K.U. Wendt, **H. Schwalbe** (2006) NMR-Characterization of kinase p38 dynamics in free and ligand bound form. *Angew. Chem. Intl. Ed.* **45**, 993-997.

C. Herbert, U. Schieborr, K. Saxena, J. Juraszek, F. De Smet, C. Alcouffe, M. Bianciotto, G. Saladino, D. Sibrac, D. Kudlinzki, S. Sreeramulu, A. Brown, P. Rigon, J.-P. Hérault, G. Lassalle, T.L. Blundell, F. Rousseau, A. Gils, J. Schymkowitz, P. Tompa, J.-M. Herbert, P. Carmeliet, F.L. Gervasio\*, **H. Schwalbe\***, F. Bono\* (2013) Molecular mechanism of SSR128129E, an extracellularly acting, small molecule, allosteric inhibitor of FGF receptor signaling. *Cancer Cell* **23**, 489-501.

## List of Publications (peer-reviewed, reviews/editorials are listed separately)

(267 original contributions, 59 reviews, 3 patents)

\*shared corresponding authorship is indicated

### 2017

267. L. Joedicke, J. Mao, G. Kuenze, C. Reinhart, T. Kalavacherla, H.R.A. Jonker, C. Richter, **H. Schwalbe**, J. Meiler, J. Preu, H. Michel, C. Glaubitz (2017) The molecular basis of subtype selectivity of human kinin G-protein-coupled receptors. *Nat. Chem. Biol.*, in press.

266. F. Lehner, D. Kudlinzki, C. Richter, H. Müller-Werkmeister, K. Eberl, J. Bredenbeck. **H. Schwalbe\***, R. Silvers\* (2017) The Impact of Azidohomoalanine Incorporation on Protein Structure and Ligand Binding. *ChemBioChem* **18**, 2340-2350 (inside cover).

265. R. Schnieders, C. Richter, S. Warhaut, V. de Jesus, S. Keyhani, E. Duchardt-Ferner, H. Keller, J. Wöhnert, L.T. Kuhn, A.L. Breeze, W. Bermel, **H. Schwalbe**, B. Fürtig (2017) Evaluation of <sup>15</sup>N-detected H-N correlation experiments on increasingly large RNAs. *J. Biomol. NMR* **69**, 31-44.

264. L. Lannes, P. Young, C. Richter, N. Morgner, **H. Schwalbe** (2017) Interaction of the N-terminal tandem domains of hnRNP LL with the BCL2 promoter i-motif DNA sequence. *ChemBiochem* **18**, 2033-2044 (ranked as "very important paper", inside cover).

263. Y. Liu, J.S. Sharp, D.H. Do, R.A. Kahn, **H. Schwalbe**, F. Buhr, J. Prestegard (2017) Mistakes in translation. Reflections on mechanism. *PLoS One* **12**, e0180566.

262. S. Heinzlmeir, J. Lohse, T. Treiber, D. Kudlinzki, V. Linhardt, S.L. Gande, S. Sreeramulu, K. Saxena, X. Liu, M. Wilhelm, **H. Schwalbe**, B. Küster, G. Médard (2017) Chemoproteomics-aided medicinal chemistry for the discovery of EPHA2 inhibitors. *ChemMedChem* **12**, 999-1011.

261. H. Steinert, F. Sochor, A. Wacker, J. Buck, C. Helmling, F. Hiller, S. Keyhani, J. Noeske, S. Grimm, M.M. Rudolph, H. Keller, R.A. Mooney, R. Landick, B. Suess, B. Fürtig\*, J. Wöhnert\*, **H. Schwalbe\*** (2017) Pausing guides RNA folding to populate transiently stable RNA structures for riboswitch-based transcription regulation. *eLife* **6**, e21297 (featured in Cell Chemical Biology).

260. D. DiGiuseppi, B. Milorey, G. Lewis, N. Kubatova, S. Farrell, **H. Schwalbe**, R. Schweitzer-Stenner, (2017) Probing the Conformation Dependent Preferential Binding of Ethanol to Cationic Glycylalanyl-glycine in Water/Ethanol by Vibrational and NMR Spectroscopy. *J. Phys. Chem. B.* **121**, 5744-5758.

259. L. Herzig, I. Elamri, **H. Schwalbe\***, J. Wachtveitl\* (2017) Light-induced antibiotic release from a coumarin-caged compound on the ultrafast timescale. *Phys Chem Chem Phys.* **19**, 14835-14844..

258. D. Barthelmes, K. Barthelmes, K. Schnorr, H.R.A. Jonker, B. Bodmer, K.N. Allen, B. Imperiali, **H. Schwalbe** (2017) Conformational dynamics and alignment properties of loop lanthanide-binding tags (LBTs) studied in interleukin-1 $\beta$ . *J. Biomol. NMR* **68**, 187-194.

257. K. Schnorr, D.B. Gophane, C. Helmling, E. Cetiner, K. Pasemann, B. Fürtig, A. Wacker, N.S. Qureshi, M. Gränz, D. Barthelmes, H.R.A. Jonker, E. Stirnal, S.Th. Sigurdsson, **H. Schwalbe** (2017) Impact of spin label rigidity on extent and accuracy of distance information from PRE data. *J. Biomol. NMR* **68**, 53-63.

256. J. Wirmer-Bartoschek, L.E. Bendel, H.R.A. Jonker, J.T. Grün, F. Papi, C. Bazzicalupi, L. Messori, P. Gratteri\*, **H. Schwalbe\*** (2017) The NMR solution structure of a ligand/hybrid-2-G-quadruplex complex reveals structural rearrangements that facilitate ligand binding. *Angew. Chem. Intl. Ed.* **56**, 7102-7106.

255. 254. X. Cai, Y.M. Shi, N. Pöhlmann, O. Revermann, I. Bahner, S.J. Pidot, F. Wesche, H. Lackner, C. Büchel, M. Kaiser, C. Richter, **H. Schwalbe**, T.P. Stinear, A. Zeeck, H.B. Bode (2017) Structure and Biosynthesis of Isatropolones, Bioactive Amine-Scavenging Fluorescent Natural Products from *Streptomyces* Gö66. *Angew. Chem. Intl. Ed.* **56**, 4945-4949.

254. H. R. Nasiri\*, K. Hohmann, M. G. Hatemler, **H. Schwalbe** (2017) in vitro production of reactive oxygen species (ROS) by sampangine. *Med. Chem. Res.* **26**, 1170-1175.

253. S. Warhaut, K.R. Mertinkus, P. Höllthaler, B. Fürtig, M. Heilemann, M. Hengesbach, **H. Schwalbe** (2017) Ligand-modulated folding of the full-length adenine riboswitch probed by NMR and single-molecule FRET spectroscopy. *Nucl. Acids Res.* **45**, 5512-5522.

252. C. Helmling, A. Wacker, M.T. Wolfinger, I.L. Hofacker, M. Hengesbach, B. Fürtig, **H. Schwalbe** (2017) NMR structural profiling of transcriptional intermediates reveals riboswitch regulation by metastable RNA conformations. *J. Am. Chem. Soc.* **139**, 2647-2656.

251. Y.B. Kim, A. Wacker, K. von Laer, V. Rogov, B. Suess, **H. Schwalbe** (2017) Ligand binding to 2'-deoxyguanosine sensing riboswitch in metabolic context. *Nucl. Acids Res.* **45**, 5375-5386.

## 2016

250. J. Henker, J. Wirmer-Bartoschek, L.E. Bendel, Y.G. Xiang, C. Fu, K. Harms, **H. Schwalbe**, E. Meggers (2016) Progress in the synthesis and bioactivity of hexacoordinate silicon(IV) complexes. *European Journal of Inorganic Chemistry* **32**, 5161-5170.

249. D. Daube, V. Aladin, J. Heiliger, J. Wittmann, D. Barthelmes, C. Bengs, **H. Schwalbe**, B. Corzilius (2016) Heteronuclear cross-relaxation under solid-state dynamic nuclear polarization. *J. Am. Chem. Soc.* **138**, 16572-16575.

248. J. Grote, D. Krysciak, K. Petersen, S. Güllert, C. Schmeisser, K.U. Förstner, H.B. Krishnan, **H. Schwalbe**, N. Kubatova, W.R. Streit (2016) The absence of the N-acyl-homoserine-lactone autoinducer synthase genes *tral* and *ngri* increases the copy number of the symbiotic plasmid in *Sinorhizobium fredii* NGR234. *Front. Microbiol.* **7**, 1848.

247. J. Hahn, S. Thalmann, A. Migur, R. Freiherr von Boeselager, N. Kubatova, E. Kubareva, **H. Schwalbe**, E. Evguenieva-Hackenberg (2016) Conserved small mRNA with an unique extended Shine-Dalgarno sequence. *RNA Biol.*, in press.

246. S. Heinzlmeir, D. Kudlinzki, S. Sreeramulu, S. Klaeger, S.L. Gande, V. Linhardt, M. Wilhelm, H. Qiao, D. Helm, B. Ruprecht, K. Saxena, G. Medard, **H. Schwalbe\***, B. Küster\* (2016) Chemical proteomics and structural biology define EPHA2 inhibition by clinical kinase drugs. *ACS Chem. Biol.* **11**, 3400-3411.

245. L. Andernach, L. Sandjo, J. Liermann, R. Schlämann, C. Richter, J. Ferner, **H. Schwalbe**, A. Schöffler, E. Thines, T. Opatz (2016) Terphenyl Derivatives from *Allantophomopsis lycopodina*. *J. Nat. Prod.* **79**, 2718-2725.

244. S.L. Gande, K. Saxena, S. Sreeramuulu, V. Linhard, D. Kudlinzki, S. Heinzlmeir, A. J. Reichert, A. Skerra, B. Küster, **H. Schwalbe** (2016) Expression and purification of EPHA2 tyrosine kinase domain for crystallographic and NMR studies. *ChemBioChem* **17**, 2257-2263.

243. K. Stellos, A. Gatsiou, K. Stamatelopoulos, L.P. Matic, D. John, F.F. Lunella, N. Jaé, O. Roszbach, C. Amrhein, F. Sigala, R.A. Boon, B. Fürtig, Y. Manavski, X. You, S. Uchida, T. Keller, J.N. Boeckel, A. Franco-Cereceda, L. Maegdefessel, W. Chen, **H. Schwalbe**, A. Bindereif, P. Eriksson, U. Hedin, A.M. Zeiher, S. Dimmeler (2016) Adenosine-to-inosine RNA editing controls cathepsin S expression in atherosclerosis by enabling HuR-mediated post-transcriptional regulation. *Nature Med.* **22**, 1140-1150.

242. M. Kaushik, T. Bahrenberg, T.V. Can, M.A. Caporini, R. Silvers, J. Heiliger, A.A. Smith, **H. Schwalbe**, R.G. Griffin, B. Corzilius (2016)  $Gd^{III+}$  and  $Mn^{II+}$  complexes for dynamic nuclear polarization: small molecular chelate polarizing agents and applications with site-directed spin labeling of proteins. *Phys Chem Chem Phys.* **18**, 27205-27218 (in-side cover).

241. A. Chauhan, R. Paul, M. Debnath, I. Bessi, S. Mandal, **H. Schwalbe**, J. Dash (2016) Synthesis of fluorescent binaphthyl amines that bind c-myc G-quadruplex DNA and repress c-myc expression. *J. Med. Chem.* **59**, 7275-81.

240. W. Zhu, R. Silvers, **H. Schwalbe**, T. Keiderling (2016) Reduced and mutant lysozyme refolding with lipid vesicles. Model study of impact of disulfides on equilibria and dynamics. *Biochim. Biophys. Acta* **1864**, 1083-1092.

239. A.H. Nasiri, K. Saxena, J. W. Bats, H.R. Nasiri\*, **H. Schwalbe\*** (2016) Biophysical investigation and conformational analysis of p38 $\alpha$  kinase inhibitor doramapimod and its analogues. *MedChemCom*, **7**, 1421-1428.
238. M. Debnath, S. Ghosh, D. Panda, I. Bessi, **H. Schwalbe**, K. Bhattacharyya, J. Dash (2016) Small Molecule Regulated Dynamic Structural changes of Human G-quadruplexes. *Chemical Science* **7**, 3279-3285.
237. B. Fürtig\*, R. Schnieders, C. Richter, H. Zetzsche, S. Keyhani, C. Helmling, H. Kovacs, **H. Schwalbe\*** (2016) Direct <sup>13</sup>C-detected NMR Experiments for Mapping and Characterization of Hydrogen Bonds in RNA. *J. Biomol. NMR* **64**, 207-21.
236. J. Thevarpadam, I. Bessi, O. Binas, D.G. Schmidt, C. Slavov, H.R.A. Jonker, J. Wachtveitl, **H. Schwalbe\***, A. Heckel\* (2016) Photoresponsive Formation of an Intermolecular Minimal G-Quadruplex Motif. *Angew. Chem. Int. Ed.* **55**, 2738-2742.
235. F. Buhr, S. Jha, M. Thommen, J. Mittelstaet, F. Kutz, **H. Schwalbe\***, M. Rodnina\*, A. Komar\* (2016) Synonymous codons direct co-translational folding towards different protein conformations. *Mol. Cell* **61**, 341-351 (recommended by faculty1000).
234. Y. Pavan Kumar, P. Saha, D. Saha, I. Bessi, **H. Schwalbe**, S. Chowdhury, J. Dash (2016) Fluorescent Dansyl-guanosine conjugates that bind c-myc promotor G-quadruplex and down-regulate c-myc expression. *Chembiochem* **17**, 388-393.
233. F. Sochor, R. Silvers, D. Müller, C. Richter, B. Fürtig, **H. Schwalbe** (2016) <sup>19</sup>F-labeling of the adenine H2-site to study large RNAs by NMR spectroscopy. *J. Biomol. NMR* **64**, 63-74.
232. J. Heering, H.R.A. Jonker, F. Löhr, **H. Schwalbe**, V. Dötsch (2016) Structural investigations of the p53/p73 homologs from the tunicate species *Ciona intestinalis* reveal the sequence requirements for the formation of a tetramerization domain. *Protein Sci.* **25**, 410-22.
- 2015**
231. O. Schimming, V.L. Challinor, N.J. Tobias, H. Adihou, P. Grün, L. Pöschel, C. Richter, **H. Schwalbe**, H.B. Bode (2015) Structure, Biosynthesis, and Occurrence of Bacterial Pyrrolizidine Alkaloids. *Angew. Chem. Int. Ed.* **54**, 12702-5.
230. D. Chatterjee, C.E. Eckert, C. Slavov, K. Saxena, B. Fürtig, C.R. Sanders, V.V. Gurevich, J. Wachtveitl\*, **H. Schwalbe\*** (2015) Influence of arrestin on the photodecay of bovine rhodopsin. *Angew. Chem. Int. Ed.* **54**, 13555-60 (ranked as "very important paper")
229. D. Barthelmes, M. Gränz, K. Barthelmes, K.N. Allen, B. Imperiali, T. Prisner\*, **H. Schwalbe\*** (2015) Encoded Loop-Lanthanide-Binding Tags for Long-Range Distance Measurements in Proteins by NMR and EPR Spectroscopy. *J. Biomol. NMR* **63**, 275-82.
228. A. Scharow, M. Raab, K. Saxena, S. Sreeramulu, D. Kudlinzki, S. Gande, C. Dötsch, E. Kurunci-Csacsko, S. Kläger, B. Küster, **H. Schwalbe**, K. Strebhardt, T. Berg (2015) Optimized PIK1 PBD inhibitors based on Poloxin induce mitotic arrest and apoptosis in tumor cells. *ACS Chem Biol.* **10**, 2570-79.
227. D. Kudlinzki\*, V.L. Linhard, K. Saxena, S. Sreeramulu, S. Gande, U. Schieborr, M. Dreyer, **H. Schwalbe\*** (2015) High-resolution crystal structure of cAMP-dependent protein kinase from *Cricetulus griseus*. *Acta Crystallogr F Struct Biol Commun.* **71**, 1088-93.
226. D. Panda, M. Debnath, S. Mandal, I. Bessi, **H. Schwalbe**, J. Dash (2015) A Nucleus-Imaging Probe That Selectively Stabilizes a Minor Conformation of c-MYC G-quadruplex and Down-regulates c-MYC Transcription in Human Cancer Cells. *Sci Rep.* **5**, 13183.
225. J. Becker-Baldus, C. Bamann, K. Saxena, H. Gustmann, L.J. Brown, R.C.D. Brown, C. Reiter, E. Bamberg, J. Wachtveitl, **H. Schwalbe**, C. Glaubitz (2015) Enlightening the photoactive site of channelrhodopsin-2 by DNP-enhanced MAS NMR. *Proc. Natl. Acad. Sci. USA* **112**, 9896-901.

224. C. Helmling, S. Keyhani, F. Sochor, B. Fürtig, M. Hengesbach, **H. Schwalbe** (2015) Rapid NMR screening of RNA secondary structure and binding. *J. Biomol. NMR* **63**, 67-76..
223. D. Chatterjee, D. Kudlinzki, V. Linhard, K. Saxena, U. Schieberr, S.L. Gande, J.P. Wurm, J. Wöhnert, R. Abele, V.V. Rogov, V. Dötsch, H. Osiewacz, S. Sreeramulu\*, **H. Schwalbe\*** (2015) Structure and Biophysical Characterization of the S-adenosylmethionine Dependent O-methyltransferase PaMTH1, a Putative Enzyme Accumulating during Senescence of *Podospora anserina*. *J. Biol. Chem.* **290**, 16415-30.
222. L. Lannes, S. Halder, Y. Krishnan, **H. Schwalbe** (2015) Tuning the pH-response of i-motif DNA oligonucleotides. *ChemBioChem* **16**, 1647-1656.
221. I. Bessi, H.R.A. Jonker, C. Richter, **H. Schwalbe** (2015) Involvement of Long-Lived Intermediate States in the Complex Folding Pathway of the Human Telomeric G-Quadruplex. *Angew. Chem. Int. Ed.* **54**, 8444-8448.
220. D. Wagner, J. Rinnenthal, F. Narberhaus, **H. Schwalbe** (2015) Mechanistic insights into temperature-dependent regulation of the simple cyanobacterial hsp17 RNA thermometer at base pair-resolution. *Nucl. Acids Res.* **43**, 5572-5585.
219. R. Silvers, H. Keller, **H. Schwalbe\***, M. Hengesbach\* (2015) Differential Scanning Fluorimetry for Monitoring RNA Stability. *ChemBioChem* **16**, 1109-1114 (inside cover).
218. H.R. Nasiri\*, J. Ferner, C. Tükek, R. Krishnathas, **H. Schwalbe\*** (2015) A concise one-step synthesis of primin and iso-primin. *Tetrahedron Lett.* **56**, 2231-2233.  
(featured in <http://pubs.acs.org/doi/pdf/10.1021/jacs.6b08856>)
217. C. Özçoban, T. Halbritter, S. Steinwand. L.-M. Herzig, J. Kohl-Landgraf, N. Askari, F. Groher, B. Fürtig, C. Richter, **H. Schwalbe**, B. Suess, J. Wachtveitl, A. Heckel (2015) Water-Soluble Py-BIPS Spiropyrans as Photoswitches for Biological Applications. *Organic Letters* **17**, 1517-20.
216. N. Bruns, W. Collisi, S. Bernecker, M. Stadler, C. Richter, **H. Schwalbe**, M. Kalesse (2015) Spirangien Derivatives from the Myxobacterium *Sorangium cellulosum*: Isolation, Structure Elucidation, and Biological Activity. *European Journal of Organic Chemistry* **4**, 847-857.
215. S. Toal, N. Kubatova, C. Richter, V. Linhardt, **H. Schwalbe**, R. Schweitzer-Stenner (2015) Randomizing the unfolded state of peptides (and proteins) by nearest neighbor interactions between unlike residues. *Chemistry* **21**, 5173-5192 (hot paper).
214. F. Buhr, J. Kohl-Landgraf, S. tom Dieck, C. Hanus, D. Chatterjee, A. Hegelein, E.M. Schuman, J. Wachtveitl, **H. Schwalbe** (2015) Design of photocaged puromycin for nascent polypeptide release and spatiotemporal monitoring of translation. *Angew. Chem. Intl. Ed.* **54**, 3717-21.
213. L. Danne, M. Aktas, J. Gleichhagen, D. Wagner, **H. Schwalbe**, B. Hoffknecht, N. Metzler-Nolte, F. Narberhaus (2015) Membrane-binding mechanism of a bacterial phospholipid *N*-methyltransferase. *Molecular Microbiology* **95**, 313-331.
212. V. Zickermann, C. Wirth, H. Nasiri, K. Siegmund, **H. Schwalbe**, C. Hunte, U. Brandt (2015) Mechanistic insight from the crystal structure of mitochondrial complex I. *Science* **347**, 44-49.
211. J. Rinnenthal, D. Wagner, T. Marquardsen, A. Krahn, F. Engelke, **H. Schwalbe** (2015) A temperature-jump NMR probe setup using rf heating optimized for the analysis of temperature-induced biomacromolecular kinetic processes. *J. Magn. Reson.* **251**, 84-93.
- 2014**
210. M. Zeiger, S. Stark, E. Kalden, B. Ackermann, J. Ferner, U. Scheffer, F. Shoja-Bazargani, V. Erdel, **H. Schwalbe**, M.W. Göbel (2014) Fragment based search for small molecule inhibitors of HIV-1 Tat-TAR. *Bioorg. Med. Chem. Lett.* **24**, 5576-80.
209. P. Rehbein, **H. Schwalbe** (2014) Integrated protocol for reliable and fast quantification and documentation of electrophoresis gels from expression screenings. *Prot. Exp. Purif.* **S1046-5928**, 00291-5.

208. S. Nozinovic, A. Reining, Y.-B. Kim, J. Noeske, K. Schlepckow, J. Wöhnert, **H. Schwalbe** (2014) The importance of helix P1 stability for structural pre-organization and ligand binding affinity of the adenine riboswitch aptamer domain. *RNA Biology* **11**, 655-666.
207. P. Rehbein, K. Saxena, K. Schlepckow\*, **H. Schwalbe\*** (2014) Protocol for aerosol-free recombinant production and NMR analysis of prion proteins. *J. Biomol. NMR* **59**, 111-117.
206. J. Schilder, F. Löhr, **H. Schwalbe**, M. Ubbink (2014) The cytochrome c peroxidase and cytochrome c encounter complex: The other side of the story. *FEBS Letters* **588**, 1873-1878. See also: Corrigendum: *FEBS Lett* (2015) **589**, 2169.
205. C. Helmling, I. Bessi, A. Wacker, K. A. Schnorr, H.R.A. Jonker, C. Richter, D. Wagner, M. Kreibich, **H. Schwalbe** (2014) Non-covalent spin labeling of riboswitch RNA to obtain long-range NMR structural restraints. *ACS Chem. Biol.* **9**, 1330-1339.
204. P. Sripakdeevong, M. Cevec, A. Chang, M. Erat, M. Ziegeler, Q. Zhao, G. Fox, X. Gao, S. Kennedy, R. Kierzek, E. Nikonowicz, **H. Schwalbe**, R. Sigel, D. Turner, R. Das (2014) Structure determination of noncanonical RNA motifs guided by <sup>1</sup>H NMR chemical shifts. *Nature Methods* **11**, 413-416.
203. J. Kohl-Landgraf, F. Buhr, D. Lefrancois, J. Mewes, **H. Schwalbe**, J. Wachtveitl, A. Dreuw (2014) Mechanism of the Photoinduced Uncaging Reaction of Puromycin Protected by a 6-Nitroveratryloxycarbonyl Group. *J. Am. Chem. Soc.* **136**, 3430-3438.
202. J. Stehle, R. Silvers, K. Werner, D. Chatterjee, S. Gande, F. Scholz, A. Dutta, J. Wachtveitl, J. Klein-Seetharaman, **H. Schwalbe** (2014) Solution NMR characterization of simultaneous meta II and meta III decay kinetics in rhodopsin. *Angew. Chem. Intl. Ed.* **53**, 2078-2084.
201. H. Steinert, F. Schäfer, H. R.A. Jonker, A. Heckel\*, **H. Schwalbe\*** (2014) Influence of the absolute configuration of NPE-caged cytosine on DNA single base pair stability. *Angew. Chem. Intl. Ed.* **53**, 1072-1075.
- 2013**
200. H. Nasiri, M. Madej, R. Panisch, J. Bats, M. Lafontaine, C.R. Lancaster, **H. Schwalbe** (2013) Design, Synthesis and Biological Testing of Novel Naphthoquinones as Substrate-Based Inhibitors of the Quinol:Fumarate Reductase from *Wolinella succinogenes*. *J. Med. Chem.* **56**, 9530-9541.
199. K. Schlepckow, **H. Schwalbe** (2013) Molecular Mechanism of Prion Protein Oligomerization at Atomic Resolution. *Angew. Chem. Intl. Ed.* **52**, 10002-10005 (VIP paper).
198. Y. Hiruma, M.A.S. Hass, Y. Kikui, W.-M. Liu, B. Ölmez, S.P. Skinner, A. Blok, A. Klosterman, H. Koteishi, F. Löhr, **H. Schwalbe**, M. Nojiri, M. Ubbink (2013) The Structure of the Cytochrome P450cam-Putidaredoxin Complex Determined by Paramagnetic NMR Spectroscopy and Crystallography. *J. Mol. Biol.* **425**, 4353-4365.
197. U. Schieborr, S. Sreeramulu, B. Elshorst, M. Maurer, K. Saxena, D. Kudlinzki, S. Gande, **H. Schwalbe** (2013) MOTOR: Model assisted Software for NMR Structure Determination. *Proteins* **81**, 2007-2022 (cover of the journal).
196. Y. P. Kumar, S. Bhowmik, R. N. Das, I. Bessi, S. Paladhi, R. Ghosh, **H. Schwalbe**, J. Dash (2013) A fluorescent guanosine dinucleoside as a selective switch-on sensor for c-myc G-quadruplex DNA with potent anticancer activities. *Chemistry – A European Journal* **19**, 11502-11506 (cover of the journal).
195. A. Reining, S. Nozinovic, K. Schlepckow, F. Buhr, B. Fürtig, **H. Schwalbe** (2013) Three-state mechanism couples ligand and temperature sensing in riboswitches. *Nature* **499**, 355-359 (see also highlighted in *Nature*: R. Micura: RNA biophysics: A three-state balancing act 499, 289-290, see also highlighted in *Nature*: F. Narberhaus: RNAs at fiver pitch 502, 178-9, see also: recommended by Faculty 1000).
194. G. Nielsen, H.R.A. Jonker, N. Vajpaj, S. Grzesiek, **H. Schwalbe** (2013) Kinase in motion: insights into the dynamic nature of p38 $\alpha$  by high pressure NMR spectroscopic studies. *ChemBioChem* **14**, 1799-1806.
193. A.L. Lieblein, B. Fürtig, **H. Schwalbe** (2013) Optimizing kinetics and thermodynamics of DNA i-motif folding. *ChemBioChem* **14**, 1226-1230.



192. C. Herbert, U. Schieborr, K. Saxena, J. Juraszek, F. De Smet, C. Alcouffe, M. Bianciotto, G. Saladino, D. Sibrac, D. Kudlinzki, S. Sreeramulu, A. Brown, P. Rigon, J.-P. Herault, G. Lassalle, T.L. Blundell, F. Rousseau, A. Gils, J. Schymkowitz, P. Tompa, J.-M. Herbert, P. Carmeliet, F.L. Gervasio\*, **H. Schwalbe\***, F. Bono\* (2013) Molecular mechanism of SSR128129E, an extracellularly acting, small molecule, allosteric inhibitor of FGF receptor signaling. *Cancer Cell* **23**, 489-501 (featured in *Nat. Chem. Biol.*).

191. F. Bono, F. De Smet, C. Herbert, K. De Bock, M. Georgiadou, P. Fons, M. Tjwa, C. Alcouffe, A. Ny, M. Bianciotto, B. Jonckx, M. Murakami, A. A. Lanahan, C. Michielsen, D. Sibrac, F. Dol-Gleizes, M. Mazzone, S. Zacchigna, J.-P. Herault, C. Fischer, P. Rigon, C. Ruiz de Almodovar, F. Claes, I. Blanc, K. Poesen, J. Zhang, I. Segura, G. Gueguen, M.-F. Bordes, D. Lambrechts, R. Broussy, M. van de Wouwer, C. Michaux, T. Shimada, I. Jean, S. Blacher, A. Noel, P. Motte, E. Rom, J.-M. Rakic, S. Katsuma, P. Schaeffer, A. Yayon, A. Van Schepdael, **H. Schwalbe**, F.L. Gervasio, G. Carmeliet, J. Rozensky, M. Dewerchin, M. Simons, A. Christopoulos, J.-M. Herbert, P. Carmeliet (2013) Inhibition of tumor angiogenesis and growth by a small – molecule multi-FGF receptor blocker with allosteric blockers. *Cancer Cell* **23**, 477-488.

190. J.A. Guan, P. Keizers, W.-M. Liu, F. Löhr, S. Skinner, E. Heeneman, **H. Schwalbe**, M. Ubbink, G. Siegal (2013) Small molecule binding sites on proteins established by paramagnetic NMR spectroscopy. *J. Am. Chem. Soc.* **135**, 5859-5869 (special significance by Faculty 1000).

189. R. Schweizer-Stenner, A. Hagarmann, S. Toal, D. Mathieu, **H. Schwalbe** (2013) Disorder and order in unfolded and disordered peptides and proteins: A view derived from tripeptide conformational analysis. I. Tripeptides with long and predominantly hydrophobic side chains. *Proteins* **81**, 955-967.

188. K. Rybka, S.E. Toal, D.J. Verbaro, D. Mathieu, **H. Schwalbe**, R. Schweizer-Stenner (2013) Disorder and order in unfolded and disordered peptides and proteins: A view derived from tripeptide conformational analysis. II. Tripeptides with short side chains populating  $\alpha$  and  $\beta$ -type like turn conformation. *Proteins* **81**, 968-983.

187. U. Schieborr, K. Saxena, B. Elshorst, **H. Schwalbe** (2013)  $^1\text{H}$ ,  $^{13}\text{C}$ , and  $^{15}\text{N}$  assignment of D2 domain of human fibroblast growth factor receptor 4. *Biomolecular NMR Assignments* **7**, 179-182.

## 2012

186. J. Stehle, F. Scholz, F. Löhr, S. Reckel, C. Roos, M. Blum, M. Braun, C. Glaubitz, V. Dötsch, J. Wachtveitl, **H. Schwalbe** (2012) Characterization of the ground state dynamics of proteorhodopsin by NMR and Optical Spectroscopies. *J. Biomol. NMR* **54**, 401-413.

185. R. Silvers, K. Saxena, D. Kudlinzki, **H. Schwalbe** (2012) Recombinant expression and purification of human TATA binding protein using a chimeric fusion. *Protein Expression and Purification* **85**, 142-147.

184. T. Stehle, Sridhar Sreeramulu, Frank Löhr, Christian Richter, Krishna Saxena, H.R.A. Jonker, **H. Schwalbe** (2012) The apo-structure of the low-molecular-weight protein tyrosine phosphatase A (MtpA) from *Mycobacterium tuberculosis* allows for better target-specific drug development. *J. Biol. Chem.* **287**, 34569-34582.

183. M. Ziegeler, M. Cevec, C. Richter, **H. Schwalbe** (2012) NMR Studies of HAR1 RNA Secondary Structures Reveal Conformational Dynamics in the Human RNA. *ChemBioChem* **13**, 2100-2112. (inside cover)

182. D.J. Verbaro, D. Mathieu, S.E. Toal, **H. Schwalbe**, R. Schweitzer-Stenner (2012) Ionized Trilycine: A Model System for Understanding the Non-Random Structure of Poly-L-Lysine and Lysine-Containing Motifs in Proteins. *J. Phys. Chem. B*, **116**, 8084-8094.

181. P. Rogne, P. Ozdowy, C. Richter, K. Saxena, **H. Schwalbe**, L. Kuhn (2012) Atomic-level structure characterization of an ultrafast folding mini-protein denatured state. *Plos One* **7**, e41301.

180. I. Bessi, C. Bazzicalupi, C. Richter, H.R.A. Jonker, K. Saxena, C. Sissi, M. Chioccioli, S. Bianco, A.R. Billia, **H. Schwalbe**, P. Gratteri (2012) Spectroscopic, molecular modeling and NMR-spectroscopic investigation of the binding mode of the natural alkaloids berberine and sanguinarine to human telomeric G-quadruplex DNA. *ACS Chemical Biology* **7**, 1109-1119.

179. A. Wacker, J. Buck, C. Richter, **H. Schwalbe**, J. Wöhnert (2012) Mechanisms for differentiation between cognate and near-cognate ligands by purine riboswitches. *RNA Biology* **9**, 672-680.
178. F. Sziegat, R. Silvers, M. Hähnke, M. Jensen, M. Blackledge, J. Wirmer-Bartoschek, **H. Schwalbe** (2012) Disentangling the coil: New insights into non-native protein states investigated by nuclear magnetic resonance spectroscopy. *Biochemistry* **51**, 3361-3372.
177. H. Angerer, H. R. Nasiri, V. Niedergesäß, S. Kirscher, **H. Schwalbe**, U. Brandt (2012) Tracing the tail of ubiquinone in mitochondrial complex I. *BBA Bioenergetics* **85**, 142-147.
176. R. Silvers, F. Sziegat, H. Tachibana, S.-I. Segawa, S. Whittaker, U. Günther, F. Gabel, J. Huang, M. Blackledge, J. Wirmer-Bartoschek, **H. Schwalbe** (2012) Modulation of Structure and Dynamics by Disulfide Bond Formation in Unfolded States. *J. Am. Chem. Soc.* **134**, 6846-6854 (special significance by Faculty 1000).
175. A.L. Lieblein, M. Krämer, A. Dreuw, B. Fürtig, **H. Schwalbe** (2012) The nature of the hydrogen bonds in Cytidine-H<sup>+</sup>-Cytidine DNA base pairs. *Angew. Chem. Int. Ed. Engl.* **51**, 4067-4070.
174. H. Steinert, J. Rinnenthal, **H. Schwalbe** (2012) Individual basepair stability of DNA and RNA studied by NMR-detected solvent exchange. *Biophysical J.* **102**, 2564-2574.
173. A.L. Lieblein, J. Buck, K. Schlepckow, B. Fürtig, **H. Schwalbe** (2012) Time-resolved NMR studies of DNA i-motif folding reveal kinetic partitioning. *Angew. Chem. Int. Ed. Engl.* **51**, 250-253. Zeitaufgelöste NMR-Untersuchungen zeigen einen kinetischen Partitionierungsmechanismus während der Faltung des DNA i-Motifs. *Angew. Chem.* **124**, 255-259.
172. A. Rosato, J.M. Aramini, C. Arrowsmith, A. Bagaria, D. Baker, A. Cavalli, J.F. Doreleijers, A. Eletsy, A. Giachetti, P. Guerry, A. Gutmanas, P. Güntert, Y. He, T. Herrmann, Y.J. Huang, V. Jaravine, H.R.A. Jonker, M.A. Kennedy, O.F. Lange, G. Liu, T.E. Malliavin, R. Mani, B. Mao, G.T. Montelione, M. Nilges, P. Rossi, G. van der Schot, **H. Schwalbe**, T.A. Szyperski, M. Vendruscolo, R. Vernon, W.F. Vranken, S. de Vries, G.W. Vuister, B. Wu, Y. Yang, A.M.J.J. Bonvin (2012) Blind testing of routine, fully automated determination of protein structures from NMR data. *Structure* **20**, 227-236.
- 2011**
171. J. Kortmann, S. Sczodrok, J. Rinnenthal, **H. Schwalbe**, F. Narberhaus (2011) Translation on demand by a simple RNA-based thermosensor. *Nucleic Acids Res.* **39**, 2855-2868.
170. K. Barthelmes, A. Reynolds, E. Peizach, H.R.A. Jonker, N. Denunzio, K. Allen\*, B. Imperiali\*, **H. Schwalbe\*** (2011) Engineering encodable lanthanide-binding tags (LBTs) into loop positions of proteins. *J. Am. Chem. Soc.* **133**, 808-819 (special significance by Faculty 1000).
169. N.E. Englert, C. Richter, J. Wiesner, M. Hintz, H. Jomaa, **H. Schwalbe** (2011) NMR studies of DOXP reductoisomerase and its inhibitor complexes. *ChemBioChem*, **12**, 468-476.
168. H.R.A. Jonker, S. Baumann, A. Wolf, S. Schoof, F. Hiller, K.W. Schulte, K.N. Kirschner, **H. Schwalbe**, H.-D. Arndt (2011) NMR structures of thiostrepton derivatives report target shape recognition. *Angew. Chem. Int. Ed. Engl.* **50**, 3308-3312.
167. A. Hagarman, D. Mathieu, S. Toal, T.J. Measey, **H. Schwalbe**, R. Schweitzer-Stenner (2011) Amino Acids with Hydrogen Bonding Side Chains have an Intrinsic Tendency to Sample Various Turn Conformations in Aqueous Solution. *Chemistry, A European Journal* **17**, 6789-97.
166. S. Nozinovic, P. Gupta, B. Fürtig, C. Richter, S. Tüllmann, E. Ferner-Duchardt, M. Holthausen, **H. Schwalbe** (2011) 2'-OH group conformation in RNA derived from NMR spectroscopy and DFT calculations. *Angew. Chem. Int. Ed. Engl.* **50**, 5397-400; Konformationsbestimmung der 2'OH-Gruppe in RNA durch NMR-Spektroskopie und Dichtefunktionalrechnungen. *Angew. Chem.* **123**, 5509-5512.
165. F. Sziegat, J. Wirmer-Bartoschek, **H. Schwalbe** (2011) Unfolded state characteristics of Human Lysozyme and its disease related mutants. *Angew. Chem. Int. Ed. Engl.* **50**, 5514-5518.

164. A. Wacker, J. Buck, D. Mathieu, C. Richter, J. Wöhnert, **H. Schwalbe** (2011) Structure and dynamics of the deoxyguanosine-sensing riboswitch studied by NMR spectroscopy. *Nucleic Acids Res.* **39**, 6802-6812.
163. J. Rinnenthal, Birgit Klinkert, F. Narberhaus, **H. Schwalbe** (2011) Modulation of the stability of the Salmonella fourU-type RNA thermometer. *Nucleic Acids Res.* **39**, 8258-8270
162. J. Buck, A. Wacker, E. Warkentin, J. Wöhnert, J. Wirmer-Bartoschek, **H. Schwalbe** (2011) Influence of ground-state structure and Mg<sup>2+</sup> binding on folding kinetics of the guanine-sensing riboswitch aptamer domain. *Nucleic Acids Res.* **39**, 9768-9778
161. D. B. Salvatore, N. Duraffourg, A. Favier, B.A. Persson, M. Lund, M. Delage, R. Silvers, **H. Schwalbe**, T. Croguennec, S. Bouhallab, V. Forge (2011) Investigation at residue level of the early steps during the assembly of two proteins into supramolecular objects. *Biomacromolecules* **12**, 2200-2210.
160. G. Nielsen, **H. Schwalbe** (2011) NMR spectroscopic investigations of the activated p38alpha mitogen-activated kinase. *ChemBioChem* **12**, 2599-2607.
159. S. Reckel, D. Gottstein, J. Stehle, F. Löhr, M.-K. Verhoefen, M. Takeda, R. Silvers, M. Kainosho, C. Glaubitz, J. Wachtveitl, F. Bernhard, **H. Schwalbe**, P. Güntert, V. Dötsch (2011) Solution NMR structure of proteorhodopsin. *Angew. Chem. Int. Ed. Engl.* **50**, 11942-11946.
- 2010**
158. A. Hagarman, T. Measey, D. Mathieu, **H. Schwalbe**, R. Schweitzer-Stenner (2010) Intrinsic Propensities of Amino Acid Residues in GXG peptides Inferred from Amide I' Band Profiles and NMR Scalar Coupling Constants. *J. Am. Chem. Soc.* **132**, 540–551.
157. S. Nozinovic, B. Fürtig, H.R.A. Jonker, C. Richter, **H. Schwalbe** (2010) High-Resolution NMR Structure of a RNA model system: the 14mer cUUCGg tetraloop hairpin RNA. *Nucleic Acids Res.* **38**, 683-694.
156. M. Hähnke, C. Richter, F. Heinicke, **H. Schwalbe** (2010) The HN(COCA)HAHB-NMR Experiment for the Stereospecific Assignment of Hbeta-Protons in Non-native States of Proteins. *J. Am. Chem. Soc.* **132**, 918-919.
155. A. Doller, K. Schlepckow, **H. Schwalbe**, J. Pfeilschifter, W. Eberhardt (2010) Tandem phosphorylation of serine 221 and 318 by PKC d coordinates mRNA binding and nucleo-cytoplasmic shuttling of HuR. *Mol. Cell. Biol.* **30**, 1397-1410. See also: Corrigendum: doi: 10.1128/MCB.00151-17
154. J. Buck, J. Noeske, J. Wöhnert, **H. Schwalbe** (2010) Mg<sup>2+</sup> compensates for a missing long-range tertiary interaction in the guanine-sensing riboswitch aptamer domain. *Nucleic Acids Res.* **38**, 4143-4153.
153. J. Rinnenthal, B. Klinkert, F. Narberhaus, **H. Schwalbe** (2010) Direct observation of the temperature induced melting process of the Salmonella fourU RNA thermometer at base-pair resolution. *Nucleic Acids Res.* **38**, 3834–3847. (cover, featured article).
152. J. Kumar, S. Sreeramulu, T.-L. Schmidt, C. Richter, J. Vonck, A. Heckel, C. Glaubitz, **H. Schwalbe** (2010) Structural rearrangement during amyloid fibril formation of the human prion protein. *ChemBioChem* **11**, 1208-1213.
151. S. Nozinovic, C. Richter, J. Rinnenthal, B. Fürtig, E. Duchardt-Ferner, J.E. Weigand, **H. Schwalbe** (2010) Quantitative 2D and 3D Gamma-HCP Experiments for the Determination of the Angles alpha and zeta in the Phosphodiester Backbone of Oligonucleotides. *J. Am. Chem. Soc.* **132**, 10318-10329.
150. A. Cherepanov, C. Glaubitz, **H. Schwalbe** (2010) Hochauflösende Festkörper-NMR-Spektroskopie an <sup>13</sup>C,<sup>15</sup>N-markierter RNA. *Angew. Chem.* **122**, 4855–4859. A. Cherepanov, C. Glaubitz, **H. Schwalbe** (2010) High-Resolution Studies of Uniformly <sup>13</sup>C,<sup>15</sup>N-labeled RNA by Solid State NMR Spectroscopy. *Angew. Chem. Int. Ed. Engl.* **48**, 4747-4750.
149. C. Gerum, K. Schlepckow, **H. Schwalbe** (2010) The Unfolded State of the Murine Prion Protein and Properties of single-point mutants related to human prion diseases. *J. Mol. Biol.* **401**, 7-12.

148. C. Richter, H. Kovacs, J. Buck, A. Wacker, B. Fürtig, **H. Schwalbe** (2010)  $^{13}\text{C}$ -direct detected NMR experiments for the sequential J-based resonance assignment of RNA oligonucleotides. *J. Biomol. NMR* **47**, 259-269.

147. K. Saxena, U. Schieborr, O. Anderka, E. Duchardt-Ferner, B. Elshorst, S.L. Gande, J. Janzon, D. Kudlinzki, S. Sreeramulu, M.K. Dreyer, K.U. Wendt, C. Herbert, P. Duchaussoy, M. Bianciotto, P-A. Dirguez, G. Lassalle, P. Savi, M. Mohammadi, F. Bono, **H. Schwalbe** (2010) Influence of heparin mimetics on the assembly of the FGF - FGFR4 signaling complex. *J. Biol. Chem.* **283**, 26628-26640.

146. B. Fürtig, P. Wenter, S. Pitsch, **H. Schwalbe** (2010) Probing mechanism and transition state of RNA refolding. *ACS Chemical Biology* **5**, 753-765.

145. R. Dastvan, B. Bode, M.P.R. Karuppijaj, A. Marko, S. Lyubenova, **H. Schwalbe**, T. Prisner (2010) Optimization of Transversal Relaxation of Nitroxides for PELDOR Spectroscopy in Phospholipid Membranes. *J. Phys. Chem. B* **114**, 13507-16.

144. S. Cao, B. Fürtig, **H. Schwalbe**, S.J. Chen (2010) Folding Kinetics for the Conformational Switch between Alternative RNA Structures. *J. Phys. Chem. B* **114**, 13609-13615.

## 2009

143. H.D. Juhnke, H. Hiltcher, H.R. Nasiri, **H. Schwalbe**, C.R.D. Lancaster (2009) Production, Characterization, and Determination of the Real Catalytic Properties of the Putative 'Succinate Dehydrogenase' from *Wolinella succinogenes*. *Molecular Microbiology* **71**, 1088-1101.

142. H.R. Nasiri, R. Panisch, M.G. Madej, J.W. Bats, C.R.D. Lancaster, **H. Schwalbe** (2009) The Correlation of Cathodic Peak Potentials of Vitamin K3 Derivatives and Their Calculated Electron Affinities. The Role of Hydrogen Bonding and Conformational Changes. *Biochim Biophys Acta.* **1787**, 601-608.

141. S. Rehm, S. Han, I. Hassani, A. Sokocevic, H.R.A. Jonker, J.W. Engels, **H. Schwalbe** (2009) The high resolution NMR structure of Parvulostat (Z-2685) from *Streptomyces parvulus* FH-1641. Comparison with Tendamistat from *Streptomyces tendae* 4158. *ChemBioChem* **10**, 119-127.

140. S. Sreeramulu, H.R.A. Jonker, T. Langer, C. Richter, C.R.D. Lancaster, **H. Schwalbe** (2009) The human CDC37-HSP90 Complex studied by heteronuclear NMR spectroscopy. *J. Biol. Chem.* **284**, 3885-3896.

139. S. Tayefeh, T. Kloss, M. Kreim, M. Gebhardt, D. Baumeister, B. Hertel, C. Richter, **H. Schwalbe**, A. Moroni, G. Thiel, S.M. Kast (2009) Model Development for the viral Kcv potassium channel. *Biophysical J.* **96**, 485-498.

138. F.G. Hermann, L. Egerer, F. Brauer, C. Gerum, **H. Schwalbe**, U. Dietrich, D. von Laer (2009) Mutations in gp120 contribute to resistance of 1 HIV-1 against the membrane-anchored C-peptide maC46. *J. Virol.* **83**, 4844-4853.

137. V. Manoharan, B. Fürtig, A. Jäschke, **H. Schwalbe** (2009) Metal-induced folding of Diels-Alderase ribozymes studied by static and time-resolved NMR spectroscopy. *J. Am. Chem. Soc.* **131**, 6261-6270.

136. J. Ferner, M. Suhartono, S. Breitung, H.R.A. Jonker, M. Hennig, J. Wöhnert, M. Göbel, **H. Schwalbe** (2009) Structures of HIV TAR RNA-ligand complexes reveal higher stoichiometries. *ChemBioChem* **15**, 1490-1494.

135. J. Rinnenthal, **H. Schwalbe** (2009) HNHC: a triple resonance experiment for correlating the H2, N1(N3) and C2 resonances in adenine nucleobases of  $^{13}\text{C}$ ,  $^{15}\text{N}$ -labeled RNA oligonucleotides. *J. Biomol. NMR* **44**, 101-105.

134. S. Sreeramulu, S.L. Gande, M. Göbel, **H. Schwalbe** (2009) Molecular mechanism of inhibition of the human protein complex Cdc37-Hsp90, a kinome chaperone-cochaperone, by triterpene celastrol. *Angew. Chem. Intl. Ed. Engl.* **48**, 5853-5855.

133. J. Rinnenthal, C. Richter, S. Nozinovic, B. Fürtig, J.J. Lopez, C. Glaubitz, **H. Schwalbe** (2009) RNA phosphodiester backbone dynamics of a perdeuterated cUUCGg tetraloop RNA from phosphorus-31 NMR relaxation analysis. *J. Biomol. NMR* **45**, 143-155.

132. J. Buck, Y.-L. Li, C. Richter, J. Vergne, M.-C. Maurel, **H. Schwalbe** (2009) NMR-spectroscopic characterization of the adenine-dependent hairpin ribozyme. *ChemBioChem* **10**, 2100-2110.

131. C. Gerum, R. Silvers, J. Wirmer-Bartoschek, **H. Schwalbe** (2009) Unfolded State Structure and Dynamics Influence Fibril Formation of Human Prion Protein. *Angew. Chem.* **121**, 9616-9620.

130. R. Hänsel, S. Foldynova-Trantarkova, F. Löhr, J. Buck, E. Bongartz, E. Bamberg, **H. Schwalbe**, V. Doetsch, L. Trantirek (2009) Evaluation of parameters critical for observing nucleic acids inside living *Xenopus laevis* oocytes by in-cell NMR spectroscopy. *J. Am. Chem. Soc.* **31**, 15761-15768.

## 2008

129. J. Dietz, J. Koch, A. Kaur, C. Raja, S. Stein, M. Grez, A. Pustowka, S. Mensch, J. Ferner, L. Müller, N. Bannert, R. Tampé, G. Divita, Y. Mely, **H. Schwalbe**, U. Dietrich (2008) Inhibition of HIV-1 by a peptide ligand of the genomic RNA packaging signal psi. *ChemMedChem* **3**, 749-755.

128. J. Ferner, A. Villa, E. Duchardt, E. Widjajakusuma, J. Wöhnert, G. Stock, **H. Schwalbe** (2008) NMR and MD studies of the temperature-dependent dynamics of RNA YNMG-tetraloops. *Nucleic Acids Res.* **36**, 1928-1940.

127. B. Fürtig, C. Richter, P. Schell, P. Wenter, S. Pitsch, **H. Schwalbe** (2008) NMR-spectroscopic characterization of phosphodiester bond cleavage catalyzed by the minimal hammerhead ribozyme. *RNA Biology* **5**, 41-48.

126. A. Nören-Müller, W. Wilk, K. Saxena, **H. Schwalbe**, M. Kaiser, H. Waldmann (2008) Discovery of a new class of mycobacterium tuberculosis protein tyrosine phosphatase B inhibitors by Biology driven synthesis (BIOS). *Angew. Chem. Int. Ed. Engl.* **47**, 5973-5977.

125. N. Cramer, S. Helbig, A. Baro, S. Laschat, R. Diestel, F. Sasse, D. Mathieu, C. Richter, G. Kummerlöwe, B. Luy, **H. Schwalbe** (2008) Synthesis and biological properties of cylindramide derivatives: evidence for Calcium-dependent cytotoxicity of tetramic acid lactams. *ChemBioChem* **9**, 2474-2486.

124. K. Werner, C. Richter, J. Klein-Seetharaman, **H. Schwalbe** (2008) Isotope labeling of mammalian GPCRs in HEK293 cells and characterization of the C-terminus of bovine rhodopsin by high-resolution liquid NMR spectroscopy. *J. Biomol. NMR* **40**, 49-53.

123. J.J. Lopez, A.K. Shukla, C. Reinhart, **H. Schwalbe**, H. Michel, C. Glaubitz (2008) The structure of the neuropeptide bradykinin bound to the human G-protein coupled receptor bradykinin B2 as determined by solid-state NMR. *Angew. Chem. Intl. Ed. Engl.* **47**, 1668-1671.

122. A. Gieldon, J.J. Lopez, C. Glaubitz, **H. Schwalbe** (2008) A Molecular Dynamics Study of the Human Bradykinin - Bradykinin B2 Receptor Complex Supported by Solid-State NMR Spectroscopy Data. *ChemBioChem* **9**, 2487-2497.

121. N. R. Silvaggi, L.J. Martin, **H. Schwalbe**, B. Imperiali, K.N. Allen (2008) Double lanthanide-binding tags for macromolecular crystallographic structure determination. *J. Am. Chem. Soc.* **129**, 7114-7120.

120. A.N. Koller, **H. Schwalbe**, H. Gohlke (2008) Starting structure dependence of NMR order parameters derived from MD simulations: Implications for judging force field quality. *Biophysical J.* **95**, L04-6.

119. K. Schlepckow, J. Wirmer, A. Bachmann, T. Kiefhaber, **H. Schwalbe** (2008) Conserved folding pathways of alpha-lactalbumin and lysozyme revealed by kinetic CD, fluorescence, NMR and interrupted refolding experiments. *J. Mol. Biol.* **378**, 686-698.

118. C. Schroeder, K. Werner, H. Otten, S. Krätzig, **H. Schwalbe**, L.-O. Essen (2008) Influence of a joining helix on the BLUF Domain of the YcgF photoreceptor from *Escherichia coli*. *ChemBioChem* **9**, 2463-2473.

117. H.R. Nasiri, M. Bolte, **H. Schwalbe** (2008) Electrochemical and crystal structural analysis of alpha- and dehydro-alpha-lapachones. *Nat Prod Res.* **22**, 1231-1236.

## 2007

116. S. Haber-Pohlmeier, K. Abarca-Heidemann, H.G. Körschen, H. Kaur Dhiman, J. Heberle, **H. Schwalbe**, J. Klein-Seetharaman, U.B. Kaupp, A. Pohlmeier (2007) Binding of  $\text{Ca}^{2+}$  to glutamic Acids rich polypeptides from the rod outer segment. *Biophysical J.* **92**, 3207-3214.

115. J. Graf, P.H. Nguyen, G. Stock, **H. Schwalbe** (2007) Structure and Dynamics of the Homologous Series of Alanine Peptides: A Joint Molecular-Dynamics/NMR Study. *J. Am. Chem. Soc.* **129**, 1179-1189.

114. O.I. Obolensky, K. Schlepckow, **H. Schwalbe**, A.V. Solovjov (2007) Theoretical framework of NMR residual dipolar couplings in unfolded proteins. *J. Biomol. NMR* **39**, 1-16.

113. E. Duchardt, A. B. Sigalov, D. Aivazian, L.J. Stern, **H. Schwalbe** (2007) Structural changes of the T-cell receptor Zeta-chain upon lipid binding investigated by NMR. *ChemBioChem* **8**, 820-827.

112. J. Noeske, J. Buck, B. Fürtig, H. Nasiri, **H. Schwalbe**, J. Wöhnert (2007) Interplay of 'induced fit' and preorganization in the ligand-induced folding of the aptamer domain of the guanine binding riboswitch. *Nucleic Acids Res.* **35**, 572-583.

111. H.R.A. Jonker, S. Ilin, S.K. Grimm, J. Wöhnert, **H. Schwalbe** (2007) L11 domain rearrangement upon binding to RNA and thiostrepton studied by NMR spectroscopy. *Nucleic Acids Res.* **35**, 441-454.

110. J. Noeske, **H. Schwalbe**, J. Wöhnert (2007) Metal-ion binding and metal-ion induced folding of the adenine-sensing riboswitch aptamer domain. *Nucleic Acids Res.* **35**, 5262-5273.

109. J. Buck, B. Fürtig, J. Noeske, J. Wöhnert, **H. Schwalbe** (2007) Time-resolved NMR methods resolving ligand-induced RNA folding at atomic resolution. *Proc. Natl. Acad. Sci. U.S.A.* **104**, 15699-15704.

108. B. Fürtig, P. Wenter, L. Reymond, C. Richter, S. Pitsch, **H. Schwalbe** (2007) Conformational Dynamics of bistable RNAs studied by time-resolved NMR spectroscopy. *J. Am. Chem. Soc.* **129**, 16222-16229.

107. V. Ludwig, A. Krebs, M. Stoll, U. Dietrich, J. Ferner, **H. Schwalbe**, U. Scheffer, G. Dürner, M.W. Göbel (2007) Tripeptides from synthetic amino acids block the Tat-Tar association and slow down HIV spread in cell cultures. *ChemBioChem* **8**, 1850-1856.

106. I.R. Correa Jr., A. Nören-Müller, H.D. Ambrosi, S. Jakupovic, K. Saxena, **H. Schwalbe**, M. Kaiser, H. Waldmann (2007) Identification of Inhibitors for mycobacterial protein tyrosine phosphatase B (MptpB) by Biology-oriented synthesis. *Chem. Asian J.* **2**, 1109-1126.

105. K. Werner, I. Lehner, H. Kaur Dhiman, C. Richter, C. Glaubitz, **H. Schwalbe**, J. Klein-Seetharaman, H.G. Khorana (2007) Assignment of tryptophan residues in the G protein-coupled receptor rhodopsin by NMR. *J. Biomol. NMR* **37**, 303-312.

104. L.J. Martin, M.J. Hähnke, M. Nitz, J. Wöhnert, N.R. Silvaggi, K.R. Allen, **H. Schwalbe**, B. Imperiali (2007) Double lanthanide-binding tags: Design, photophysical properties and NMR applications. *J. Am. Chem. Soc.* **129**, 7106-7113.

103. J. Rinnenthal, C. Richter, J. Ferner, E. Duchardt, **H. Schwalbe** (2007) Quantitative gamma-HCNCH: determination of the glycosidic torsion angle chi in RNA oligonucleotides from the analysis of CH dipolar cross-correlated relaxation by solution NMR spectroscopy. *J. Biomol. NMR* **39**, 1-29.

## 2006

102. J. Wirmer, W. Peti, **H. Schwalbe** (2006) Motional properties of unfolded ubiquitin: A model for a random coil protein. *J. Biomol. NMR*, **35**, 175-186.

101. C. Schlörb, S. Mensch, C. Richter, **H. Schwalbe** (2006) Photo-CIDNP reveals differences in compaction of non-native states of lysozyme. *J. Am. Chem. Soc.* **128**, 1802-1803.

100. J. Wirmer, H. Berk, R. Ugolini, C. Redfield, **H. Schwalbe** (2006) Characterization of the unfolded state of bovine alpha-lactalbumin and comparison with unfolded states of homologous proteins. *Protein Science* **15**, 1397-1407.
99. I. Landrieu, L. Lacosse, A. Leroy, J.-M. Wiesruszeski, X. Trivelli, N. Sibille, **H. Schwalbe**, K. Saxena, T. Langer, G. Lippens (2006) NMR analysis of a Tau phosphorylation pattern. *J. Am. Chem. Soc.* **128**, 3575-3583.
98. R. Batra-Safferling, K. Abarca Heidemann, H. G. Körschen, C. Tziatzios, M. Stoldt, I. Budyak, D. Willbold, **H. Schwalbe**, J. Klein-Seetharaman, U. B. Kaupp (2006) Glutamic Acids-Rich Proteins of Rod Photoreceptors are Natively Unfolded. *J. Biol. Chem.* **281**, 1449-1460.
97. P. Wenter, B. Fürtig, A. Hainard, **H. Schwalbe**, S. Pitsch (2006) A caged Uridine for the selective Preparation of an RNA fold and determination of its refolding kinetics by real-time NMR. *ChemBioChem* **7**, 417-420.
96. C. Raja, J. Ferner, U. Dietrich, S. Avilov, D. Ficheux, J. Darlix, H. de Rocquigny, **H. Schwalbe**, Y. Mély (2006) Inhibition by a Trp-rich hexapeptide of the nucleic acid destabilization chaperoned by the HIV-1 nucleocapsid protein. *Biochemistry* **45**, 9254-9265.
95. J. Noeske, C. Richter, E. Stiral, **H. Schwalbe**, J. Wöhnert (2006) Phosphate group recognition by the aptamer domain of the thiamine pyrophosphate sensing riboswitch. *ChemBioChem* **7**, 1451-1456.
94. M. Vogtherr, K. Saxena, S. Hoelder, S. Grimme, M. Betz, U. Schieborr, B. Pescatore, M. Robin, T. Langer, K.U. Wendt, **H. Schwalbe** (2006) NMR-Characterization of kinase p38 dynamics in free and ligand bound form. *Angew. Chemie Intl. Ed. Engl.* **45**, 993-997.
93. N. Cramer, M. Buchweitz, S. Laschat, W. Frey, D. Mathieu, C. Richter, **H. Schwalbe** (2006) Total synthesis and NMR Investigations of Cylindramide. *Chemistry* **12**, 2488-2503.
92. D. Müller, A. Krick, S. Kehraus, M. Hart, F.C. Küpper, H. Prinz, P. Janning, H. Waldmann, K. Saxena, **H. Schwalbe**, G.M. König (2006) Brunsvicamide A-C, Sponge-related Cyanobacterial Peptides with Mycobacterium Tuberculosis Protein Tyrosine Phosphatase Inhibitory Activity. *J. Med. Chem.* **49**, 4871-4878.
91. A. Nören-Müller, I. Reis Correa Jr., H. Prinz, C. Rosenbaum, K. Saxena, **H. Schwalbe**, D. Vestweber, S. Schunk, O. Schwarz, H. Schiewe, H. Waldmann (2006) Discovery of New Protein Phosphatase Inhibitor Classes by Biology Oriented Synthesis (BIOS). *Proc. Natl. Acad. Sci. U.S.A.* **103**, 10606-10611.
90. D. M. Jacobs, B. Elshorst, K. Saxena, K.M. Fiebig, M. Vogtherr, T. Langer, **H. Schwalbe** (2006) NMR backbone assignment of the N-terminal domain of human HSP90. *J. Biomol. NMR* **36**, 52
89. M.G. Madej, H.R. Nasiri, N.S. Hilgendorff, **H. Schwalbe**, C.R.D. Lancaster (2006) Evidence for transmembrane H<sup>+</sup> transfer in a dihaem-containing membrane protein complex. *EMBO J.* **25**, 4963-4970.
88. M.G. Madej, H.R. Nasiri, N.S. Hilgendorff, **H. Schwalbe**, G. Unden, C.R.D. Lancaster (2006) Experimental evidence for proton-motive force-dependent catalysis by the diheme-containing succinate:menaquinone oxidoreductase from the Gram-positive bacterium *Bacillus licheniformis*. *Biochemistry* **45**, 14049-14055.
87. H.R. Nasiri, M.G. Madej, C.R.D. Lancaster, **H. Schwalbe**, M. Bolte (2006) 2-Hydroxy-3-(3-oxobutyl)-naphthalene-1,4-dione, a monoclinic but twinned triclinic structure. *Acta Cryst* **C62**, o671-o673.
86. S. Rehm, M. O. Lenz, S. Mensch, **H. Schwalbe**, J. Wachtveitl (2006) Ultrafast spectroscopy of a photoswitchable 30 amino-acid de-novo synthesized peptide. *Chem. Phys.* **323**, 28-35.
- 2005**
85. E. Collins, J. Wirmer, K. Hirai, H. Tachibana, S. Segawa, C.M. Dobson, **H. Schwalbe** (2005) Characterization of Disulfide Bond Dynamics in Non-native States of Lysozyme and its Disulfide Deletion Mutants by NMR. *ChemBioChem* **6**, 1619-1627.

84. C. Schlörb, K. Ackermann, C. Richter, J. Wirmer, **H. Schwalbe** (2005) Heterologous expression of hen egg white lysozyme and resonance assignment of tryptophan side chains in its non-native states. *J. Biomol. NMR* **33**, 95-104.
83. I. Bertini, Y.K. Gupta, C. Luchinat, G. Parigi, C. Schlörb, **H. Schwalbe** (2005) Protein Proton NMR Detection and Longitudinal Relaxation Rates between 0.01 and 50 MHz. *Angew. Chemie Intl. Edit. Engl.* **44**, 2223-2225.
82. J. Noeske, C. Richter, M.A. Grundl, H.R. Nasiri, **H. Schwalbe**, J. Wöhnert (2005) An intermolecular base triple as the basis of ligand specificity and affinity in the guanine and adenine sensing riboswitch RNAs. *Proc. Natl. Acad. Sci. USA* **102**, 1372-1377.
81. E. Duchardt, **H. Schwalbe** (2005) Residue specific dynamic investigation of the cUUCGg tetraloop motif by NMR  $^{13}\text{C}$  relaxation. *J. Biomol. NMR* **32**, 295-308.
80. P. Wenter, B. Fürtig, A. Hainard, **H. Schwalbe**, S. Pitsch (2005) Kinetic investigation of photoinduced RNA refolding by realtime NMR spectroscopy. *Angew. Chemie* **117**, 2656-2659.
79. J. Koplín, Y. Mu, C. Richter, **H. Schwalbe**, G. Stock (2005) Structure and dynamics of an RNA tetraloop: A joint molecular-dynamics and NMR study. *Structure* **13**, 1255-1267.
78. S. Ilin, A. Hoskin, O. Ohlenschläger, **H. Schwalbe**, J. Wöhnert (2005) Domain reorientation and induced fit upon RNA binding: solution structure and dynamics of ribosomal protein L11 from *Thermotoga maritima*. *ChemBioChem* **6**, 1611-1618.
77. N. Cramer, S. Laschat, A. Baro, **H. Schwalbe**, C. Richter (2005) Enantioselektive Totalsynthese von Cylinamid. *Angew. Chem. Int. Ed. Engl.* **44**, 820-822.
76. U. Schieborr, M. Vogtherr, B. Elshorst, M. Betz, S. Grimme, B. Pescatore, T. Langer, K. Saxena, **H. Schwalbe** (2005) How much NMR-Data is required for the Determination of a Protein-Ligand Complex? *ChemBioChem* **6**, 1891-1898.
75. M. Vogtherr, K. Saxena, S. Grimme, M. Betz, U. Schieborr, B. Pescatore, T. Langer, **H. Schwalbe** (2005) NMR backbone assignment of the mitogen-activated protein (MAP) kinase p38. *J. Biomol. NMR* **32**, 175.
74. K. Saxena, D.M. Jacobs, M. Vogtherr, S. Grimme, B. Elshorst, B. Pescatore, M. Betz, U. Schieborr, T. Langer, **H. Schwalbe**, K. Fiebig (2005) Backbone assignment of the human E2 ubiquitin conjugating enzyme UbcH5alpha (F72K,F82S) double mutant. *J. Biomol. NMR* **32**, 338.
73. S. Sreeramulu, J. Kumar, C. Richter, M. Vogtherr, K. Saxena, T. Langer, **H. Schwalbe** (2005)  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{15}\text{N}$  backbone resonance assignment of the Hsp90 binding domain of human Cdc37. *J. Biomol. NMR* **32**, 262.
72. D.M. Jacobs, S. Grimme, B. Elshorst, B. Pescatore, M. Vogtherr, M. Betz, U. Schieborr, T. Langer, K. Saxena, **H. Schwalbe**, K. Fiebig (2005) Backbone NMR assignment of the C-terminal haemopexin-like domain (HPLD) of human matrix metalloproteinase MMP-13. *J. Biomol. NMR* **32**, 556.
71. M. Manger, M. Scheck, H. Prinz, F. Feyen, T. Langer, K. Saxena, **H. Schwalbe**, A. Fürstner, H. Waldmann (2005) Discovery of Natural Product Derived Inhibitors of *Mycobacterium tuberculosis* Protein Tyrosine Phosphatase (MtpA). *ChemBioChem* **6**, 1749-1753.
70. T. Langer, S. Sreeramulu, M. Vogtherr, B. Elshorst, M. Betz, U. Schieborr, K. Saxena, **H. Schwalbe** (2005) Folding and activity of cAMP-dependent protein kinase (PKA) mutants. *Febs Lett.* **57**, 4049-4054.
69. K. Saxena, B. Elshorst, H. Berk, M. Betz, S. Grimme, T. Langer, B. Pescatore, U. Schieborr, M. Vogtherr, **H. Schwalbe** (2005) Backbone NMR assignment of the low-molecular-weight protein tyrosine phosphatase (MtpA) from *Mycobacterium tuberculosis*. *J. Biomol. NMR* **33**, 136.
68. C.R.D. Lancaster, U.S. Sauer, R. Groß, A.H. Haas, J. Graf, **H. Schwalbe**, W. Mäntele, J. Simon, M.G. Madej (2005) Experimental Support for the "E-pathway hypothesis" of coupled transmembrane e- and H+ transfer in dihemic quinol:fumarate reductase. *Proc. Natl. Acad. Sci. USA* **102**, 18869-18865.



## 2004

67. J. Wirmer, C. Schlörb, J. Klein-Seetharaman, R. Hirano, T. Ueda, T. Imoto, **H. Schwalbe** (2004) Modulation of Compactness and Long-range Interactions of Unfolded Lysozyme by Single Point Mutations. *Angew. Chem.* **116**, 5904-5909.
66. T. Giroglou, Ch. Drosten, **H. Schwalbe**, H. Rabenau, D. von Laer (2004) Retroviral vectors pseudotyped with severe acquired respiratory syndrome (SARS) Coronavirus S protein. *J. Virol.* **78**, 9007-9015.
65. B. van Buuren, J. Schleucher, V. Wittmann, C. Griesinger, **H. Schwalbe**, S.S. Wijmenga (2004) NMR Spectroscopic Determination of the Solution Structure of a Branched Nucleic Acids from Residual Dipolar Couplings by Using Isotopically Labeled Nucleotides. *Angew. Chem.* **116**, 189-194.
64. B. Fürtig, C. Richter, W. Bermel, **H. Schwalbe** (2004) New NMR Experiments for Complete Resonance Assignment of an RNA UUCG Tetraloop. *J. Biomol. NMR* **28**, 69-79.
63. E. Duchardt, C. Richter, O. Ohlenschläger, M. Görlach, J. Wöhnert, **H. Schwalbe** (2004) Determination of angle  $\chi$  in RNA from cross-correlated relaxation of CH-dipolar coupling and N-chemical shift anisotropy. *J. Am. Chem. Soc.* **126**, 1962-1970.
62. T. Giroglou, Ch. Drosten, **H. Schwalbe**, H. Rabenau, D. von Laer (2004) Retroviral vectors pseudotyped with severe acquired respiratory syndrome (SARS) Coronavirus S protein. *J. Virol.* **78**, 9007-9015.
61. T. Langer, M. Vogtherr, B. Elshorst, M. Betz, U. Schieborr, K. Saxena, **H. Schwalbe** (2004) NMR backbone assignment of a protein kinase catalytic domain by a combination of several approaches: Application to the catalytic subunit of cAMP-dependent kinase. *ChemBioChem* **5**, 1508-1516.
60. J. Klein-Seetharaman, P.J. Reeves, E.V. Getmanova, **H. Schwalbe**, H.G. Khorana (2004) Backbone versus side-chain dynamics in  $^{15}\text{N}$ -Tryptophan Labeled Rhodopsin in Dodecyl Maltoside Micelles. *Proc. Natl. Acad. Sci. USA* **101**, 3409-3413.

## 2003

59. S. Ilin, A. Hoskins, **H. Schwalbe**, J. Wöhnert (2003) Letter to the Editor: NMR assignment of the full-length ribosomal protein L11 from *Thermotoga maritima*. *J. Biomol. NMR* **25**, 163-164.
58. S. Ilin, C. Bosques, C. Turner, **H. Schwalbe** (2003) Gamma-HMBC: An NMR experiment for the conformational analysis of the o-glycosidic linkage in glycopeptides. *Angew. Chem.* **115**, 1394-1397.
57. J. Wöhnert, M. Görlach, **H. Schwalbe** (2003) HCCNH-TOCSY experiments for the simultaneous correlation of exchangeable and H6/H5 base proton resonance in pyrimidines. *J. Biomol. NMR* **26**, 79-83.
56. B. Elshorst, D.M. Jacobs, **H. Schwalbe**, T. Langer (2003) Letter to the Editor:  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{15}\text{N}$  backbone resonance assignment of the integrin  $\alpha 2$  I-domain. *J. Biomol. NMR* **27**, 191-192.
55. M. Vogtherr, S. Grimme, B. Pescatore, **H. Schwalbe** (2003) Letter to the Editor:  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{15}\text{N}$  backbone resonance assignment of the VASP EVH1 domain. *J. Biomol. NMR* **27**, 189-190.
54. A. Pustowka, J. Dietz, M. Baumann, M. Landersz, C. Königs, **H. Schwalbe**, U. Dietrich (2003) Identification of peptide ligands for target RNA structures derived from the HIV-1 packaging signal *psi* ( $\Psi$ ) by screening phage displayed peptide libraries. *ChemBioChem* **4**, 1093-1097.
53. J. Wöhnert, K.J. Franz, M. Nitz, B. Imperiali, **H. Schwalbe** (2003) Protein alignment by a coexpressed lanthanide-binding tag for the measurement of residual dipolar couplings. *J. Am. Chem. Soc.* **125**, 13338-13339.

## 2002

52. S. Ilin, I. Schlönvogt, M.-O. Ebert, B. Jaun, **H. Schwalbe** (2002) Comparison of the NMR Solution Structures of Pyranosyl-RNA and its Nucleo- $\delta$ -peptides Analogues. *ChemBioChem* **3**, 93-99.

51. P.J. Gee, F.A. Hamprecht, L.D. Schuler, W.F. Van Gunsteren, E. Duchardt, **H. Schwalbe**, M. Albert, D. Seebach (2002) A molecular dynamics simulation study of the conformational preferences of oligo-(3-hydroxyalkanoic acids) in chloroform solution. *Helv. Chim. Acta* **85**, 618-632.

50. M. Albert, D. Seebach, E. Duchardt, **H. Schwalbe** (2002) Synthesis and NMR Analysis in Solution of Oligo(3-hydroxyalkanoates) with the Side Chains of Alanine, Valine, and Leucine – Coming Full Circle from PHB to  $\beta$ -Peptides to PHB. *Helv. Chim. Acta* **85**, 633-658.

49. J. Klein-Seetharaman, P.J. Reeves, M.C. Loewen, E.V. Getmanova, J. Chung, P.E. Wright, **H. Schwalbe**, H.G. Khorana (2002) Application of Solution NMR Spectroscopy to  $\alpha$ - $^{15}\text{N}$ -Lysine Labeled Rhodopsin. *Proc. Natl. Acad. Sci. USA* **99**, 3452-3457.

48. J. Klein-Seetharaman, M. Oikawa, S.B. Grimshaw, J. Wirmer, E. Duchardt, T. Ueda, T. Imoto, L.J. Smith, C.M. Dobson, **H. Schwalbe** (2002) Long-range interactions within a non-native protein. *Science* **265**, 1917-1921.

47. J. Wirmer, **H. Schwalbe** (2002) Torsion Angle and Sequence Dependence of  $^1\text{J}(\text{N}_i, \text{C}\alpha_i)$  and  $^2\text{J}(\text{N}_i, \text{C}\alpha_{i-1})$  coupling constants. Comparison for Folded and Unfolded Ubiquitin. *J. Biomol. NMR* **23**, 47-55.

## 2001

46. W. Peti, L. Smith, C. Redfield, **H. Schwalbe** (2001) Chemical Shifts in Denatured Proteins: Resonance Assignments for Denatured Ubiquitin and Comparisons with other Denatured Proteins. *J. Biomol. NMR* **19**, 153-165.

45. **H. Schwalbe**, S.B. Grimshaw, A. Spencer, M. Buck, J. Boyd, C.M. Dobson, C. Redfield, and L.J. Smith (2001) A refined solution structure of hen lysozyme determined using residual dipolar coupling data. *Protein Science* **10**, 677-688.

44. M.C. Loewen, J. Klein-Seetharaman, E.V. Getmanova, P.J. Reeves, **H. Schwalbe**, H.G. Khorana (2001) Solution  $^{19}\text{F}$  NOE effects in structural studies of the cytoplasmic domain of mammalian rhodopsin. *Proc. Natl. Acad. Sci. USA* **98**, 4888-4892.

43. J.C. Mareque Rivas, **H. Schwalbe**, S.J. Lippard (2001) Inter-chain hydrogen bonding interactions may facilitate translocation of  $\text{K}^+$  ions across the potassium channel selectivity filter as suggested by synthetic modeling chemistry. *Proc. Natl. Acad. Sci. USA* **98**, 9478-9483.

42. A. Abiko, T. Inoue, H. Furuno, W. Davies, C. Fieres, **H. Schwalbe**, S. Masamune, (2001) The first doubly borylated enolate as an intermediate of the double aldol reaction. *J. Am. Chem. Soc.* **123**, 4605-4606.

41. Elke Duchardt, Christian Richter, Bernd Reif, Steffen J. Glaser, Joachim W. Engels, Christian Griesinger, **H. Schwalbe** (2001) Measurement of  $^1\text{J}(\text{H}, \text{C})$ -Coupling Constants by  $\alpha/\beta$  selective HC(C)H-TOCSY in Uniformly  $^{13}\text{C}$  labeled RNA. *J. Biomol. NMR* **21**, 117-126.

40. M. Waser, M. Rueping, D. Seebach, E. Duchardt, **H. Schwalbe** (2001) On the solution structure of PHB – Preparation and NMR Analysis of Isotopically Labeled Oligol ((R)-3-hydroxybutanoic acids) (OHBs). *Helv. Chim. Acta* **84**, 1821-45.

39. J. Wirmer, T. Kühn, **H. Schwalbe** (2001) Millisecond Time Resolved Photo-CIDNP NMR Reveals a Non-native Folding Intermediate on the Ion Induced Refolding Pathway of Bovine  $\alpha$ -Lactalbumin. *Angew. Chemie* **113**, 4378-4381.

38. C.K. Smith, J. Wöhnert, R.T. Sauer, **H. Schwalbe** (2001) Letter to the Editor:  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  Chemical Shift Assignments of Lon-1 Protein. *J. Biomol. NMR* **21**, 387-388.

## 2000

37. M. Hennig, W. Bermel, **H. Schwalbe**, C. Griesinger (2000) Determination of NMR  $\psi$  Torsion Angle Restraints from  $^3\text{J}(\text{C}_\alpha, \text{C}_\alpha)$  and  $^3\text{J}(\text{H}^{\text{N}}, \text{C}_\alpha)$  Coupling Constants in Proteins. *J. Am. Chem. Soc.* **122**, 6268-6277.

36. **H. Schwalbe**, J. Wermuth, C. Richter, S. Szalma, A. Eschenmoser, G. Quinkert (2000)  $\delta$ -Peptide Analogues of Pyranosyl-RNA Part III: Nucleo- $\delta$ -peptides Derived from Conformationally Constrained Nucleo- $\delta$ -

amino acids: NMR Study of the Duplex Formed by Self-pairing of the (1'S,2'S,4'S)-(phba)-Nucleo- $\delta$ -peptide-(AATAT). *Helvetica Chimica Acta* **83**, 1079-1107.

35. T. Kühn, **H. Schwalbe** (2000) Monitoring the Kinetics of Ion Dependent Protein Folding by Time Resolved NMR at Atomic Resolution. *J. Am. Chem. Soc.* **122**, 6169-6174.

34. W. Peti, M. Hennig, L.J. Smith, **H. Schwalbe** (2000) NMR Spectroscopic Investigation of  $\psi$  Torsion Angle Distribution in Unfolded Ubiquitin from Analysis of  $^3J(C_{\alpha},C_{\alpha})$  Coupling Constants and Cross-Correlated Relaxation Rates. *J. Am. Chem. Soc.* **122**, 12017-12018.

33. C. Richter, B. Reif, C. Griesinger, **H. Schwalbe** (2000) NMR-Spectroscopic Determination of Angles  $\alpha$  and  $\zeta$  in RNA from CH-Dipolar Coupling, P-CSA Cross-Correlated Relaxation. *J. Am. Chem. Soc.* **122**, 12728-12731.

#### 1999

32. I.C. Felli, Christian Richter, C. Griesinger, **H. Schwalbe** (1999) Determination of RNA Sugar Pucker Mode from Cross Correlated Relaxation in Solution NMR Spectroscopy. *J. Am. Chem. Soc.* **121**, 1956-1957.

31. M. Hennig, W. Bermel, A. Spencer, C.M. Dobson, L.J. Smith, **H. Schwalbe** (1999) Determination of Side Chain Conformations in Unfolded Proteins:  $\chi_1$  Distribution for Lysozyme by Heteronuclear  $^{13}C,^{15}N$  NMR spectroscopy. *J. Mol. Biol.* **288**, 705-723.

30. B. Elshorst, M. Hennig, H. Försterling, A. Diener, M. Maurer, P. Schulte, J. Krebs, H. Schmid, T. Vorherr, E. Carafoli, **H. Schwalbe**, C. Griesinger (1999) NMR Solution Structure of a Complex of Calmodulin with a Binding Peptide of the  $Ca^{2+}$ -Pump. *Biochemistry* **38**, 12320-12332.

29. C. Richter, C. Griesinger, I.C. Felli, P.T. Cole, G. Varani, **H. Schwalbe** (1999) Determination of Sugar Conformation in Large RNA Oligonucleotides from Analysis of Dipole, Dipole Cross Correlated Relaxation by Solution NMR Spectroscopy. *J. Biomol. NMR* **15**, 241-250.

#### 1998

28. C. Richter, B. Reif, K. Wörner, S. Quant, J.W. Engels, C. Griesinger, **H. Schwalbe** (1998) New Experiment for the Measurement of  $^3J(C,P)$  Coupling Constants including  $^3J(C4'_i,P_i)$  and  $^3J(C4'_i,P_{i+1})$  coupling constants in Oligonucleotides. *J. Biomol. NMR* **12**, 223-230.

27. T. Carlomagno, **H. Schwalbe**, A. Rexroth, O.W. Sørensen, C. Griesinger (1998) New methylene specific experiments for the measurement of scalar spin-spin coupling constants between protons attached to C-13", *J. Magn. Reson.* **135**, 216-226.

#### 1997

26. **H. Schwalbe**, K.M. Fiebig, M. Buck, J.A. Jones, S.B. Grimshaw, S.J. Glaser, L.J. Smith, C.M. Dobson (1997) Structural and Dynamical Properties of Lysozyme Denatured in 8M Urea. Heteronuclear 3D NMR Experiments and Theoretical Simulations. *Biochemistry* **36**, 8977-8991.

25. M. Hennig, D. Ott, P. Schulte, R. Löwe, J. Krebs, T. Vorherr, W. Bermel, **H. Schwalbe**, C. Griesinger (1997) Determination of Homonuclear  $^{13}C$ - $^{13}C$  J Couplings between Aliphatic Carbon Atoms in Perdeuterated Proteins. *J. Am. Chem. Soc.* **119**, 5055-5056.

24. B. Reif, V. Wittmann, **H. Schwalbe**, C. Griesinger, K. Wörner, K. Jahn-Hofmann, J.W. Engels, W. Bermel (1997) Structural Comparison of Oligoribonucleotides and Their 2'-Deoxy-2'-fluoro Analogs by Heteronuclear NMR Spectroscopy. *Helv. Chim. Acta* **80**, 1952-1971.

#### 1996

23. K.M. Fiebig, **H. Schwalbe**, M. Buck, L.J. Smith, C.M. Dobson (1996) Towards a Description of the Conformations of Denatured States of Proteins. Comparison of a Random Coil Model with NMR Measurements. *J. Phys. Chem.* **100**, 2661-2666.

22. L.J. Smith, K.M. Fiebig, **H. Schwalbe**, C.M. Dobson (1996) The concept of a random coil. Residual structure in peptides and denatured proteins. *Folding and Design* **1**, 95-106.

21. J.P. Marino, **H. Schwalbe**, S.J. Glaser, C. Griesinger (1996) Determination of  $\gamma$  and Stereospecific Assignment of H5' Protons by Measurement of  $^2J$  and  $^3J$  Coupling Constants in Uniformly  $^{13}C$  labeled RNA. J. Am. Chem. Soc. **118**, 7251-7252.

20. S.J. Glaser, **H. Schwalbe**, J.P. Marino, C. Griesinger (1996) Directed TOCSY, a Method for Selection of Directed Correlations by Optimal Combinations of Isotropic and Longitudinal Mixing. J. Magn. Reson., Series B **112**, 160-180.

#### 1995

19. J.P. Marino, **H. Schwalbe**, C. Anklin, W. Bermel, D.M. Crothers, C. Griesinger (1995) Sequential Correlation of Anomeric Ribose Protons and Intervening Phosphorous in RNA Oligonucleotides by an  $^1H$ ,  $^{13}C$ ,  $^{31}P$  Triple Resonance Experiment: HCP-CCH-TOCSY. J. Biomol. NMR **5**, 87-92.

18. **H. Schwalbe**, J.P. Marino, S.J. Glaser, C. Griesinger (1995) Measurement of all H,H-Coupling Constants associated with  $\nu_1$ ,  $\nu_2$ , and  $\nu_3$  in uniformly  $^{13}C$  labeled RNA by HCC-TOCSY-CCH-E.COSY. J. Am. Chem. Soc. **117**, 7251-7252.

17. A. Rexroth, S. Szalma, R. Weisemann, W. Bermel, **H. Schwalbe**, C. Griesinger (1995) Determination of  $^1J(N_i, C'_{i-1})$ ,  $^2J(H^N, C'_{i-1})$ , and  $^3J(H^N, C'_i)$  Coupling Constants in Proteins with the C'-FIDS Method. J. Biomol. NMR **6**, 237-244.

16. A. Rexroth, P. Schmidt, S. Szalma, T. Geppert, **H. Schwalbe**, C. Griesinger (1995) A New Principle for the Determination of Coupling Constants that largely suppresses Differential Relaxation Effects. J. Am. Chem. Soc. **117**, 10389-10390.

15. M. Buck, **H. Schwalbe**, C.M. Dobson (1995) Main-chain dynamics of a partially folded protein: N-15 NMR relaxation measurements of hen egg white lysozyme denatured in trifluoroethanol. J.Mol.Biol. **254**, 7532-7539.

14. M. Buck, **H. Schwalbe**, C.M. Dobson (1995) Characterization of Conformational Preferences in a Partly Folded Protein by Heteronuclear NMR: Assignment and Secondary Structure Analysis of Hen Egg-White Lysozyme in Trifluoroethanol. Biochemistry **34**, 13219-13232.

13. L.J. Smith, K.A. Bolin, **H. Schwalbe**, M.W. MacArthur, J.M. Thornton, C.M. Dobson (1995) Analysis of Main Chain Torsion Angles in Proteins. Predictions of NMR Coupling Constants for Native and Denatured Conformations. J.Mol.Biol. **255**, 494-506.

#### 1994

12. R. Weisemann, H. Rüterjans, **H. Schwalbe**, J. Schleucher, W. Bermel, C. Griesinger (1994) Determination of  $H^N$ ,  $H_\alpha$  and  $H^N, C'$  coupling constants in  $^{13}C$ ,  $^{15}N$ -labeled proteins. J. Biomol. NMR **4**, 231-240.

11. **H. Schwalbe**, J.P. Marino, G.C. King, R. Wechselberger, W. Bermel, C. Griesinger (1994) Determination of a complete set of coupling constants in  $^{13}C$ -labeled oligonucleotides. J. Biomol. NMR **4**, 631-644.

10. Y. Karimi-Nejad, J.M. Schmidt, H. Rüterjans, **H. Schwalbe**, C. Griesinger (1994) Conformation of Valine Side Chains in Ribonuclease T<sub>1</sub> Determined by NMR Studies of Homonuclear and Heteronuclear  $^3J$  Coupling Constants. Biochemistry **33**, 5481-5492.

9. S.S.P. Quant, R.W. Wechselberger, M.A. Wolter, K. Wörner, P. Schell, J.W. Engels, C. Griesinger, **H.J. Schwalbe** (1994) Chemical Synthesis of  $^{13}C$  labeled RNA and DNA monomers for the solid phase and template controlled enzymatic synthesis of DNA and RNA oligomers. Tetrahedron Lett. **35**, 6649-55.

8. John P. Marino, **H. Schwalbe**, Clemens Anklin, Wolfgang Bermel, Donald M. Crothers, and Christian Griesinger (1994) A three-dimensional Triple Resonance HCP Experiment: Sequential Through Bond Correlation of Ribose Protons and Intervening Phosphorous along the RNA Oligonucleotide Backbone. J. Am. Chem. Soc. **116**, 6472-6473.

#### 1993

7. P. Schmidt, **H. Schwalbe**, S.J. Glaser, C. Griesinger (1993) Exclusive Tailored Correlation Spectroscopy (E-TACS). J. Magn. Reson. Series B **101**, 328-333.

6. **H. Schwalbe**, W. Samstag, J.W. Engels, W. Bermel, C. Griesinger (1993) Determination of  $^3J(C,P)$  and  $^3J(H,P)$  Coupling Constants in Nucleotide Oligomers. *J. Biomol. NMR* **3**, 479-486.

5. **H. Schwalbe**, A. Rexroth, U. Eggenberger, T. Geppert, C. Griesinger (1993) Measurement of  $C',C$  Coupling Constants in  $^{13}C$  Labeled Proteins, A New Method for Stereospecific Assignment of  $\gamma$ -Methyl Groups in Valine Residues. *J. Am. Chem. Soc.* **115**, 7878-7879.

4. A. Berkessel, T. Schwenkreis, G. Huttner, B. Schiemenz, C. Griesinger, **H. Schwalbe**, M. Bolte, T. Neumann (1993) Konformationsanalyse an Nickel(II)-Modellkomplexen für die Methyl-Coenzym-M-Reduktase methanogener Bakterien: Ein Vergleich von Kristall- und Lösungsstrukturen. *Angew. Chem.* **105**, 1776-80.

#### 1992

3. M. Sattler, **H. Schwalbe**, C. Griesinger (1992) Stereospecific Assignment of Leucine  $\delta$ -Methylgroups with  $^{13}C$  in Natural Abundance or Random  $^{13}C$  Labelling. *J. Am. Chem. Soc.* **114**, 1127-28.

2. C.H. Schein, E. Boix, M. Haugg, K.P. Holliger, S. Hemmi, G. Frank, **H. Schwalbe** (1992) Secretion of Mammalian Ribonucleases from Escherichia-Coli using the Signal Sequence of Murine Spleen Ribonuclease. *Biochemical Journal* **283**, 137-144.

1. L.E. Kay, T.E. Bull, L.K. Nicholson, C. Griesinger, **H. Schwalbe**, A. Bax, D.A. Torchia, (1992) On the Measurement of Heteronuclear Transverse Relaxation Times in  $AX_3$  Spin Systems Via Polarization Transfer Techniques. *J. Magn. Reson.* **100**, 538-558.

## List of Review Articles, Book Chapters, Highlights, Commentaries

### 2017

59. A.C. Kruse, B.T. Lobingier, R. Hüttenhain, M. von Zatrow, N. J. Kogan, T.P. Tyler, P.H. Opgenorth, J. U. Bowie, P. J. Hergenrother, M. F. Richter, C. Ye, B.P. Tu, B. Fürtig, J. Wöhnert, **H. Schwalbe** (2017) Principles of Chemical Biology: APEX, cell-free enzyme systems, new antibiotics, epigenetic-membrane relationship, and metastable transcription. *Cell Chemical Biology* **24**, in press.

58. **H. Schwalbe** (2017) 1.2 GHz NMR spectrometers – new Horizons? *Angew. Chem. Int. Ed.* **56**, 10252-10253.

57. M. Hutchison, **H. Schwalbe** (2017) Protein misfolding in Modern Magnetic Resonance, 2<sup>nd</sup> edition.

56. J. Wirmer-Bartoschek, I. Bessi, J. Dash, **H. Schwalbe** (2017) Targeting G-quadruplex with small molecules: an NMR view. in *Modern Magnetic Resonance*, 2<sup>nd</sup> edition.

55. G. Pinter, **H. Schwalbe** (2017) Unprecedented carbon signal enhancement in liquid-state NMR spectroscopy. *Angew. Chem. Int. Ed.* **56**, 8332-8334.

### 2016

54. J. Wirmer-Bartoschek, **H. Schwalbe** (2016) Understanding how DNA enzymes work. *Angew. Chem. Int. Ed.* **55**, 5376-7.

### 2015

53. M. Göbel, **H. Schwalbe** (2015) Gerhard Quinkert (1927-2015) *Angew. Chem. Int. Ed.* **54**, 8597.

52. K. Saxena, **H. Schwalbe** (2015) The role of NMR in target identification and validation for pharmaceutical R&D. *eMagRes* **4**, 305-314.

51. B. Fürtig, S. Nozinovic, A. Reining, **H. Schwalbe** (2015) Multiple conformational states of riboswitches fine-tune gene regulation. *Curr. Opin. Struct. Biol.* **30**, 112-124.

50. J.-H. Ardenkjaer-Larsen, G.S. Boebinger, A. Comment, S. Duckett, A. Edison, F. Engelke, C. Griesinger, R.G. Griffin, C. Hilty, H. Maeda, G. Parigi, T. Prisner, E. Ravera, J. van Bentum, S. Vega, A. Webb, C. Luchinat\*, **H. Schwalbe\***, L. Frydman\* (2015) Facing and Overcoming Biomolecular NMR's sensitivity challenges. *Angew. Chem. Int. Ed. Engl.* **54**, 9162-85.

### 2014

49. **H. Schwalbe** (2014) Author Profile Harald Schwalbe. *Angew. Chem. Int. Ed. Engl.* **53**, 10576 – 10577.

48. **H. Schwalbe**, B. Fürtig (2014) RNA refolding studied by light-coupled NMR spectroscopy. *Meth. Mol. Biol.* vol. 1086, 309-19.

47. M. Hengesbach, **H. Schwalbe** (2014) Structural basis for regulation of ribosomal RNA 2'-O-methylation. *Angew. Chem. Int. Ed. Engl.* **53**, 1742-4.

46. B. Fürtig, A. Reining, F. Sochor, E. M. Oberhauser, A. Heckel, **H. Schwalbe** (2014) Characterization of the conformational dynamics of bistable RNA by equilibrium and non-equilibrium NMR methods. *Curr. Prot. in Nucl. Acid Chem.* **55**, 11.13.1-11.13.16. doi: 10.1002/0471142700.nc1113s55

### 2013

45. **H. Schwalbe**, J. Teller (2013) Magnetic Resonance Spectroscopy in bio(in)organic chemistry and mechanistic systems biology: A tribute to Ivano Bertini, *ChemBioChem* **14**, 1671-1675.

44. R. Silvers, **H. Schwalbe** (2013) Detecting Intracellular Cysteine Redox States by In-Cell NMR spectroscopy. *ChemBioChem* **14**, 1705-1707.

### 2012

44. G. Nielsen, **H. Schwalbe** (2012) Protein NMR Spectroscopy: Hydrogen bonds under pressure. *Nature Chemistry* **4**, 693-695.

43. B. Fürtig, J. Buck, C. Richter, **H. Schwalbe** (2012) Functional dynamics of RNA ribozymes studied by NMR spectroscopy. *Methods Mol. Biol.* **848**, 185-199. (peer-reviewed)

42. K. Saxena, A. Dutta, J. Klein-Seetharaman, **H. Schwalbe** (2012) Isotope labeling in insect cells. *Methods Mol. Biol.* **831**, 37-54. (peer-reviewed)

41. A. Dutta, K. Saxena, **H. Schwalbe**, J. Klein-Seetharaman (2012) Isotope labeling in mammalian cells. *Methods Mol Biol.* **831**, 55-69. (peer-reviewed)

40. U. Schieborr, S. Sreeramulu, **H. Schwalbe** (2012) NMR structure determination of protein-ligand complexes, in *NMR of Biomolecules: Towards Mechanistic Systems Biology*, Edited by I. Bertini, K.S. McGreevy, G. Parigi 34, 549-561. (peer-reviewed)

39. J. Ferner, E. Duchardt-Ferner, J. Rinnenthal, J. Buck, J. Wöhnert, **H. Schwalbe** (2012) RNA as drug target, in *NMR of Biomolecules: Towards Mechanistic Systems Biology*, Edited by I. Bertini, K.S. McGreevy, G. Parigi 34, 299-314. (peer-reviewed)

38. D. Mathieu, K. Rybka, J. Graf, **H. Schwalbe** (2012) Mapping conformational dynamics in unfolded polypeptide chains using short model peptides by NMR spectroscopy, in press.

37. M. Cevec, H.R.A. Jonker, S. Nozinovic, **H. Schwalbe** (2012) Nucleic Acids, in *NMR of Biomolecules: Towards Mechanistic Systems Biology*, Edited by I. Bertini, K.S. McGreevy, G. Parigi 34, 21-32. (peer-reviewed)

## 2011

36. R. Silvers, K. Schlepckow, J. Wirmer-Bartoschek, **H. Schwalbe** (2011) NMR-spectroscopic investigation of Disulfide Dynamics in Unfolded States of Proteins.

35. **H. Schwalbe** (2011) Commentary: Double Take on PiWi Protein/piRNA Complex Structure. *Structure* **19**, 141-142.

34. B. Fürtig, J. Buck, J. Rinnenthal, A. Wacker, **H. Schwalbe** (2011) NMR-Spektroskopie zum Verständnis RNA-basierter Regulation. *Biospektrum* **17**, 174-177.

33. K. Schlepckow, B. Fürtig, **H. Schwalbe** (2011) Nonequilibrium NMR methods for monitoring protein and RNA folding. *Z. Phys. Chem.* **225**, 611-636. (peer-reviewed)

32. J. Rinnenthal, J. Buck, J. Ferner, A. Wacker, **H. Schwalbe** (2011) Mapping the landscape of RNA dynamics by NMR spectroscopy. *Acc. Chem. Res.*, **44**, 1292-1301. (peer-reviewed)

## 2010

31. **H. Schwalbe**, J. Rinnenthal (2010) Thermodynamics: the world is flat. *Nat. Chem. Biol.* **6**, 312-313.

30. R. Silvers, F. Buhr, **H. Schwalbe** (2010) Highlight: The molecular mechanism of spider silk formation. *Angew. Chem. Int. Ed. Engl.* **49**, 5410-5412; R. Silvers, F. Buhr, **H. Schwalbe** (2010) Highlight: Der molekulare Mechanismus der Bildung von Spinnenseide. *Angew. Chem.* **122**, 5538-5540. (peer-reviewed)

## 2009

29. J. Buck, B. Fürtig, J. Noeske, J. Wöhnert, **H. Schwalbe** (2009) Time-resolved NMR spectroscopy: ligand-induced refolding of riboswitches. *Methods Mol. Biol.* **540**, 161-171. (peer-reviewed)

28. K.H. Altmann, J. Buchner, H. Kessler, F. Diederich, B. Kräutler, S. Lippard, R. Liskamp, K. Müller, E.M. Nolan, B. Samori, G. Schneider, S.L. Schreiber, **H. Schwalbe**, C. Toniolo, C.A.A. van Boeckel, H. Waldmann, C.T. Walsh (2009) Editorial: The State of the Art of Chemical Biology- *ChemBioChem.* **10**, 16-29.

27. J. Noeske, J. Buck, J. Wöhnert, **H. Schwalbe** (2009) Ligand Binding and Conformational Changes in the Purine-binding riboswitch aptamer domains. *Non-Protein Coding RNAs*, p. 229-247.

## 2008

26. B. Fürtig, **H. Schwalbe** (2008) *Nucleic Acids from A to Z*. p. 185-200.
25. G. Nielsen, M. Stadler, H.R.A. Jonker, M. Betz, **H. Schwalbe** (2008) *NMR Spectroscopy in Chemical Biology*.
24. M. Betz, M. Vogtherr, U. Schieberr, B. Elshorst, S. Grimme, B. Pescatore, T. Langer, K. Saxena, **H. Schwalbe** (2008) *Chemical Biology of Kinases Studied by NMR Spectroscopy* *Chemical Biology* 852-890. (peer-reviewed)
23. M. Pellechia, I. Bertini, D. Cowburn, C. Dalvit, E. Giralto, W. Jahnke, T.L. James, S.W. Homans, H. Kessler, C. Luchinat, B. Meyer, H. Oschkinat, J. Peng, **H. Schwalbe**, G. Siegal (2008) *Perspectives on NMR in drug discovery: a technique comes of age*. *Nat. Rev. Drug. Discov.* **7**, 738-745. (peer-reviewed)
- 2007**
22. B. Fürtig, J. Buck, V. Manoharan, W. Bermel, A. Jäschke, P. Wenter, S. Pitsch, **H. Schwalbe** (2007) *Time-resolved NMR studies of RNA folding*. *Biopolymers* **86**, 360-383. (peer-reviewed)
21. **H. Schwalbe**, J. Buck, B. Fürtig, J. Noeske, J. Wöhnert (2007) *Structures of RNA switches: insight into molecular recognition and tertiary structure*. *Angew. Chem. Int. Ed. Engl.* **46**, 1212-1219. (peer-reviewed)
- 2006**
20. M. Betz, M. Vogtherr, U. Schieberr, B. Elshorst, S. Grimme, B. Pescatore, T. Langer, K. Saxena, **H. Schwalbe** (2006) *Chemical Biology of Kinases Studied by NMR spectroscopy*. *Chemical Biology – From Small Molecules to Systems Biology and Drug Design*.
19. M. Betz, K. Saxena, **H. Schwalbe** (2006) *Biomolecular NMR: A chaperone to drug discovery*. *Curr. Opin. Chem. Biol.* **10**, 219-225 (peer-reviewed).
18. E. Ab, A.R. Atkinson, L. Banci, I. Bertini, S. Ciofi-Baffoni, K. Brunner, T. Diercks, V. Dötsch, F. Engelke, G.E. Folkers, C. Griesinger, W. Gronwald, U. Günther, M. Habeck, R.N. de Jong, H.R. Kalbitzer, B. Kieffer, B.R. Leeﬂang, S. Loss, C. Luchinat, T. Marquardsen, D. Moskau, K.P. Neidig, M. Nilges, M. Piccioli, R. Pieratelli, W. Rieping, T. Schippmann, **H. Schwalbe**, G. Travé, J. Trenner, J. Zweckstetter, R. Kaptein (2006) *NMR in the Spine Structural Proteomics project*. *Acta Crystallogr D Biol Crystallogr.* **62**, 1150-1161.
- 2005**
17. **H. Schwalbe**, H.U. Stiliz, H. Kessler (2005) *Editorial: NMR spectroscopy of Biomacromolecules in Drug Discovery and Beyond*. *ChemBioChem* **6**, 1475-1478.
16. J. Wirmer, C. Schlörb, **H. Schwalbe** (2005) *Conformation and Dynamics of Nonnative States of Proteins studied by NMR spectroscopy*. In *Protein Folding Handbook*, p. 737-808.
15. **H. Schwalbe**, J. Wirmer (2005) *Protein Misfolding Disease: Overview of liquid and solid state high resolution NMR studies*. *Handbook of Modern Magnetic Resonance*.
14. S. Nozinovic, B. Nachtsheim, S. Scheuermann, J. Schnorr, R. Silvers, M. Wagner, **H. Schwalbe** (2005) *Learning problem-solving thinking in group work*. *Nachrichten aus der Chemie* **53**, 978-980.
- 2004**
13. **H. Schwalbe**, G. Wess (2004) *Editorial: Molecules as modulators: systems biology challenges chemistry*. *ChemBioChem* **5**, 1311-1313.
- 2003**
12. **H. Schwalbe**, M. Göbel, G. Wess (2003) *Editorial: RNA Targeting*. *ChemBioChem* **4**, 915-917.
11. **H. Schwalbe**, H. Kessler (2003) *900-MHz NMR-Spektrometer in München und Frankfurt*. *Nachrichten aus der Chemie*.
10. B. Fürtig, C. Richter, J. Wöhnert, **H. Schwalbe** (2003) *NMR spectroscopy of RNA*. *ChemBioChem* **4**, 936-962. (peer-reviewed)



9. **H. Schwalbe** (2003) Kurt Wüthrich, the ETH Zürich, and the Development of NMR Spectroscopy for the Investigation of Structure, Dynamics and Folding of Proteins. *ChemBioChem* **4**, 135-142. (peer-reviewed)

#### 2002

8. **H. Schwalbe** (2002) Editorial: Dissecting G-protein coupled receptors: structure, function, and ligand interaction. *ChemBioChem* **3**, 915-919.

7. C. Griesinger, M. Hennig, J. Marino, B. Reif, C. Richter, **H. Schwalbe** (2002) Methods for the determination of torsion angle restraints in biomacromolecules. in *Modern Techniques in Protein NMR*, p. 259-367.

#### 2001

6. **H. Schwalbe**, A. Bielecki (2001) Recent Advances in High-Resolution Solid-State NMR Spectroscopy. *Angew. Chem. Int. Ed. Engl.* **40**, 2045-2050 (peer-reviewed).

5. **H. Schwalbe**, T. Carlomagno, M. Hennig, J. Junker, B. Reif, C. Richter, C. Griesinger (2001) Cross-correlated relaxation measurement of angles between tensorial interactions. *Methods Enzymol.* **338**, 35-81 (peer-reviewed).

#### 1999

4. C. Griesinger, M. Hennig, J.P. Marino, B. Reif, C. Richter, **H. Schwalbe** (1999) Methods for the Determination of Torsion Angle Restraints in Biomacromolecules. in *Modern Techniques in Protein NMR*, Eds.: N.R. Krishna and L.J. Berliner in Plenum Press **16** 259-367.

3. J.P. Marino, **H. Schwalbe**, C. Griesinger (1999) J-coupling restraints in RNA Structure Determination. *Acc. Chem. Res.* **32**(7), 614-623 (peer-reviewed).

#### 1995

2. **H. Schwalbe**, P. Schmidt, C. Griesinger (1995) Determination of Coupling Constants with E.COSY related methods. *Encyclopedia of NMR*, chapter 14, p. 177-196.

#### 1994

1. C. Griesinger, **H. Schwalbe**, J. Schleucher, M. Sattler (1994) Proton Detected Heteronuclear NMR. In *Two Dimensional NMR Spectroscopy: Applications for Chemists and Biochemists*. p. 457-580.

### Patents

#### 2017

3. Preparation and use of N-phenyl-2-(phenylamino)thiazole-5-carboxamides as protein kinase inhibitors 2016-11E03DR.

#### 2007

2. L. Mueller-Kuhrt, H. Schiewe, S. Schunk, H. Waldmann, H. Prinz, **H. Schwalbe**, K. Saxena Synthesis of 1,4:3,6-dianhydro-mannitol derivs. for use in the treatment of diabetes. *Ger.Offen.* (2007) 13pp. DE 102006018912

#### 1996

1. M. Spraul, M. Hoffmann, **H. Schwalbe** (1996) NMR-Meßzelle und Verfahren zur schnellen Mischung mindestens zweier Reaktionsfluide in der NMR-Meßzelle. DE 19548977 C 1