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## Qualifications

Physical Chemistry, PhD, Water and Protein Solutions Studied by Field-Dependent Magnetic Relaxation, Faculty of Engineering, LTH  
1998 Jan 1 → 2003 Oct 23  
Award Date: 2003 Oct 23

Physical Chemistry, Master of Science, A Nuclear Magnetic Relaxation Dispersion Study of Oxytocin Hydration, Faculty of Science  
1993 Aug 30 → 1998 Sept 3  
Award Date: 1998 Sept 3

2010 → ... Excellent Teaching Practitioner, ETP

## Employment

**Senior lecturer**  
Biophysical Chemistry  
Lund University  
Lund, Sweden  
2010 Nov 1 → present

### Assistant dean

Faculty of Engineering, LTH  
Lund University  
Lund, Sweden  
2020 Dec 17 → present

### Deputy assistant professor

Lund university: Department of Chemistry  
Lund, Sweden  
2007 Jan 7 → 2010 Oct 31

**High school teacher (programming)**  
Polhemskolan, Lund  
Lund, Sweden  
2006 Aug 11 → 2007 Jan 12

### Postdoc

University of Copenhagen

Copenhagen, Denmark  
2003 Nov 1 → 2006 Aug 15

## Research outputs

### Proton Transfer Kinetics in Histidine Side Chains Determined by pH-Dependent Multi-Nuclear NMR Relaxation

Raum, H. N., Modig, K., Akke, M. & Weininger, U., 2024 Aug, In: *Journal of the American Chemical Society*. 146, 32, p. 22284-22294 11 p.

### Ligand-induced protein transition state stabilization switches the binding pathway from conformational selection to induced fit

Stenström, O., Diehl, C., Modig, K. & Akke, M., 2024 Apr 2, In: *Proceedings of the National Academy of Sciences of the United States of America*. 121, 14, p. e2317747121

### Transition-State Compressibility and Activation Volume of Transient Protein Conformational Fluctuations

Dreydoppel, M., Dorn, B., Modig, K., Akke, M. & Weininger, U., 2021 Jun 3, In: *JACS Au*. 1, 6, p. 833-842 10 p.

### Mapping the energy landscape of protein-ligand binding via linear free energy relationships determined by protein NMR relaxation dispersion

Stenström, O., Diehl, C., Modig, K., Nilsson, U. J. & Akke, M., 2021, In: *RSC Chemical Biology*. 2, 1, p. 259-265 7 p.

### Rotamer jumps, proton exchange, and amine inversion dynamics of dimethylated lysine residues in proteins resolved by pH-dependent <sup>1</sup>H and <sup>13</sup>C nmr relaxation dispersion

Weininger, U., Modig, K., Ishida, H., Vogel, H. J. & Akke, M., 2019 Nov 21, In: *Journal of Physical Chemistry B*. 123, 46, p. 9742–9750 9 p.

### Dynamics of Aromatic Side Chains in the Active Site of FKBP12

Weininger, U., Modig, K., Geitner, A. J., Schmidpeter, P. A. M., Koch, J. R. & Akke, M., 2017 Jan 10, In: *Biochemistry*. 56, 1, p. 334-343 10 p.

### Molecular insights into substrate recognition and catalytic mechanism of the chaperone and FKBP peptidyl-prolyl isomerase SlyD

Quistgaard, E. M., Weininger, U., Ural-Blimke, Y., Modig, K., Nordlund, P., Akke, M. & Löw, C., 2016 Sept 23, In: *BMC Biology*. 14, 1, 82.

### Off-resonance rotating-frame relaxation dispersion experiment for (13)C in aromatic side chains using L-optimized TROSY-selection.

Weininger, U., Brath, U., Modig, K., Teilum, K. & Akke, M., 2014, In: *Journal of Biomolecular NMR*. 59, 1, p. 23-29

### Ring Flips Revisited: C-13 Relaxation Dispersion Measurements of Aromatic Side Chain Dynamics and Activation Barriers in Basic Pancreatic Trypsin Inhibitor

Weininger, U., Modig, K. & Akke, M., 2014, In: *Biochemistry*. 53, 28, p. 4519-4525

### High water mobility on the ice-binding surface of a hyperactive antifreeze protein.

Modig, K., Qvist, J., Marshall, C. B., Davies, P. L. & Halle, B., 2010, In: *Physical chemistry chemical physics : PCCP*. 12, Online 29th July 2010, p. 10189-10197

### Protein Flexibility and Conformational Entropy in Ligand Design Targeting the Carbohydrate Recognition Domain of Galectin-3.

Diehl, C., Engström, O., Delaine, T., Håkansson, M., Genheden, S., Modig, K., Leffler, H., Ryde, U., Nilsson, U. & Akke, M., 2010, In: *Journal of the American Chemical Society*. 132, p. 14577-14589

### Structure and Dynamics of Ribosomal Protein L12: An Ensemble Model Based on SAXS and NMR Relaxation

Bernardo, P., Modig, K., Grela, P., Svergun, D. I., Tchorzewski, M., Pons, M. & Akke, M., 2010, In: *Biophysical Journal*. 98 , 10, p. 2374-2382

**Conformational entropy changes upon lactose binding to the carbohydrate recognition domain of galectin-3.**  
Diehl, C., Genheden, S., Modig, K., Ryde, U. & Akke, M., 2009, In: Journal of Biomolecular NMR. 45, 1-2, p. 157-169

**Kursutvärderingssystemet CEQ vid LTH: uppfylls avsedda syften?**  
Björnsson, L., Dahlbom, M., Modig, K. & Sjöberg, A., 2009, Proceedings 2:a Utvecklingskonferensen för Sveriges ingenjörsutbildningar. LTH

**Students' micro cultures determine the quality of teaching!**  
Roxå, T. & Modig, K., 2009.

**Model-independent interpretation of NMR relaxation data for unfolded proteins: the acid-denatured state of ACBP**  
Modig, K. & Poulsen, F. M., 2008, In: Journal of Biomolecular NMR. 42, 3, p. 163-177

**Protein conformational transitions as seen from the solvent: magnetic relaxation dispersion studies of water, cosolvent, and denaturant interactions with nonnative proteins**  
Halle, B., Denisov, V., Modig, K. & Davidovic, M., 2005, *Protein Folding Handbook*. Buchner, J. & Kiehaber, T. (eds.). John Wiley & Sons Inc., p. 201-246

**Dynamics of protein and peptide hydration**  
Modig, K., Liepinsh, E., Otting, G. & Halle, B., 2004, In: Journal of the American Chemical Society. 126, 1, p. 102-114

**Temperature-dependent hydrogen-bond geometry in liquid water.**  
Modig, K., Pfrommer, B. G. & Halle, B., 2003, In: Physical Review Letters. 90, 7, p. 075502-1-075502-4

**Trifluoroethanol-induced beta -> alpha transition in beta-lactoglobulin: hydration and cosolvent binding studied by  $^2\text{H}$ ,  $^{17}\text{O}$ , and  $^{19}\text{F}$  magnetic relaxation dispersion.**  
Kumar, S., Modig, K. & Halle, B., 2003, In: Biochemistry. 42, 46, p. 13708-13716

**Water and protein solutions studied by field-dependent magnetic relaxation**  
Modig, K., 2003, Biophysical Chemistry (LTH), Lund University. 248 p.

**Water and urea interactions with the native and unfolded forms of a beta-barrel protein.**  
Modig, K., Kurian, E., Prendergast, F. G. & Halle, B., 2003, In: Protein Science. 12, 12, p. 2768-2781

**Water dynamics in the large cavity of three lipid-binding proteins monitored by  $^{17}\text{O}$  magnetic relaxation dispersion.**  
Modig, K., Rademacher, M., Lücke, C. & Halle, B., 2003, In: Journal of Molecular Biology. 332, 4, p. 965-977

**Proton magnetic shielding tensor in liquid water**  
Modig, K. & Halle, B., 2002, In: Journal of the American Chemical Society. 124, 40, p. 12031-12041